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23

24 **3. Materials and methods for biological studies**

25 **4. Supplementary figures for biological studies**

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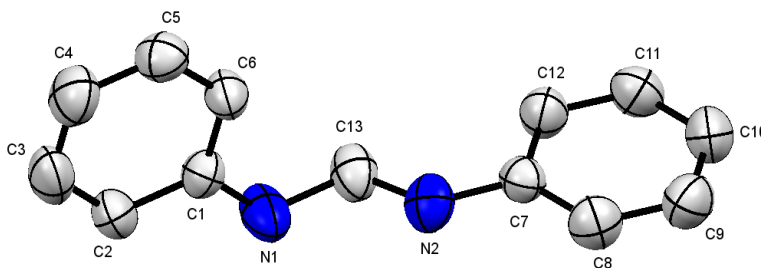
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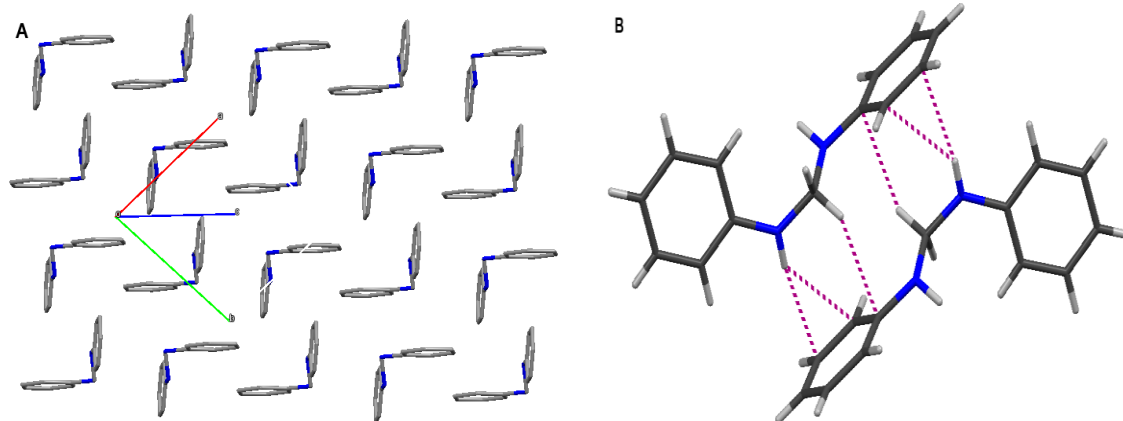
1 **1. X-ray data collection, structure resolution and model refinement of 2a**

2 The crystal data were obtained with Bruker APEX II QUAZAR three-circle
3 diffractometer. Indexing was performed using APEX2¹ Data integration and reduction
4 were carried out with SAINT.² Absorption correction was performed by multi-scan
5 method implemented in SADABS.³ The structure was solved using SHELXT⁴ and then
6 refined by full-matrix least-squares refinements on F^2 using the SHELXL⁴ in OLEX2⁵.
7 All non-hydrogen atoms were refined anisotropically using all reflections with $I > 2\sigma(I)$.
8 Aromatic and aliphatic C-bound H atoms were positioned geometrically and refined
9 using a riding mode. Crystallographic data and refinement details of the data collection
10 for **2a** are given in **Table S1** Mercury was used for visualization of the cif file.⁶
11 Additional crystallographic data with CCDC reference number 2306536 have been
12 deposited within the Cambridge Crystallographic Data Center via
13 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.

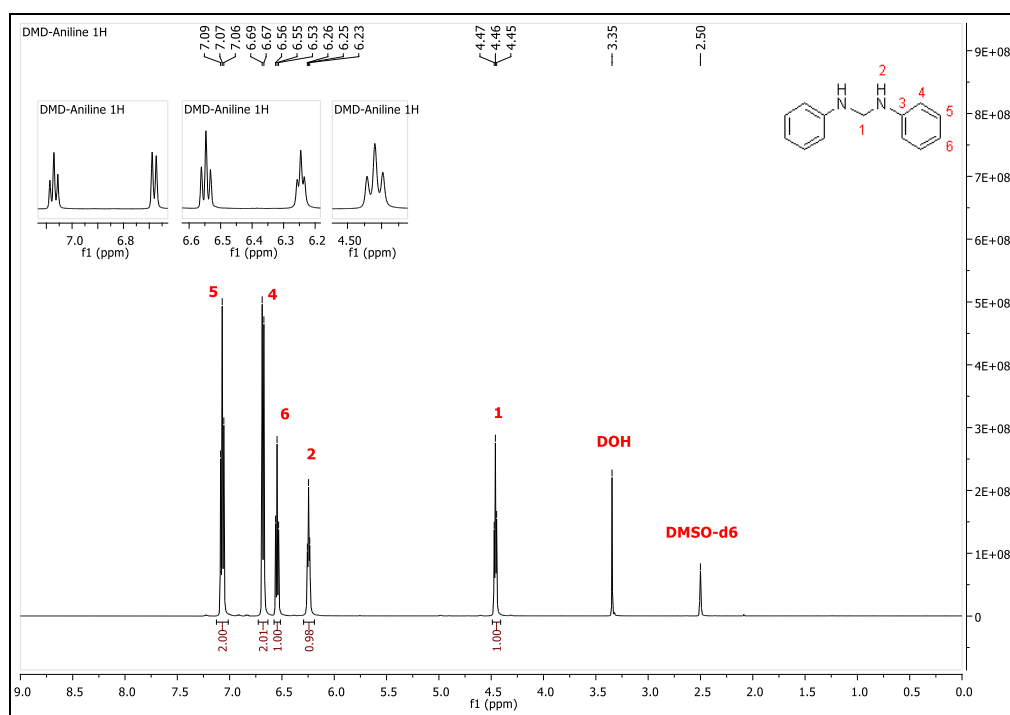


1
 2 **Figure S2** A) The pleated form of the layers, viewed in the direction of propagation of the
 3 pleats. B) The N—H··· π and C—H··· π interactions indicated by dashed lines (symmetry code: -
 4 x, -y, -z).

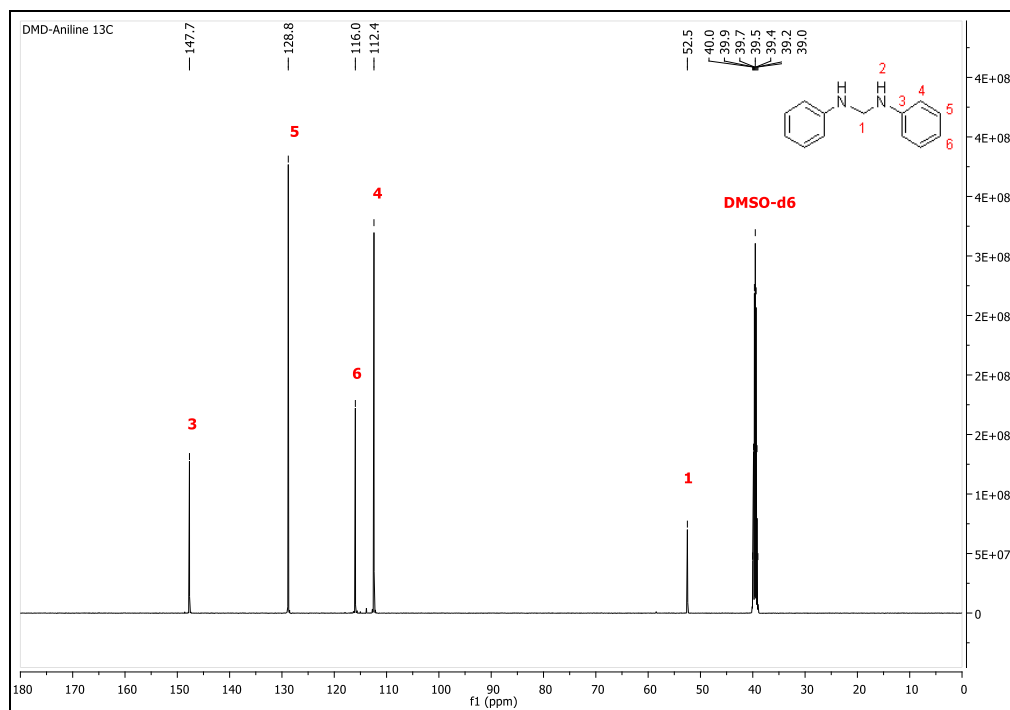
5 **Table S1** Crystal data and refinement parameters for 2a

Empirical Formula	0.5(C _{6.5} H ₇ N)
Formula weight (g. mol⁻¹)	99.13
Temperature (K)	296.15
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> (Å)	7.118(4)
<i>b</i> (Å)	7.596(4)
<i>c</i> (Å)	10.967(6)
α (°)	72.24(4)
β (°)	77.59(4)
γ (°)	85.39(4)
Crystal size (mm)	0.244 × 0.12 × 0.047
<i>V</i> (Å³)	551.5(6)
<i>Z</i>	4
ρ_{calcd} (g. cm⁻³)	1.194
μ (mm⁻¹)	0.072
<i>F</i>(000)	212.0
2 θ range for data collection (°)	3.98 to 49.996
<i>h</i>/<i>k</i>/<i>l</i>	-8 ≤ <i>h</i> ≤ 8, -6 ≤ <i>k</i> ≤ 8, -13 ≤ <i>l</i> ≤ 13
Reflections collected	4175
Independent reflections	1849 [Rint = 0.0772, Rsigma = 0.1122]
Data/restraints/parameters	1851/0/137
Goodness-of-fit on <i>F</i>²	0.892
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0748, <i>wR</i> 2 = 0.1759
<i>R</i> indices (all data)	<i>R</i> 1 = 0.1607, <i>wR</i> 2 = 0.2143
Largest diff. peak and hole (e.Å⁻³)	0.46/-0.39
CCDC	2306536

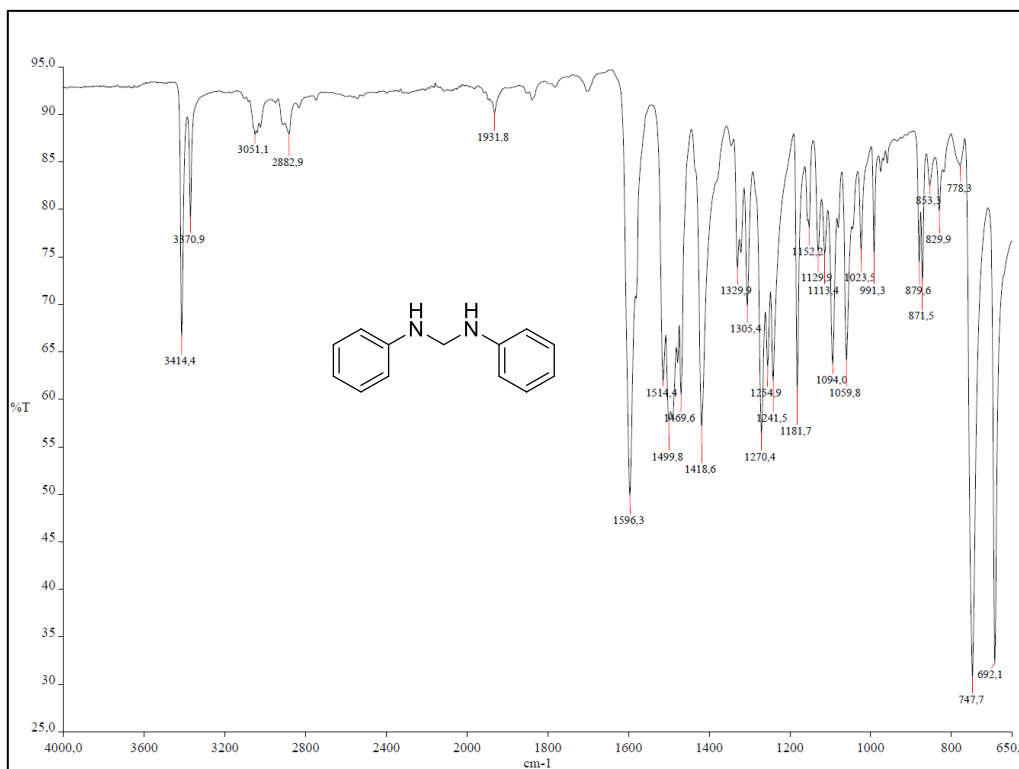
- 1 **2. Supplementary figures for synthetic parts**
- 2 **2.1 *N,N'*-diphenylmethanediamine (2a)**



3
4
5
Figure S3 ¹H NMR Spectrum of *N,N'*-diphenylmethanediamine (2a)

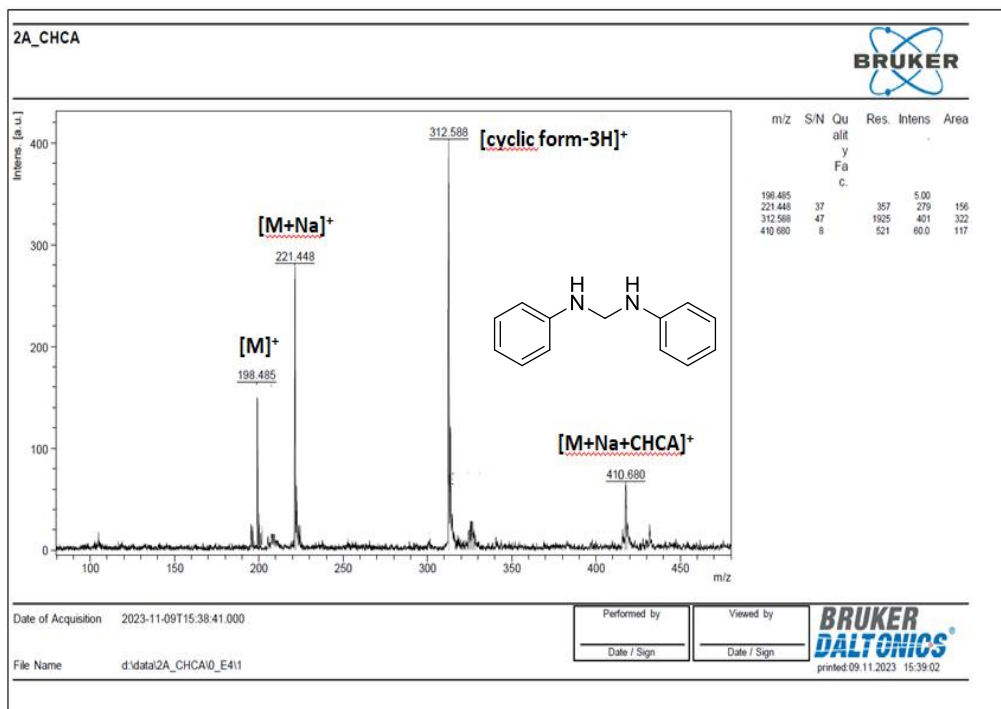


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Figure S4 ¹³C NMR Spectrum of *N,N'*-diphenylmethanediamine (2a)



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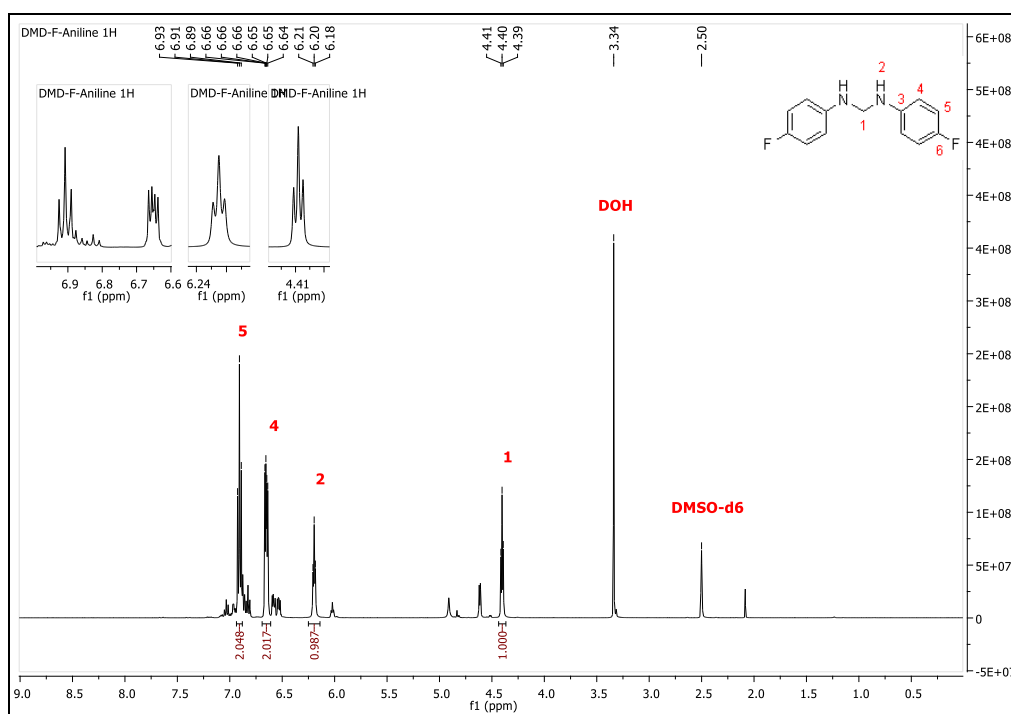
Figure S5 FT-IR Spectrum of *N,N'*-diphenylmethanediamine (2a)



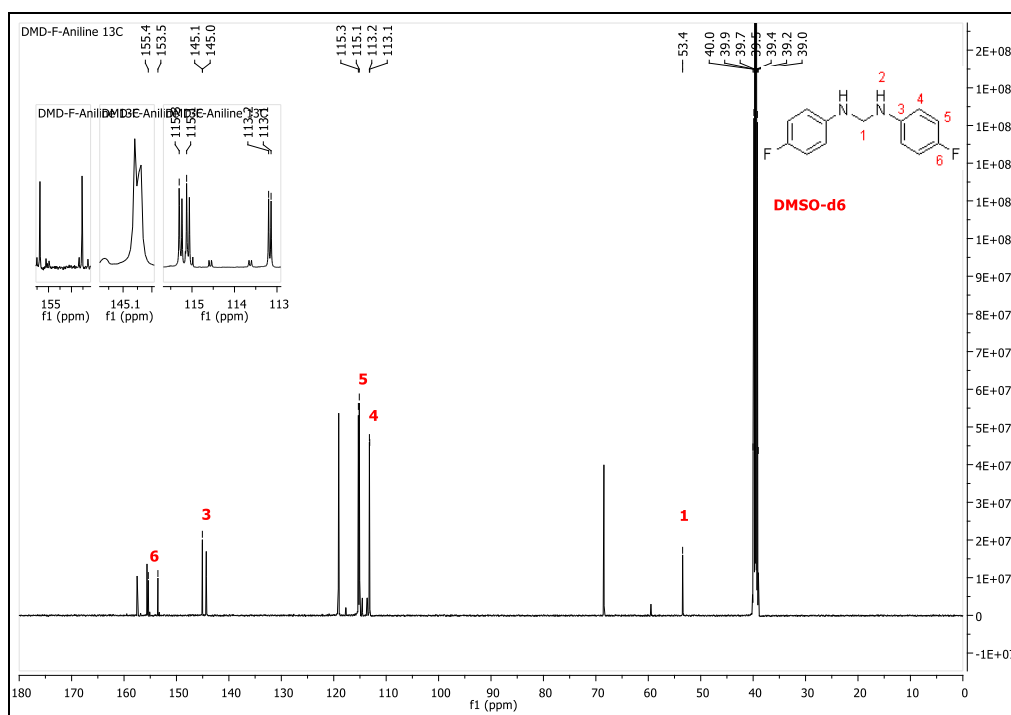
4
5

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

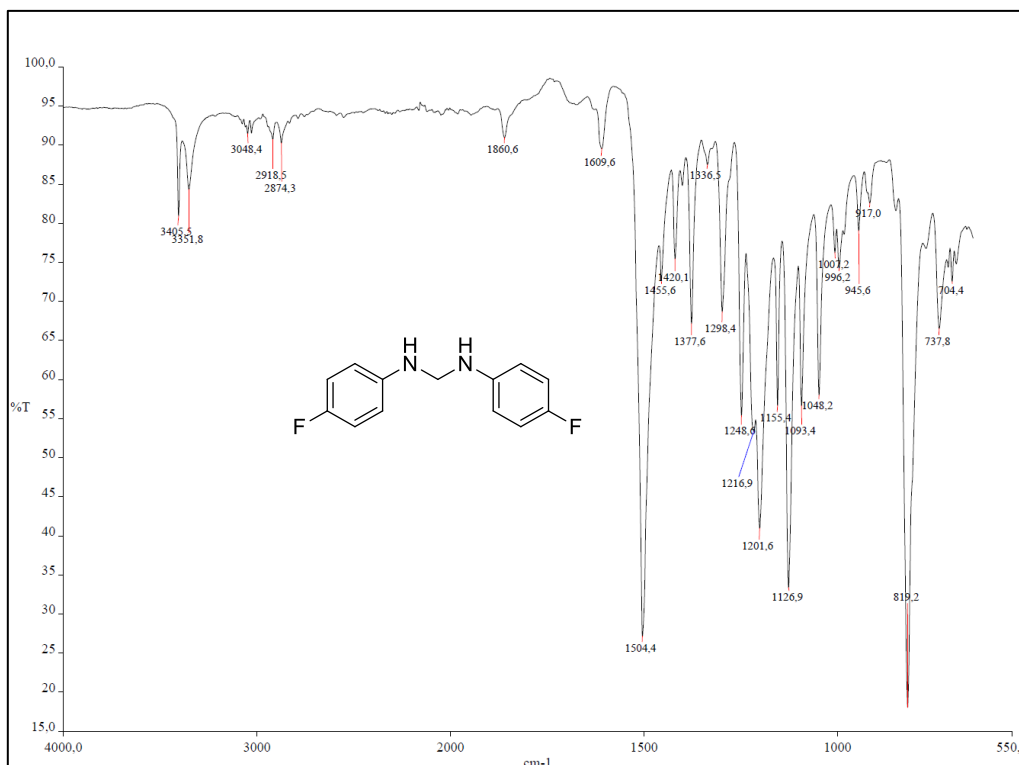
1 **2.2 *N,N'*-bis(4-fluorophenyl)methanediamine**



2
3 **Figure S7** ¹H NMR Spectrum of *N,N'*-bis(4-fluorophenyl)methanediamine (2b)



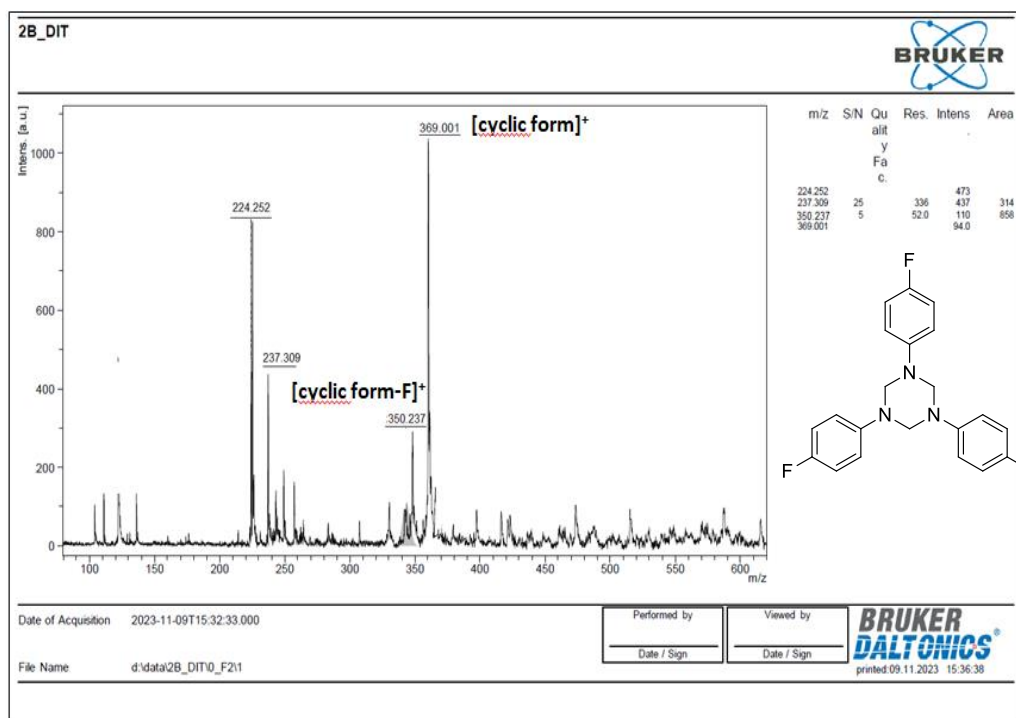
5
6 **Figure S8** ¹³C NMR Spectrum of *N,N'*-bis(4-fluorophenyl)methanediamine (2b)



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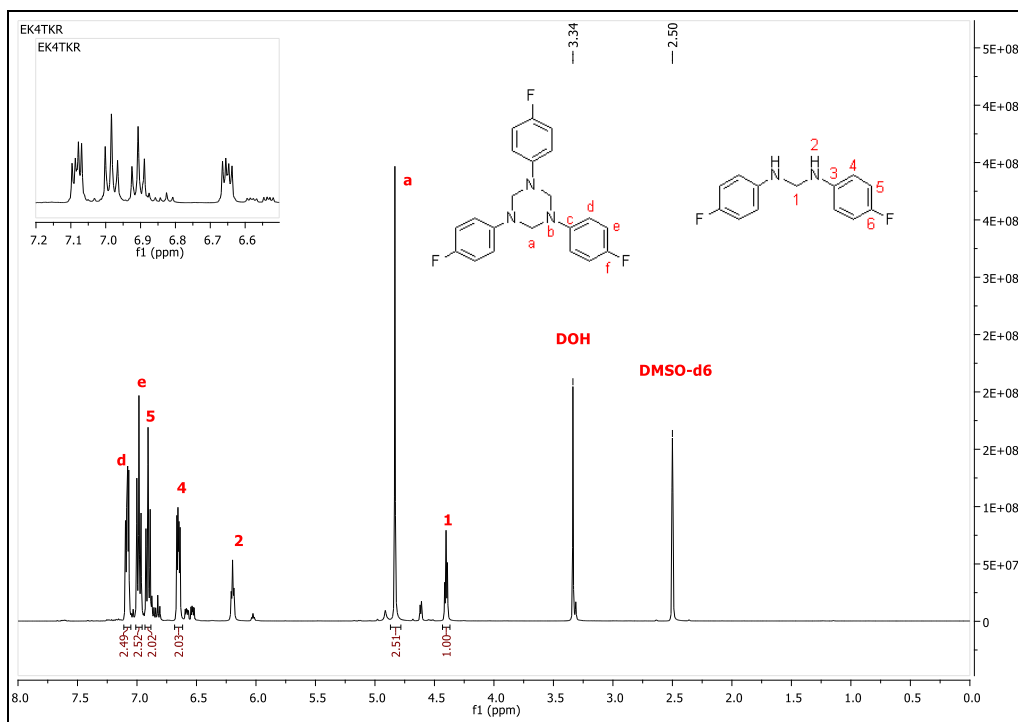
2 **Figure S9** FT-IR Spectrum of *N,N'*-bis(4-fluorophenyl)methanediamine (2b)

3

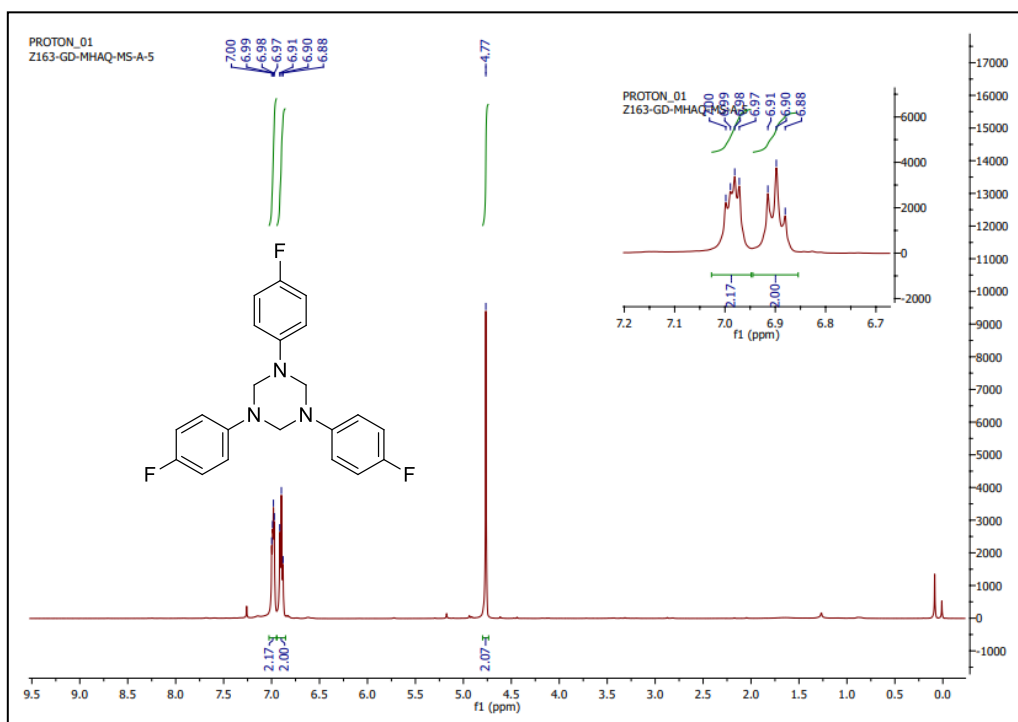


4

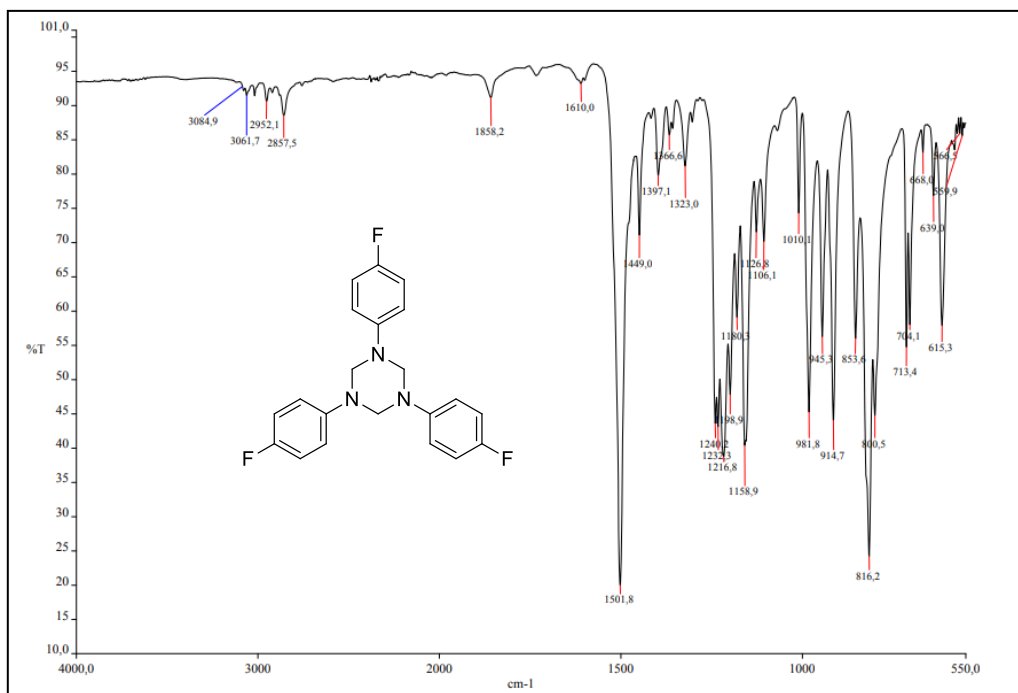
5 **Figure S10** MS Spectrum of *N,N'*-bis(4-fluorophenyl)methanediamine (2b)



1
2 **Figure S11** ^1H NMR Spectrum of N,N' -bis(4-fluorophenyl)methanedi-amine (2b) in
3 $\text{DMSO-}d_6$ after two hours

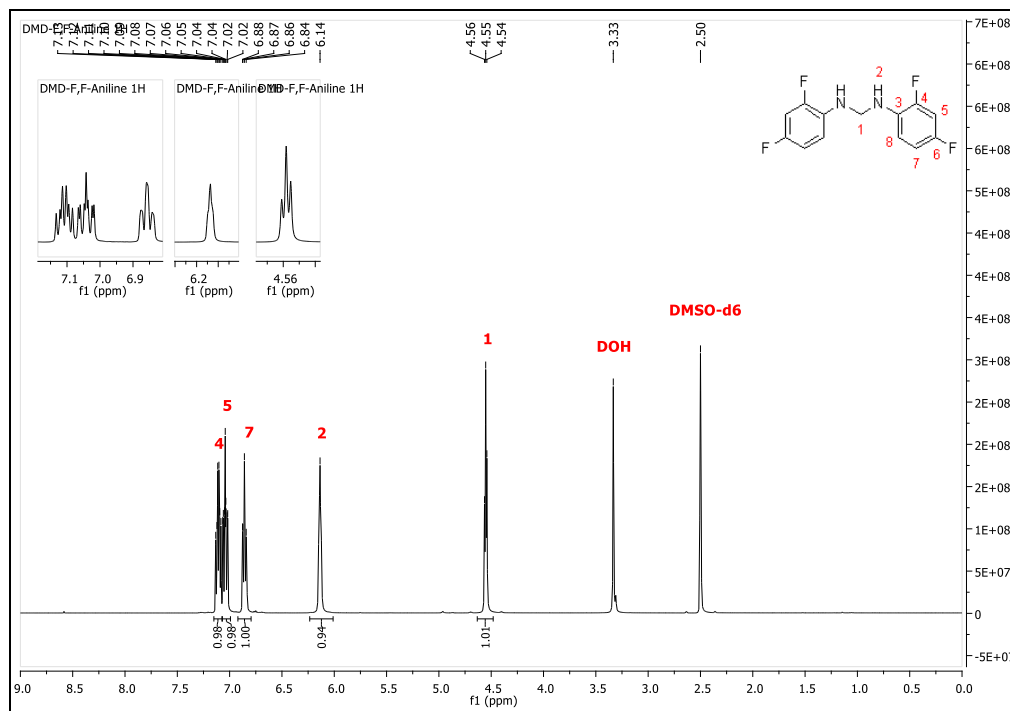


4
5 **Figure S12** ^1H NMR Spectrum of N,N' -bis(4-fluorophenyl)methanedi-amine (2b) in
6 CDCl_3 after 30 min

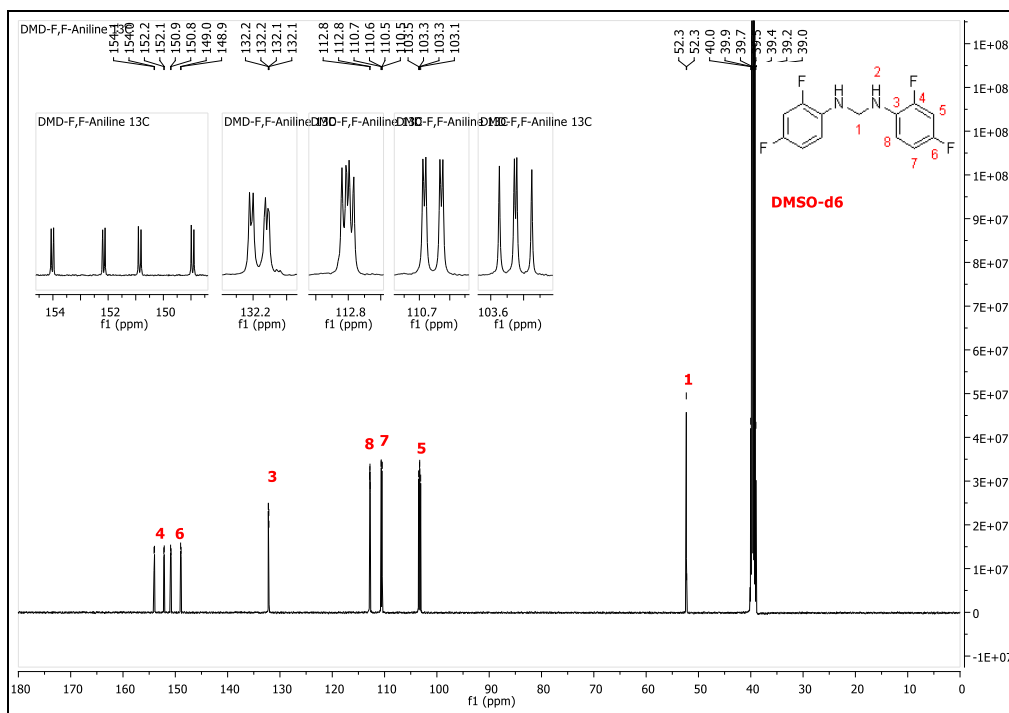


1
 2 **Figure S13** FT-IR Spectrum of *N,N'*-bis(4-fluorophenyl)methanediamine (2b) after
 3 cyclization

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



5
 6 **Figure S14** ^1H NMR Spectrum of *N,N'*-bis(2,4-difluorophenyl)methanediamine (2c)

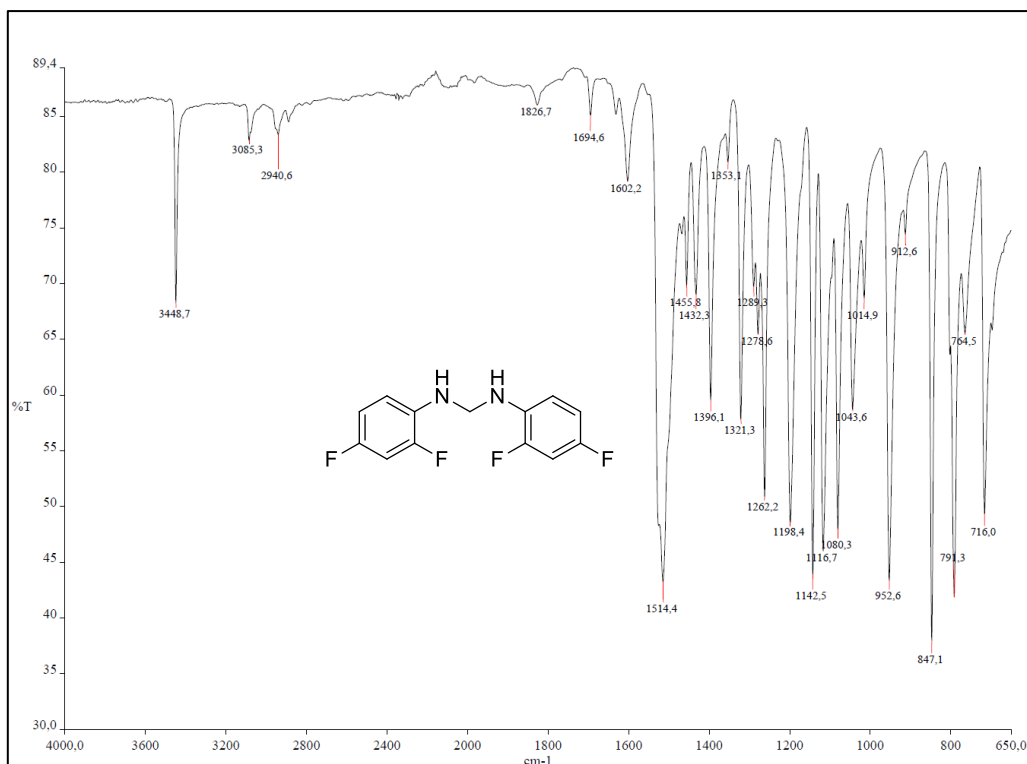


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Figure S15 ^{13}C NMR Spectrum of *N,N'*-bis(2,4-difluorophenyl)methanedi-amine (2c)

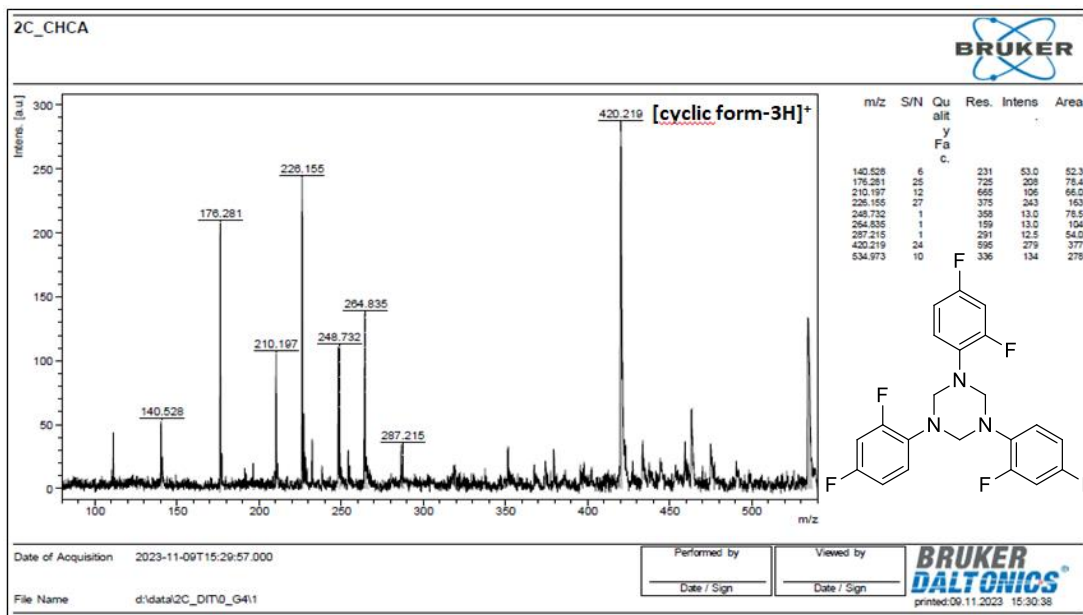
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Figure S16 FT-IR Spectrum of *N,N'*-bis(2,4-difluorophenyl)methanedi-amine (2c)



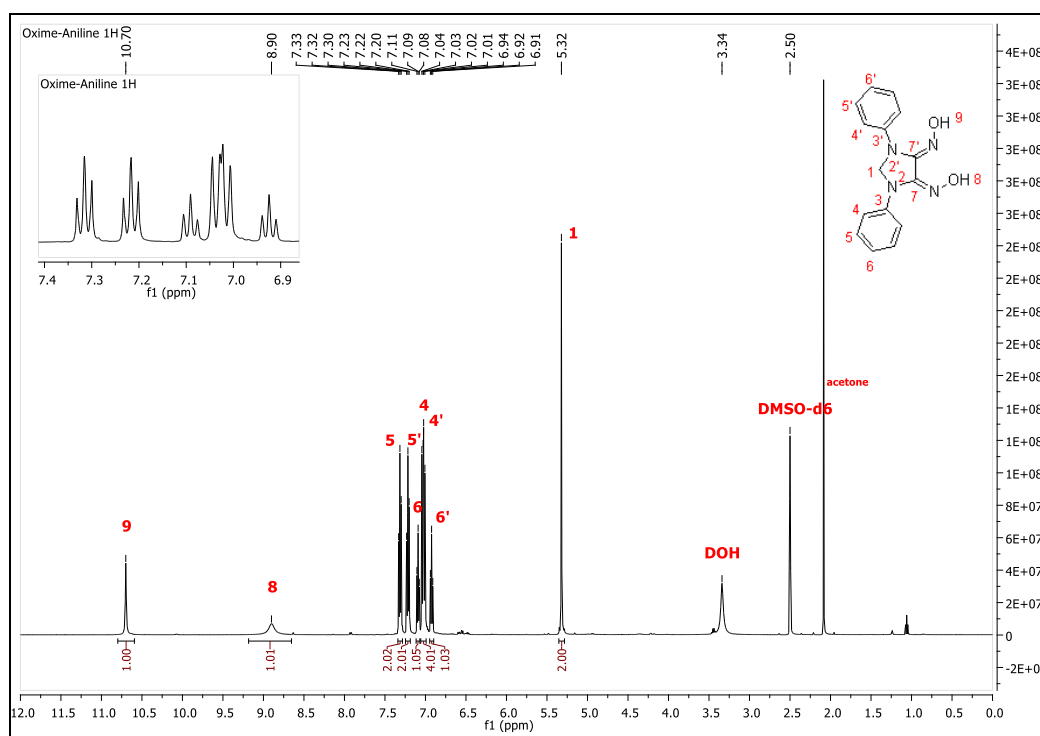
1

2

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

3

2.4 (4Z,5E)-1,3-diphenylimidazolidine-4,5-dione dioxime



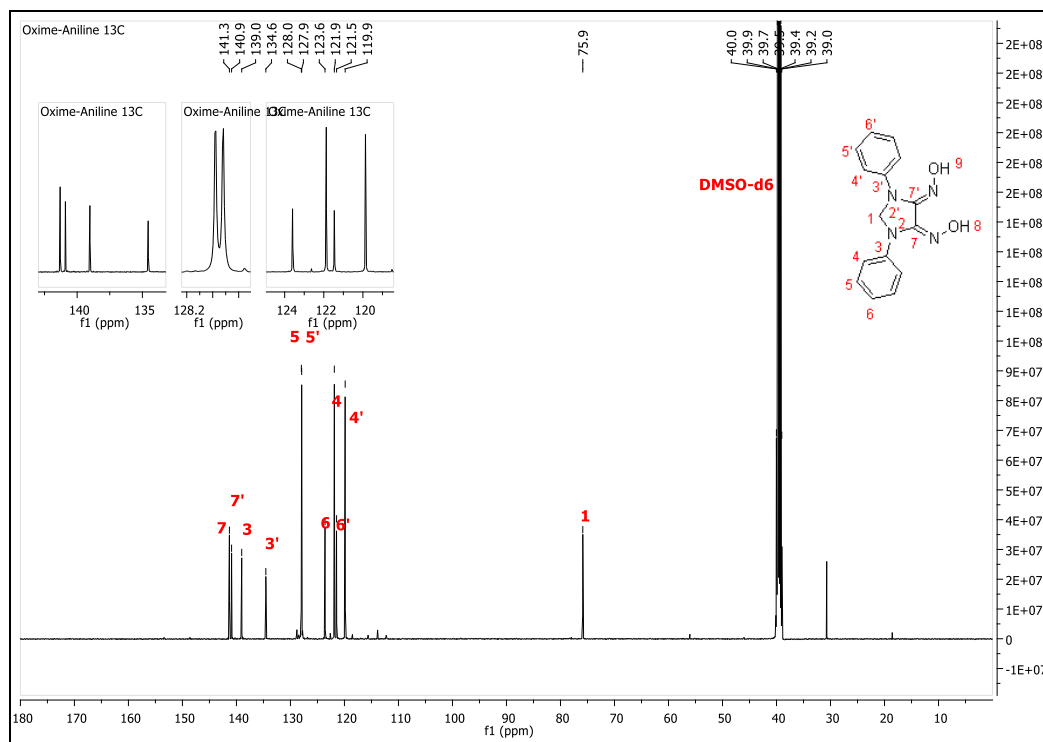
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Figure S18 ¹H NMR Spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dione

6

dioxime (*L*_{1a})



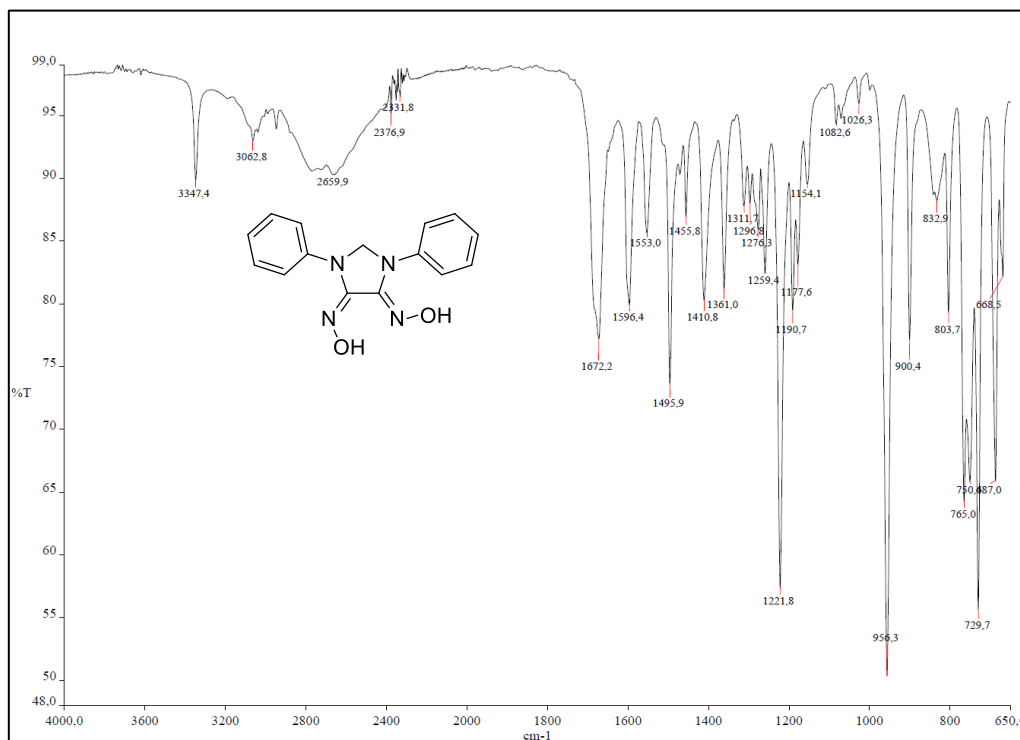
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Figure S19 ^{13}C NMR Spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dione

3

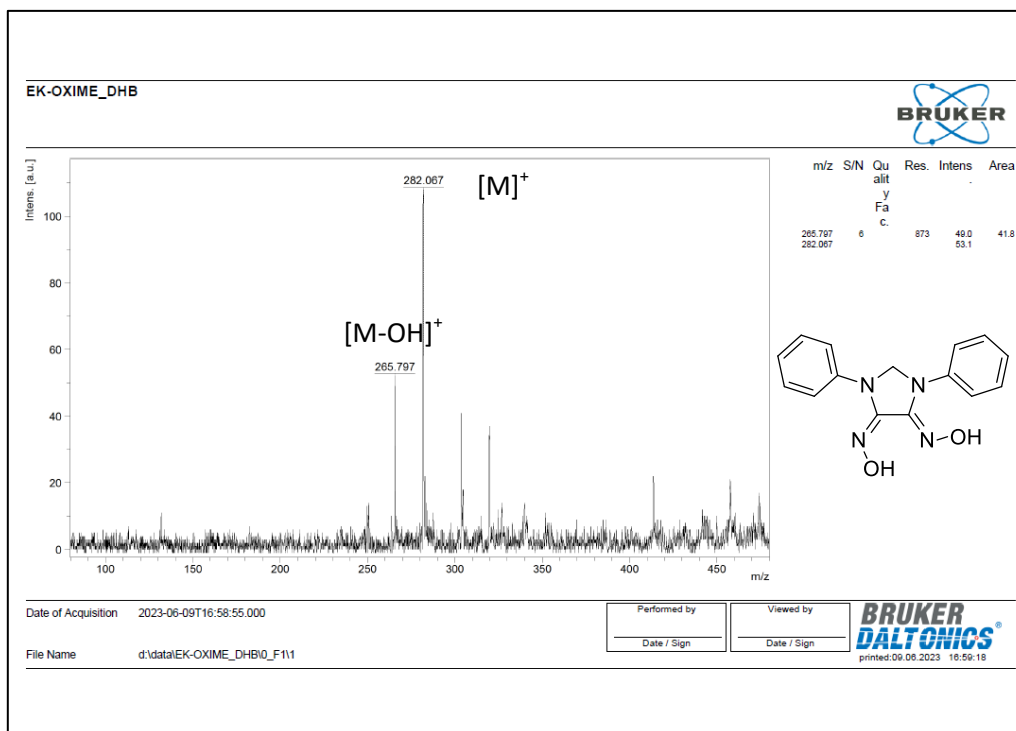
dioxime (L_{1a})



4

5

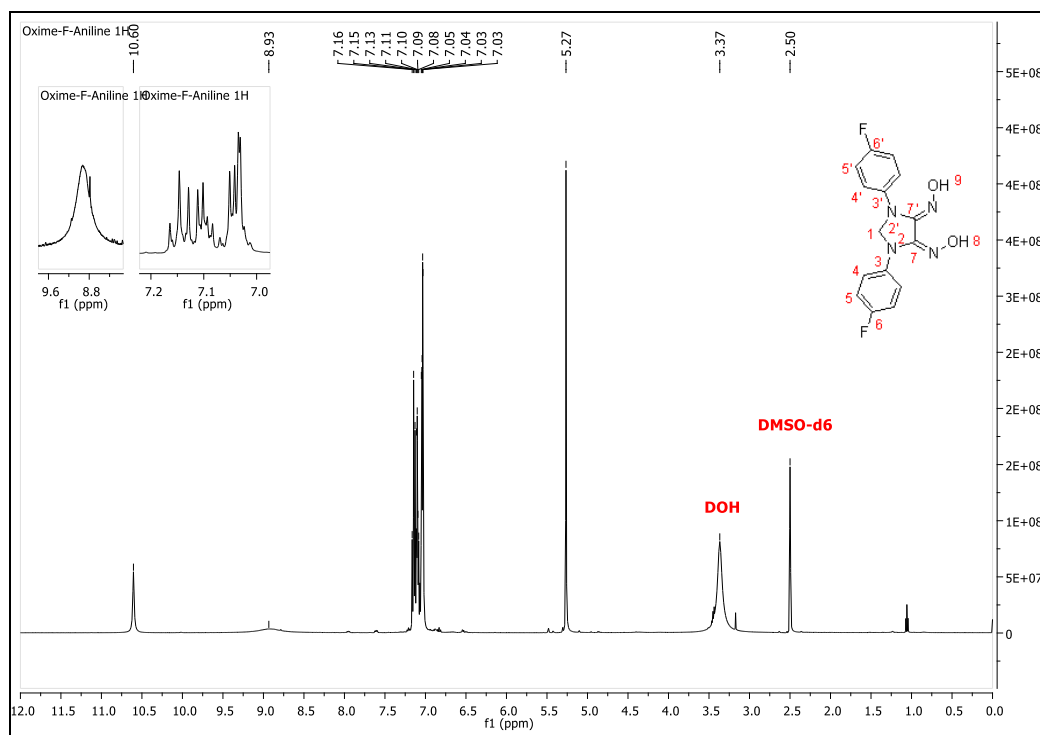
Figure S20 FT-IR Spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dione dioxime (L_{1a})



1

2 **Figure S21** MS Spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dione dioxime (L_{1a})

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



4

5 **Figure S22** ^1H NMR Spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-dione

6

dioxime (L_{1b})

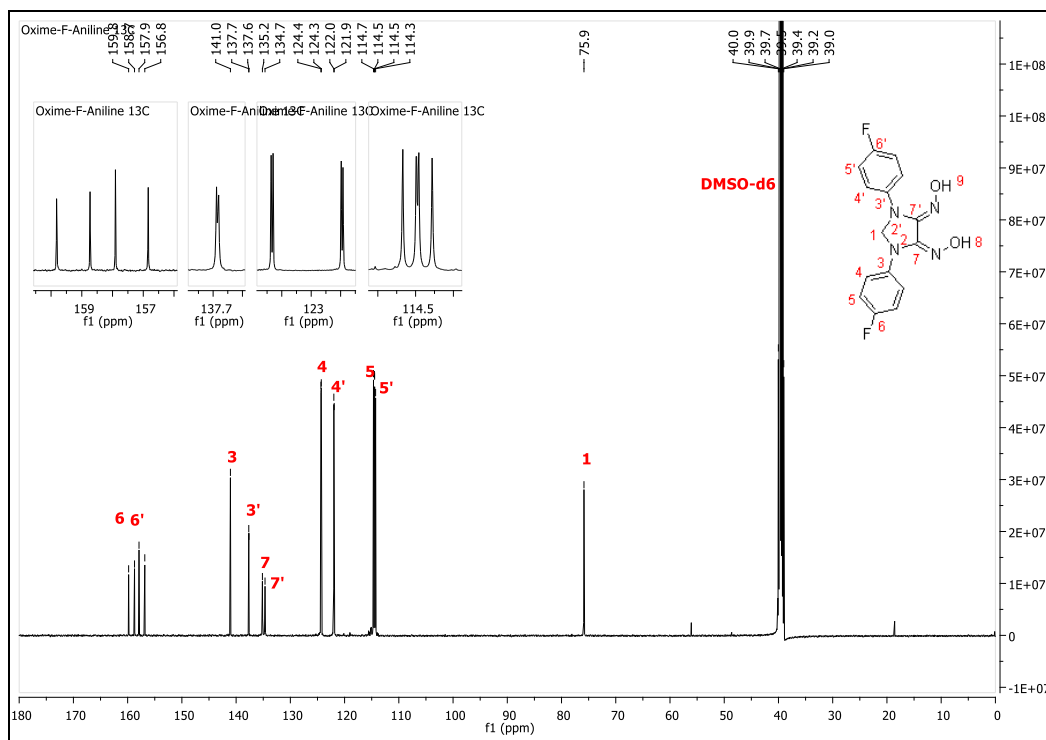


Figure S23 ^{13}C NMR Spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-dione dioxime ($\text{L}_{1\text{b}}$)

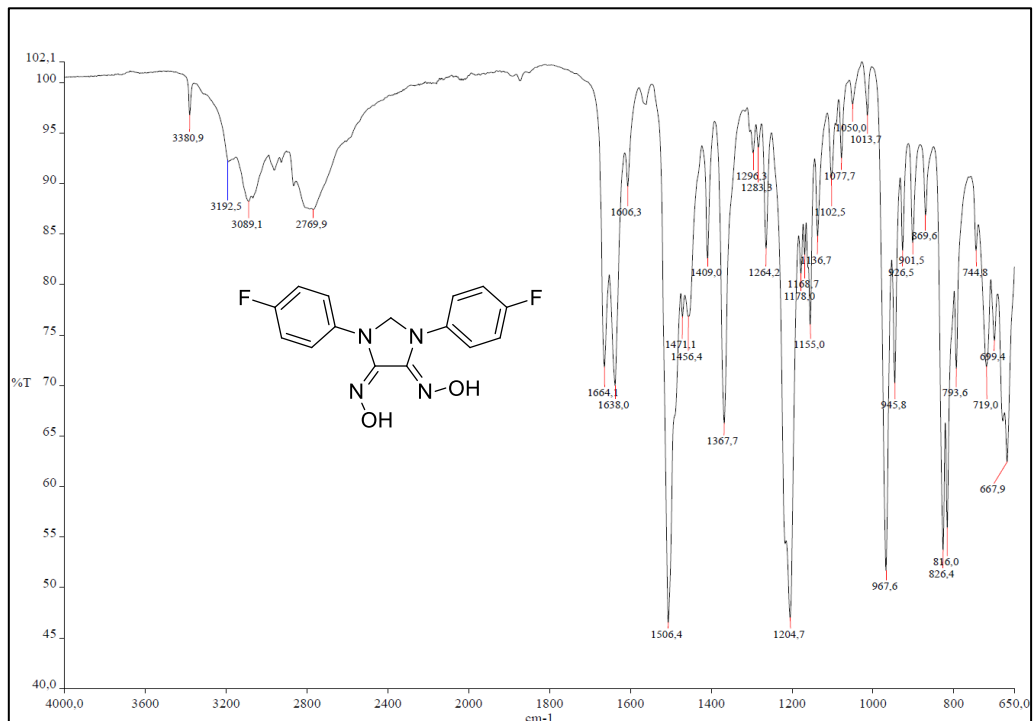
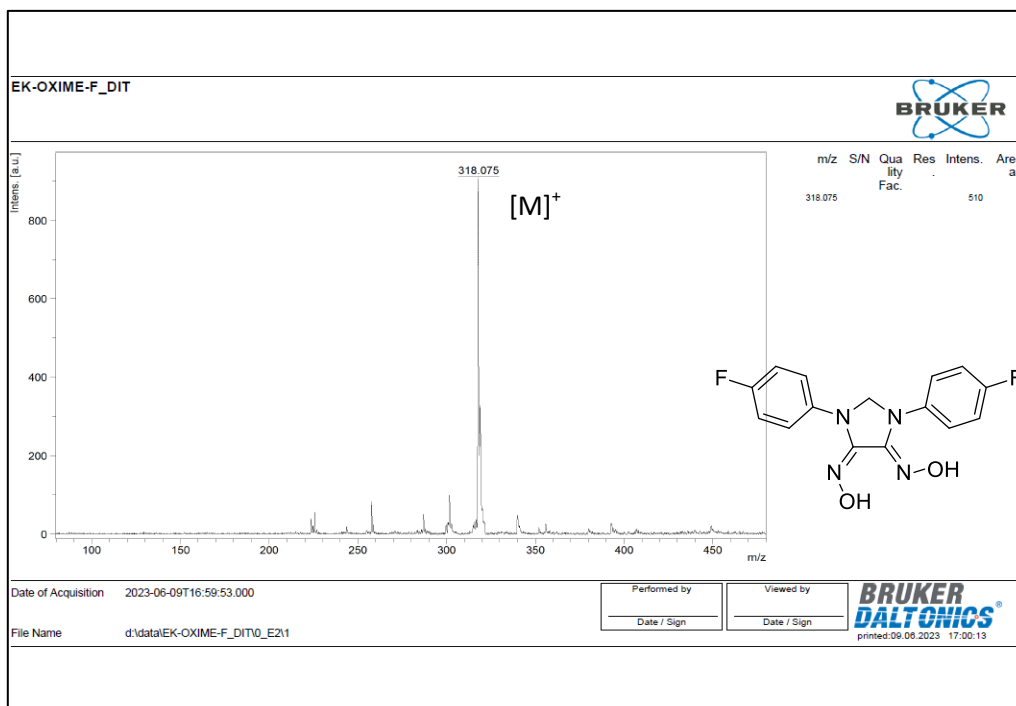


Figure S24 FT-IR Spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-dione dioxime ($\text{L}_{1\text{b}}$)



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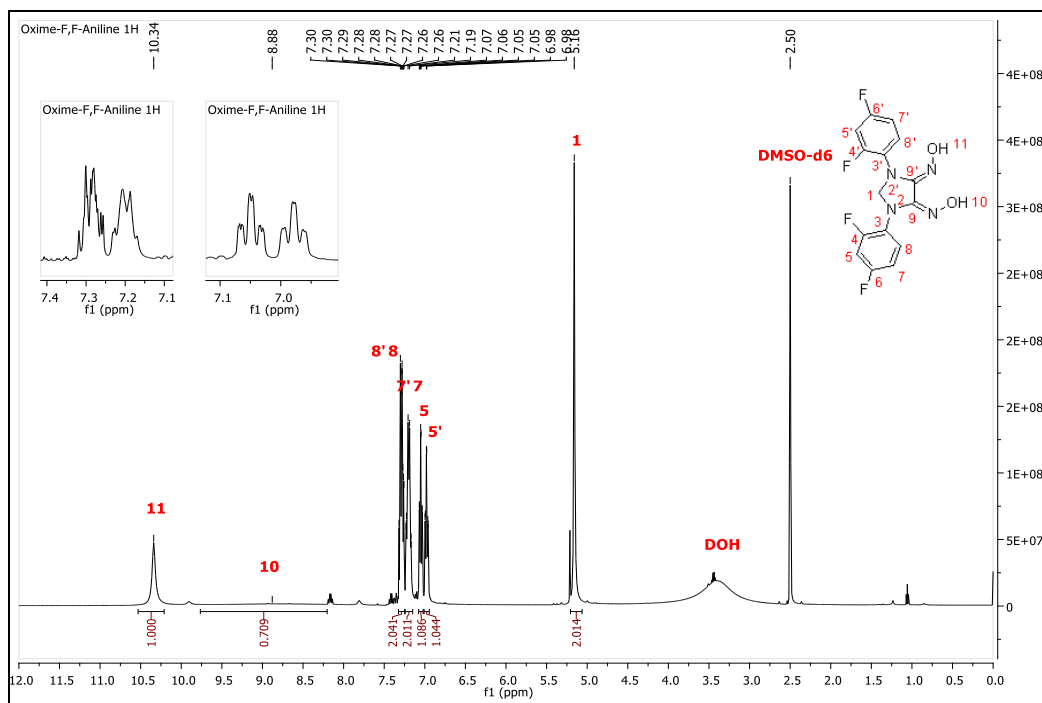
2 **Figure S25** MS Spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-dione dioxime

3

(L_{1b})

4

2.6 (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-dione dioxime



5

6 **Figure S26** ¹H NMR Spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-dione

7

dioxime (L_{1c})

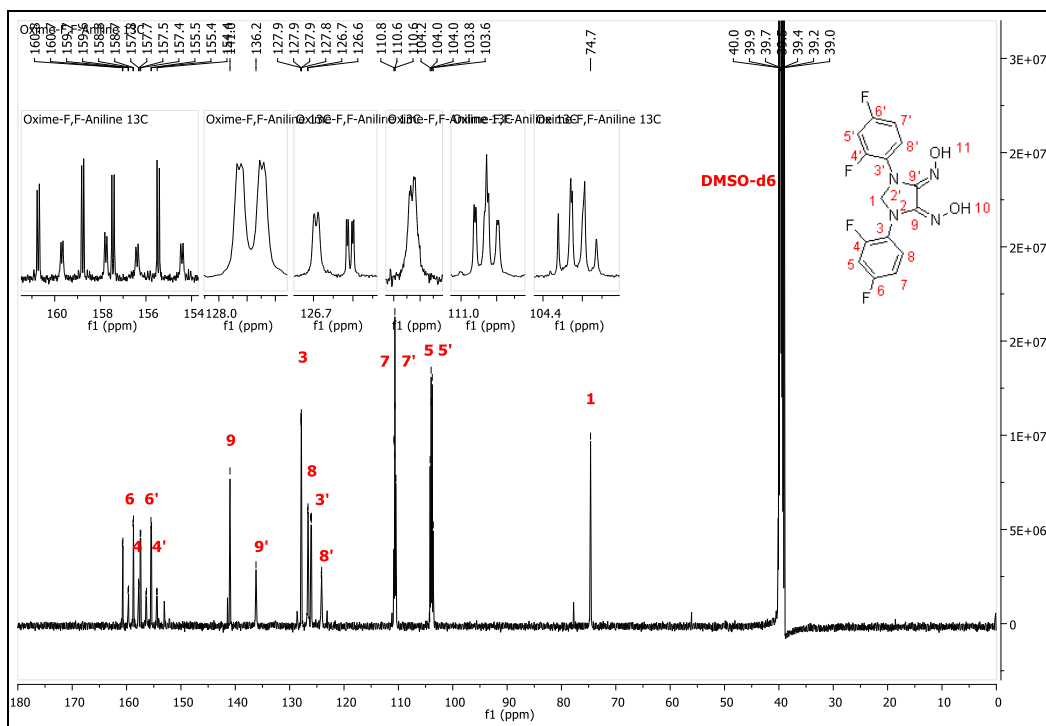


Figure S27 ^{13}C NMR Spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-dione dioxime (L_{1c})

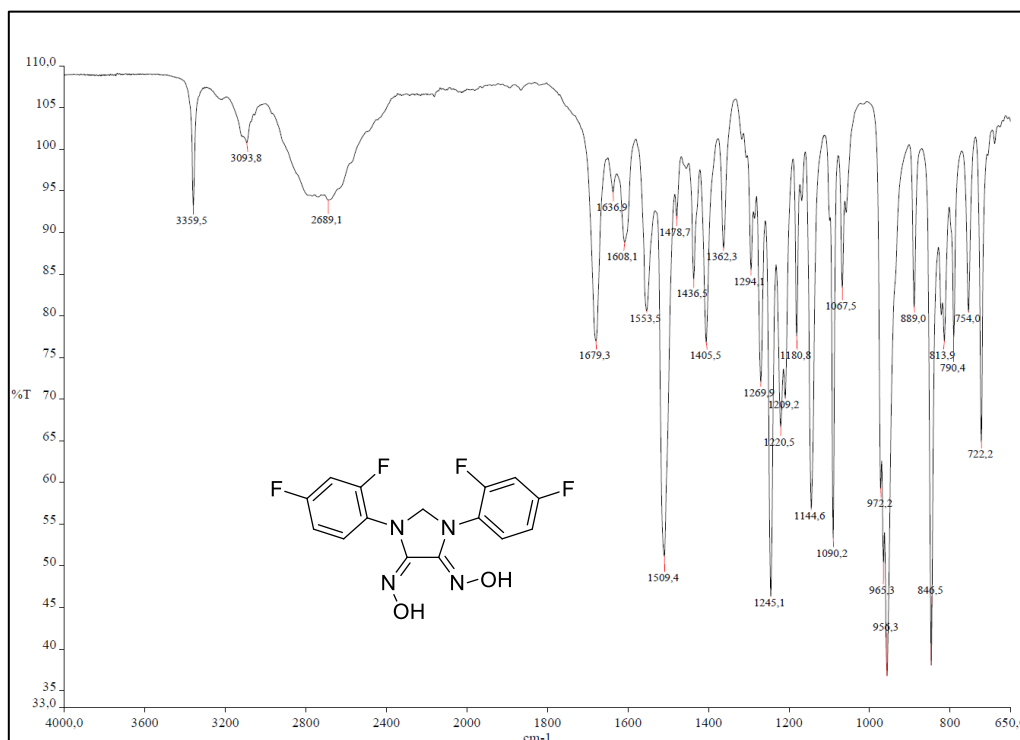
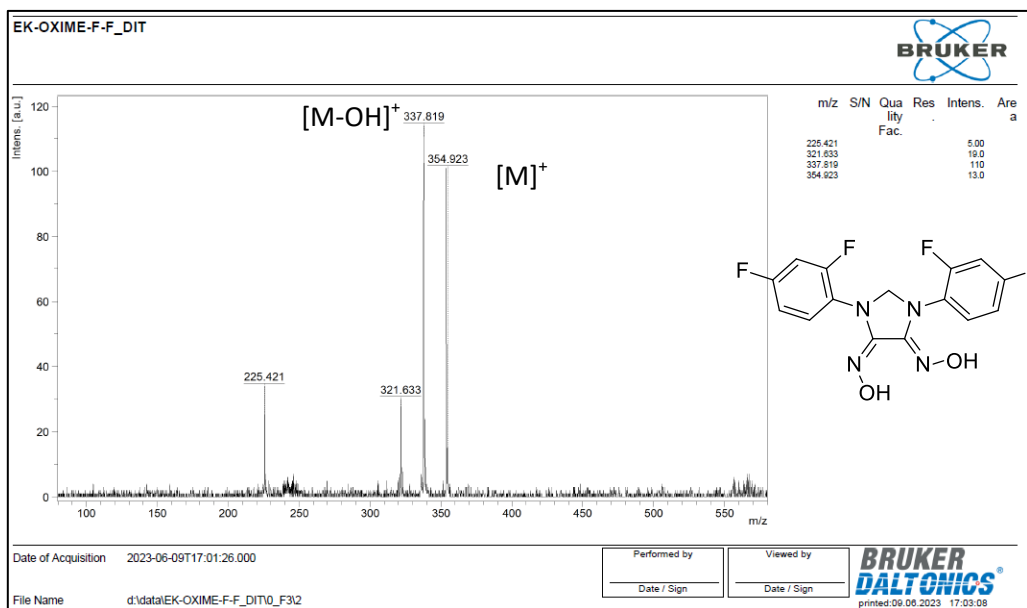


Figure S28 FT-IR Spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-dione dioxime (L_{1c})

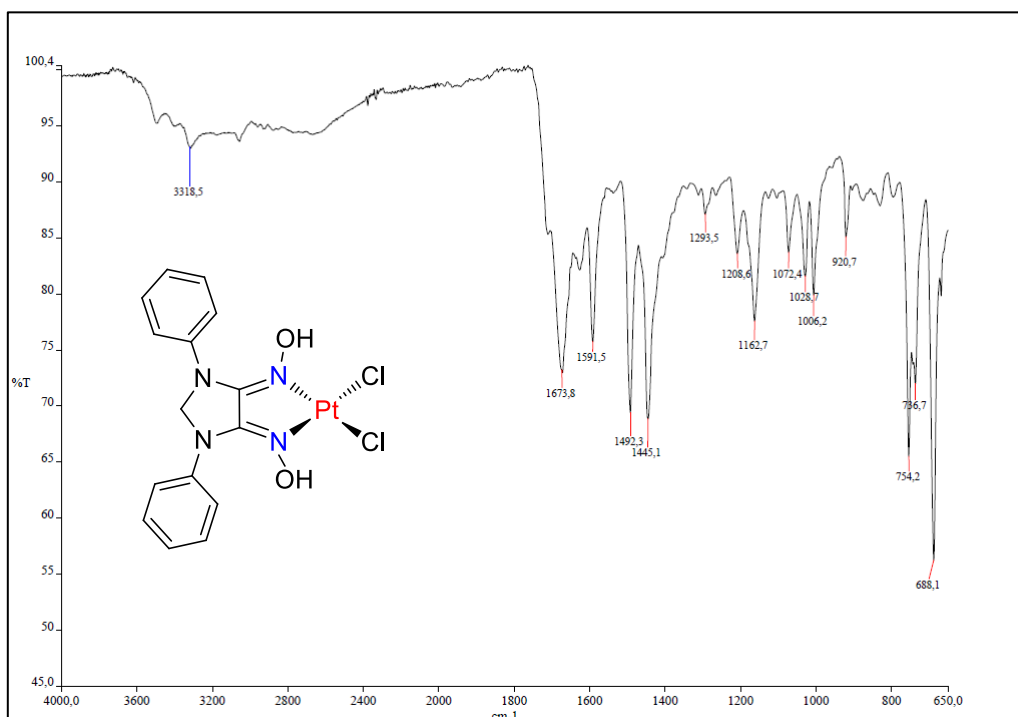


1

2 **Figure S29** MS Spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-dione
 3 dioxime (L_{1c})

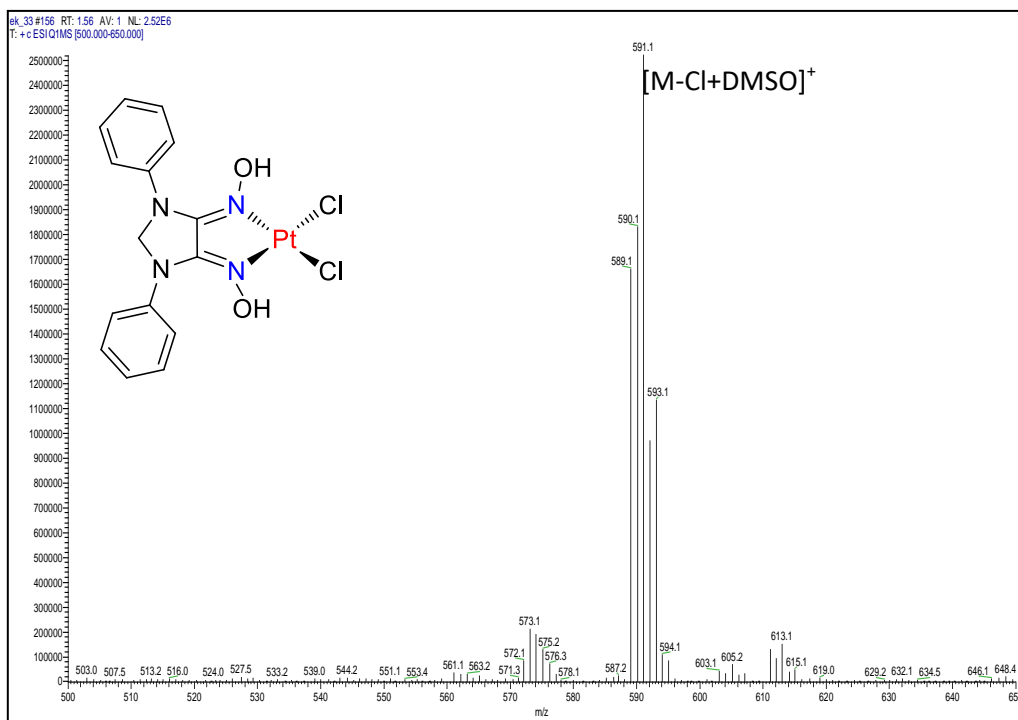
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5 **2.7 Mono-Platinum Complexes of *vic*-dioximes**



6

7 **Figure S30** FT-IR Spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dione dioxime
 8 mono-Pt(II) complex ($L_{1a}Pt-m$)



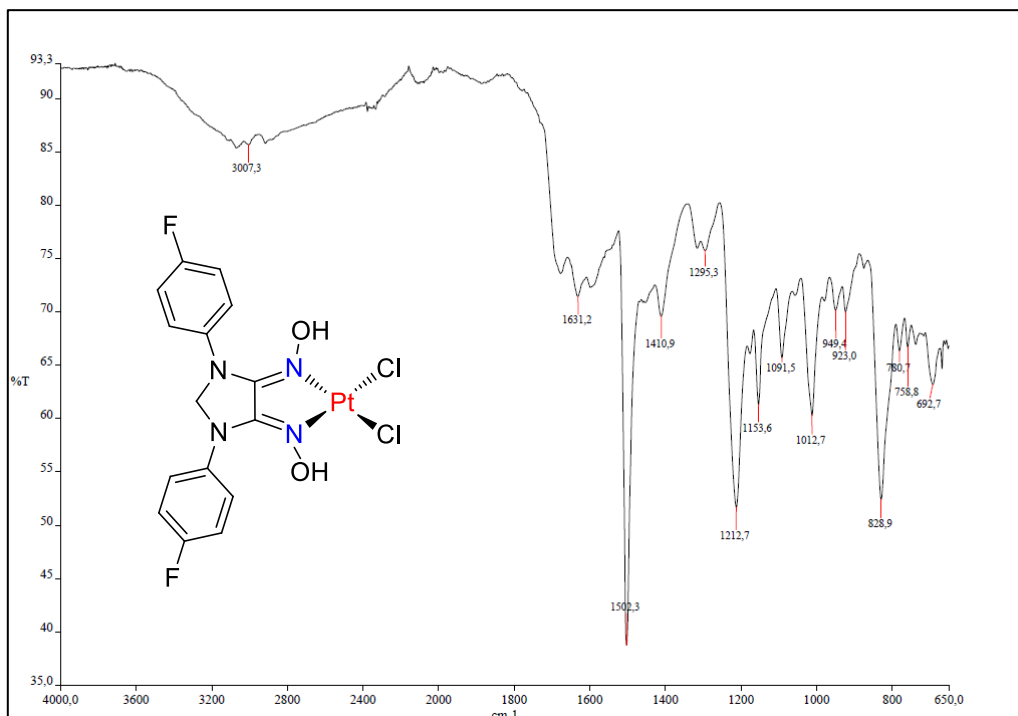
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Figure S31 MS Spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dione dioxime

3

mono-Pt(II) complex ($L_{1a}Pt-m$)



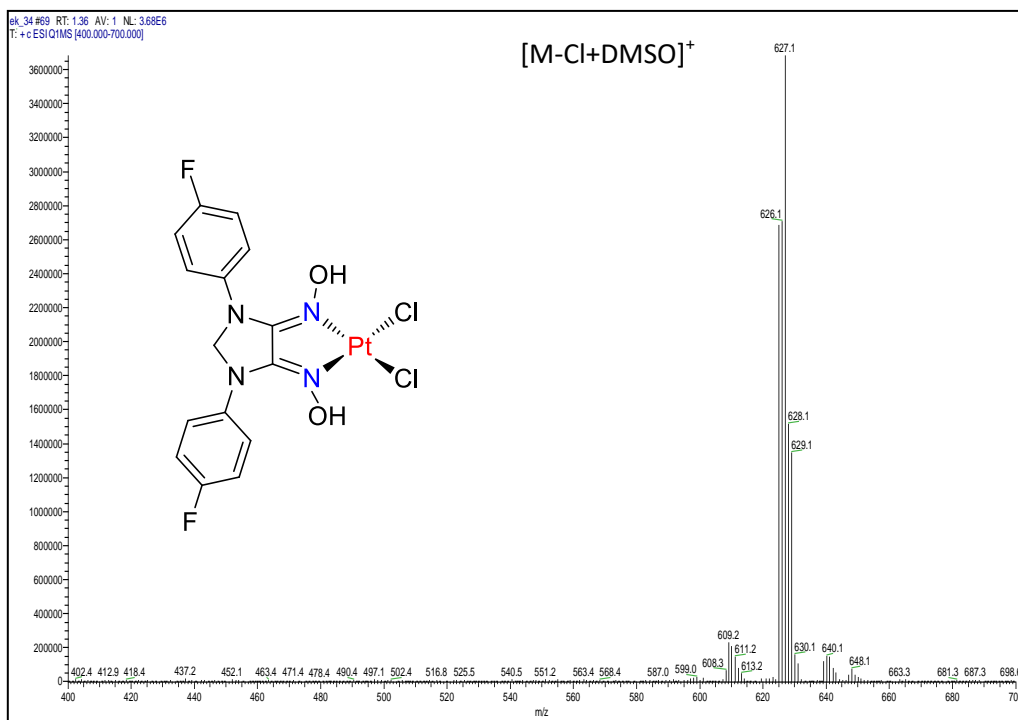
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5

Figure S32 FT-IR Spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-dione

6

dioxime mono-Pt(II) complex ($L_{1b}Pt-m$)

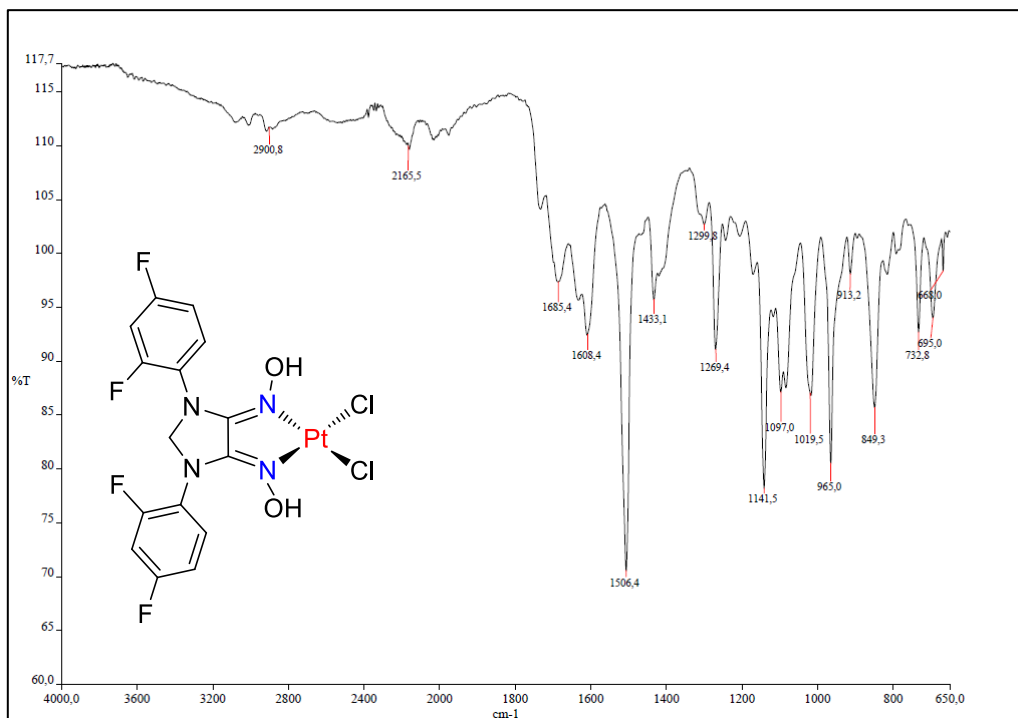


1

2 **Figure S33** MS Spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-dione

3

dioxime mono-Pt(II) complex (L_{1b}Pt-m)

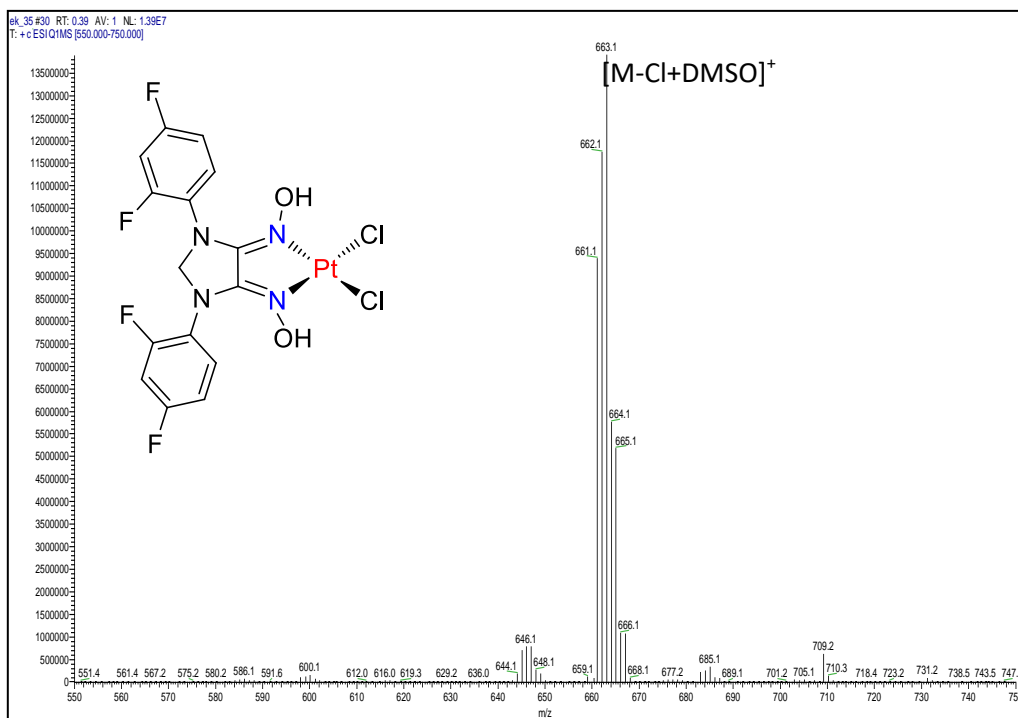


4

5 **Figure S34** FT-IR Spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-

6

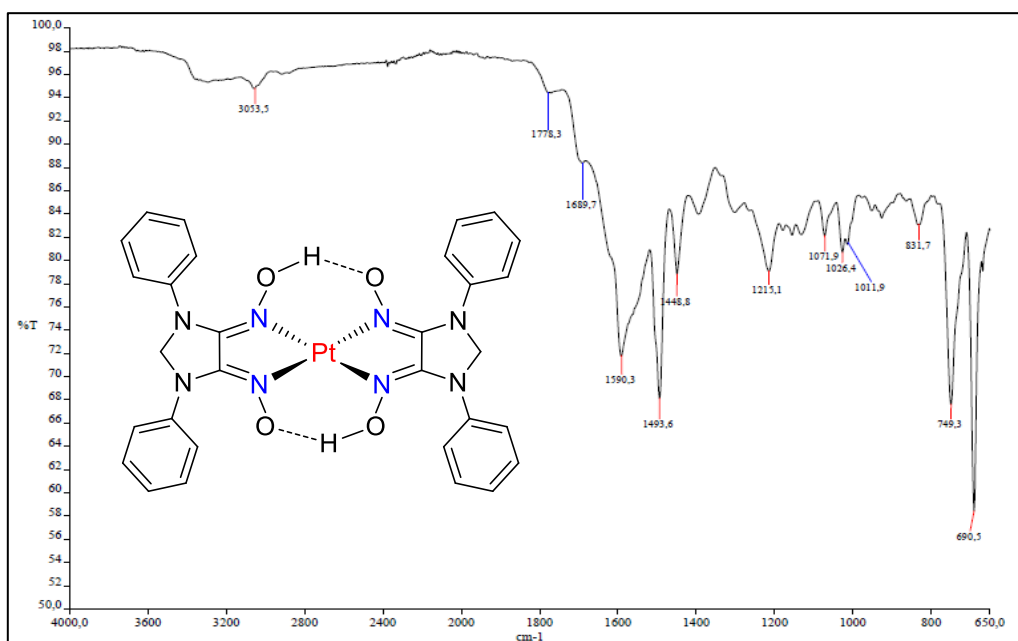
dione dioxime mono-Pt(II) complex (L_{1c}Pt-m)



1

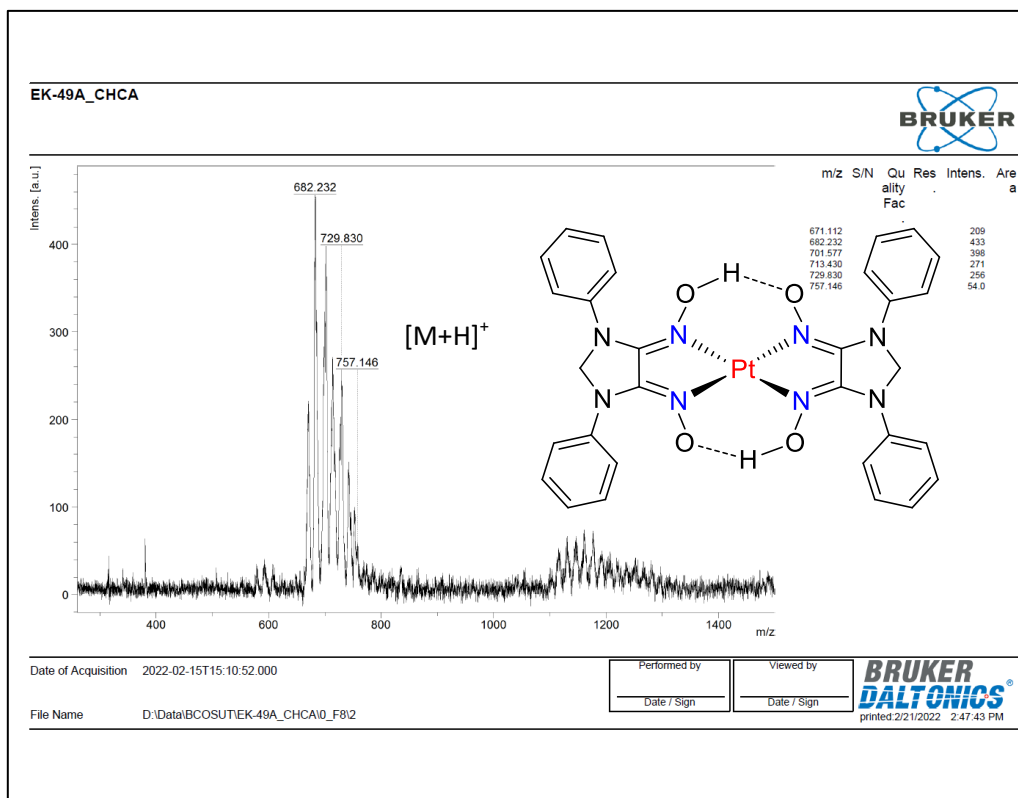
2 **Figure S35** MS Spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-
3 dione dioxime mono-Pt(II) complex ($L_{1c}Pt-m$)

4 **2.8 Bis-Platinum Complexes of *vic*-dioximes**



5

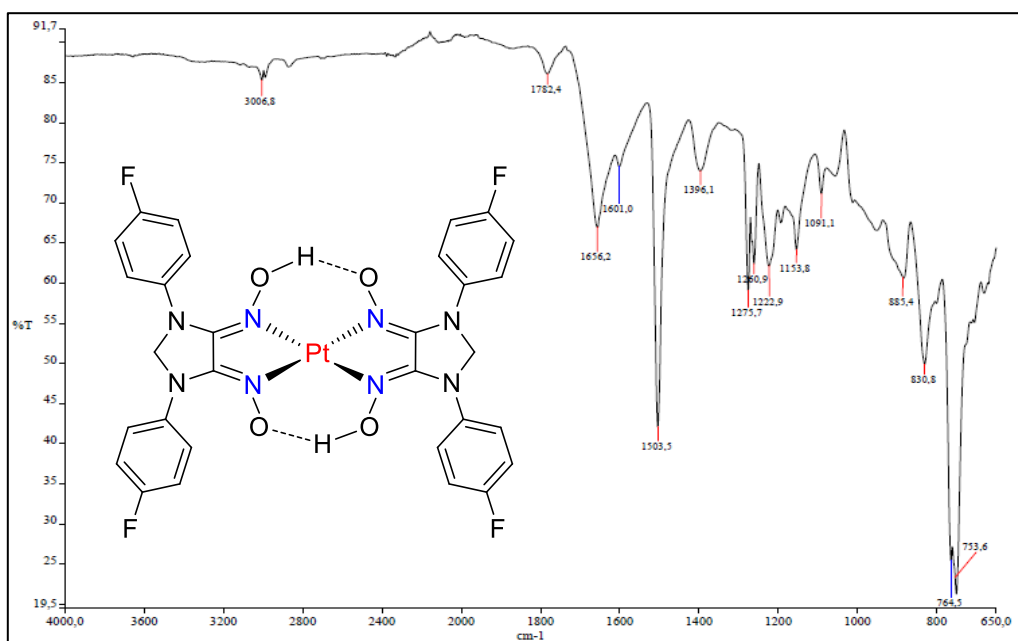
6 **Figure S36** FT-IR Spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dione dioxime
7 bis-Pt(II) complex ($L_{1a}Pt-b$)



1

2 **Figure S37** MS Spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dione dioxime bis-

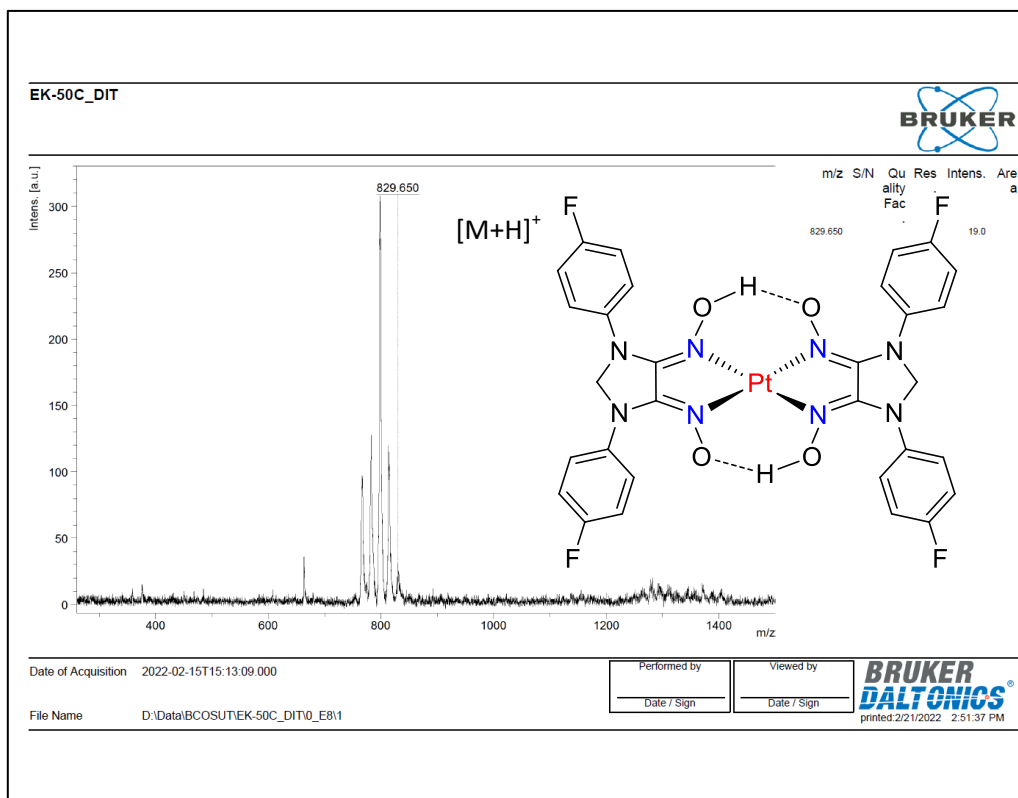
3 Pt(II) complex (L_{1a}Pt-b)



4

5 **Figure S38** FT-IR Spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-dione

6 dioxime bis-Pt(II) complex (L_{1b}Pt-b)

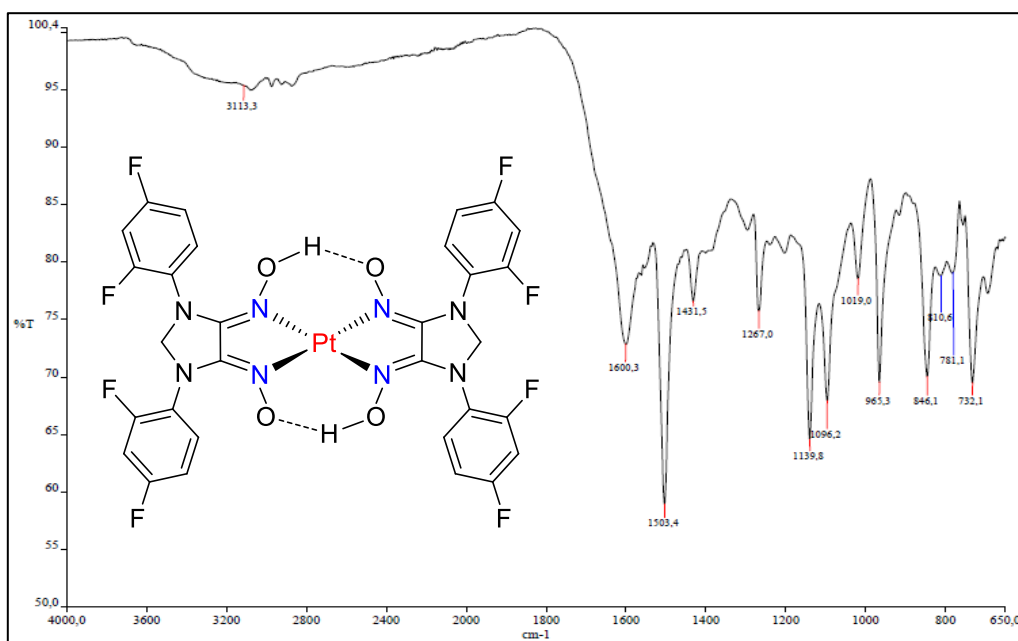


1

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

3

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

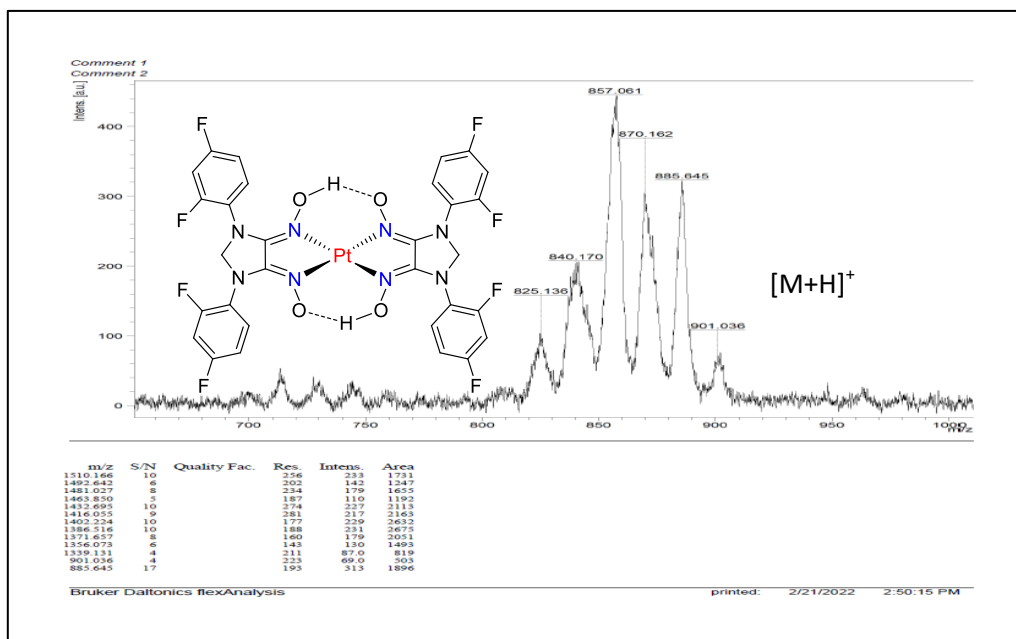


4

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

6

dione dioxime bis-Pt(II) complex ($L_{1c}Pt-b$)

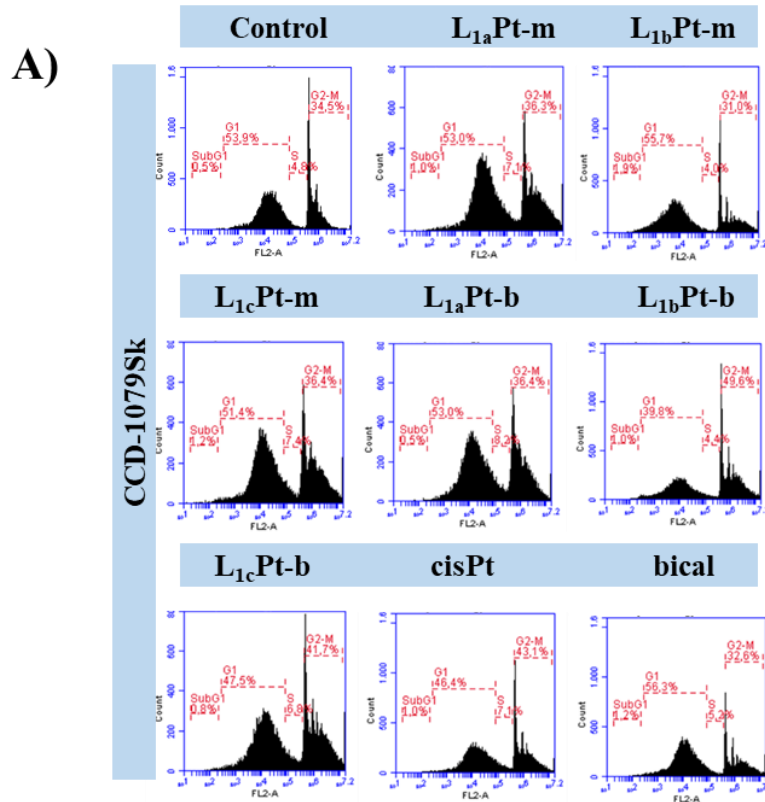


1
2 **Figure S41** MS Spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-
3 dione dioxime bis-Pt(II) complex (L_{1c}Pt-b)

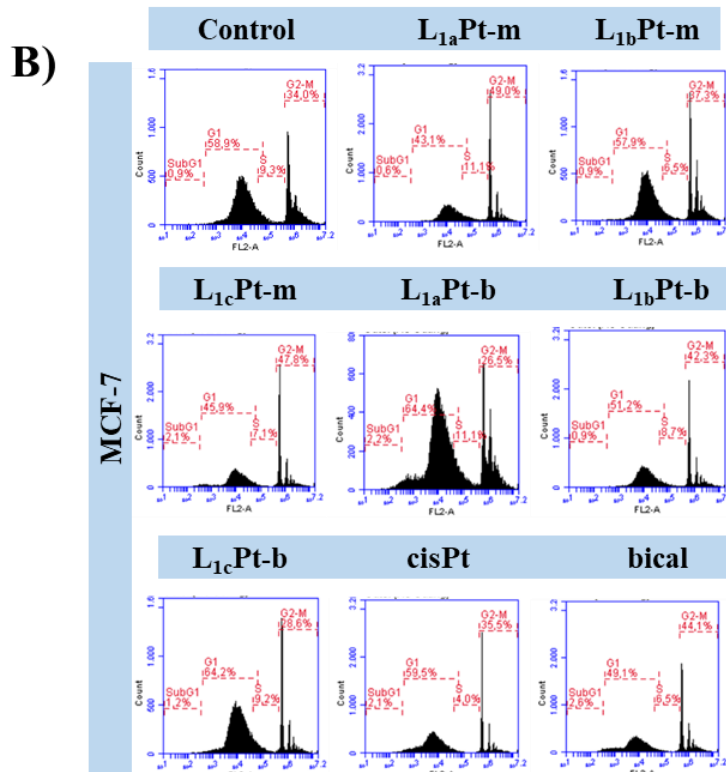
4
5 **3. Materials and methods for biological studies**

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

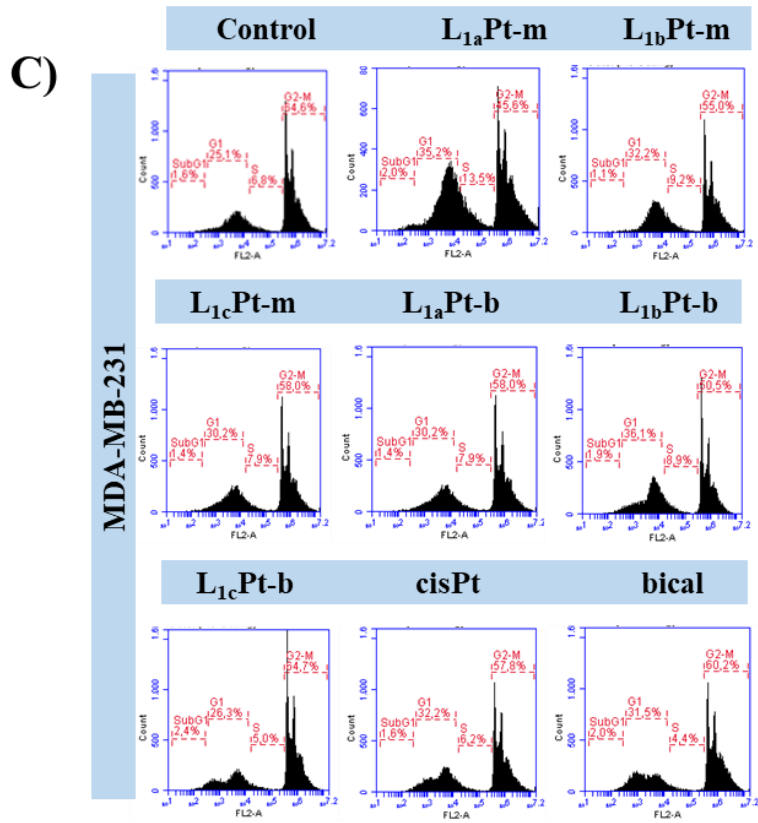
1 4. Supplementary figures for biological studies



2



3



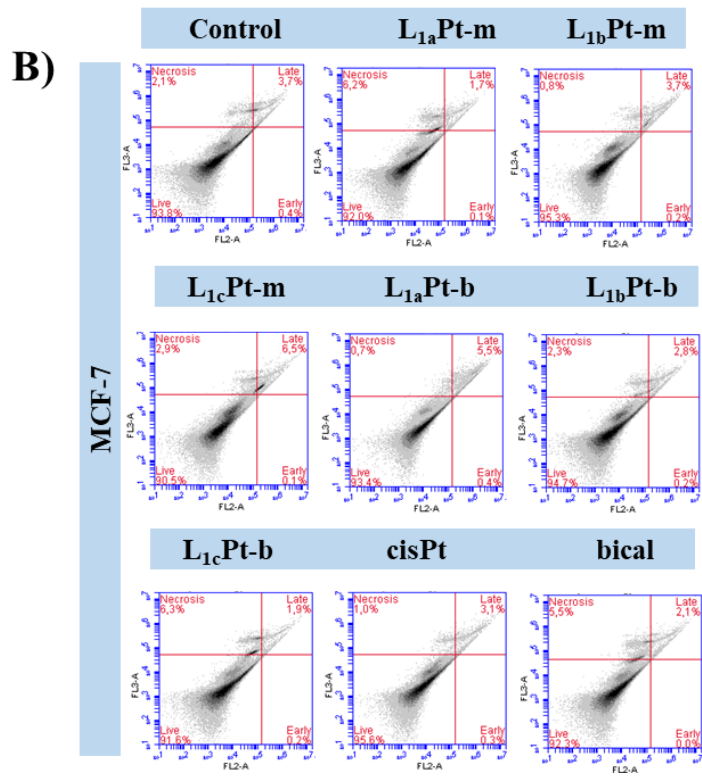
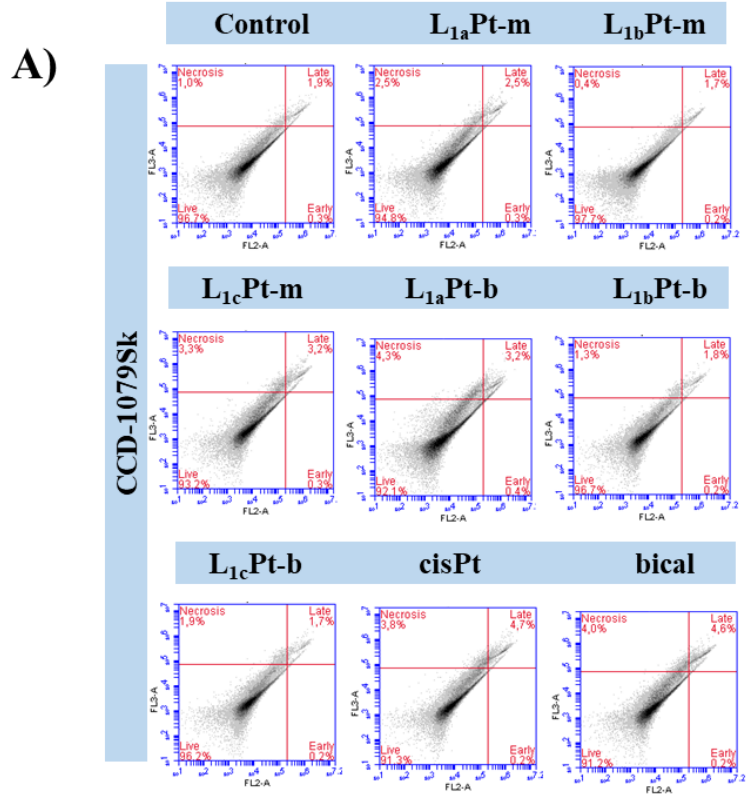
1

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

3

C) MDA-MB-231 cells.

4



1

2

3

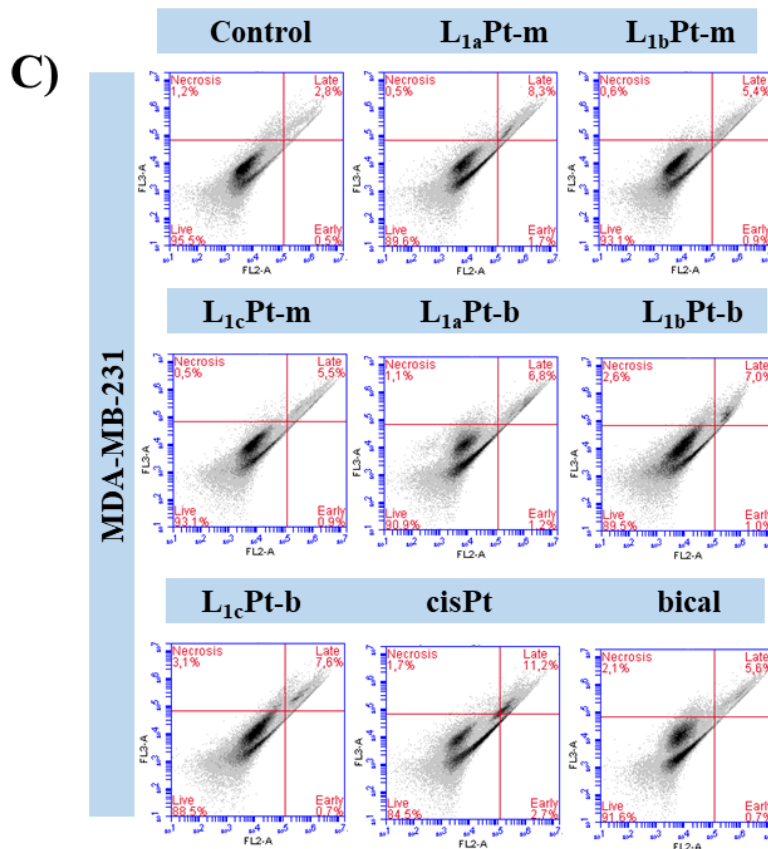


Figure S43 Apoptosis assay results of compounds treated A) CCD-1079Sk B) MCF-7 and C) MDA-MB-231 cells.

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4 <https://doi.org/10.1107/S002188980600731X>
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