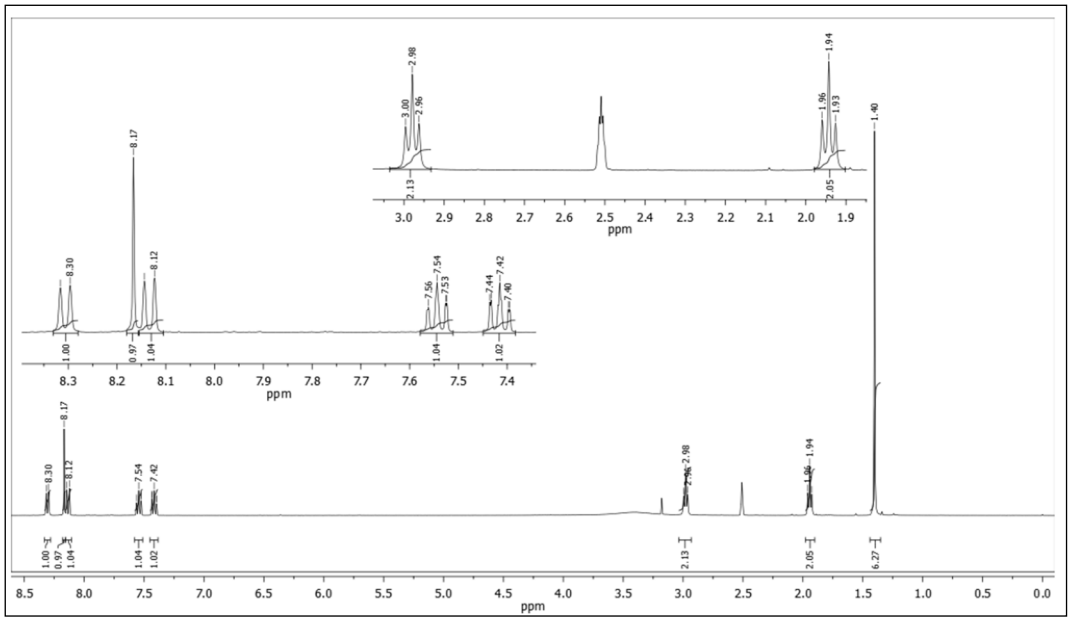
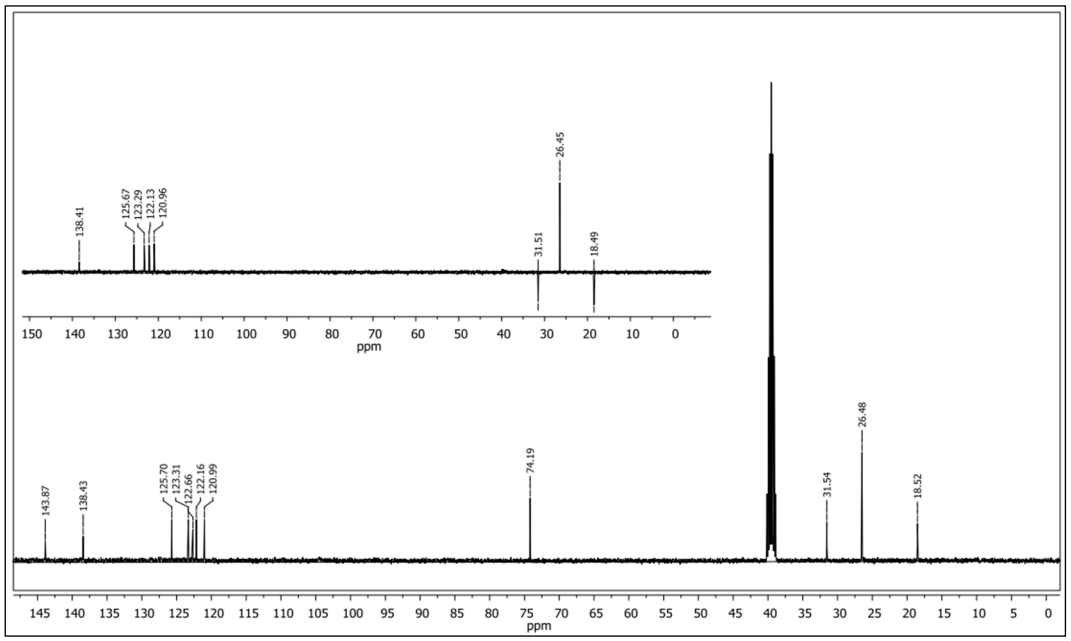
SUPPLEMENTARY INFORMATION

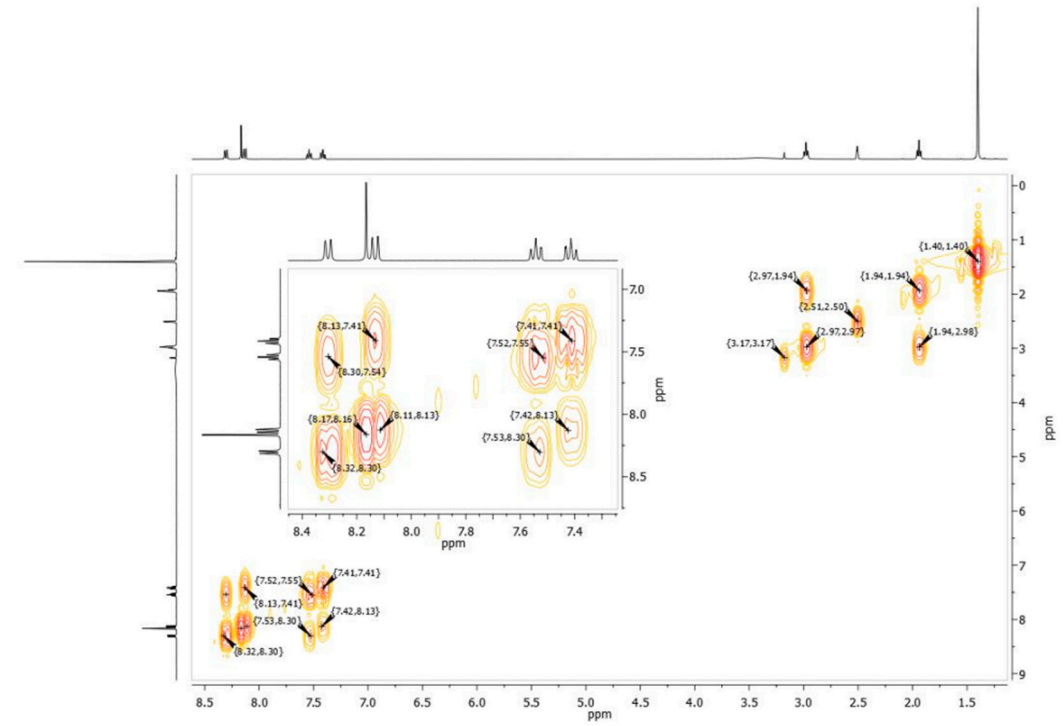
Naphth[1,2-*d*]imidazoles bioactive from β-Lapachone: fluorescent probes and cytotoxic agents to cancer cells

Victória Laysna dos Anjos Santos [1], Arlan de Assis Gonsalves [1, 2], Délis Galvão Guimarães [3], Sidney Silva Simplicio [1], Helinando Pequeno de Oliveira [2], Lara Polyana Silva Ramos [4], Marcília Pinheiro da Costa [4], Fátima de Cássia Evangelista de Oliveira [5], Claudia Pessoa [5], Cleônia Roberta Melo Araújo [1,*]

1. Molecular structure elucidation of synthesized naphth[1,2-*d*]imidazoles (IM1–IM7).



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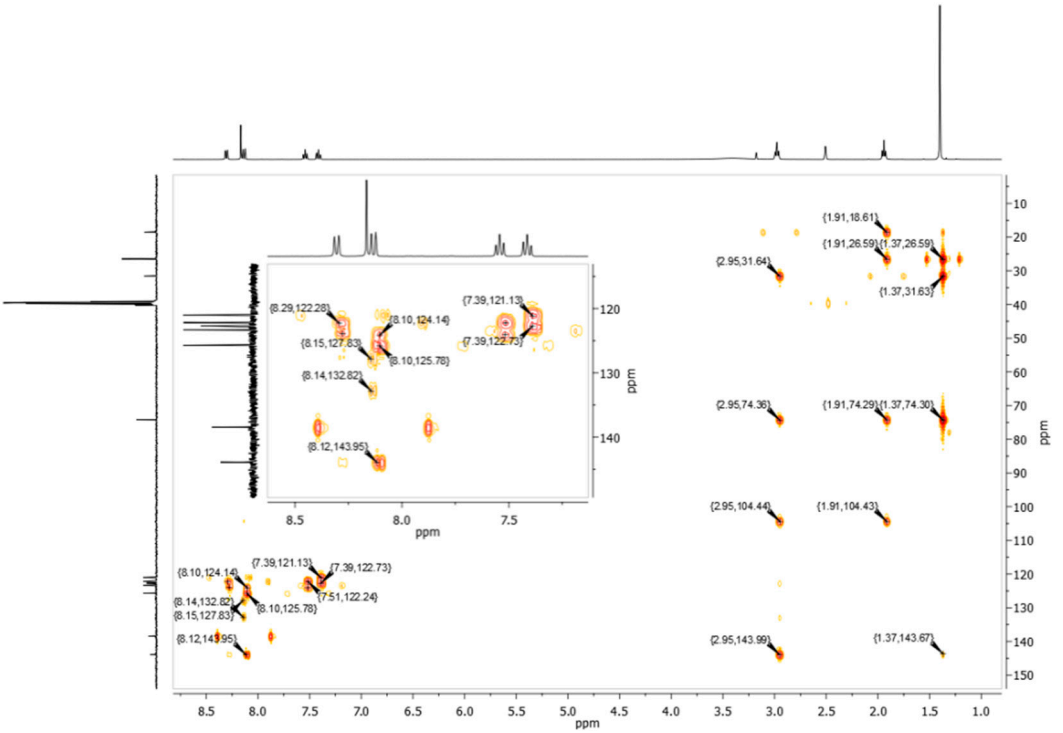
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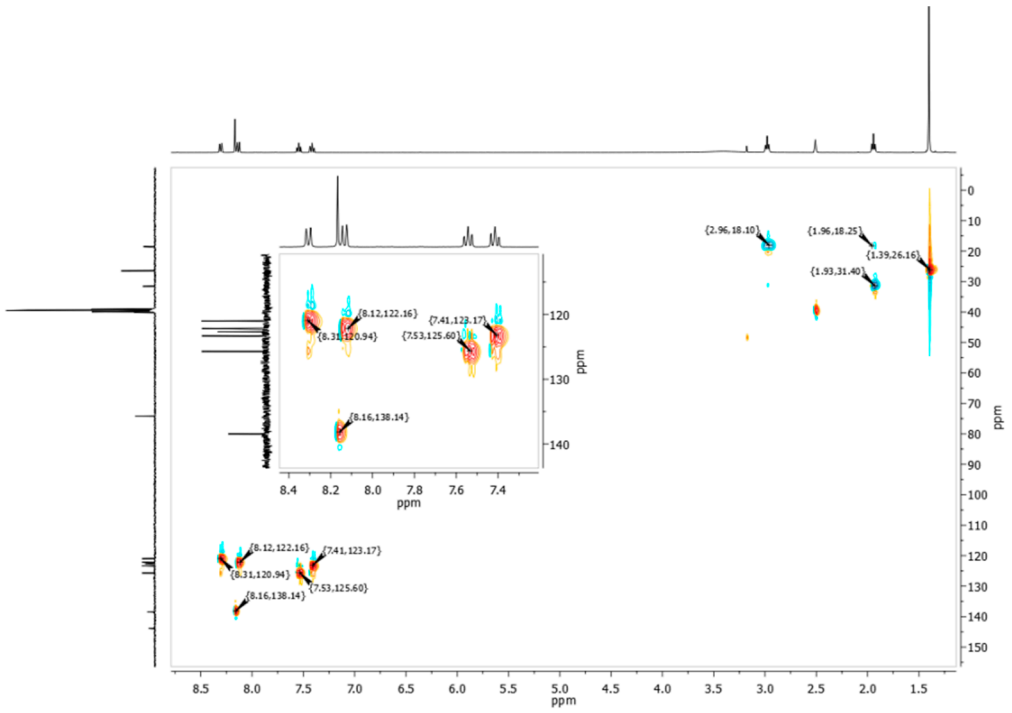
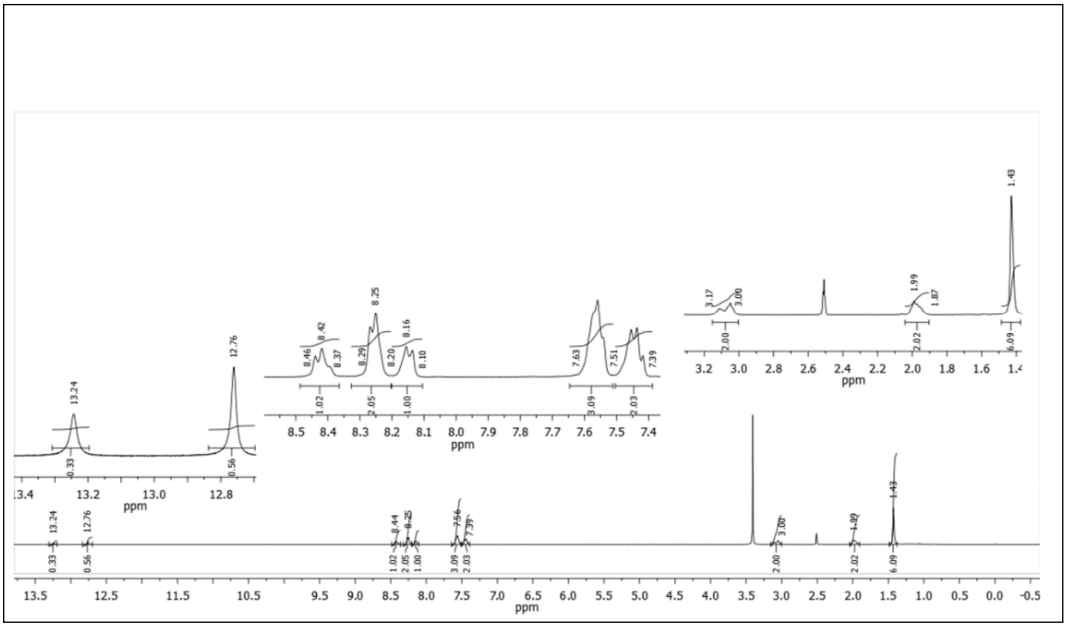
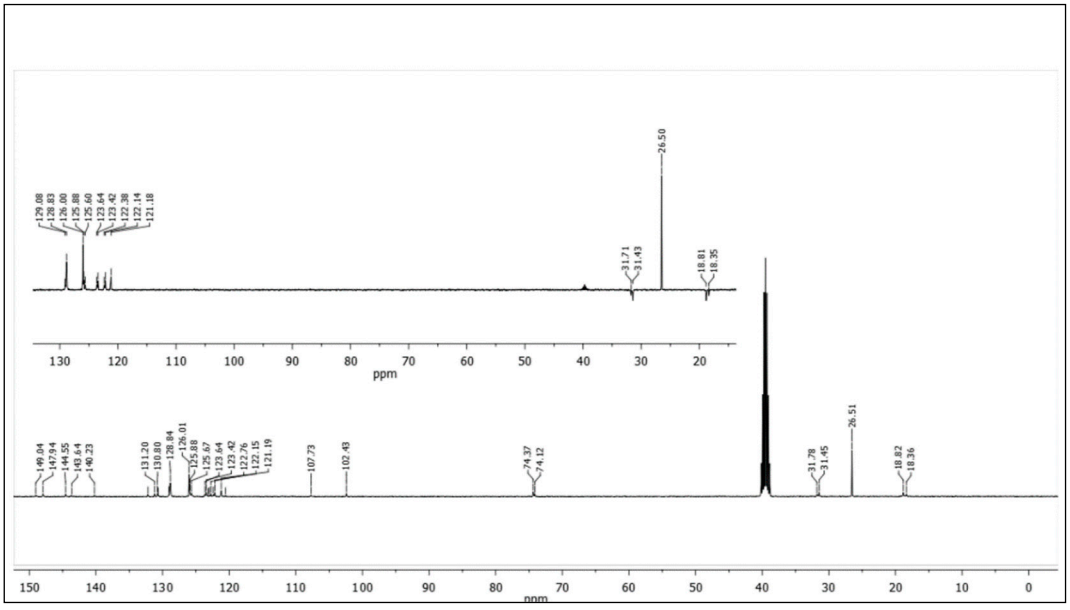
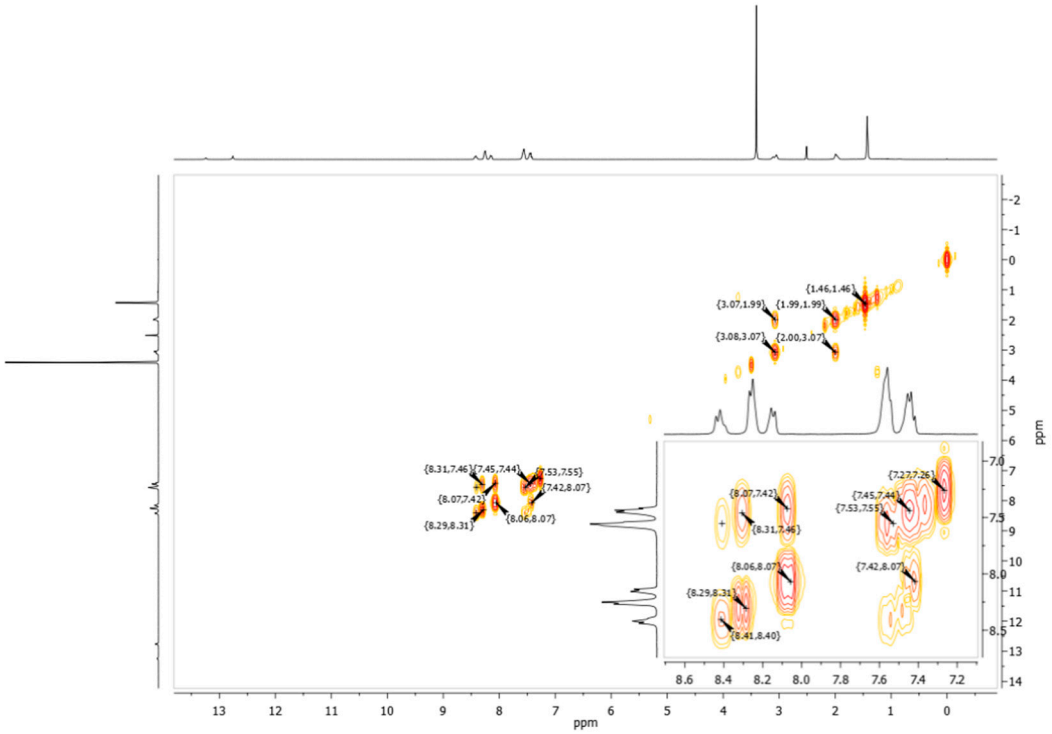


Figure S1. NMR spectra of 4,5-dihydro-6,6-dimethyl-6*H*-2-pyran[*b*-4,3]naphth[1,2-*d*]imidazole (**IM1**) in DMSO-d_6.



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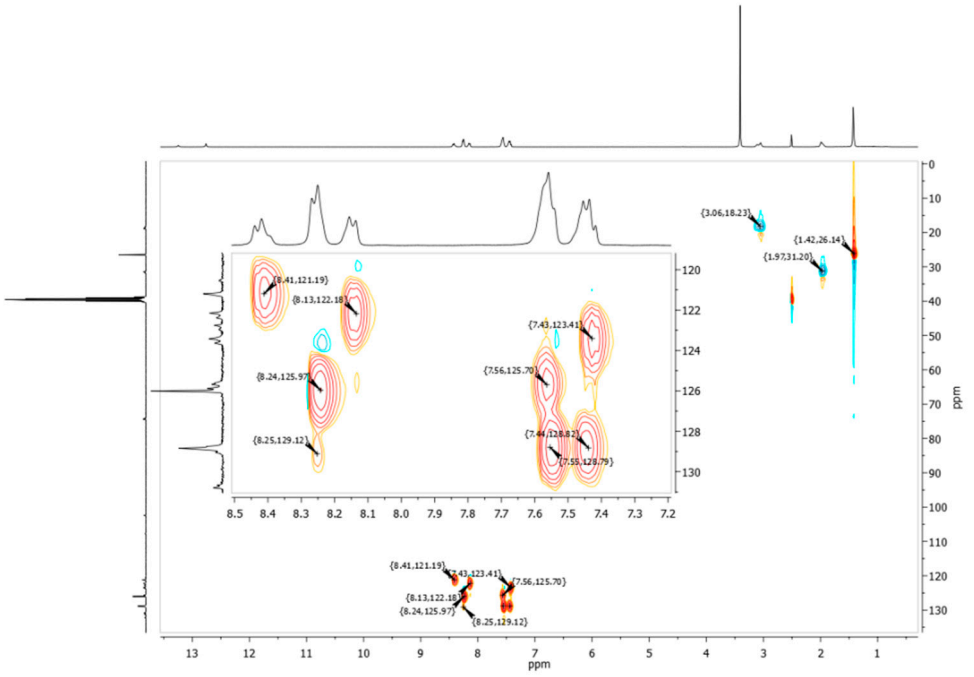
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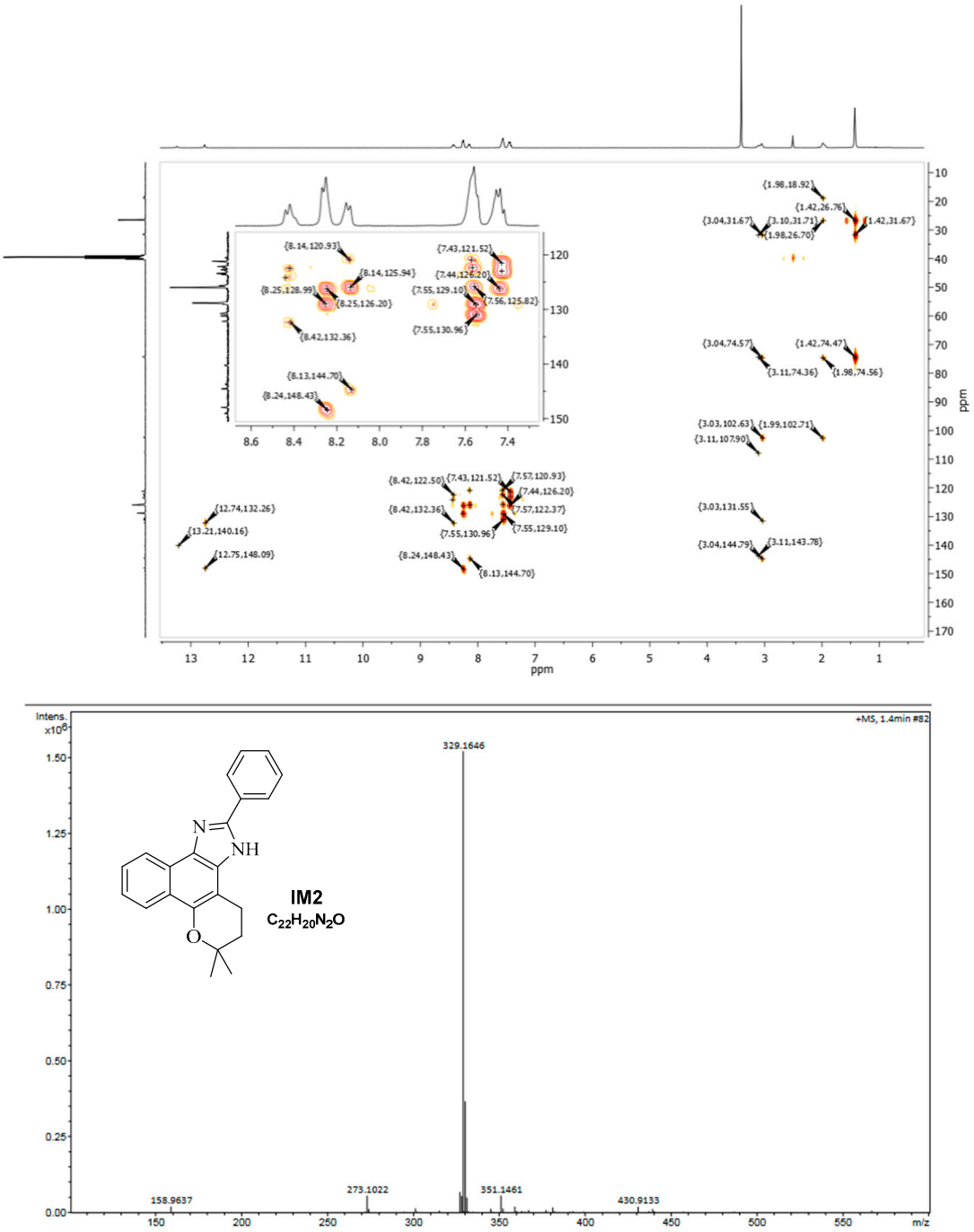
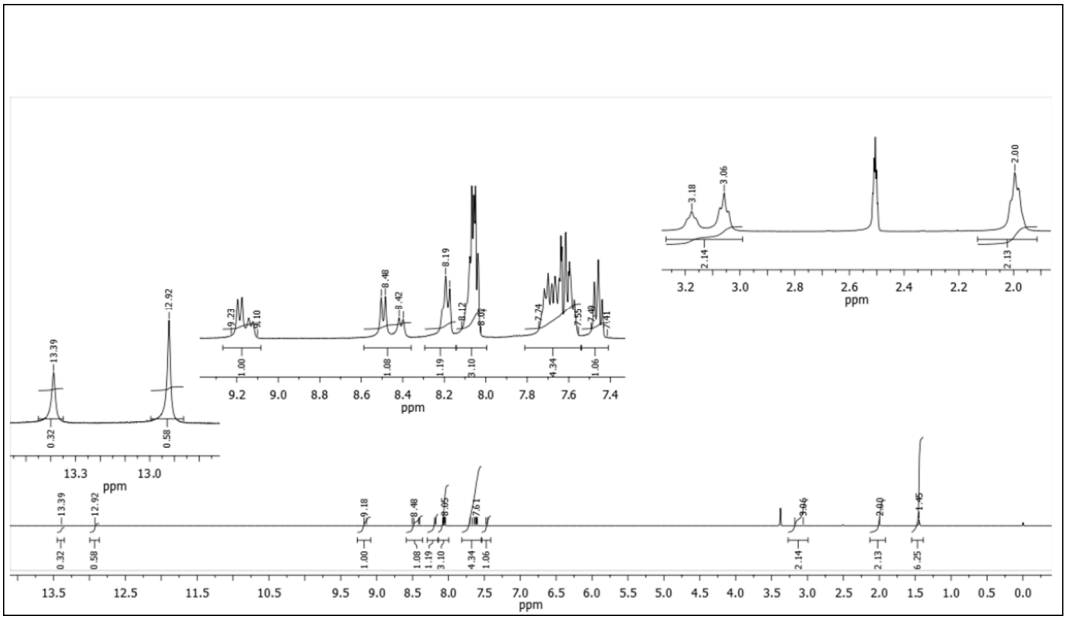


Figure S2. NMR spectra of 4,5-dihydro-6,6-dimethyl-6*H*-2-(phenyl)-pyran[*b*-4,3]naphth[1,2-*d*]imidazole (**IM2)** in DMSO-d_6 and ESI-MS.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8.05
7.61
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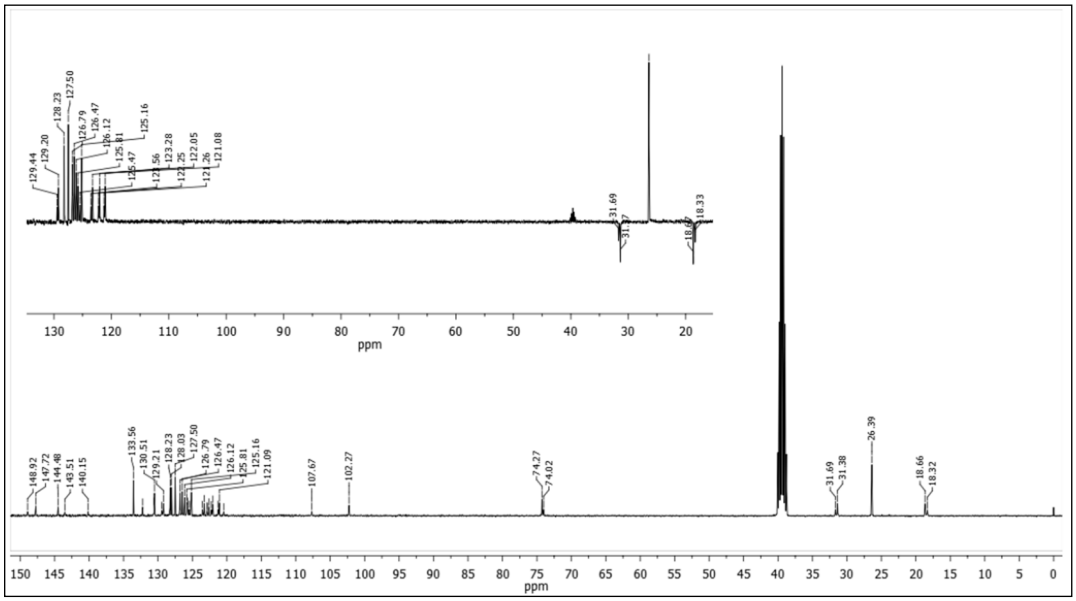
2.00
ppm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144.48
143.51
140.15
133.56
130.51
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128.23
128.03
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126.79
126.47
126.12
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74.02
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31.38
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18.32
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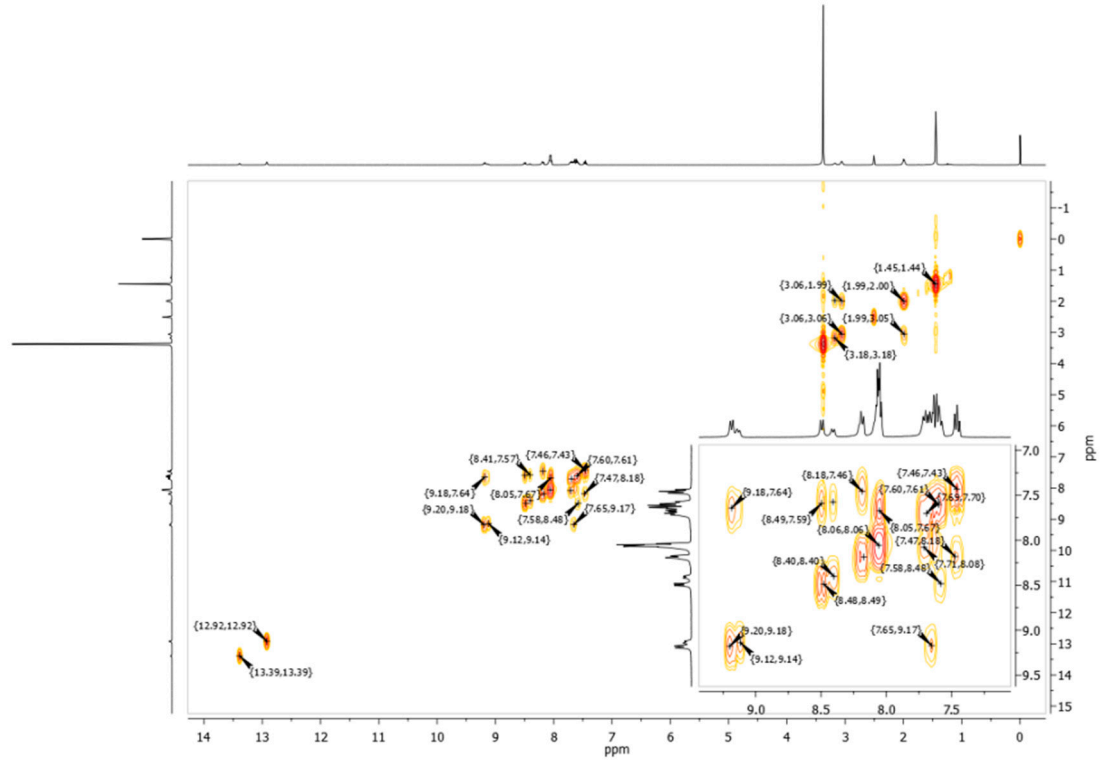
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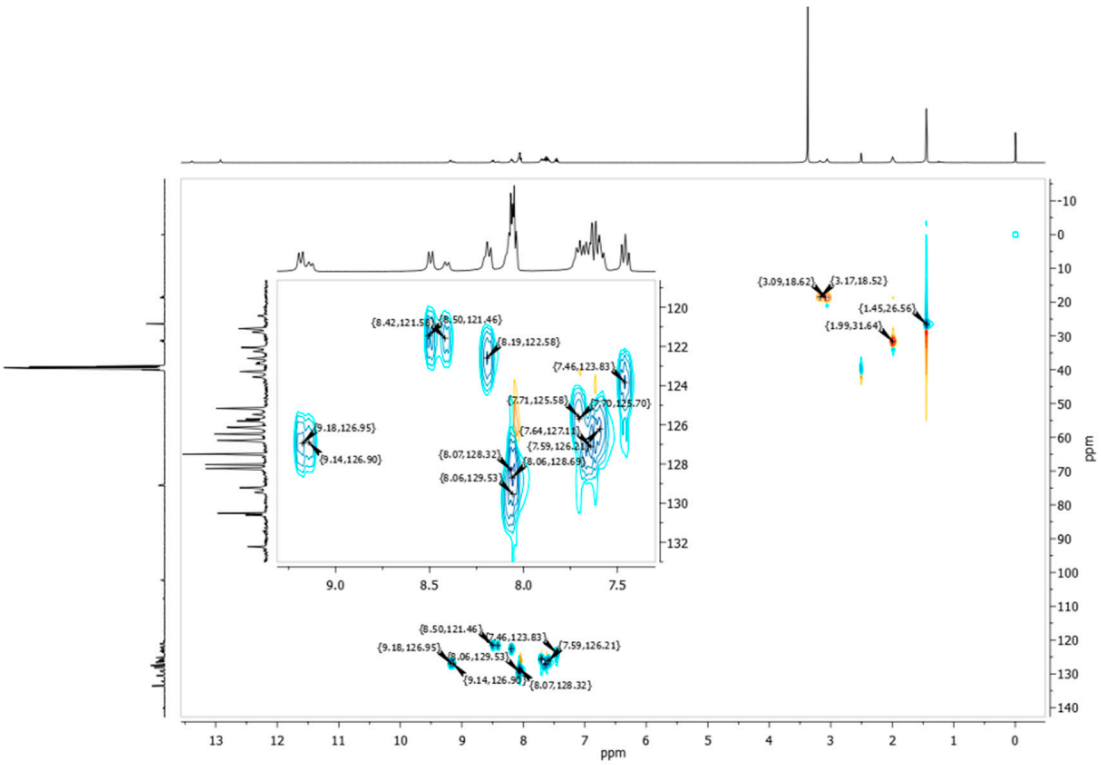
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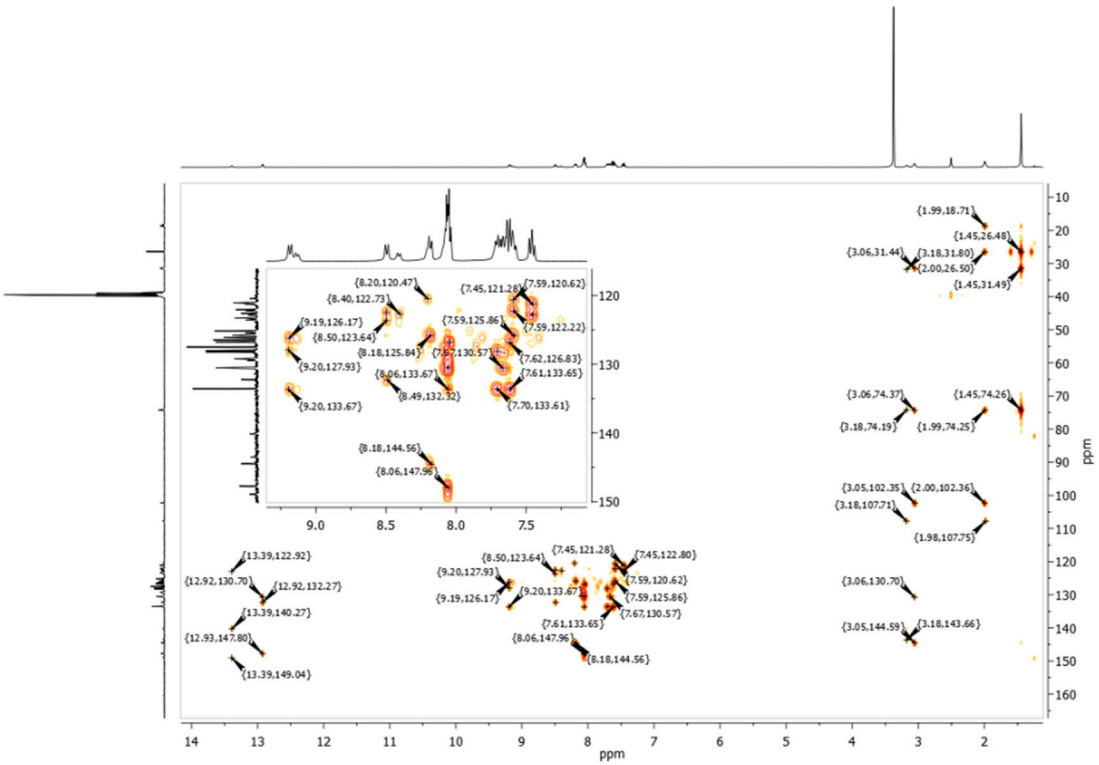


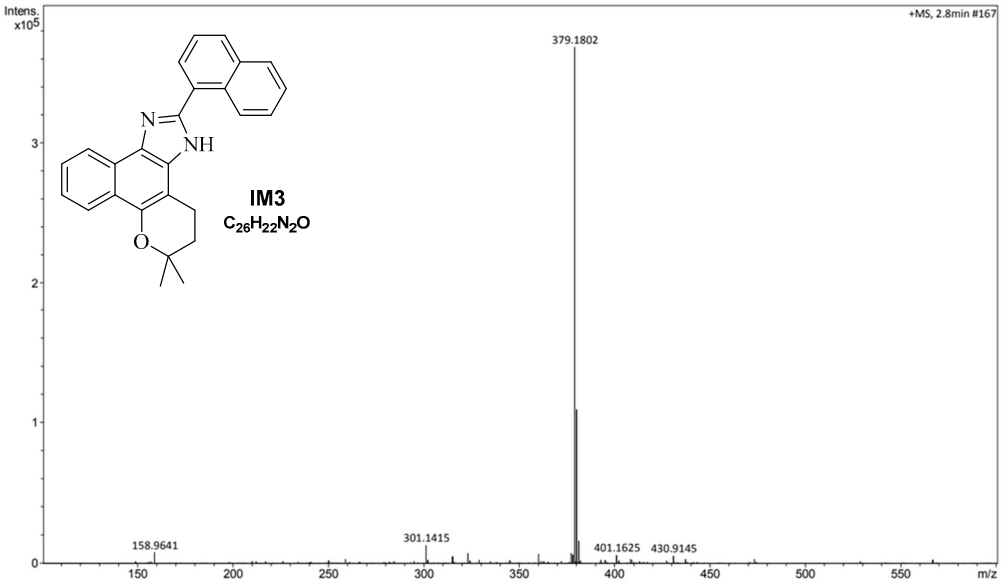
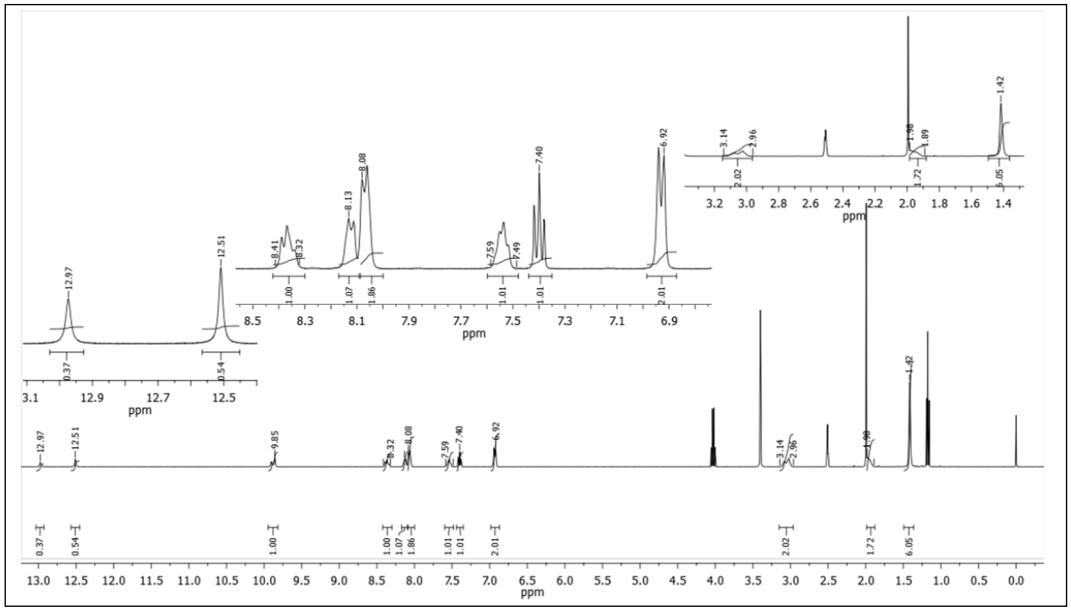
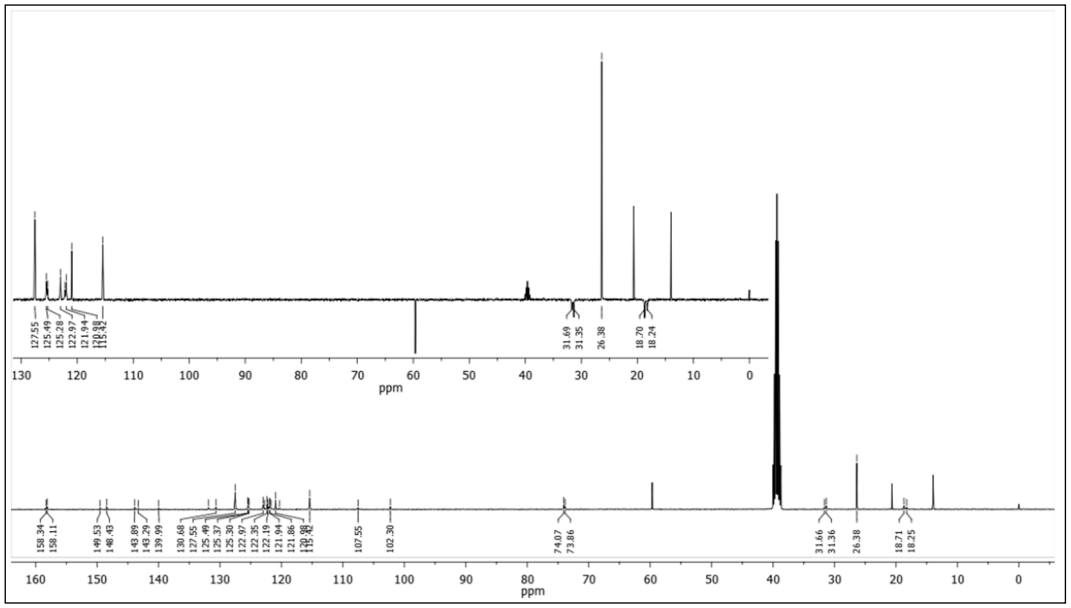
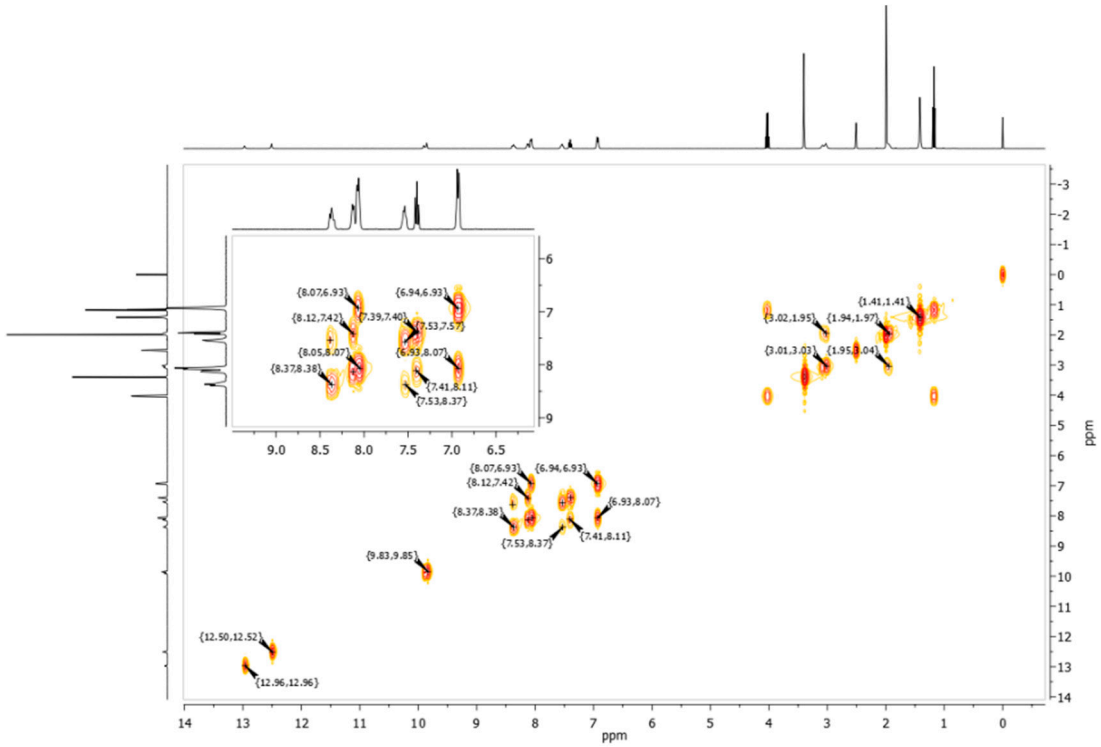


Figure S3. NMR spectra of 4,5-dihydro-6,6-dimethyl-6*H*-2-(naphthalenyl)-pyran[*b*-4,3]naphth[1,2-*d*]imidazole (**IM3)** in DMSO-d_6 and ESI-MS.



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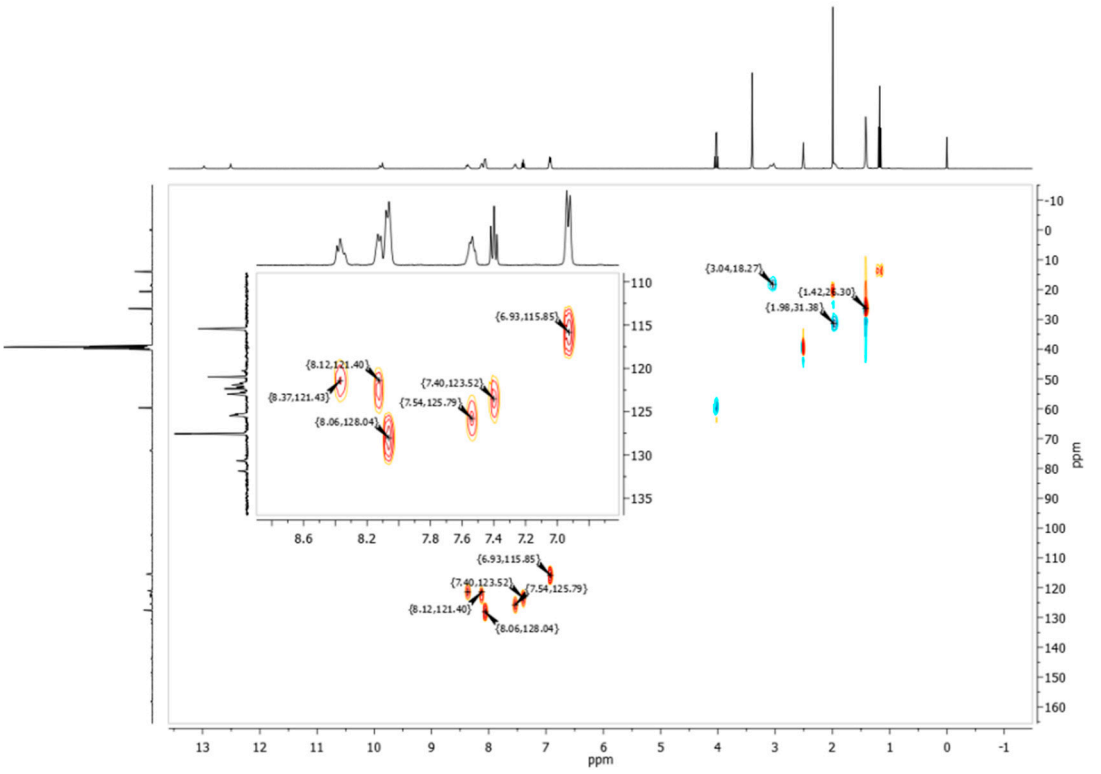
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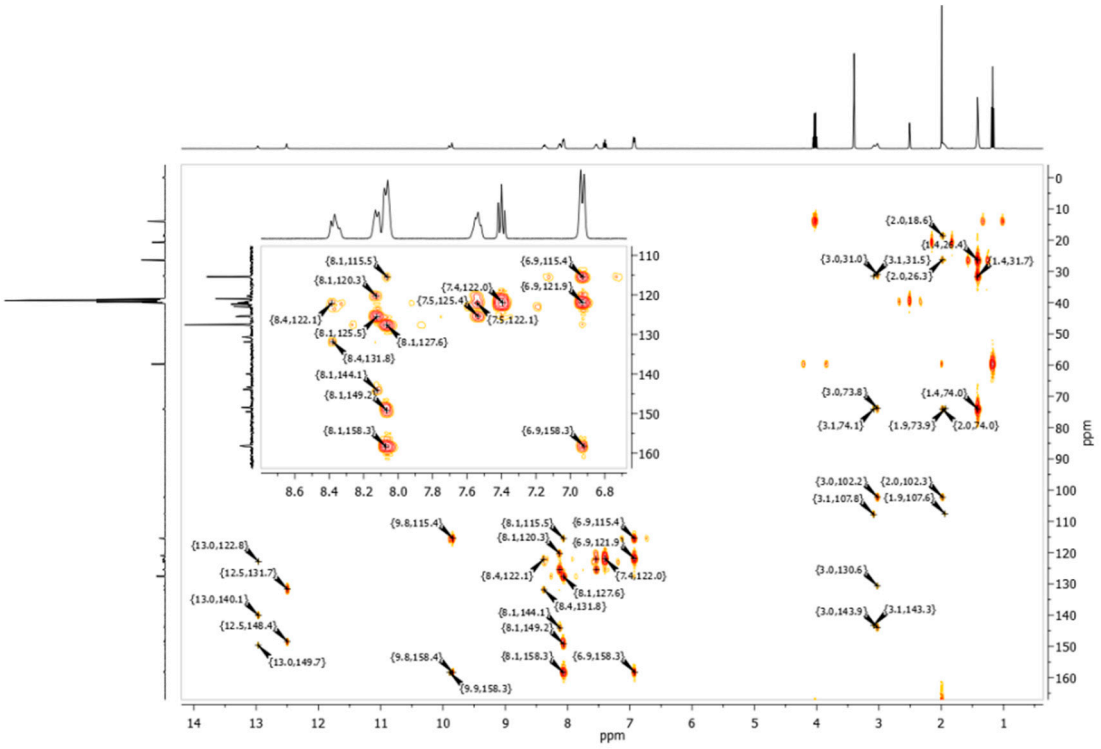


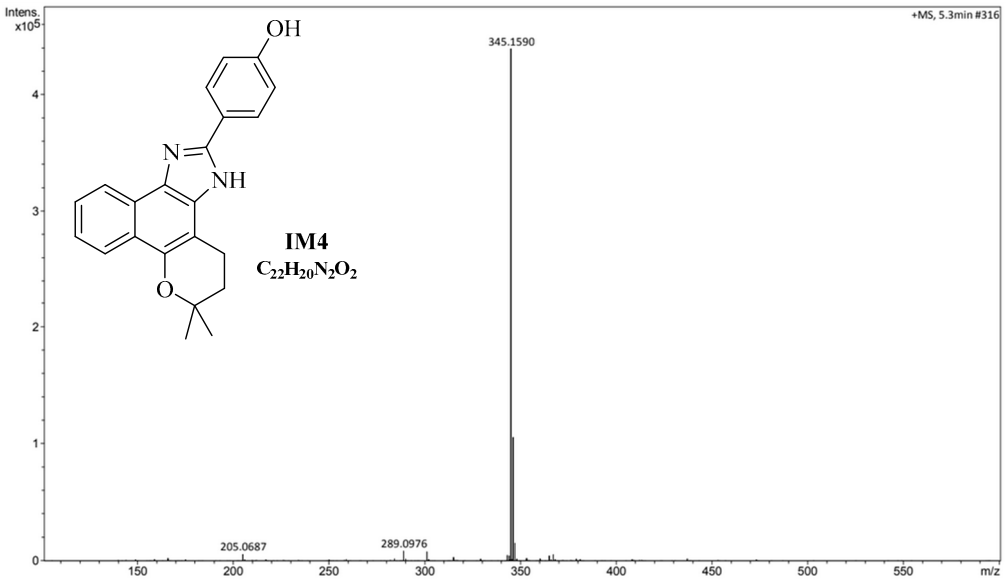
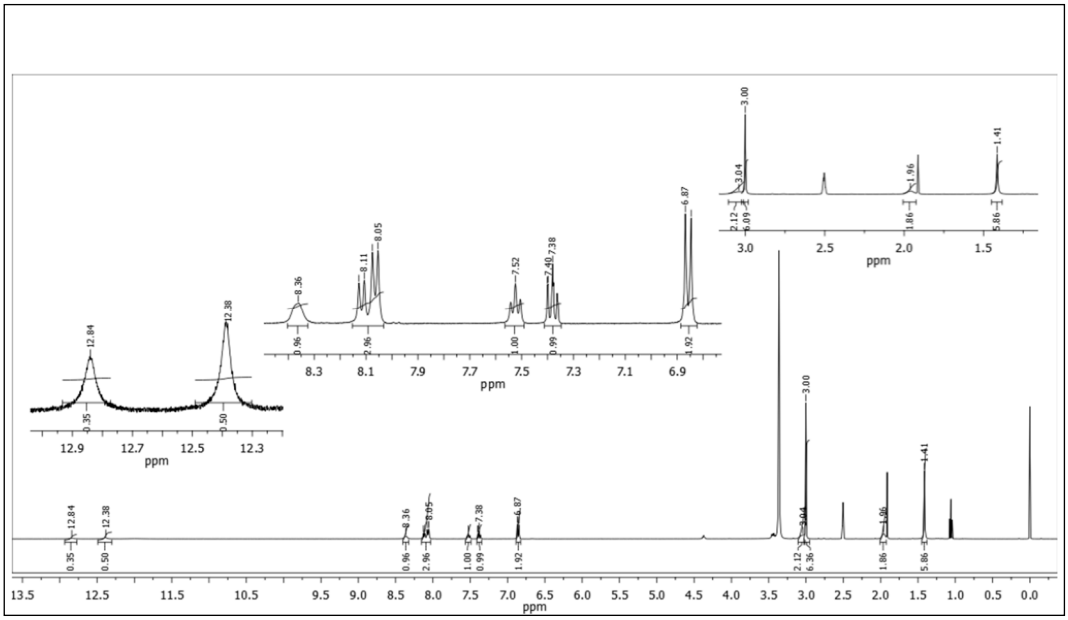


Figure S4. NMR spectra of 4,5-dihydro-6,6-dimethyl-6*H*-2-(4-hidroxyphenyl)-pyran[*b*-4,3]naphth[1,2-*d*]imidazole (**IM4**) in DMSO-d_6 and ESI-MS.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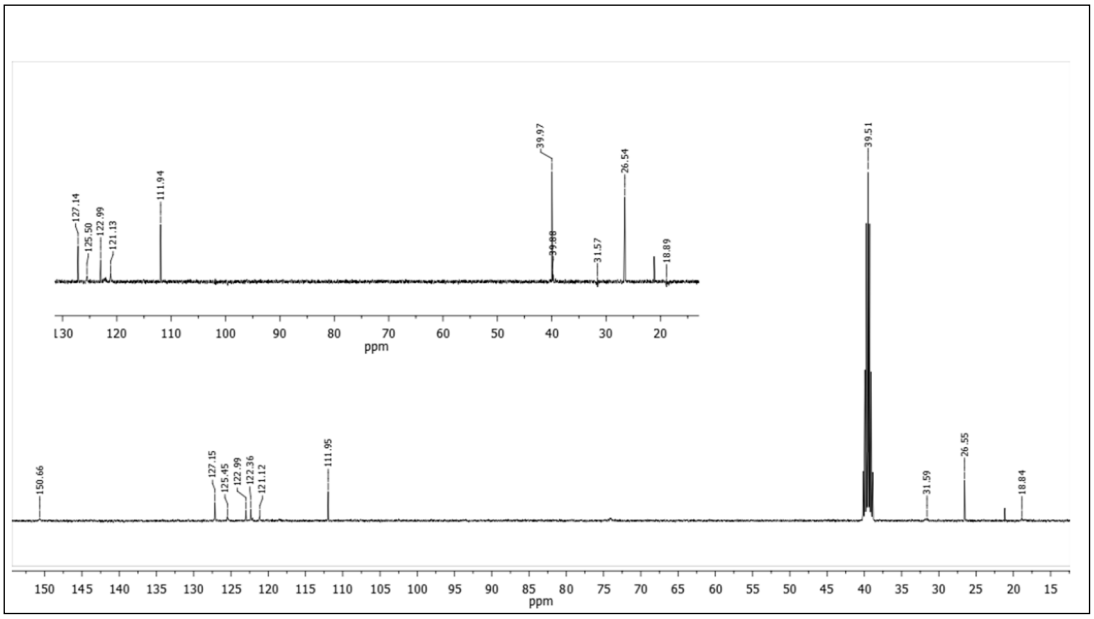
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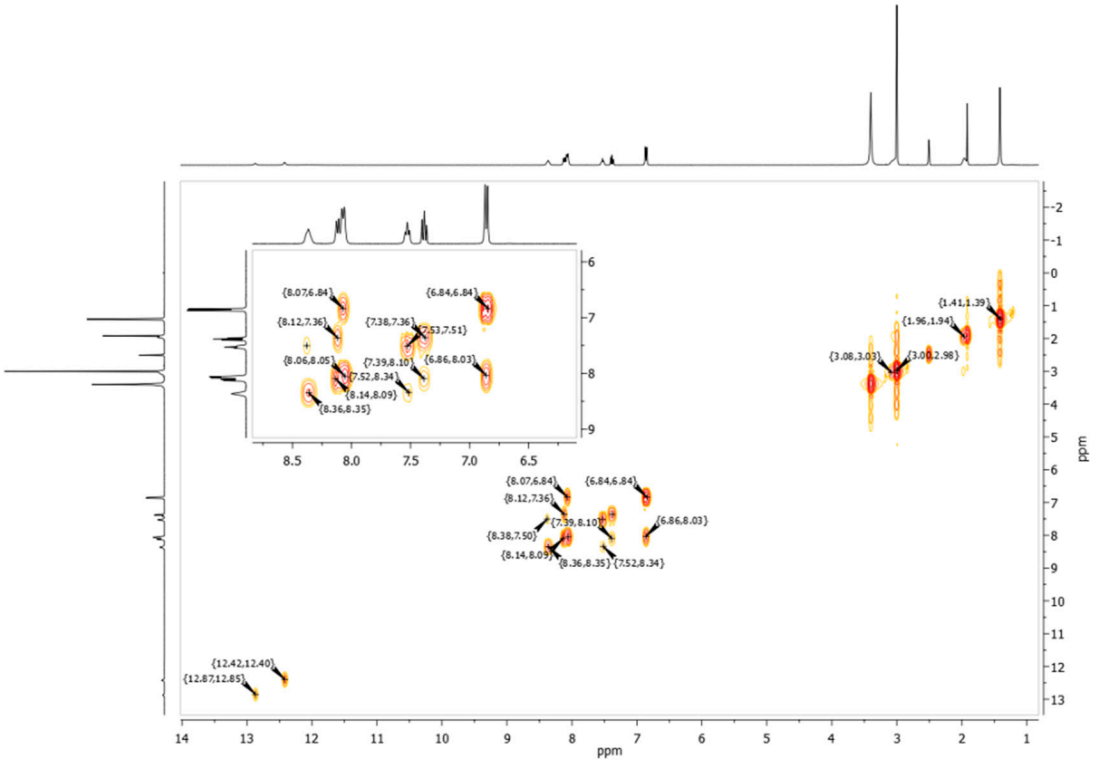
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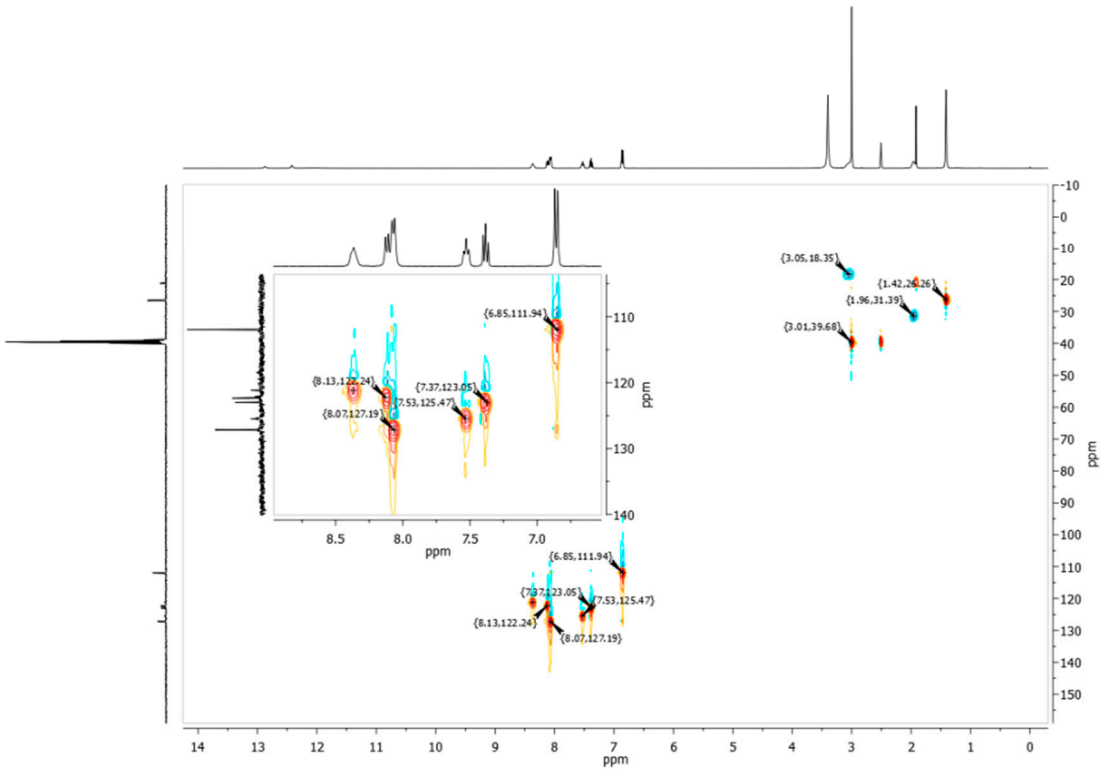
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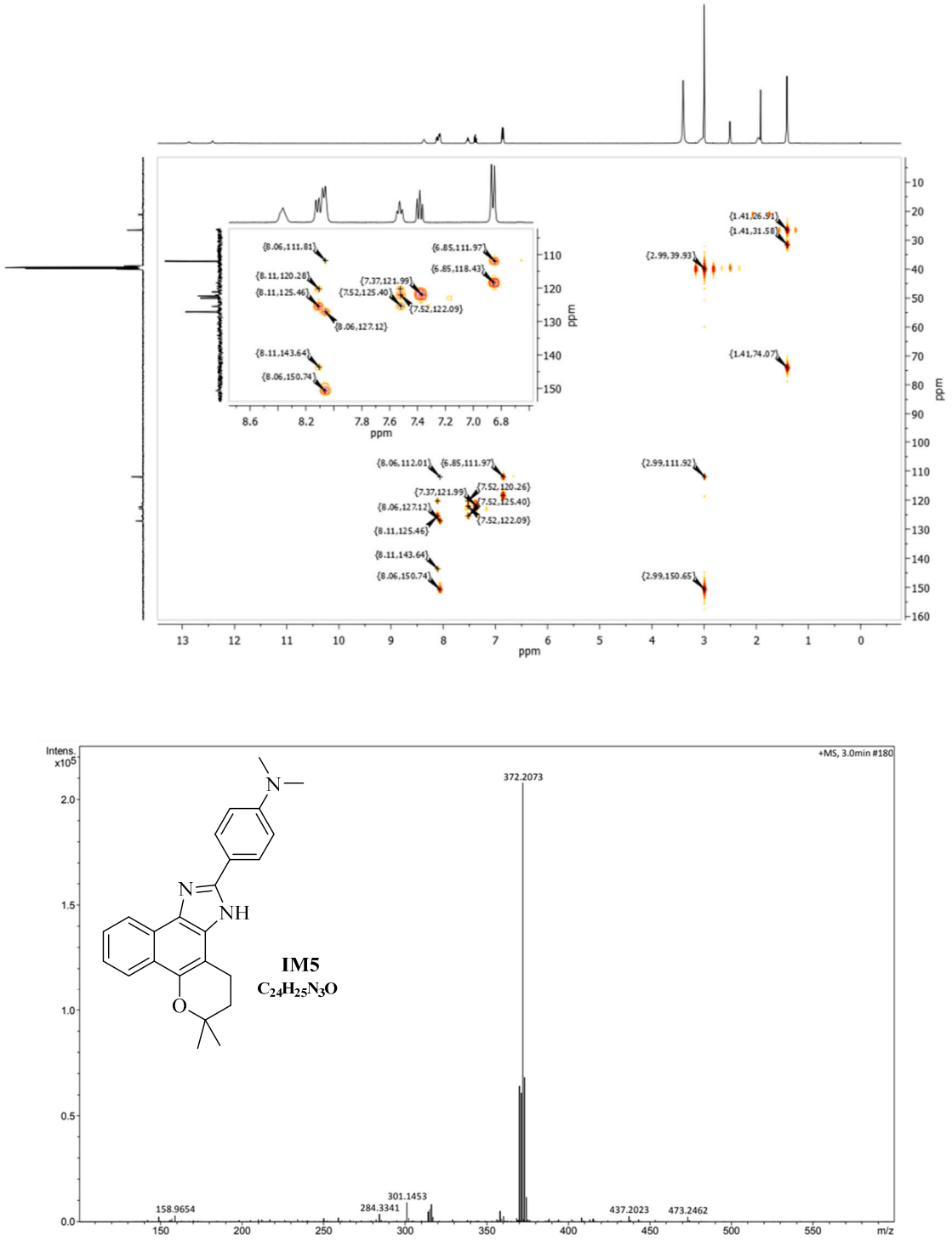
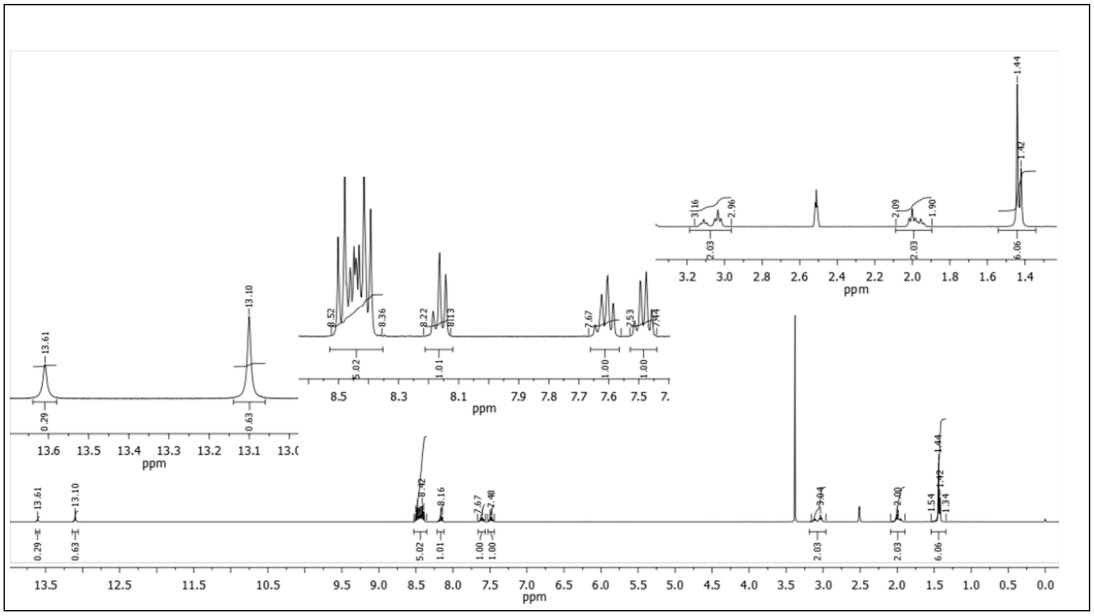
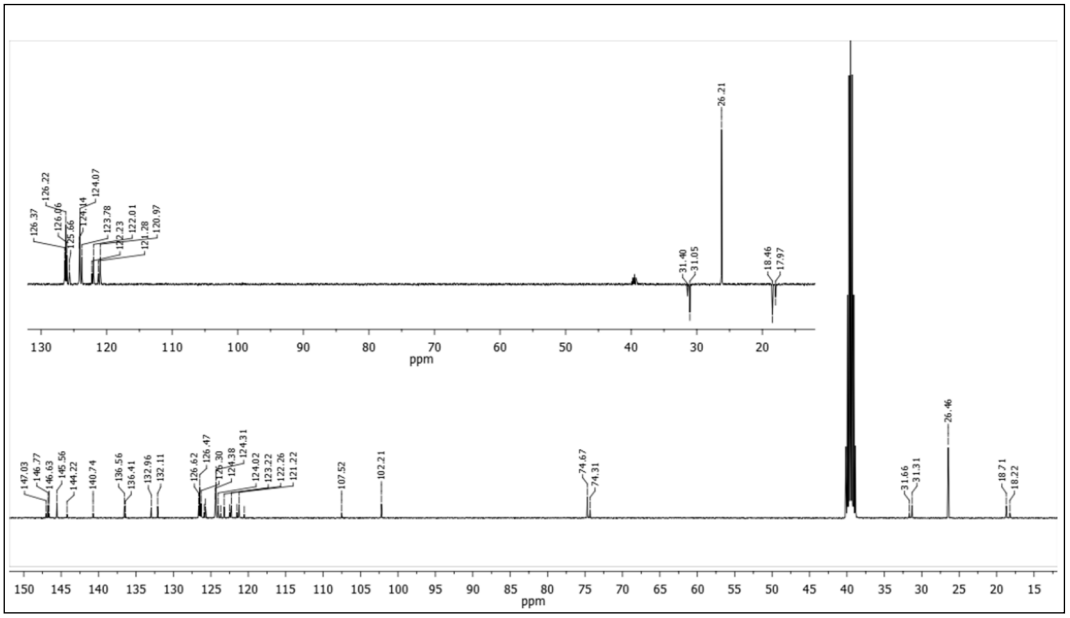
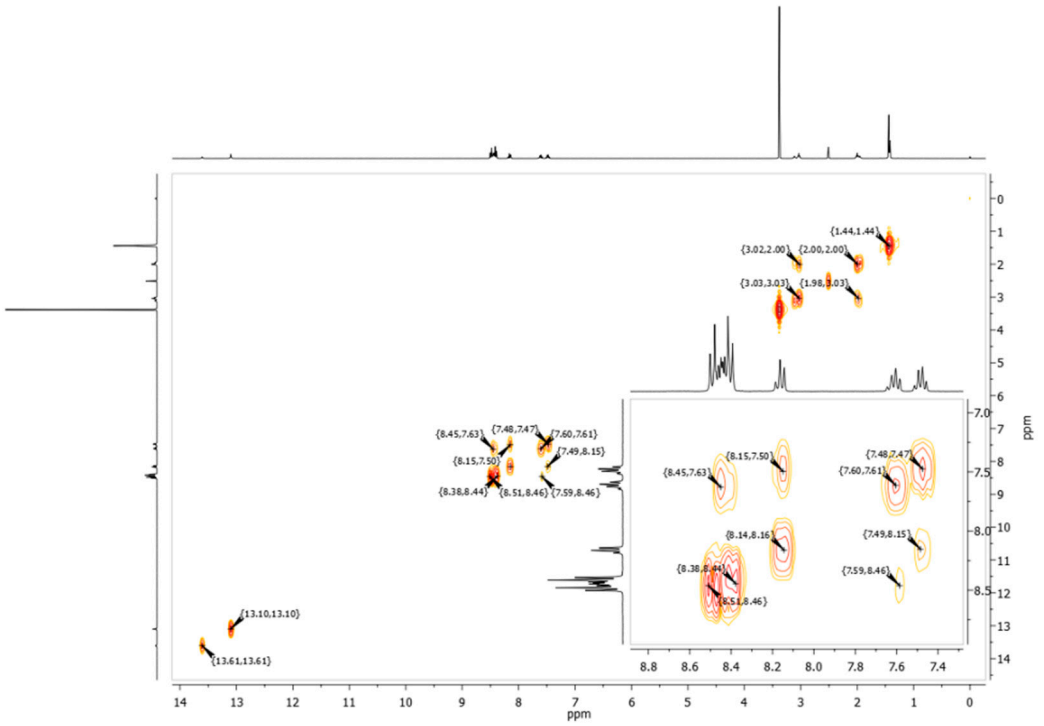


Figure S5. NMR spectra of 4,5-dihydro-6,6-dimethyl-6*H*-2-(4-dimethylaminophenyl)-pyran[*b*-4,3]naphth[1,2-*d*]imidazole **(IM5)** in DMSO-d_6 and ESI-MS.



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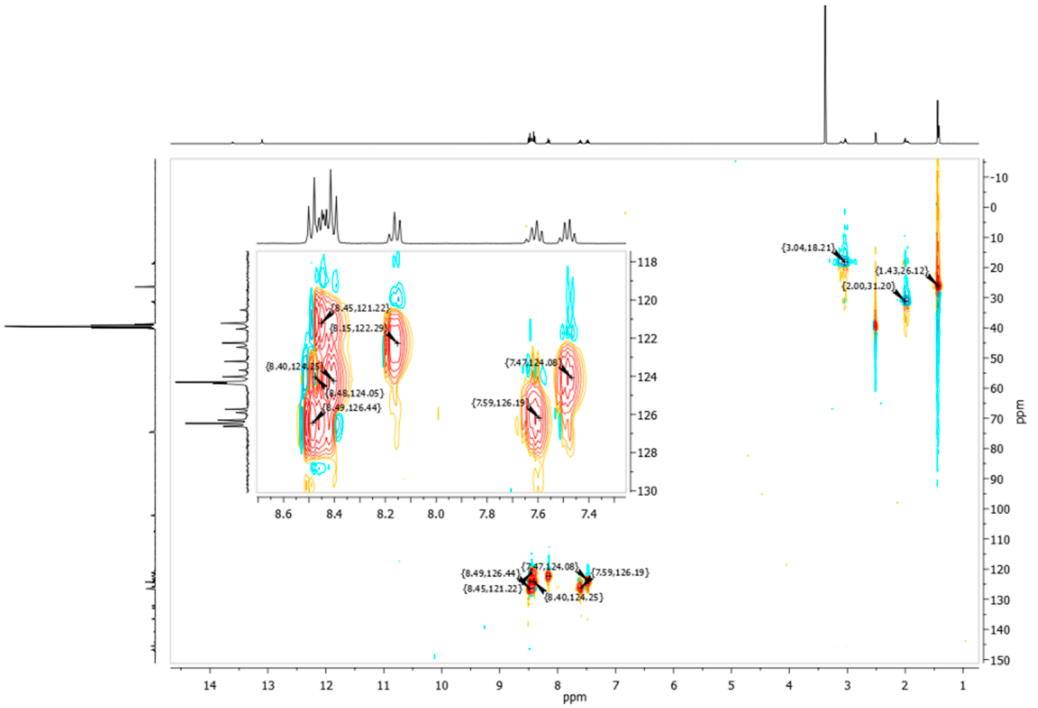
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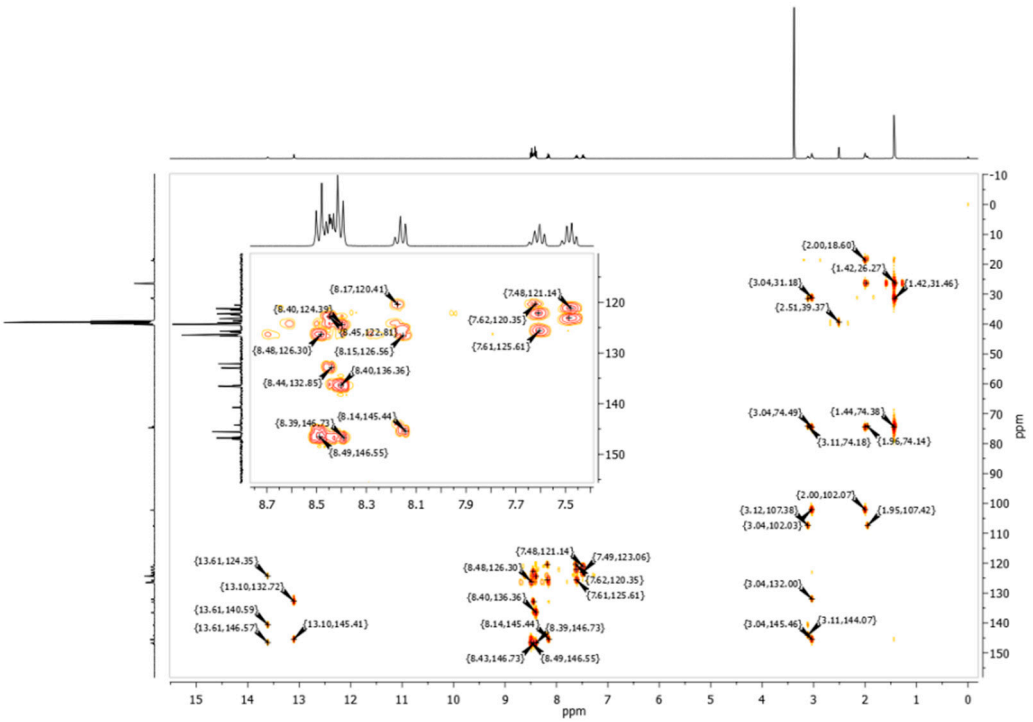


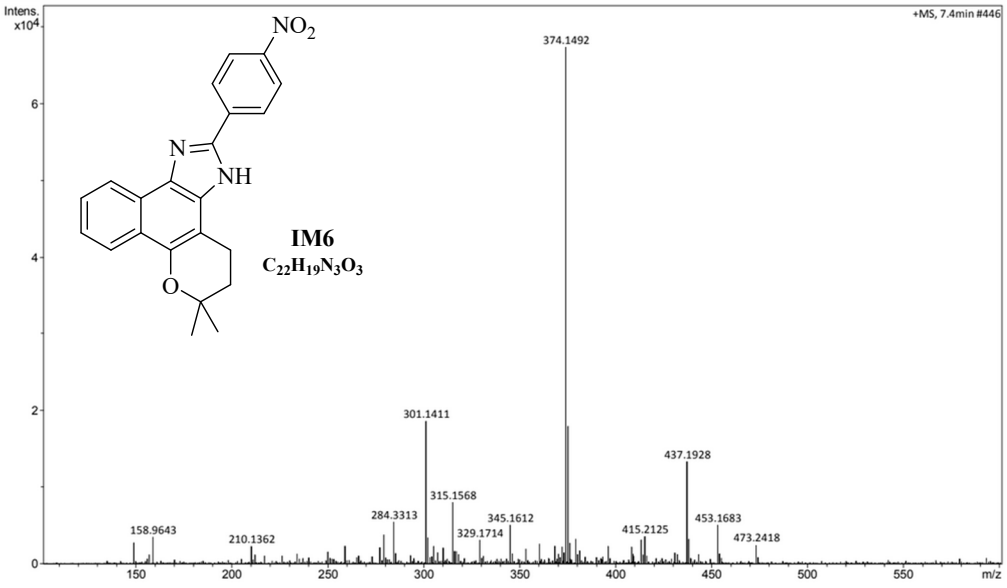
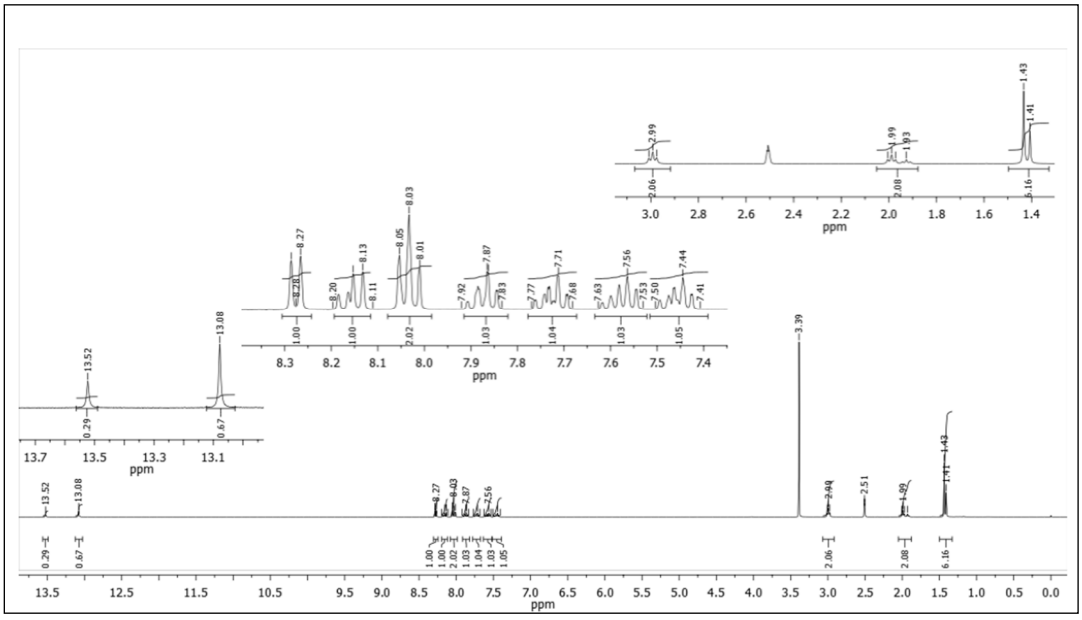
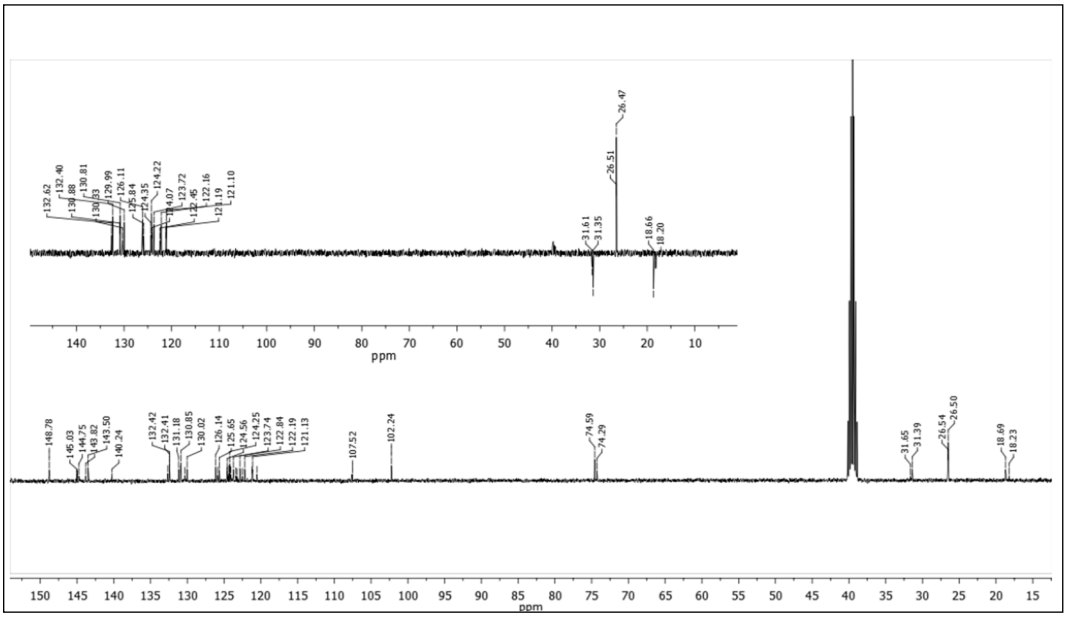
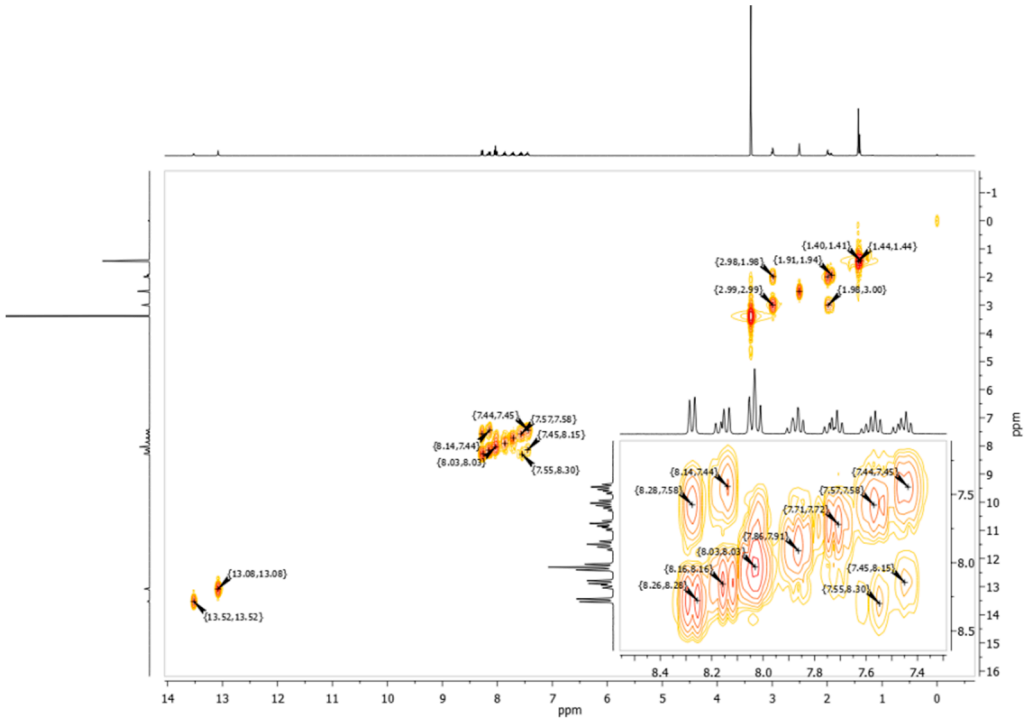


Figure S6. NMR spectra of 4,5-dihydro-6,6-dimethyl-6*H*-2-(4-nitrophenyl)-pyran[*b*-4,3]naphth[1,2-*d*]imidazole (**IM6**) in DMSO-d_6 and ESI-MS.



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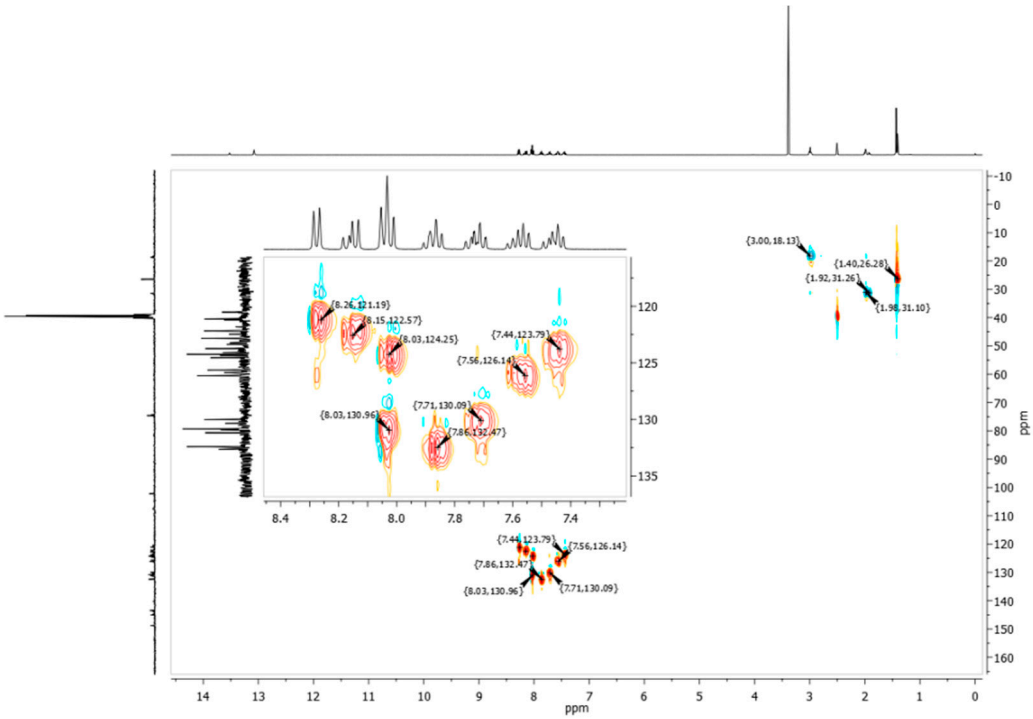
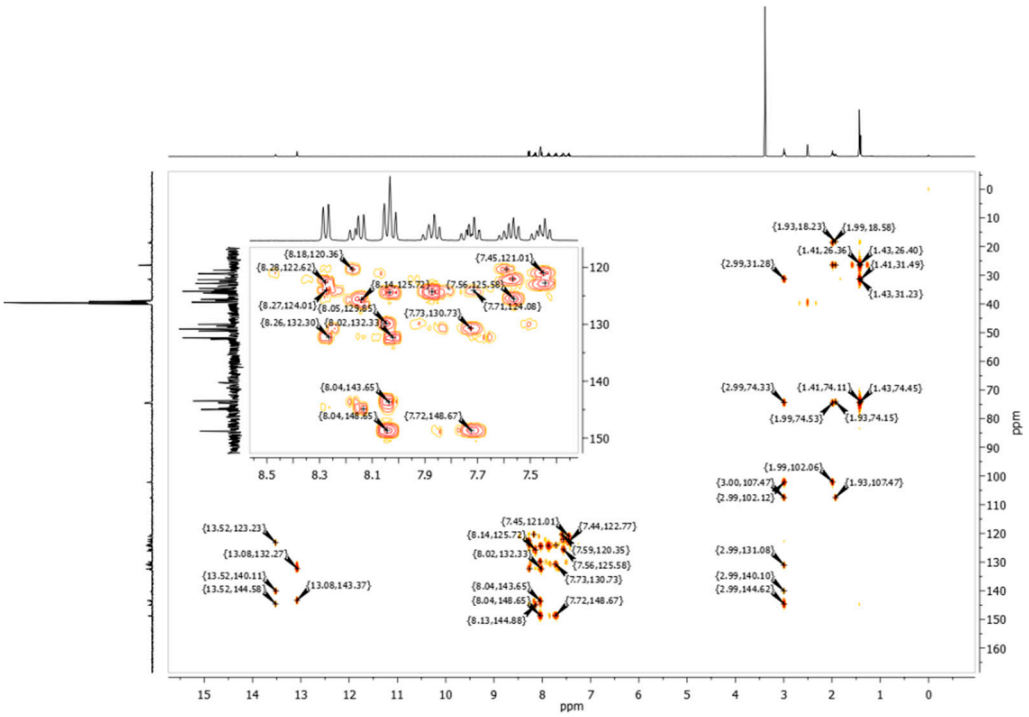
{7.55,8.30}
ppm


{8.26,121.19}
{8.15,122.57}
{8.03,124.25}
{7.44,123.79}
{7.56,126.14}
{8.03,130.96}
{7.71,130.09}
{7.86,132.47}
{3.00,18.13}
{1.40,26.28}
{1.92,31.26}
{1.96,31.10}
ppm



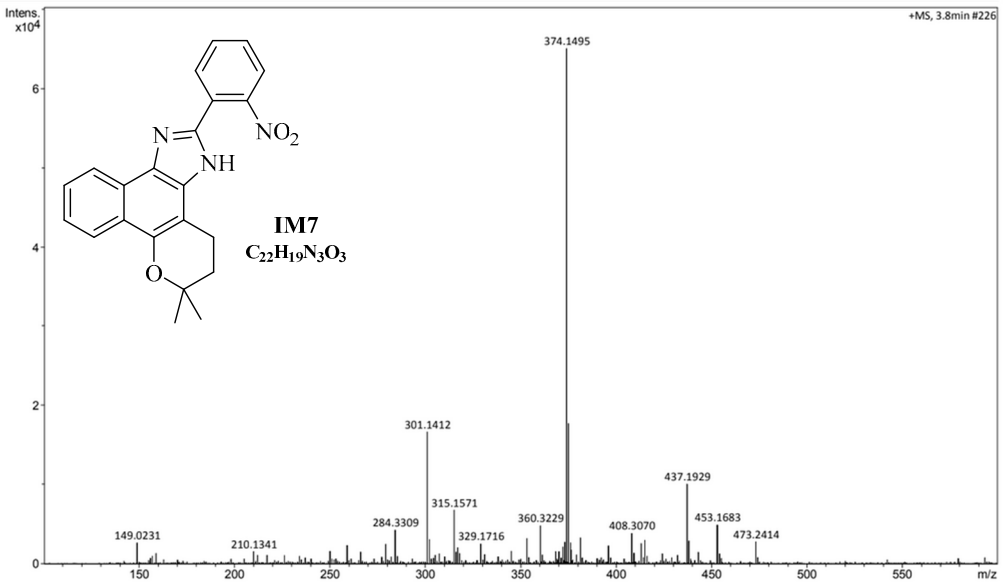


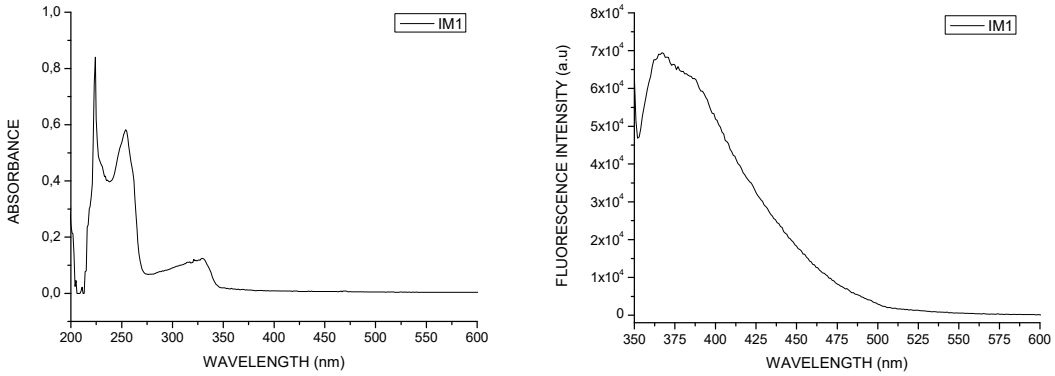
Figure S7. NMR spectra of 4,5-dihydro-6,6-dimethyl-6*H*-2-(2-nitrophenyl)-pyran[*b*-4,3]naphth[1,2-*d*]imidazole (**IM7)** in DMSO-d_6 and ESI-MS.

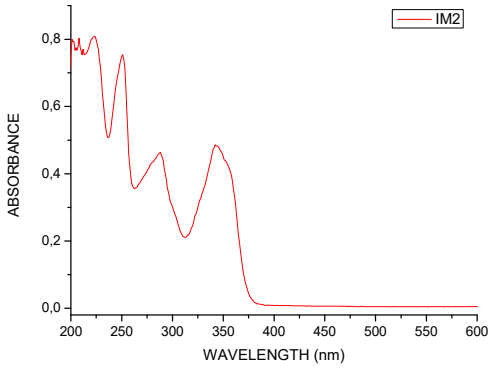
2. Solvatochromism study

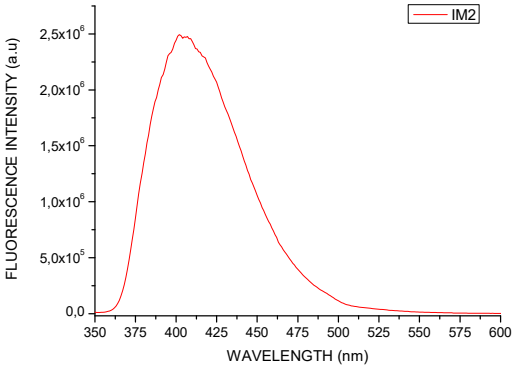
Table S1. Wavelength (nm) and absorbance of the scanning spectra of the naphth[1,2-*d*]imidazoles obtained in the solvatochromism study.

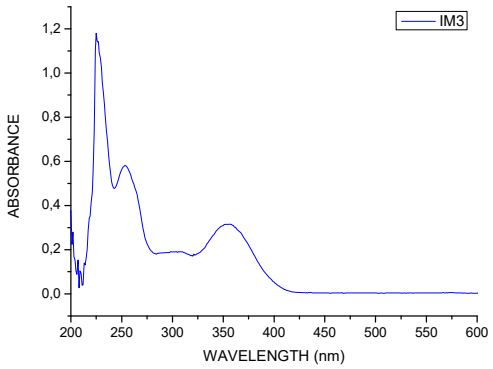
SOLVATOCHROMISM STUDY λ_{Abs} (nm) and absorbance				
COMPOUND	**HEXANE**	**CH_2Cl_2**	**DMSO**	**CH_3OH**
IM1	313 (0.088) 328 (0.068)	315 (0.107) 329 (0.117)	320 (0.111) 333 (0.102)	314 (0.068) 328 (0.077)
IM2	291 (0.228) 344 (0.203)	289 (0.333) 348 (0.330)	360 (0.125) 450 (0.149)	288 (0.355) 343 (0.375)
IM3	348 (0.152)	306 (0.209) 355 (0.334)	305 (0.189) 360 (0.313)	288 (0.243) 343 (0.320)
IM4	Not observed	360 (0.125) 450 (0.149)	346 (0.315) 362 (0.306)	342 (0.342) 352 (0.293)
IM5	302 (0.155) 352 (0.130)	321 (0.271) 374 (0.426) 485 (0.072)	307 (0.494) 357 (0.614) 375 (0.573)	300 (0.429) 353 (0.530)
IM6	290 (0.083) 413 (0.234	321 (0.096) 428 (0.226)	315 (0.098) 433 (0.235)	298 (0.088) 414 (0.234)
IM7	294 (0.235) 341 (0.241) 427 (0.088)	287 (0.220) 336 (0.238)	281 (0.256) 341 (0.229)	333 (0.184)

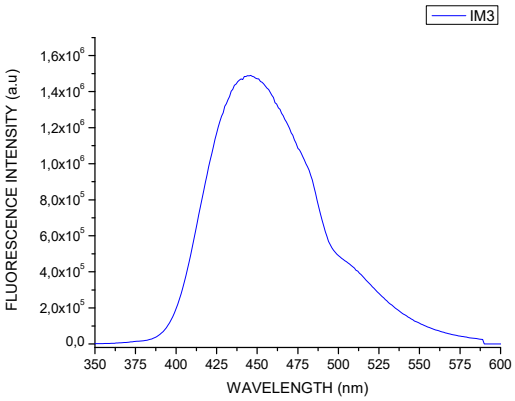
3. Absorbance and fluorescence emission spectrum

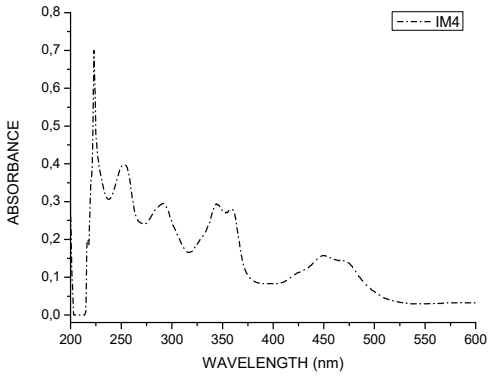


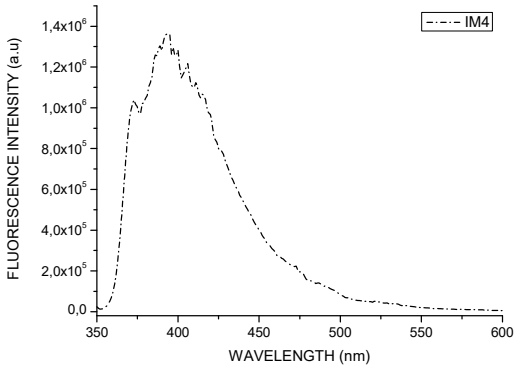

IM2
ABSORBANCE
WAVELENGTH (nm)

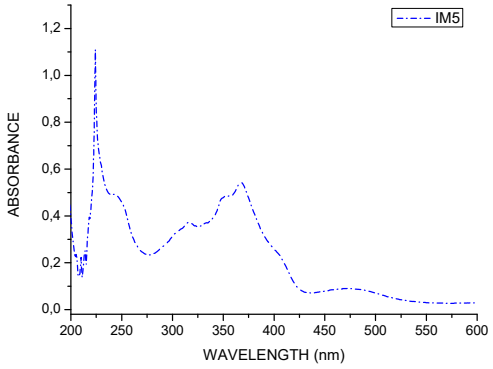

IM2
FLUORESCENCE INTENSITY (a.u)
WAVELENGTH (nm)

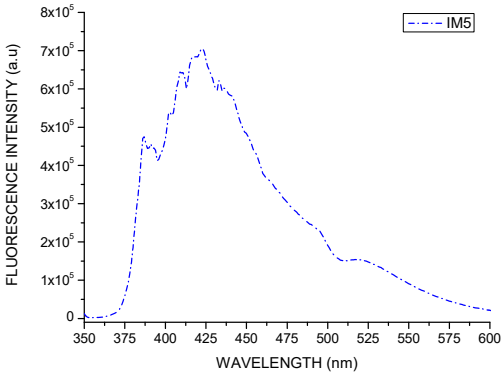

IM3
ABSORBANCE
WAVELENGTH (nm)

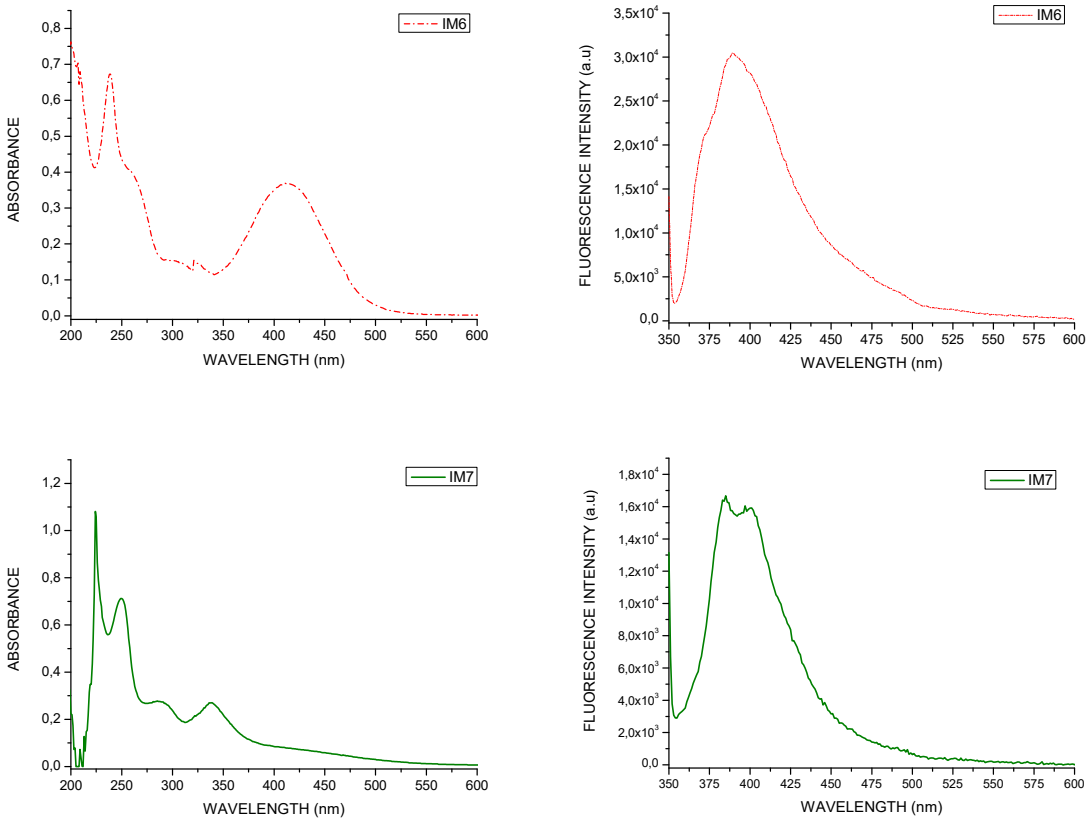

IM3
FLUORESCENCE INTENSITY (a.u)
WAVELENGTH (nm)


IM4
ABSORBANCE
WAVELENGTH (nm)


IM4
FLUORESCENCE INTENSITY (a.u)
WAVELENGTH (nm)


IM5
ABSORBANCE
WAVELENGTH (nm)


IM5
FLUORESCENCE INTENSITY (a.u)
WAVELENGTH (nm)



a. Solvents used solvents: IM2 – DMSO; IM6 - CH_3OH; IM1, IM3, IM4, IM5 - CH_2Cl_2; and IM7 hexane.
b. Excitation wavelength of 345 nm for all compounds.

Figure S8. Absorbance and emission spectra of naphth[1,2-*d*]imidazoles (**IM1–IM7)**.