



Supporting Information

for

Kinetically stabilized 1,3-diarylisobenzofurans and the possibility of preparing large, persistent isoacenofurans with unusually small HOMO–LUMO gaps

Qian Liu and Glen P. Miller

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^1H NMR stability studies for compounds 3 and 23, ^1H and ^{13}C NMR spectra for key compounds and ESI high-resolution mass spectra

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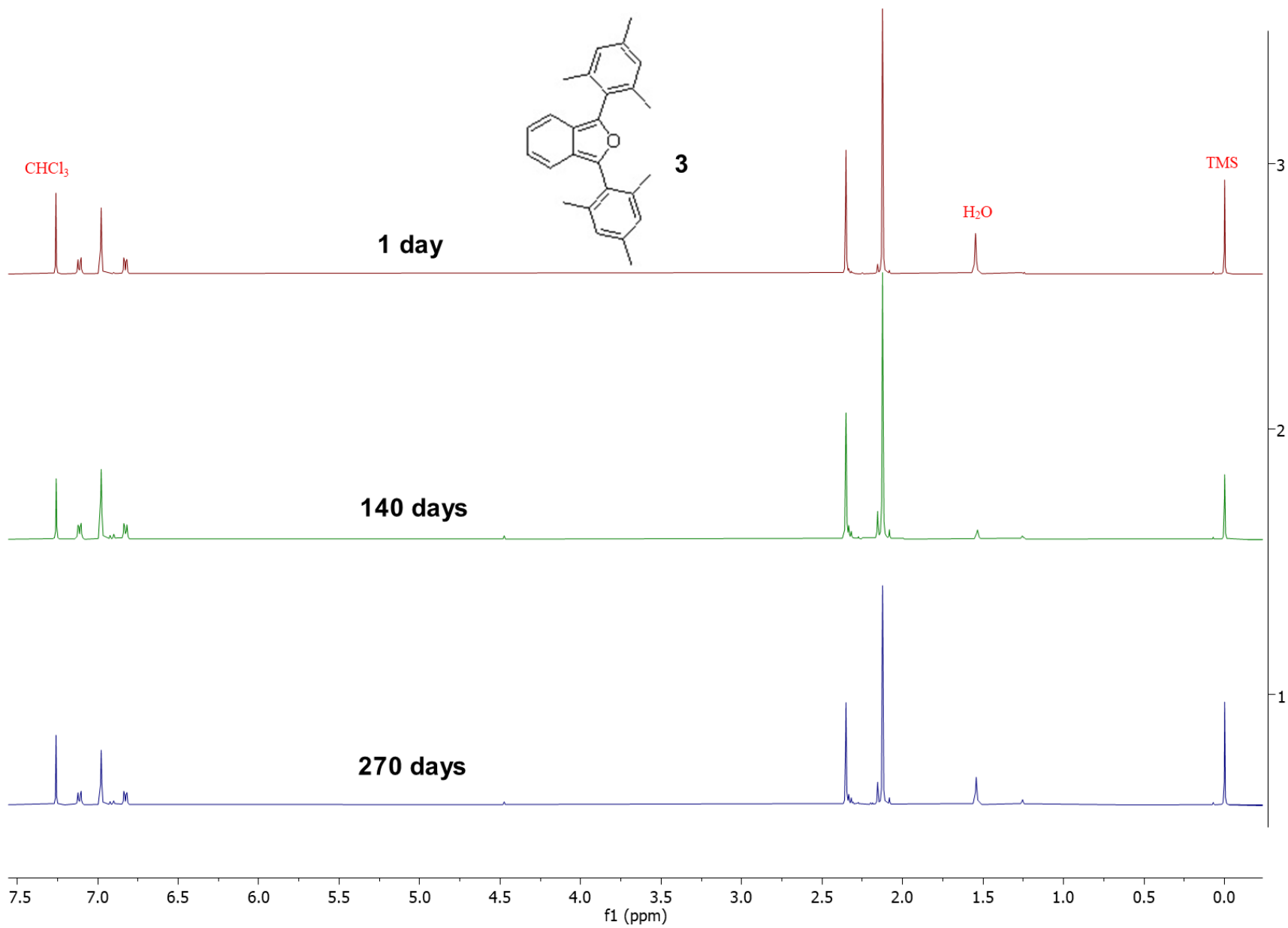
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|---|-----|
| ¹ H NMR stability study for compounds 3 and 23 | S3 |
| ¹ H and ¹³ C NMR spectra of key compounds | S8 |
| Electrospray ionization high-resolution mass spectra of new compounds | S20 |

Stability study for compounds **3** and **23** maintained in the solid state

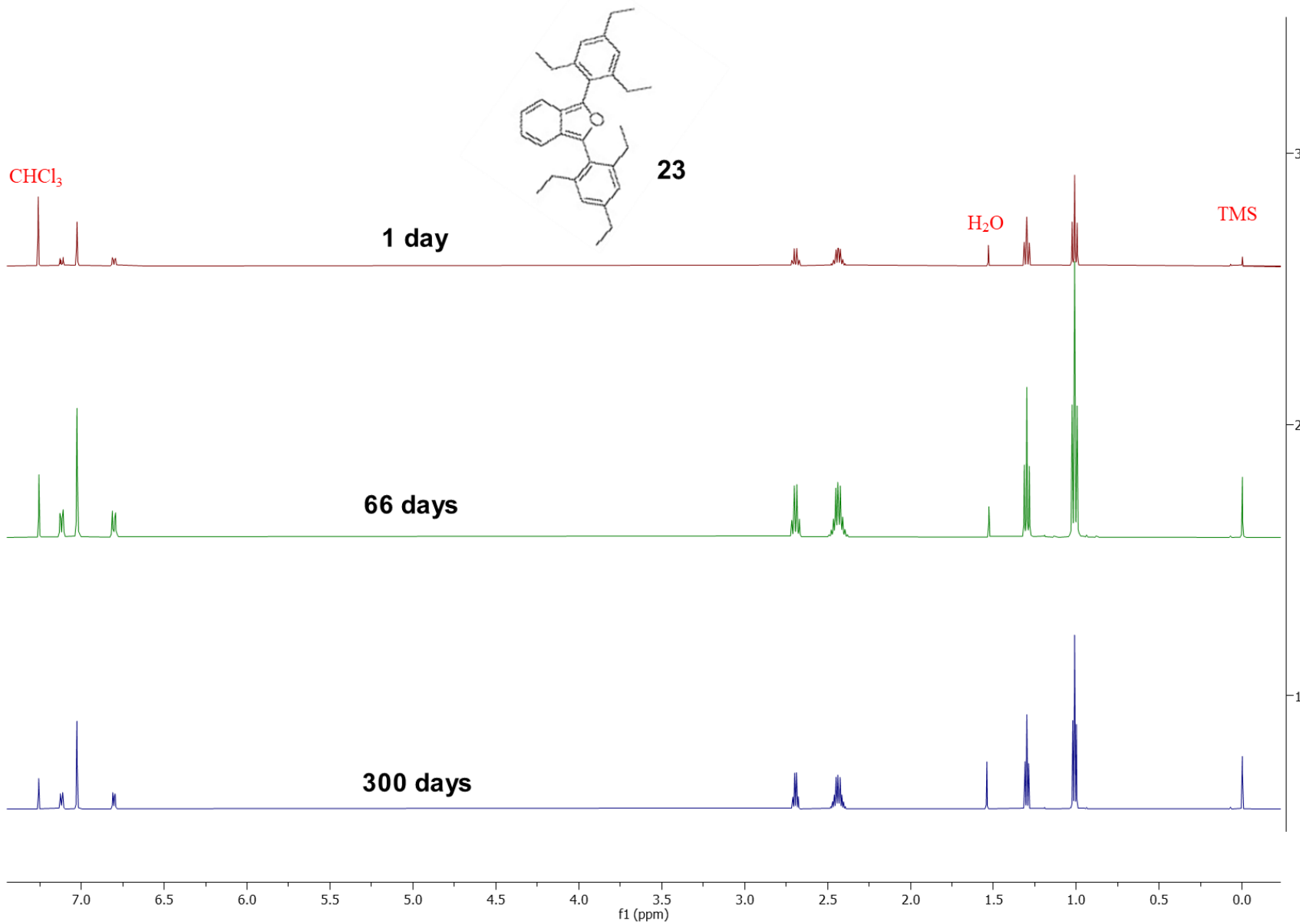
When not in use, compounds **3** and **23** were stored in vials that were capped and wrapped in foil. The samples were otherwise not protected from ambient oxygen. Periodically, samples for ^1H NMR spectroscopy were prepared.

^1H NMR samples were prepared by separately dissolving compounds **3** and **23** in CDCl_3 . The resulting solutions were placed in standard 5 mm NMR tubes and capped with standard plastic NMR tube caps.

Select spectra are displayed on the following 2 pages.



S3

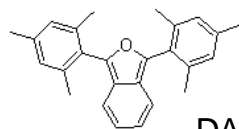


S4

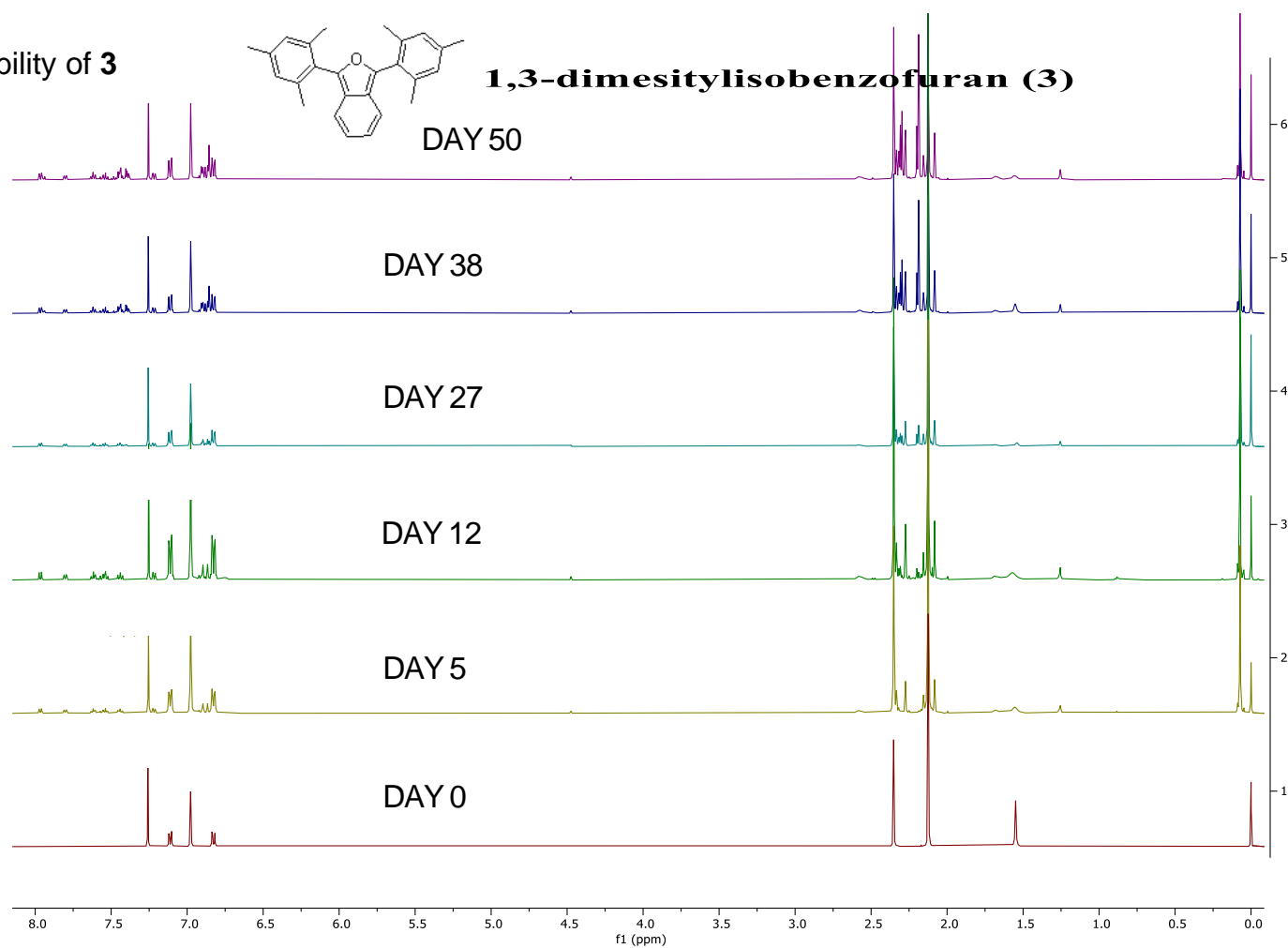
Stability study for compound **3** maintained in solution

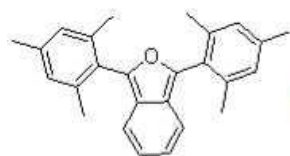
A solution composed of 15 mg of compound **3** was dissolved in 0.6 ml of CDCl₃ and placed in a 5 mm NMR tube with plastic cap. The tube was capped but otherwise not protected from air or ambient light. ¹H NMR spectra were acquired periodically over 50 days.

Solution Phase Stability of **3**



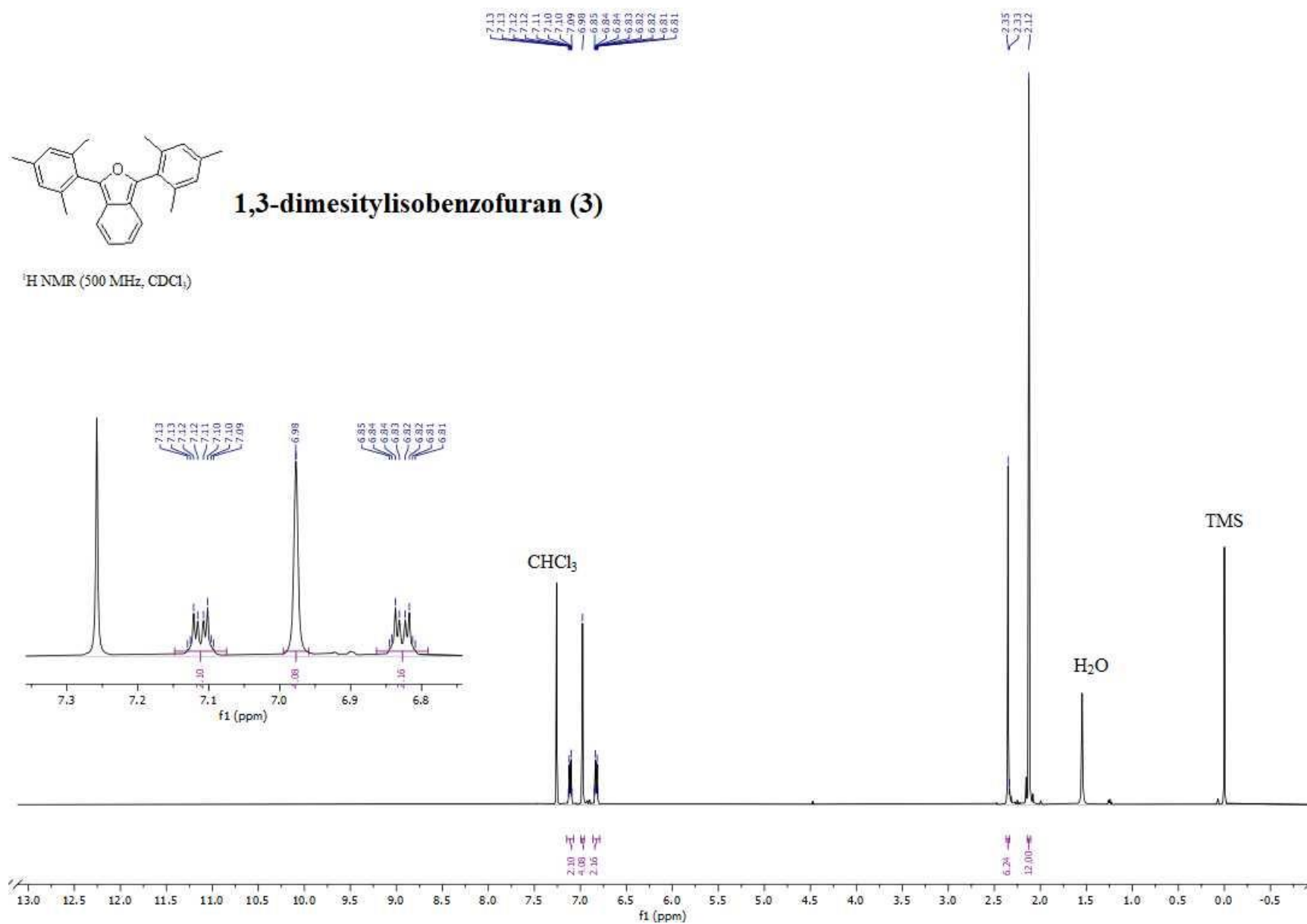
1,3-dimesitylisobenzofuran (3)



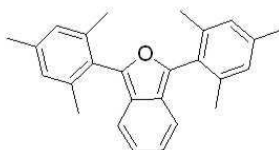


1,3-dimesitylisobenzofuran (3)

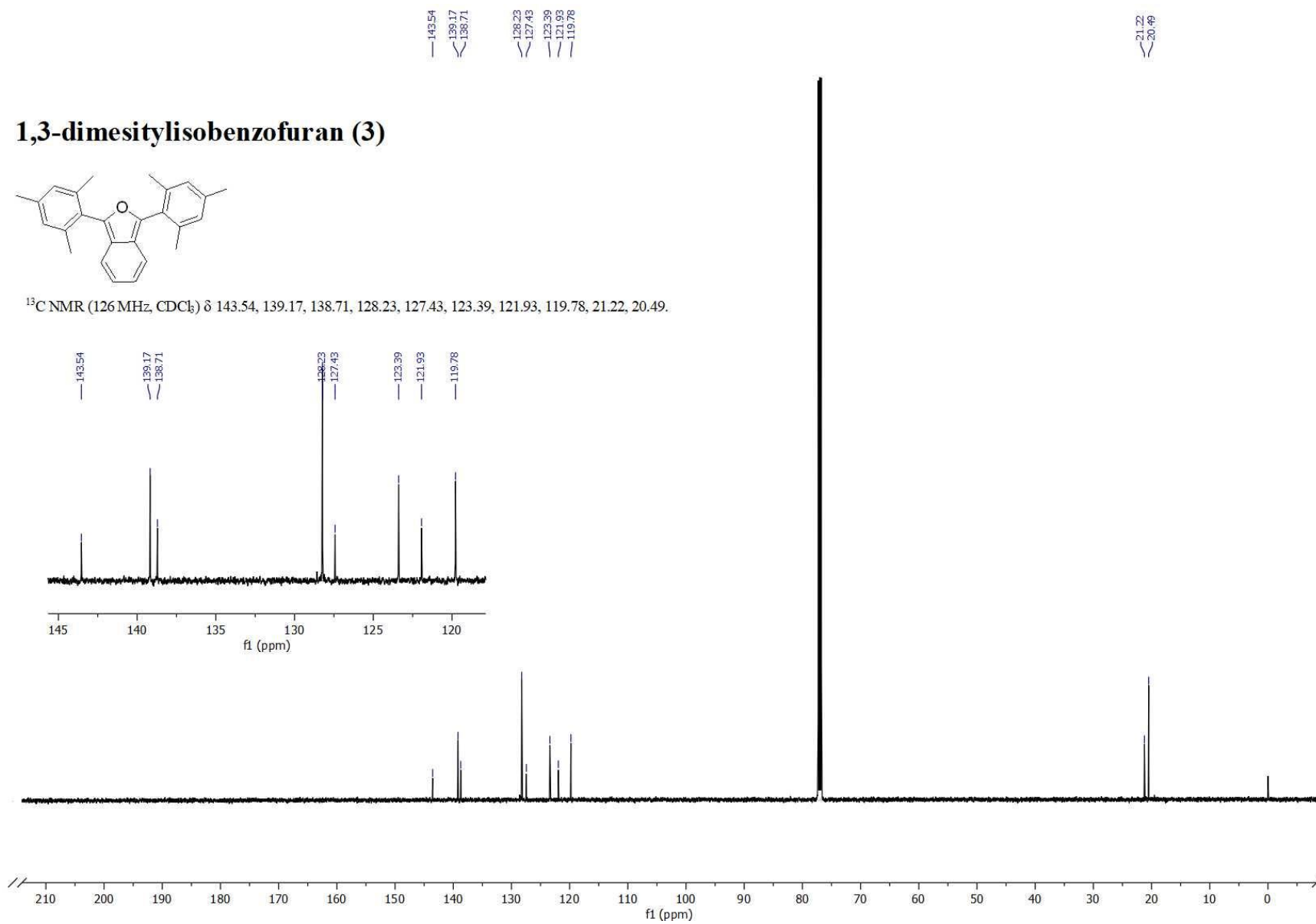
¹H NMR (500 MHz, CDCl₃)

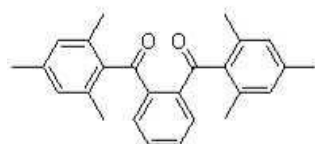


1,3-dimesitylisobenzofuran (3)



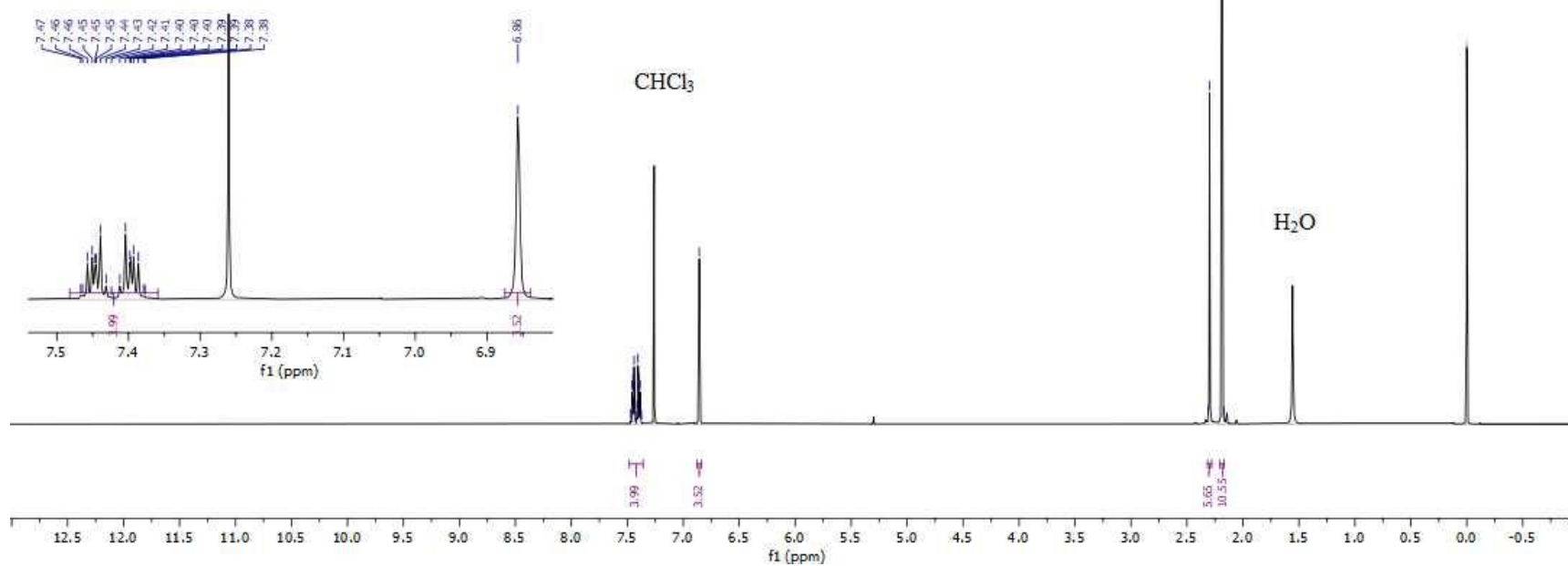
^{13}C NMR (126 MHz, CDCl_3) δ 143.54, 139.17, 138.71, 128.23, 127.43, 123.39, 121.93, 119.78, 21.22, 20.49.

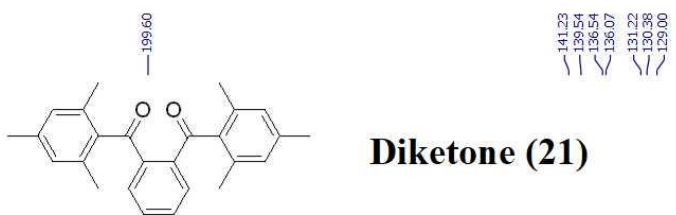




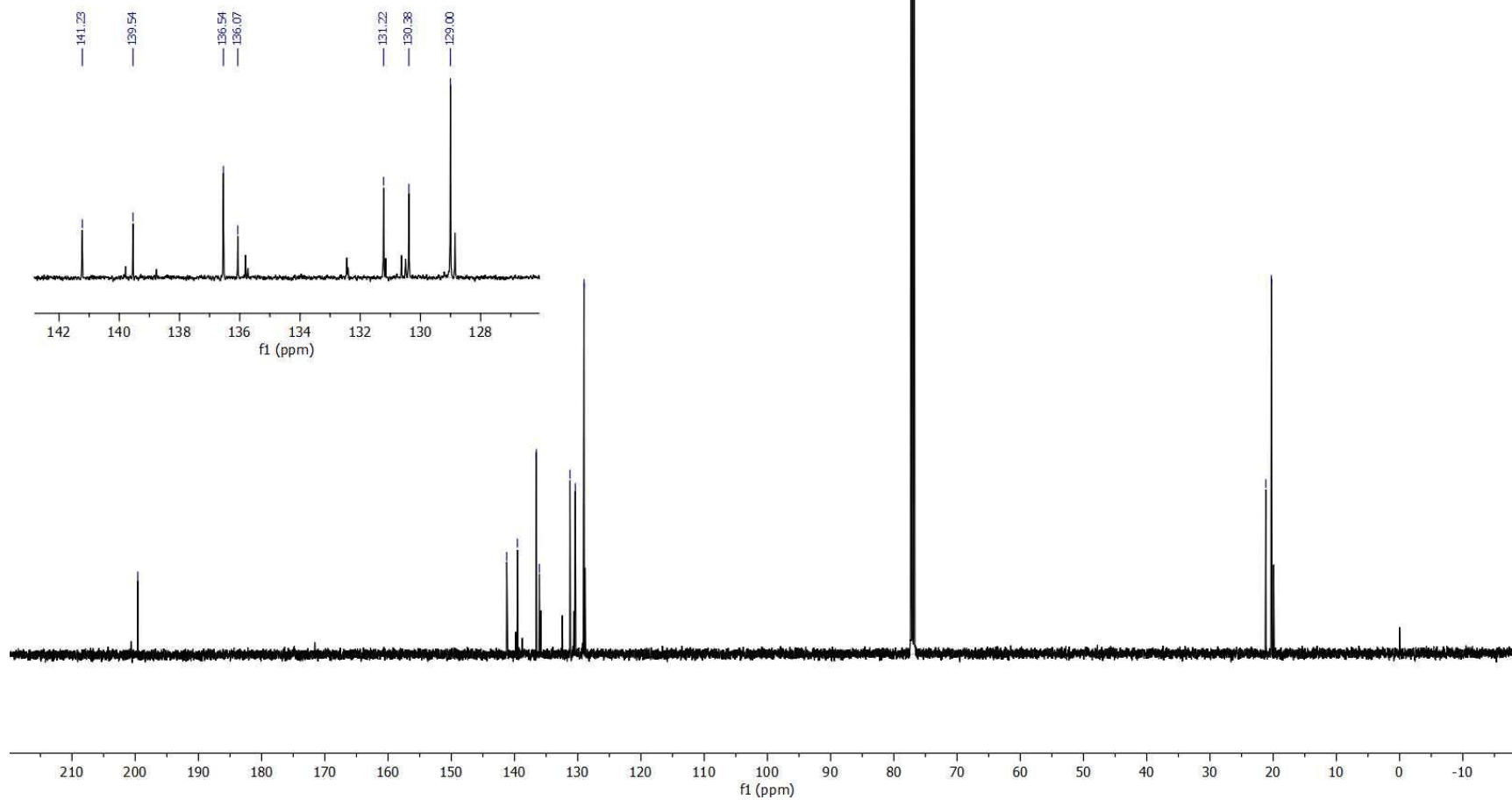
Diketone (21)

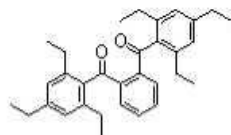
¹H NMR (500 MHz, CDCl₃)





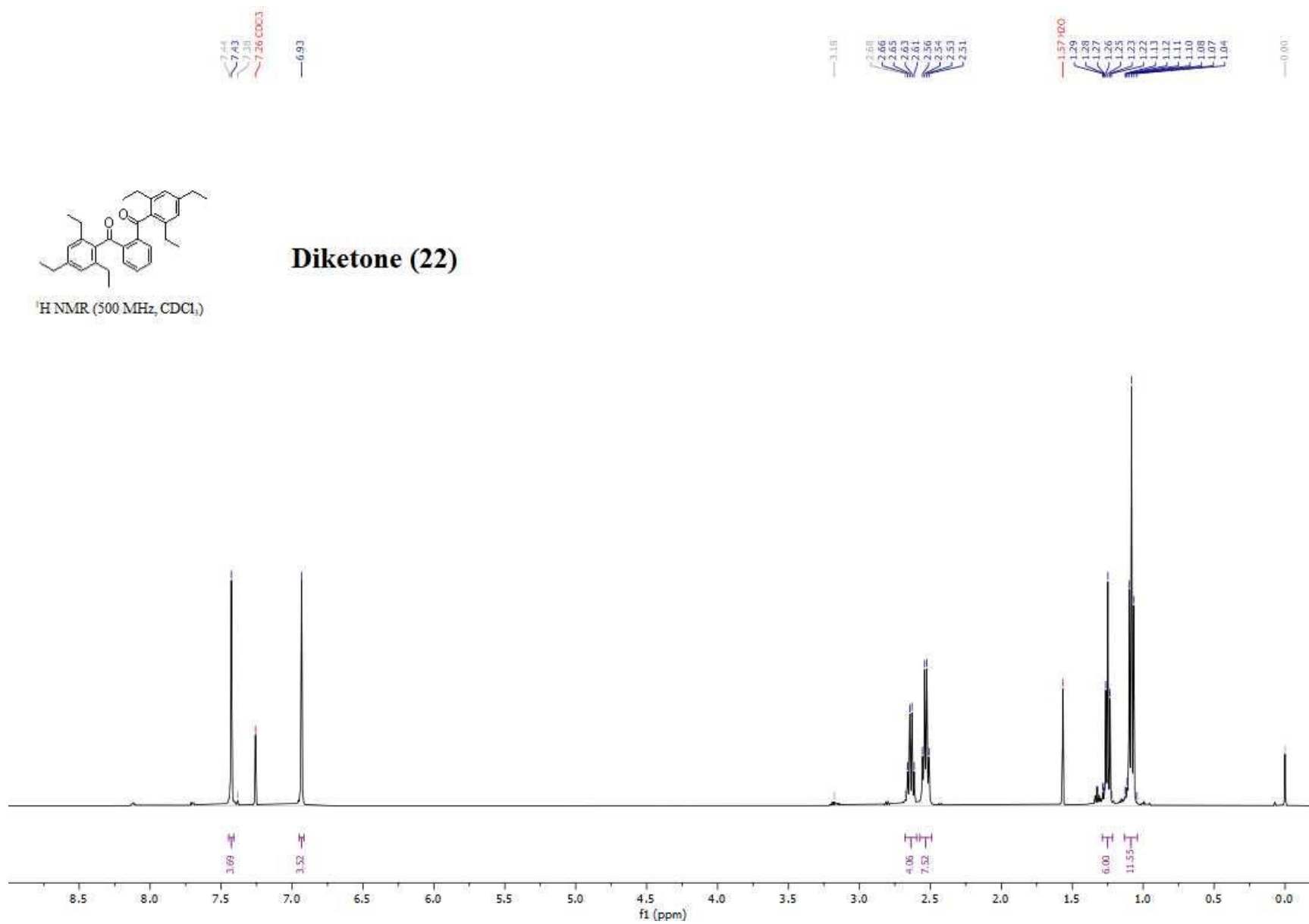
^{13}C NMR (126 MHz, CDCl_3) δ 199.60, 141.23, 139.54, 136.54, 136.07, 131.22, 130.38, 129.00, 21.17, 20.29.

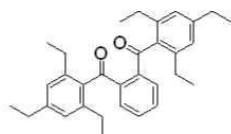




¹H NMR (500 MHz, CDCl₃)

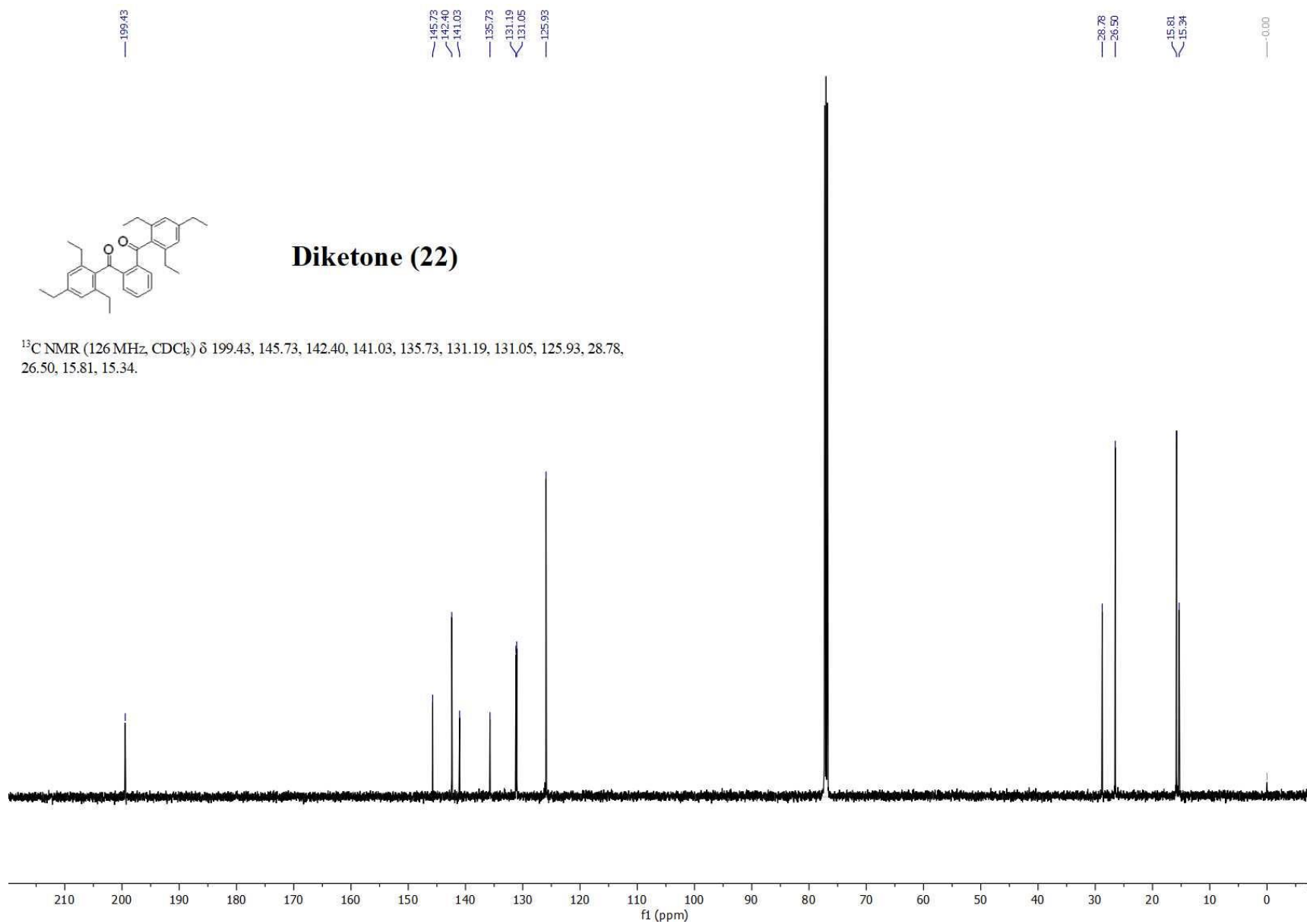
Diketone (22)

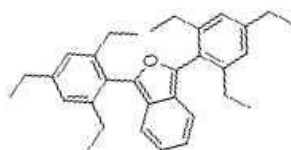




Diketone (22)

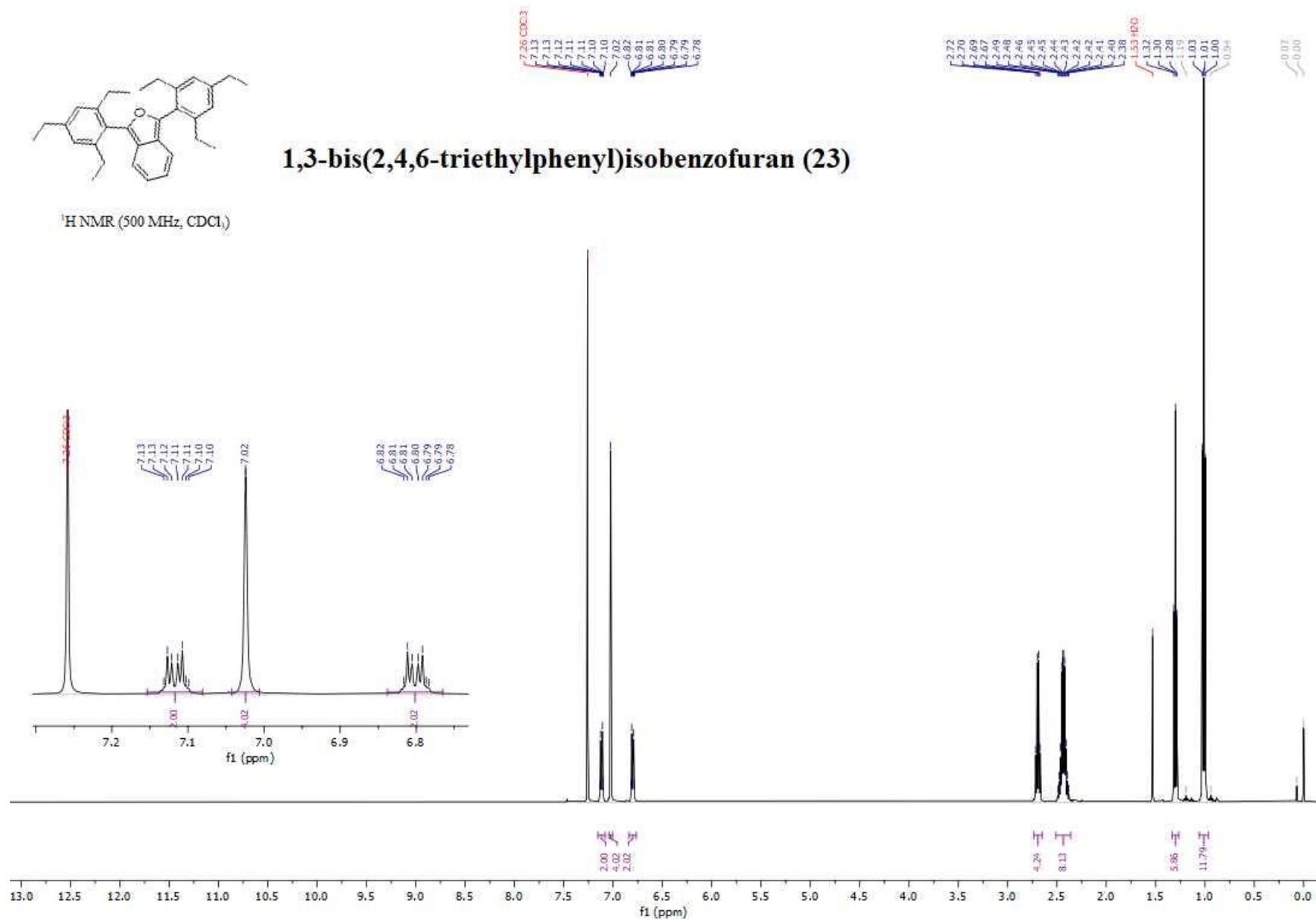
^{13}C NMR (126 MHz, CDCl_3) δ 199.43, 145.73, 142.40, 141.03, 135.73, 131.19, 131.05, 125.93, 28.78, 26.50, 15.81, 15.34.

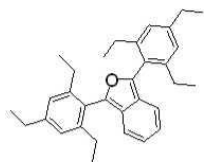




1,3-bis(2,4,6-triethylphenyl)isobenzofuran (23)

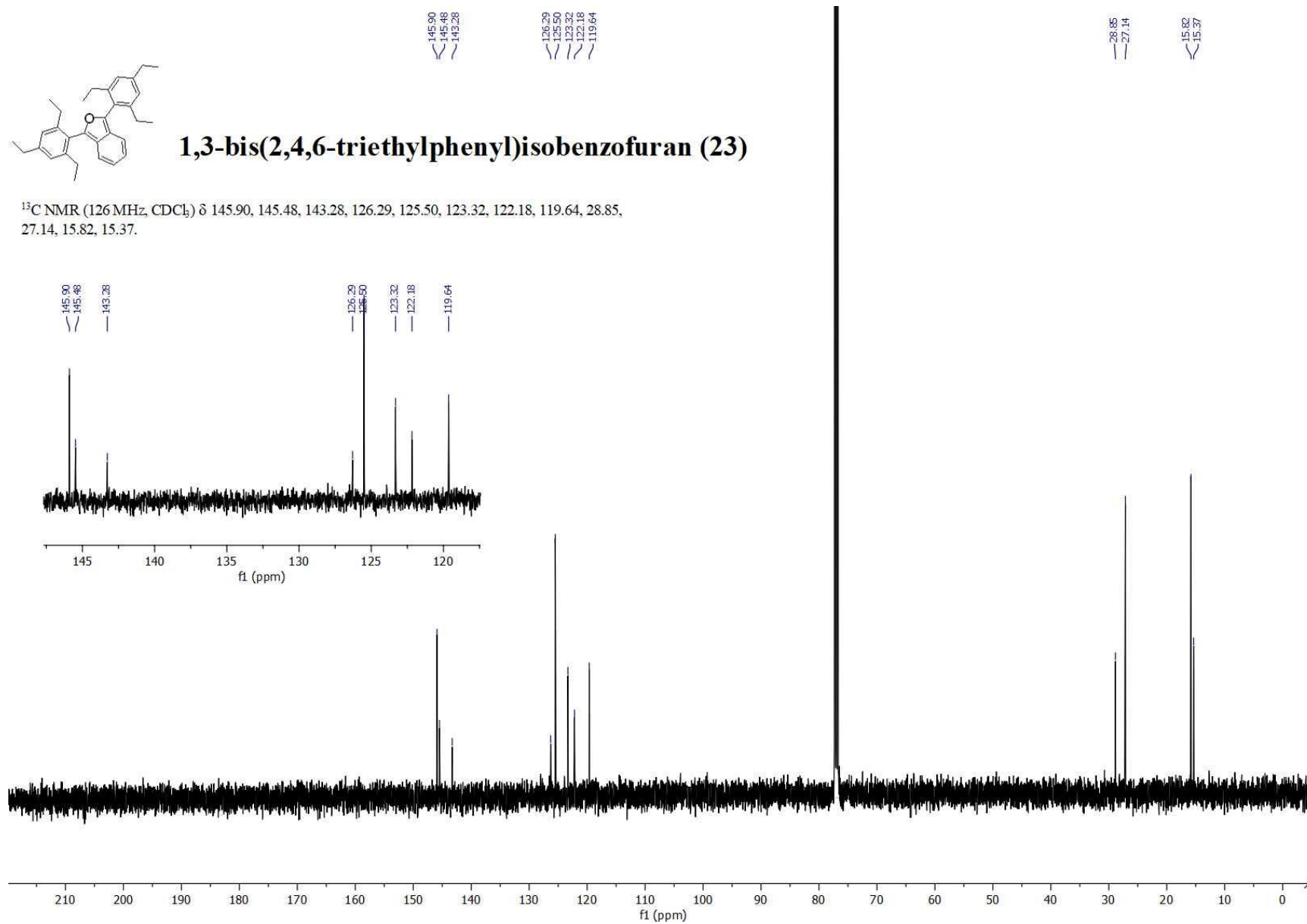
¹H NMR (500 MHz, CDCl₃)

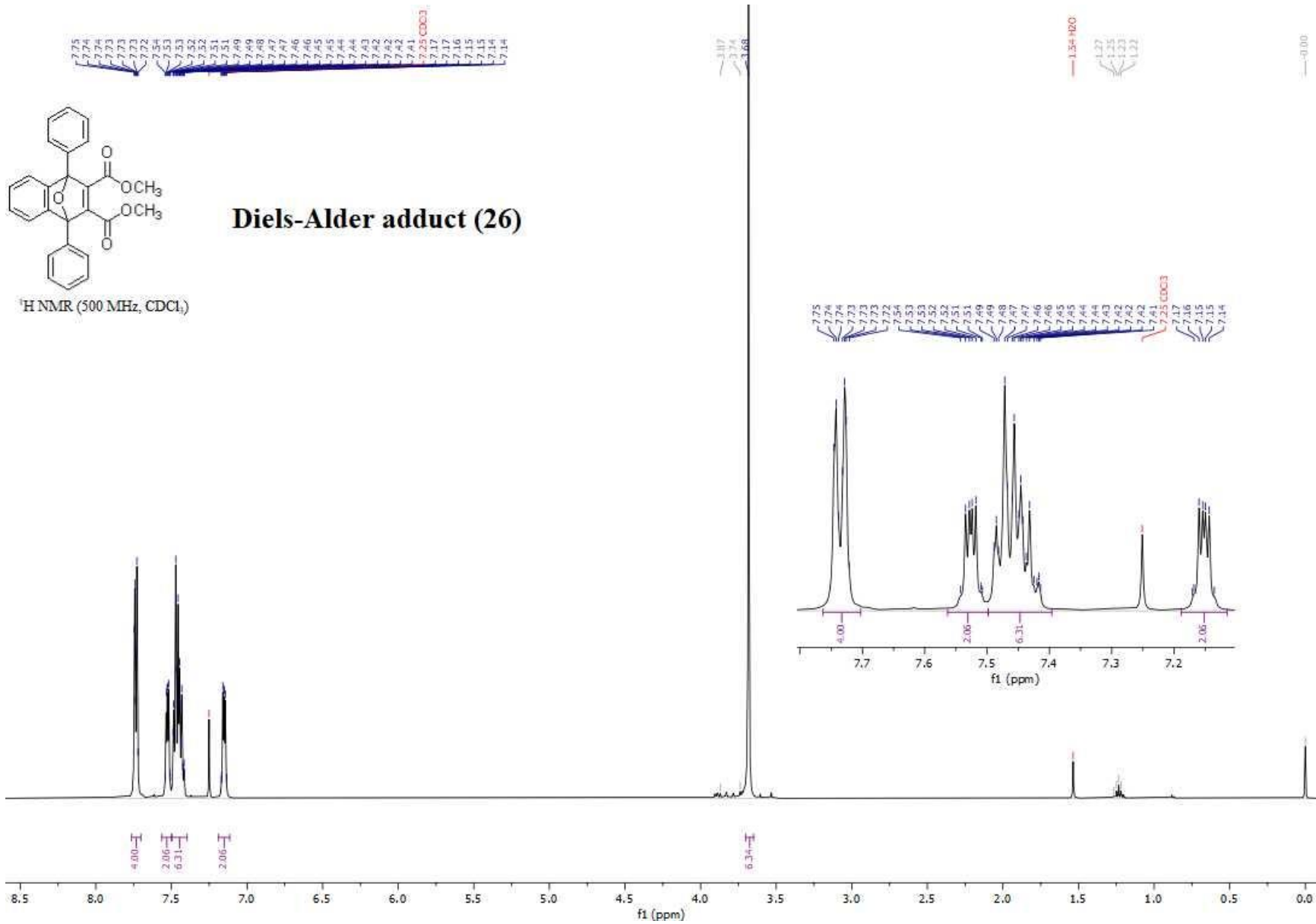


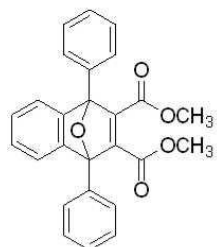


1,3-bis(2,4,6-triethylphenyl)isobenzofuran (23)

^{13}C NMR (126 MHz, CDCl_3) δ 145.90, 145.48, 143.28, 126.29, 125.50, 123.32, 122.18, 119.64, 28.85, 27.14, 15.82, 15.37.

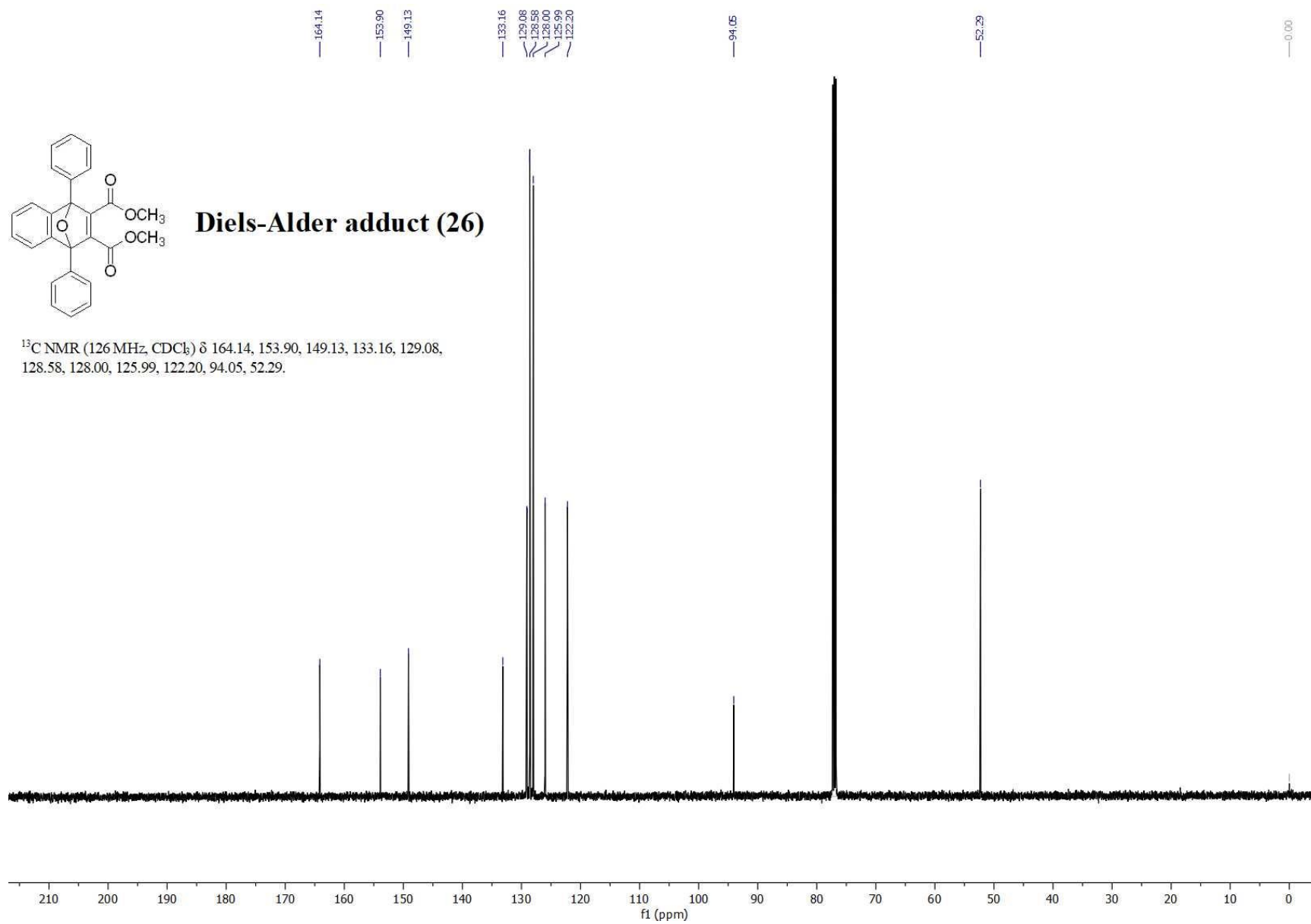


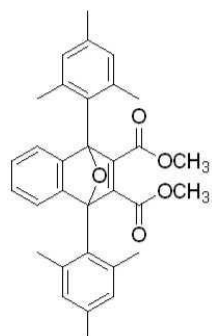




Diels-Alder adduct (26)

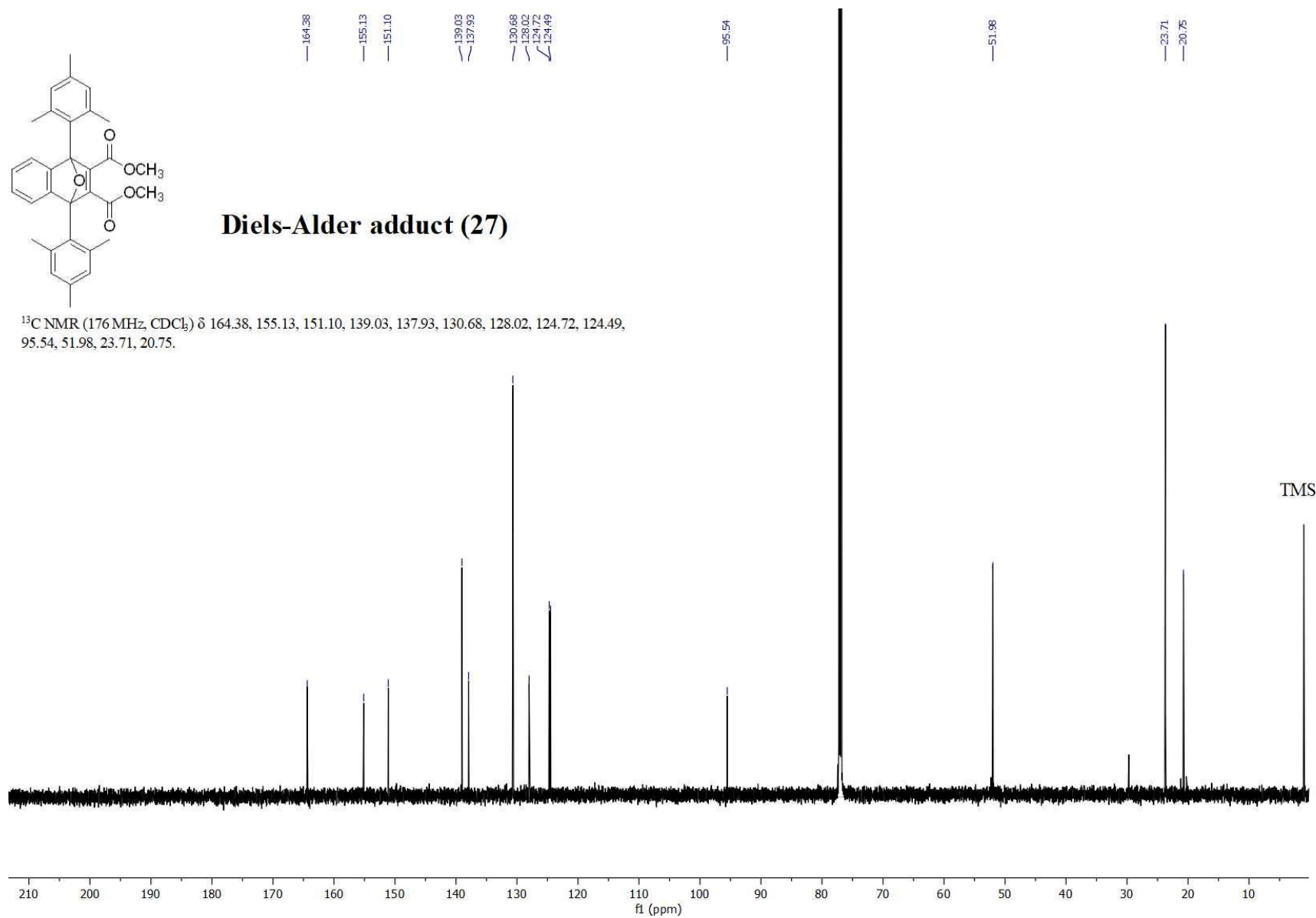
^{13}C NMR (126 MHz, CDCl_3) δ 164.14, 153.90, 149.13, 133.16, 129.08, 128.58, 128.00, 125.99, 122.20, 94.05, 52.29.



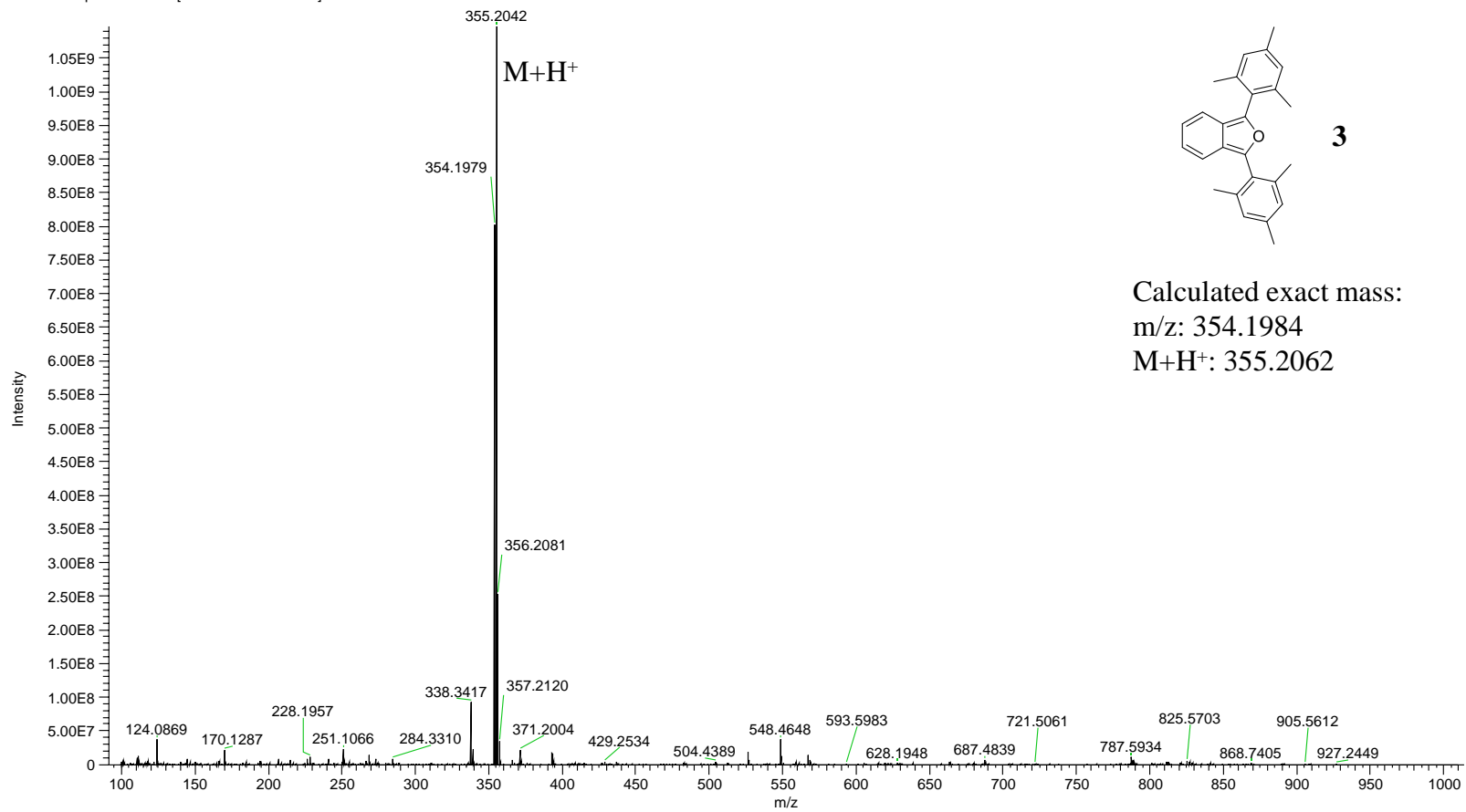


Diels-Alder adduct (27)

^{13}C NMR (176 MHz, CDCl_3) δ 164.38, 155.13, 151.10, 139.03, 137.93, 130.68, 128.02, 124.72, 124.49, 95.54, 51.98, 23.71, 20.75.

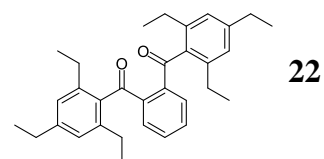
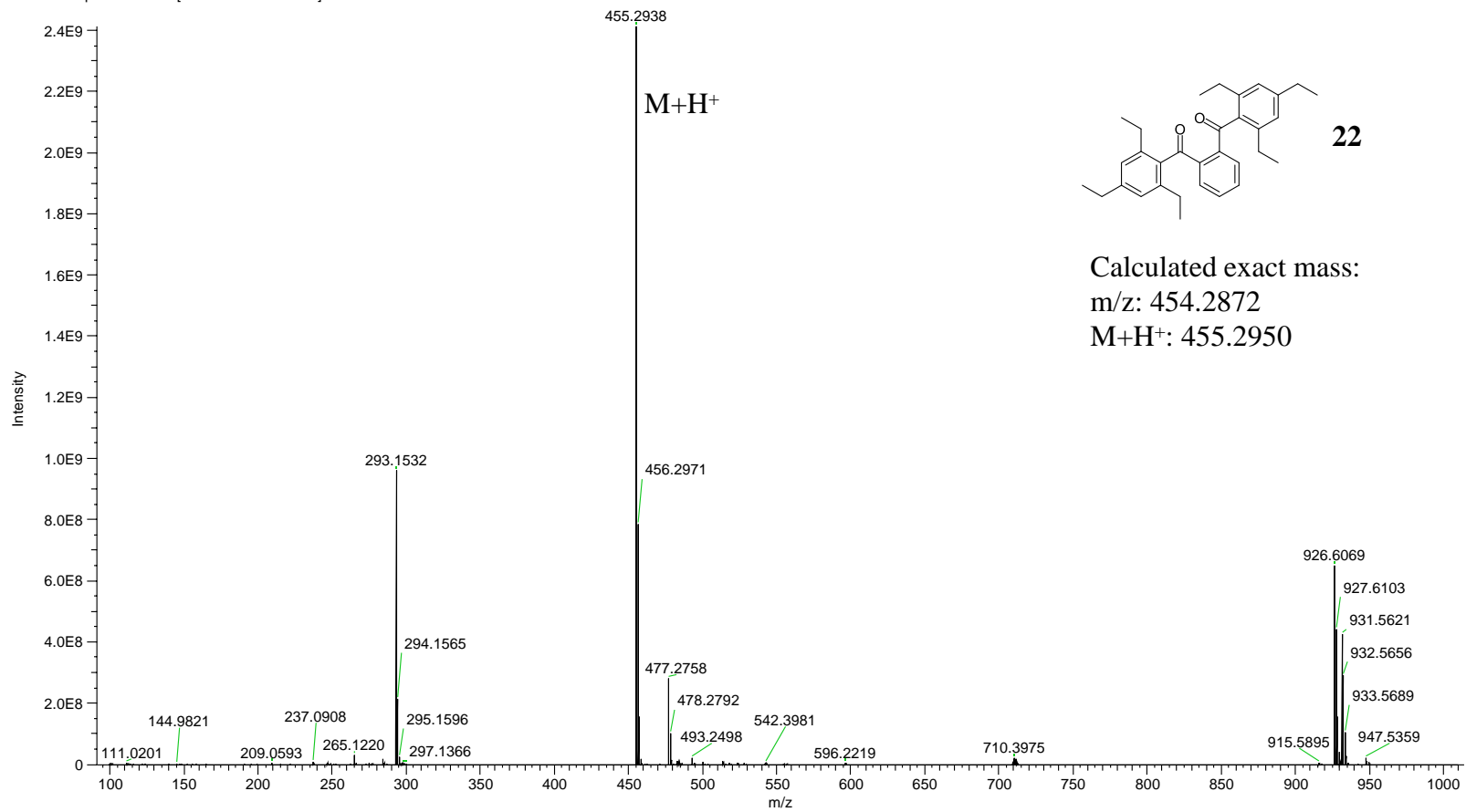


T: FTMS + p ESI Full ms [100.0000-1000.0000]



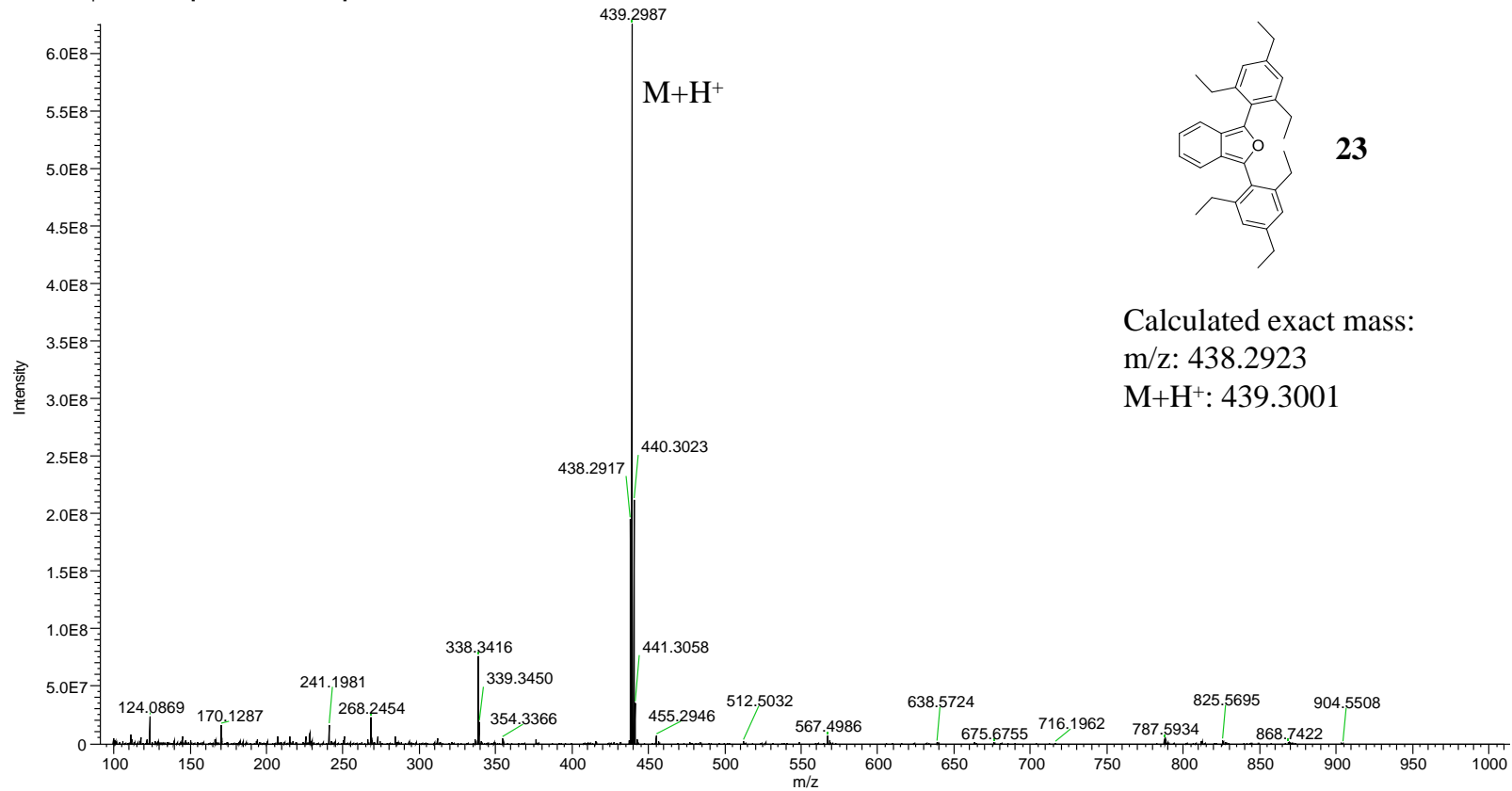
Calculated exact mass:
m/z: 354.1984
M+H+: 355.2062

T: FTMS + p ESI Full ms [100.0000-1000.0000]



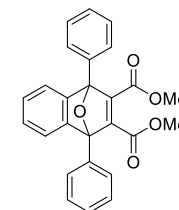
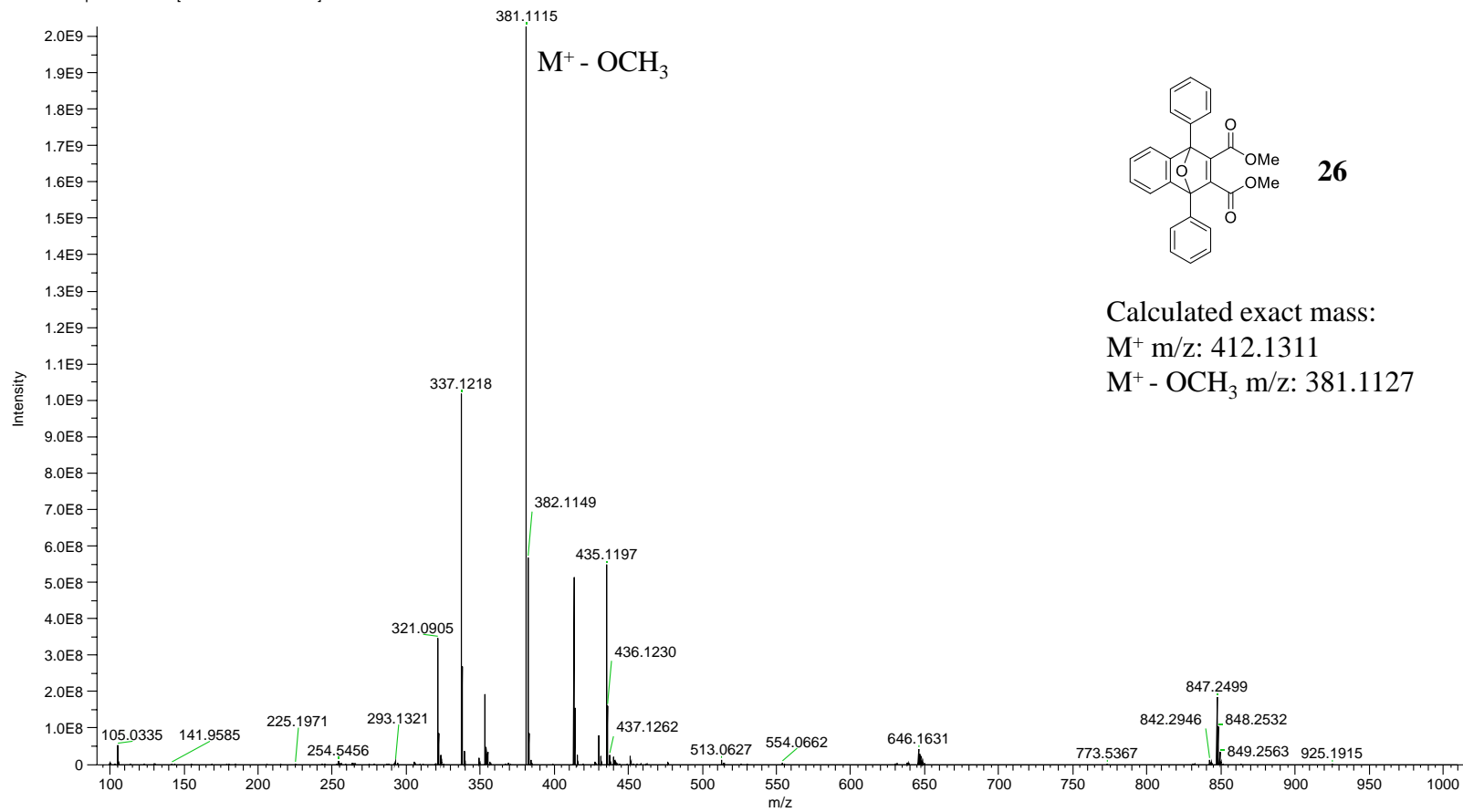
Calculated exact mass:
m/z: 454.2872
M+H⁺: 455.2950

T: FTMS + p ESI Full ms [100.0000-1000.0000]



Calculated exact mass:
m/z: 438.2923
M+H⁺: 439.3001

T: FTMS + p ESI Full ms [100.0000-1000.0000]



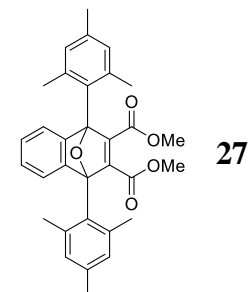
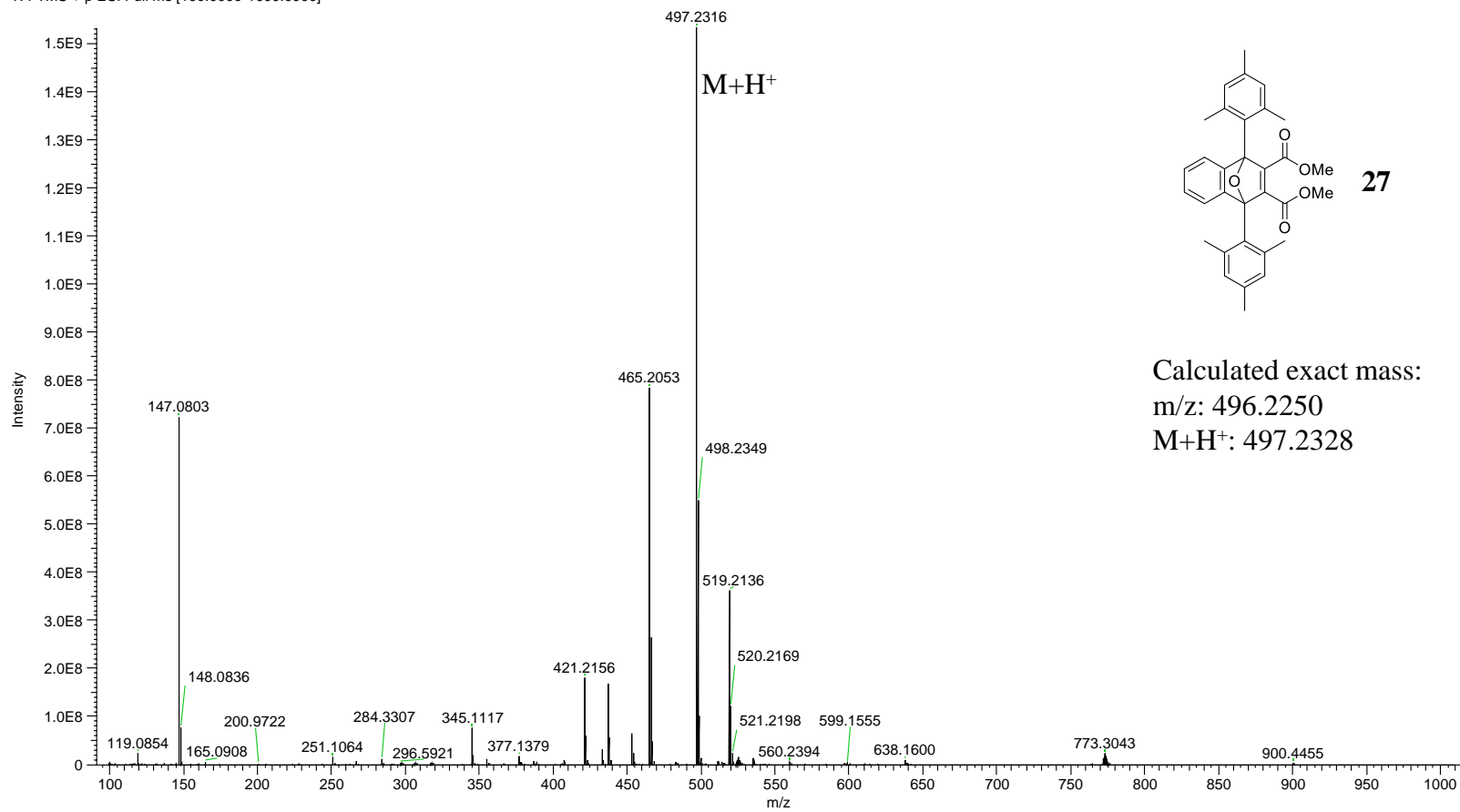
26

Calculated exact mass:

M^+ m/z: 412.1311

$M^+ - OCH_3$ m/z: 381.1127

T: FTMS + p ESI Full ms [100.0000-1000.0000]



Calculated exact mass:
m/z: 496.2250
M+H⁺: 497.2328