

*Supplementary Information for*

**Design, synthesis, and anticancer activities of new  
compounds bearing the quinone-pyran-lactone tricyclic  
pharmacophore**

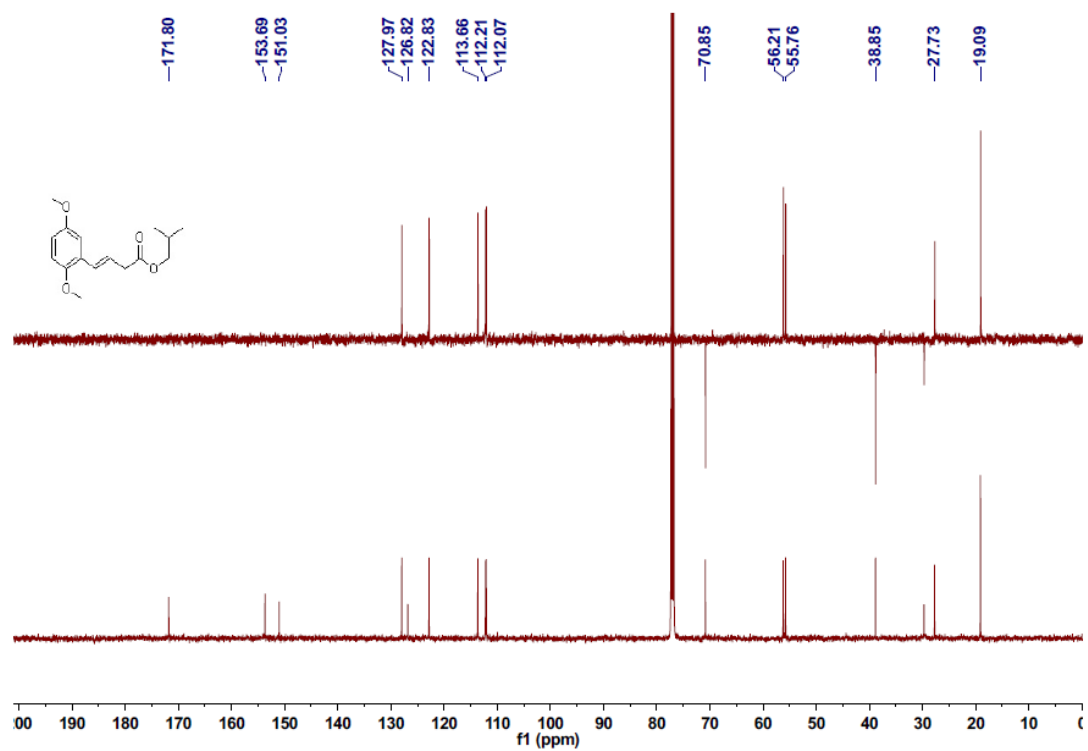
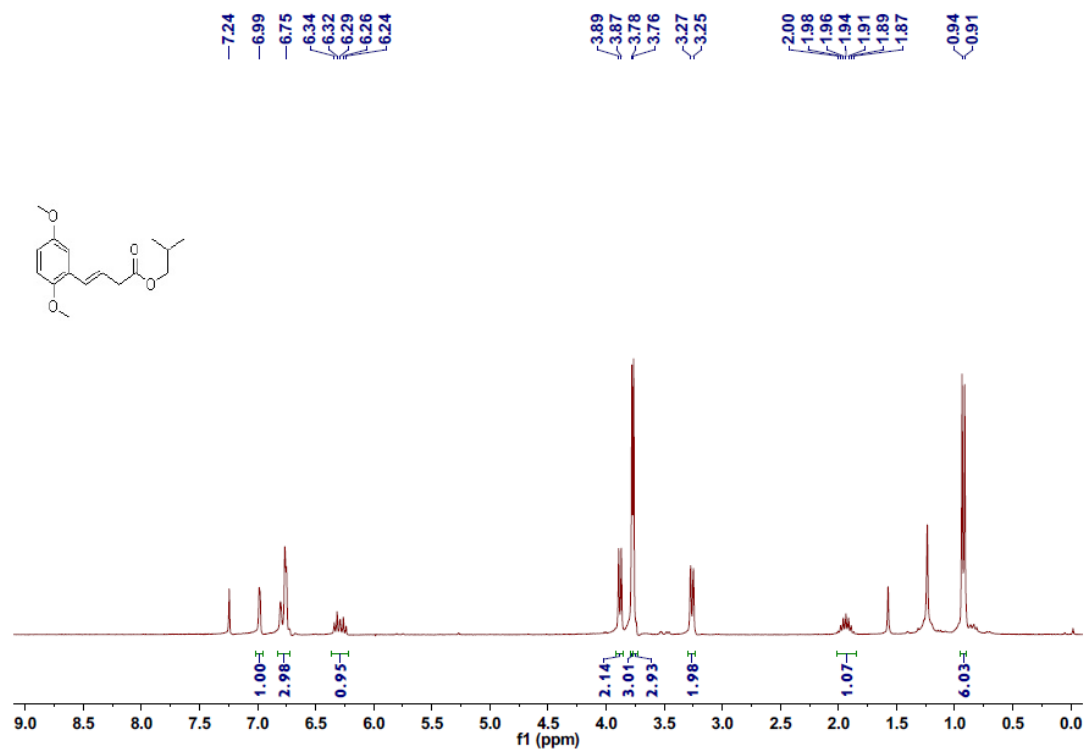
Xue Jiang,<sup>a</sup> Meining Wang,<sup>b</sup> Shanshan Song,<sup>c</sup> Youjun Xu, <sup>\*,a</sup> Zehong Miao,<sup>\*,c</sup> and Ao Zhang<sup>\*,b</sup>

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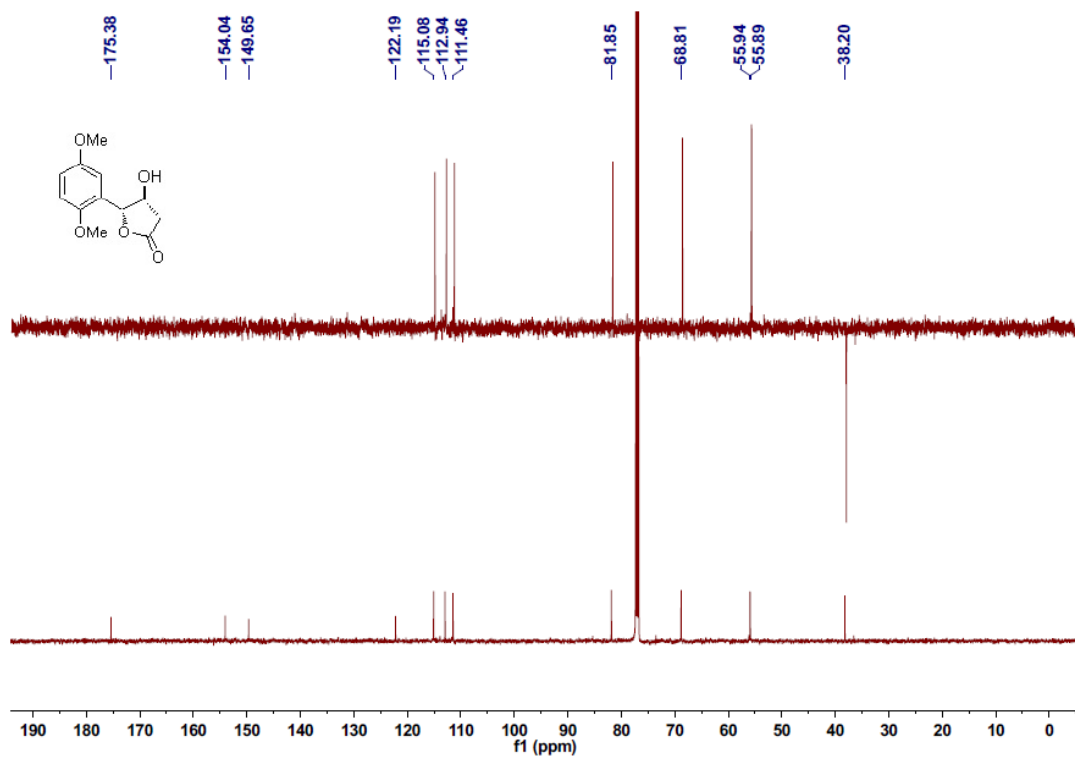
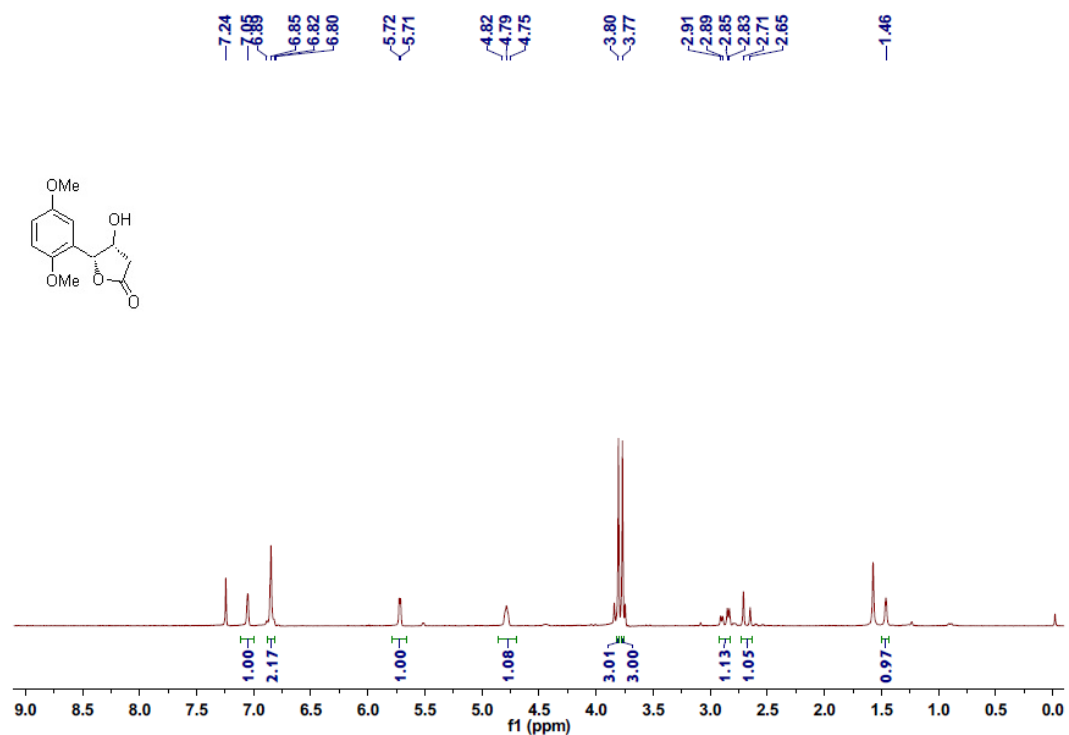
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## 1. Copies of NMR Data for All Compounds.

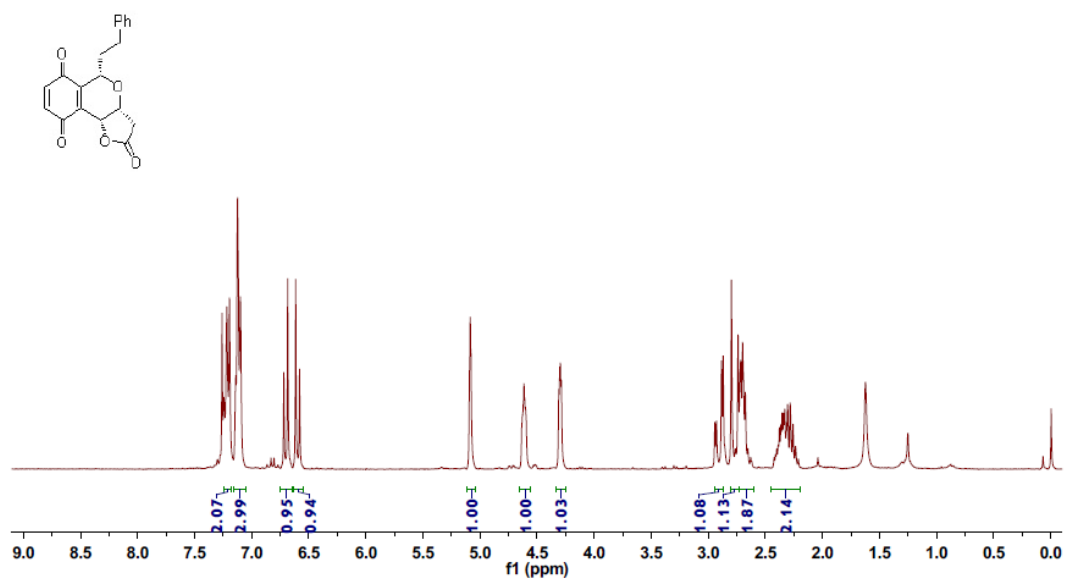
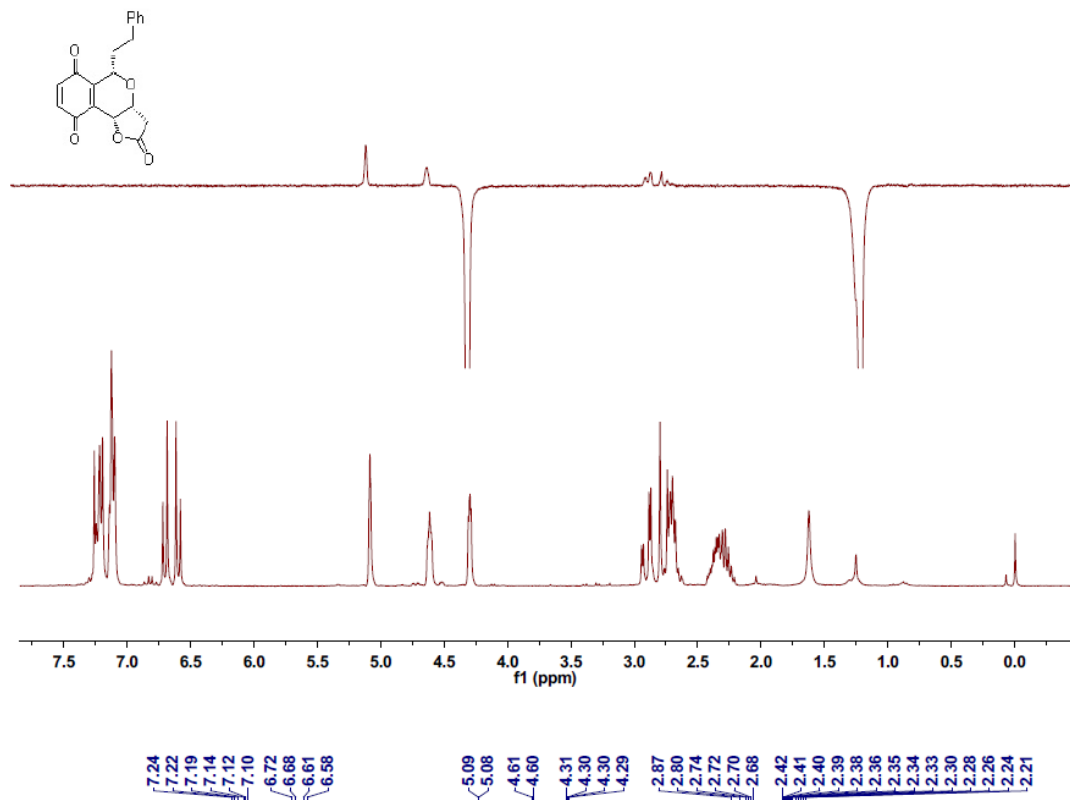
$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (126 MHz) spectra of compound **6b**.

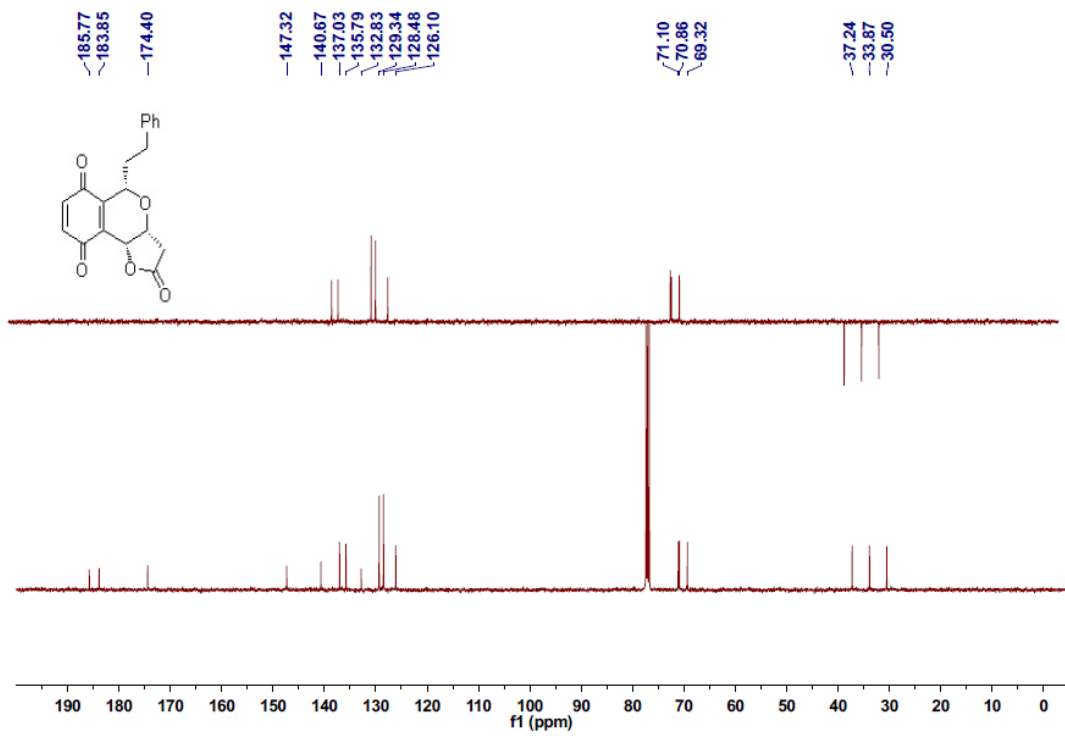


$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (126 MHz) spectra of compound 7.

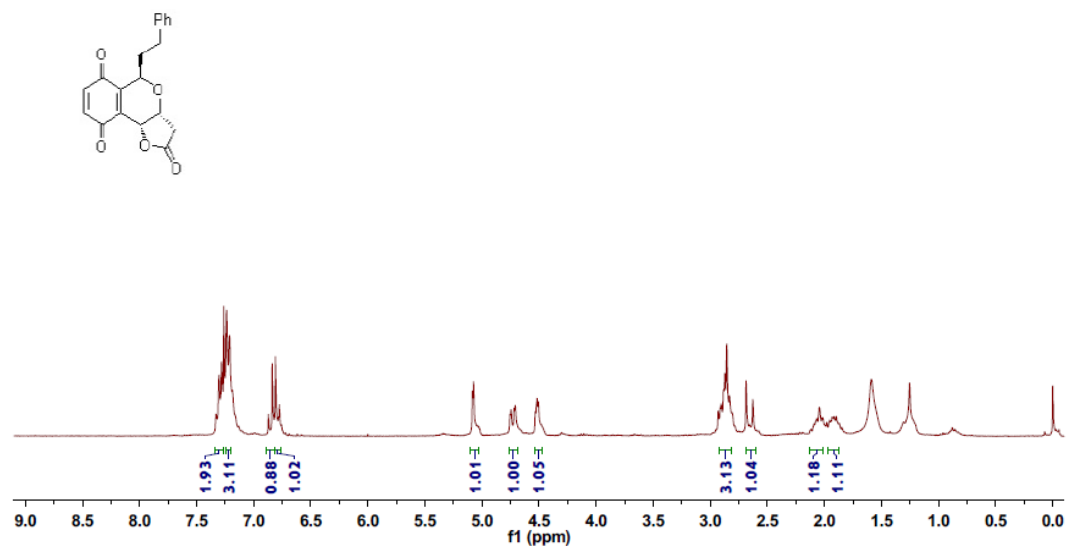
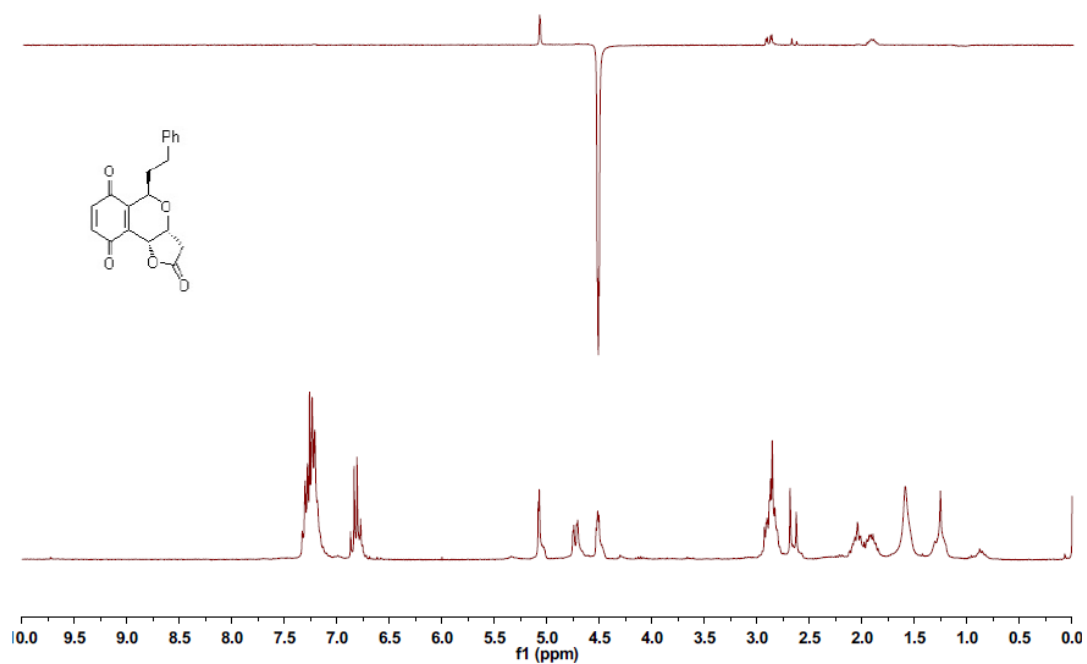


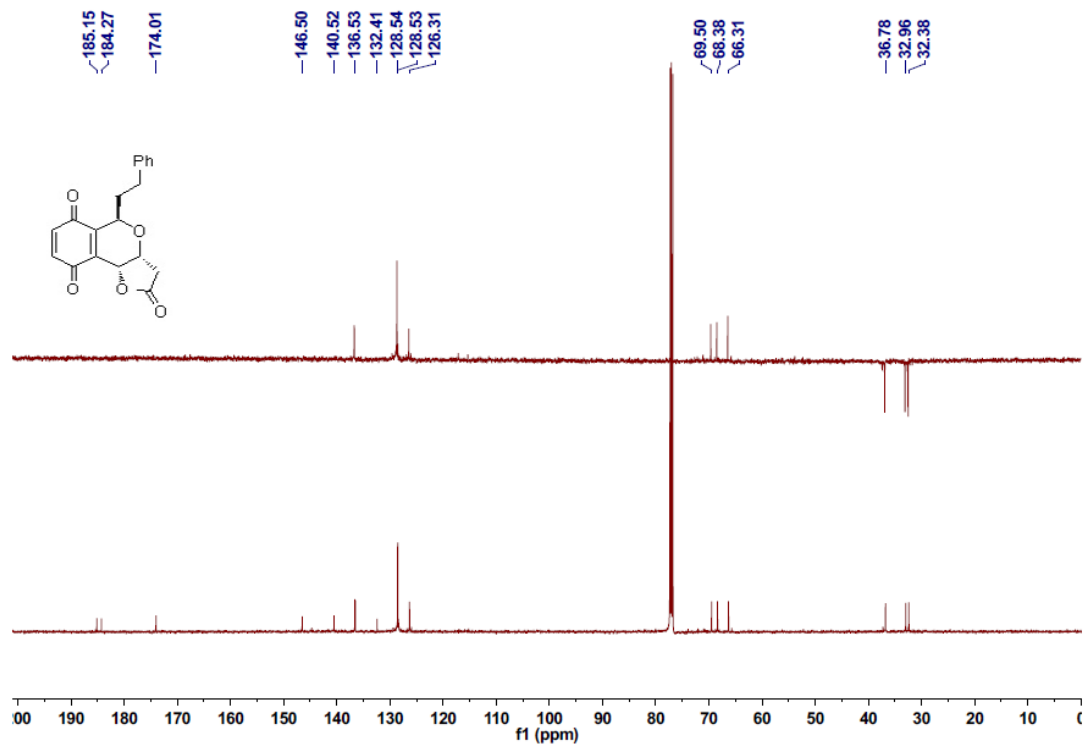
$^1\text{H}$  NMR (300 MHz),  $^{13}\text{C}$  NMR (101 MHz) and NOE spectra of compound **9a**.



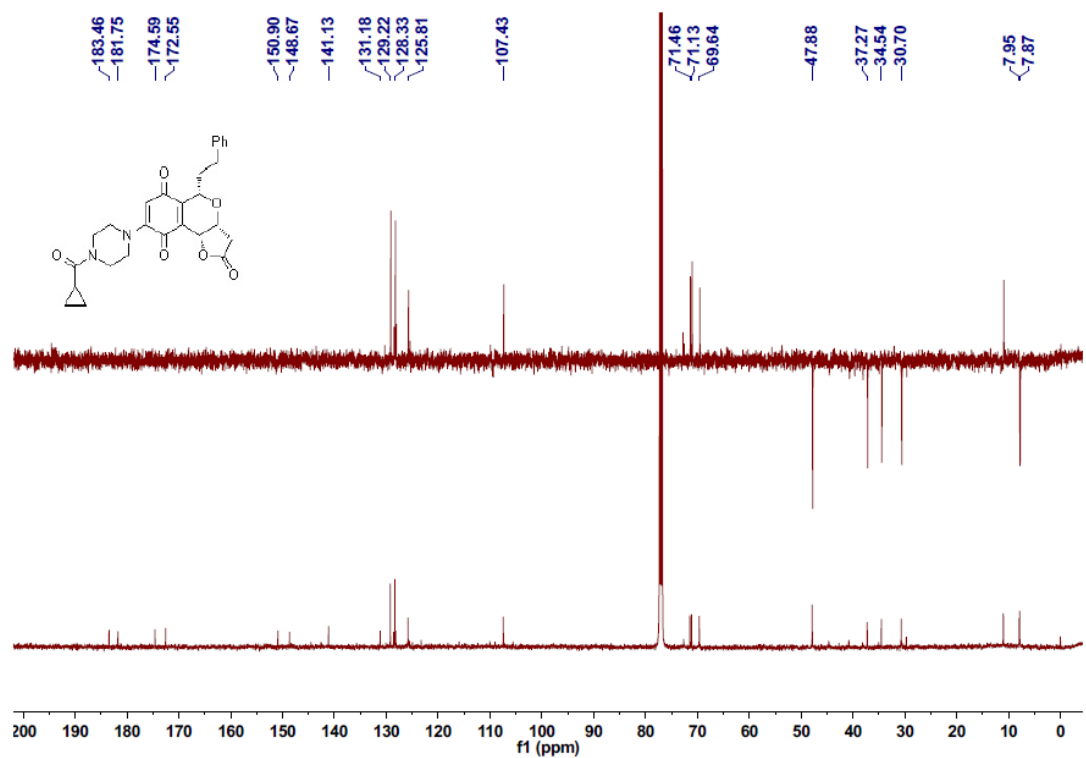
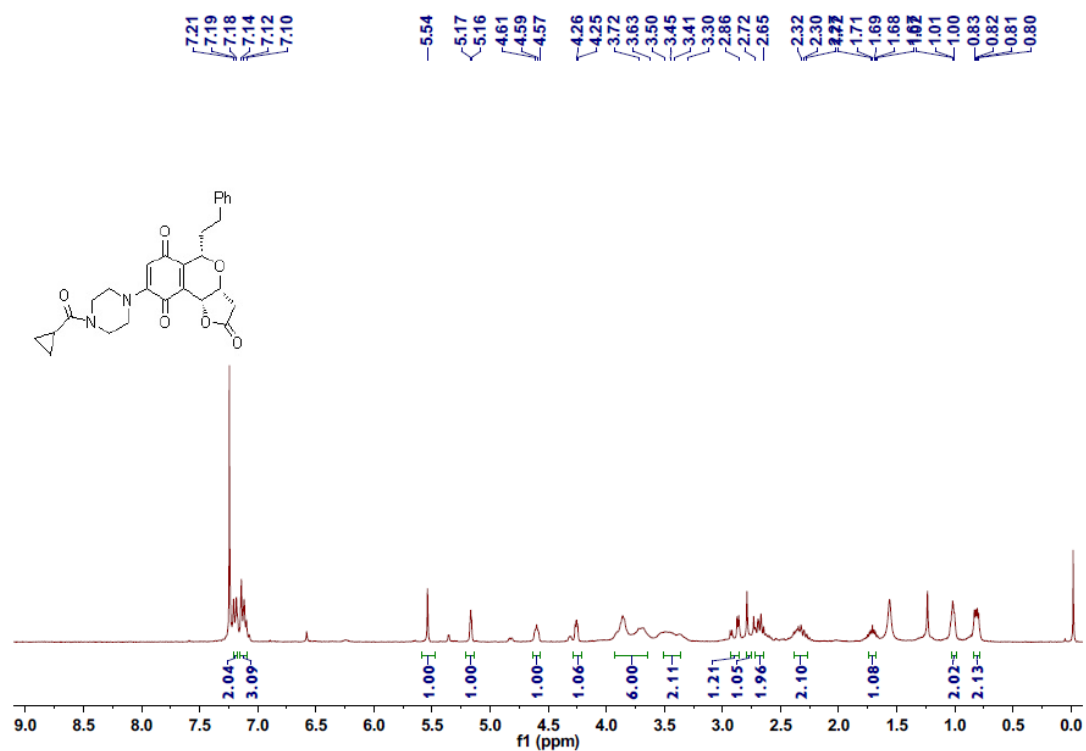


$^1\text{H}$  NMR (300 MHz),  $^{13}\text{C}$  NMR (126 MHz) and NOE spectra of compound **9a'**.



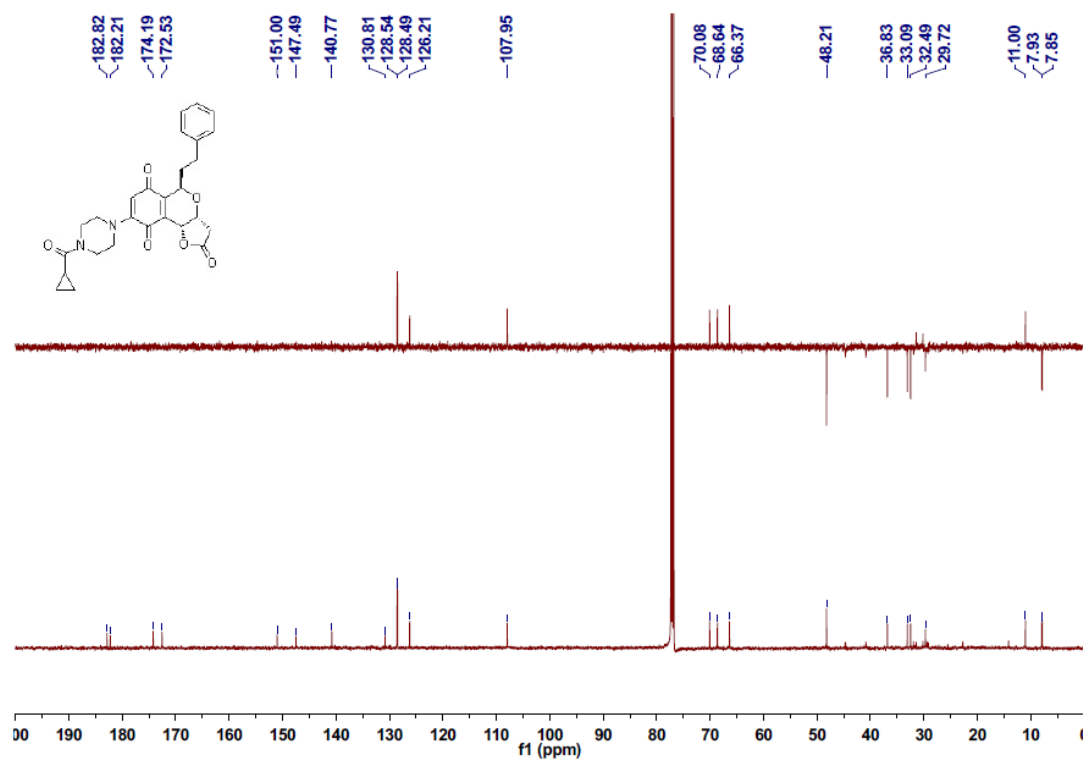
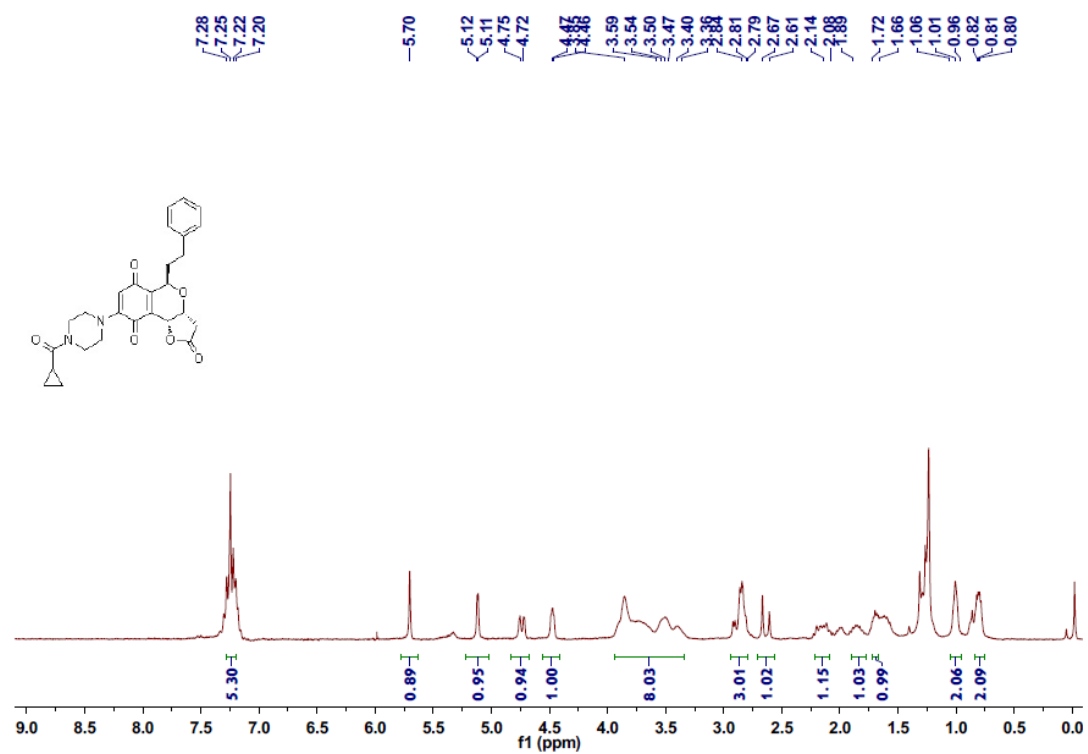


$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (126 MHz) spectra of compound **10a**.

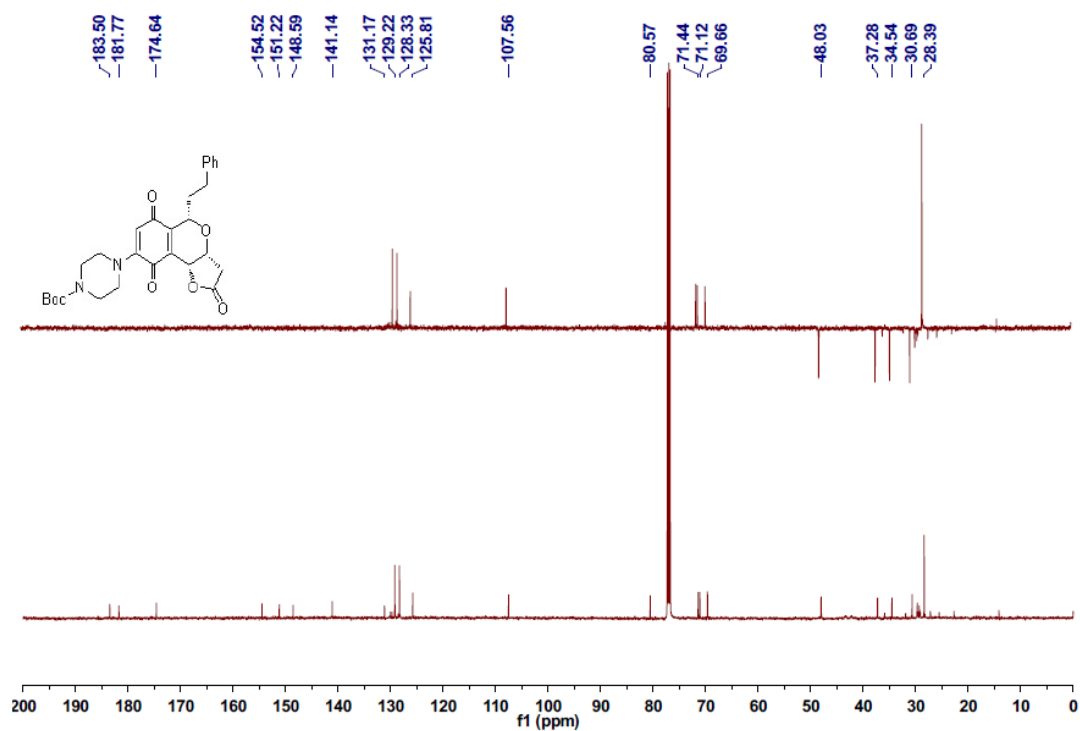
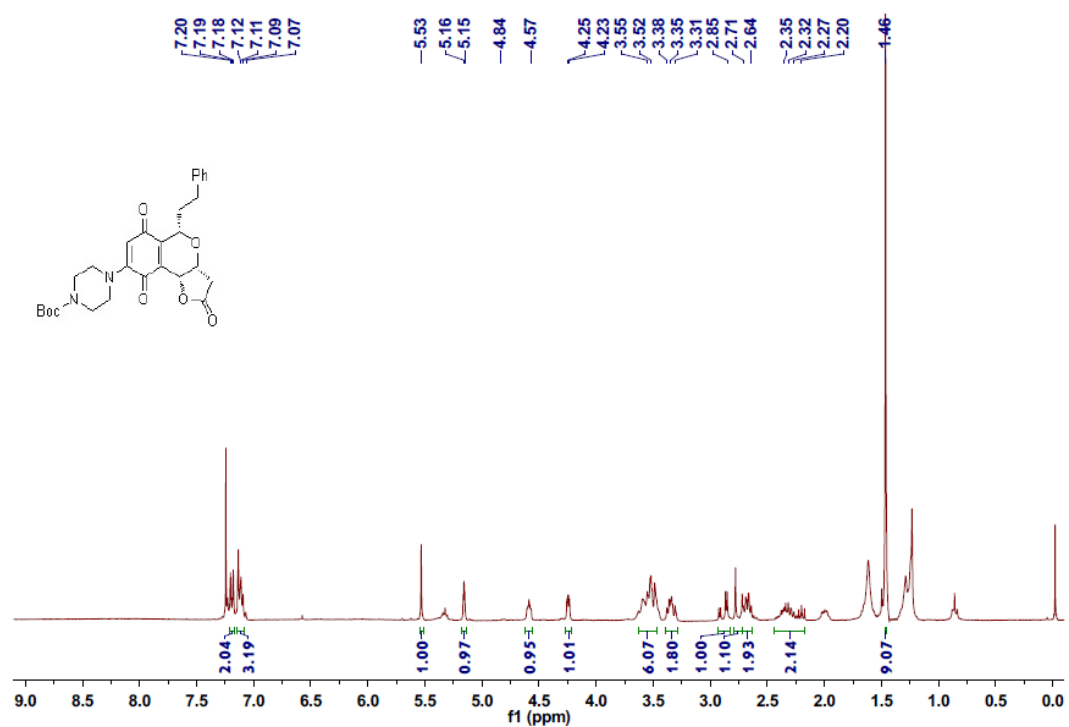




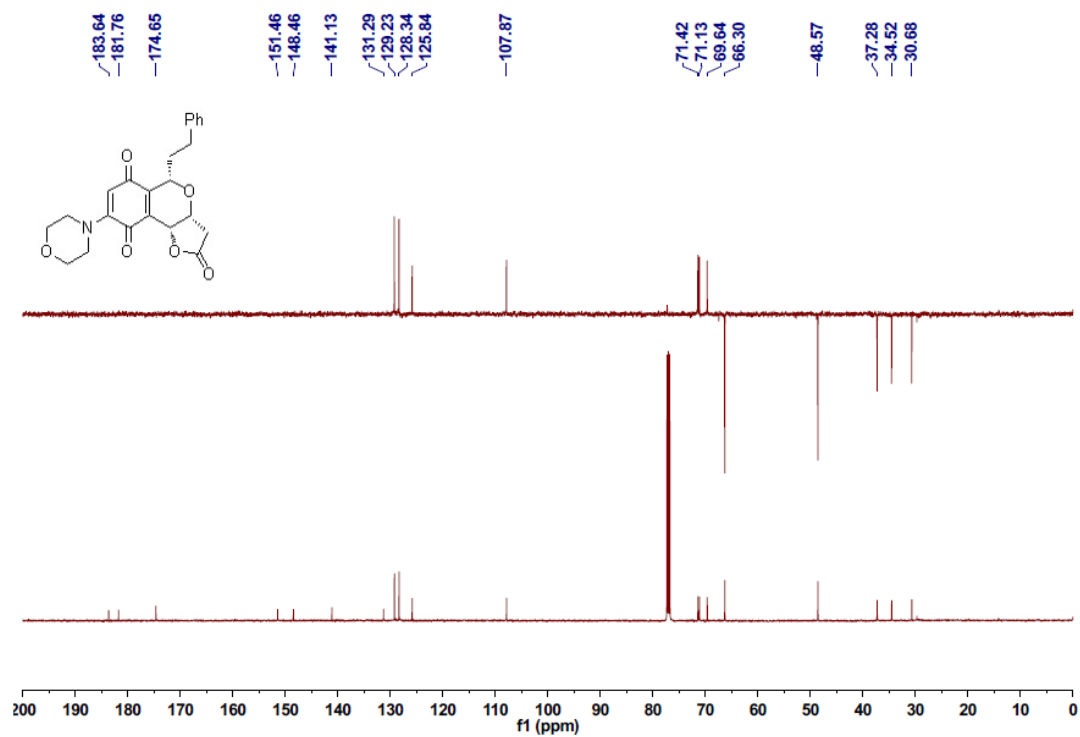
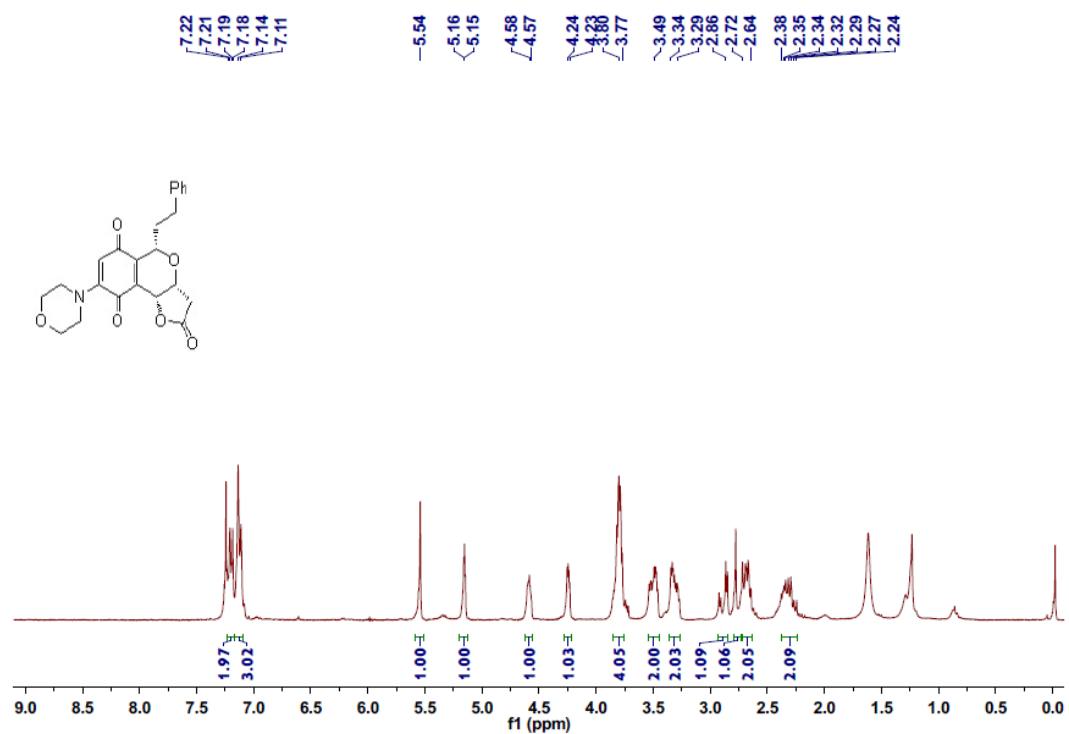
$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (126 MHz) spectra of compound **10a'**.



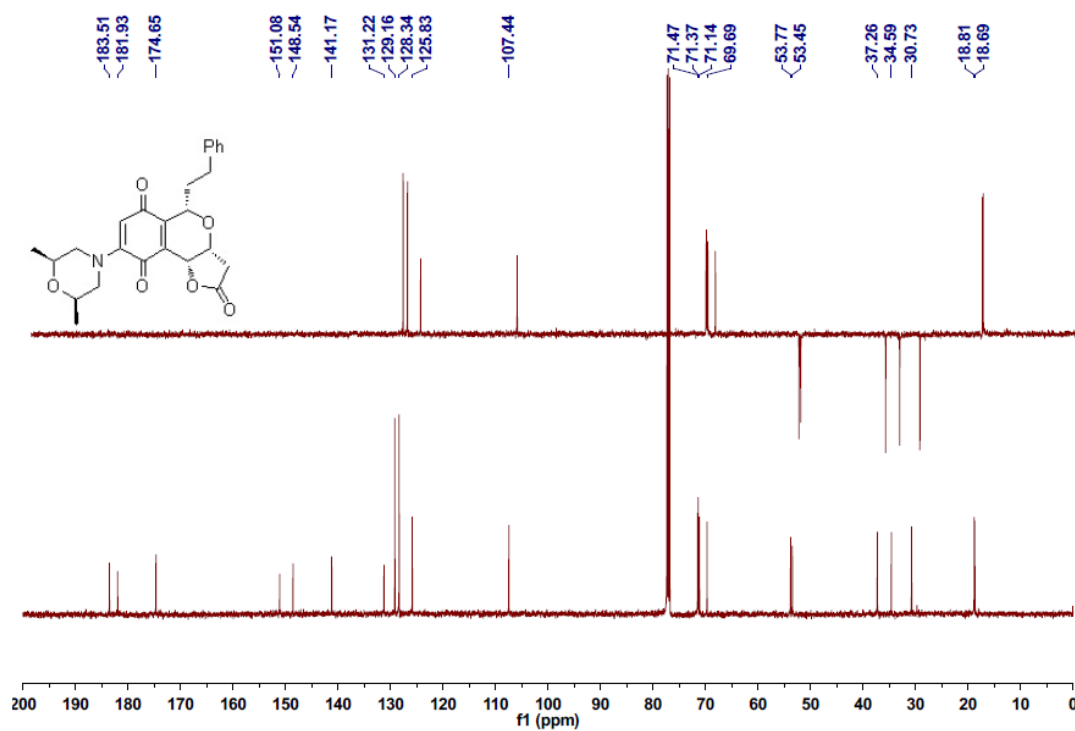
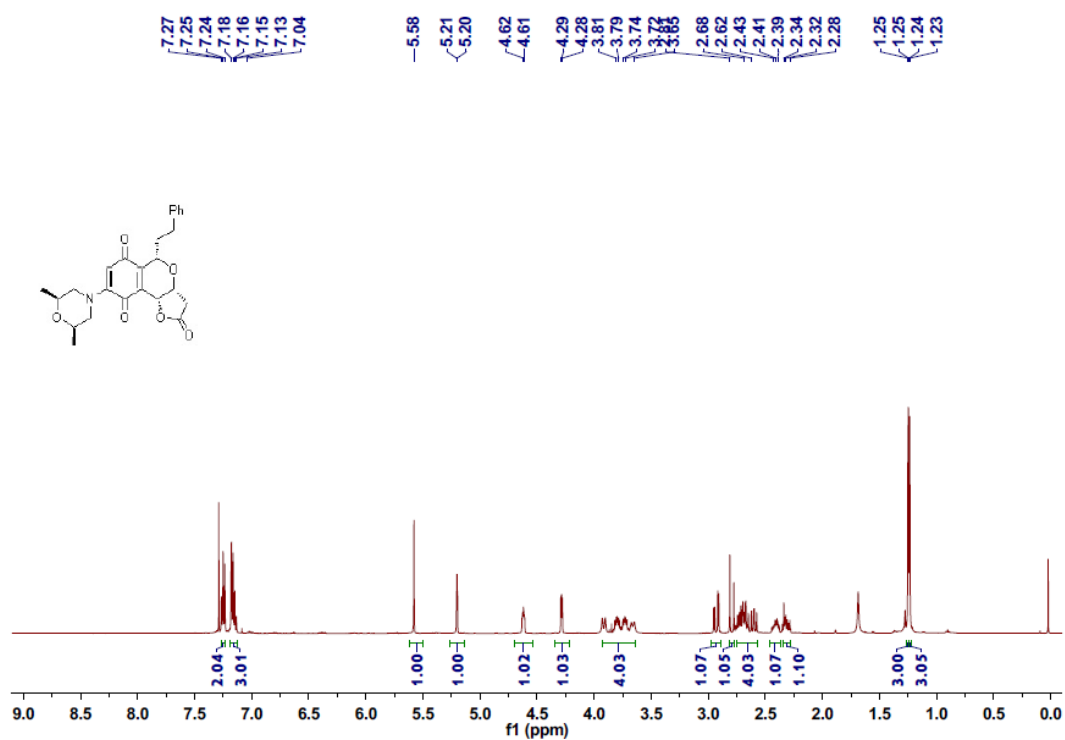
$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (126 MHz) spectra of compound **10b**.

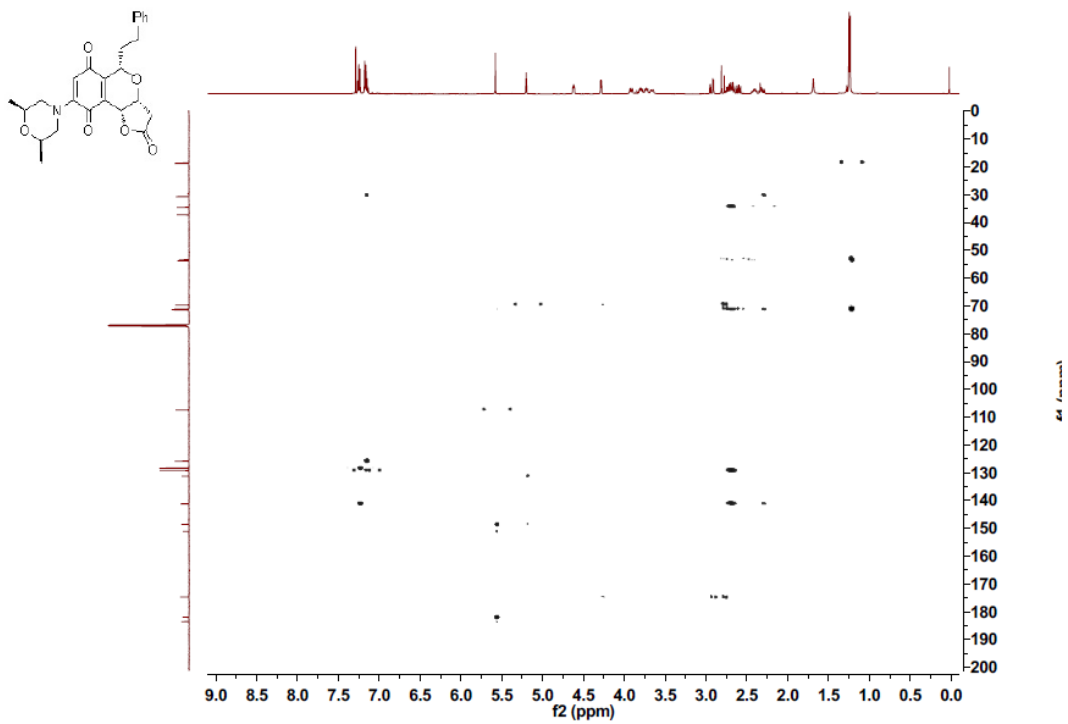


$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (126 MHz) spectra of compound **10c**.

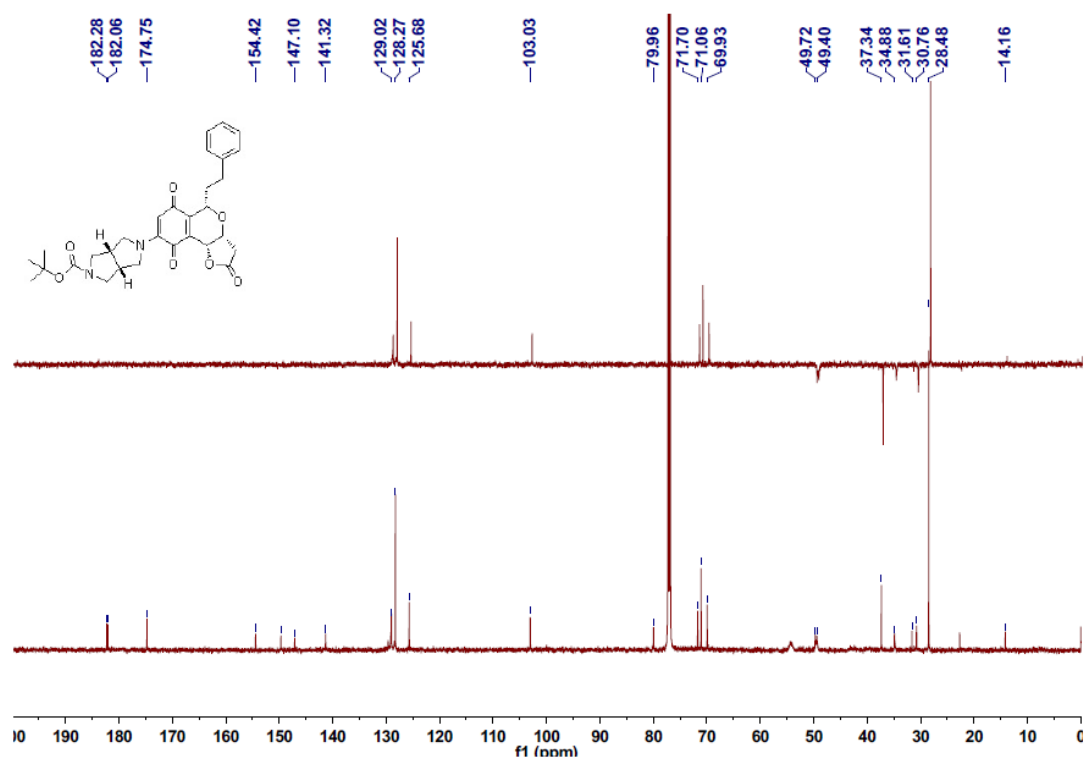
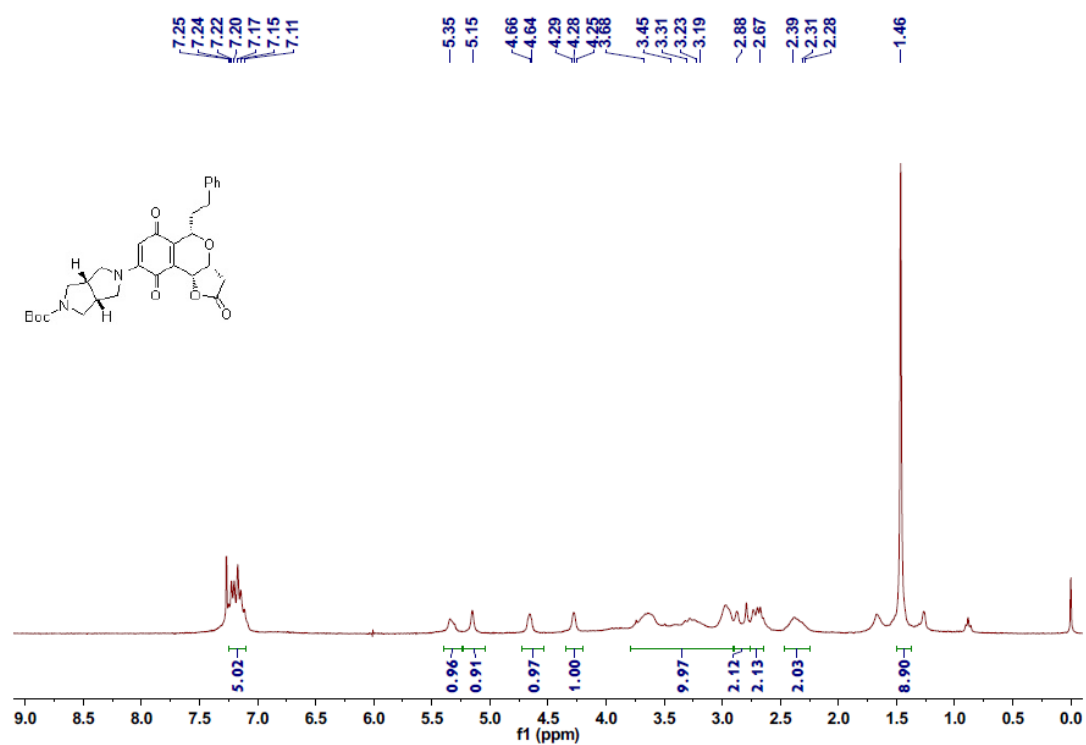


$^1\text{H}$  NMR (500 MHz),  $^{13}\text{C}$  NMR (126 MHz) and HMBC spectra of compound **10d**.

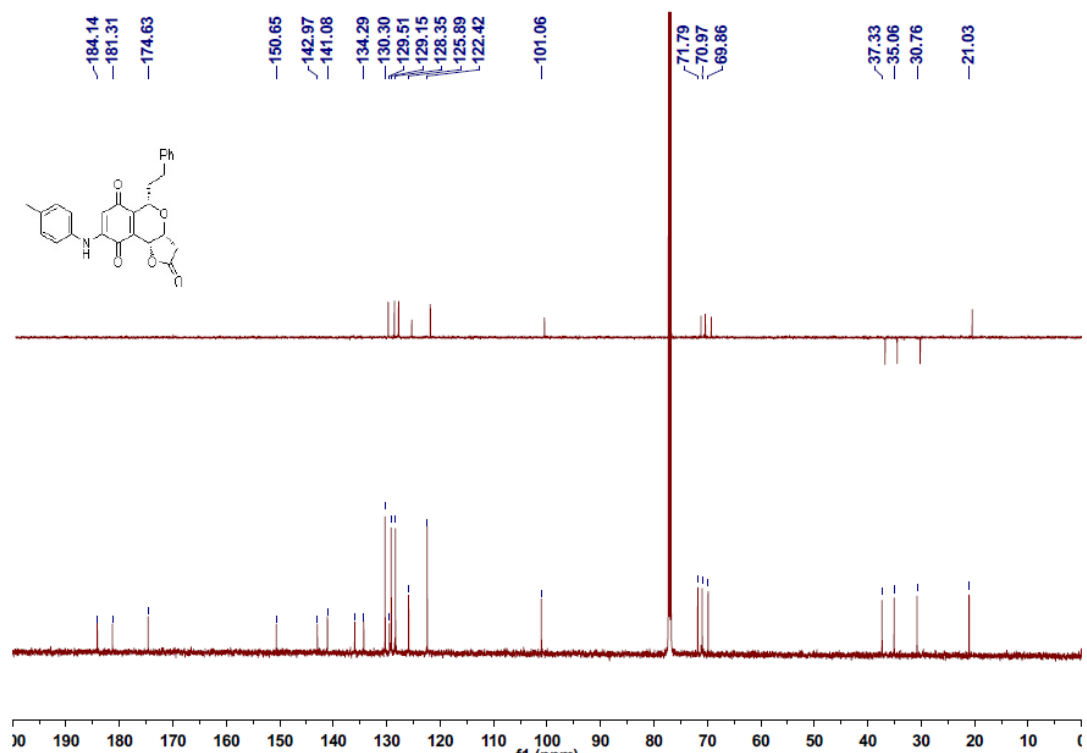
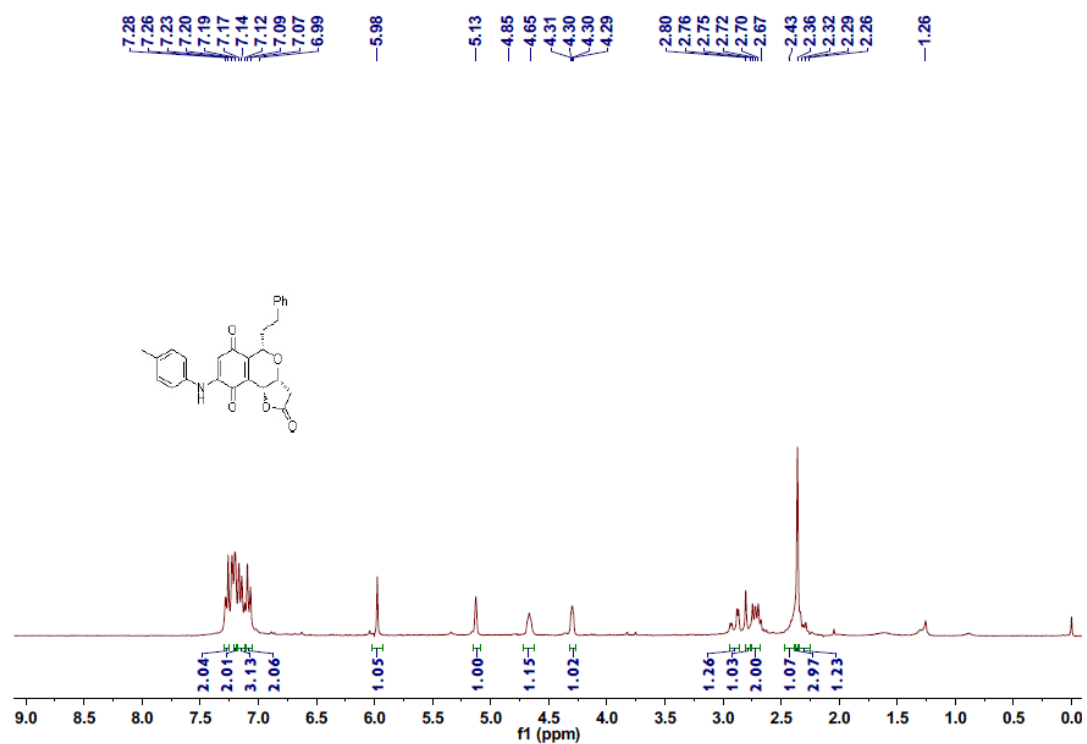




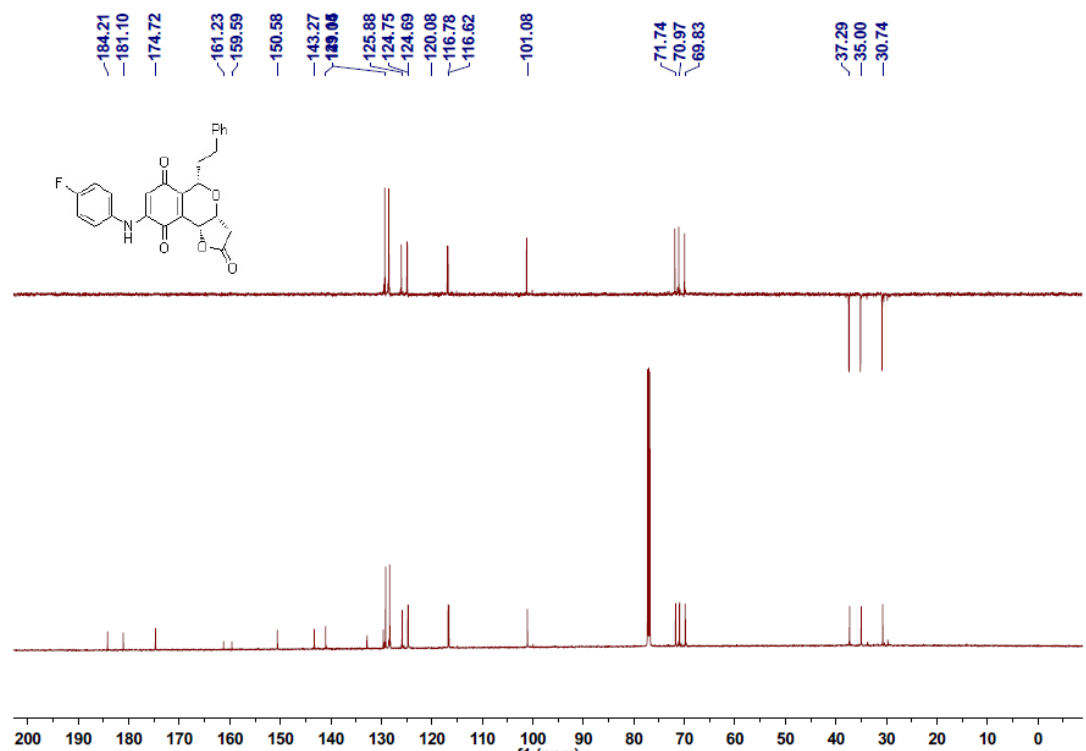
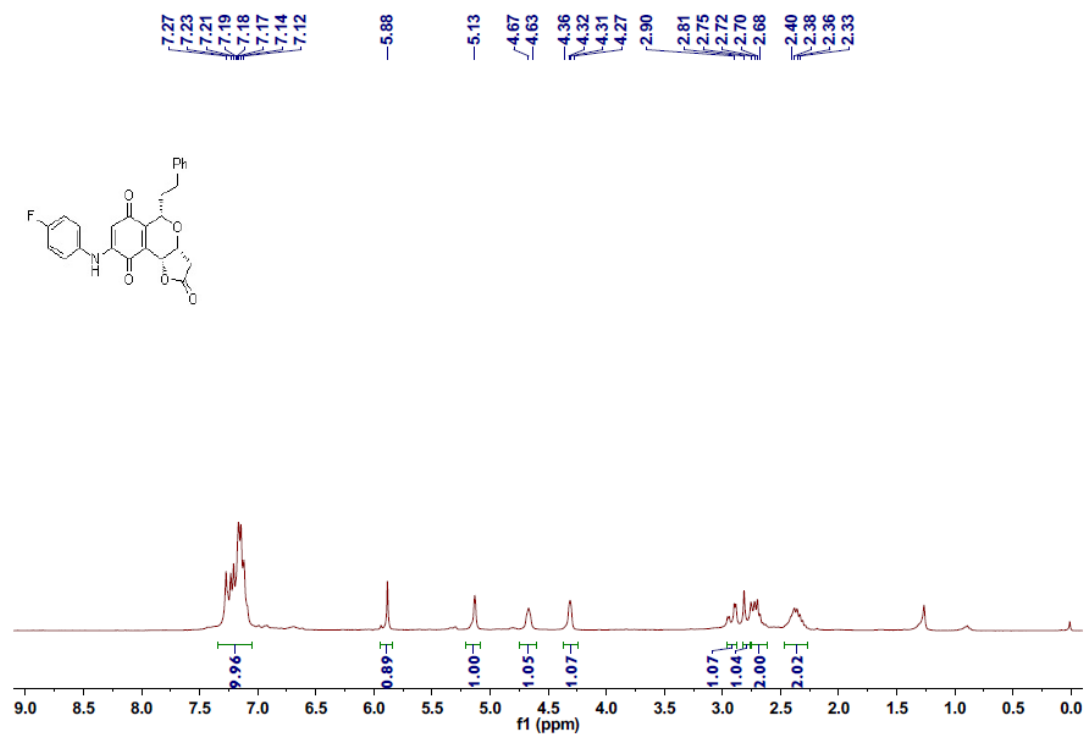
$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (151 MHz) spectra of compound **10e**.



$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (151 MHz) spectra of compound **11a**.

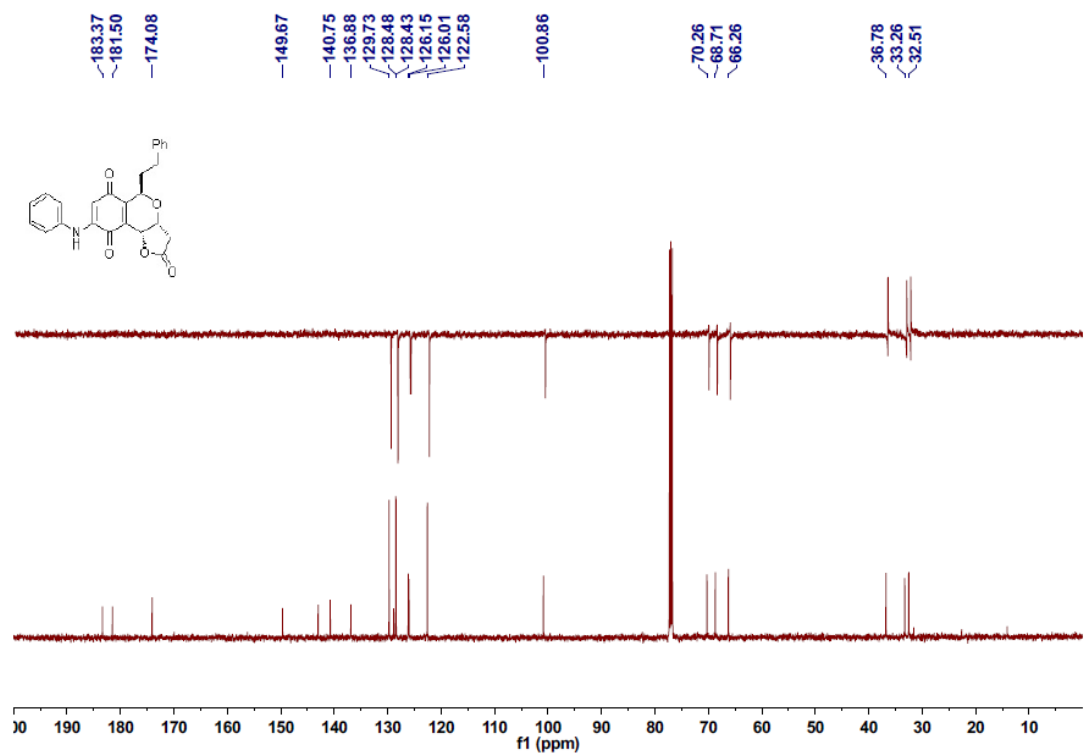
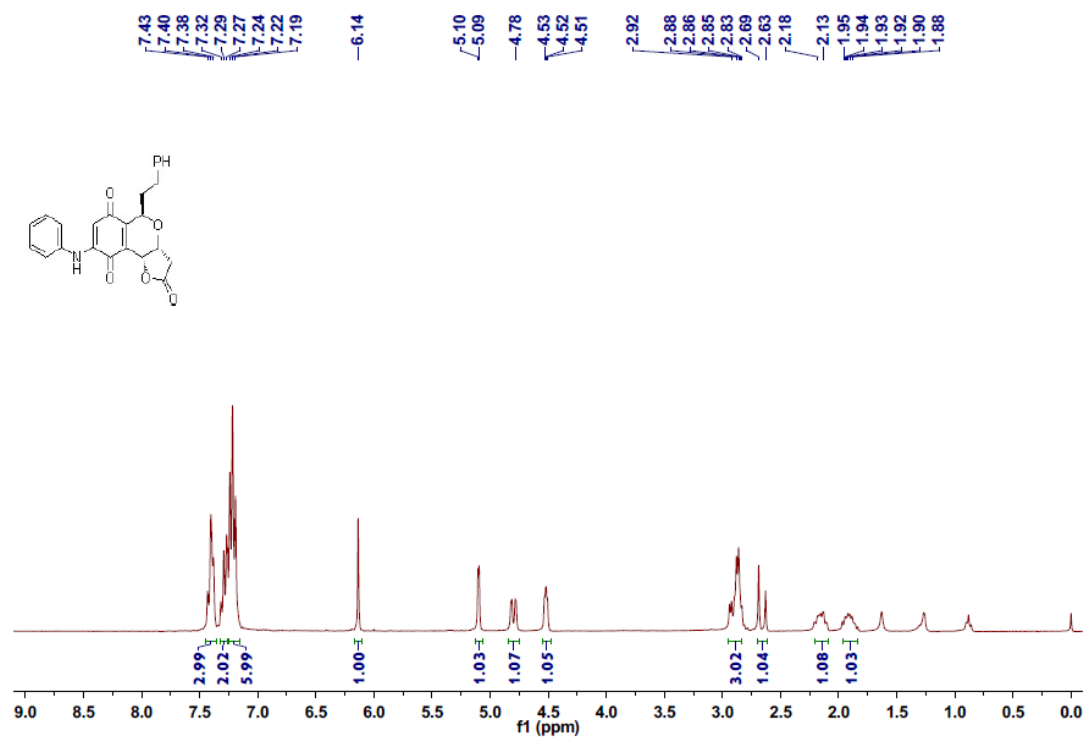


$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (151 MHz) spectra of compound **11b**.

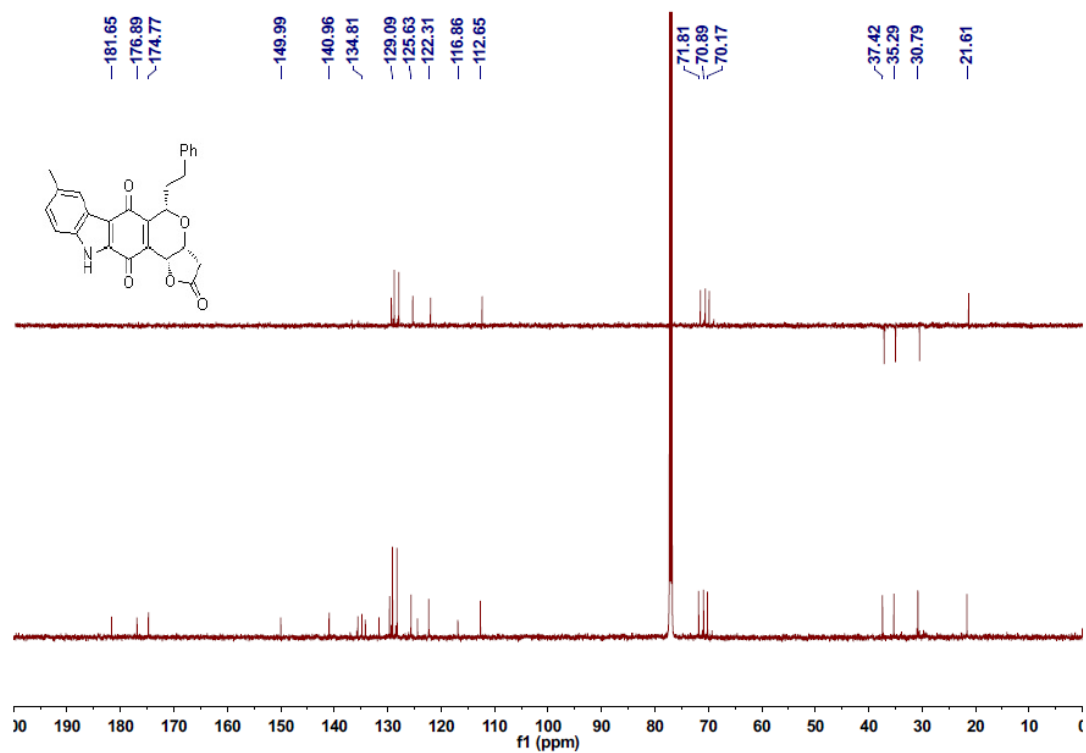
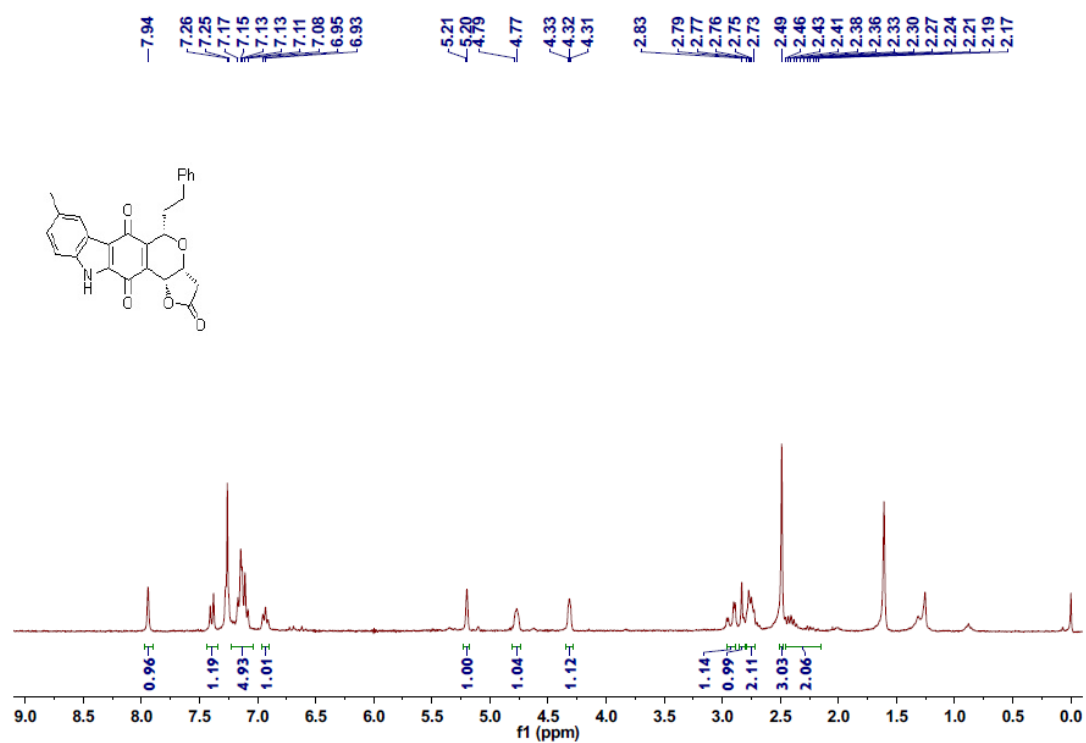




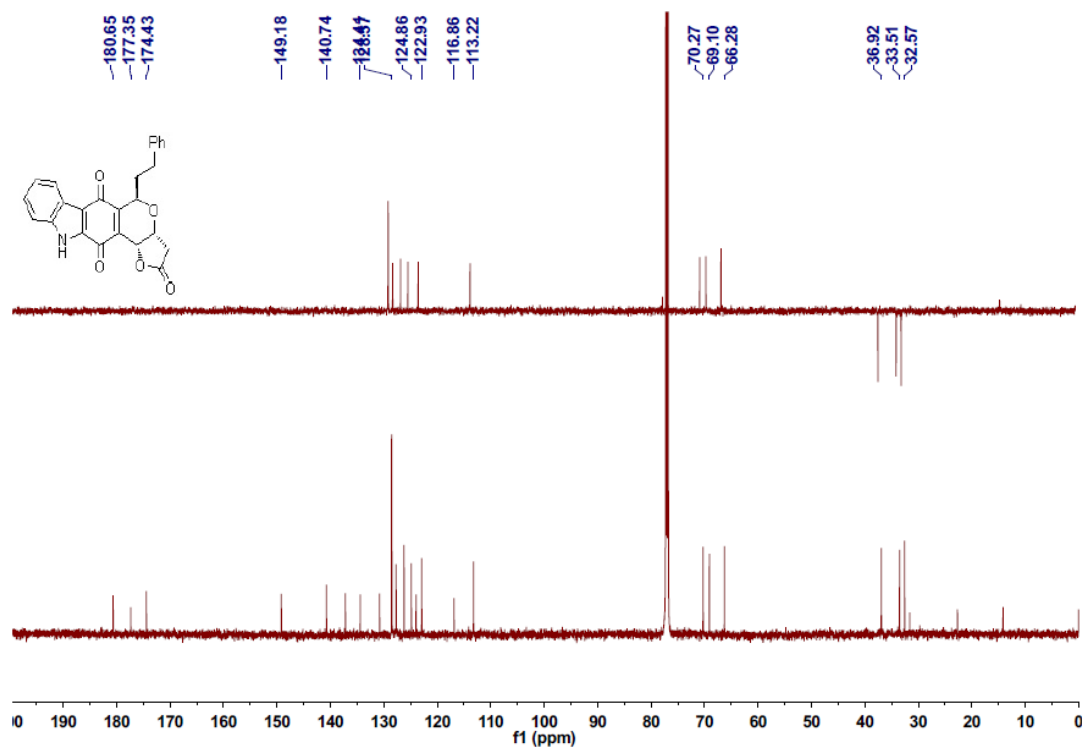
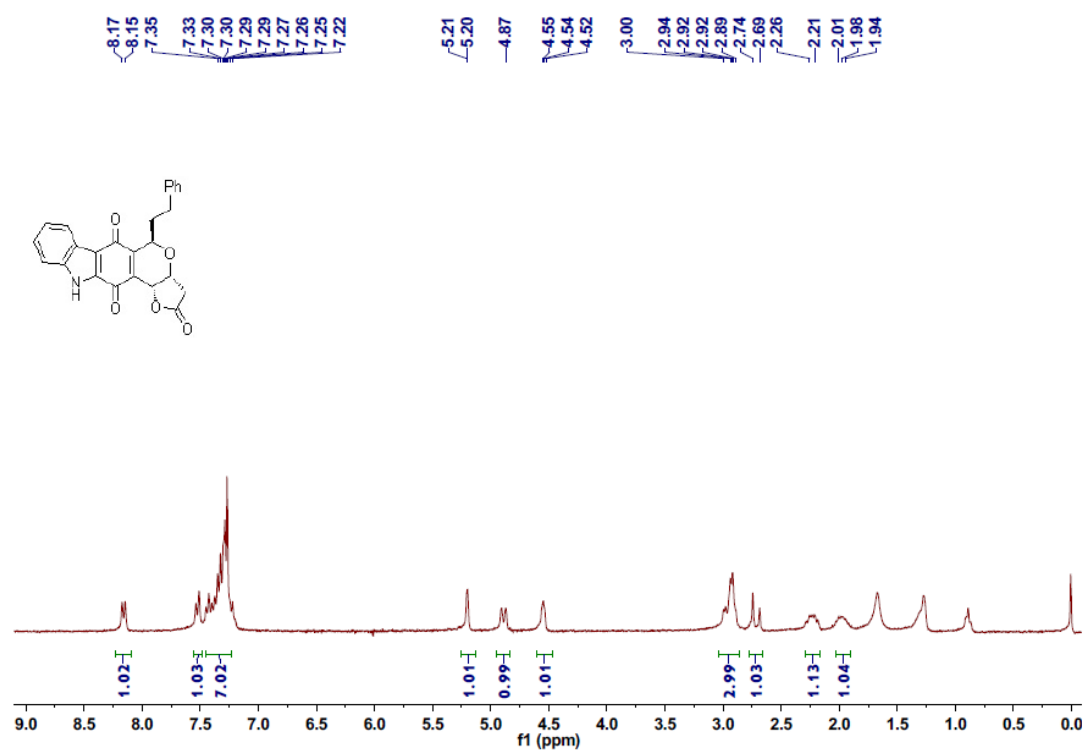
$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (126 MHz) spectra of compound **11c**.



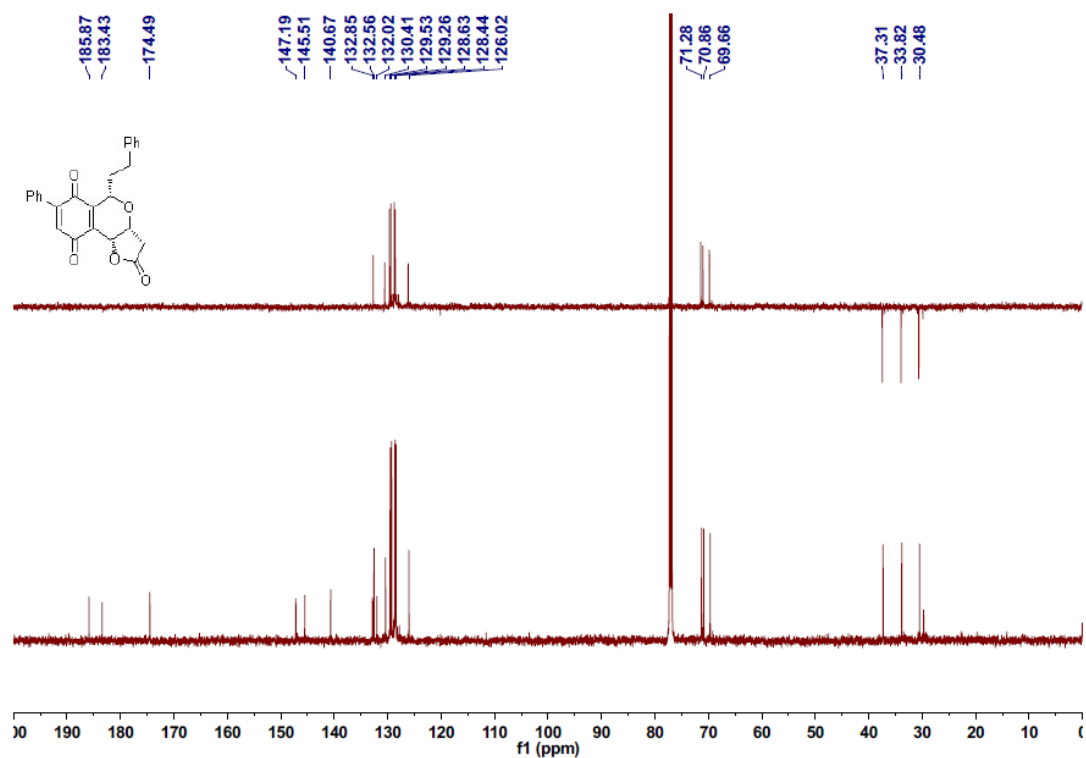
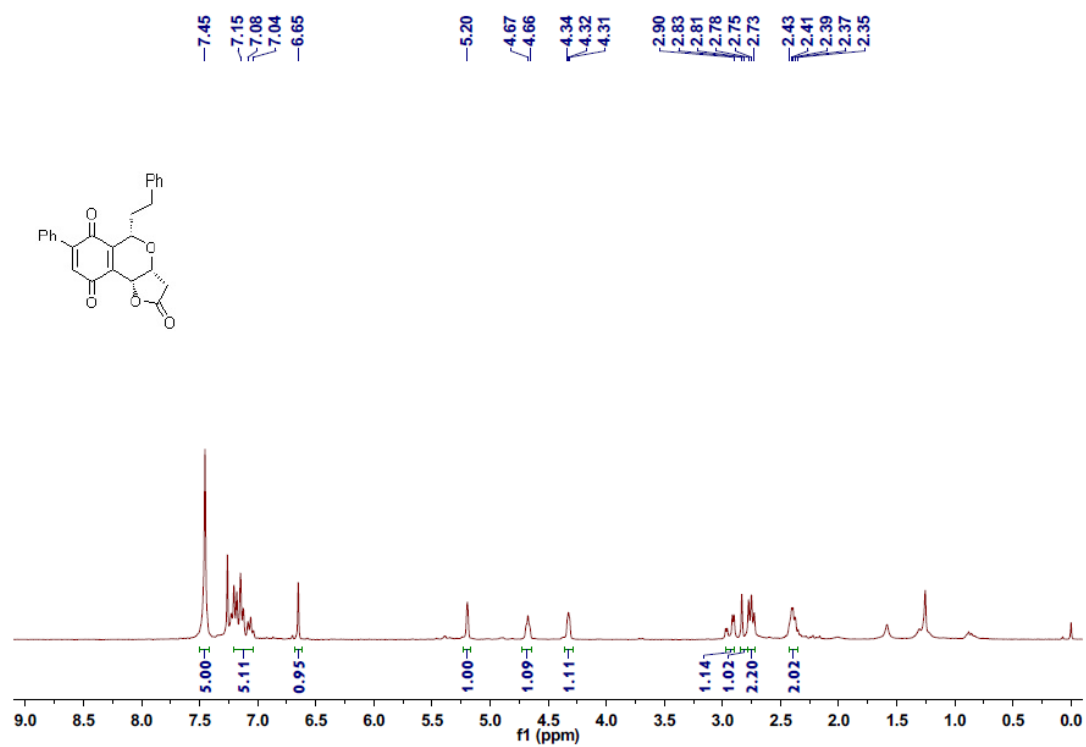
$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (151 MHz) spectra of compound **12**.

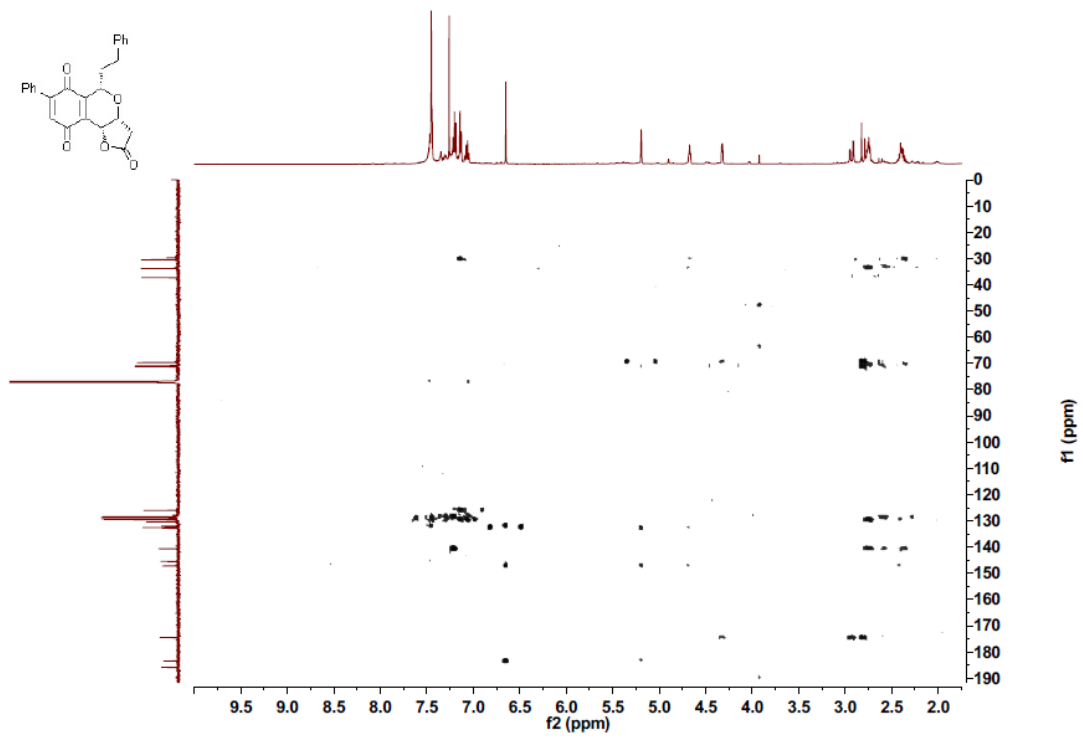


$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (151 MHz) spectra of compound **13**.



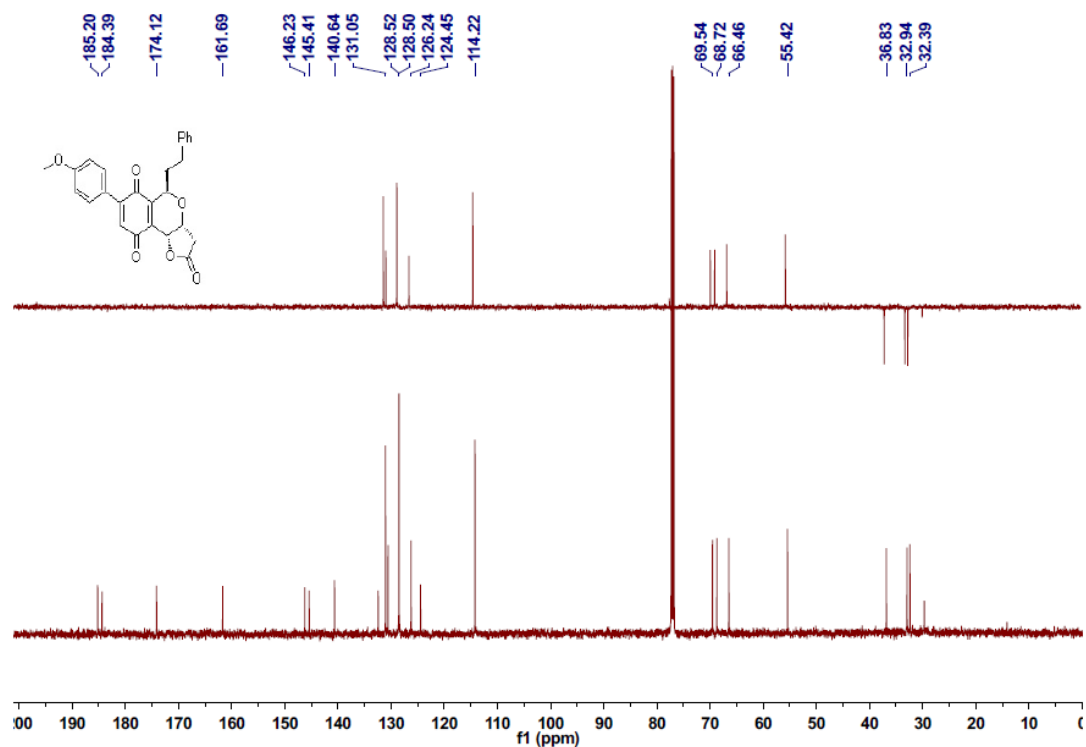
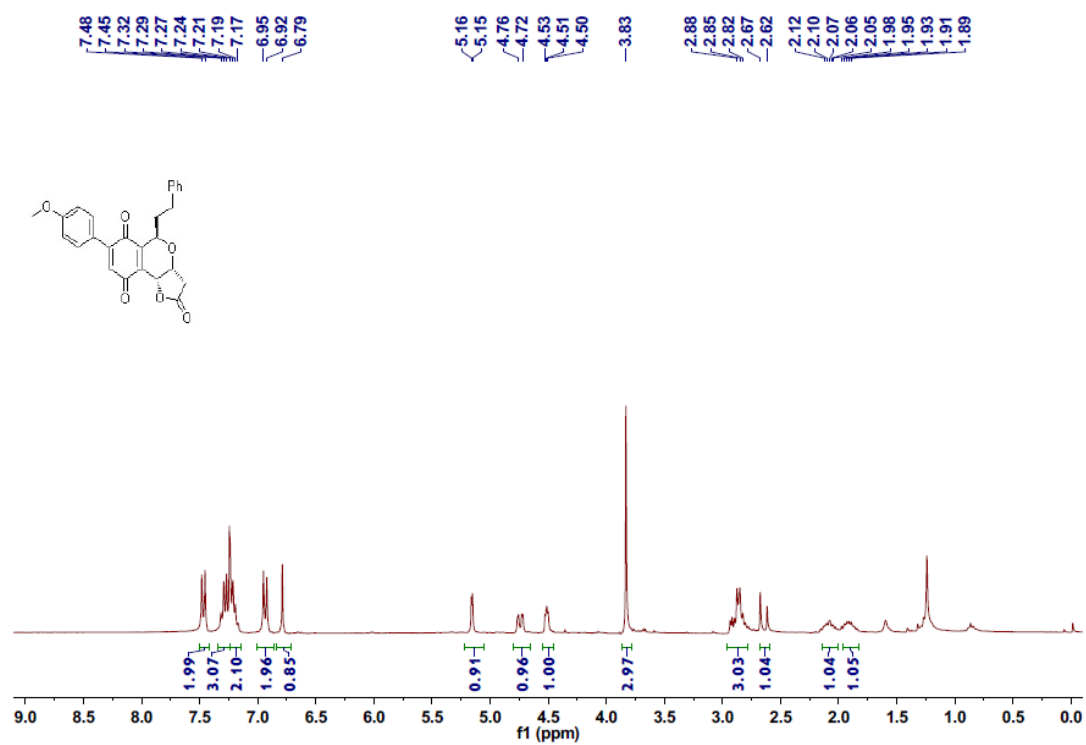
$^1\text{H}$  NMR (300 MHz),  $^{13}\text{C}$  NMR (151 MHz) and HMBC spectra of compound **14a**.



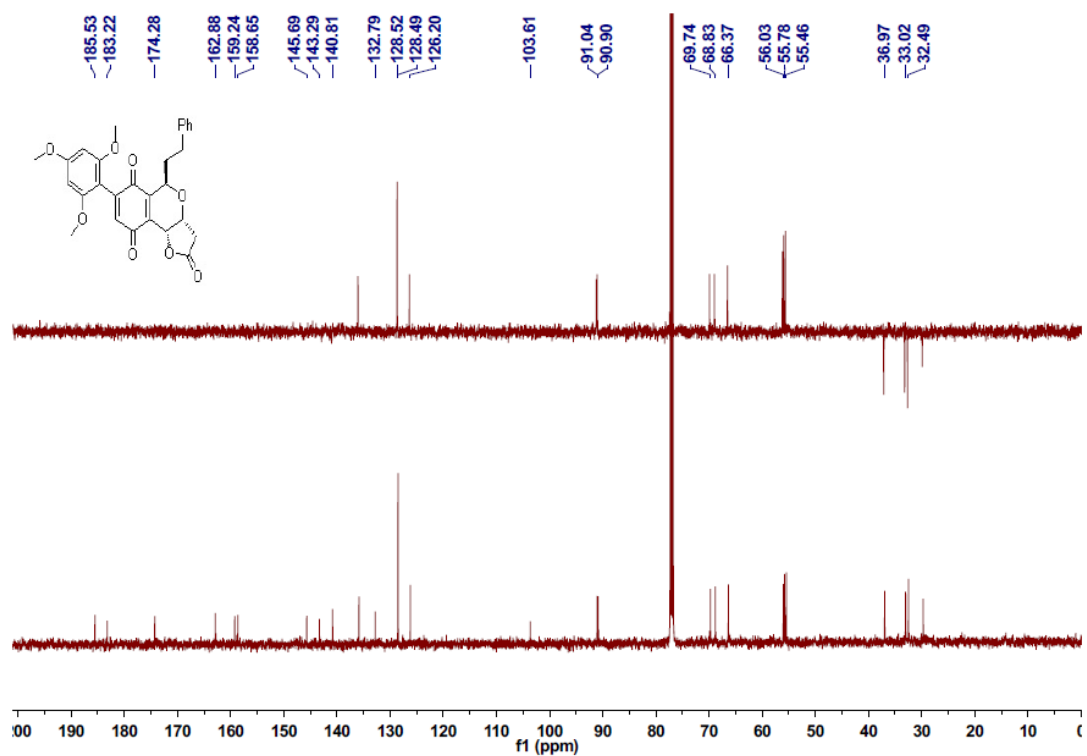
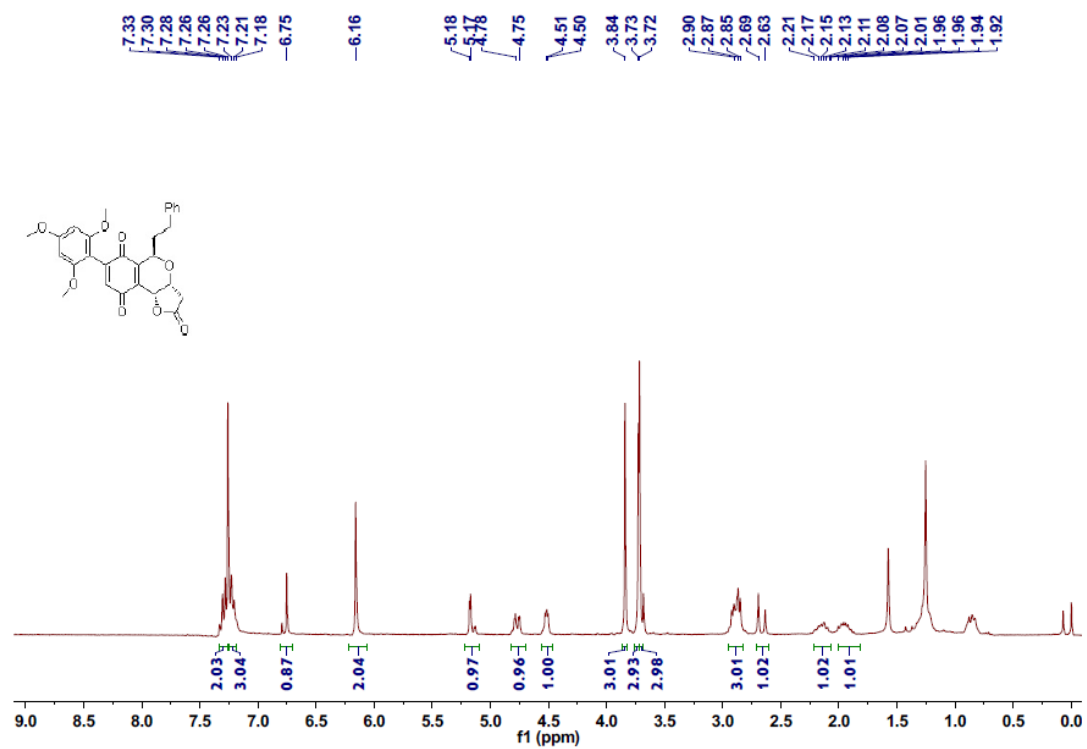




$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (126 MHz) spectra of compound **14c**.



$^1\text{H}$  NMR (300 MHz) and  $^{13}\text{C}$  NMR (126 MHz) spectra of compound **14d**.





## 2. Computational method of compound 9a

Gaussian 09<sup>1</sup> was performed at the B3LYP<sup>2</sup> level of density functional theory (DFT) for geometry optimizations. 6-31(g) basis set was used for C, H, O.<sup>3</sup>

### Cartesian coordinates

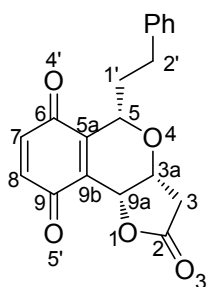
#### 9a

0 1 (charge, spin multiplicity)

C	-3.26200000	1.15200000	0.60000000
C	-3.22400000	-0.18000000	0.63300000
C	-1.94800000	-0.91500000	0.56400000
C	-0.69900000	-0.12100000	0.40700000
C	-0.73900000	1.22400000	0.38200000
C	-2.03100000	1.95400000	0.49200000
C	0.58800000	-0.90100000	0.32300000
C	1.85800000	-0.03900000	0.44000000
C	0.49000000	2.07800000	0.23300000
O	-2.09300000	3.17700000	0.49200000
O	-1.94400000	-2.13800000	0.63600000
C	2.96200000	-0.90200000	-0.18200000
H	-4.19300000	1.70400000	0.65500000
H	-4.12200000	-0.78000000	0.71800000
H	0.61500000	-1.64800000	1.13000000
H	2.08700000	0.16200000	1.49400000
H	0.73000000	2.52100000	1.20800000
H	3.52200000	-1.42000000	0.60600000
H	3.68500000	-0.30800000	-0.75200000
C	2.26500000	-1.93800000	-1.06500000
O	2.79535839	-2.85374640	-1.68663939
O	0.77800000	-1.61000000	-1.02200000
O	1.70200000	1.30200000	-0.28600000
C	0.22177700	3.24217208	-0.73878176
H	-0.49713624	2.93760978	-1.47042755
H	-0.15737798	4.08140627	-0.19396301
C	1.53395143	3.63681590	-1.44167188
H	2.33162268	3.64649755	-0.72856120
H	1.75305533	2.92756815	-2.21229572
C	1.38272927	5.03831176	-2.06178576
C	1.69621933	6.17114440	-1.31019704
C	0.93247569	5.17518948	-3.37482968
C	1.55881321	7.44055833	-1.87138291
H	2.05043191	6.06292922	-0.27479146
C	0.79591264	6.44487647	-3.93666183
H	0.68552182	4.28243917	-3.96740009

C	1.10885649	7.57750316	-3.18515671
H	1.80529176	8.33354302	-1.27882642
H	0.44127706	6.55247366	-4.97209926
H	1.00065149	8.57849064	-3.62743726

### NBO (Natural Bond Orbital) charge values



Atom	NBO charge values
O <sub>1</sub>	-0.531
O <sub>4</sub>	-0.591
O <sub>3'</sub>	-0.524
O <sub>4'</sub>	-0.484
O <sub>5'</sub>	-0.473
C <sub>2</sub>	0.773
C <sub>3</sub>	-0.593
C <sub>3a</sub>	0.054
C <sub>5</sub>	0.059
C <sub>5a</sub>	-0.040
C <sub>6</sub>	0.463
C <sub>7</sub>	-0.246
C <sub>8</sub>	-0.236
C <sub>9</sub>	0.465
C <sub>9b</sub>	-0.076
C <sub>9a</sub>	0.012

### 3. References

- (1) Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J.

- B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
- (2) Becke, A. D. *J. Chem. Phys.*, 1993, **98**, 5648.
- (3) Wadt, W. R.; Hay, P. J. *J. Chem. Phys.*, 1985, **82**, 299.