

Supporting Information
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Diels-Alder Reactions of 1,3-Dienes Incorporated into 8-Oxa- and 8-Thiabicyclo[3.2.1]octane Skeletons: A Convenient Access to Complex Tri- and Tetracyclic Compounds

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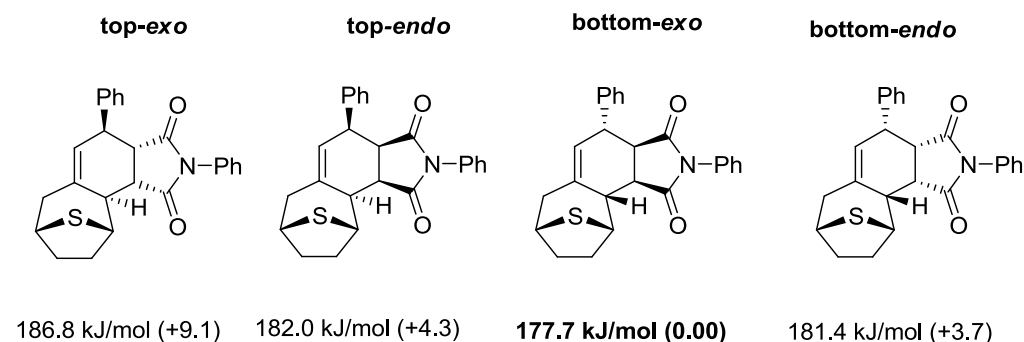
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MM2 Calculations

Molecular modeling (MM2 force-field as implemented in the ChemBio3D program package)^[1] was used to obtain the energy-minimized conformations of the generated Diels-Alder adducts.

Absolute and relative energies in kJ/mol of the four diastereomers of compound **12**



top- <i>exo</i> - 12	top- <i>endo</i> - 12	bottom- <i>exo</i> - 12	bottom- <i>endo</i> - 12
9.1	4.3	0.0	3.7

Relative energies of the other calculated compounds in kJ/mole

top- <i>exo</i> - 13	top- <i>endo</i> - 13	bottom- <i>exo</i> - 13	bottom- <i>endo</i> - 13
11.5	3.7	0.0	3.9

top- <i>exo</i> - 16	top- <i>endo</i> - 16	bottom- <i>exo</i> - 16	bottom- <i>endo</i> - 16
10.9	0.0	4.3	7.7

Calculations of **18** without methoxy group

top- <i>exo</i> - 18*	top- <i>endo</i> - 18*	bottom- <i>exo</i> - 18*	bottom- <i>endo</i> - 18*
17.4	0.0	8.2	3.5

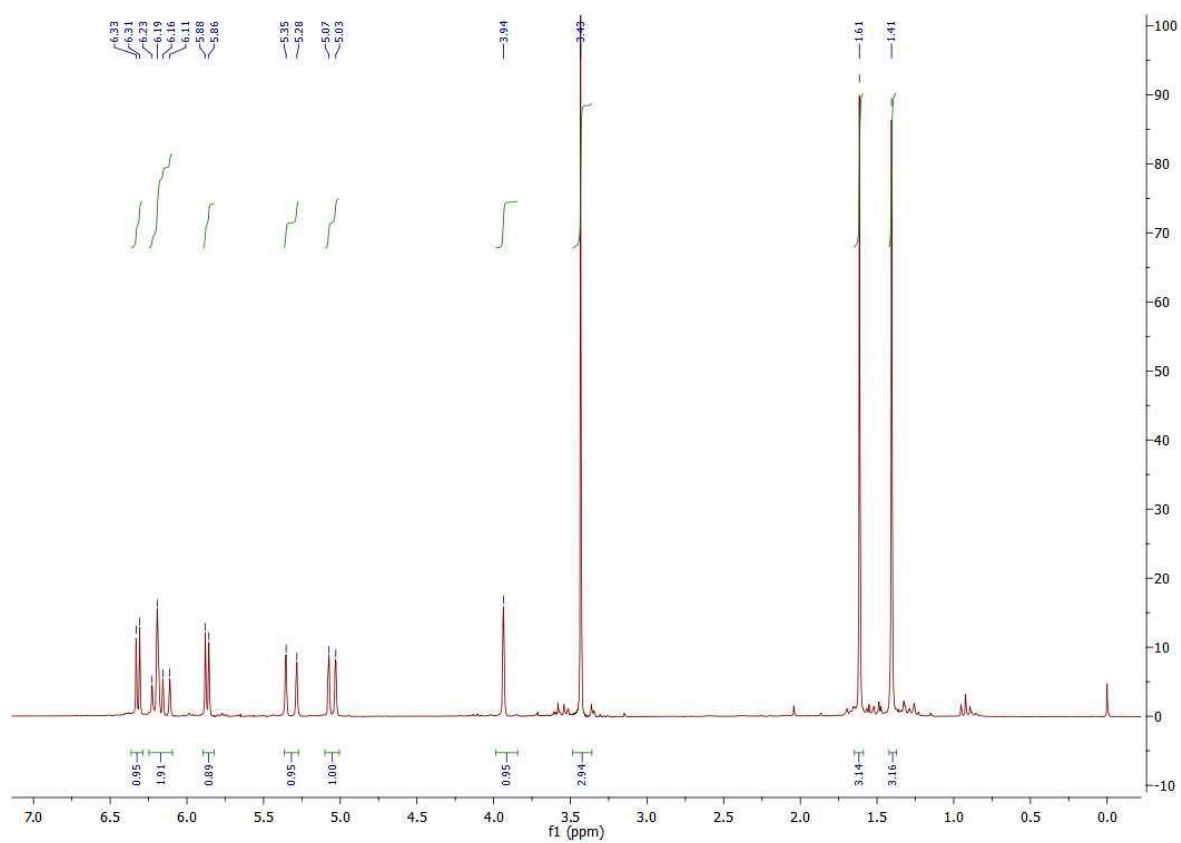
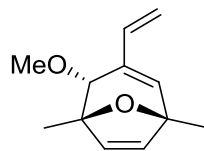
Calculations of **19** without methoxy group

top- <i>exo</i> - 19*	top- <i>endo</i> - 19*	bottom- <i>exo</i> - 19*	bottom- <i>endo</i> - 19*
14.0	0.0	4.8	1.8

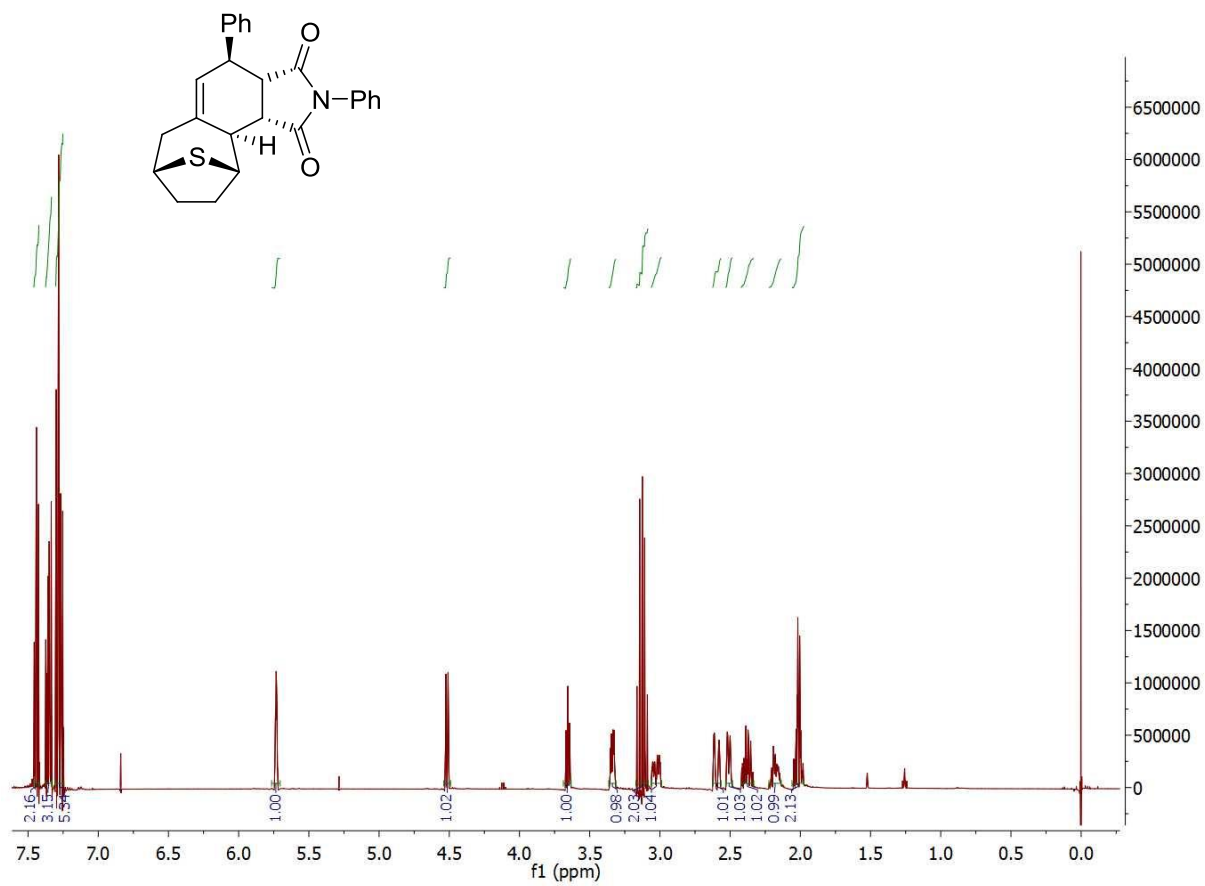
[1] ChemBio3D v.14, CambridgeSoft Corporation, PerkinElmer, Inc. Based on method of N. L. Allinger: Allinger, N. J. *J. Am. Chem. Soc.* **1977**, *99*, 8127

Selected NMR data of new compounds

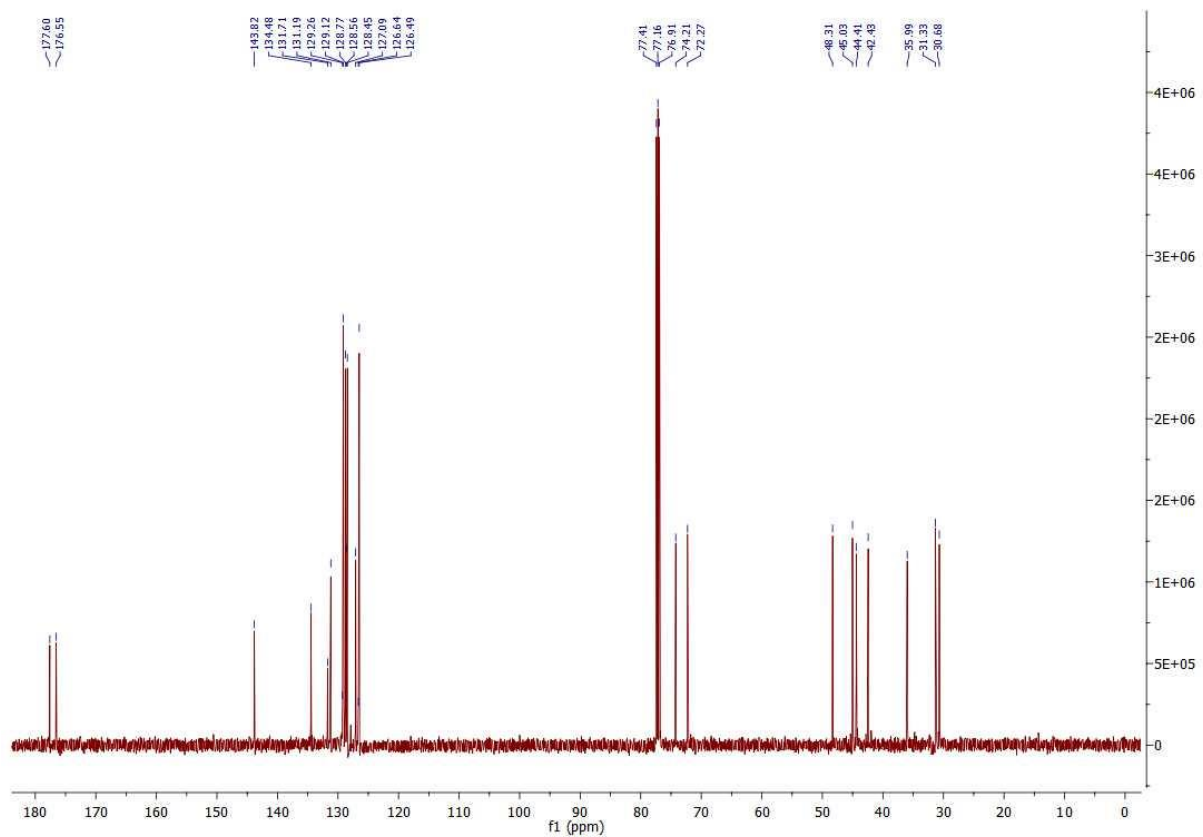
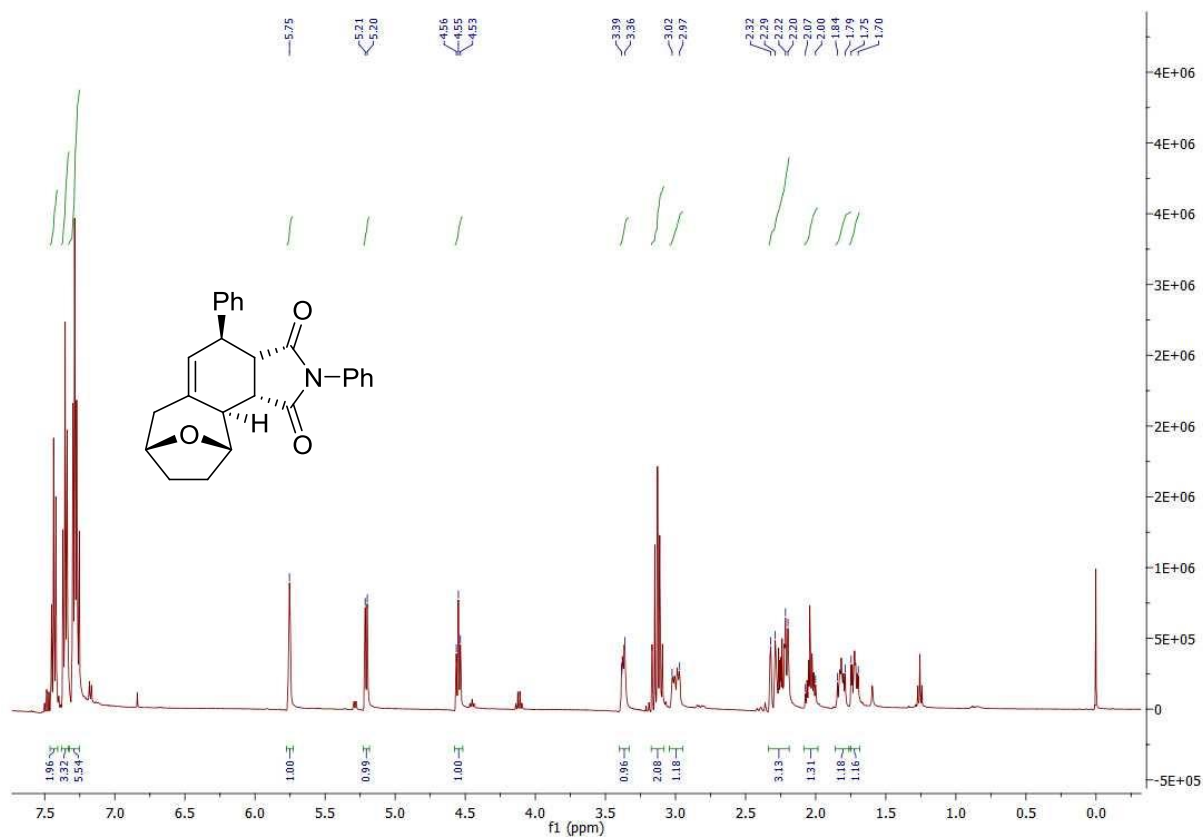
Compound 7



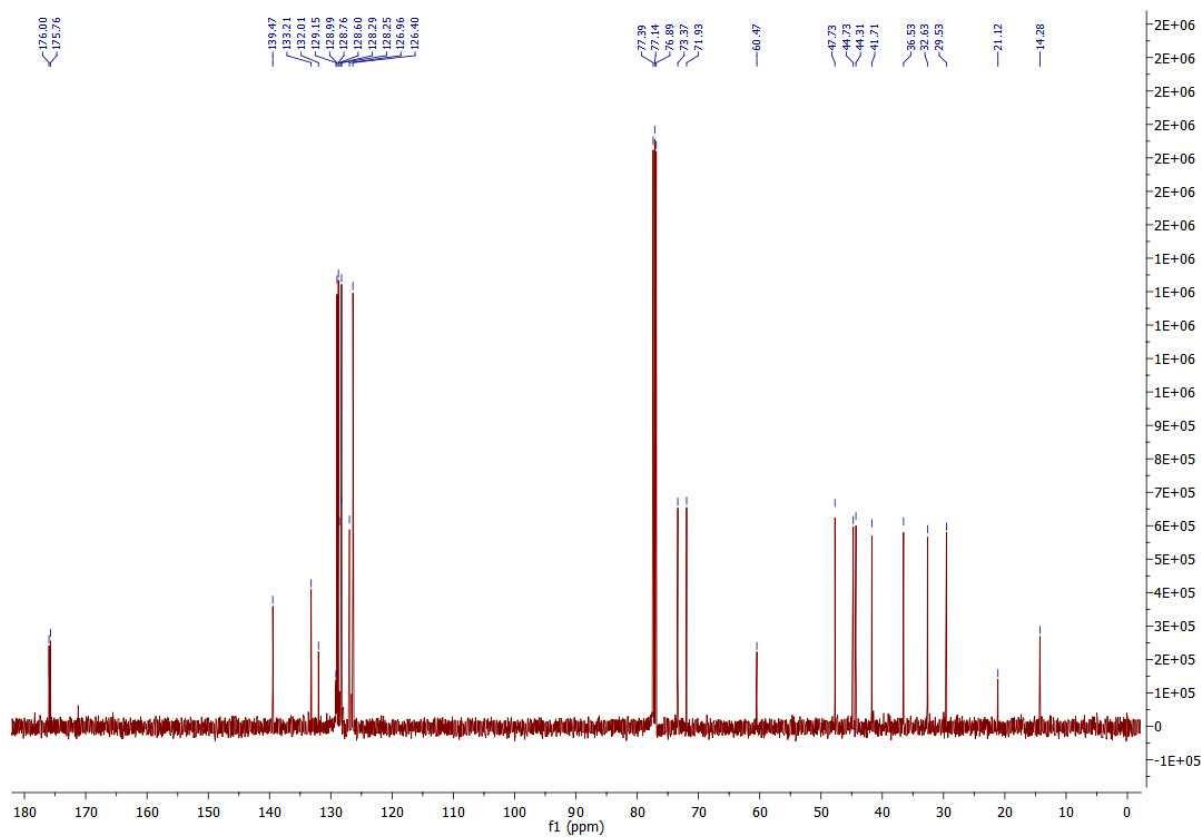
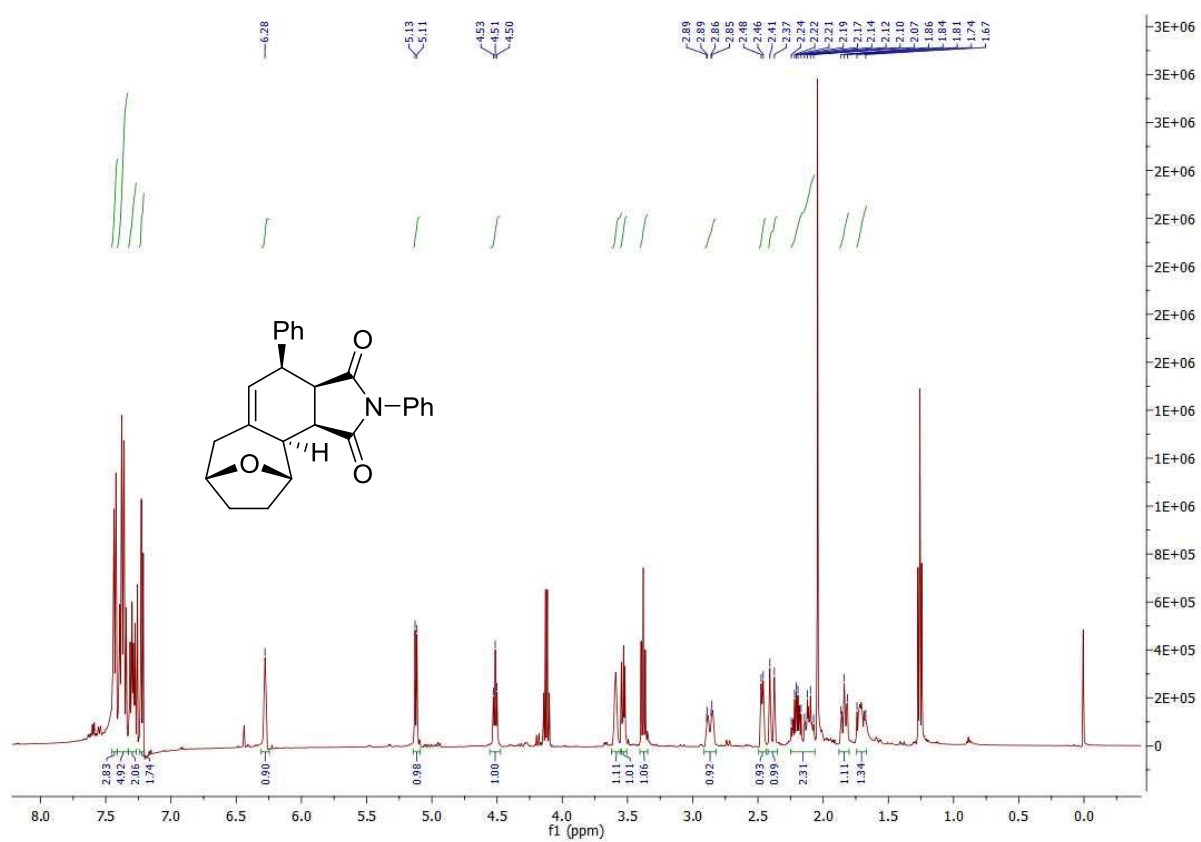
Compound *exo*-12



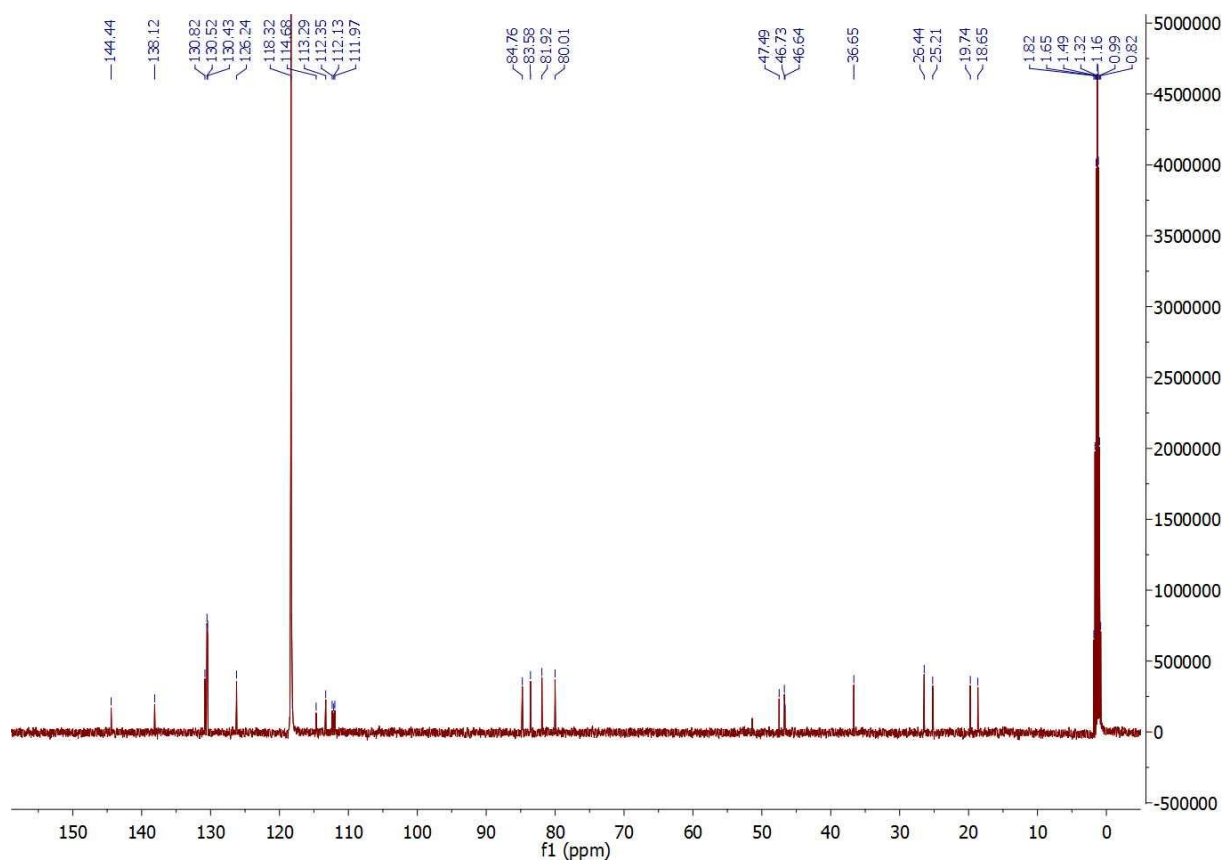
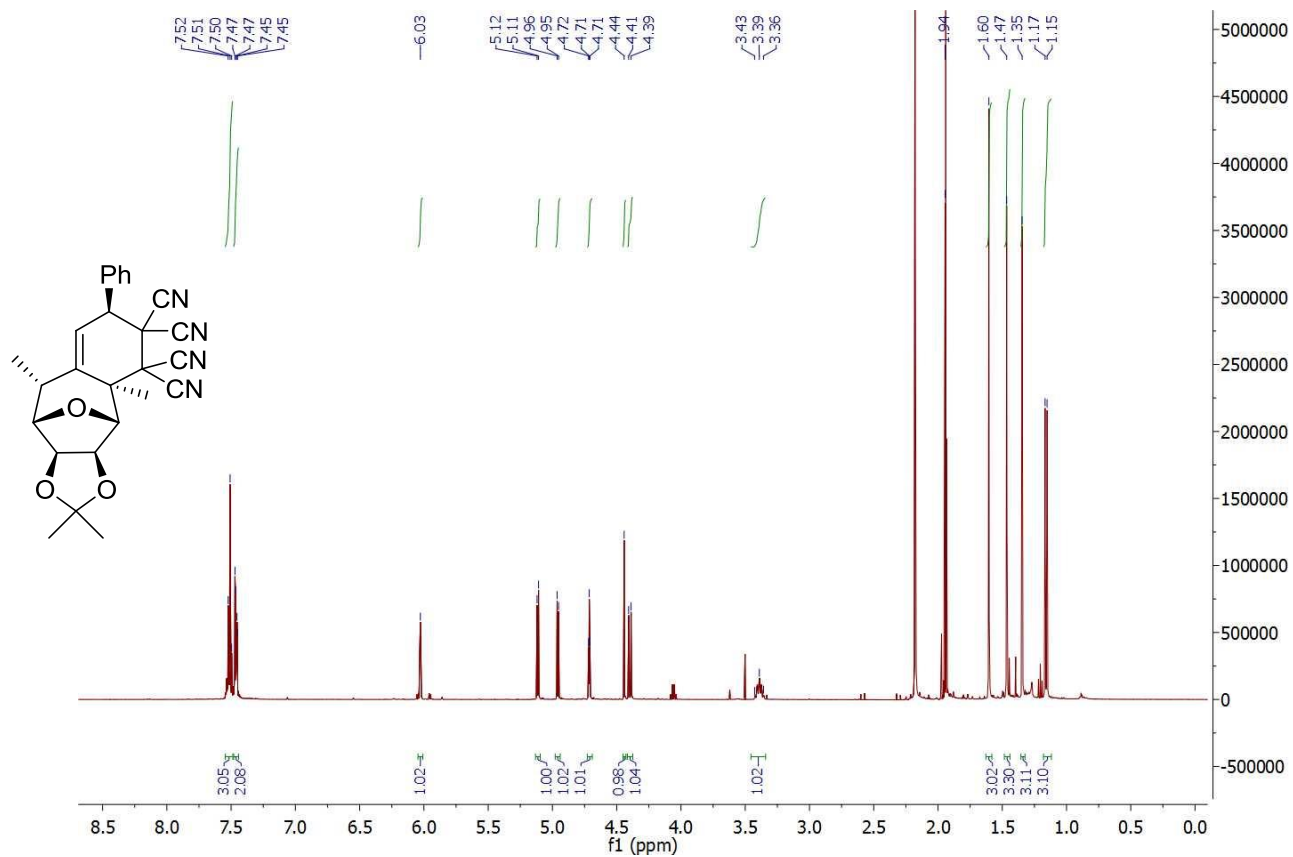
Compound *exo*-13



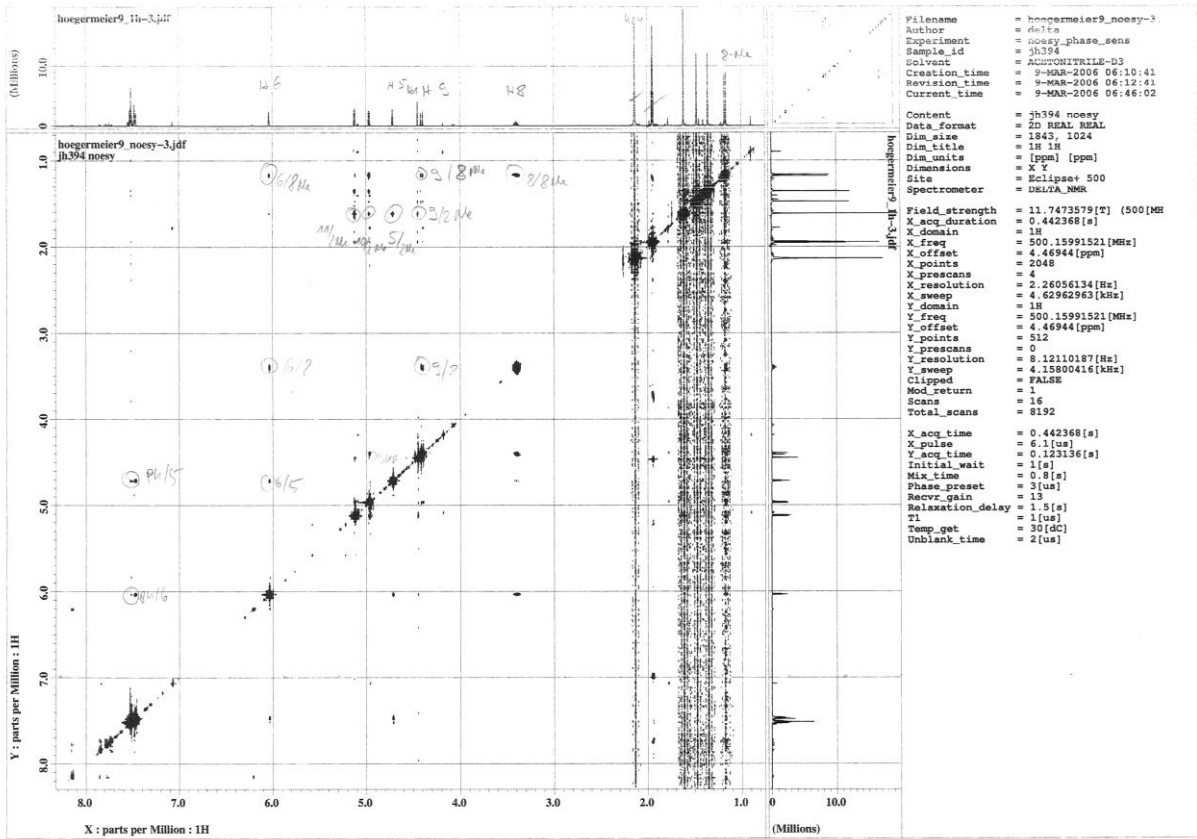
Compound *endo-13*



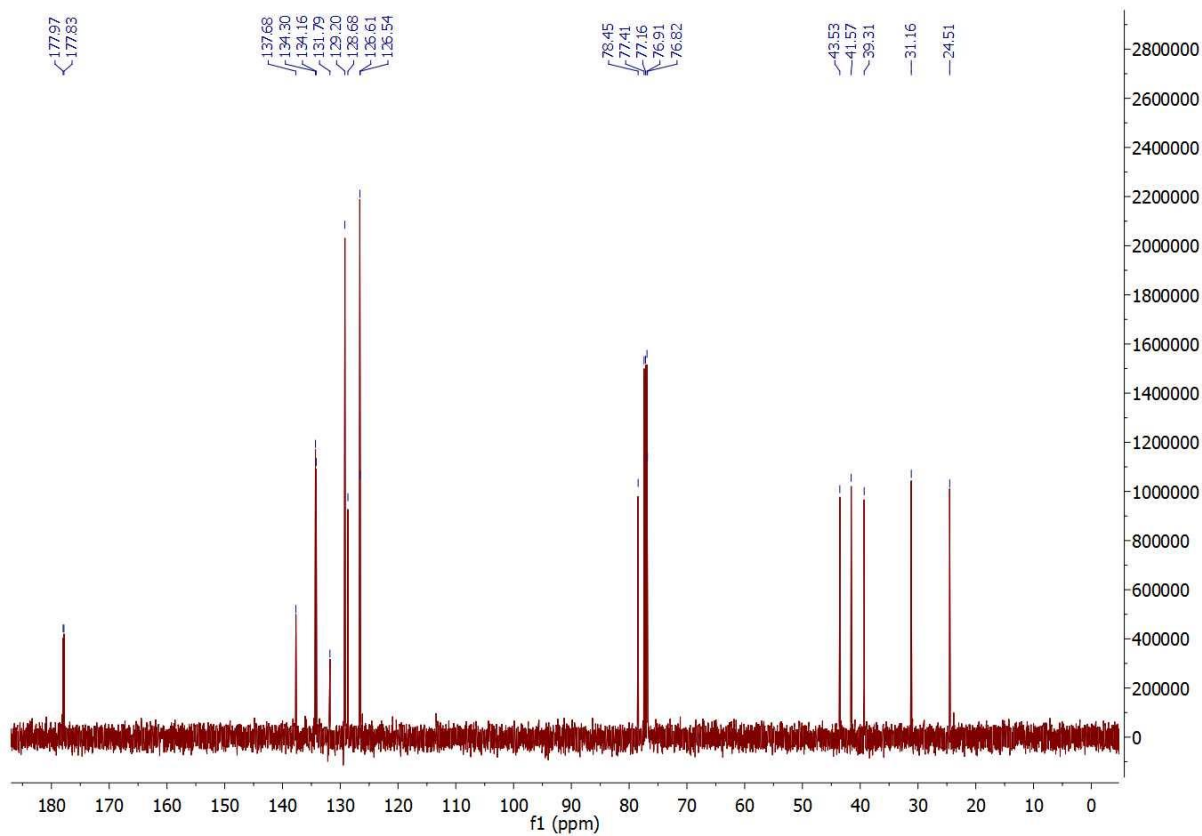
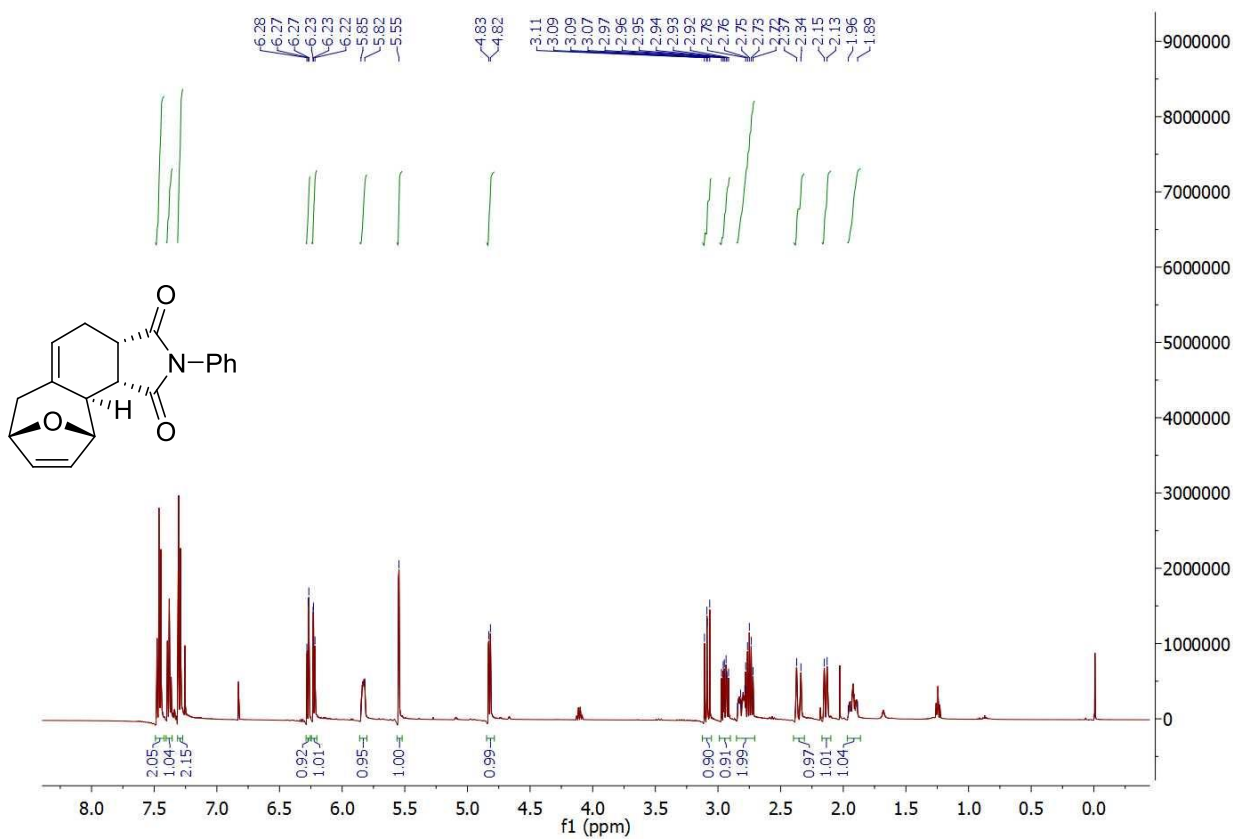
Compound 15



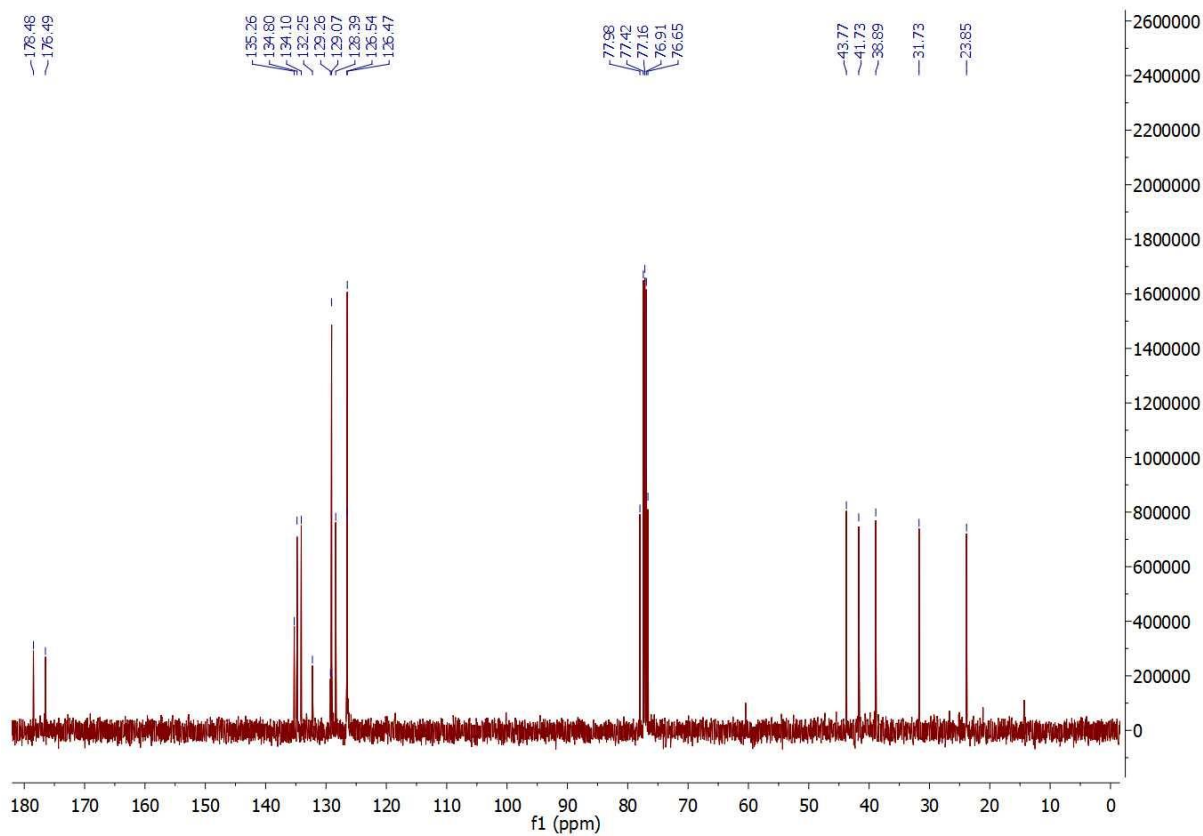
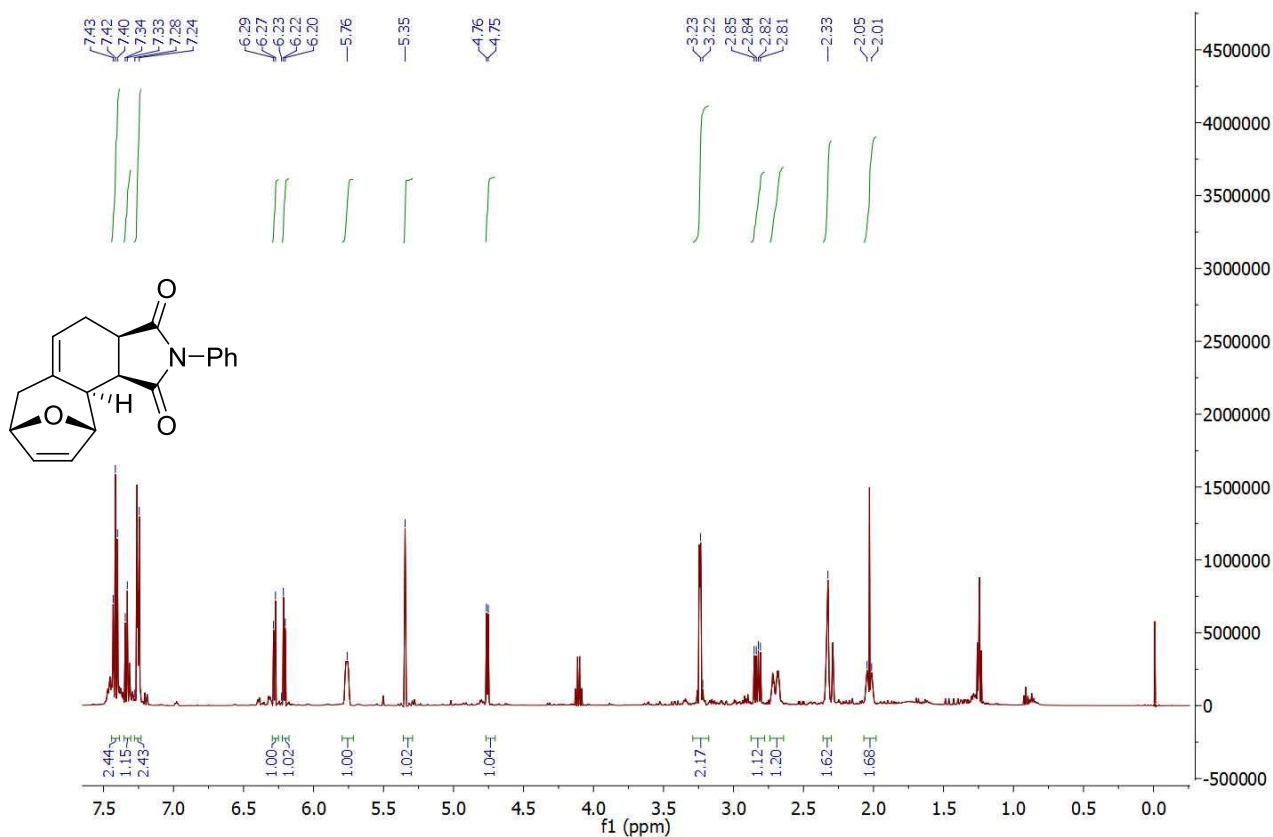
NOESY of compound 15



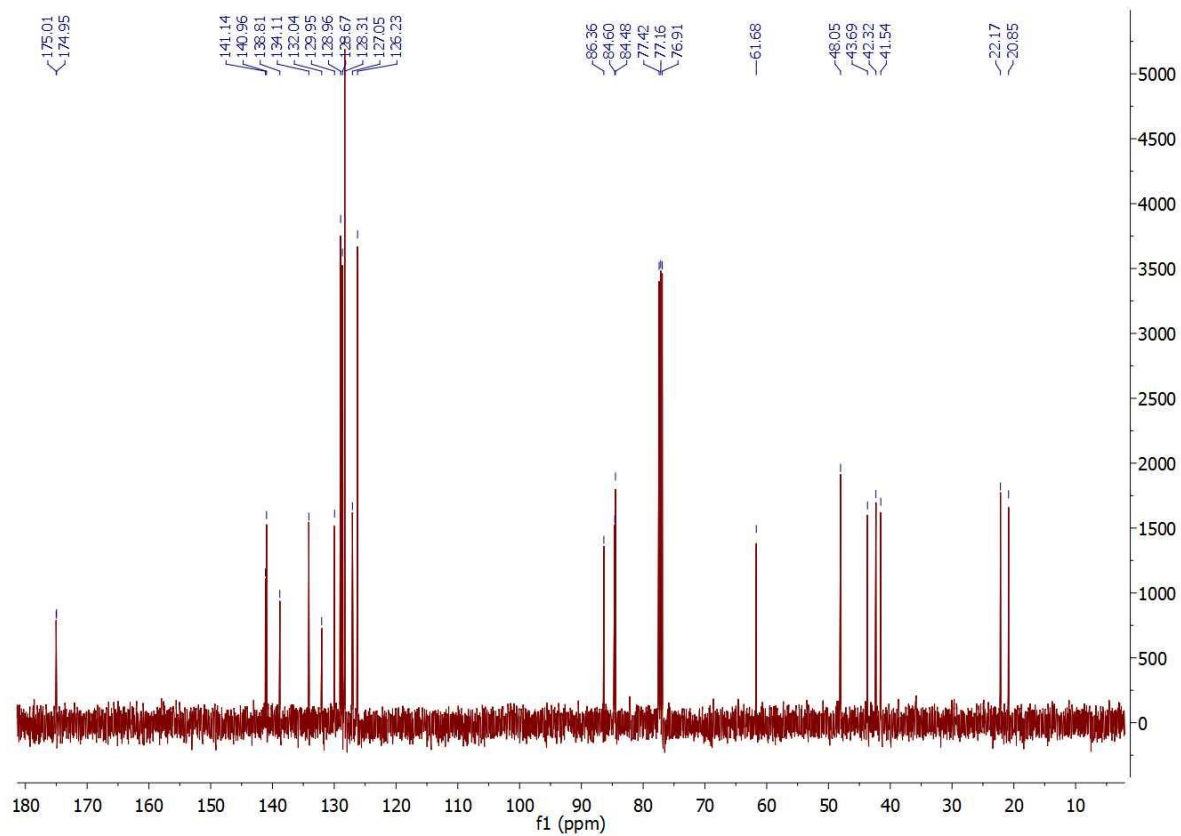
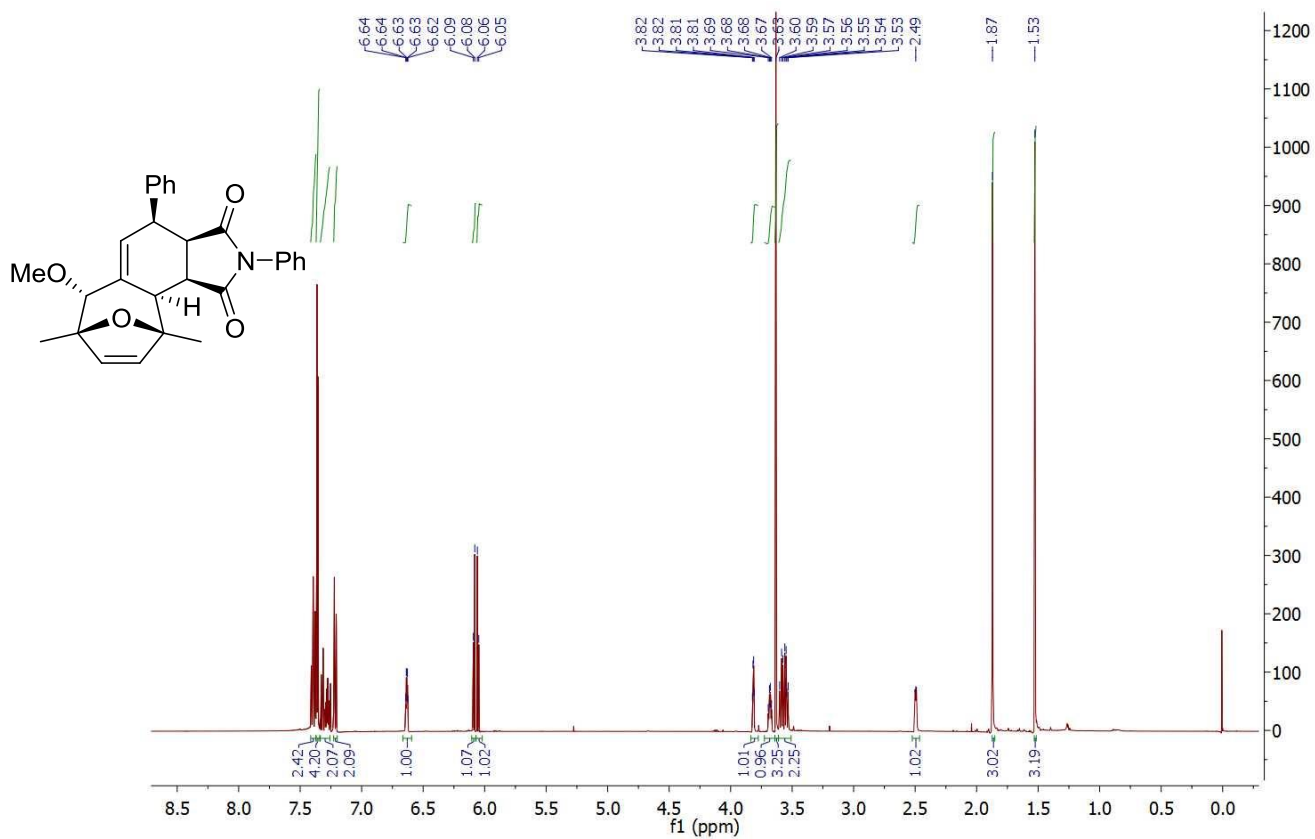
Compound exo-16



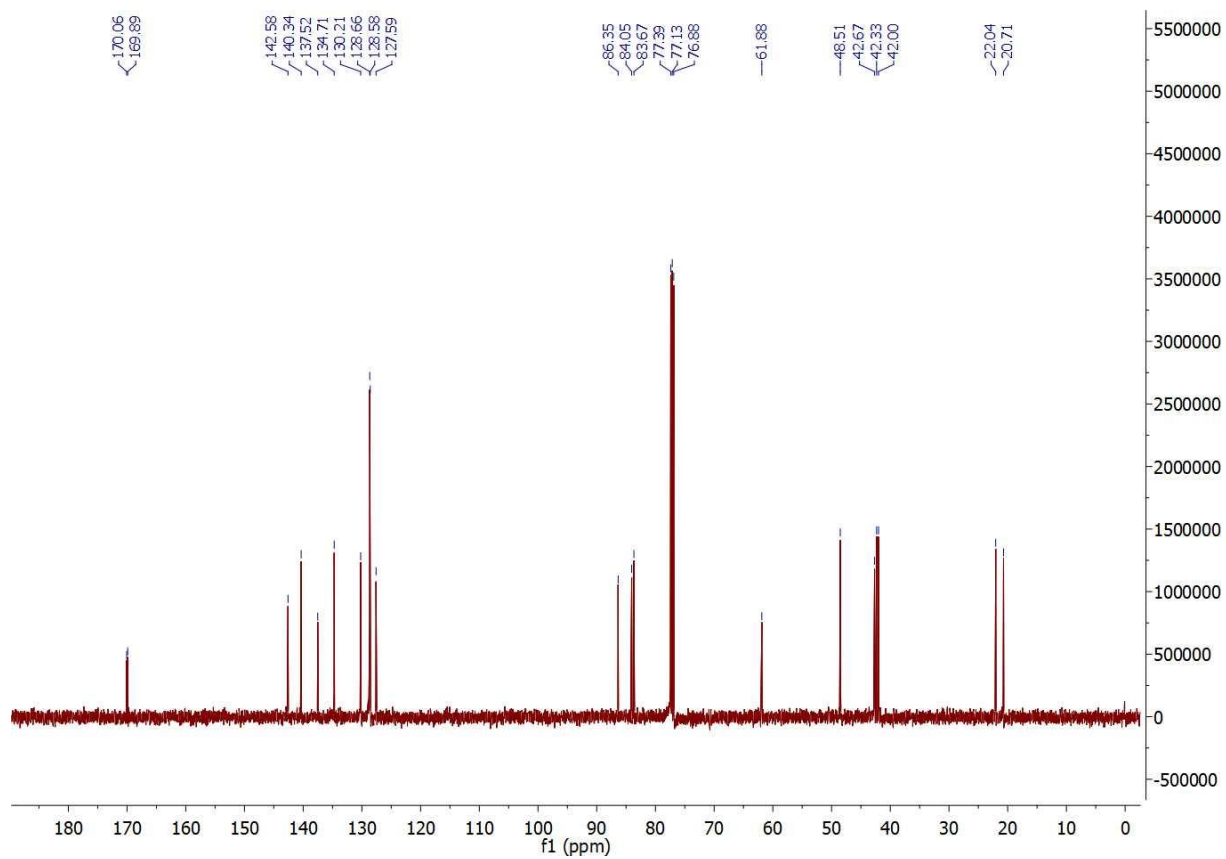
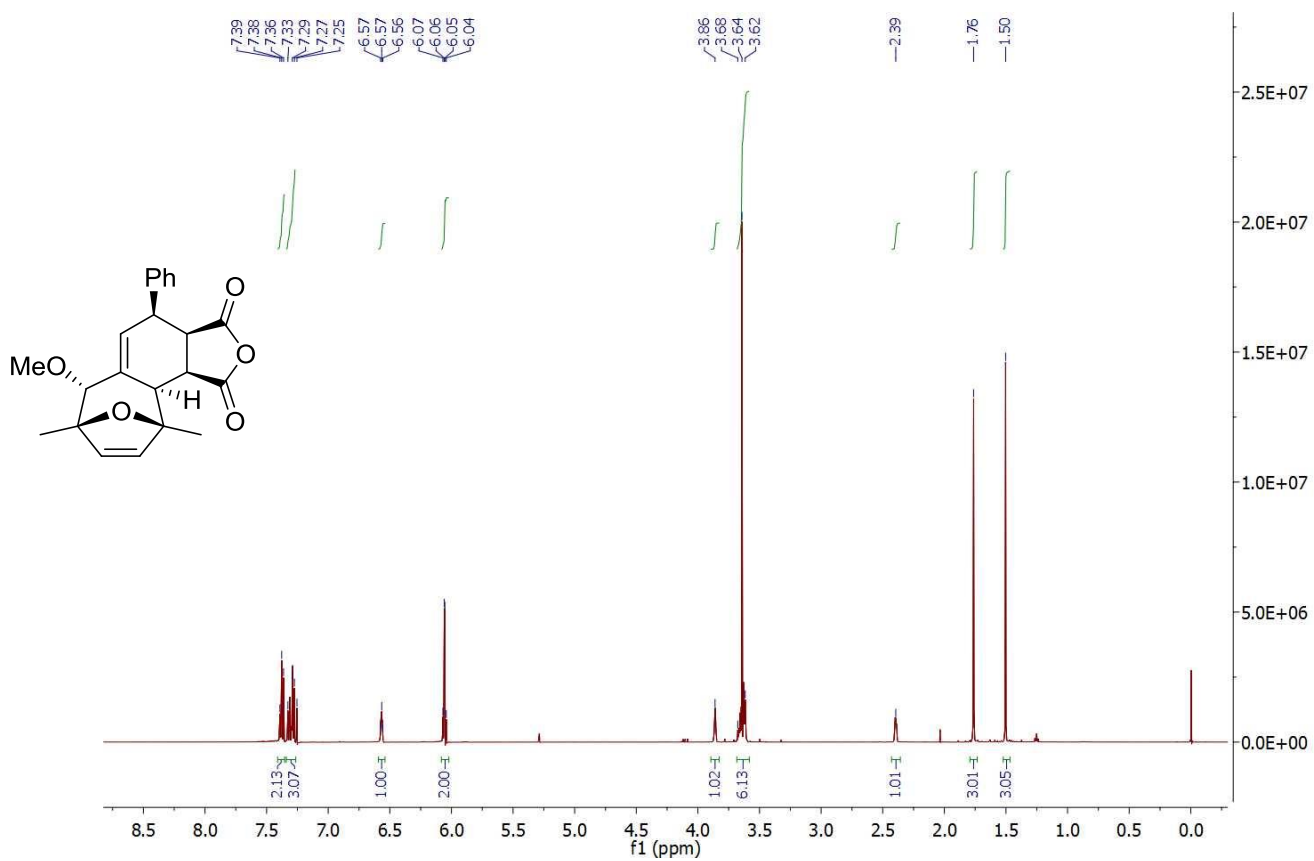
Compound *endo*-16



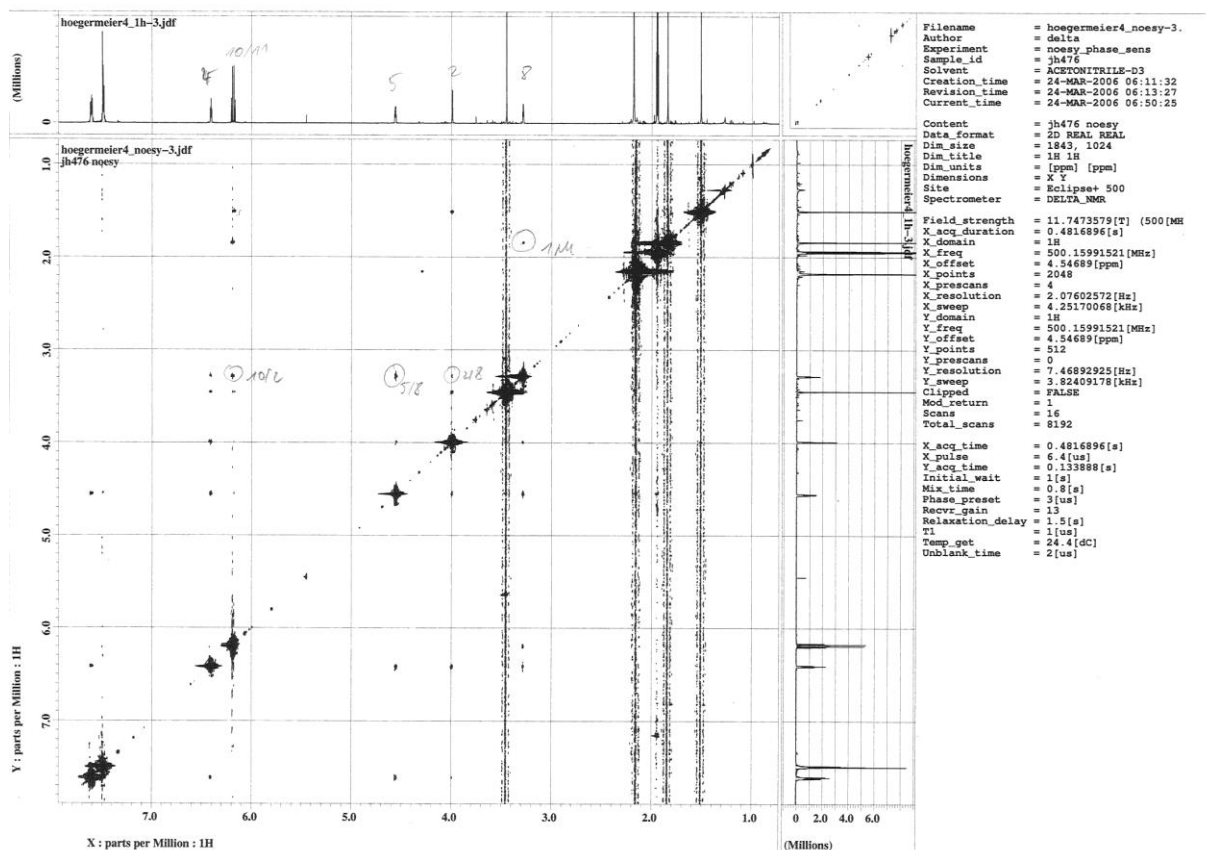
Compound *endo*-19



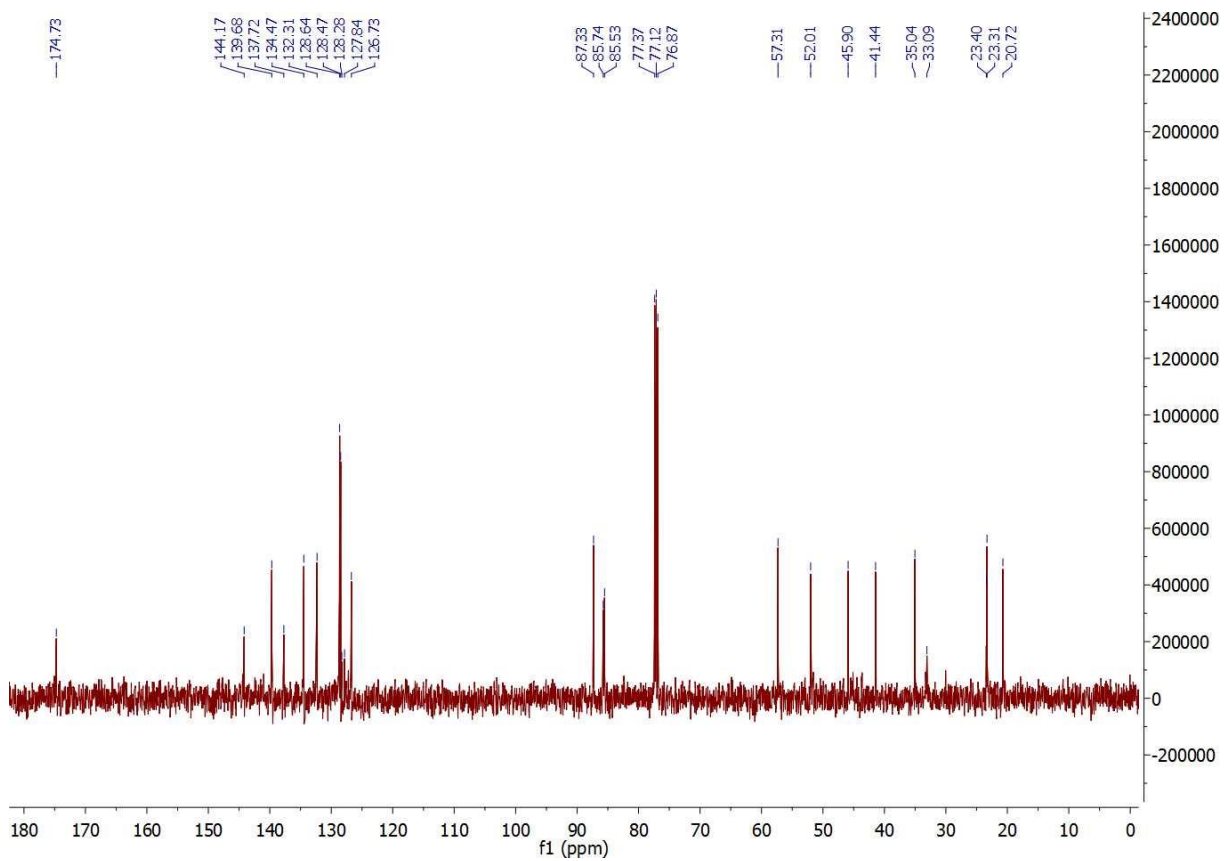
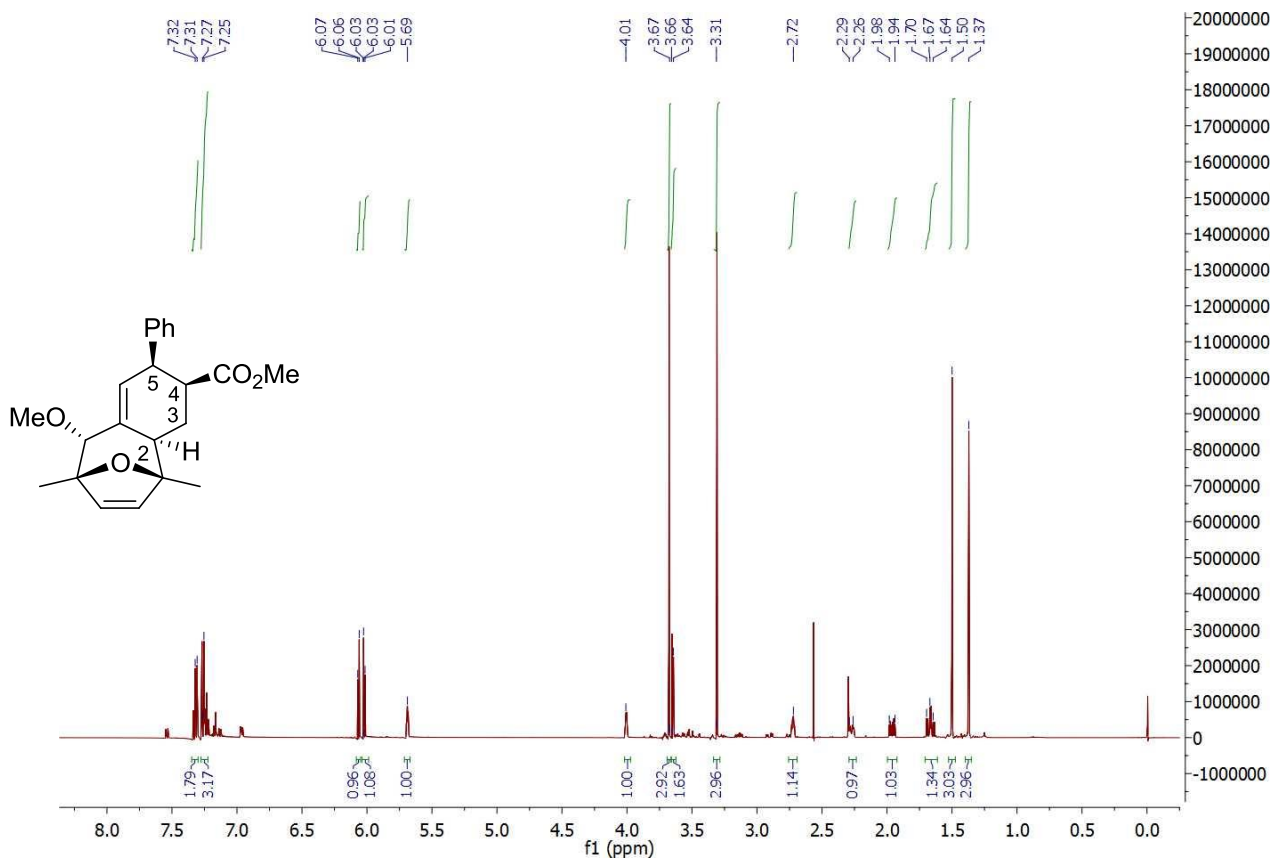
Compound *endo-20*



NOESY of compound 22



Compound *endo-23*



Compound *exo*-23

