Supporting Information for

Gold-Catalyzed Intramolecular Cyclization of *N*-Propargylic *β*-Enaminones for the Synthesis of 1,4-Oxazepine Derivatives

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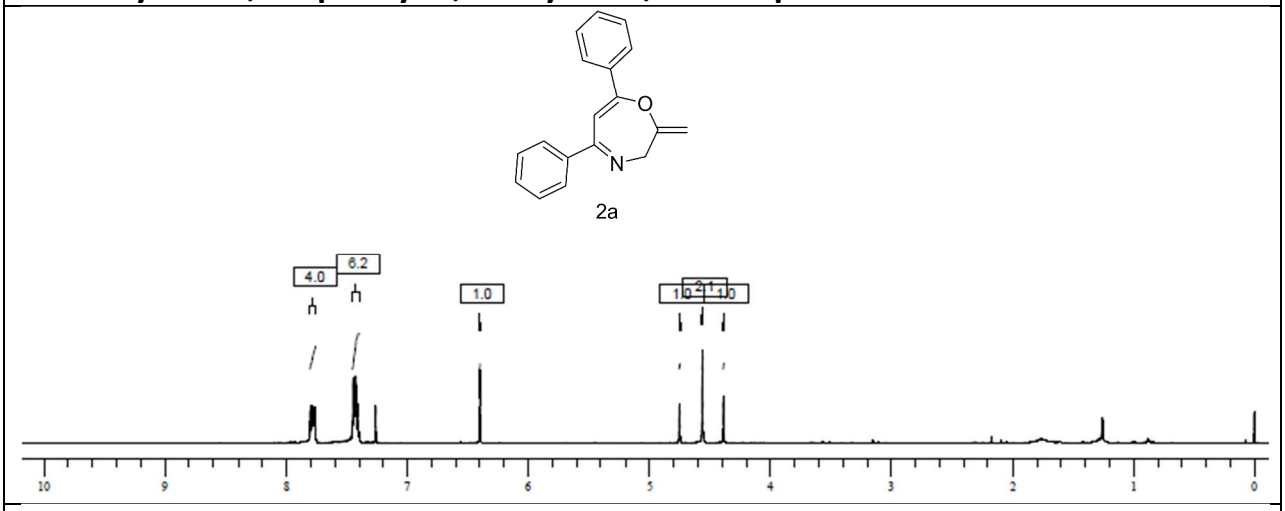
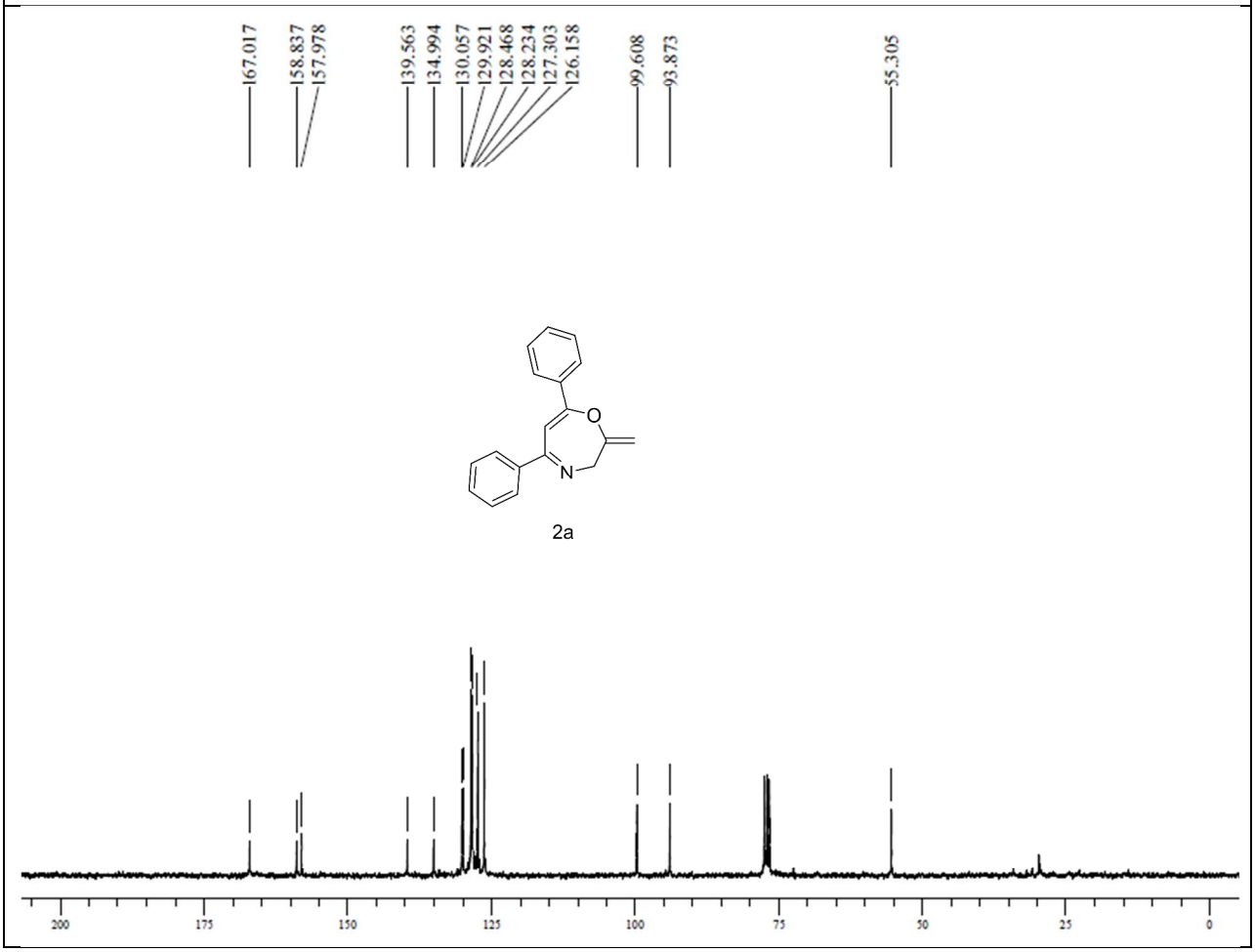
♀Dedicated to Dr. Veena Shatrugna, on the occasion of her 65th birthday.

Contents:

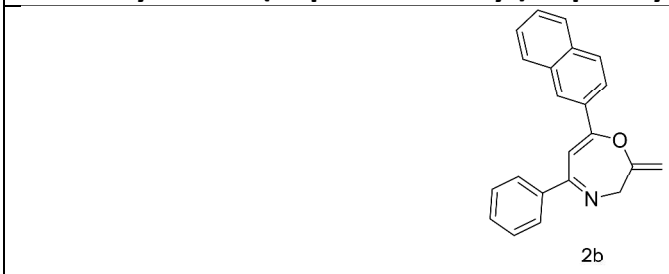
1.1 *Copies of ^{1}H and ^{13}C NMR spectra* (2a-q)

2-Methylene-5,7-diphenyl-2,3-dihydro-1,4-oxazepine: 2a





2-Methylene-7-(naphthalen-2-yl)-5-phenyl-2,3-dihydro-1,4-oxazepine: 2b



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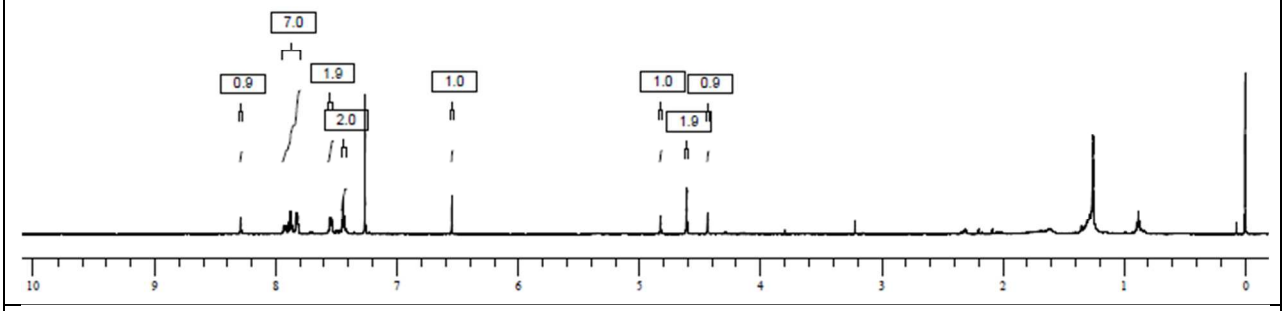

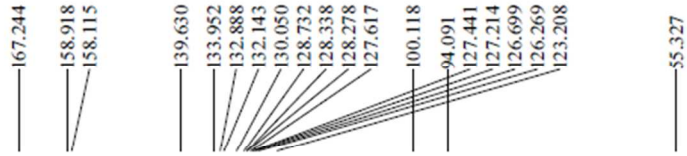

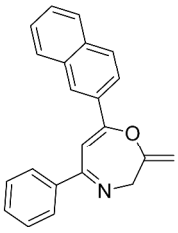

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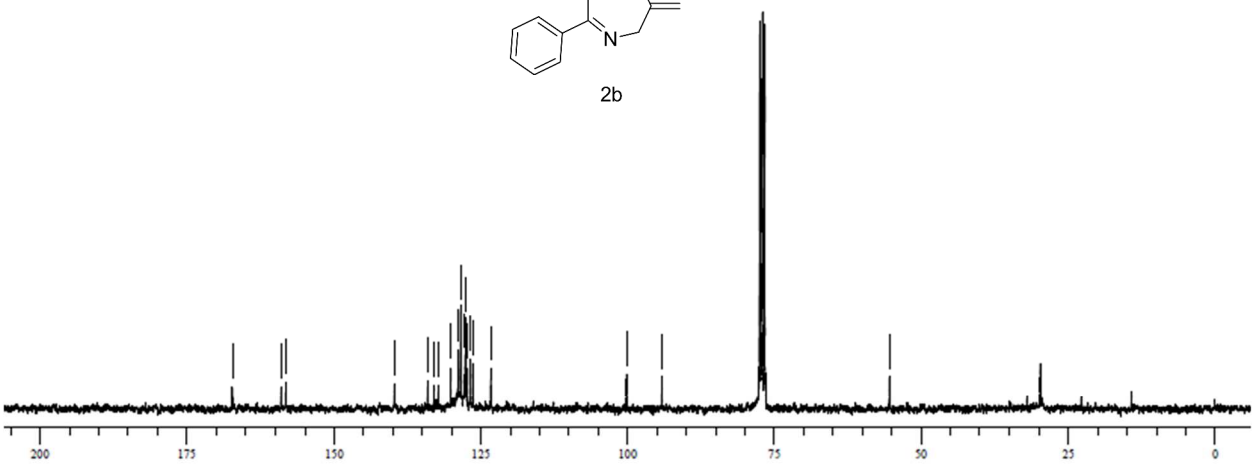
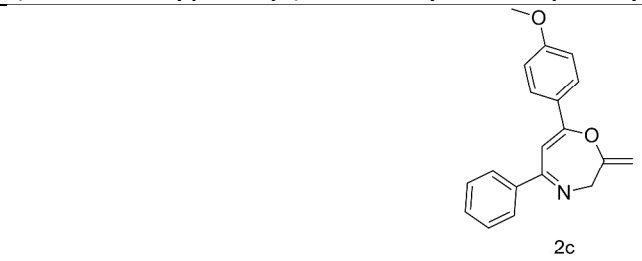


7-(4-Methoxyphenyl)-2-methylene-5-phenyl-2,3-dihydro-1,4-oxazepine: **2c**



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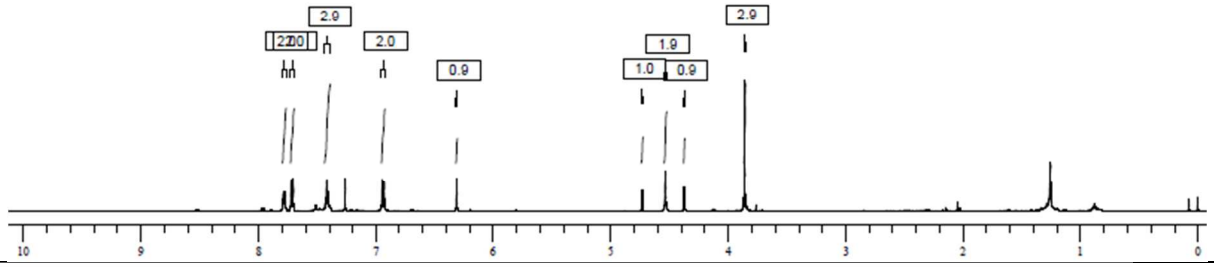

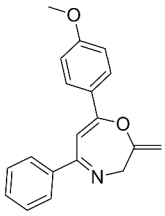

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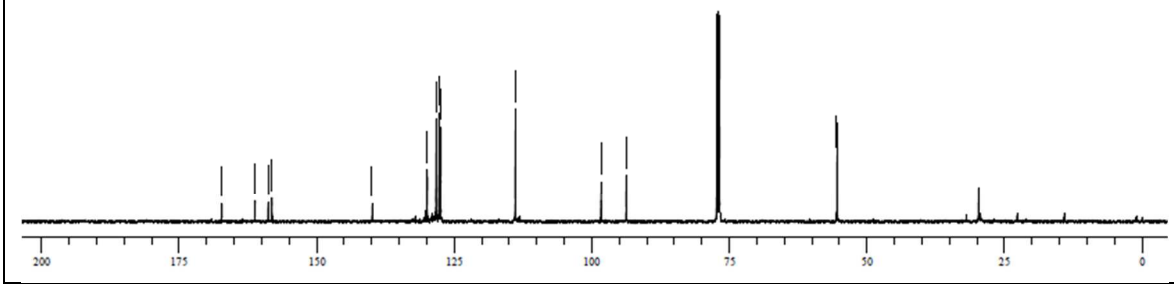
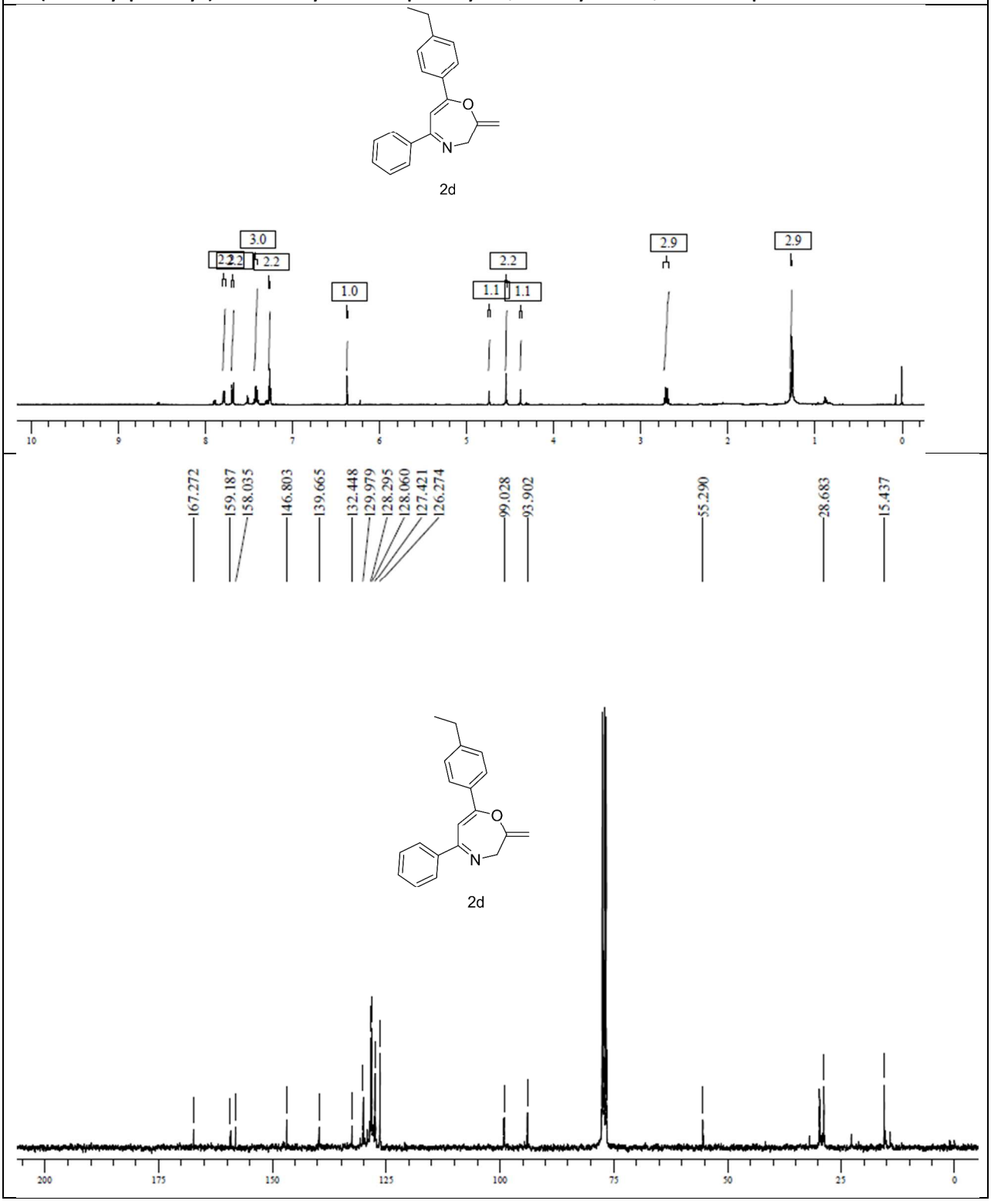


7-(4-Ethylphenyl)-2-methylene-5-phenyl-2,3-dihydro-1,4-oxazepine: **2d**



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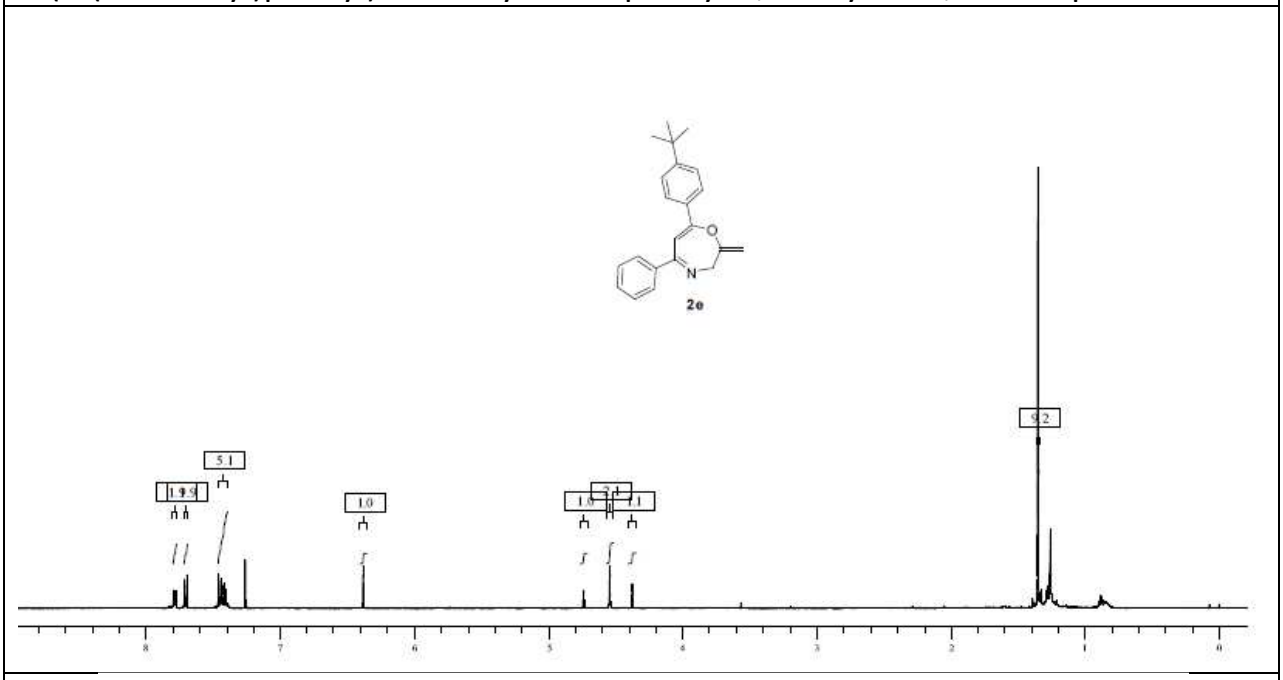
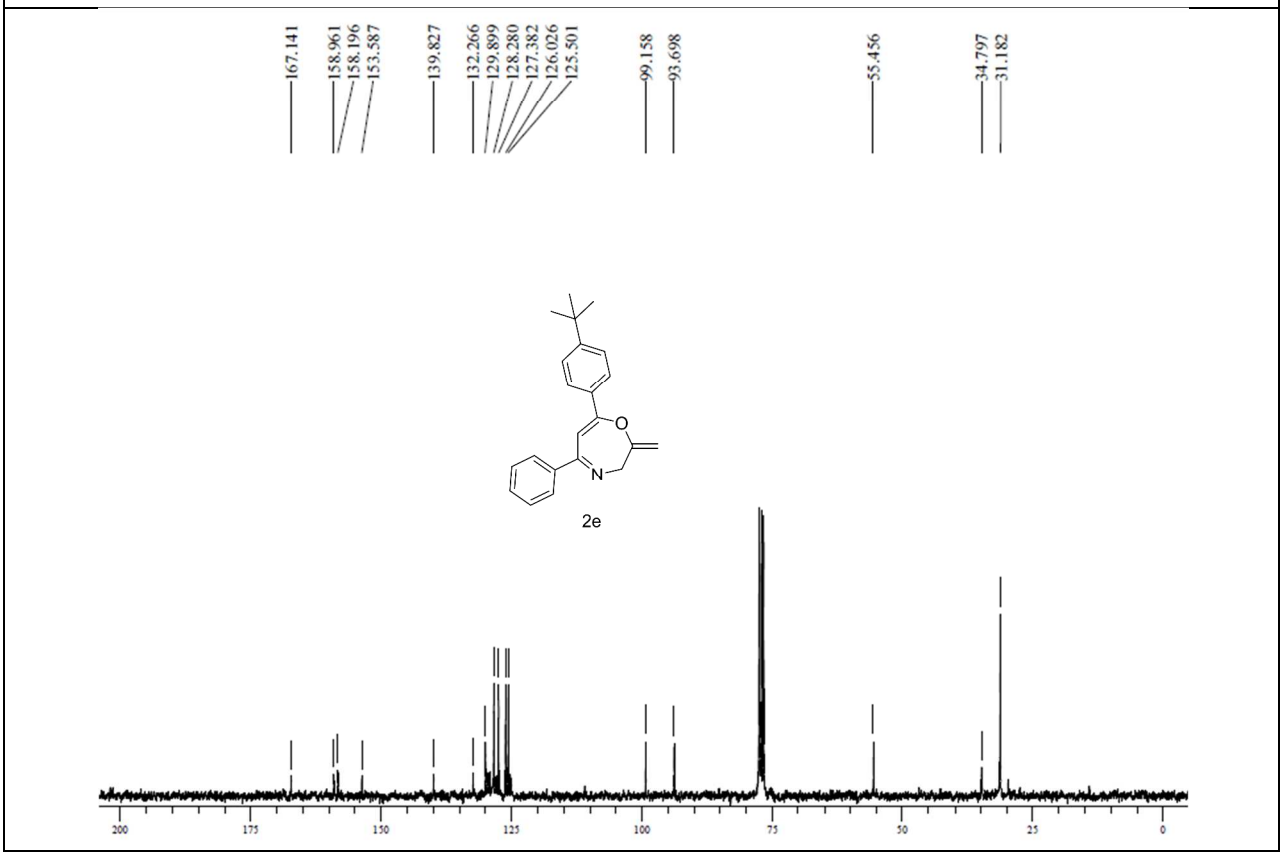
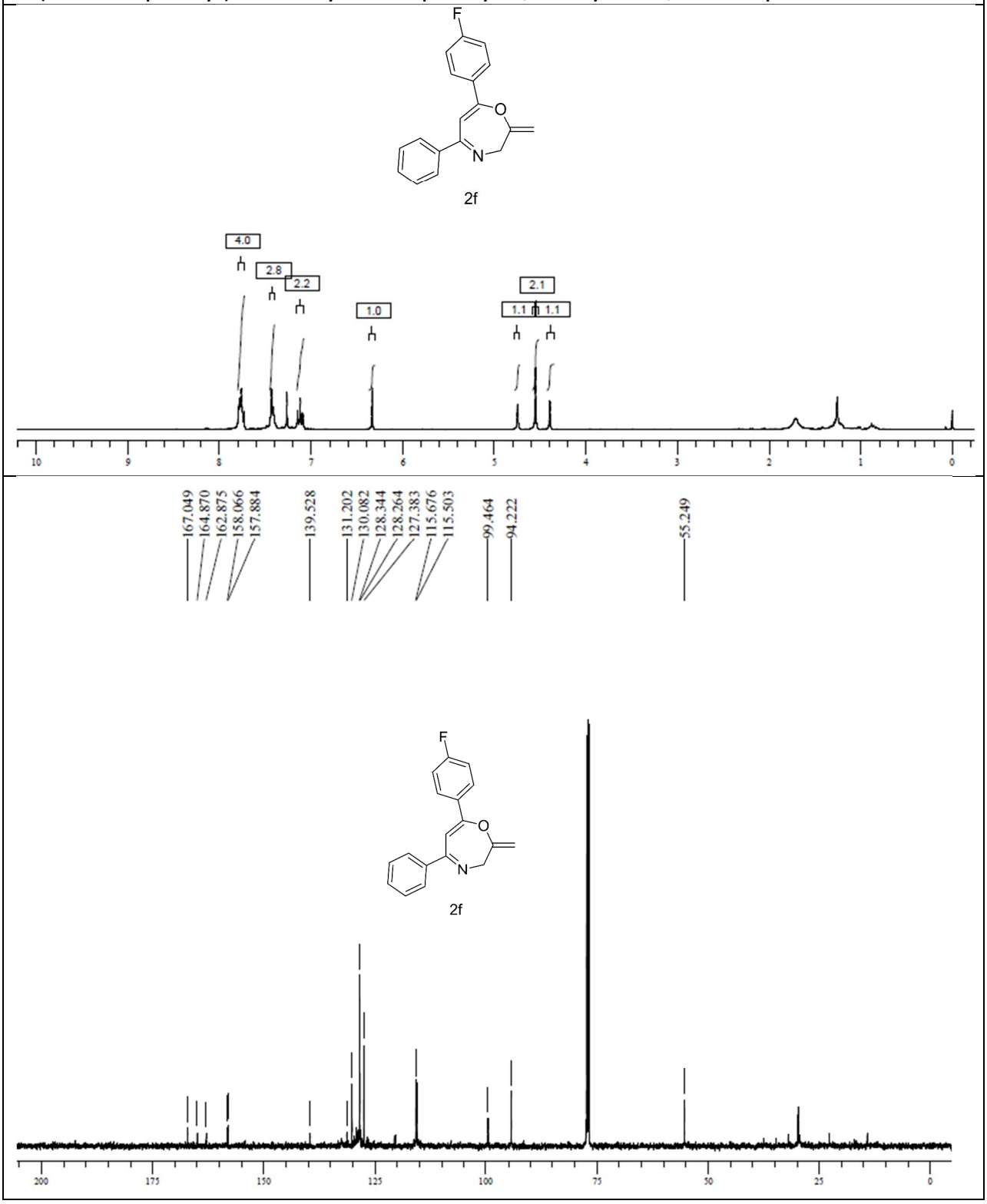
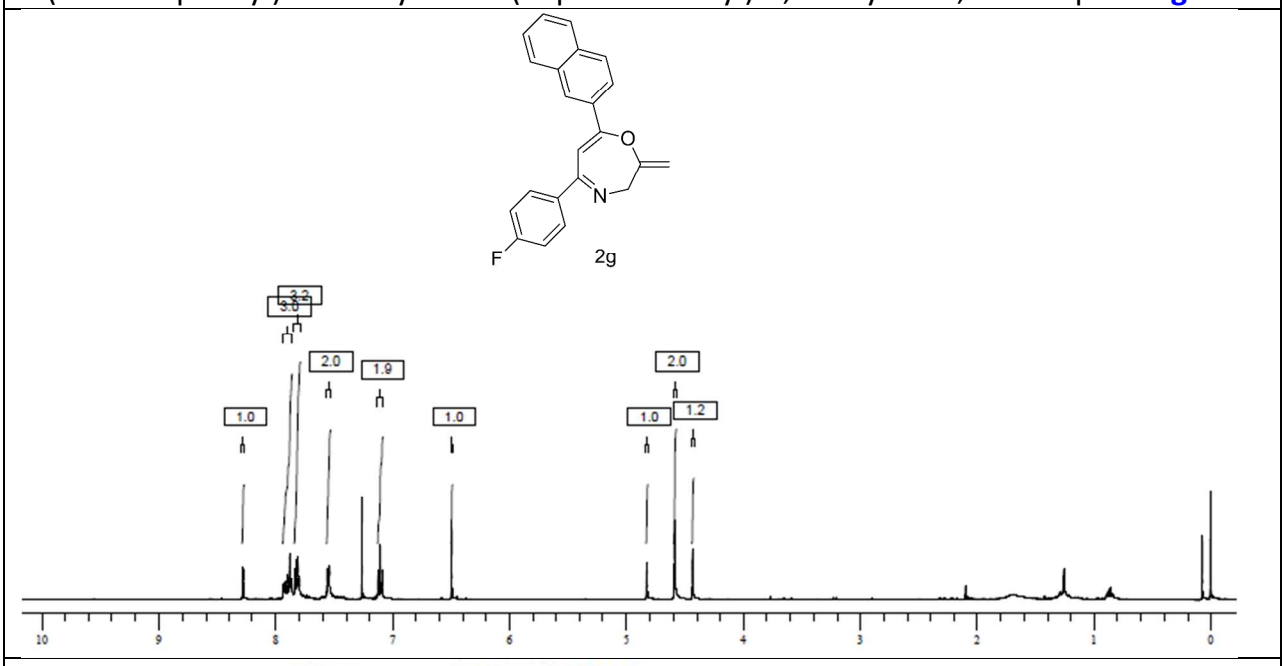


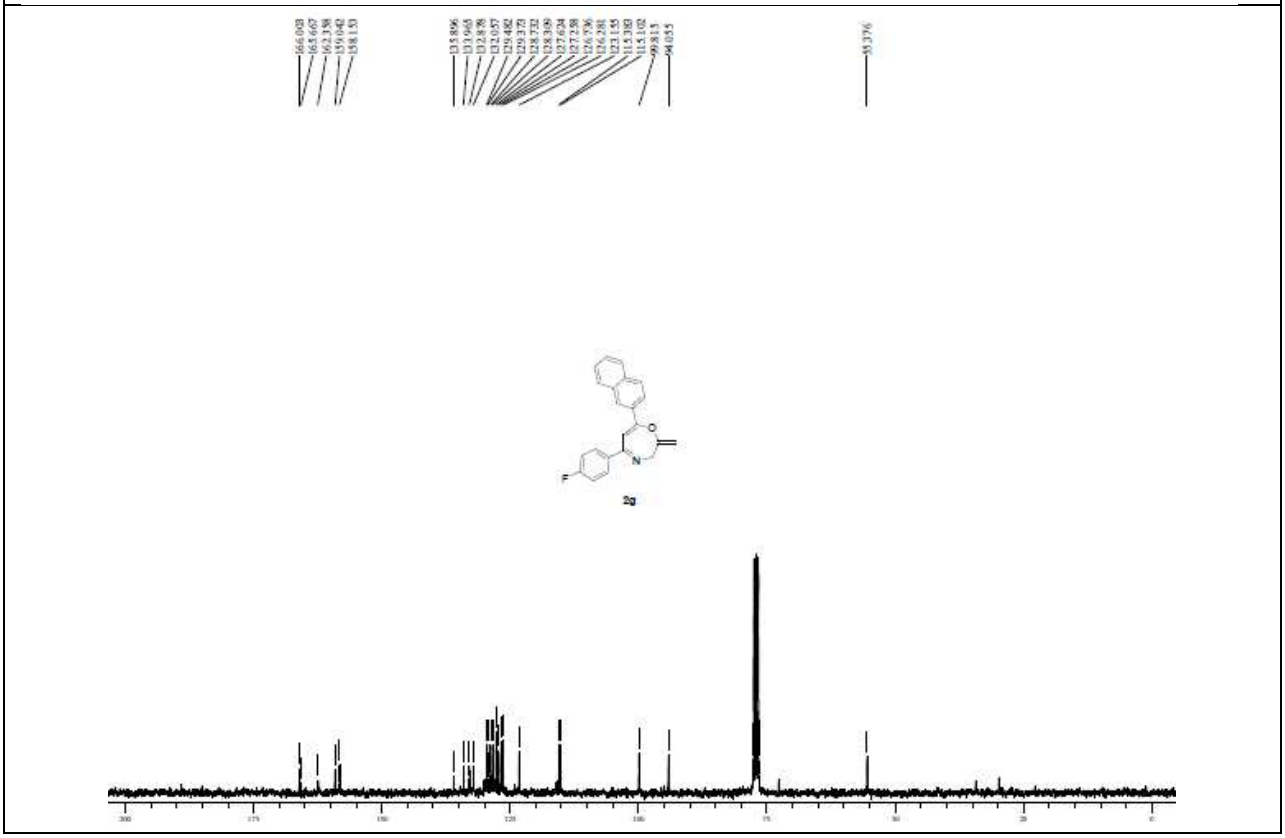


7-(4-Fluorophenyl)-2-methylene-5-phenyl-2,3-dihydro-1,4-oxazepine: **2f**

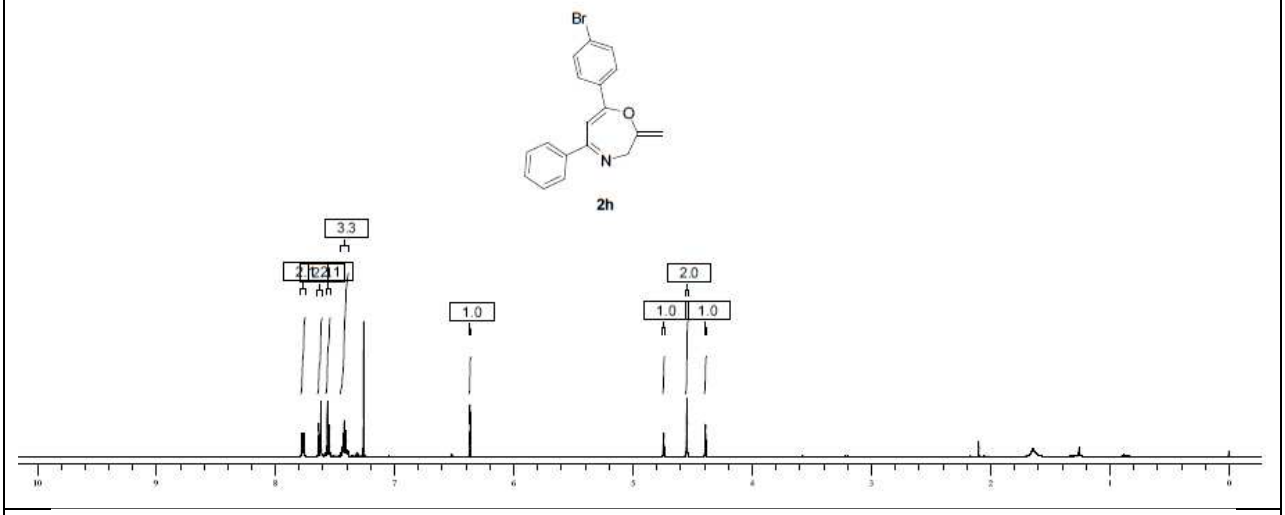


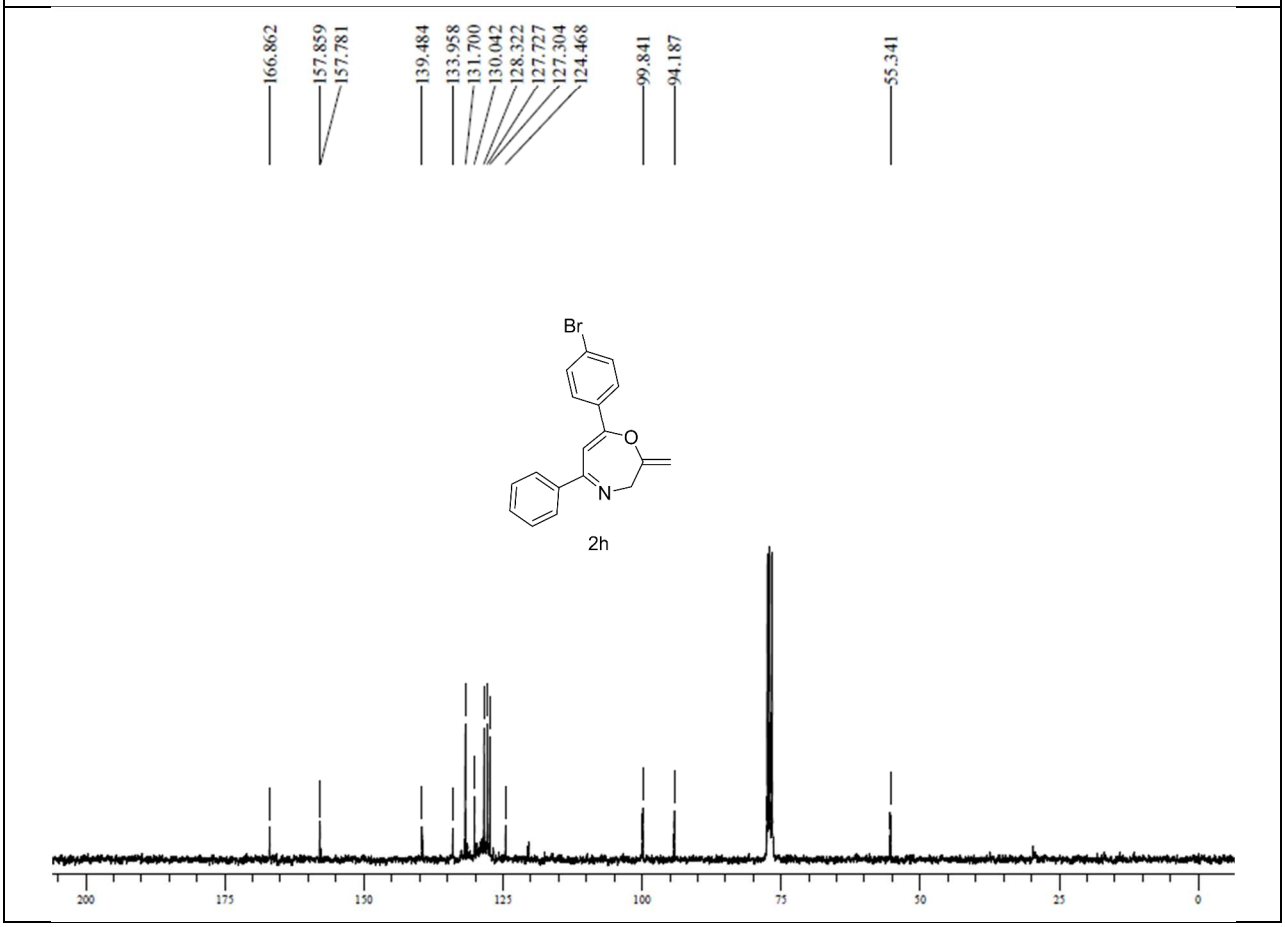
5-(4-Fluorophenyl)-2-methylene-7-(naphthalen-2-yl)-2,3-dihydro-1,4-oxazepine: **2g**



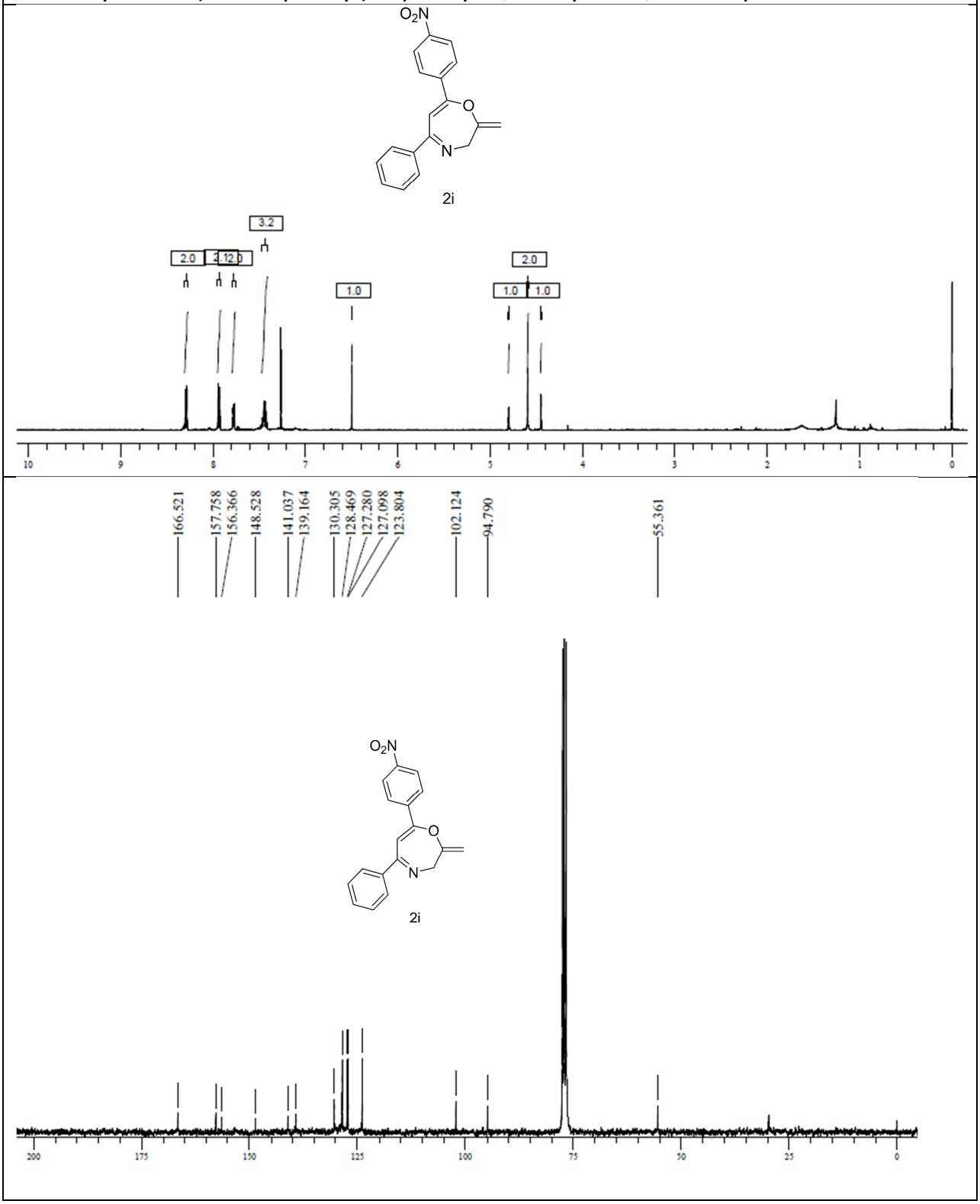


7-(4-Bromophenyl)-2-methylene-5-phenyl-2,3-dihydro-1,4-oxazepine: **2h**

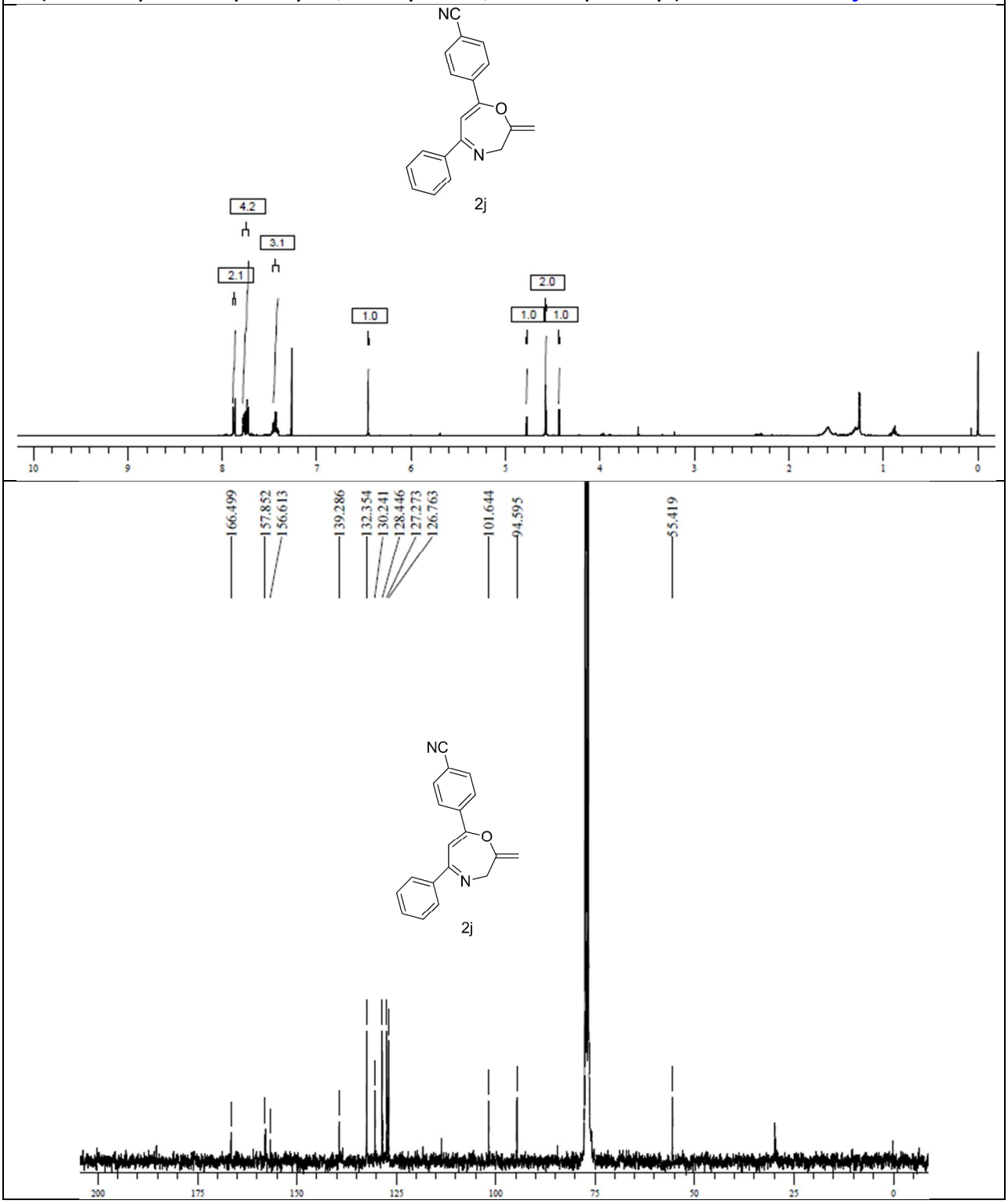




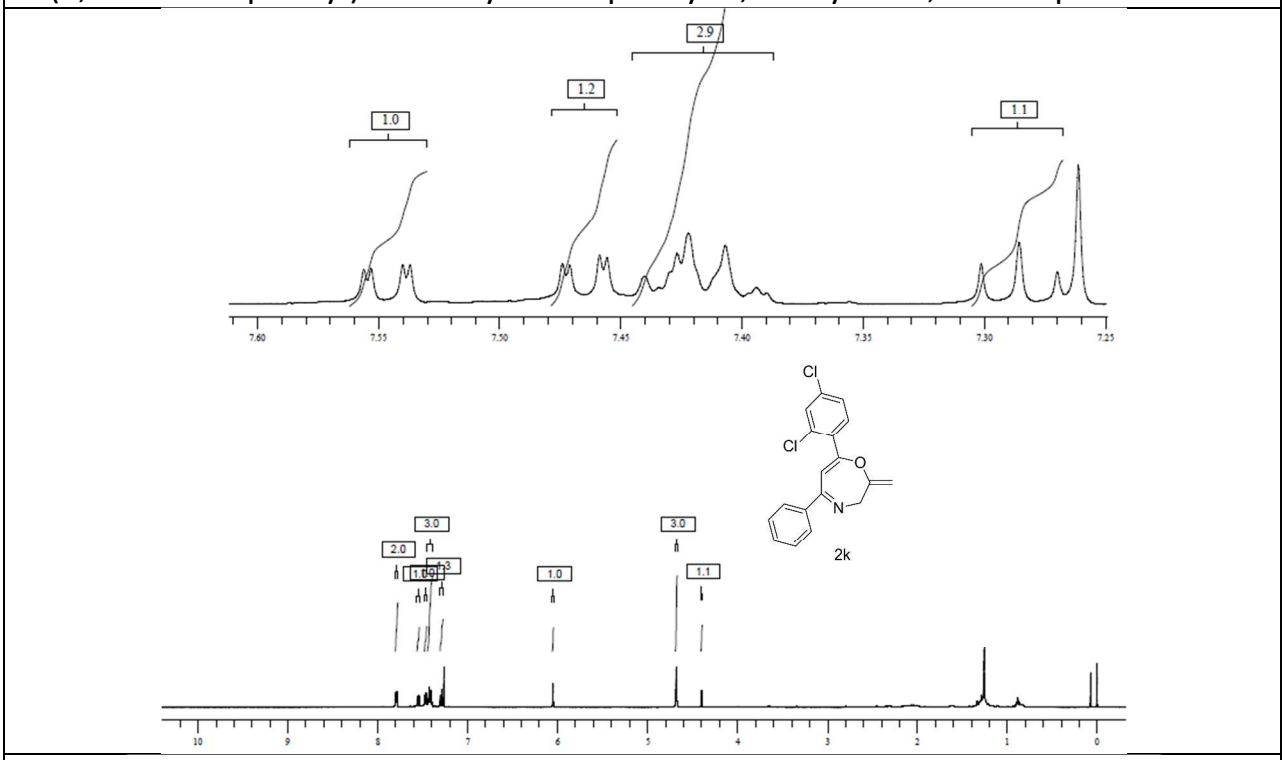
2-Methylene-7-(4-nitrophenyl)-5-phenyl-2,3-dihydro-1,4-oxazepine: **2i**

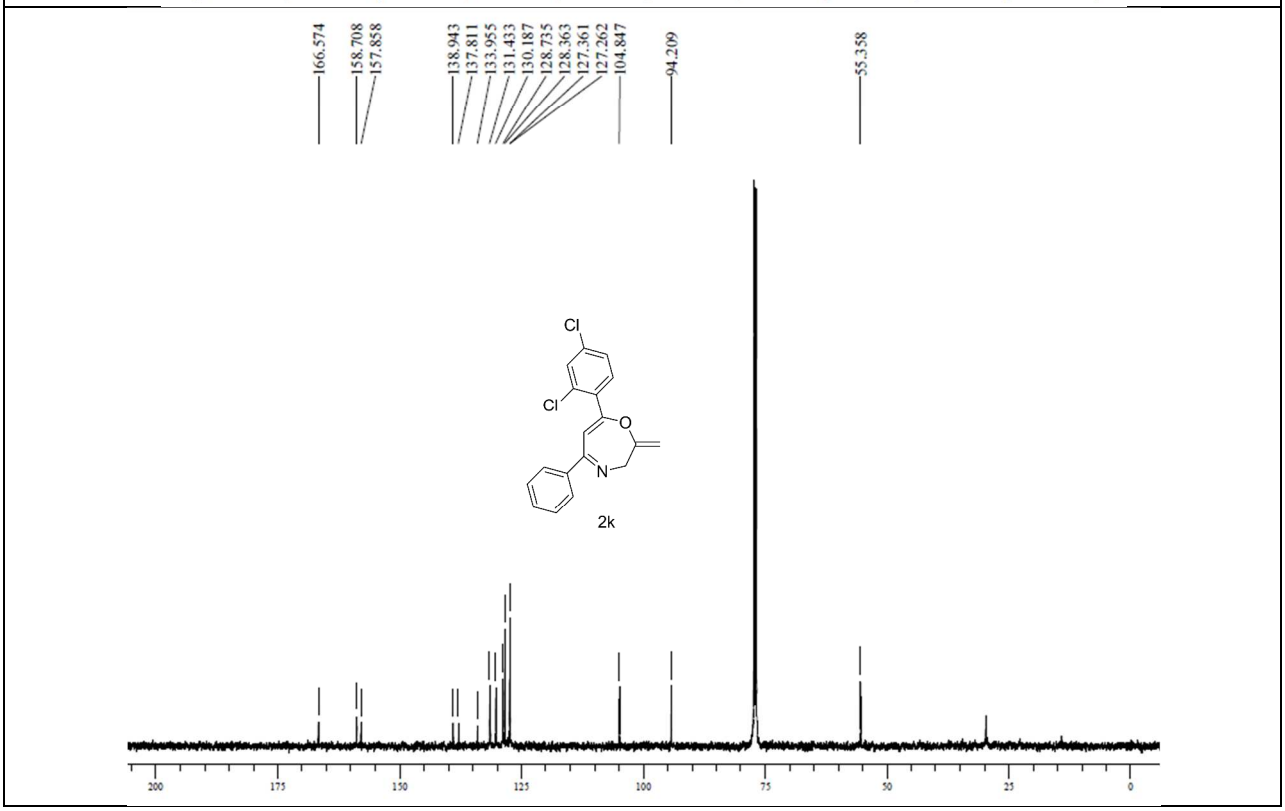


4-(2-Methylene-5-phenyl-2,3-dihydro-1,4-oxazepin-7-yl)benzonitrile: **2j**

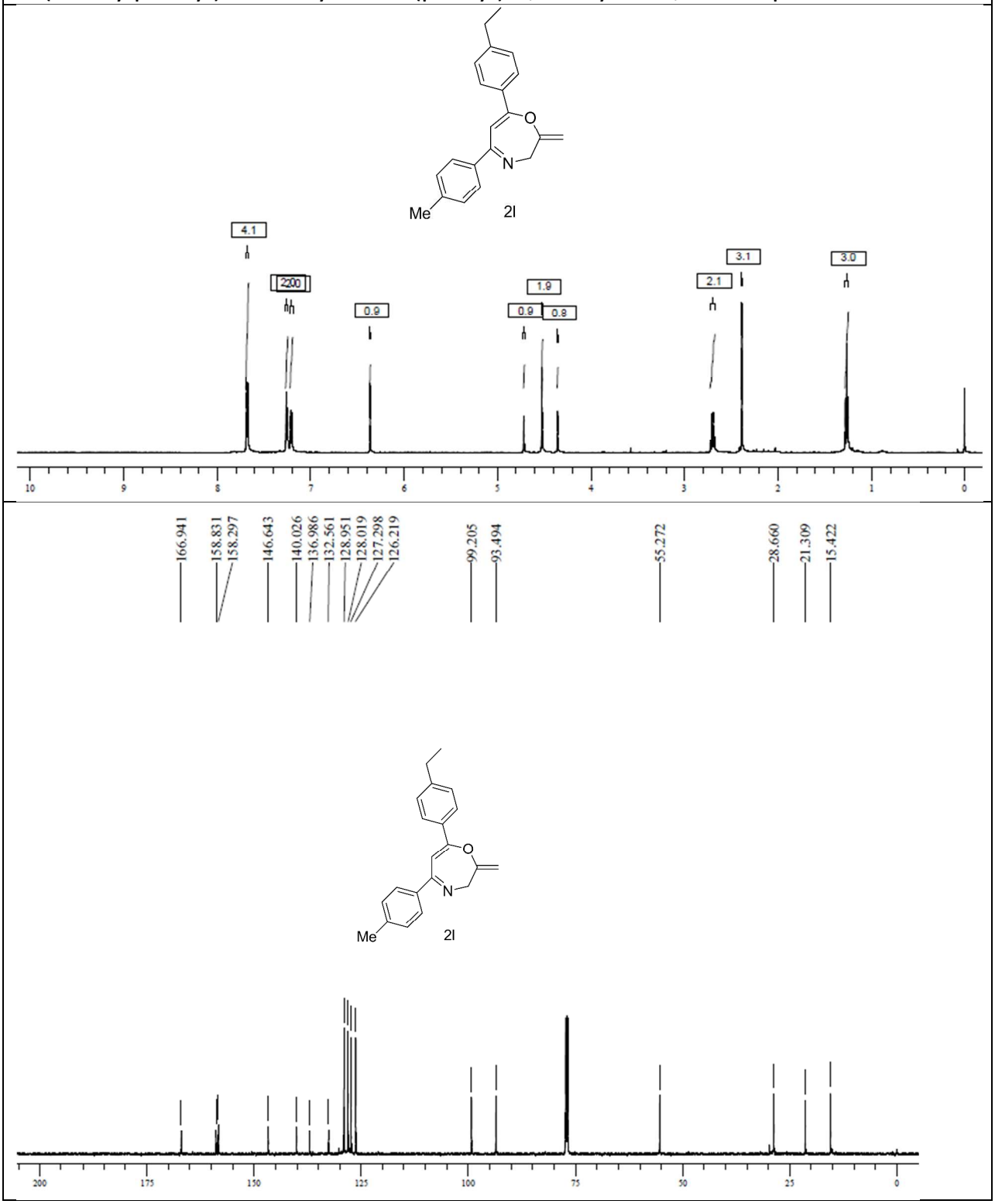


7-(2,4-Dichlorophenyl)-2-methylene-5-phenyl-2,3-dihydro-1,4-oxazepine: **2k**

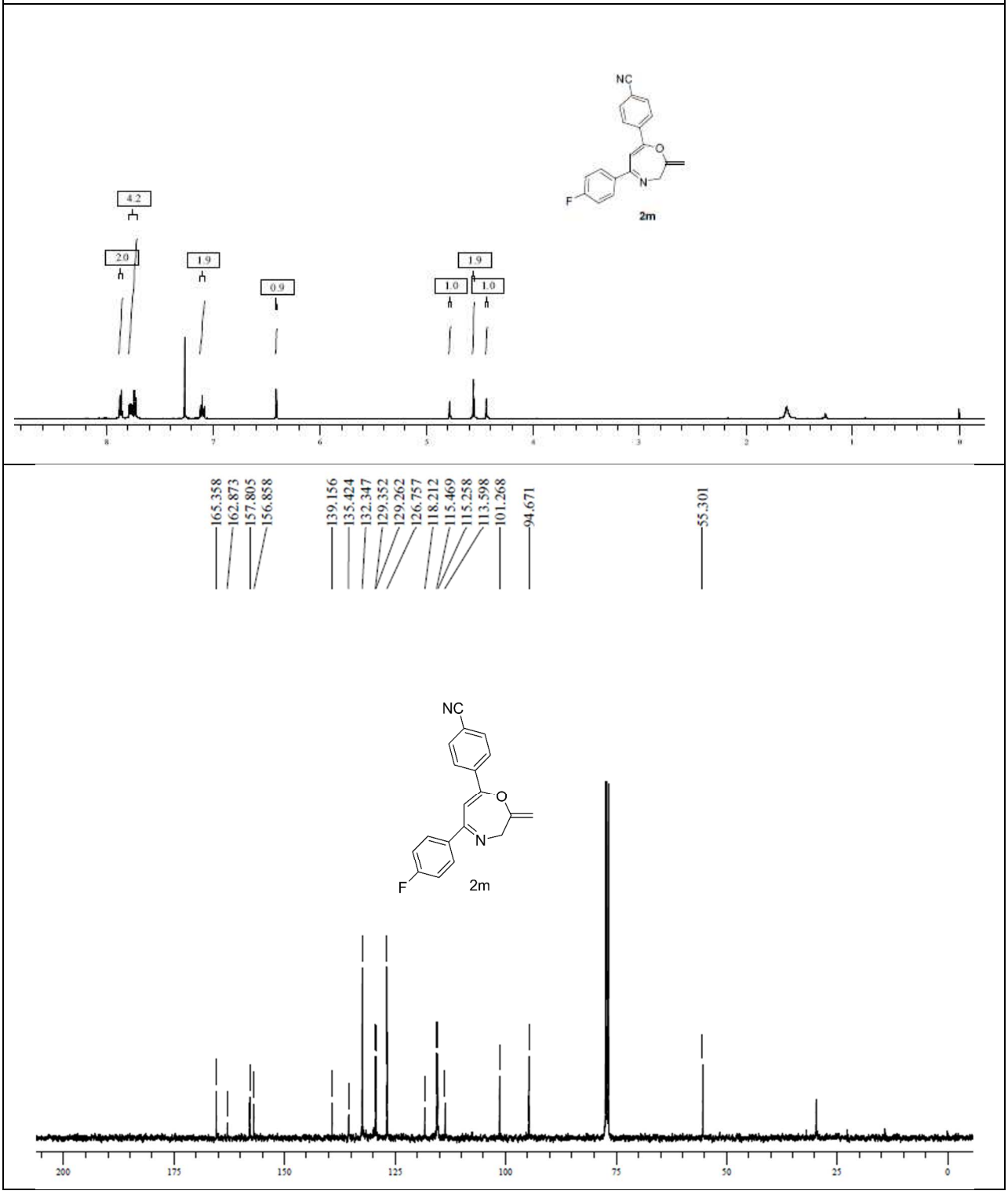




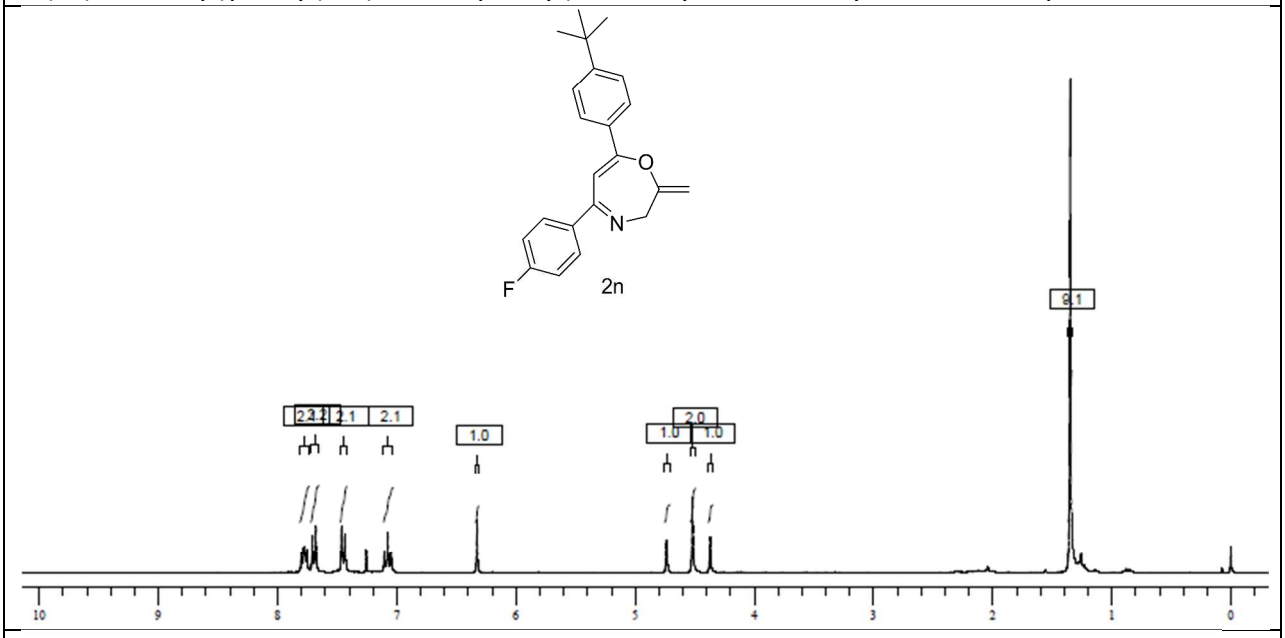
7-(4-Ethylphenyl)-2-methylene-5-(p-tolyl)-2,3-dihydro-1,4-oxazepine: **2l**

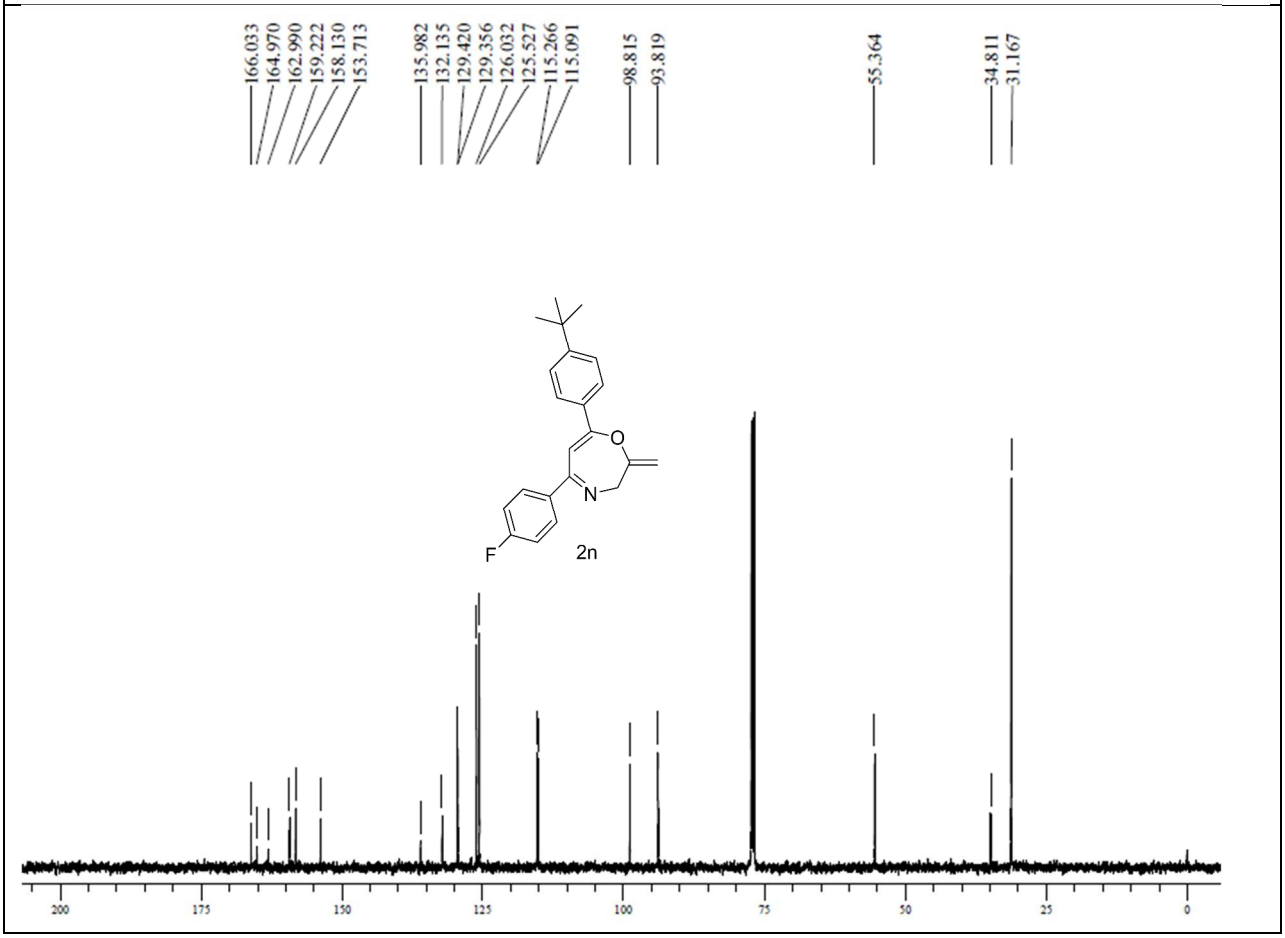


4-(5-(4-Fluorophenyl)-2-methylene-2,3-dihydro-1,4-oxazepin-7-yl)benzonitrile: **2m**

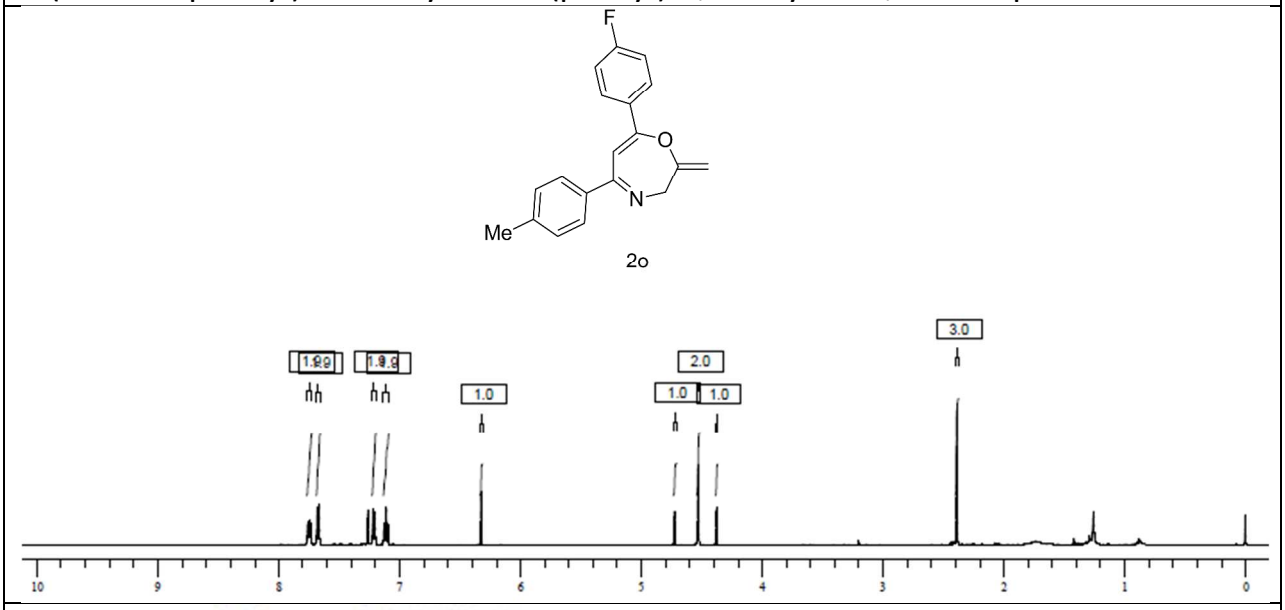


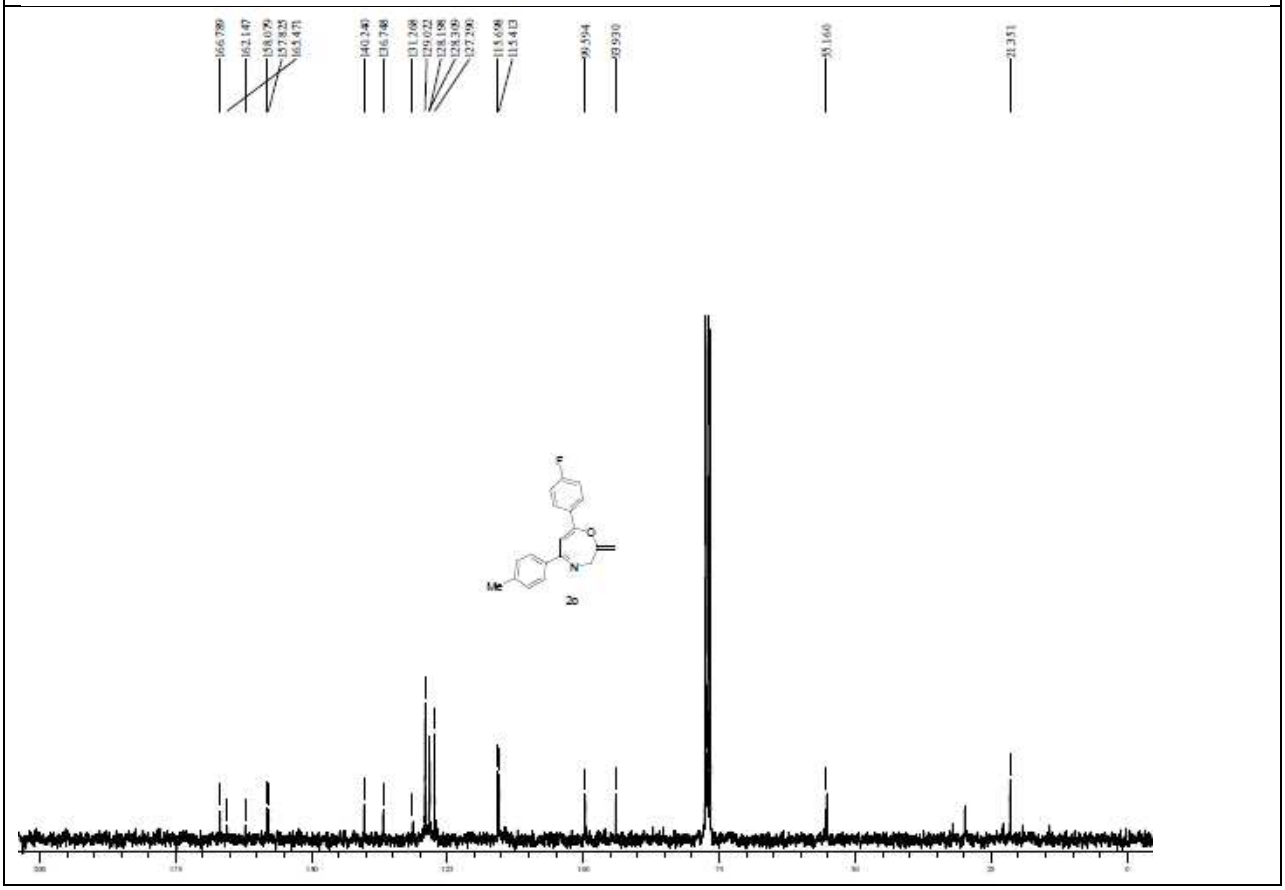
7-(4-(Tert-butyl)phenyl)-5-(4-fluorophenyl)-2-methylene-2,3-dihydro-1,4-oxazepine: **2n**



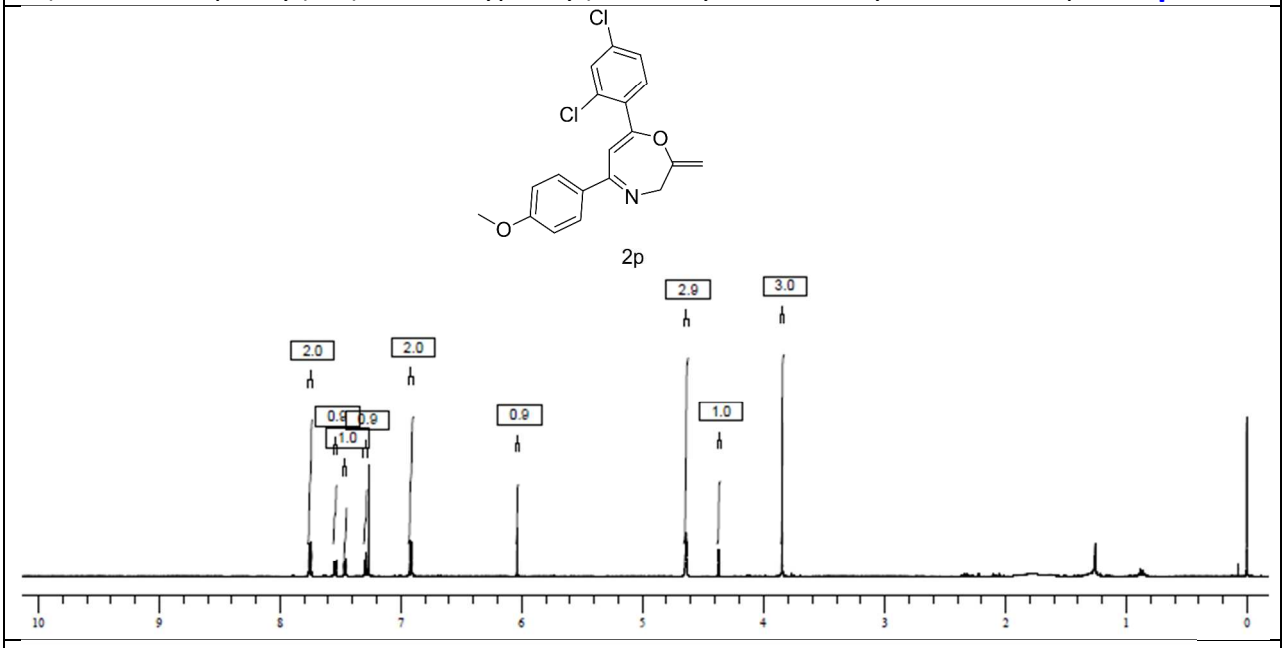


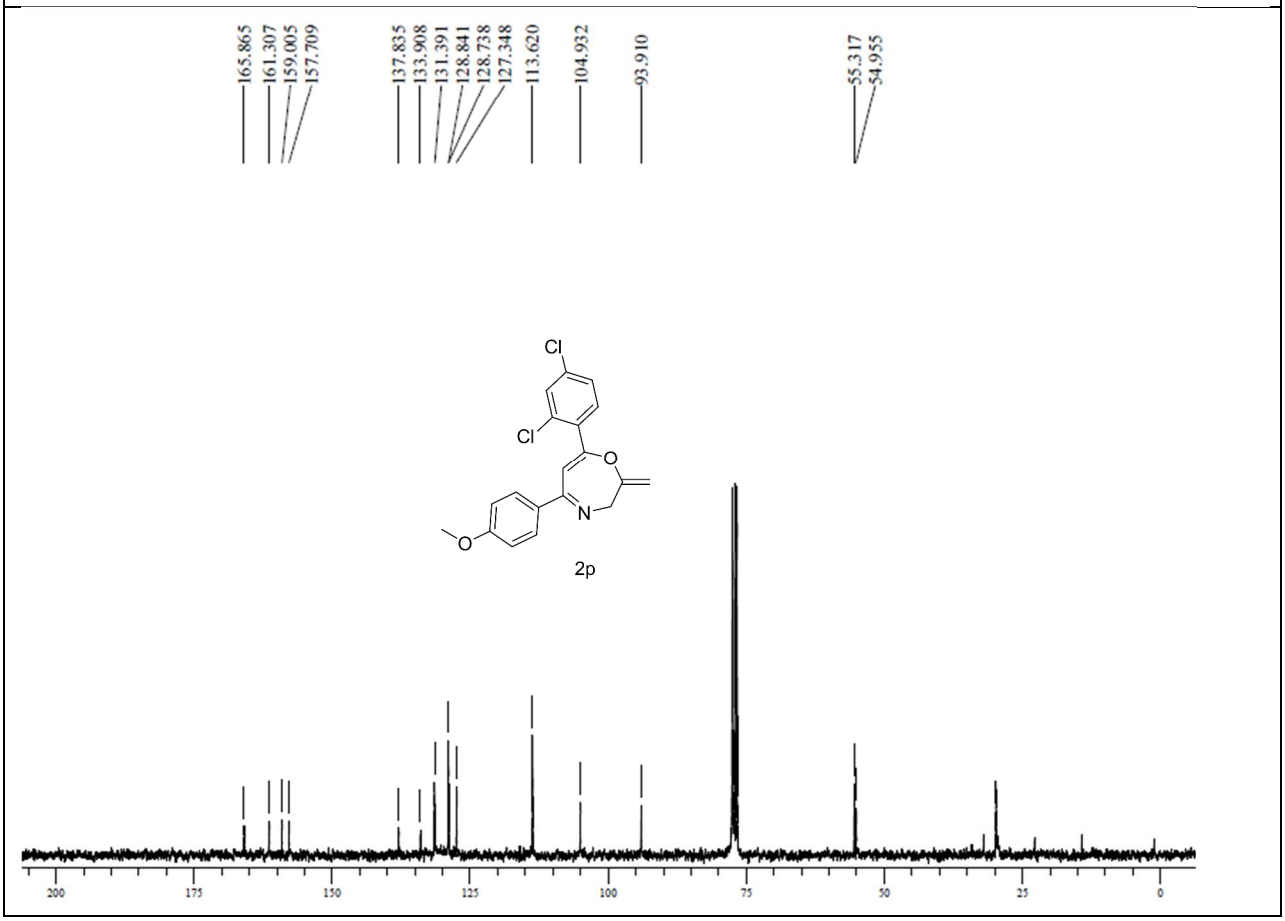
7-(4-Fluorophenyl)-2-methylene-5-(p-tolyl)-2,3-dihydro-1,4-oxazepine: **2o**



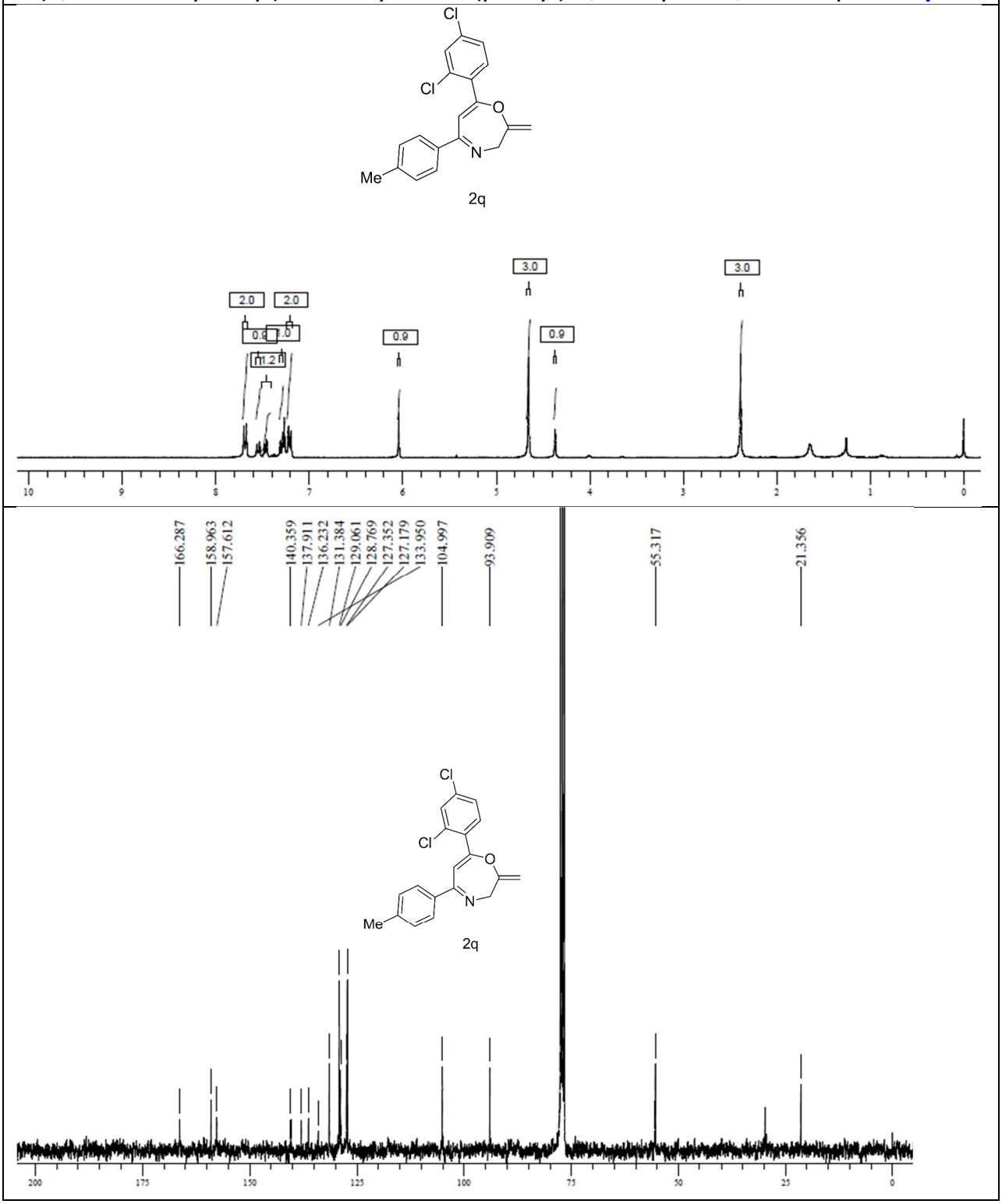


7-(2,4-Dichlorophenyl)-5-(4-methoxyphenyl)-2-methylene-2,3-dihydro-1,4-oxazepine: **2p**





7-(2,4-Dichlorophenyl)-2-methylene-5-(p-tolyl)-2,3-dihydro-1,4-oxazepine: **2q**



1.2 X-ray crystallography data

Cambridge Crystallographic Data Centre (CCDC)

This CIF contains data from an original supplementary publication deposited with the CCDC, and may include chemical, crystal, experimental, refinement, atomic coordinates, anisotropic displacement parameters and molecular geometry data, as required by the journal to which it was submitted. This CIF is provided on the understanding that it is used for bona fide research purposes only. It may contain copyright material of the CCDC or of third parties, and may not be copied or further disseminated in any form, whether machine-readable or not, except for the purpose of generating routine backup copies on your local computer system. For further information on the CCDC, data deposition and data retrieval see: www.ccdc.cam.ac.uk

Crystal structure data of 2a: Crystal structure deposition no: CCDC 1048547

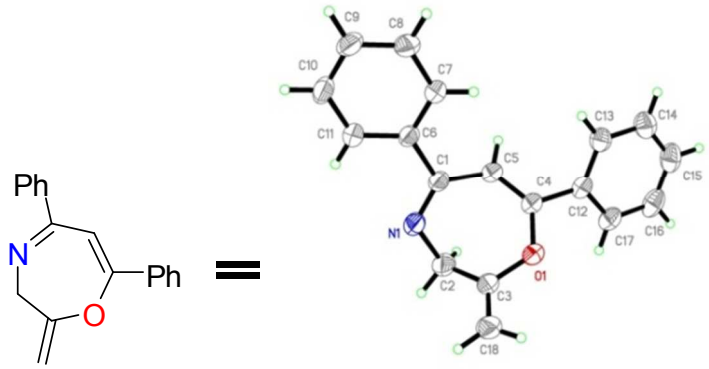


Figure 1. ORTEP representation of 1,4-oxazepine derivative (**2a**: CCDC 1048547). A view of **2a**, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary radii.

X-ray data for the compounds were collected at room temperature using a Bruker Smart Apex CCD diffractometer with graphite monochromated MoKα radiation (λ=0.71073Å) with ω-scan method.[1] Preliminary lattice parameters and orientation matrices were obtained from four sets of frames. Integration and scaling of intensity data were accomplished using SAINT program.[1] The structure was solved by direct methods using SHELXS[2] and refinement was carried out by full-matrix least-squares technique using SHELXL.[2] Anisotropic displacement parameters were

included for all non-hydrogen atoms. All H atoms were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.98 Å and $U_{iso}(H) = 1.2U_{eq}(C)$].

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1. Bruker (2001). SAINT (Version 6.28a) & SMART (Version 5.625). Bruker AXS Inc., Madison, Wisconsin, USA.
2. Sheldrick G. M. (2015**)** Acta Crystallogr C71: 3-8.