

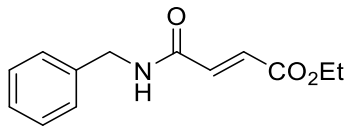
*Supporting information*

ARTIFICIAL INTELLIGENCE-DESIGNED STEREOSELECTIVE ONE-POT SYNTHESIS  
OF *TRANS*  $\beta$ -LACTAMS AND ITS APPLICATION TO CHOLESTEROL ABSORPTION  
INHIBITOR SCH 47949 SYNTHESIS

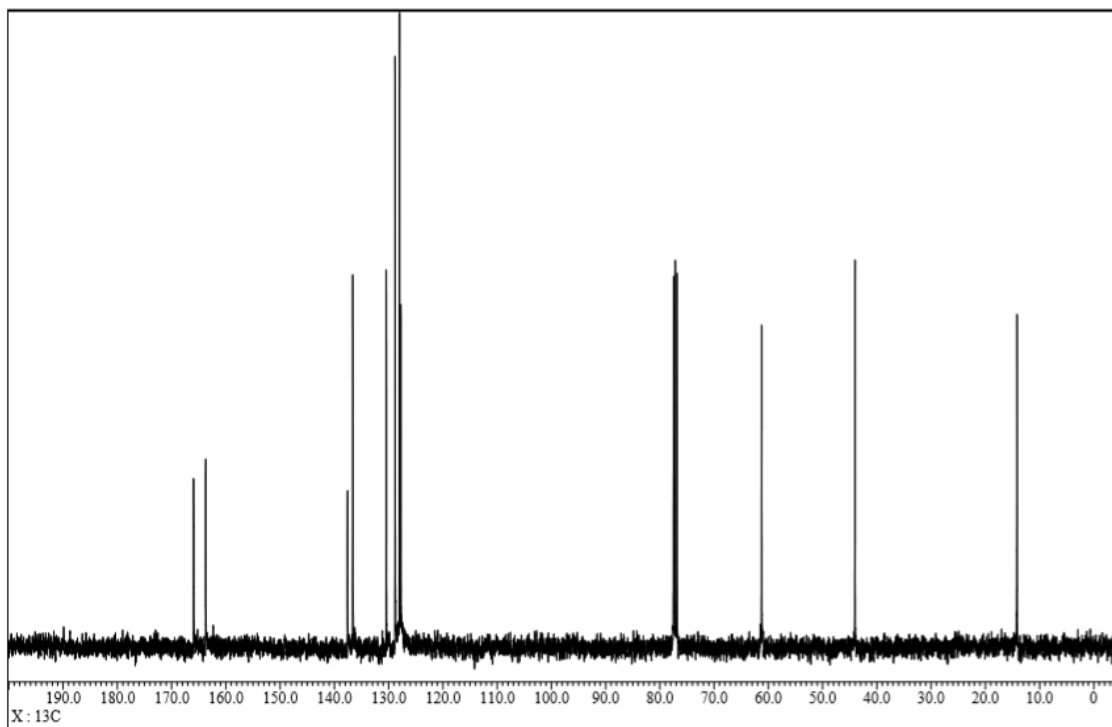
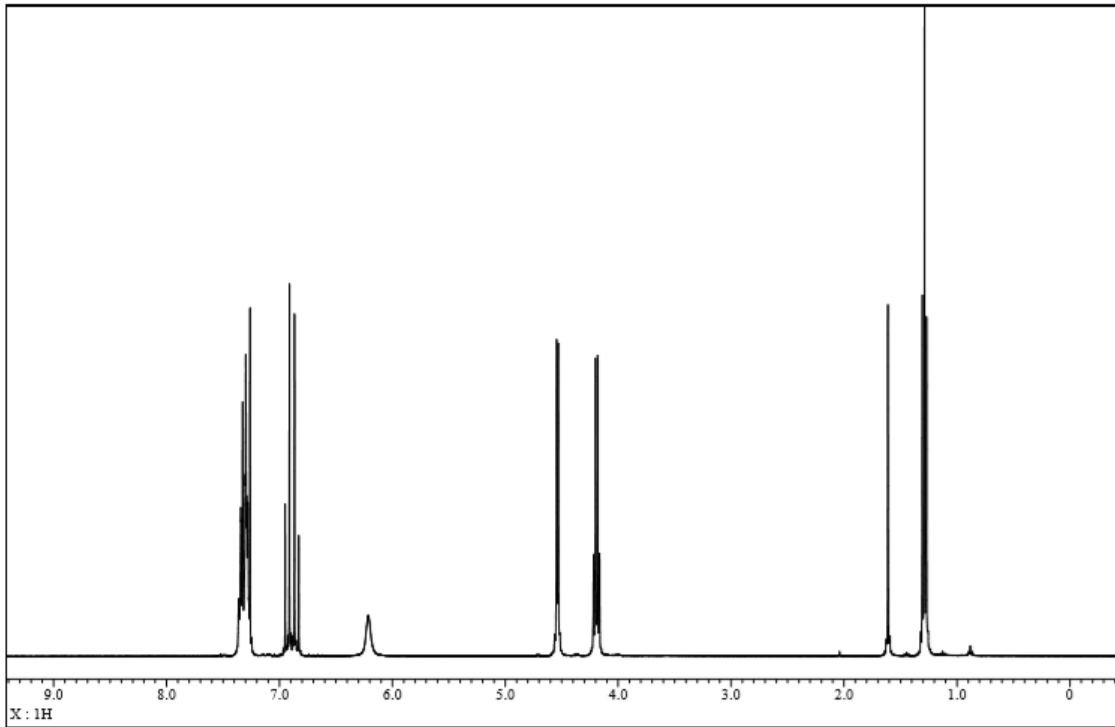
Tetsuhiko Takabatake, Takuya Yoneda, Jyo Otsuka, Natsuko Kagawa, and Masahiro Toyota\*

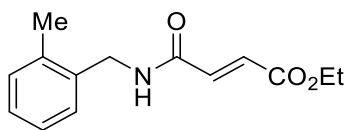
*Spectral data*

2 - 39

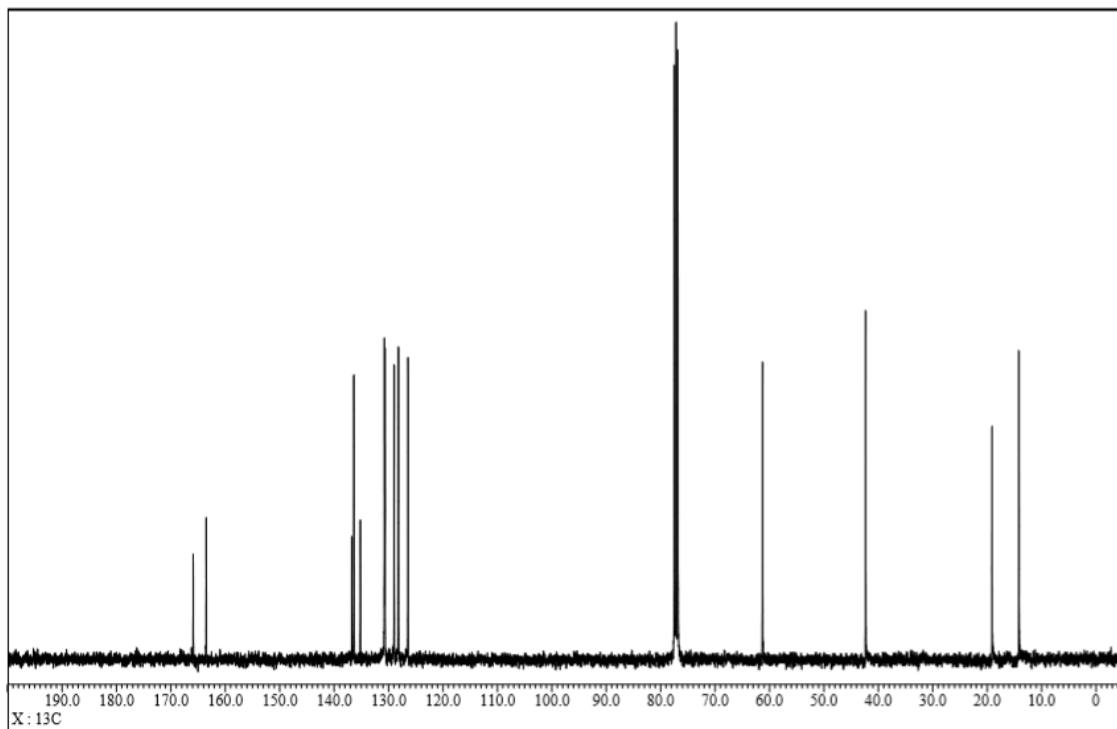
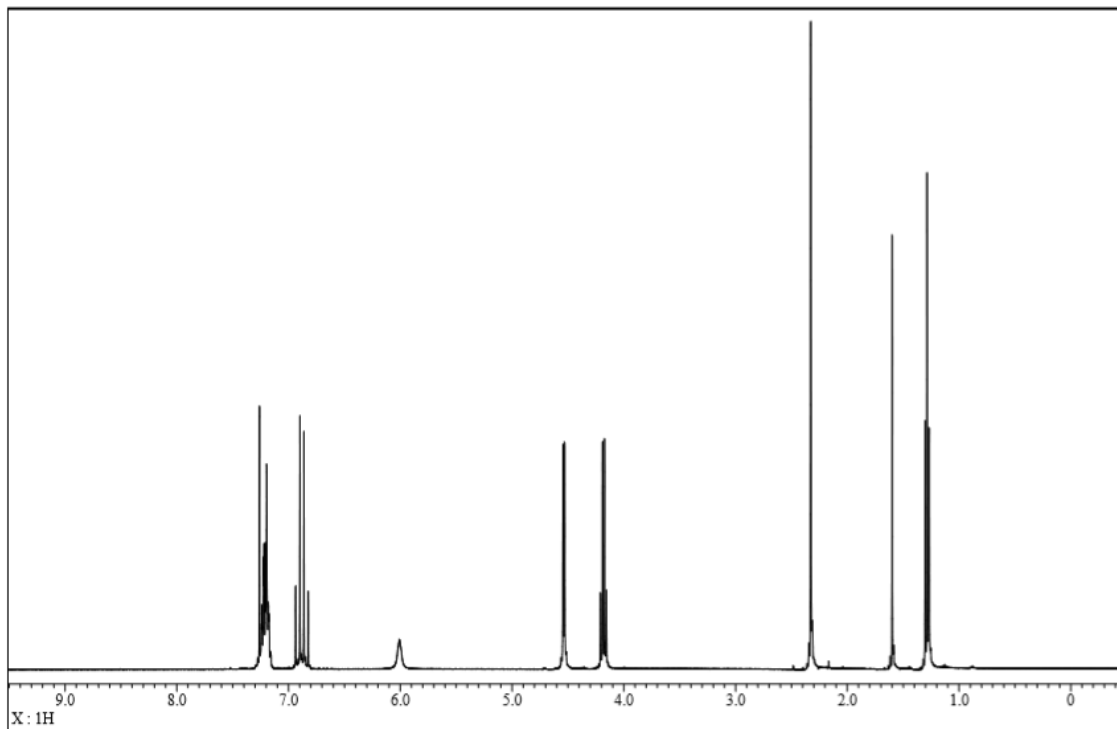


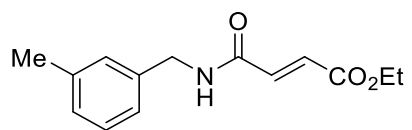
**Ethyl (*E*)-4-(benzylamino)-4-oxobut-2-enoate (4a)**



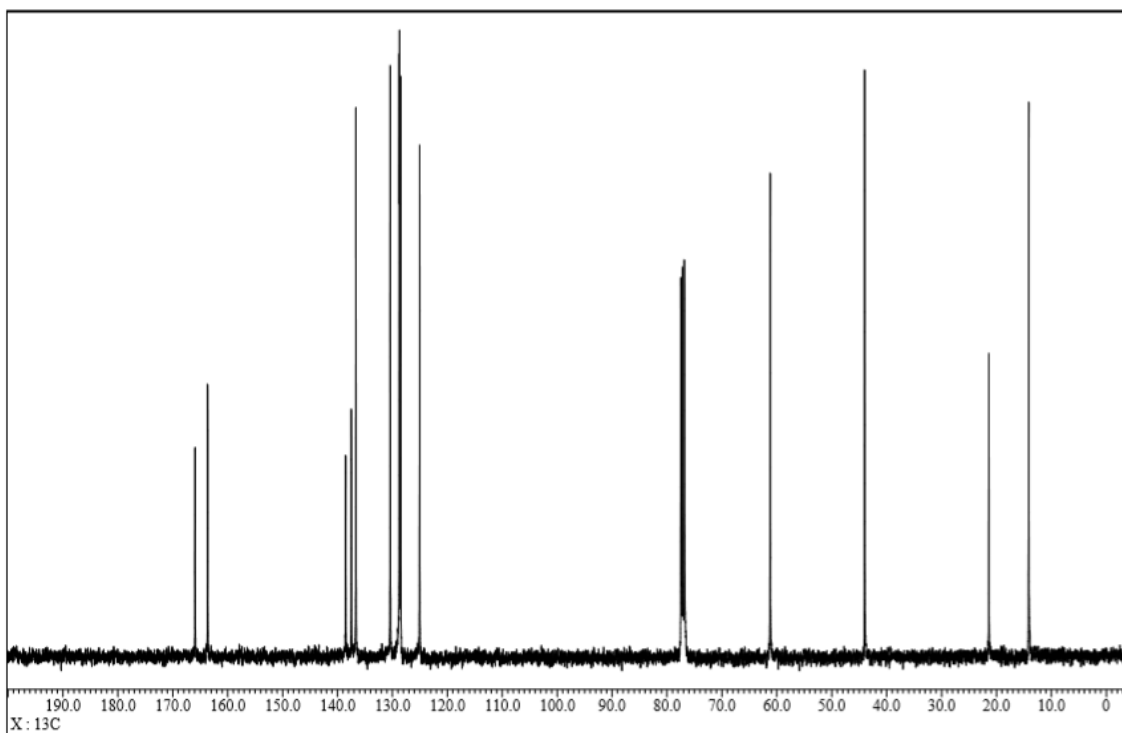
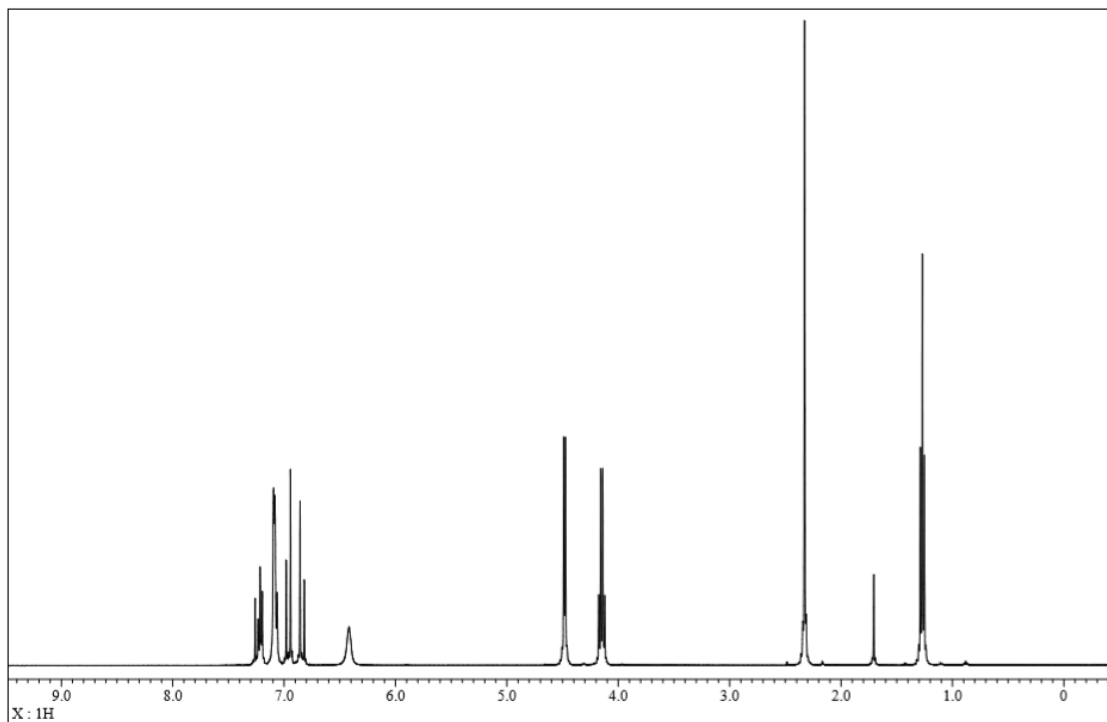


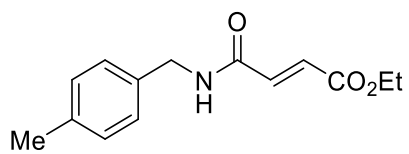
**Ethyl (*E*)-4-[(2-methylbenzyl)amino]-4-oxobut-2-enoate (4b)**



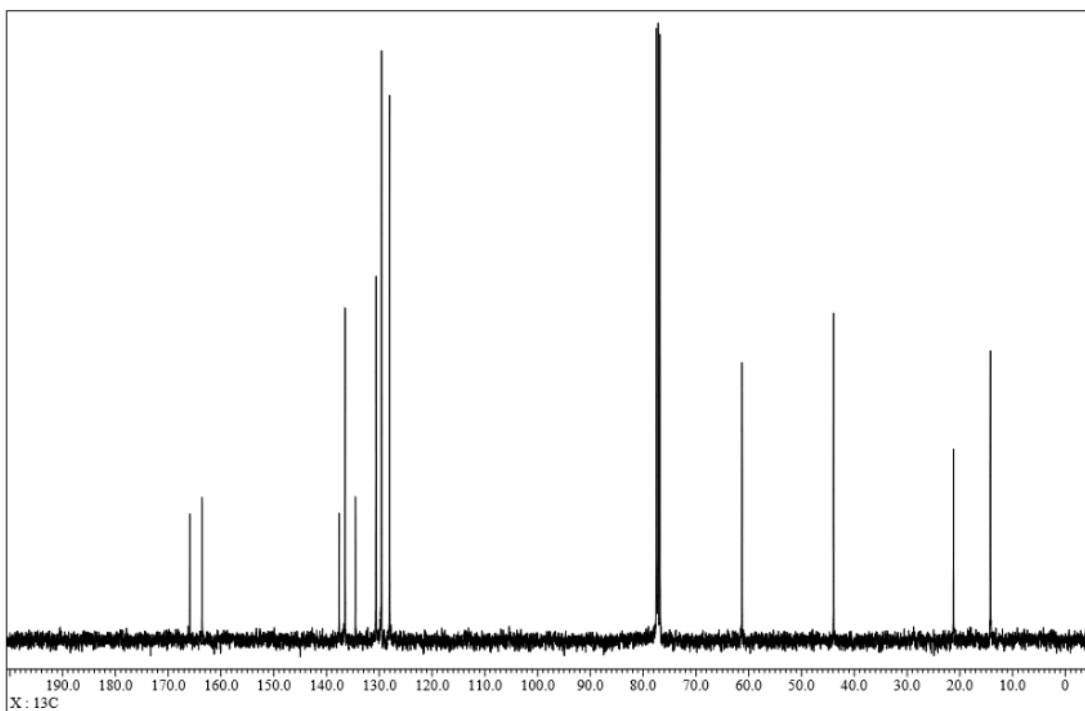
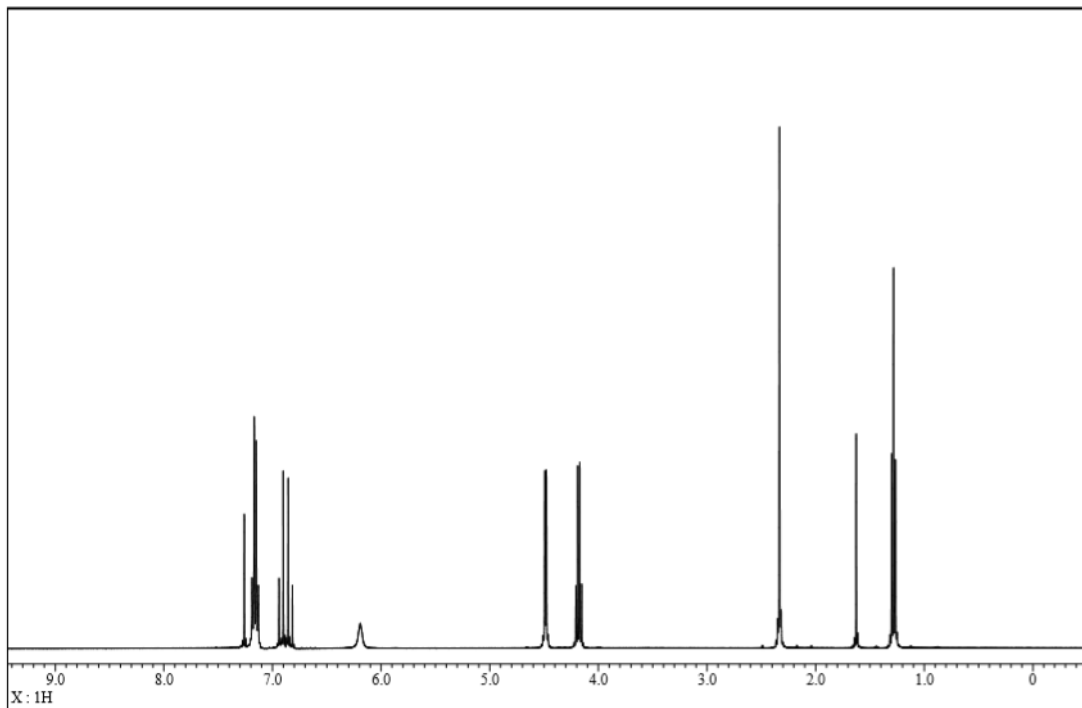


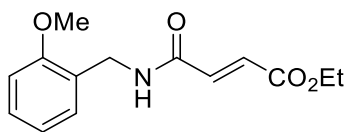
**Ethyl (*E*)-4-[(3-methylbenzyl)amino]-4-oxobut-2-enoate (4c)**



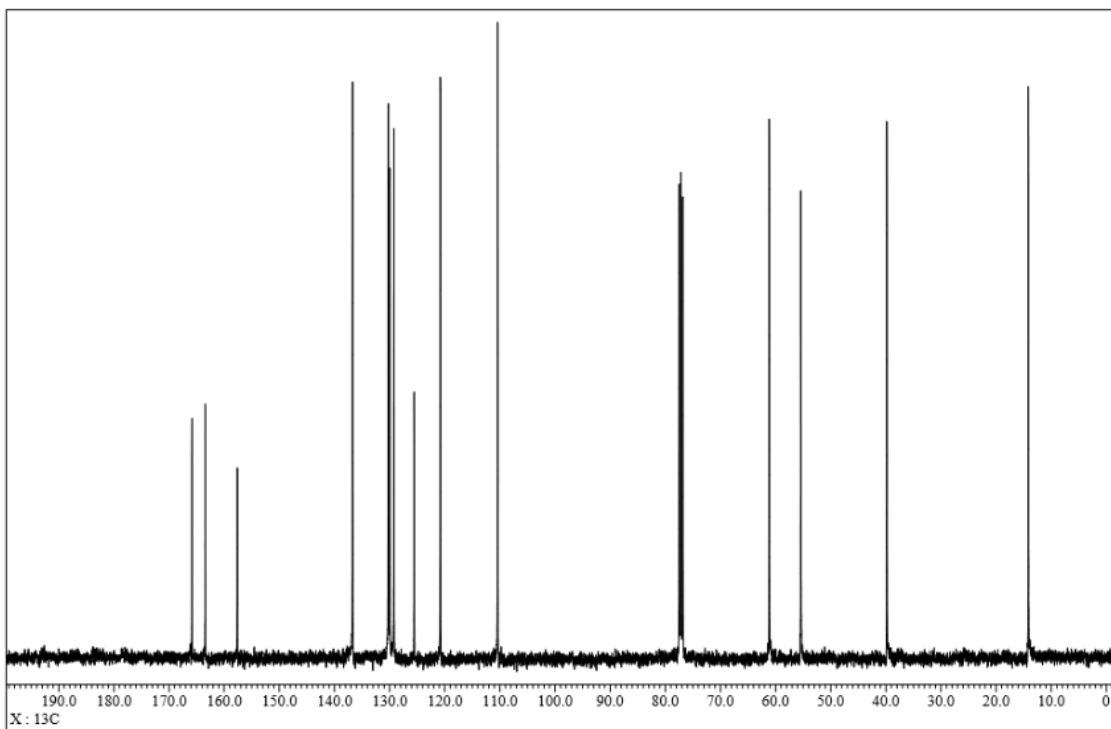
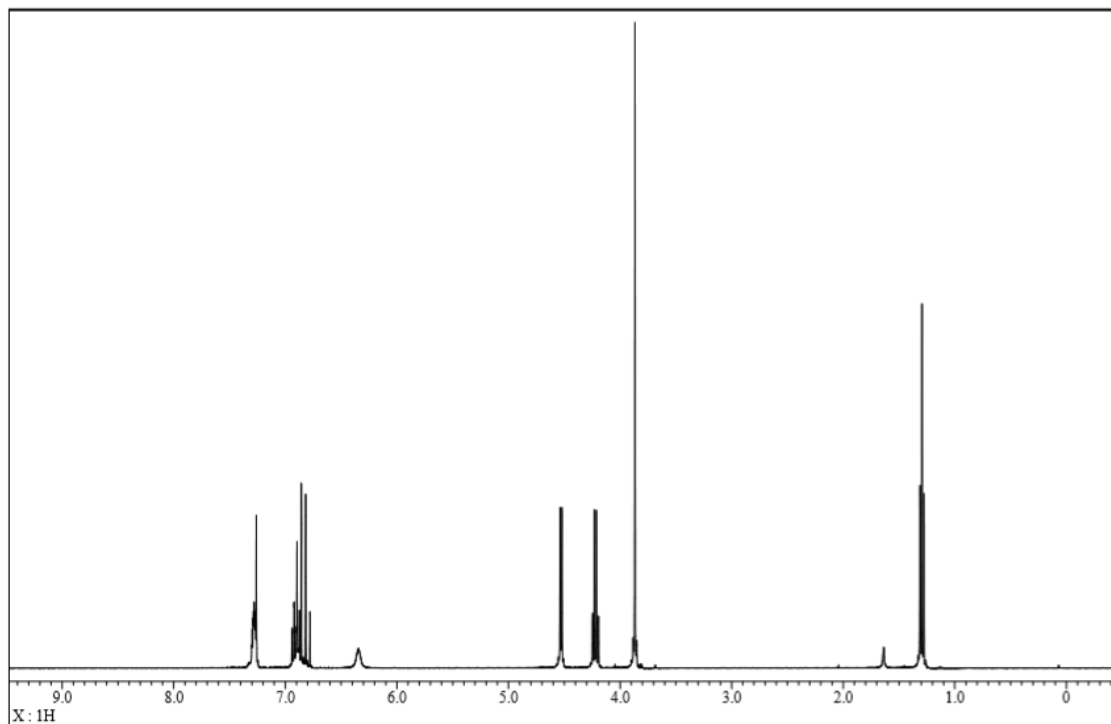


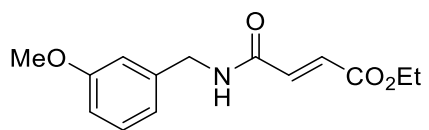
**Ethyl (*E*)-4-[(4-methylbenzyl)amino]-4-oxobut-2-enoate (4d)**



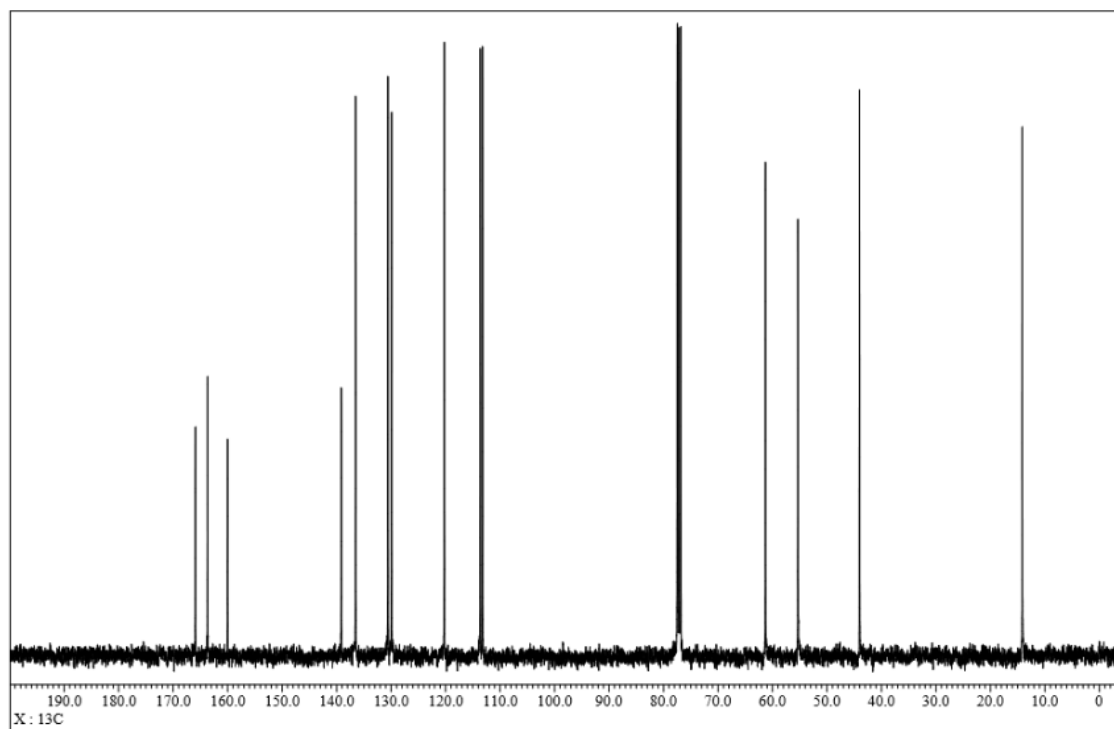
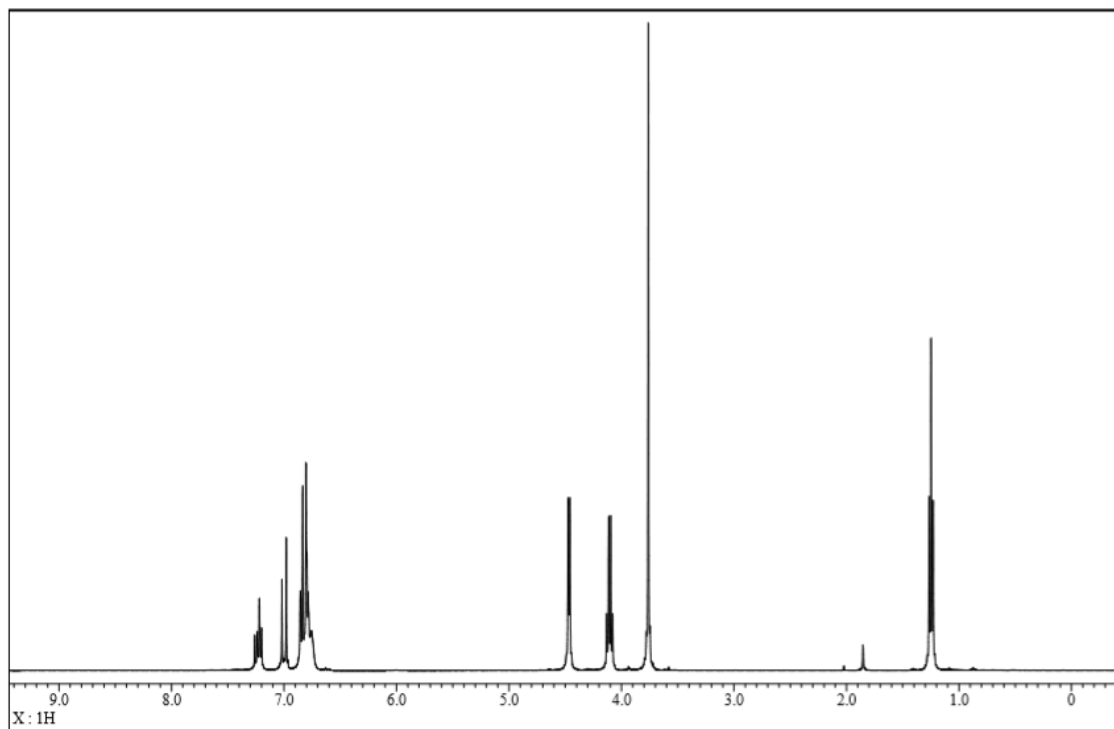


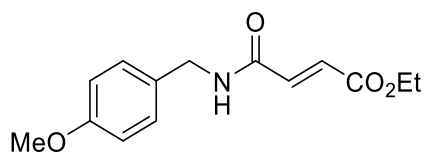
**Ethyl (*E*)-4-[(2-methoxybenzyl)amino]-4-oxobut-2-enoate (4e)**



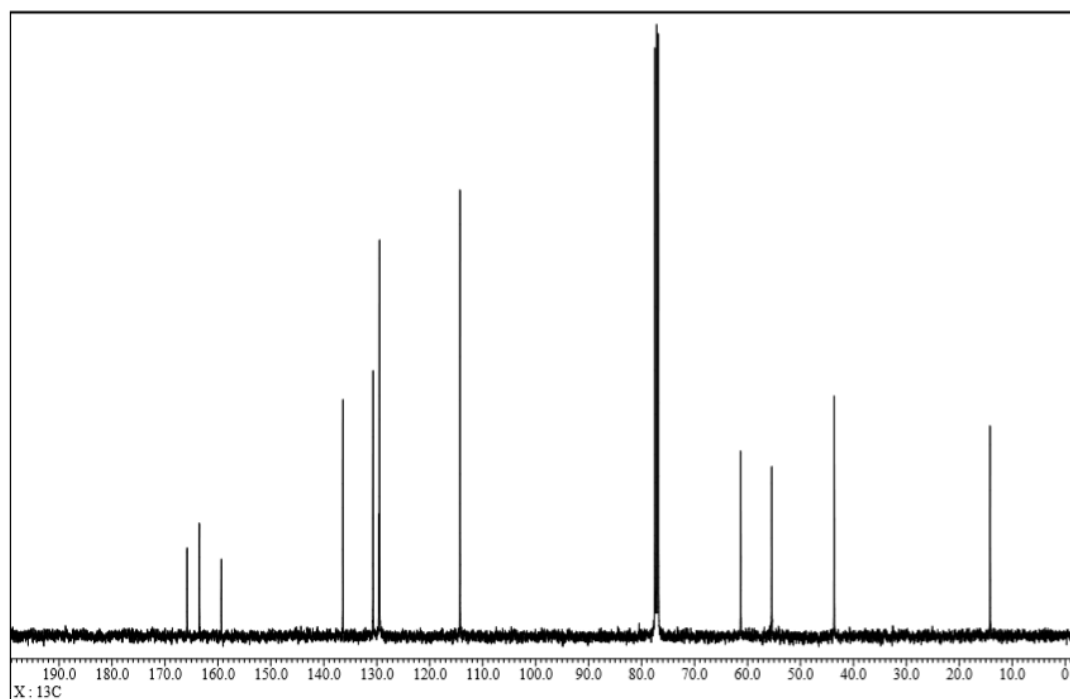
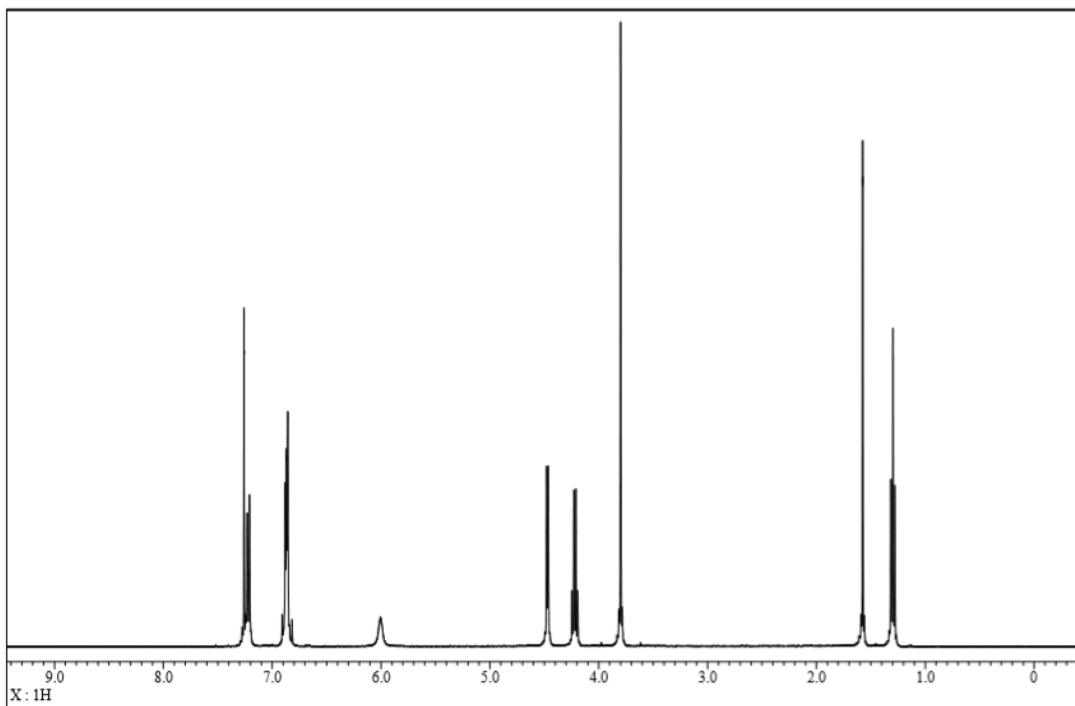


**Ethyl (*E*)-4-[(3-methoxybenzyl)amino]-4-oxobut-2-enoate (4f)**

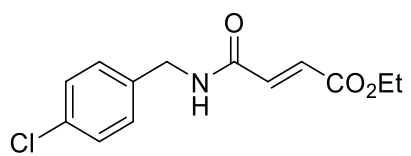




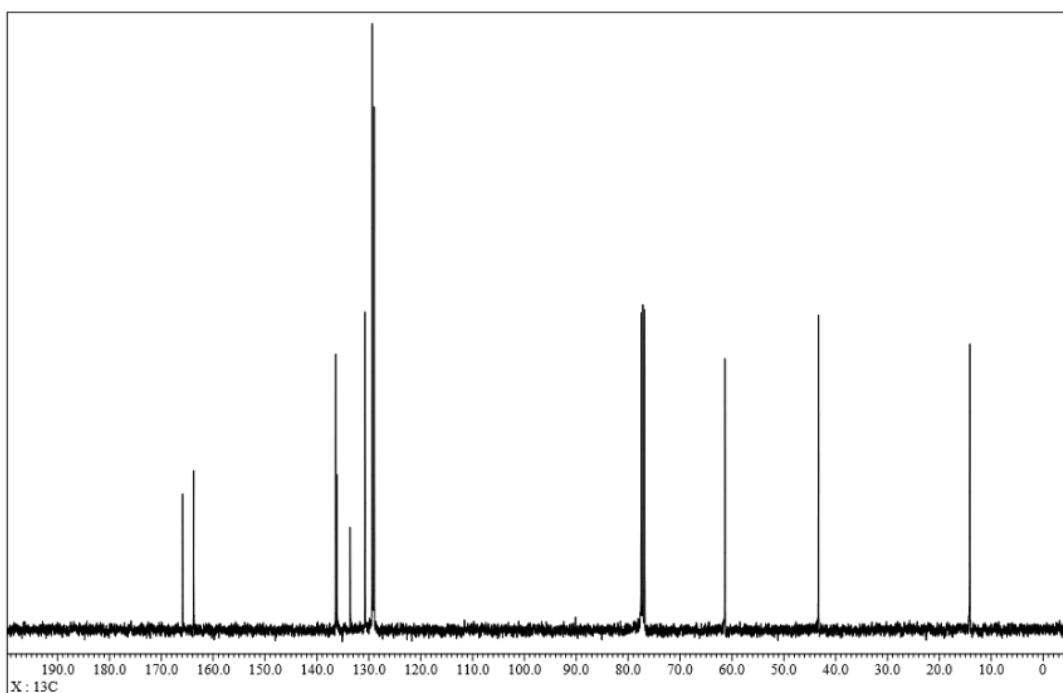
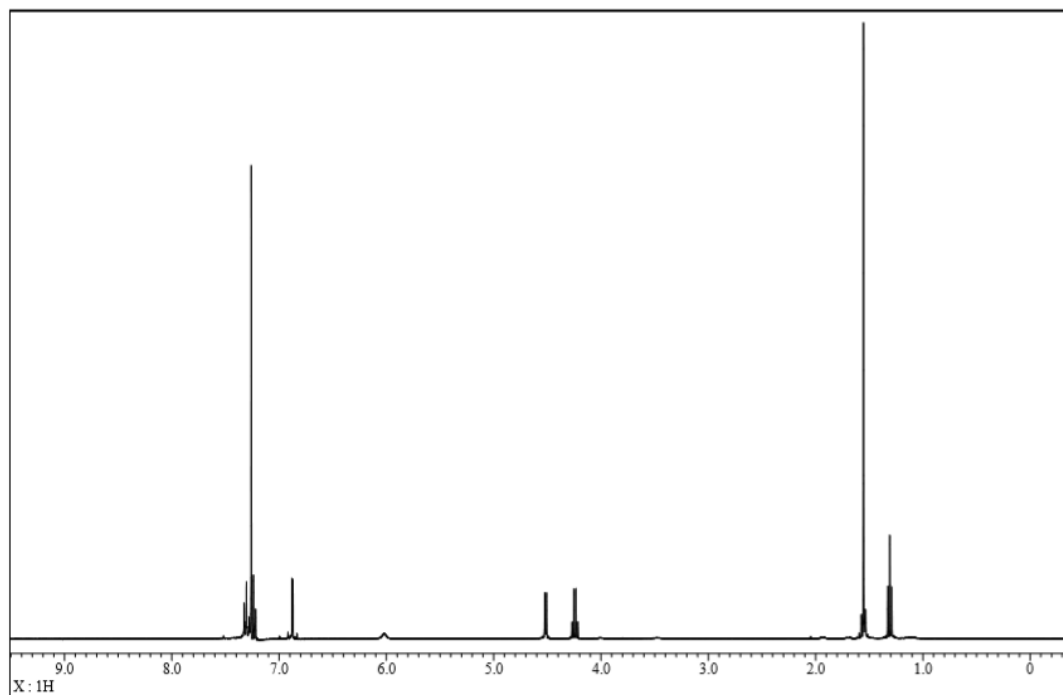
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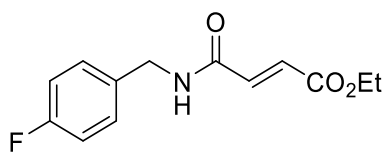




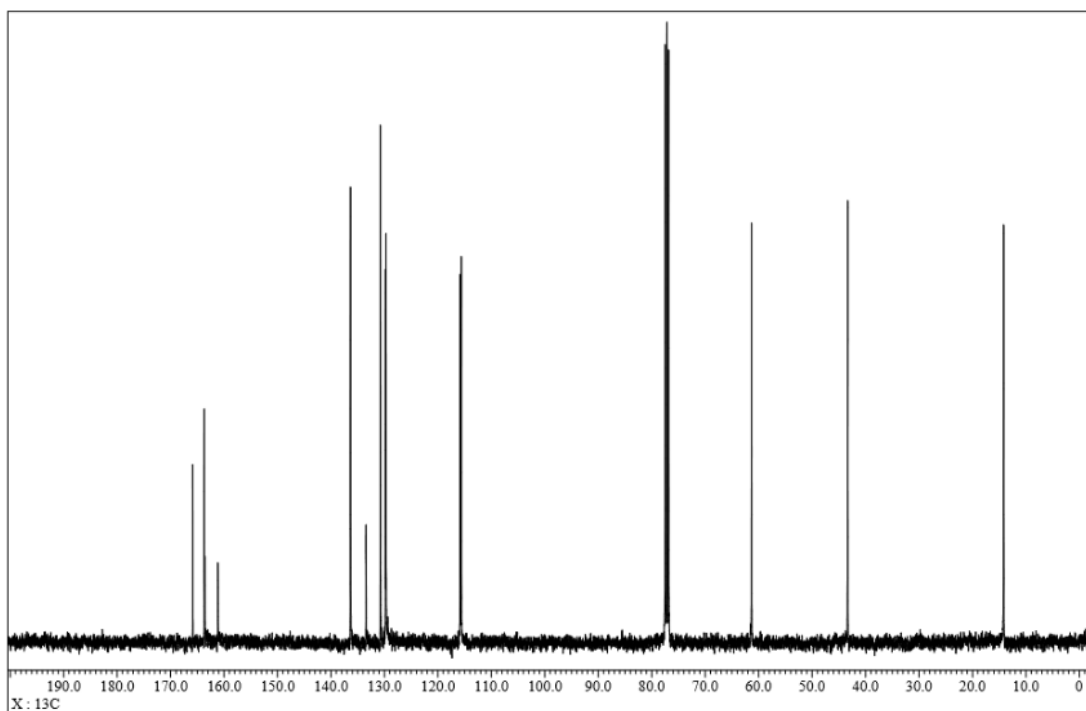
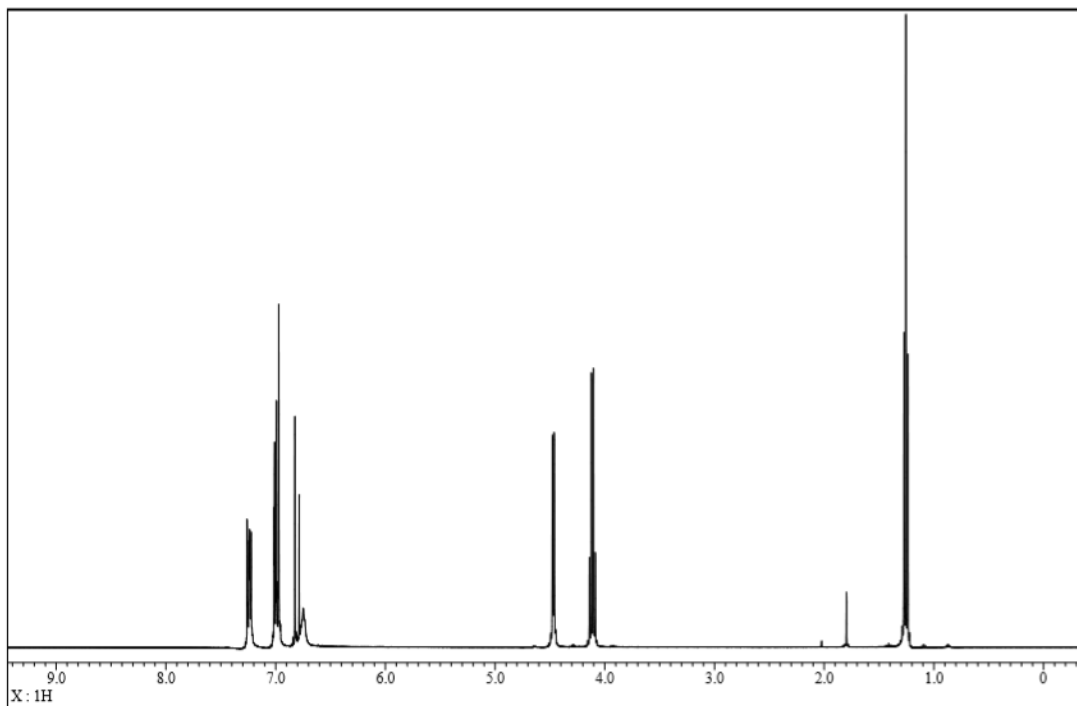


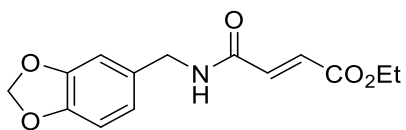
**Ethyl (E)-4-[(4-chlorobenzyl)amino]-4-oxobut-2-enoate (4i)**



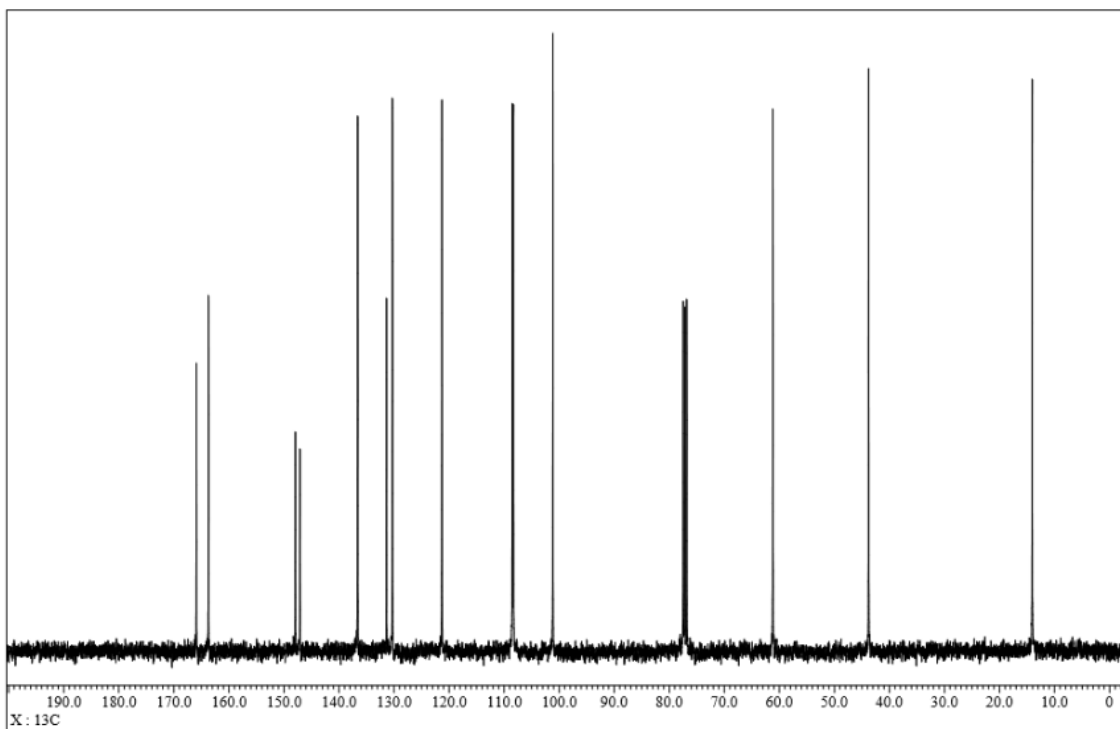
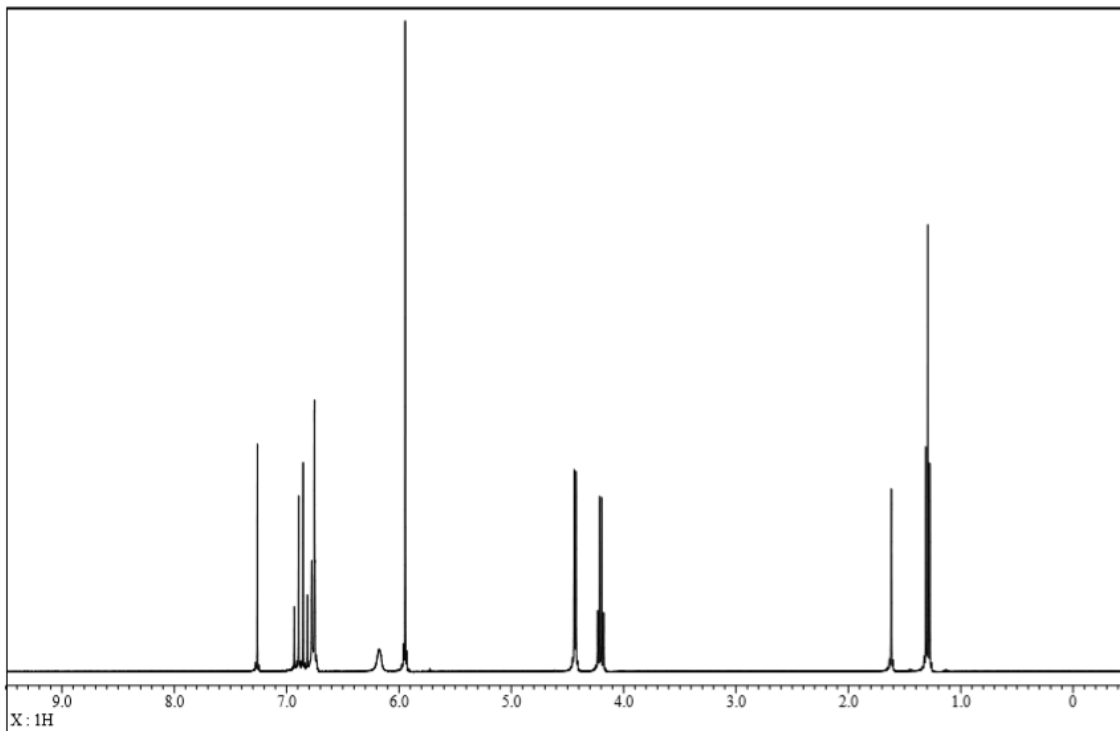


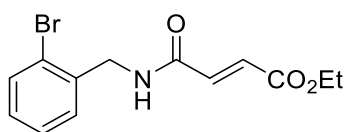
**Ethyl (*E*)-4-[(4-fluorobenzyl)amino]-4-oxobut-2-enoate (4j)**



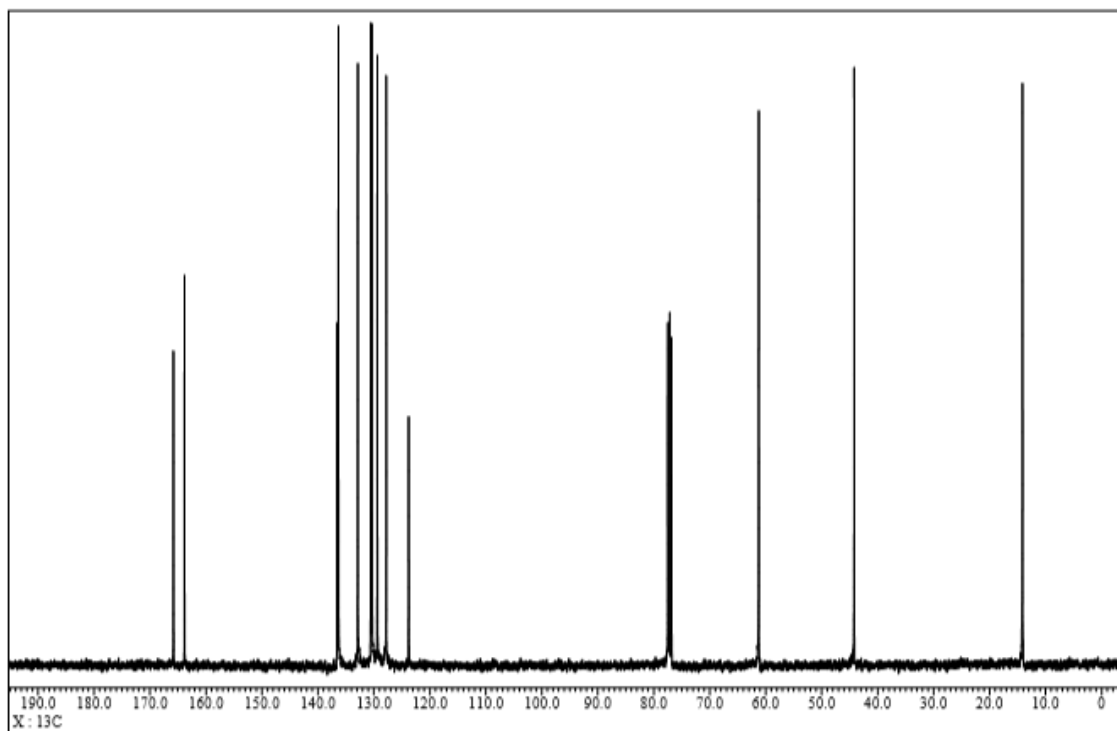
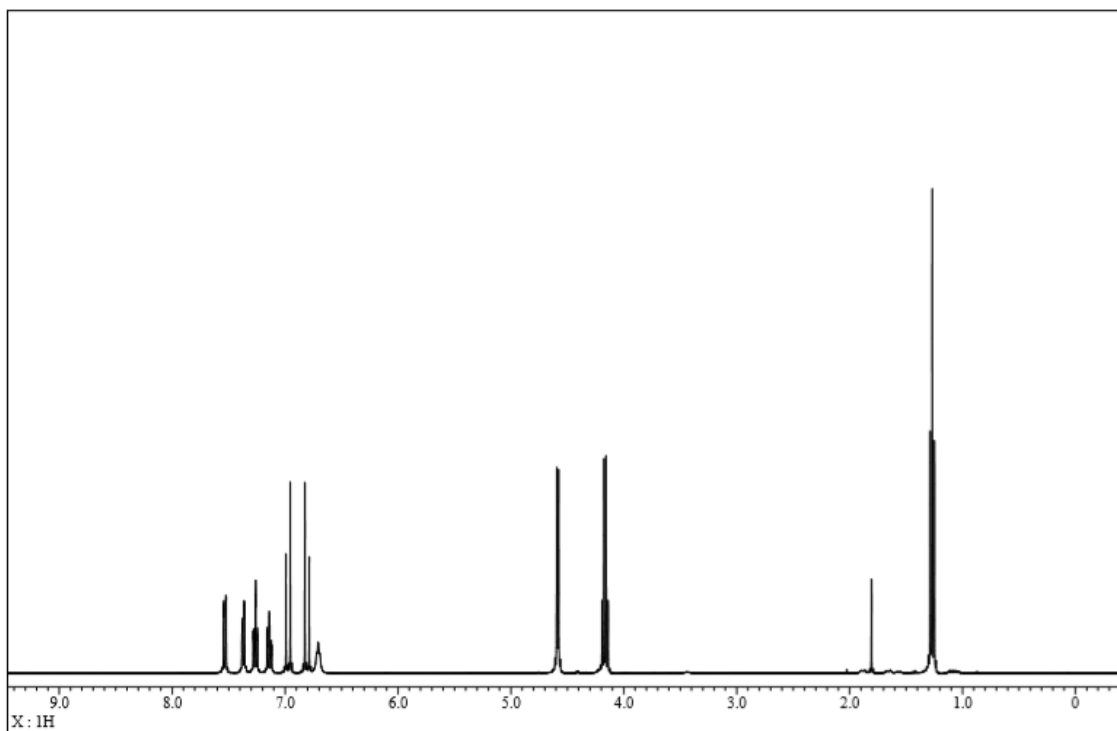


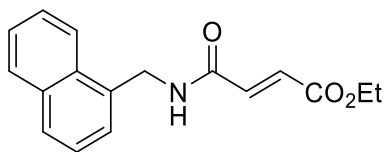
**Ethyl (*E*)-4-[(benzo[d][1,3]dioxol-5-ylmethyl)amino]-4-oxobut-2-enoate (4k)**



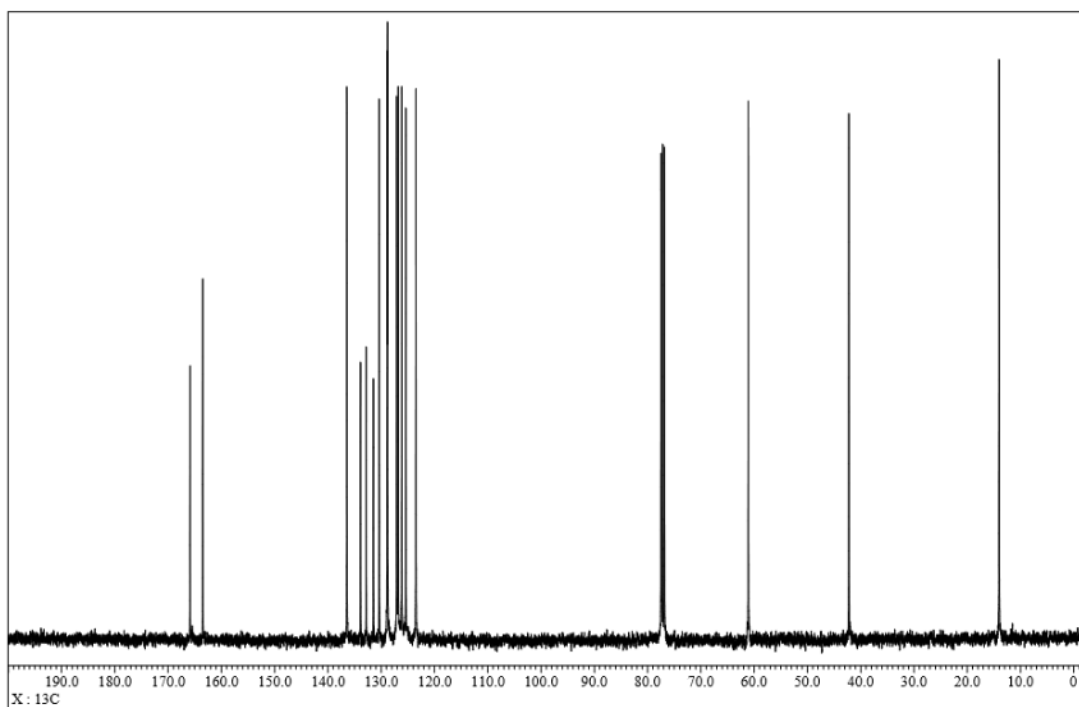
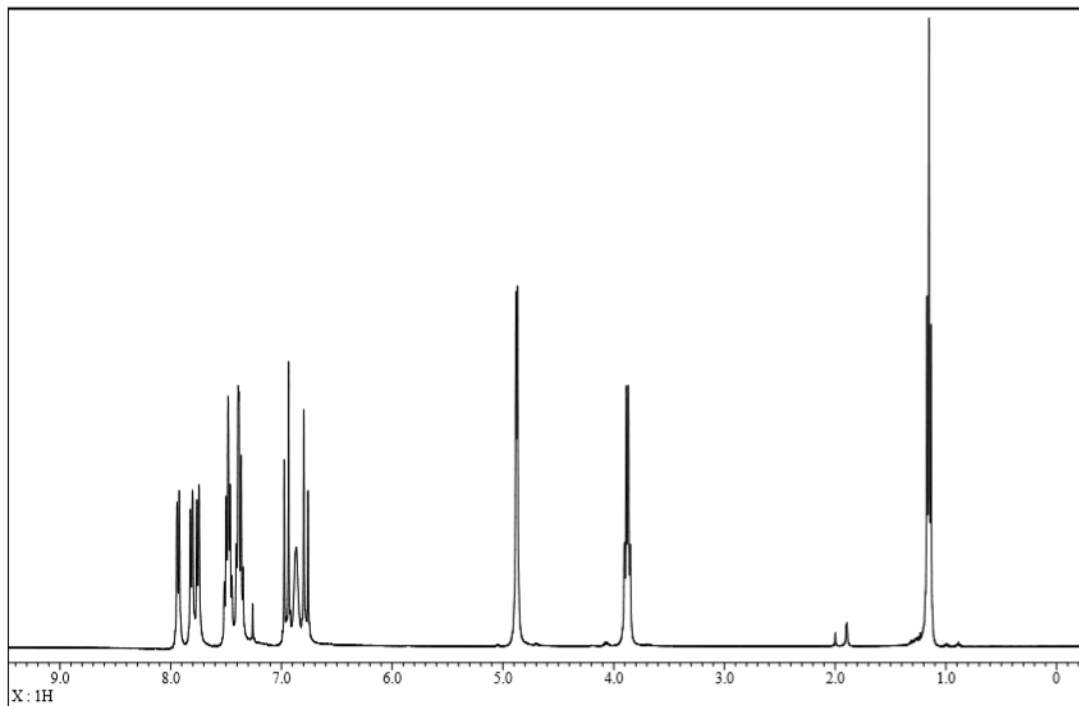


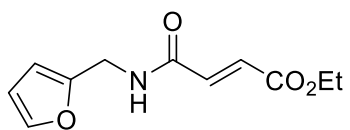
**Ethyl (*E*)-4-[(2-bromobenzyl)amino]-4-oxobut-2-enoate (4l)**



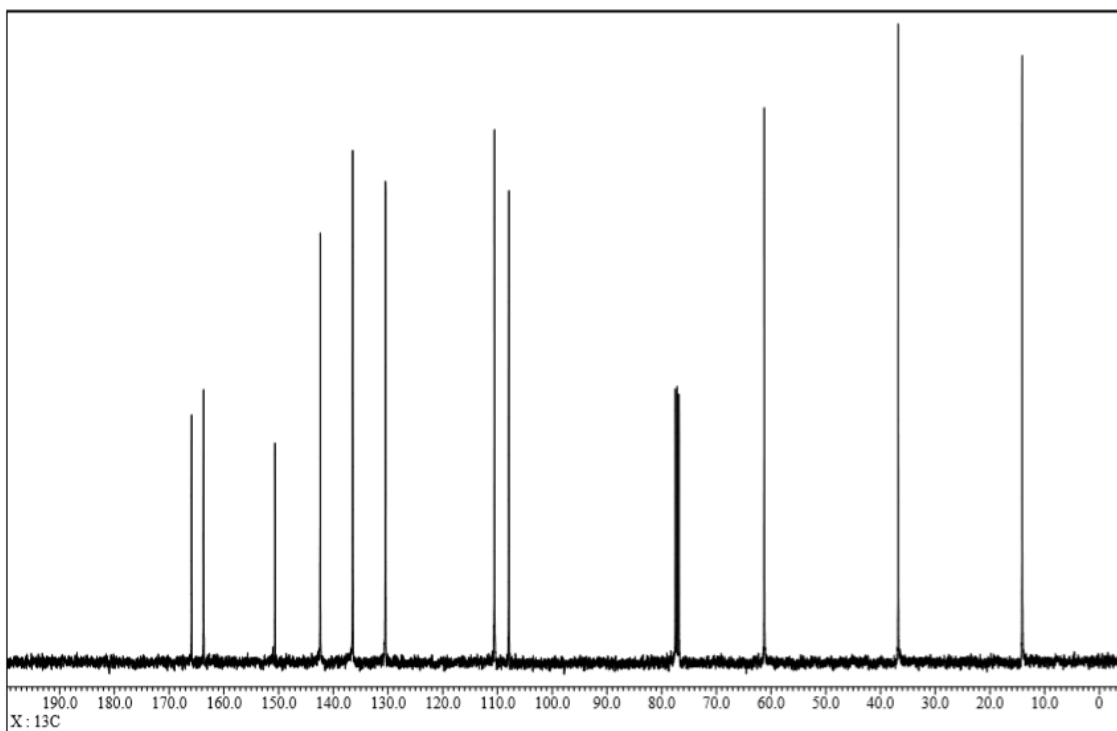
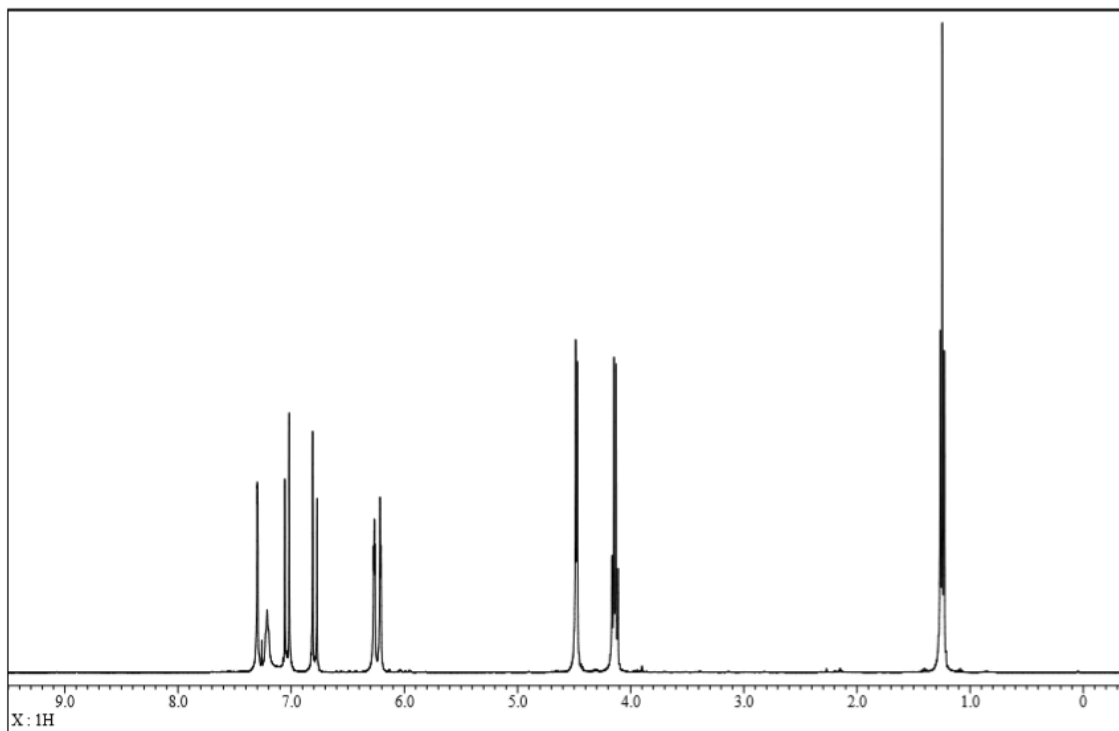


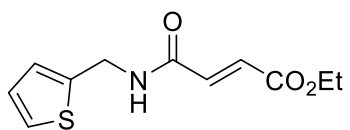
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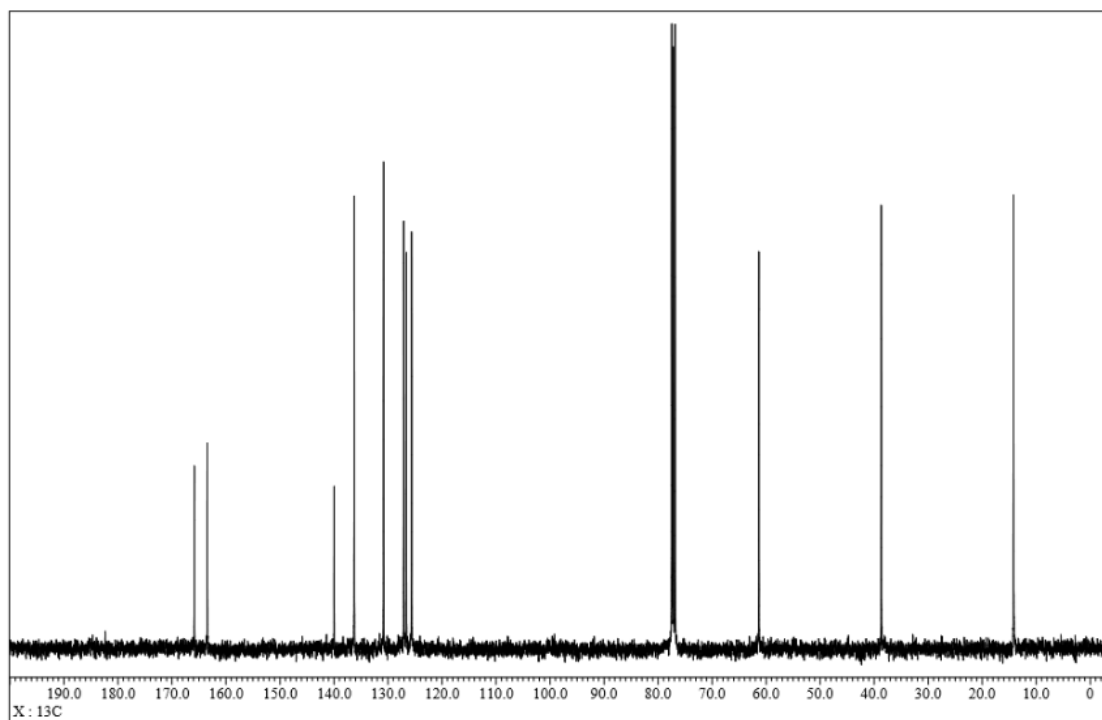
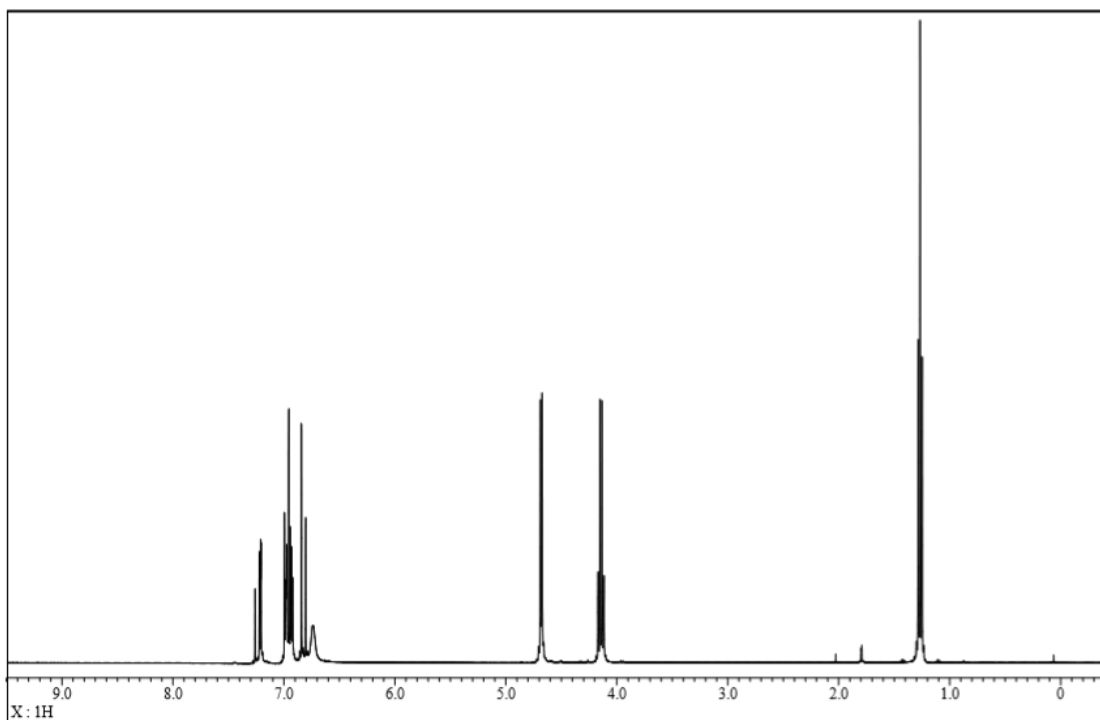


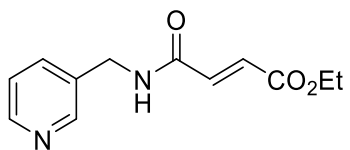
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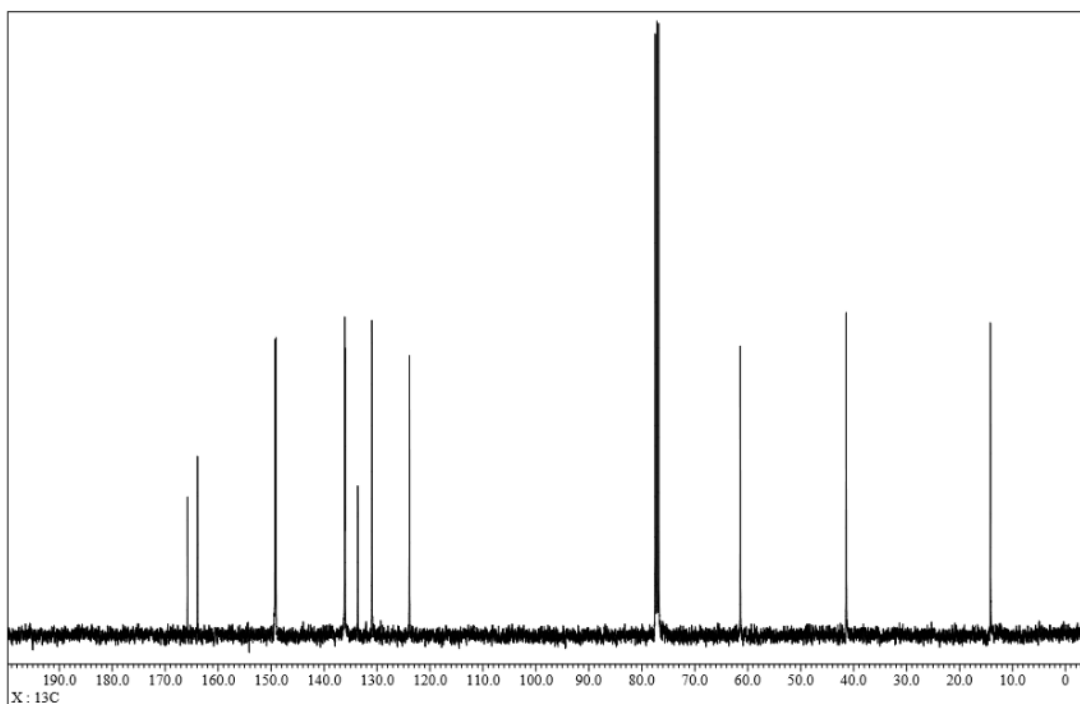
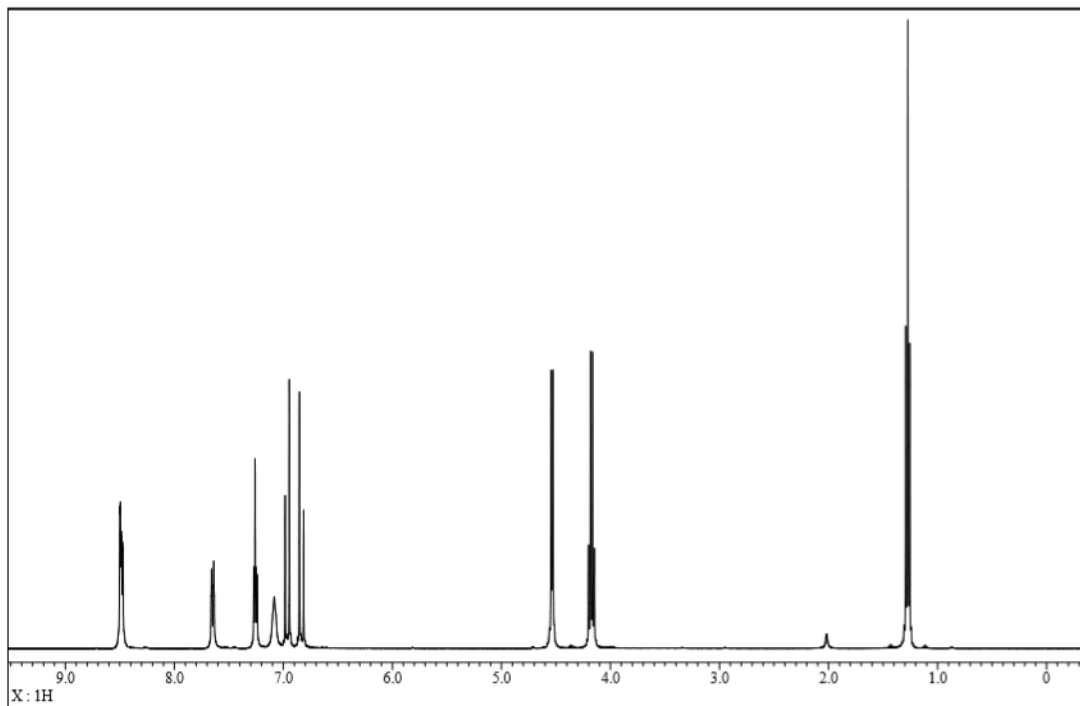


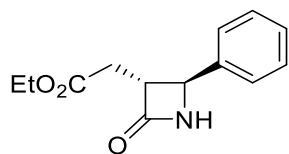
**Ethyl (*E*)-4-oxo-4-[(thiophen-2-ylmethyl)amino]but-2-enoate (4o)**



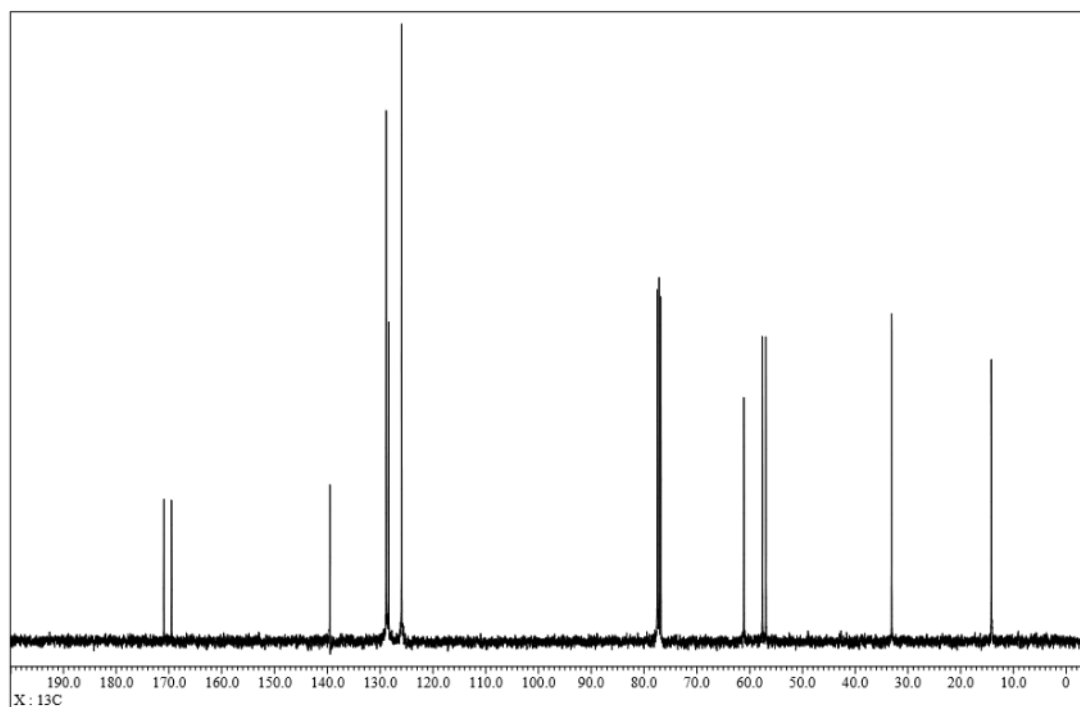
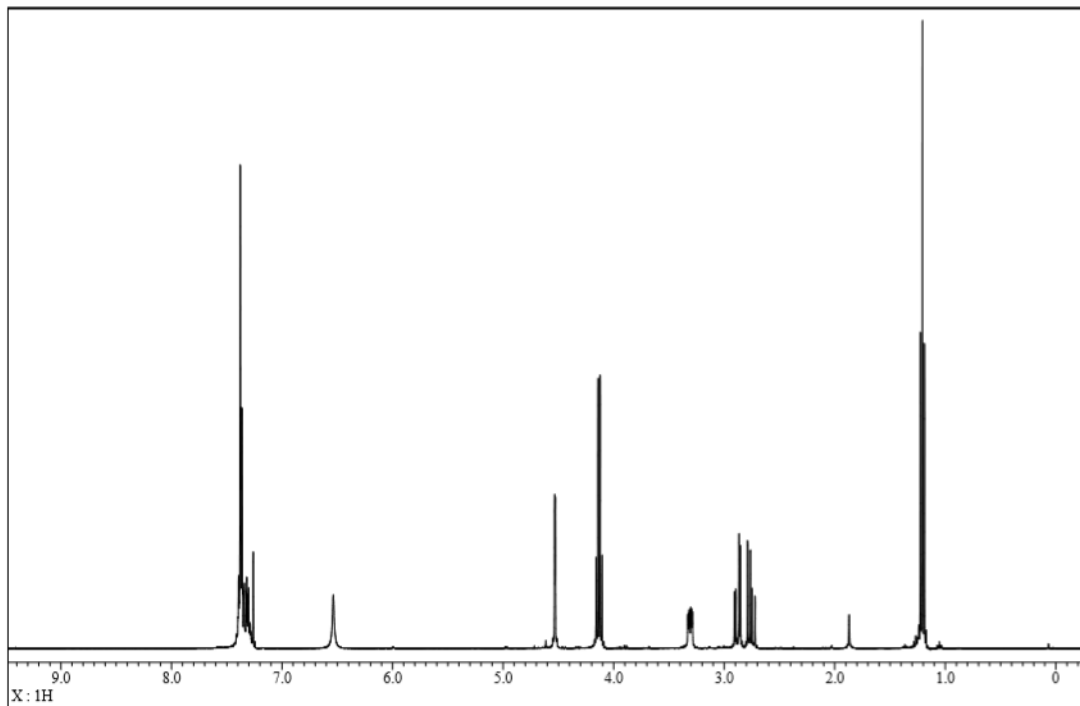


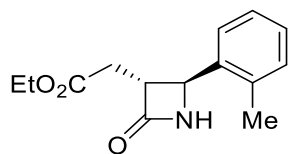
**Ethyl (*E*)-4-oxo-4-[(pyridin-3-ylmethyl)amino]but-2-enoate (4p)**



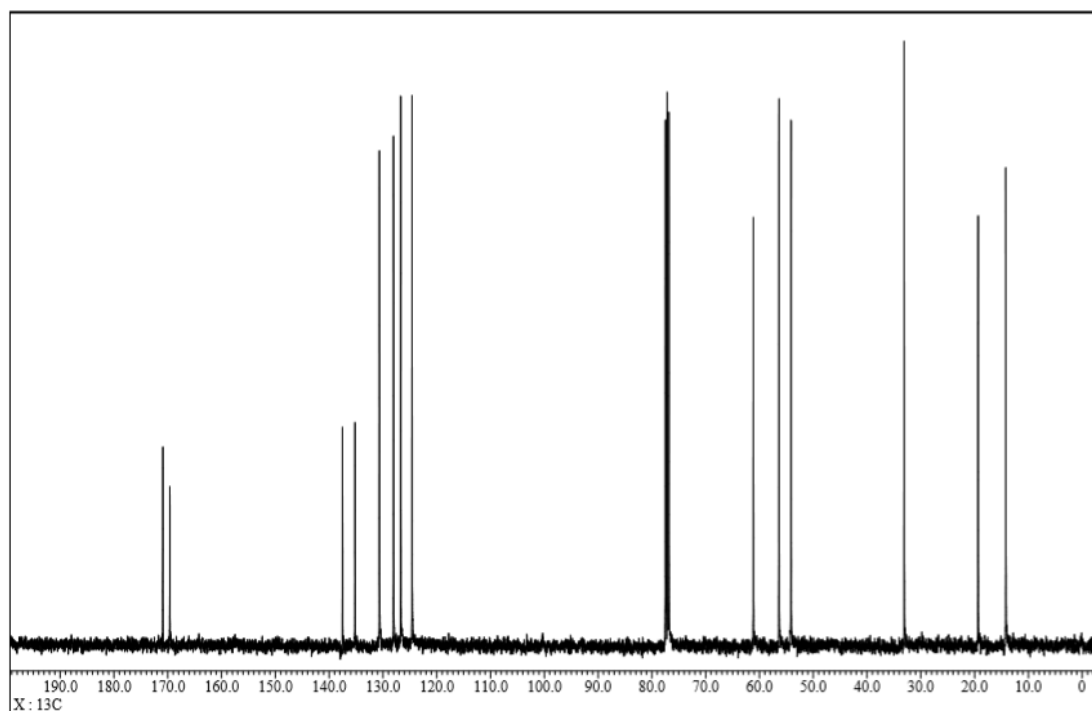
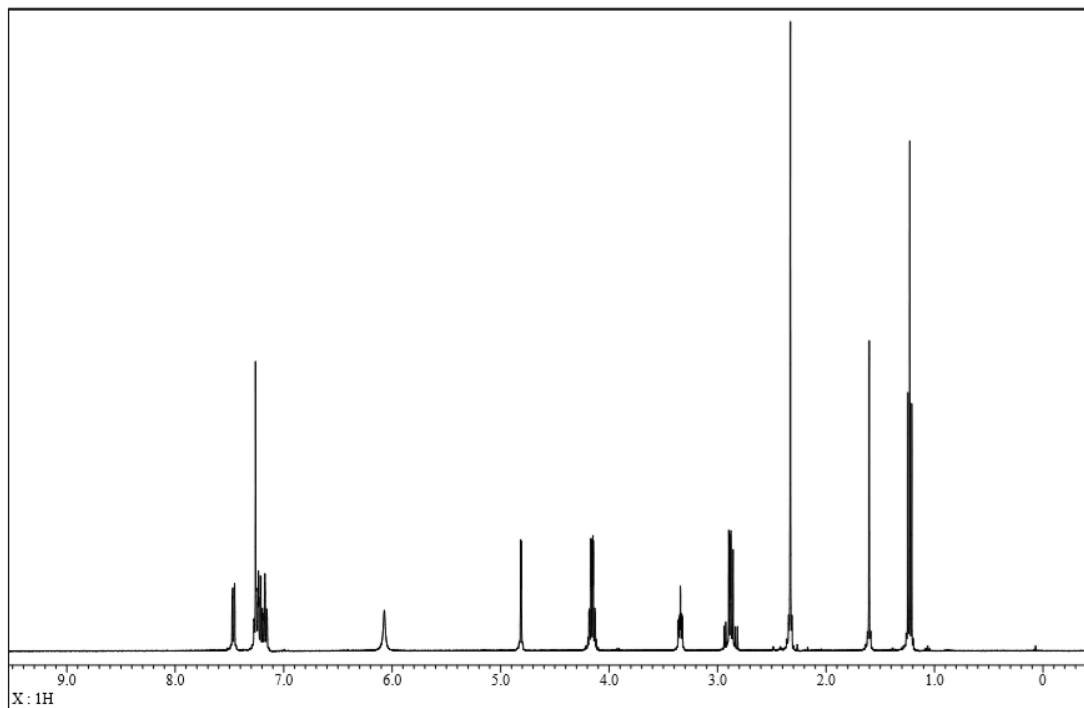


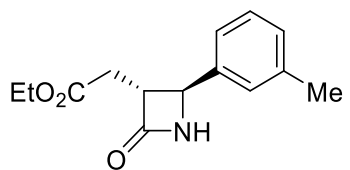
**Ethyl 2-((3*R*\*,4*S*\*)-2-oxo-4-phenylazetidin-3-yl)acetate (5a)**



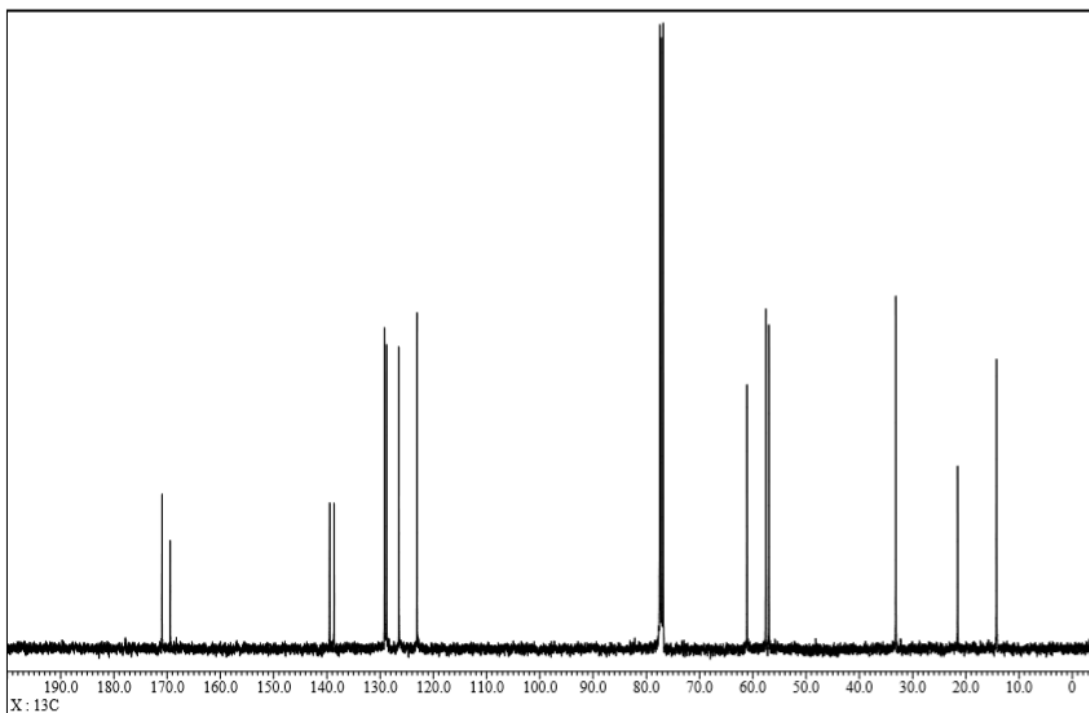
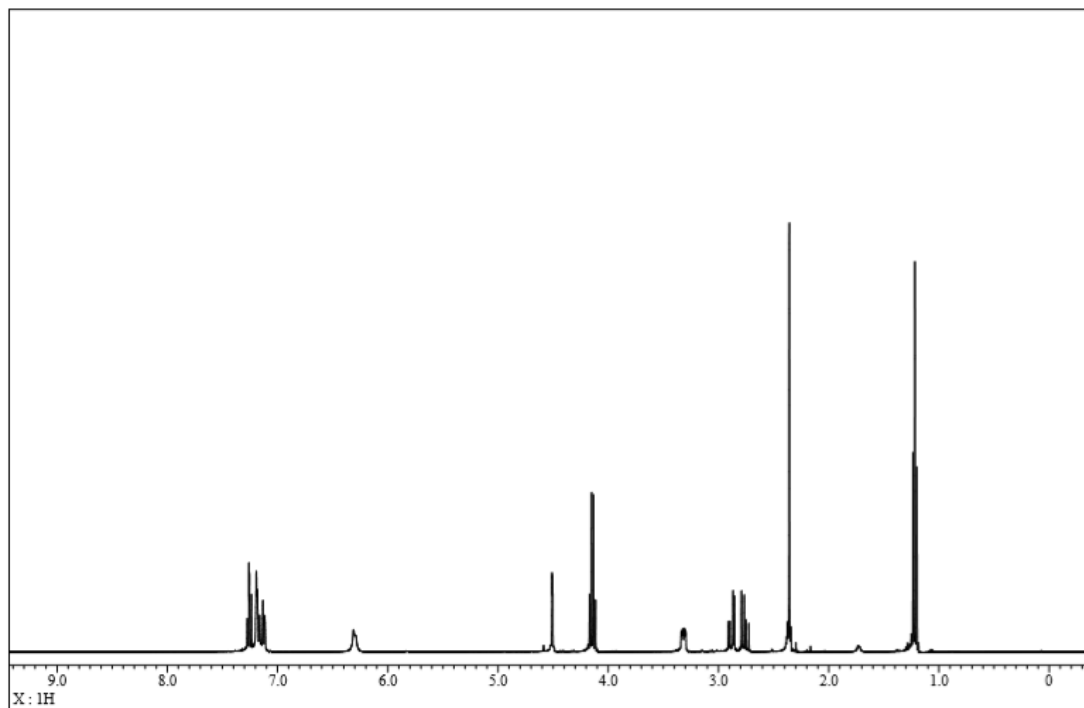


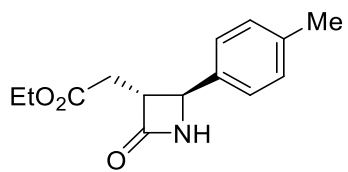
**Ethyl 2-((3*R*\*,4*S*\*)-2-oxo-4-(2-tolyl)azetidin-3-yl)acetate (5b)**



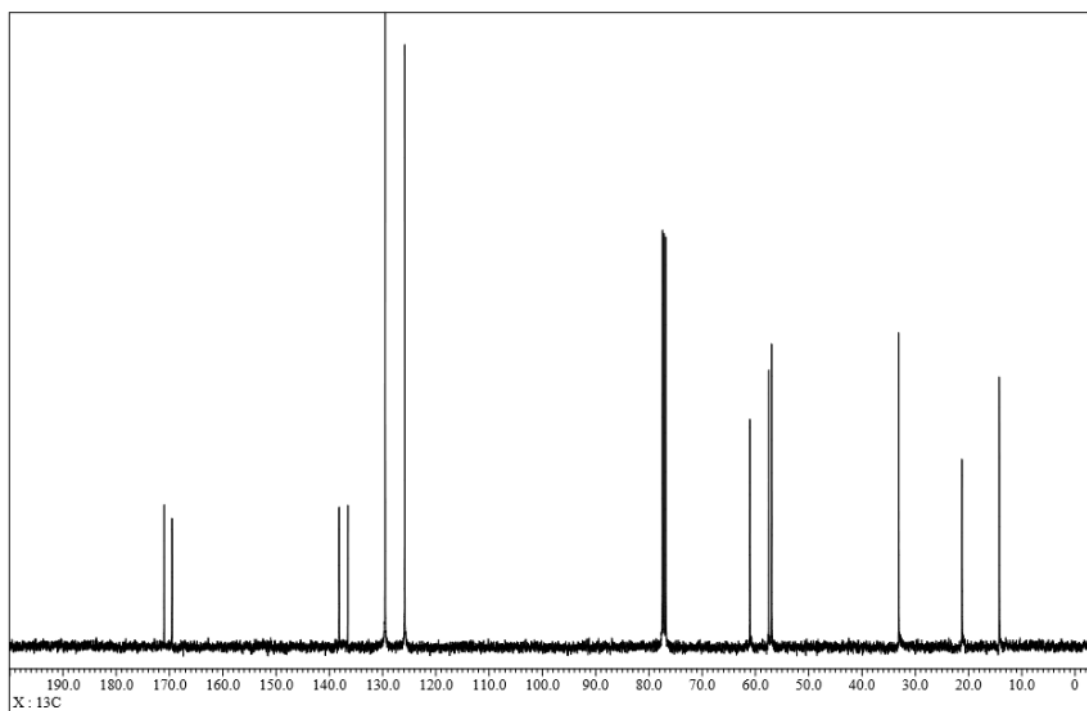
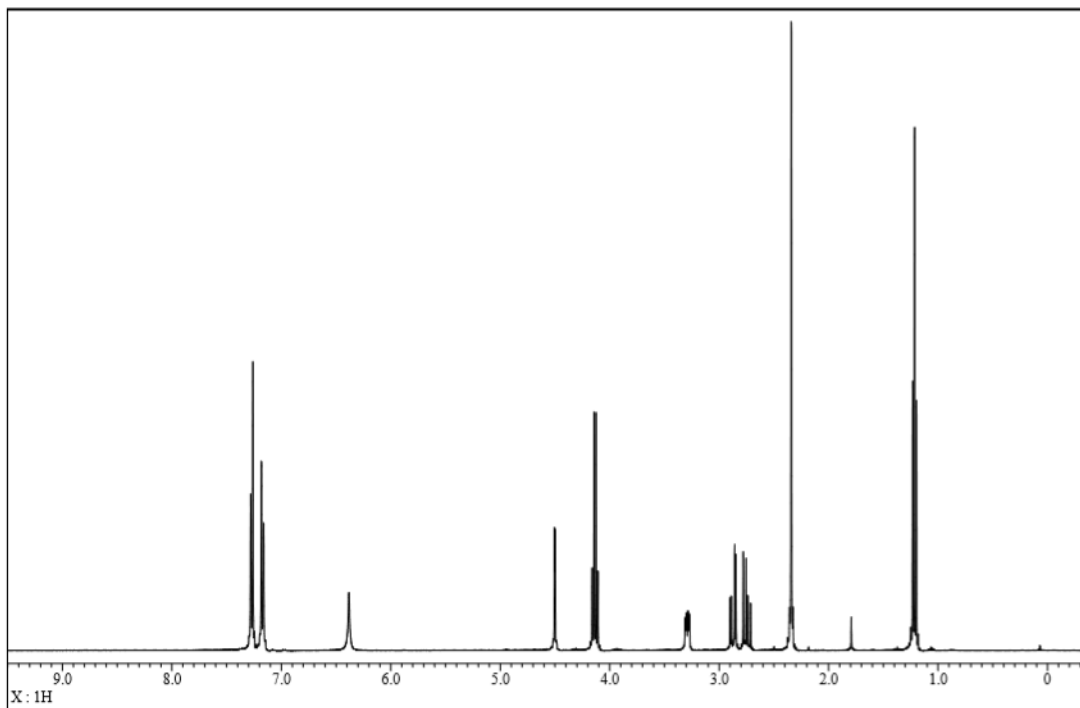


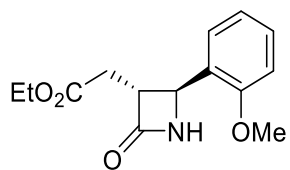
**Ethyl 2-((3*R*\*,4*S*\*)-2-oxo-4-(3-tolyl)azetidin-3-yl)acetate (5c)**



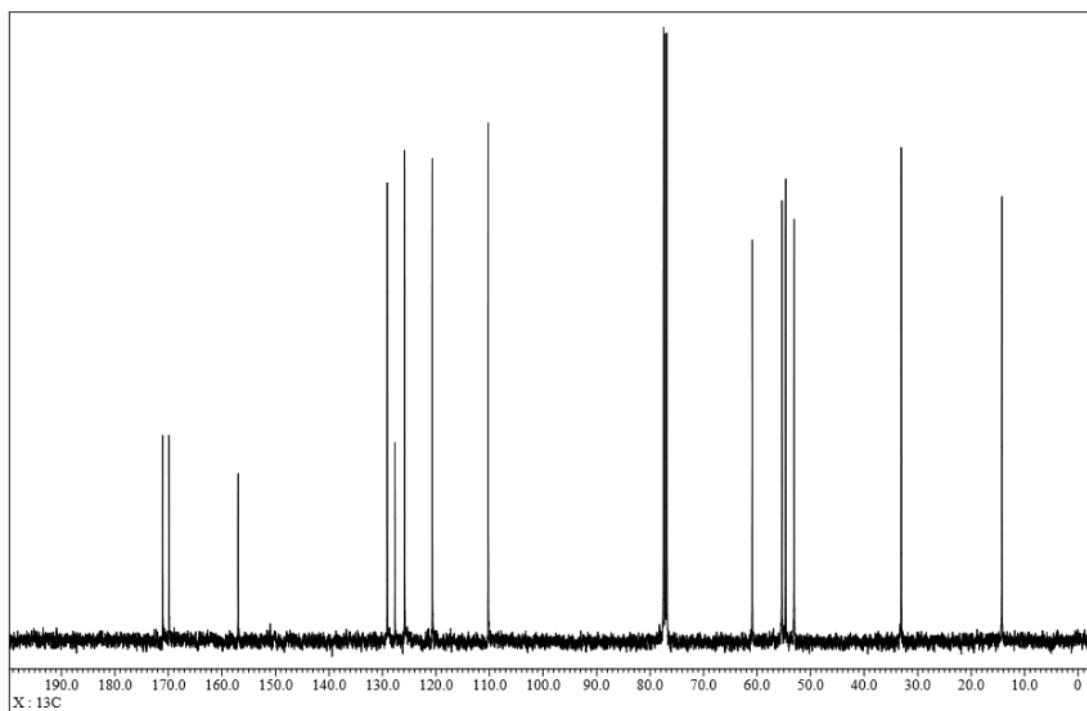
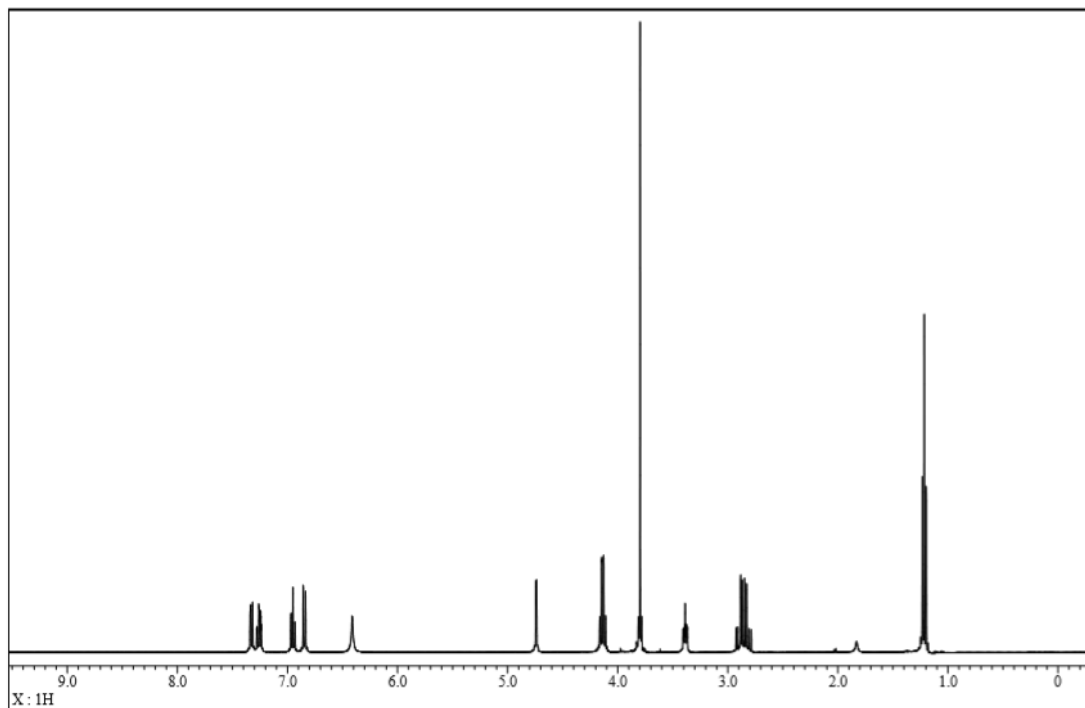


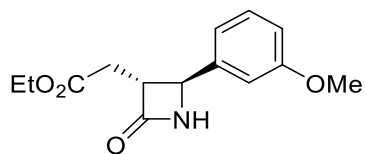
**Ethyl 2-((3*R*\*,4*S*\*)-2-oxo-4-(4-tolyl)azetidin-3-yl)acetate (5d)**



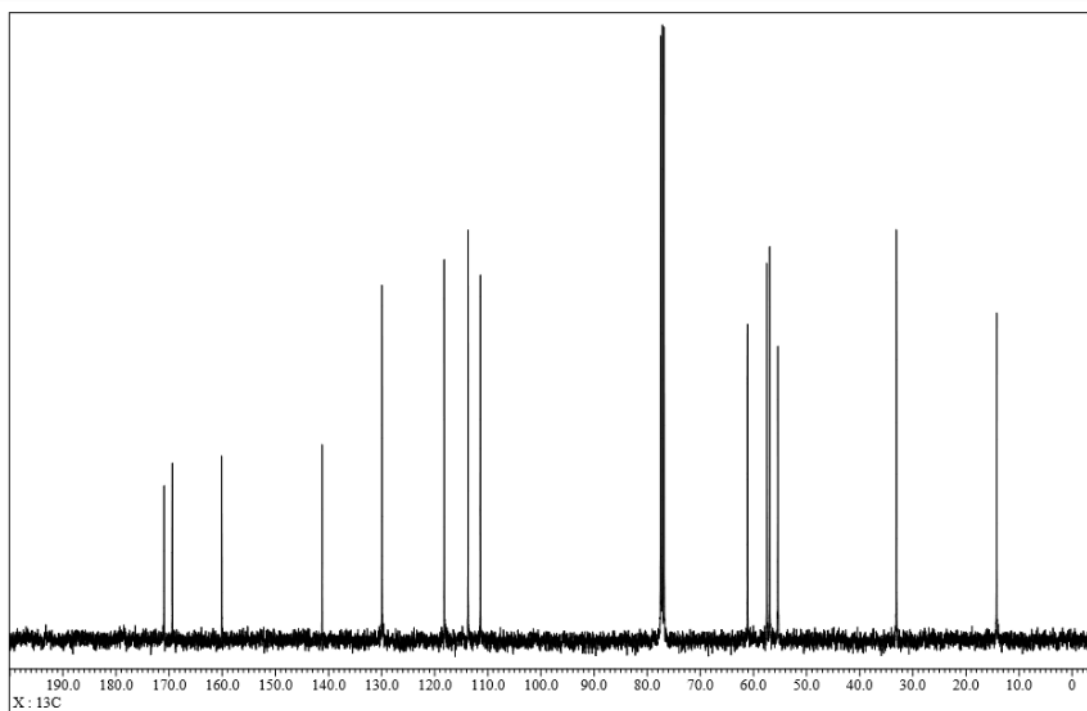
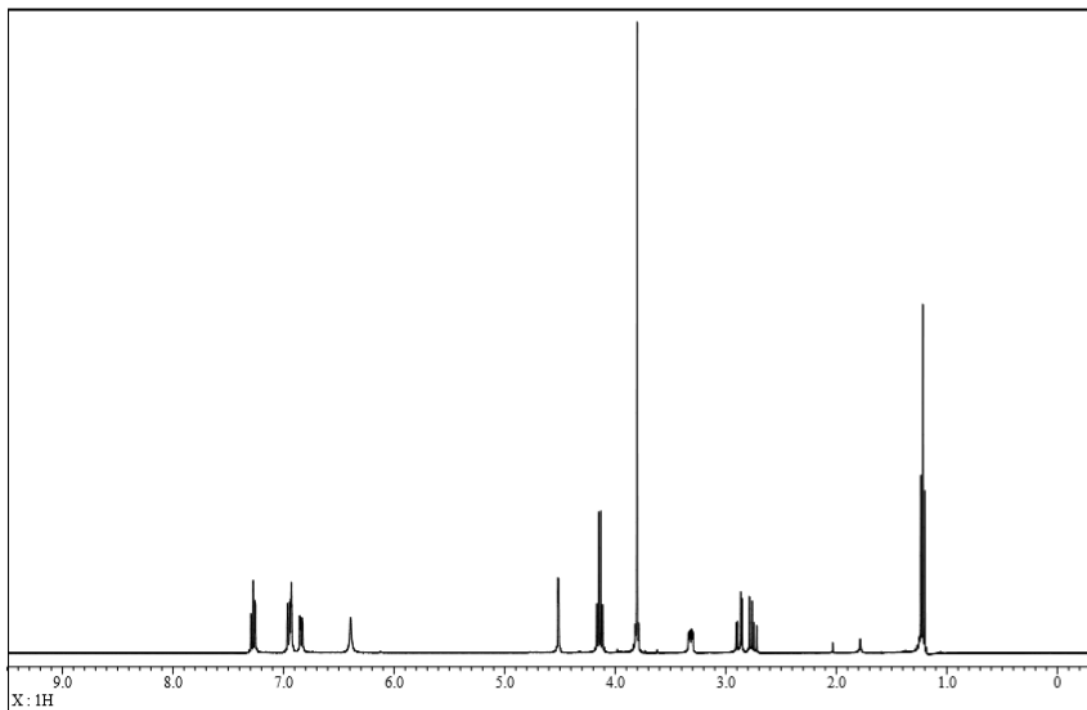


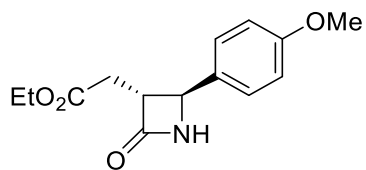
**Ethyl 2-((3*R*\*,4*S*\*)-2-(2-methoxyphenyl)-4-oxoazetidin-3-yl)acetate (5e)**



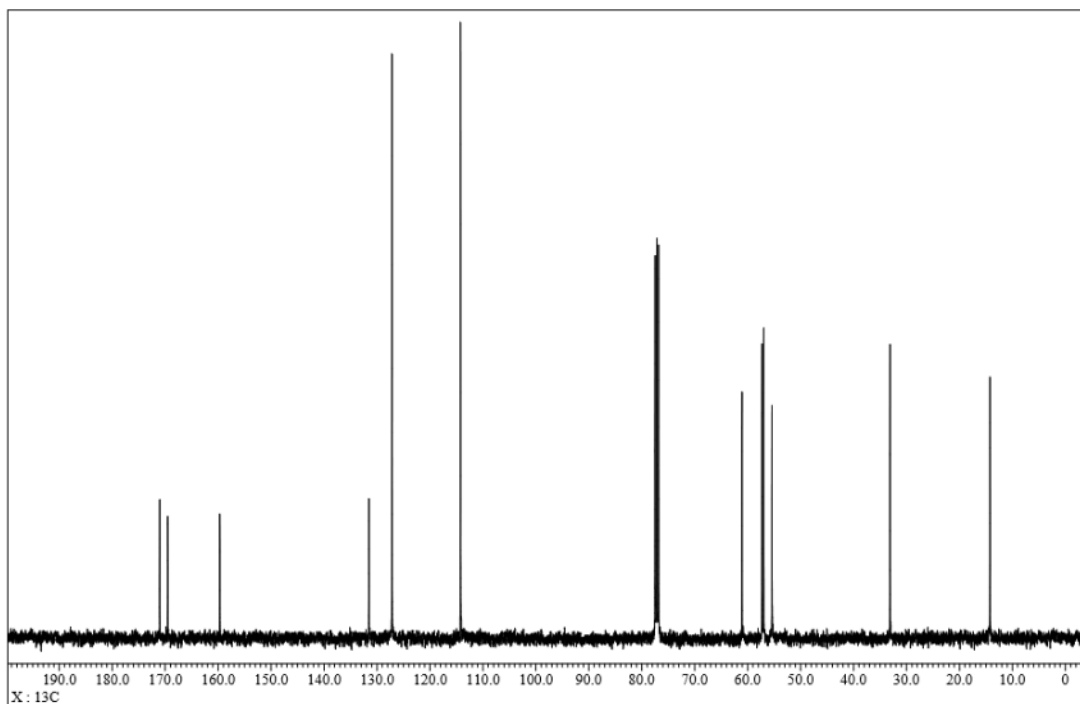
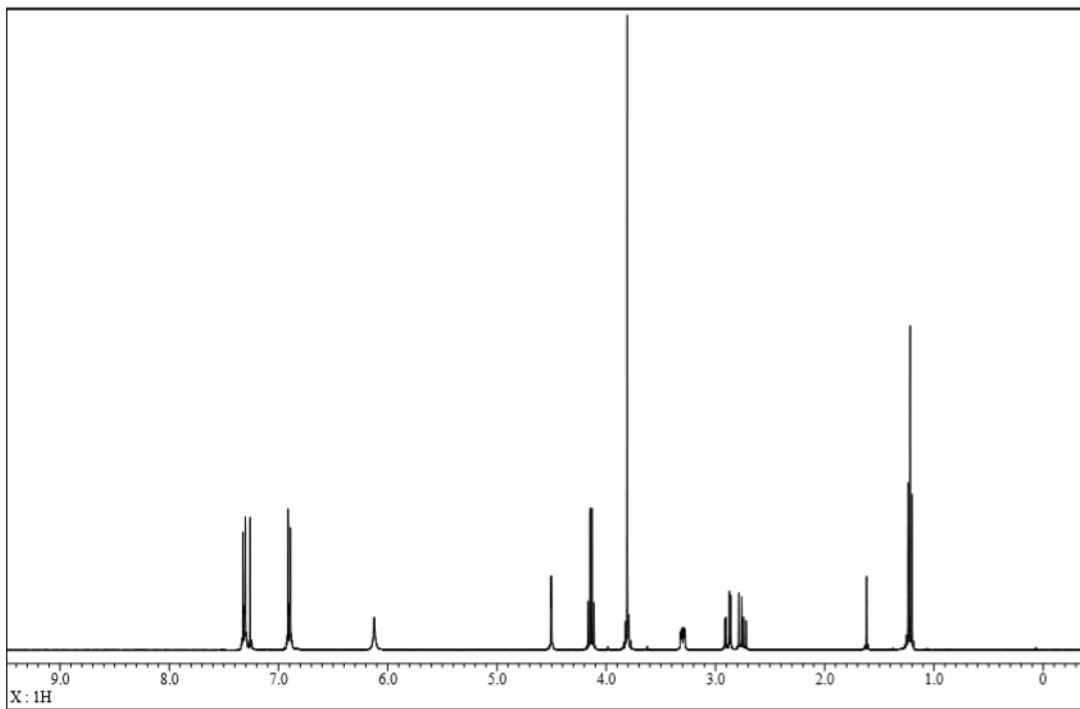


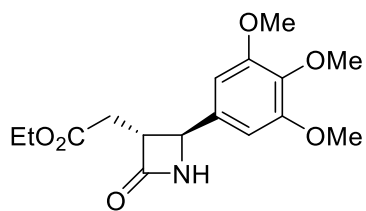
**Ethyl 2-((3*R*\*,4*S*\*)-2-(3-methoxyphenyl)-4-oxoazetidin-3-yl)acetate (5f)**



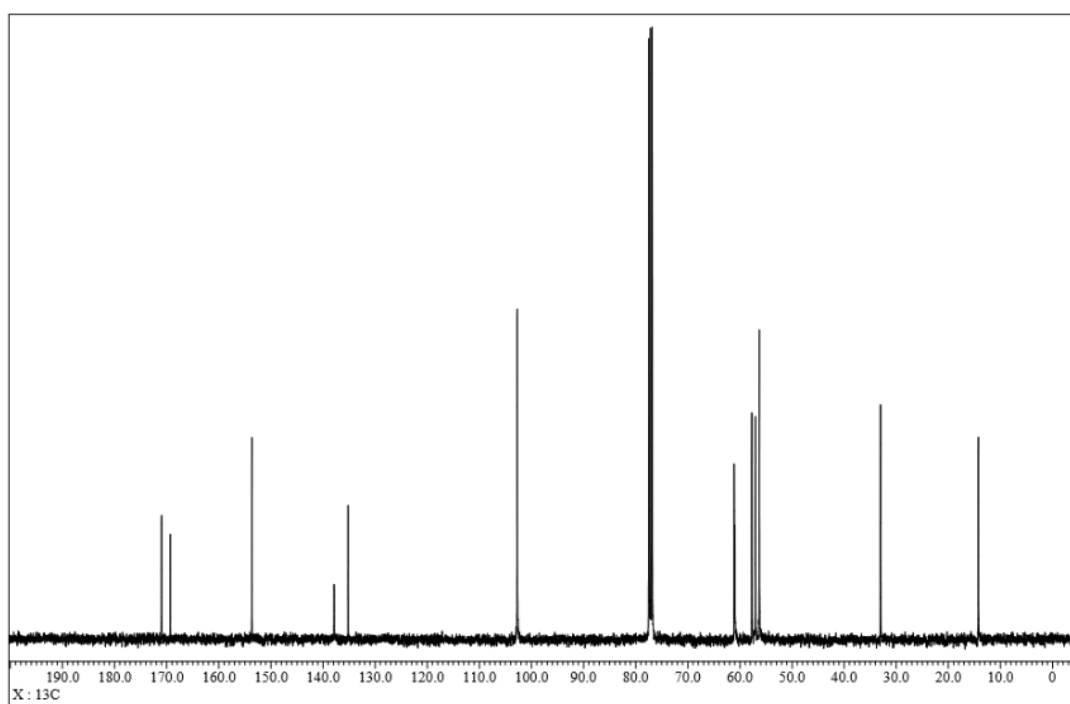
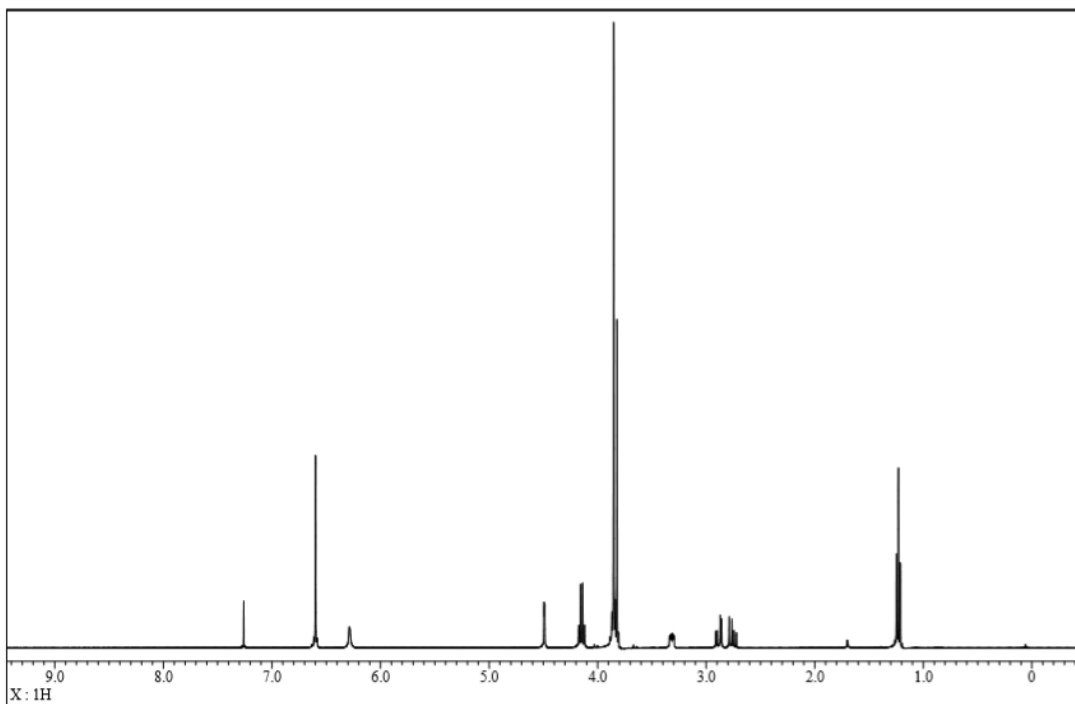


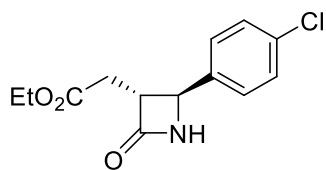
**Ethyl 2-((3*R*\*,4*S*\*)-2-(4-methoxyphenyl)-4-oxoazetidin-3-yl)acetate (5g)**



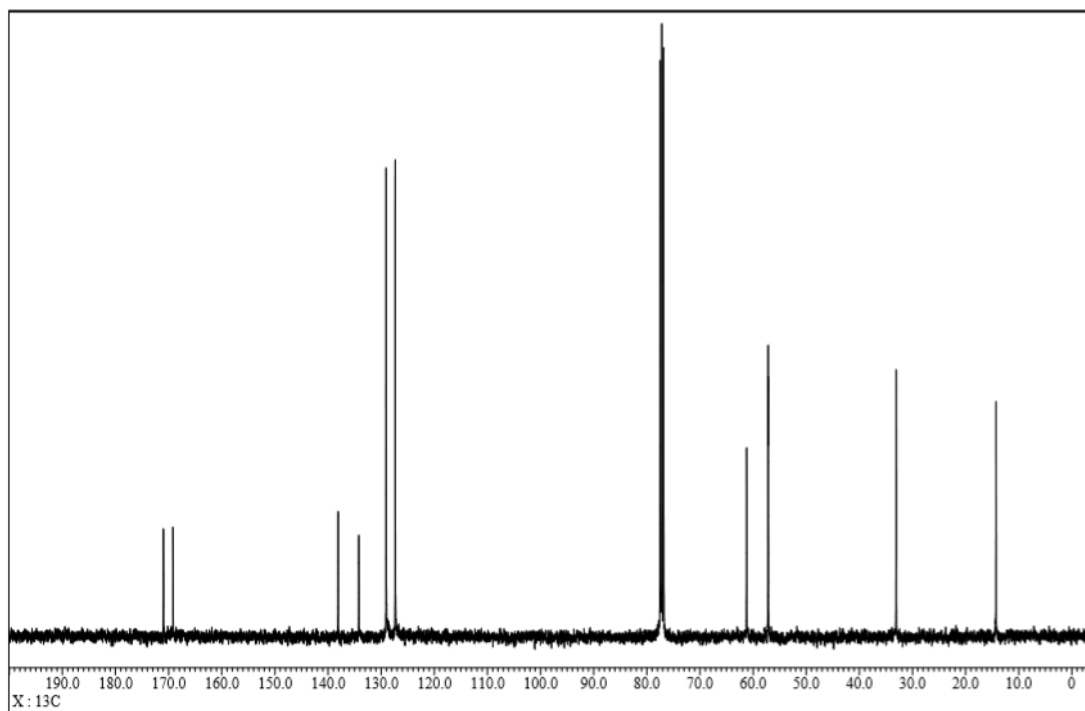
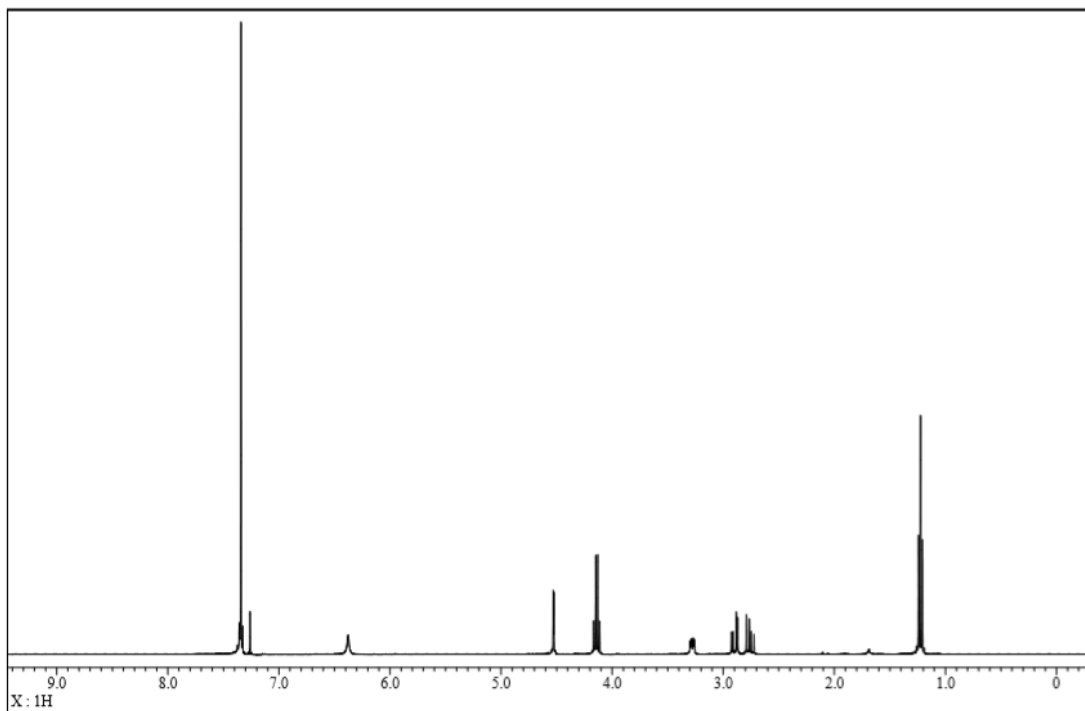


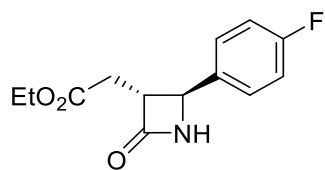
**Ethyl 2-((3*R*\*,4*S*\*)-2-oxo-4-(3,4,5-trimethoxyphenyl)azetidin-3-yl)acetate (5h)**



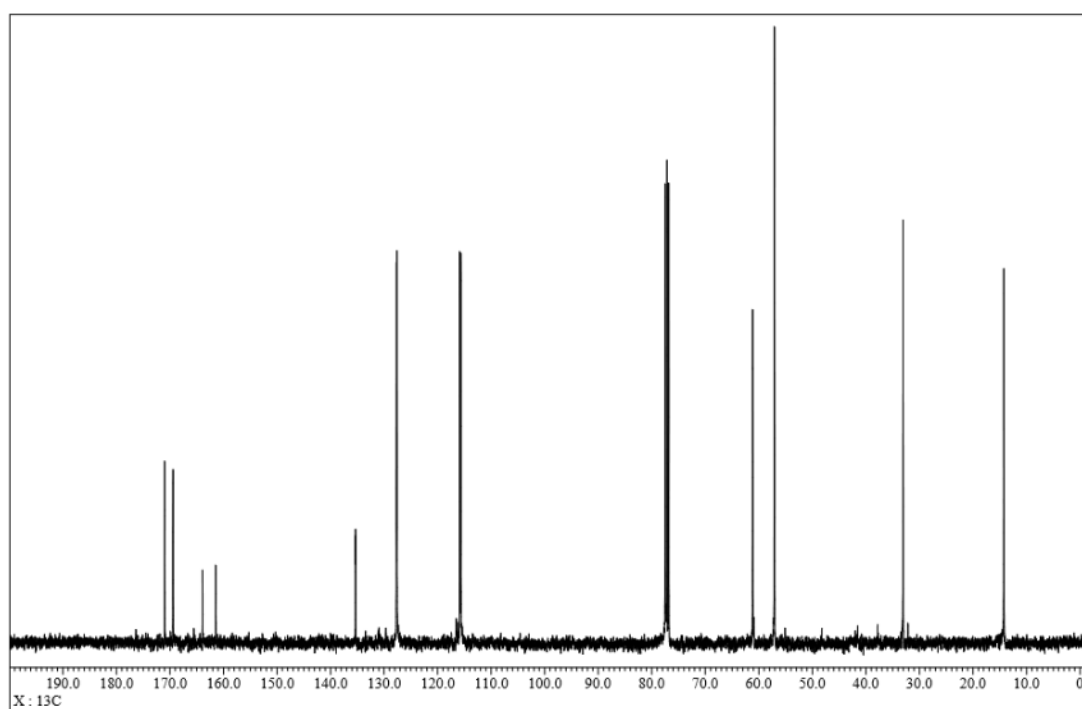
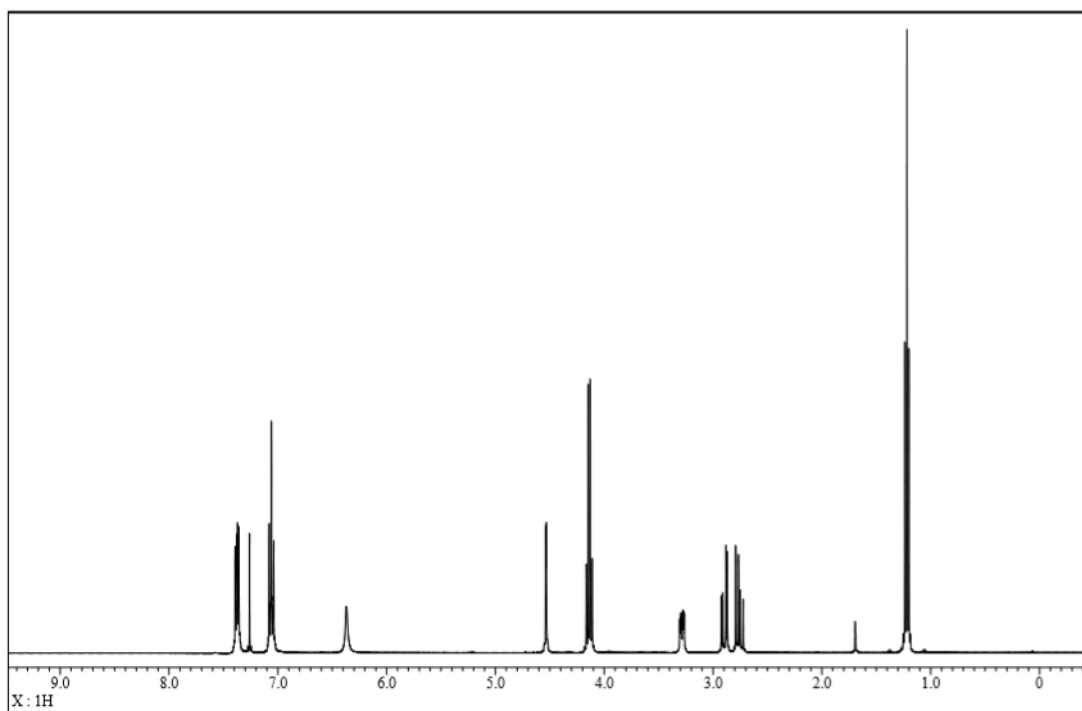


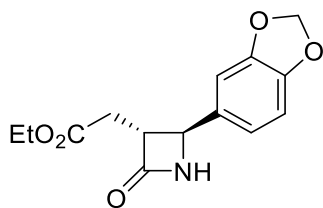
**Ethyl 2-((3*R*\*,4*S*\*)-2-(4-chlorophenyl)-4-oxoazetidin-3-yl)acetate (5j)**



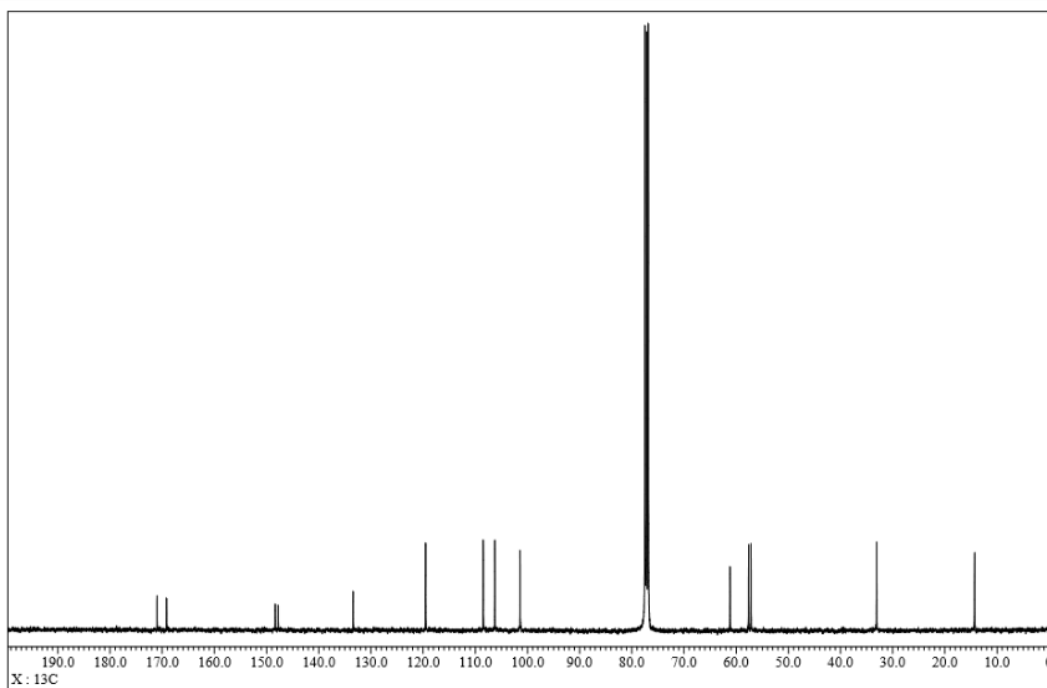
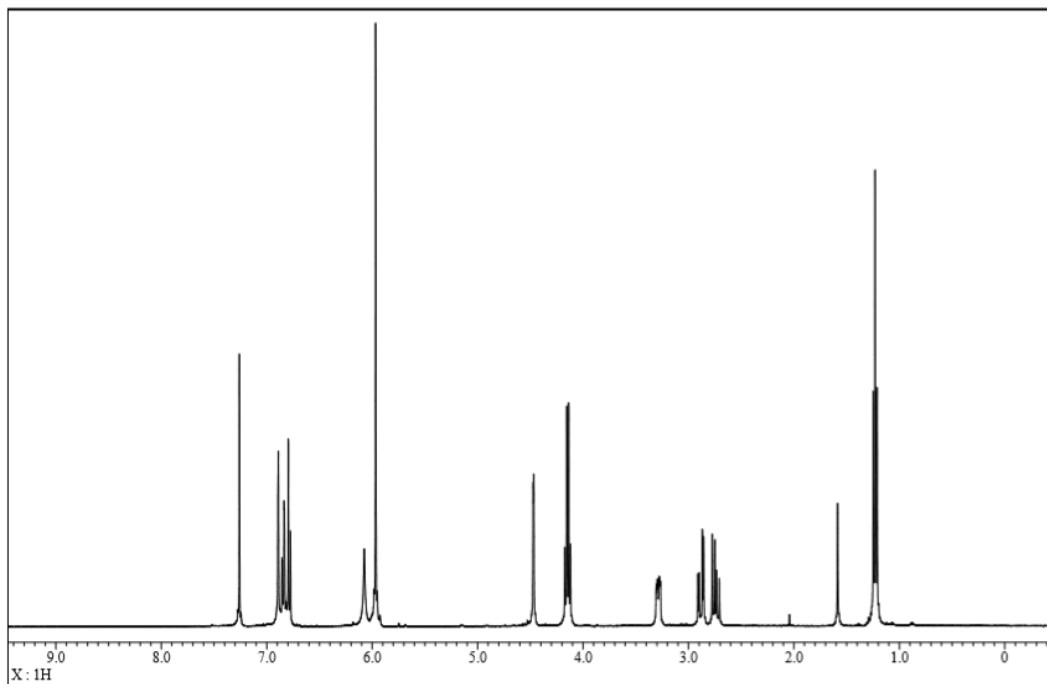


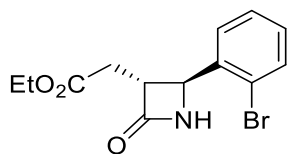
**Ethyl 2-((3*R*\*,4*S*\*)-2-(4-fluorophenyl)-4-oxoazetidin-3-yl)acetate (5k)**



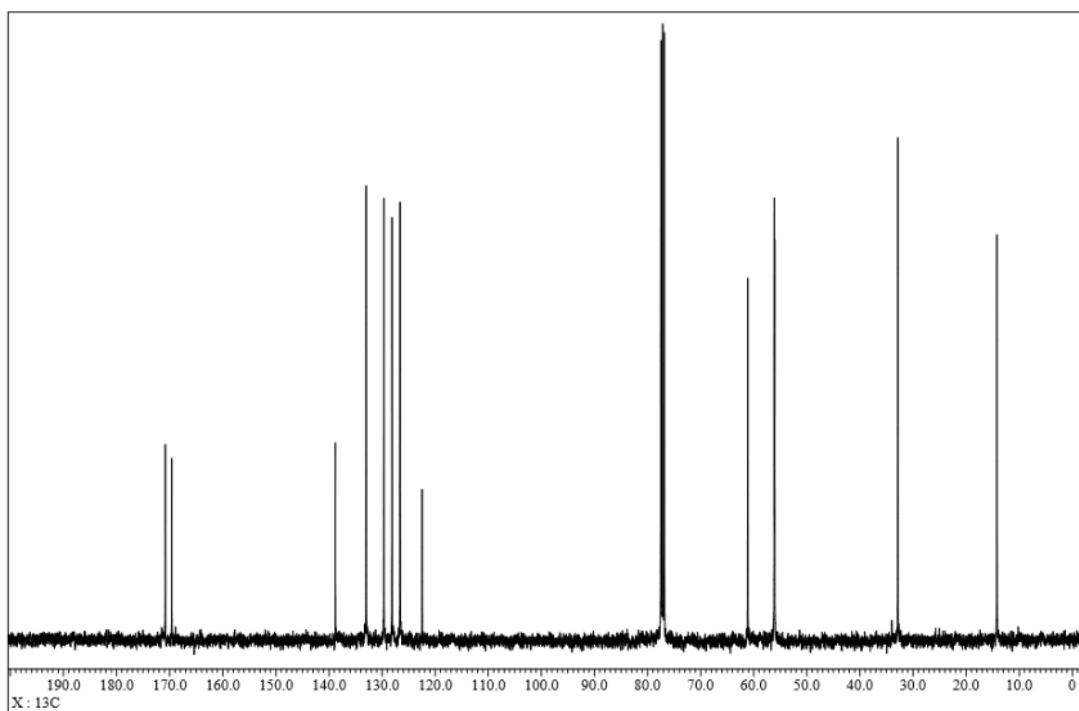
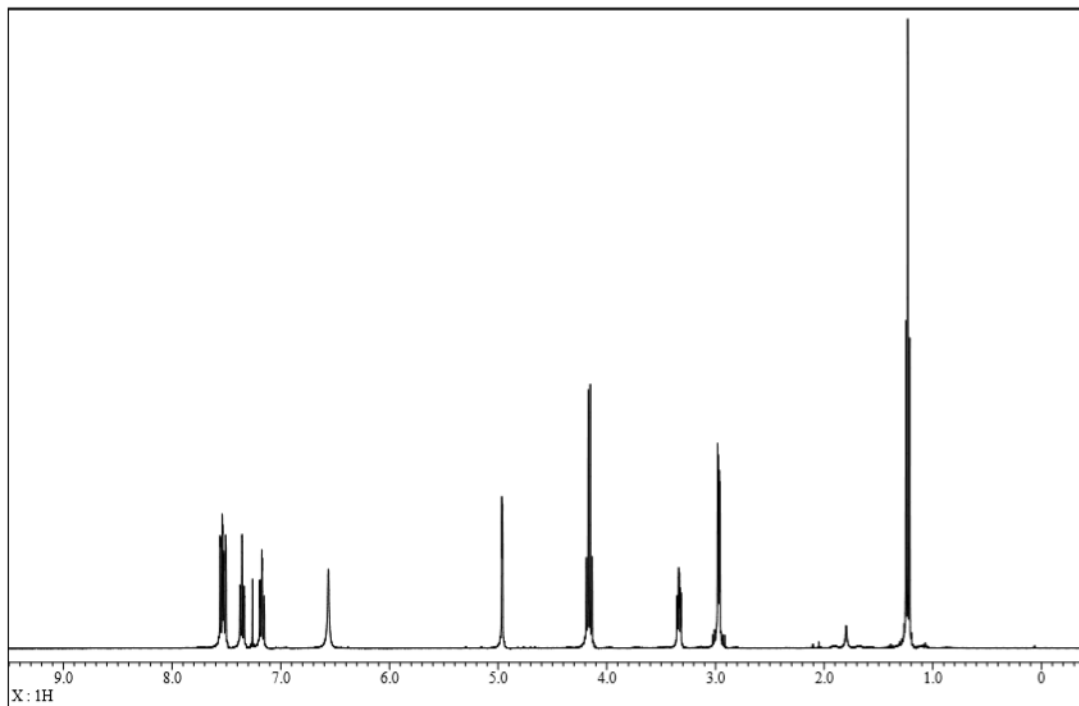


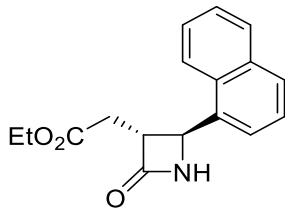
**Ethyl 2-((3*R*\*,4*S*\*)-2-(benzo[d][1,3]dioxol-5-yl)-4-oxoazetidin-3-yl)acetate (5i)**



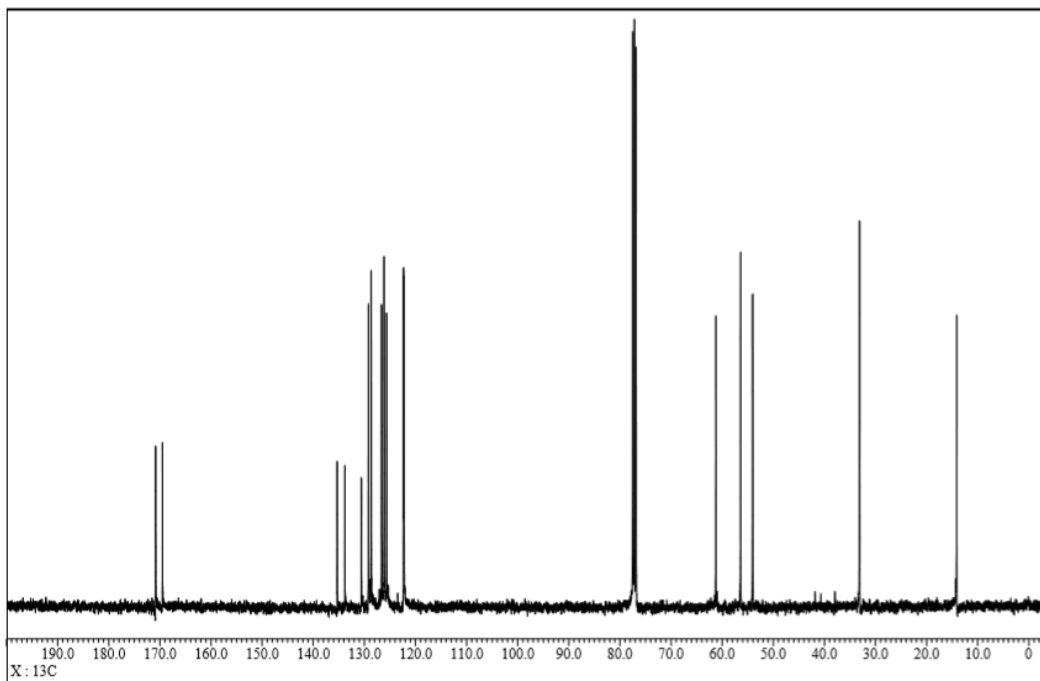
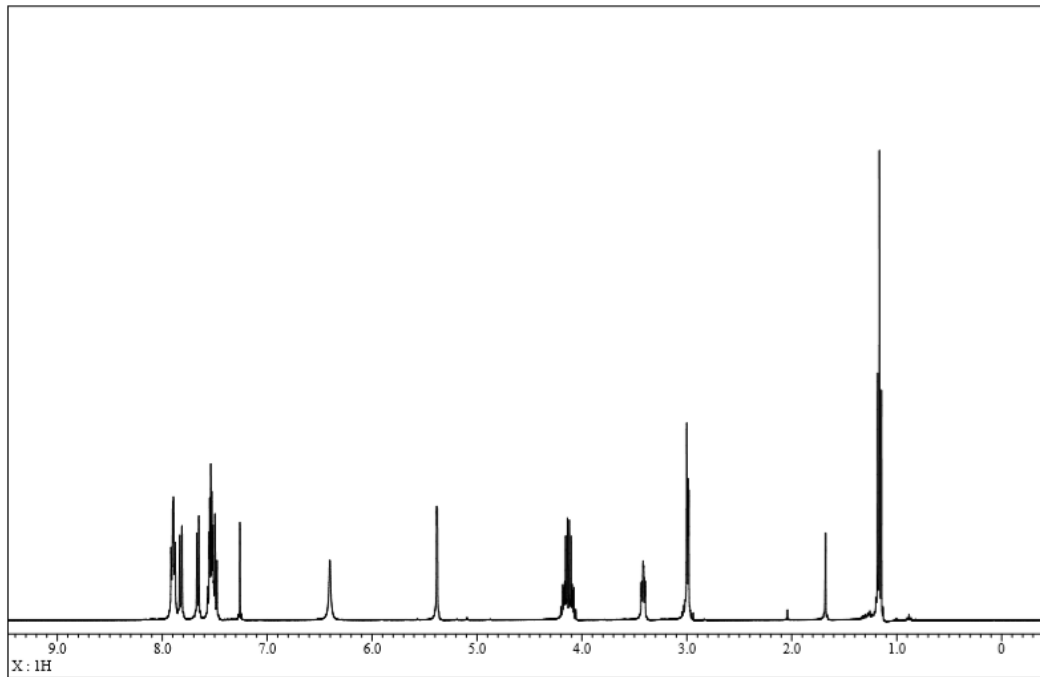


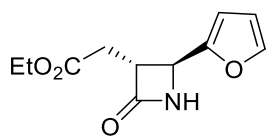
**Ethyl 2-((3*R*\*,4*S*\*)-2-(2-bromophenyl)-4-oxoazetidin-3-yl)acetate (5l)**



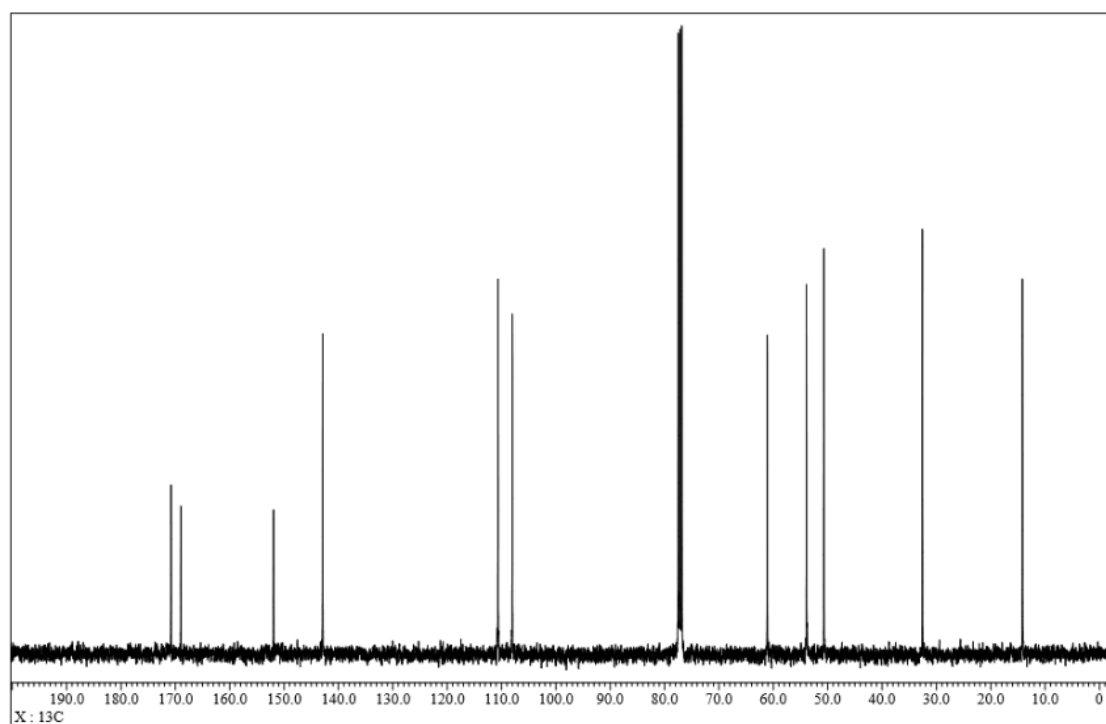
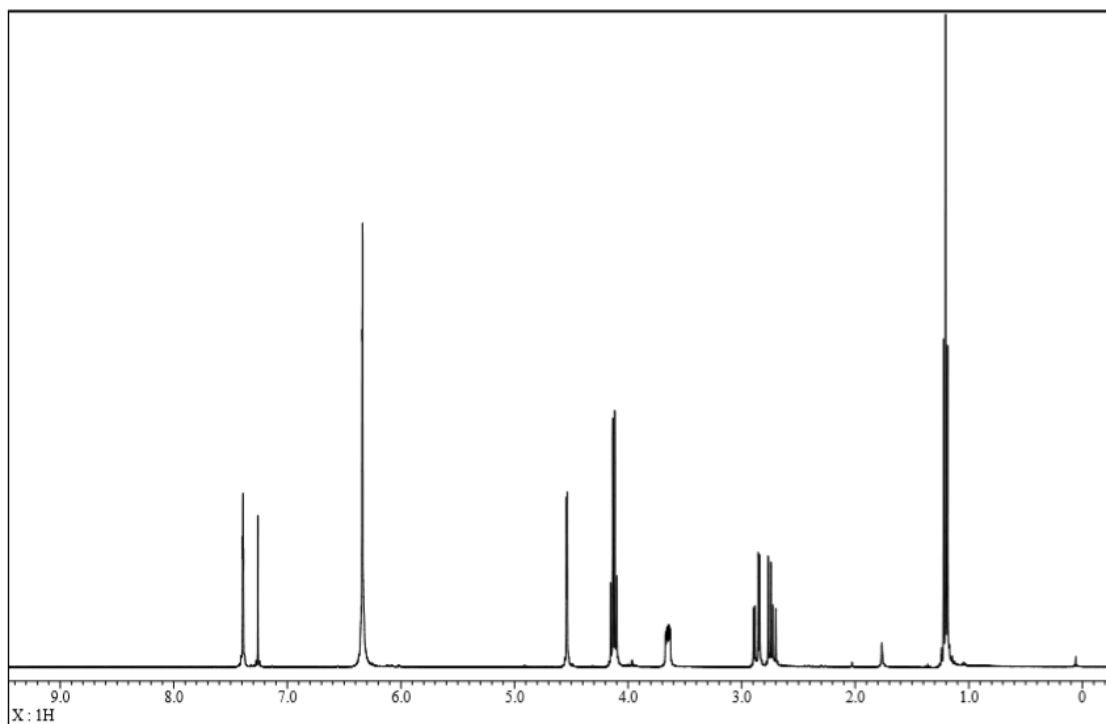


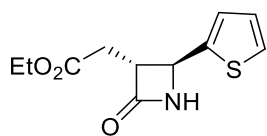
**Ethyl 2-((3*R*\*,4*S*\*)-2-(naphthalen-1-yl)-4-oxoazetidin-3-yl)acetate (5m)**



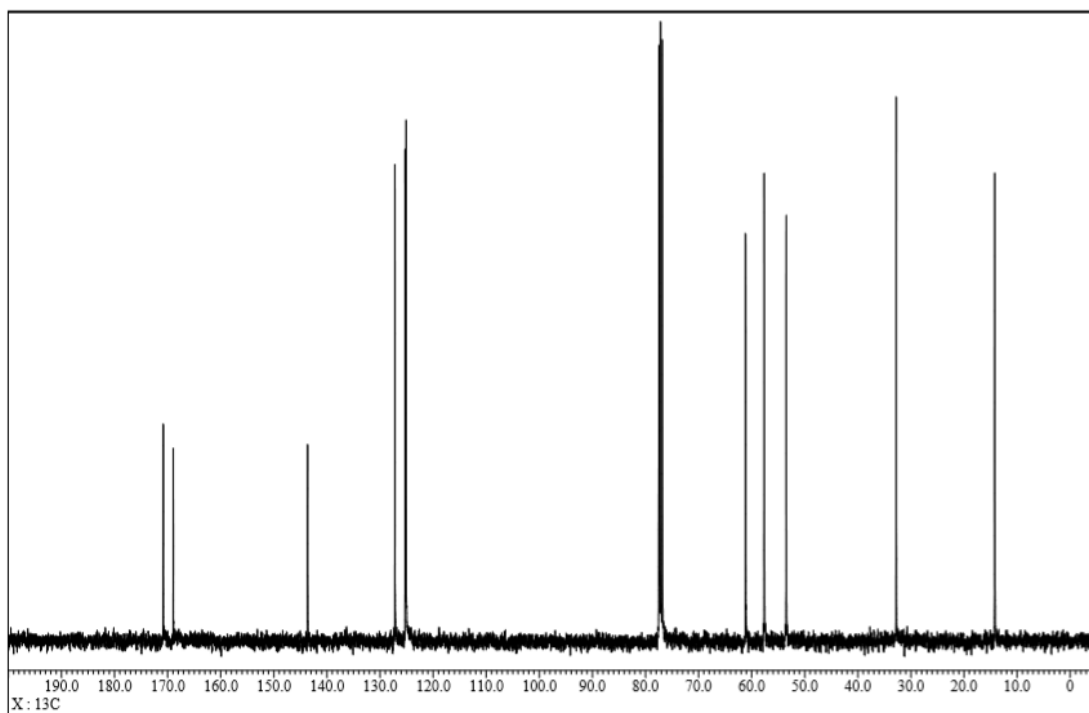
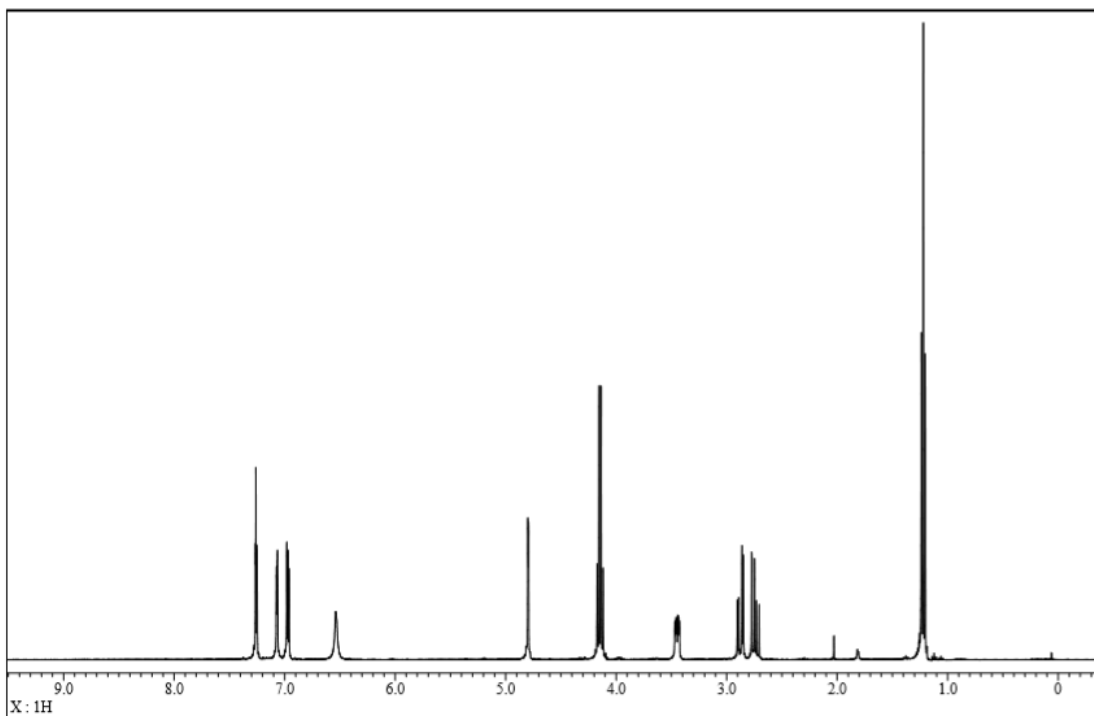


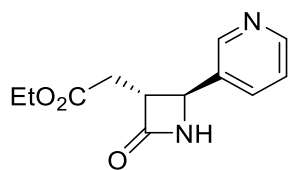
**Ethyl 2-((3*R*\*,4*S*\*)-2-(furan-2-yl)-4-oxoazetidin-3-yl)acetate (5n)**



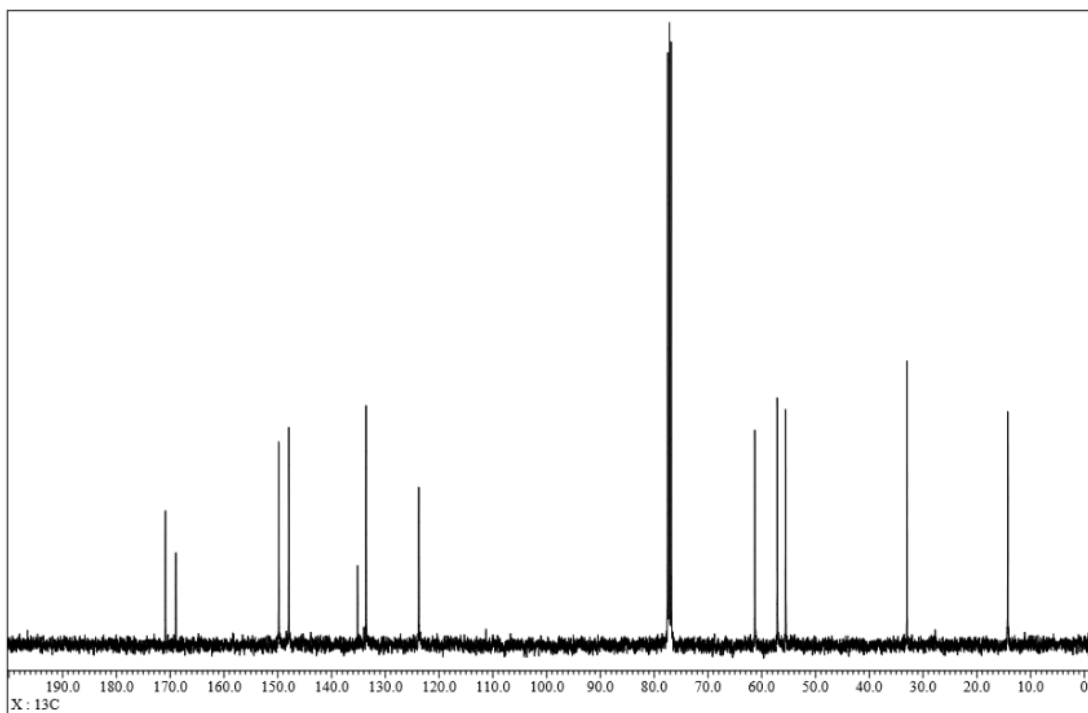
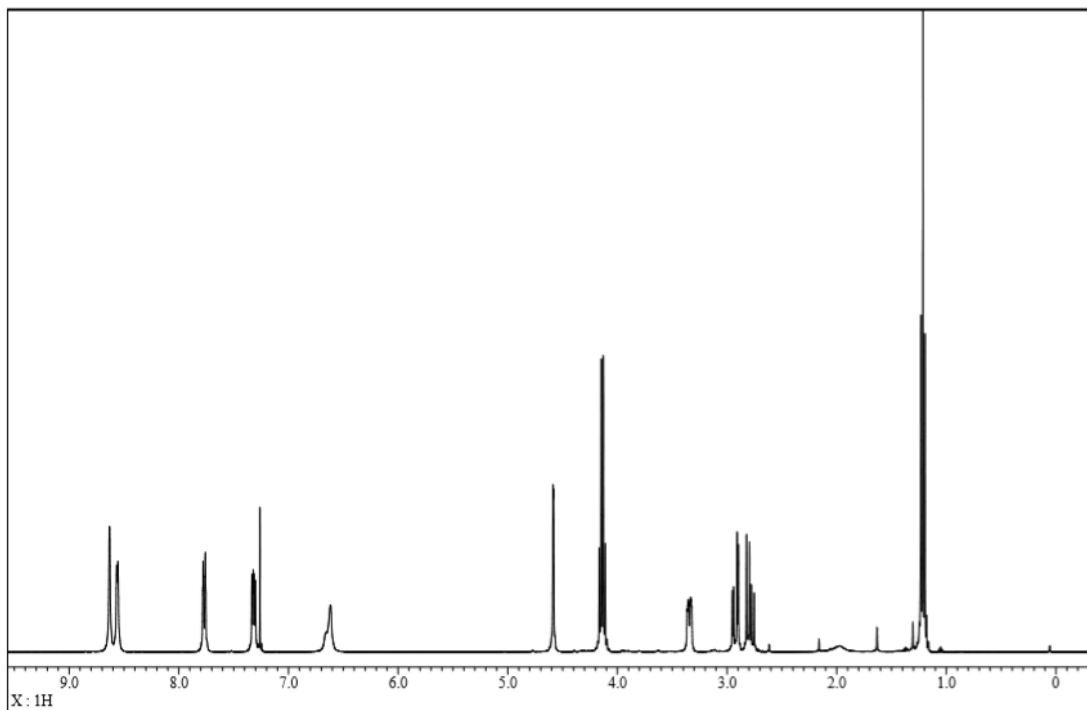


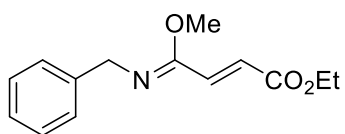
**Ethyl 2-((3*R*\*,4*S*\*)-2-oxo-4-(thiophen-2-yl)azetidin-3-yl)acetate (5o)**



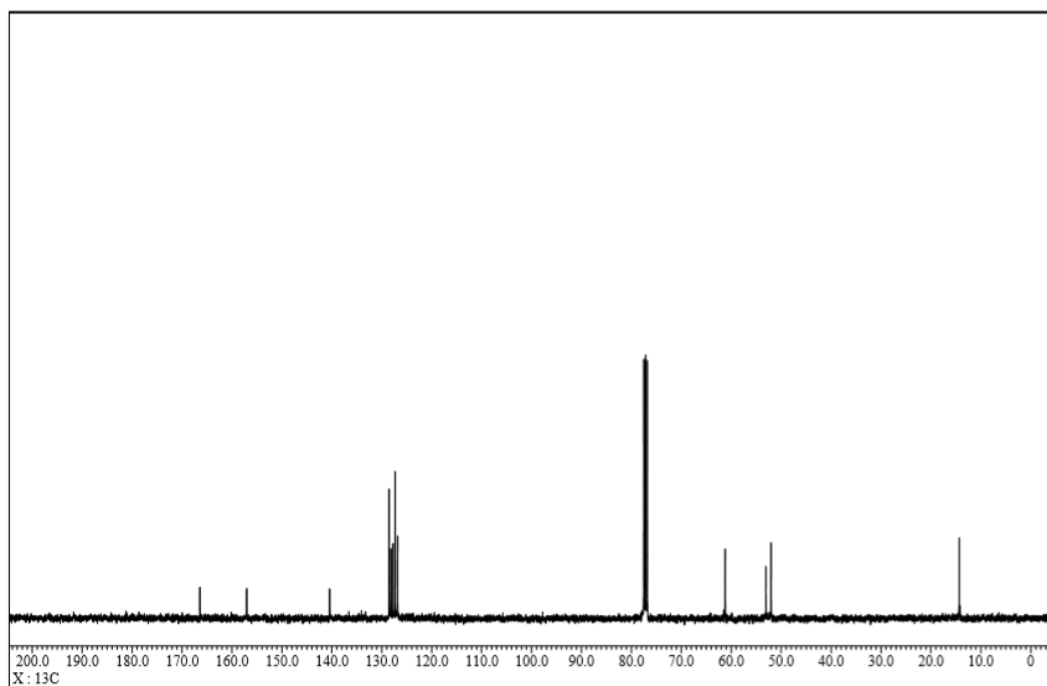
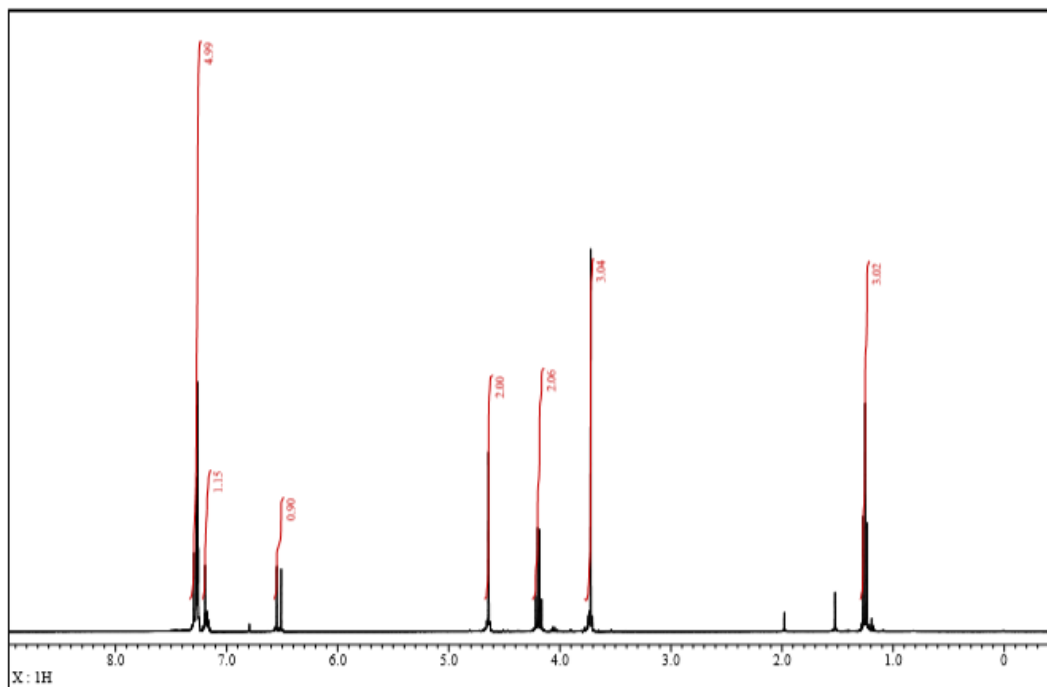


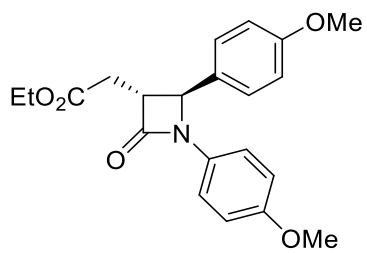
**Ethyl 2-((3*R*\*,4*S*\*)-2-oxo-4-(pyridin-3-yl)azetidin-3-yl)acetate (5p)**



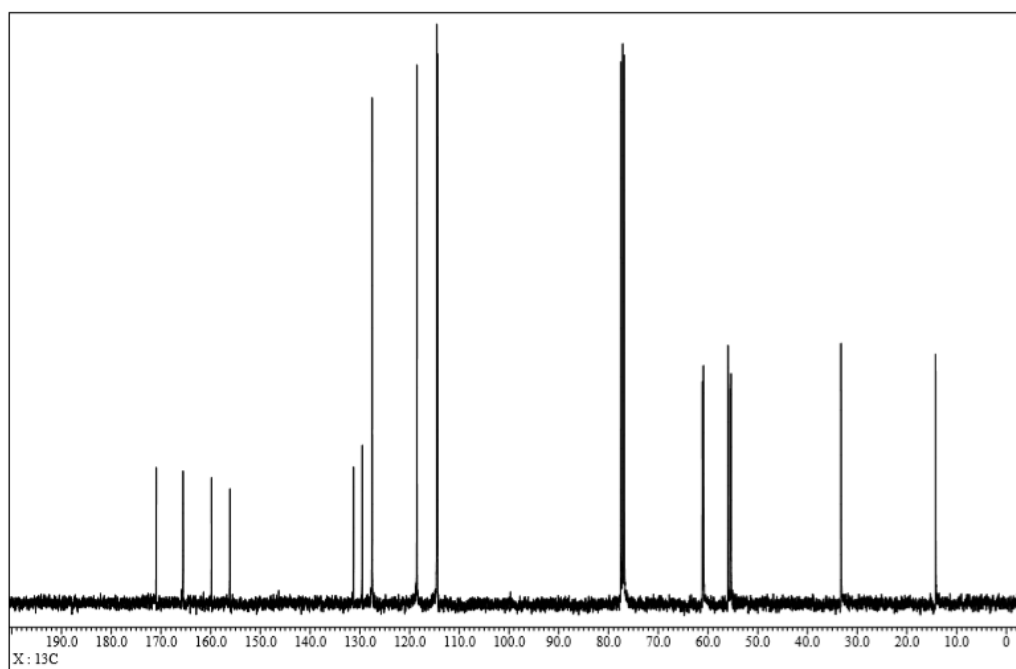
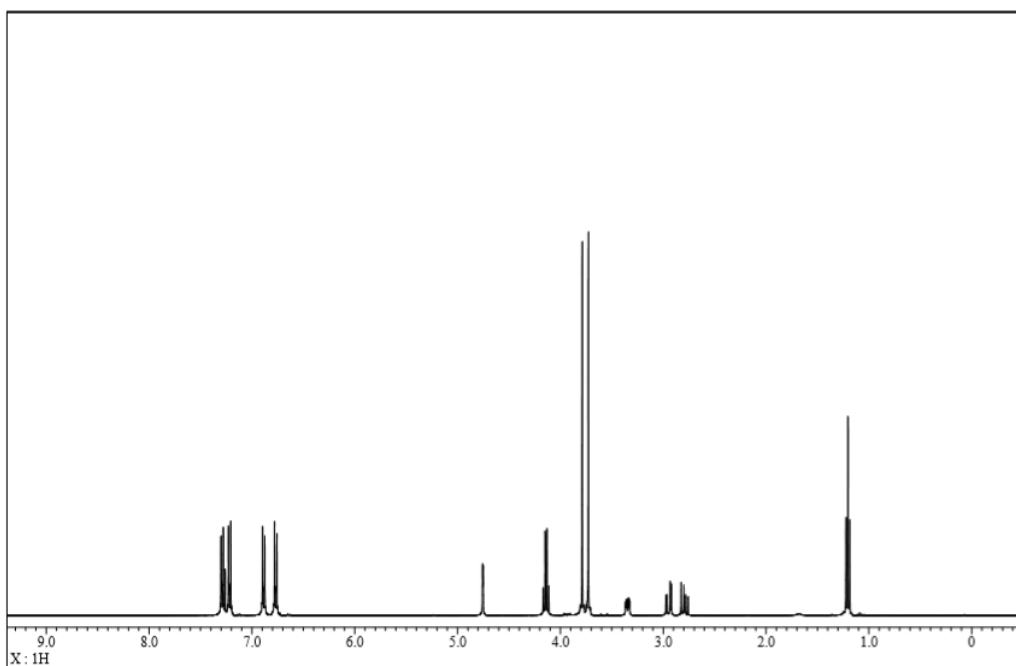


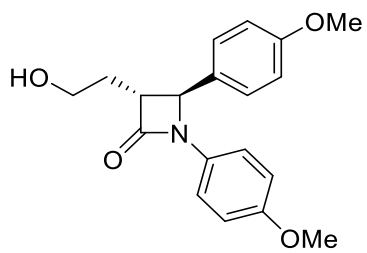
**Ethyl (2*E*,4*Z*)-4-(benzylimino)-4-methoxybut-2-enoate (8')**



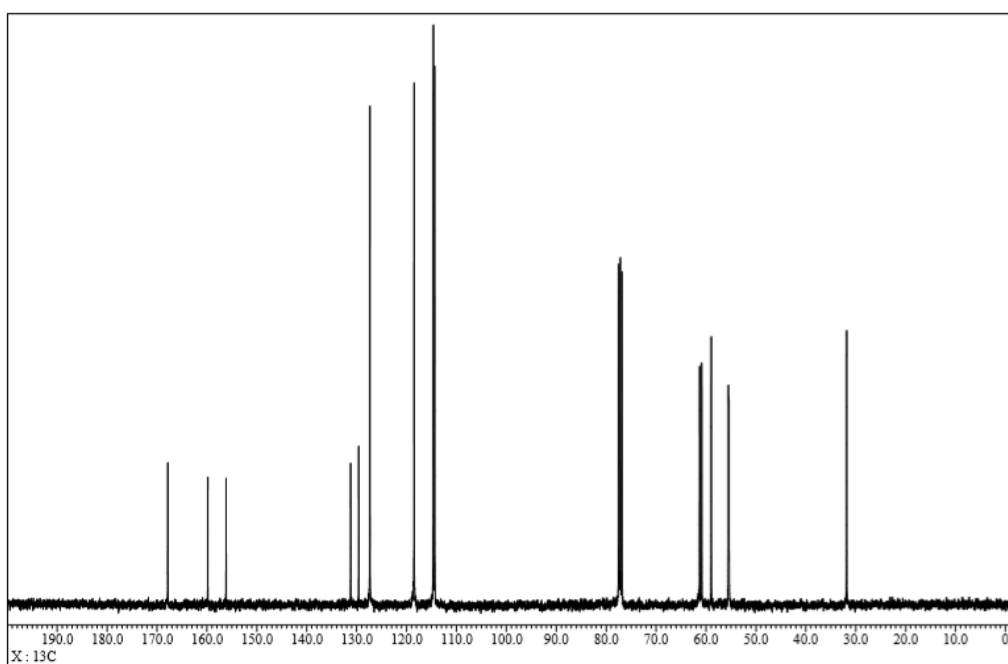
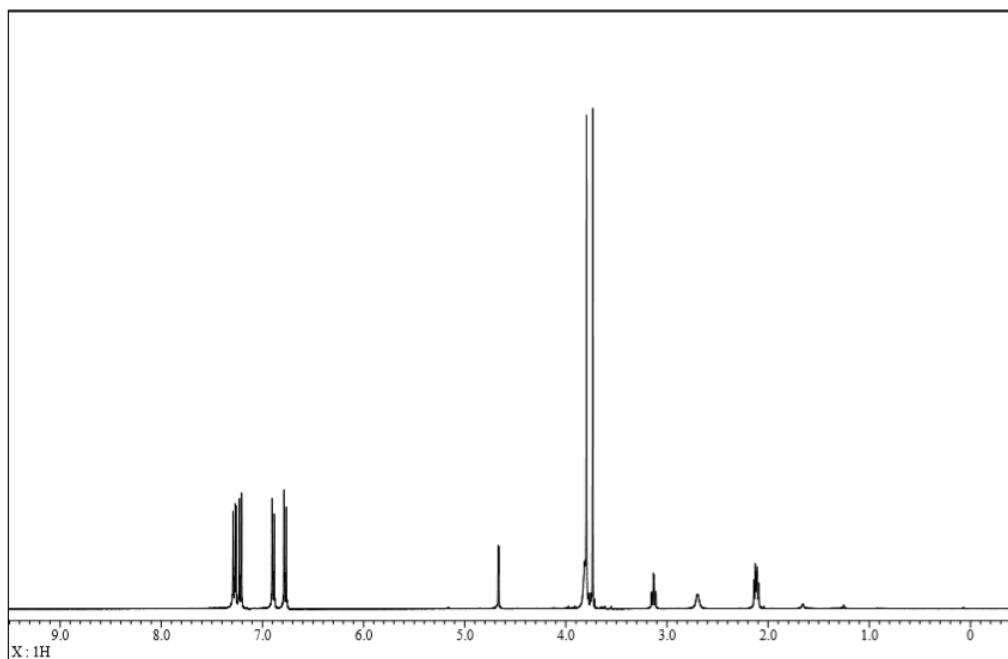


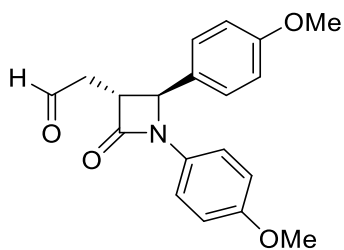
**Ethyl 2-((2*S*\*,3*R*\*)-1,2-bis(4-methoxyphenyl)-4-oxoazetidin-3-yl)acetate (6)**



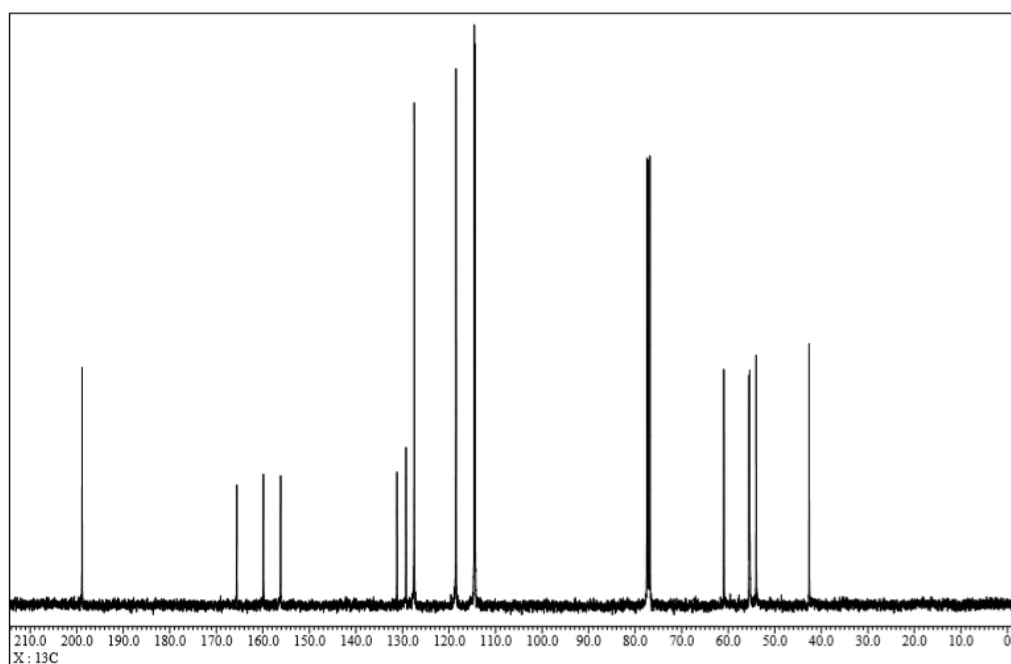
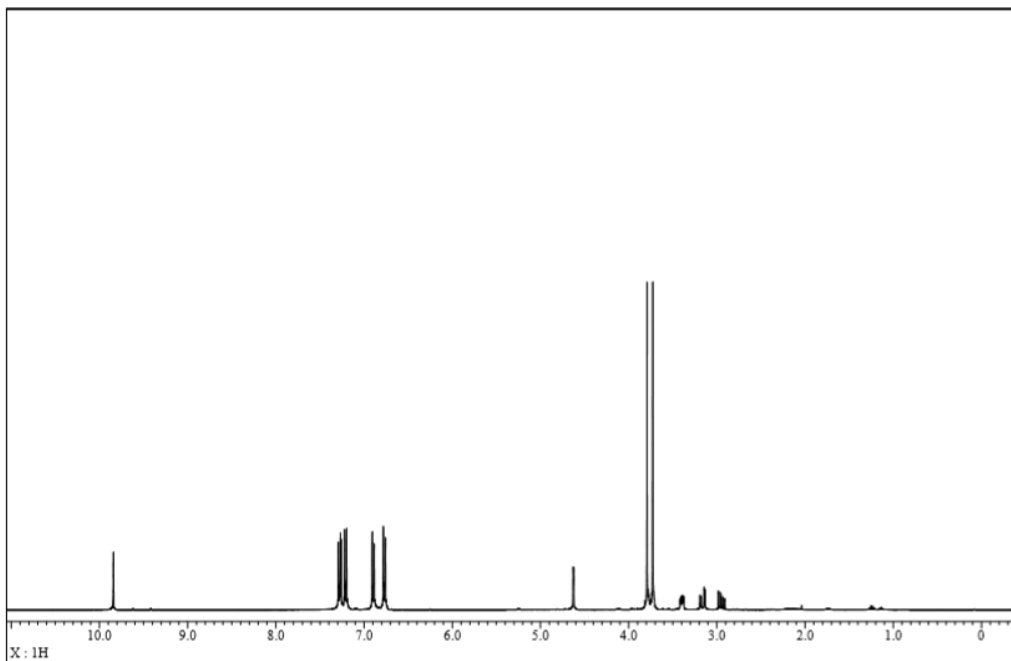


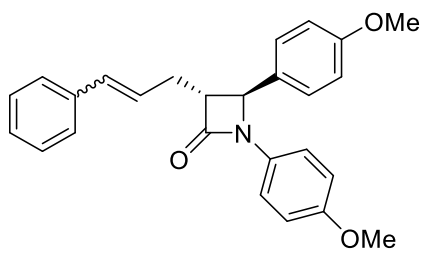
Intermediate



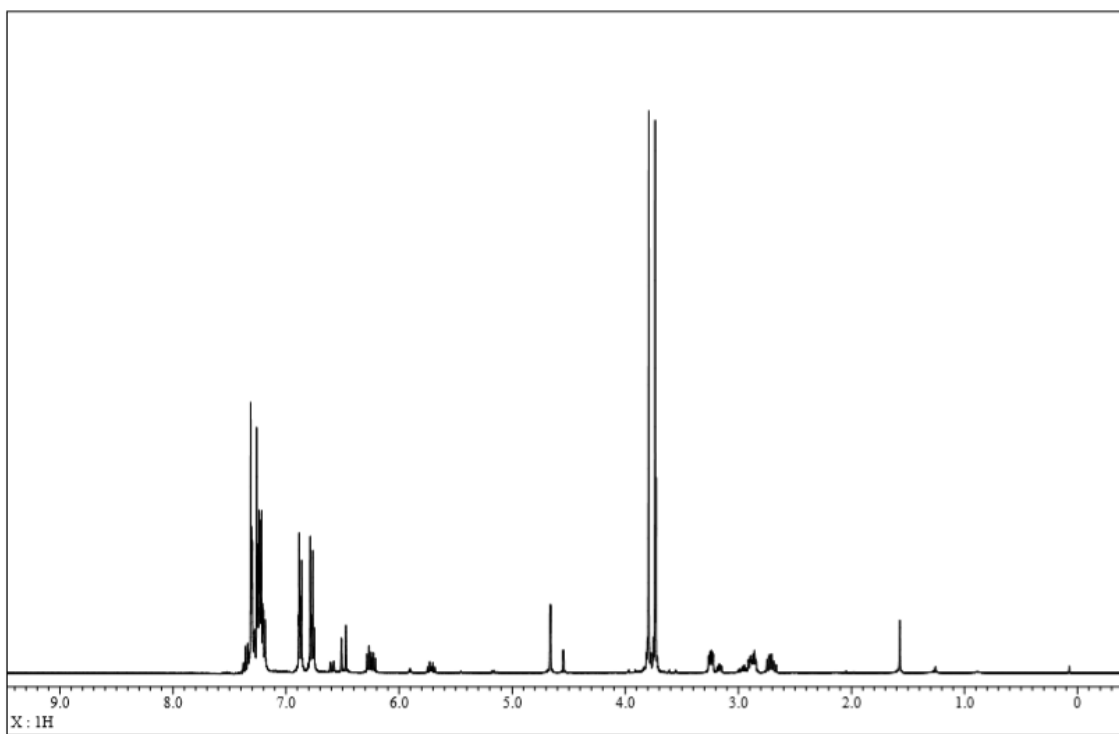


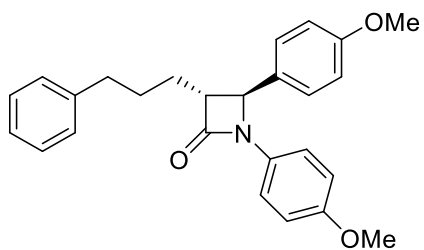
**2-((2*S*\*,3*R*\*)-1,2-bis(4-methoxyphenyl)-4-oxoazetidin-3-yl)acetaldehyde (7)**





Intermediate





**(3*R*\*,4*S*\*)-1,4-bis(4-methoxyphenyl)-3-(3-phenylpropyl)azetidin-2-one (1)**

