

# Studies on Chemoselective Synthesis of 1,4- and 1,2-Dihydropyridine Derivatives by Hantzsch-Like Reaction: A Combined Experimental and DFT Study

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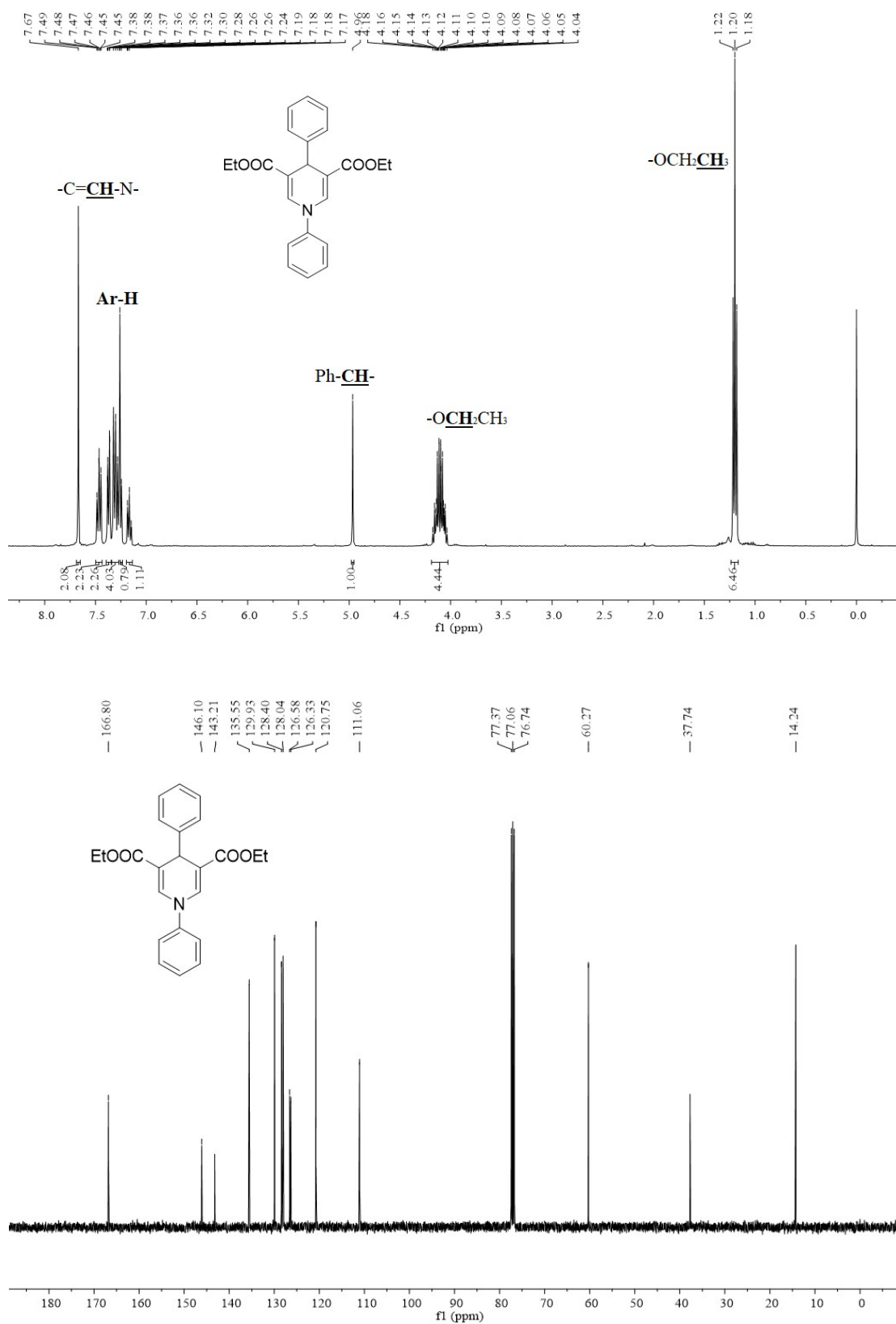
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## Support Information

1. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of all compounds .....s2
2. Cartesian coordinates, the number of imaginary frequencies, computed total energies of every stationary points .....s23

**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of all compounds**



**Figure S1 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of 4a.**

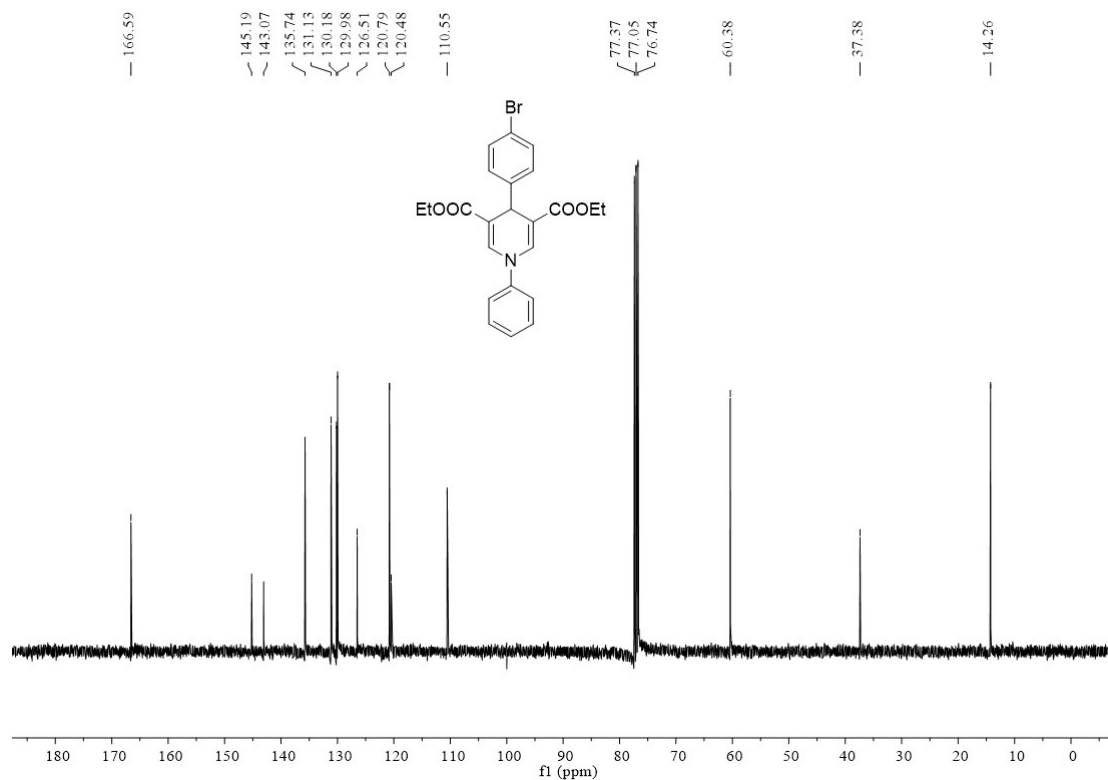
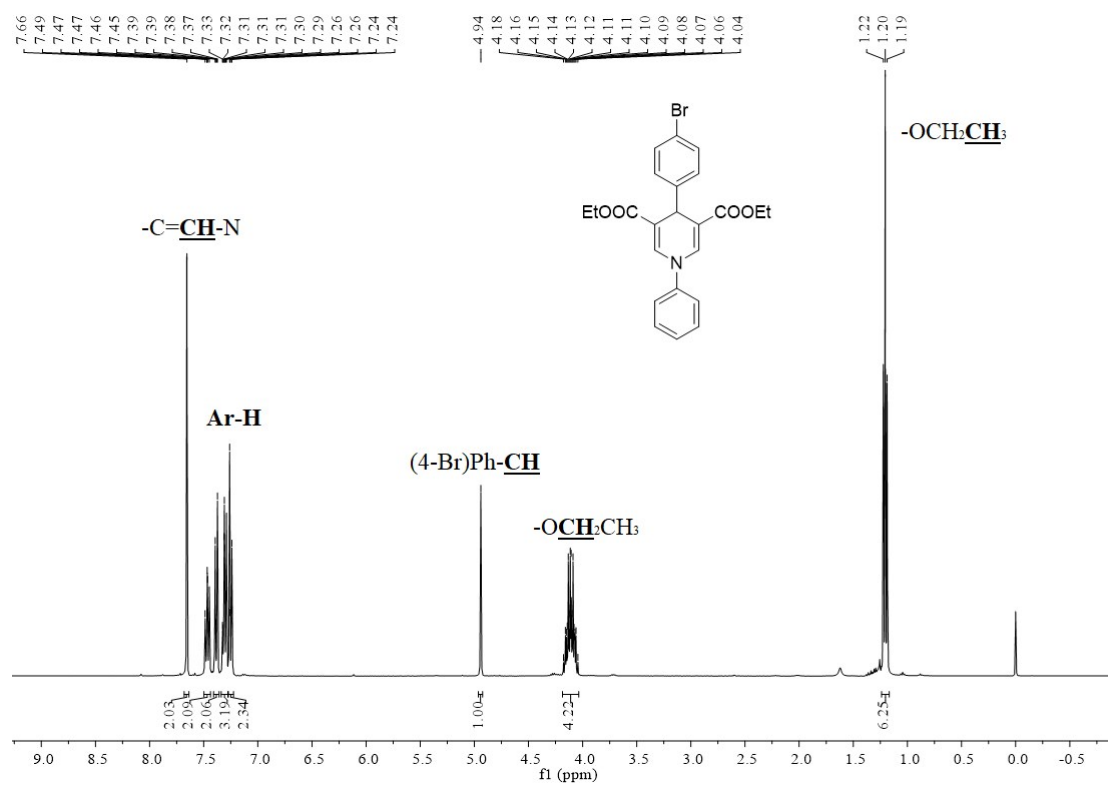


Figure S2 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of **4b**.

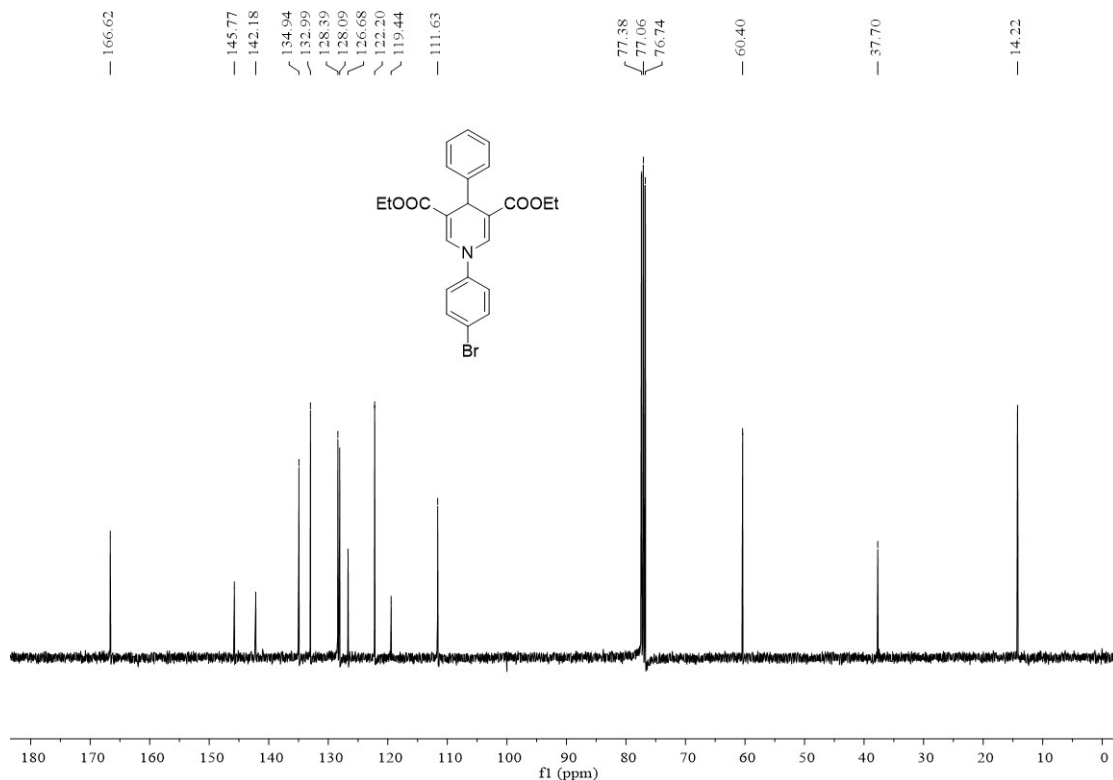
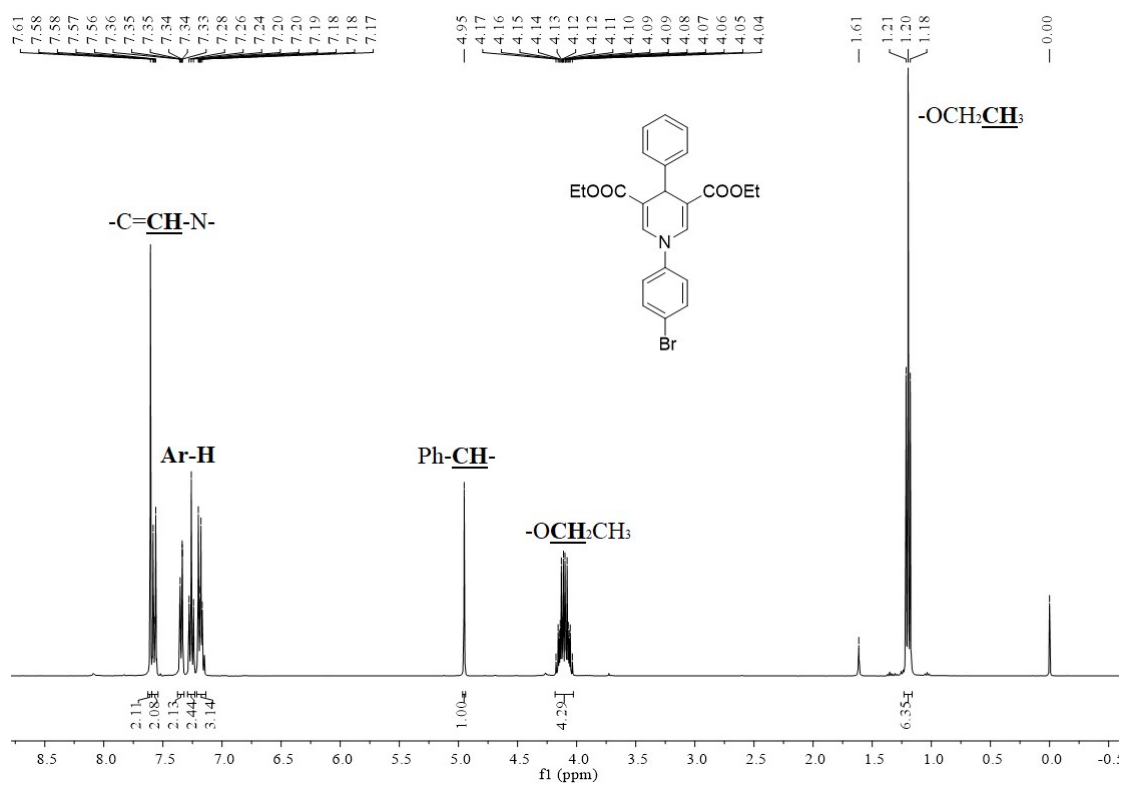


Figure S3  $^1\text{H NMR}$  and  $^{13}\text{C NMR}$  spectra of 4c.

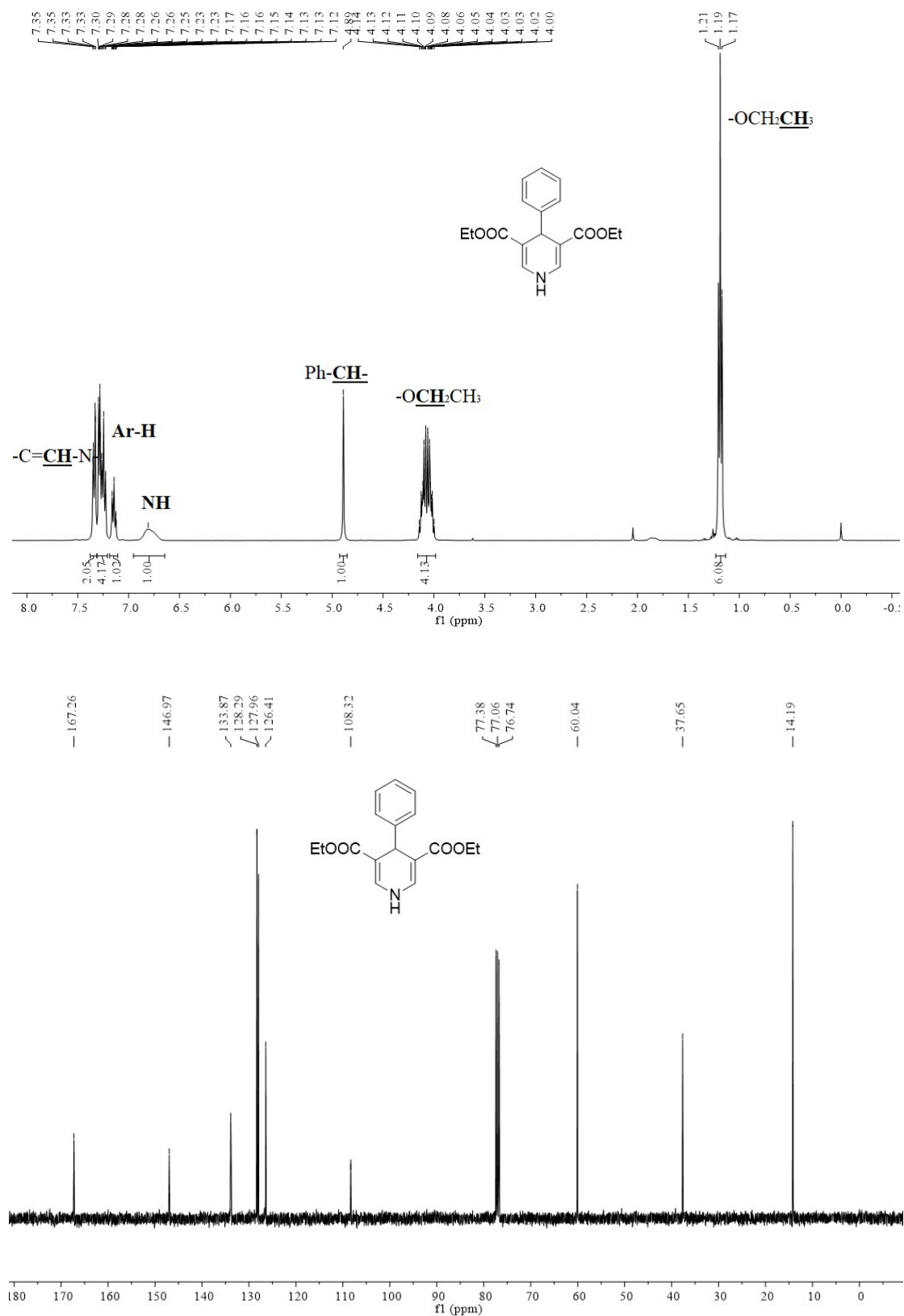


Figure S4 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of 4d.

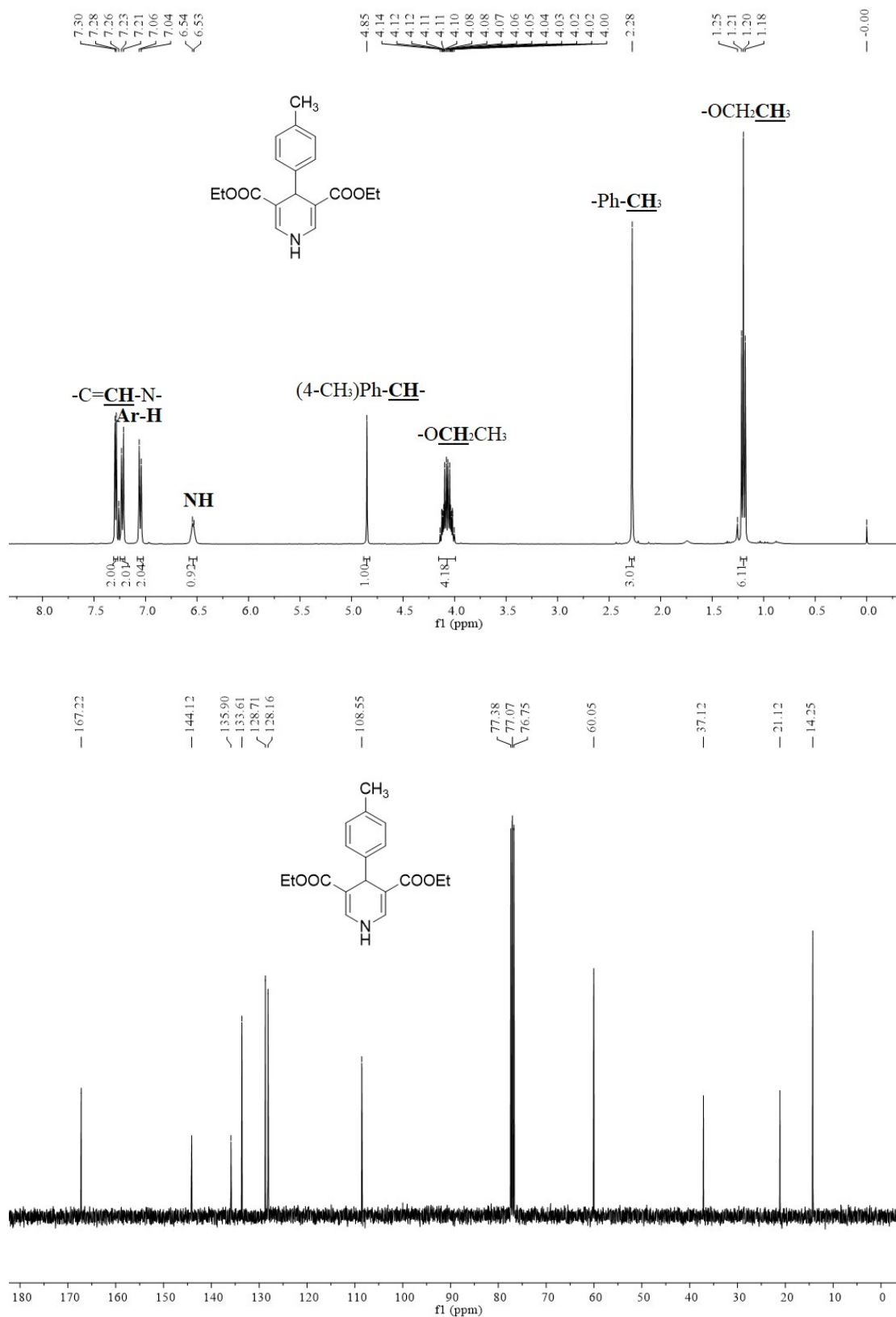


Figure S5 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of 4e.

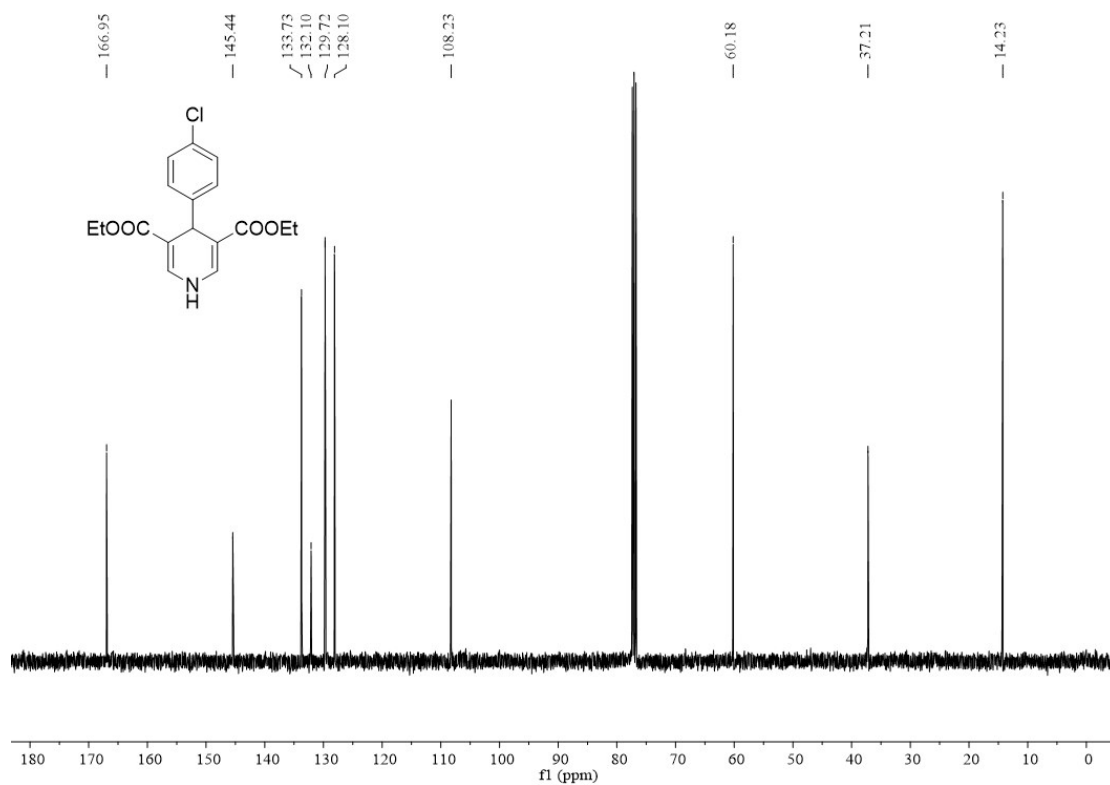
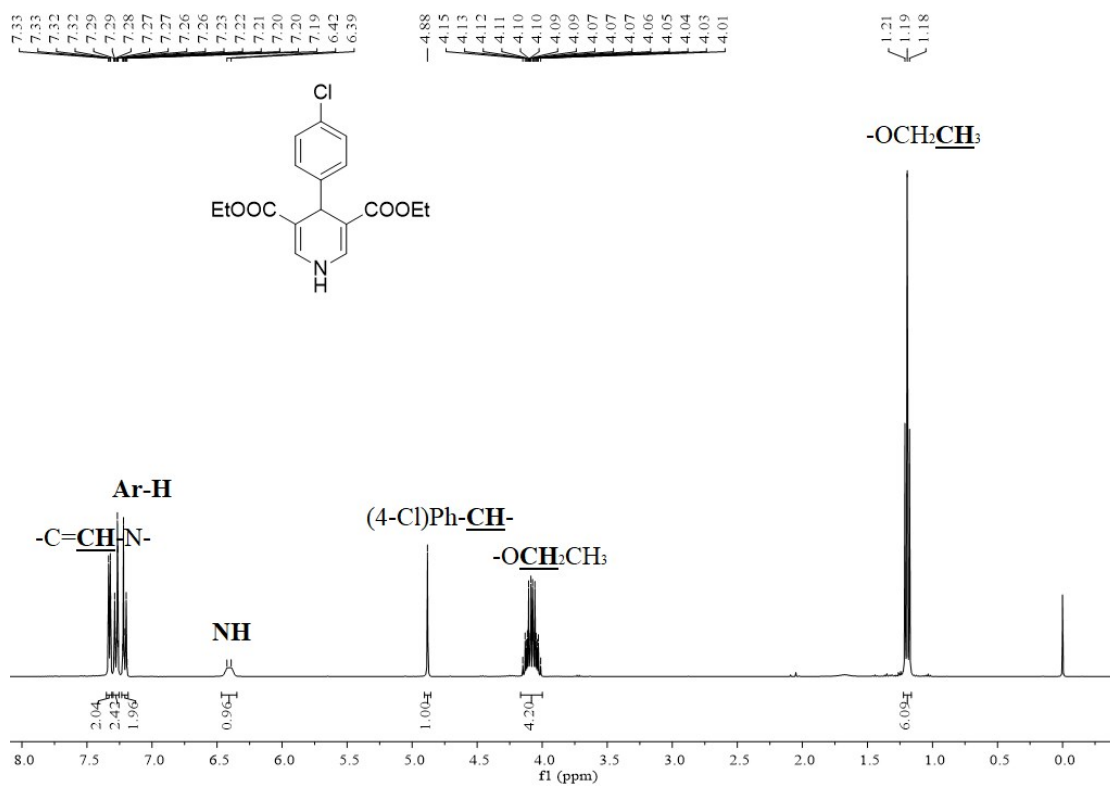


Figure S6  $^1\text{H NMR}$  and  $^{13}\text{C NMR}$  spectra of 4f

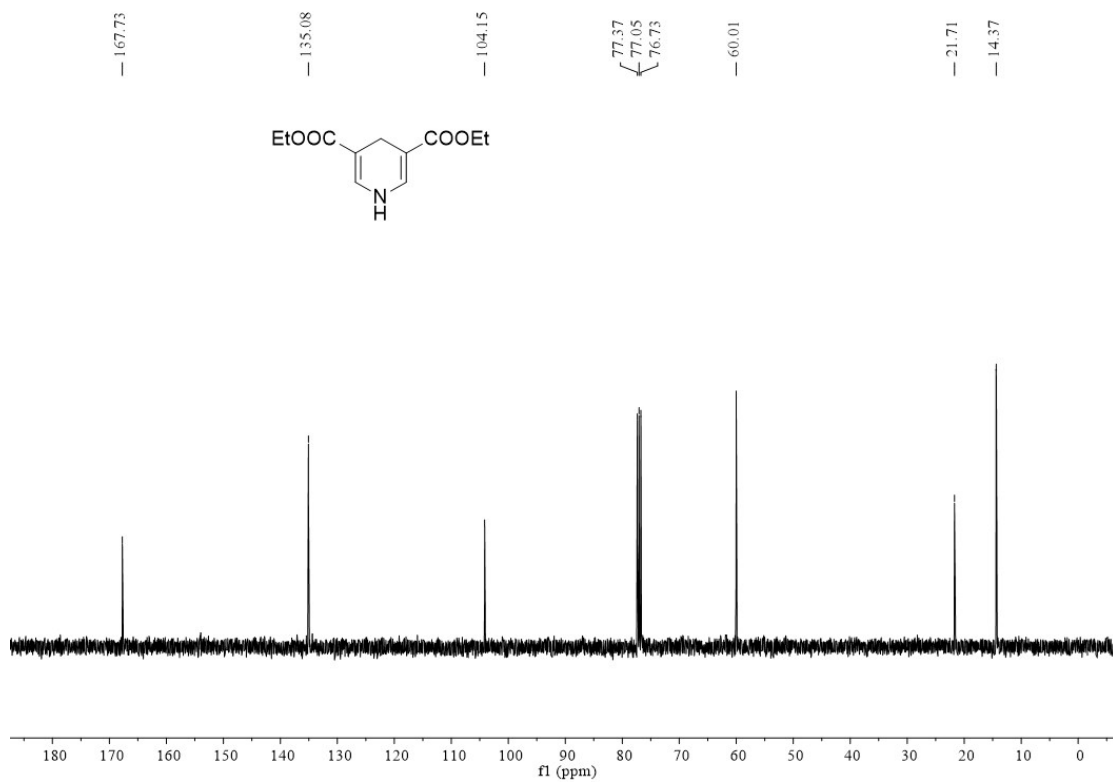
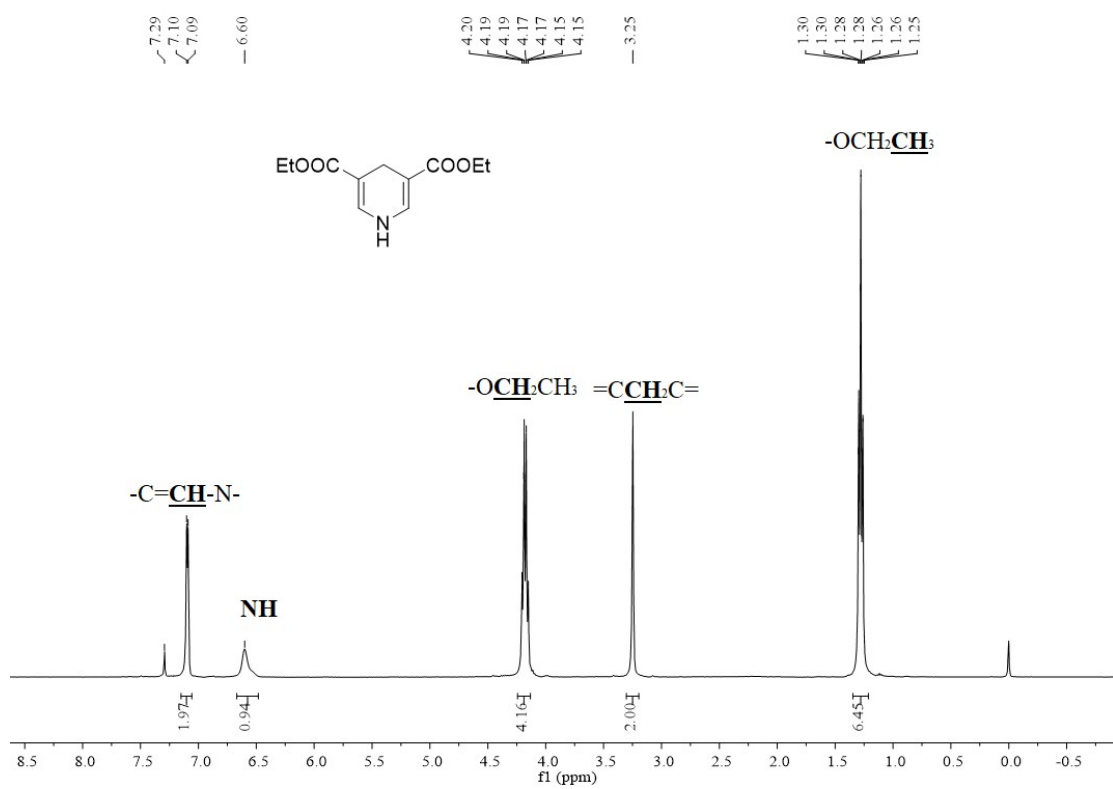


Figure S7 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of 4g.



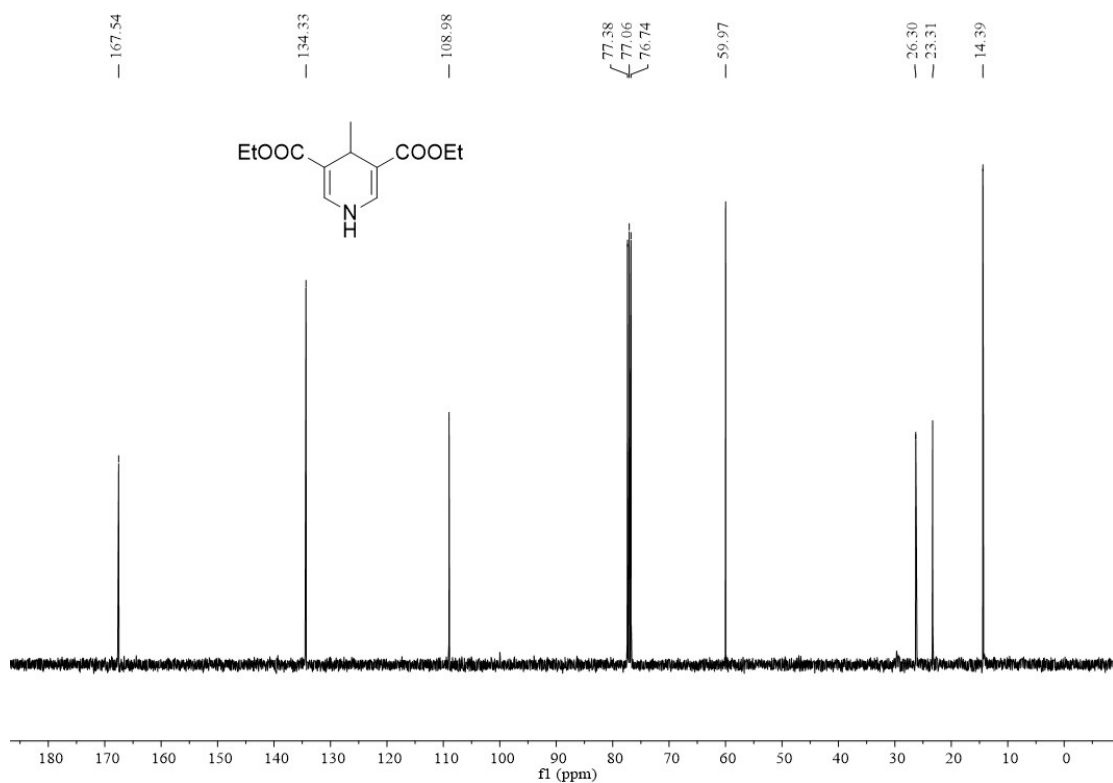
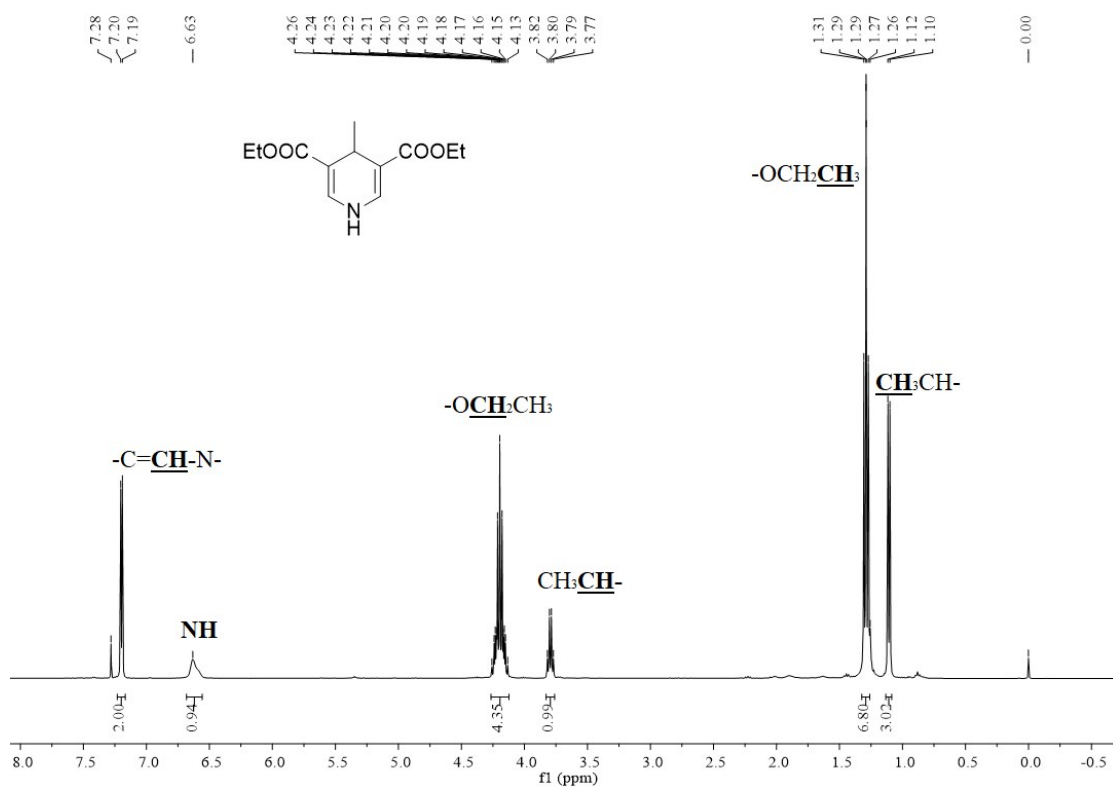


Figure S8  $^1\text{H NMR}$  and  $^{13}\text{C NMR}$  spectra of **4h**.

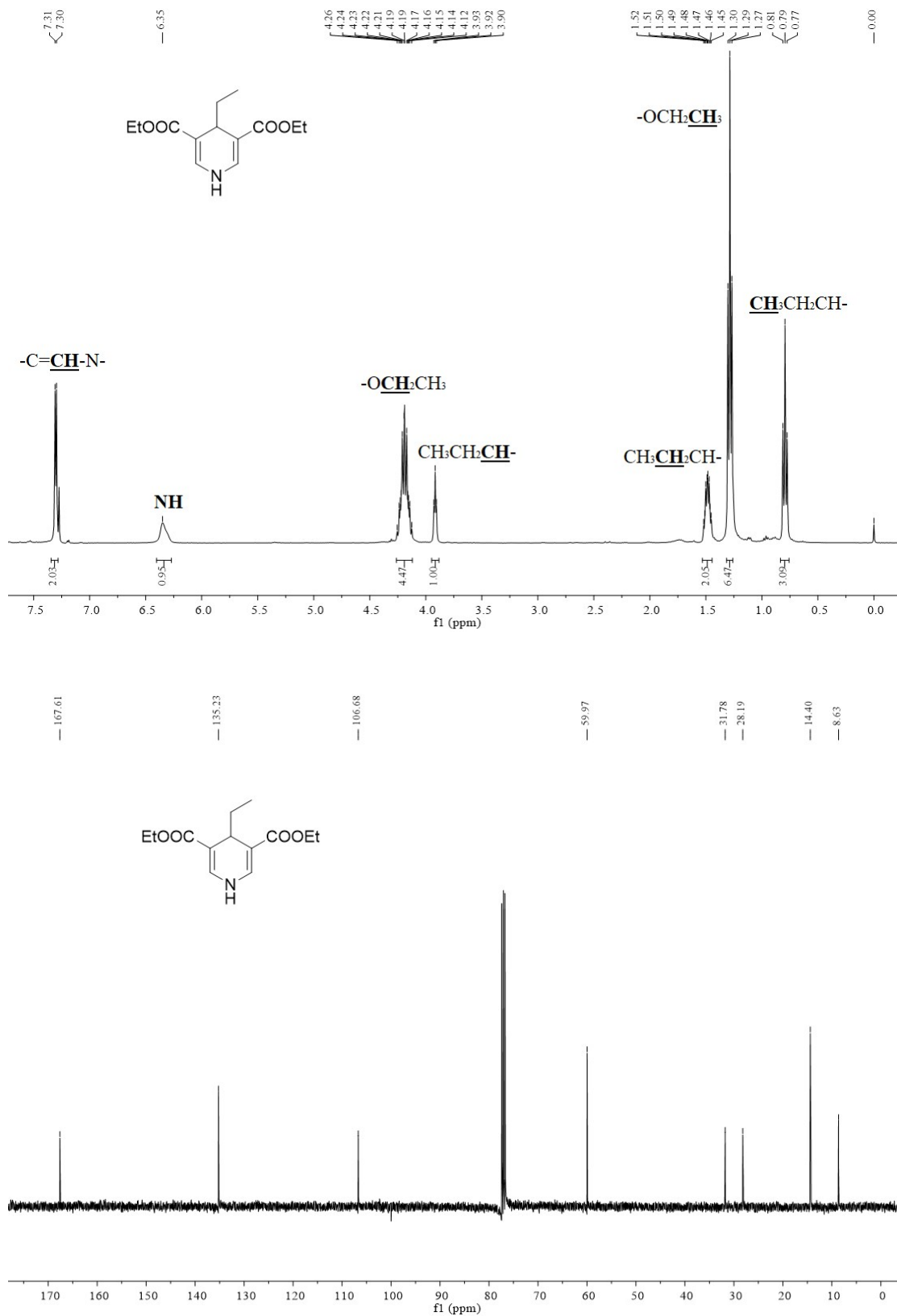


Figure S9 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of 4i.

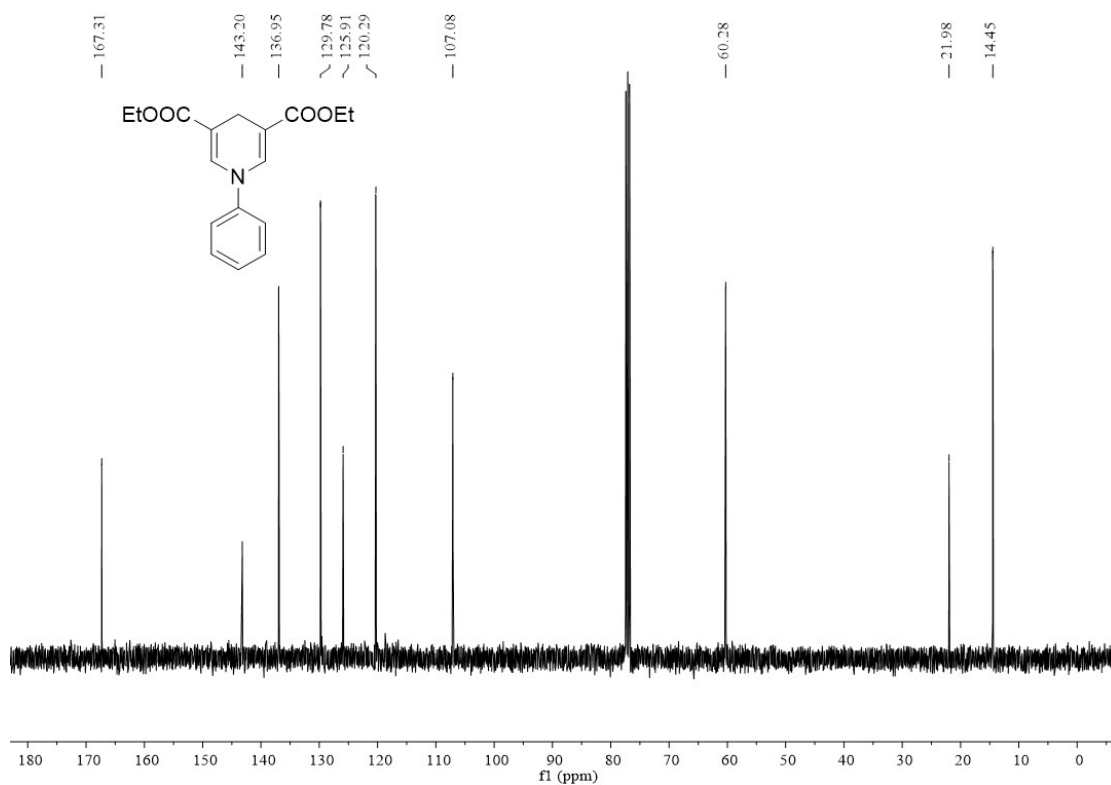
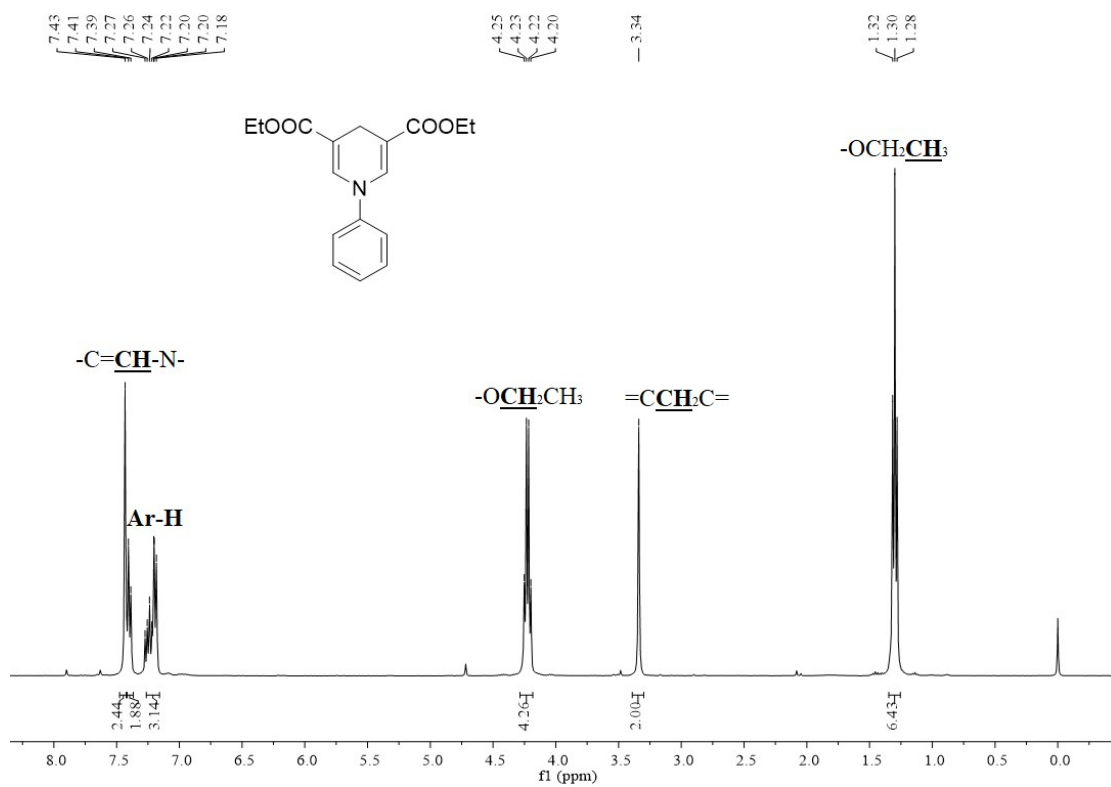


Figure S10  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra of **4j**.

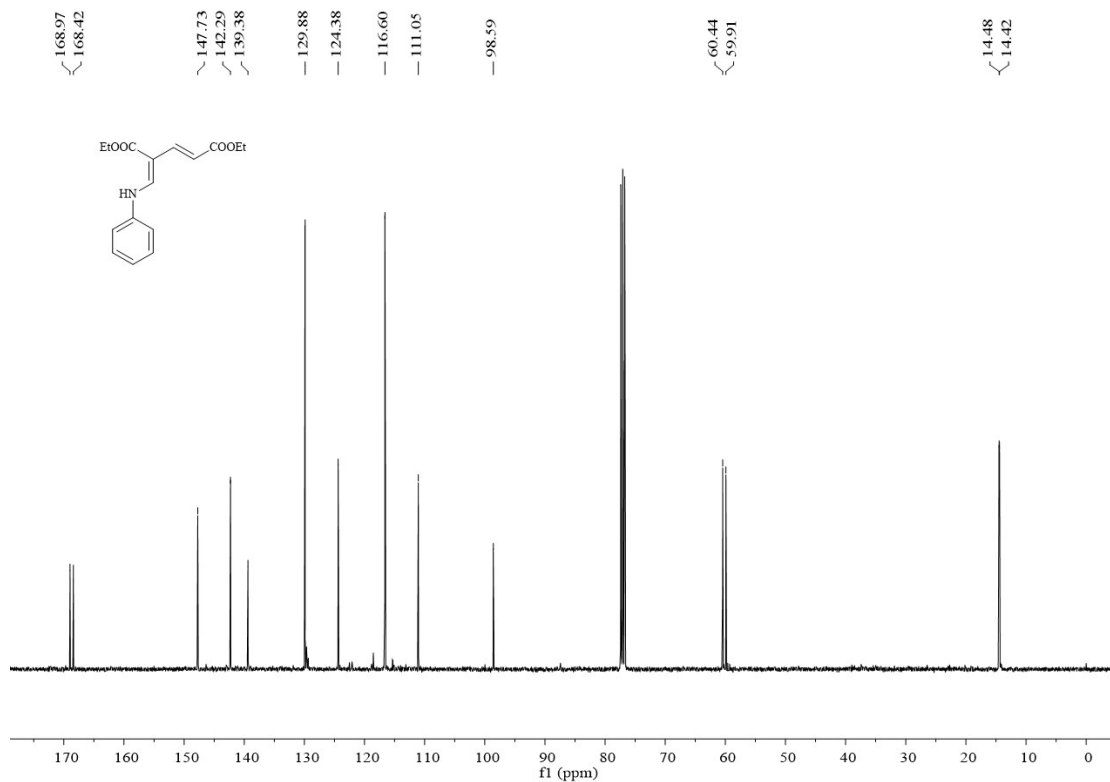
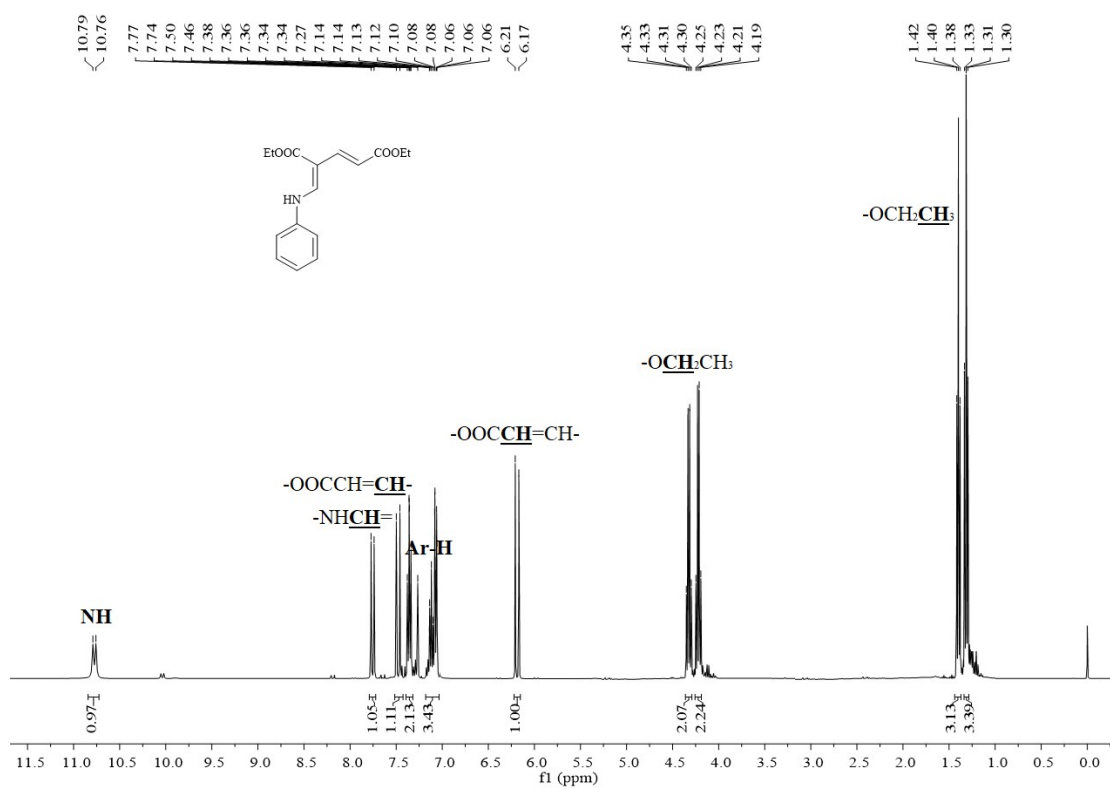


Figure S11 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of 6a.

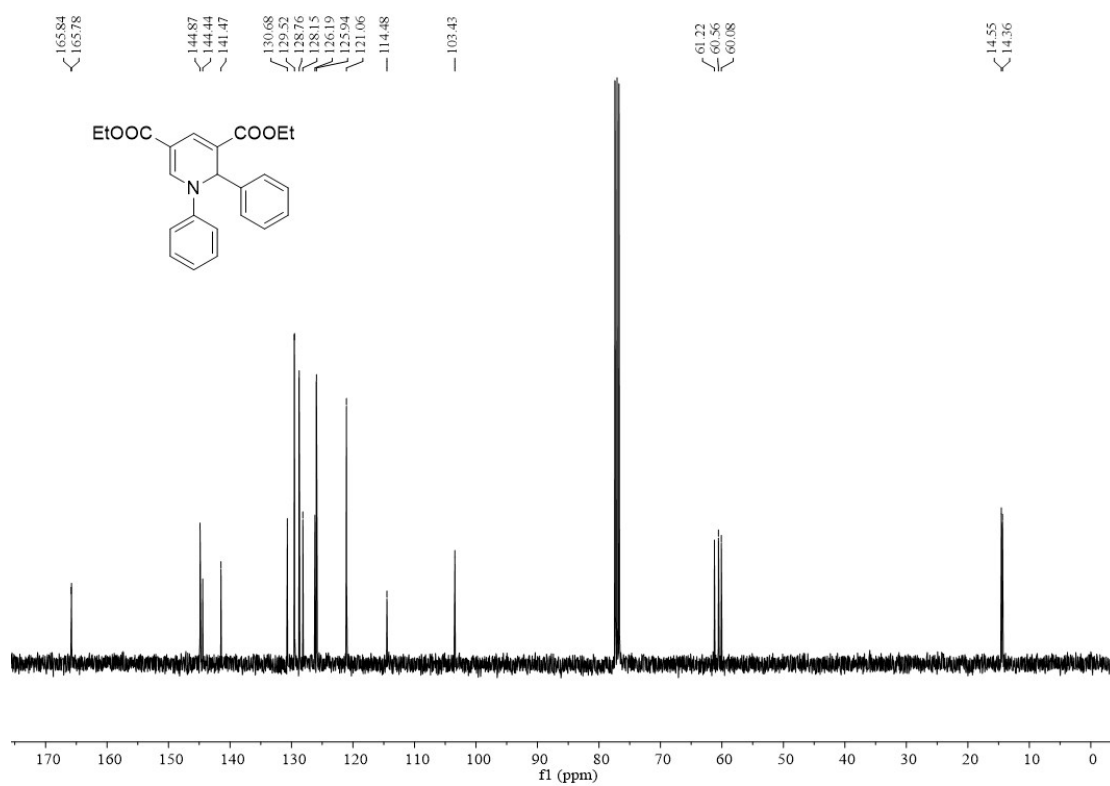
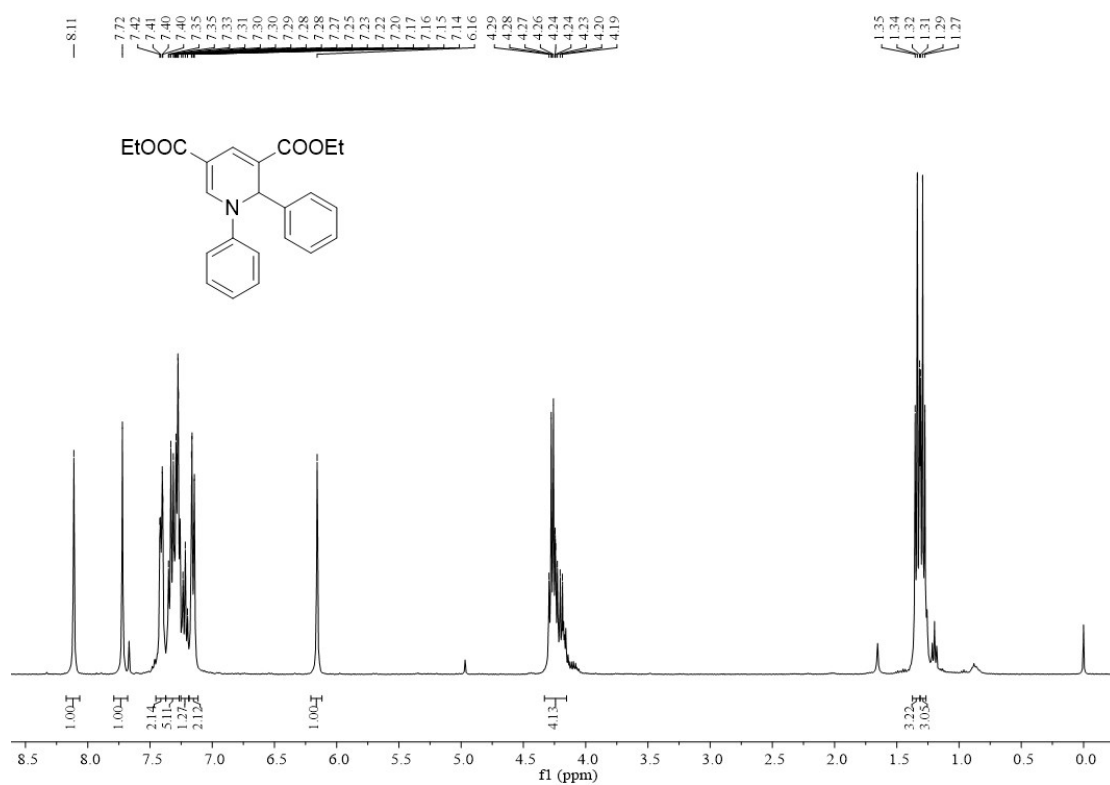


Figure S12 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of **5a**.

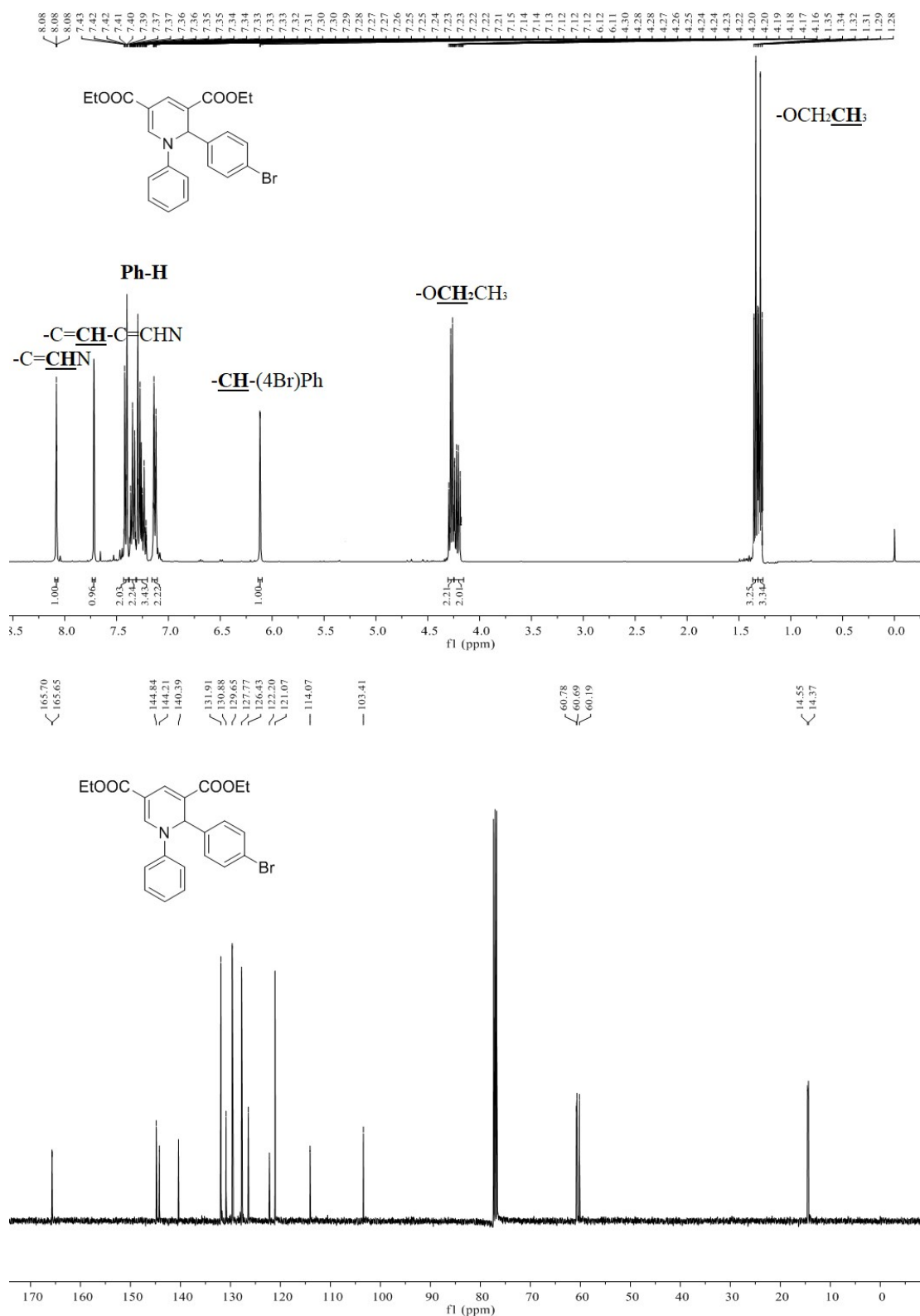


Figure S13 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of 5b.

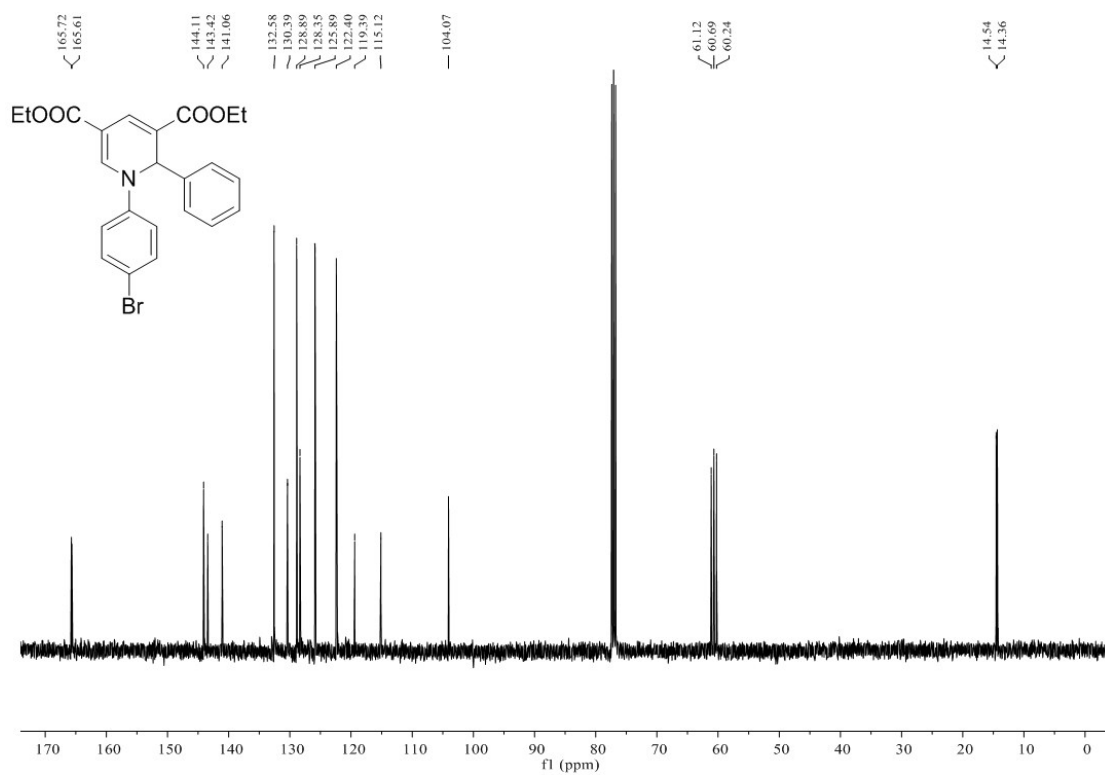
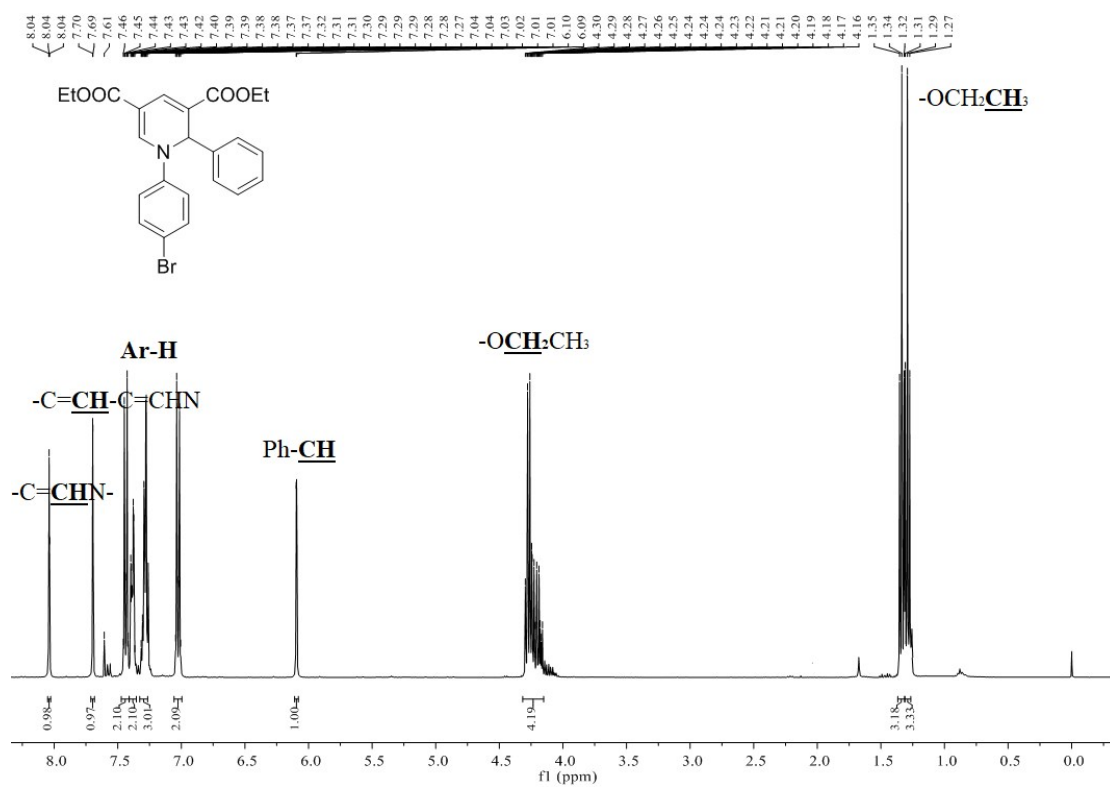


Figure S14 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of 5c.

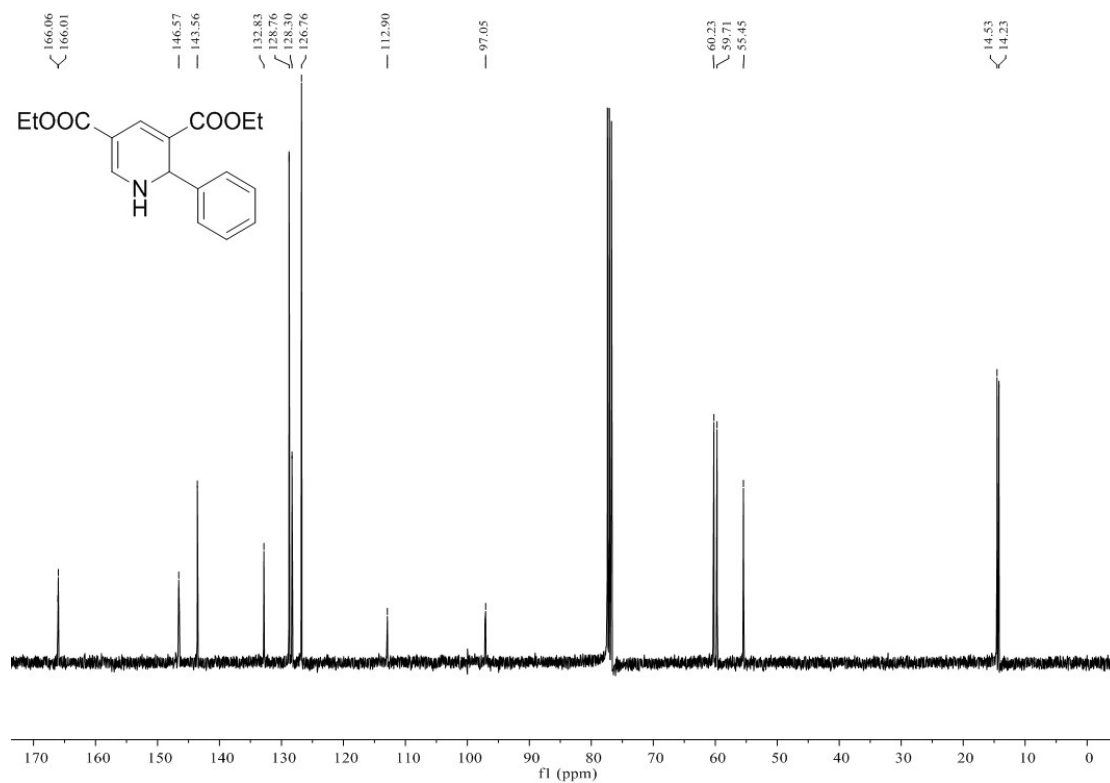
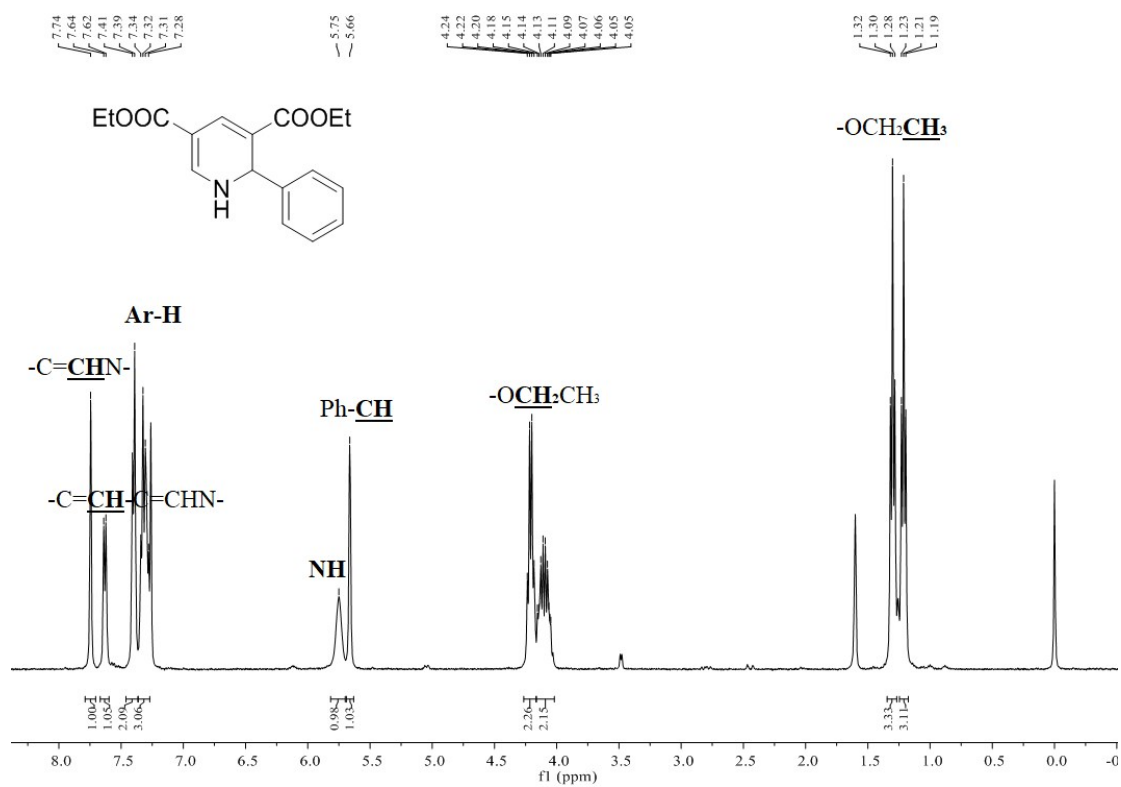


Figure S15 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of 5d.



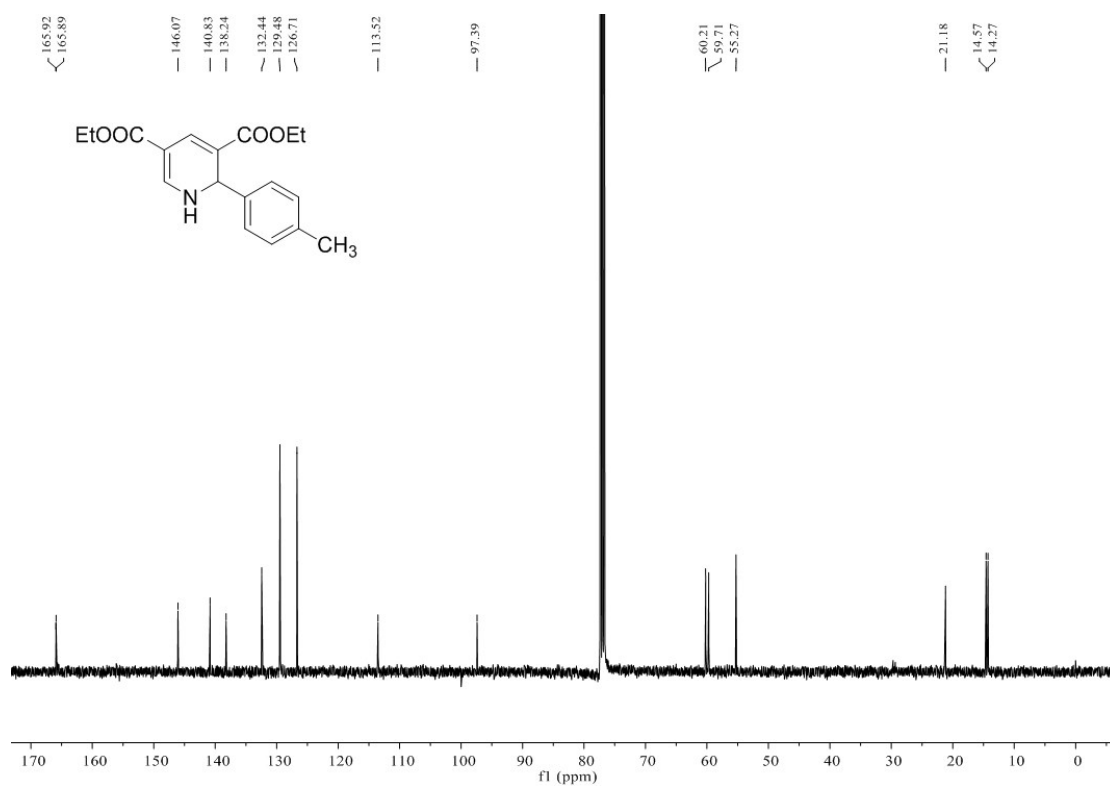
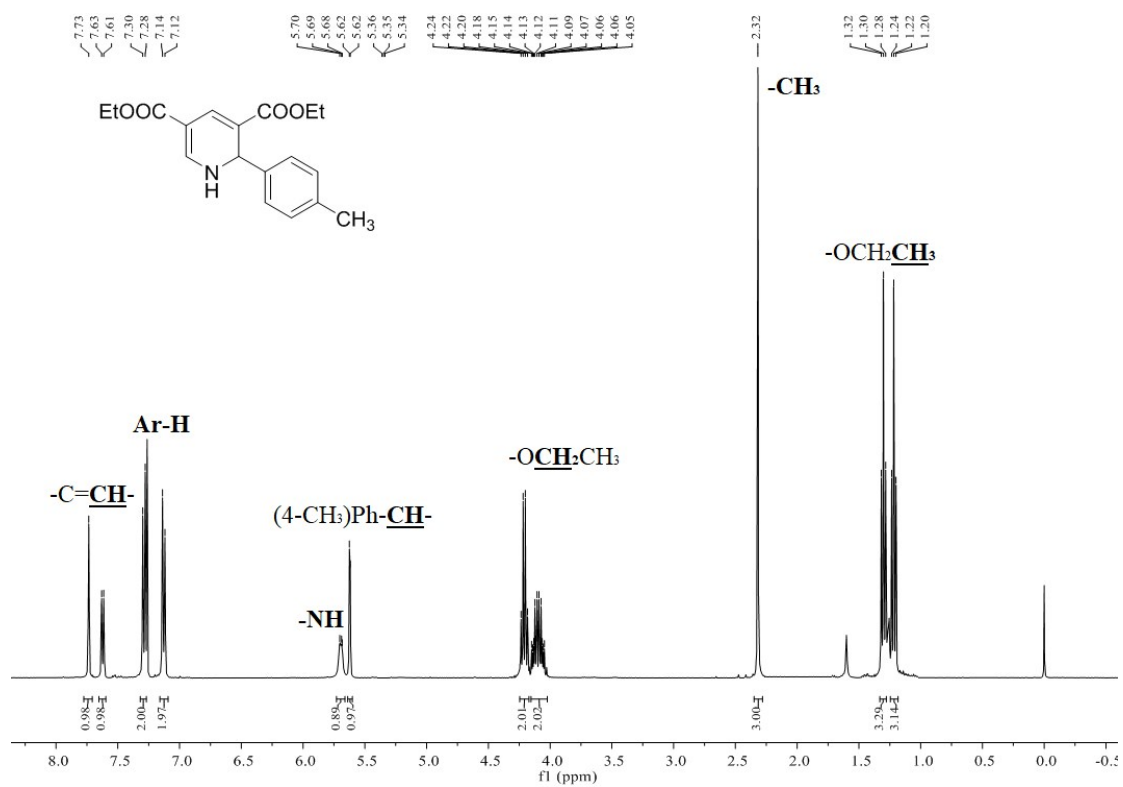


Figure S16 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of **5e**.

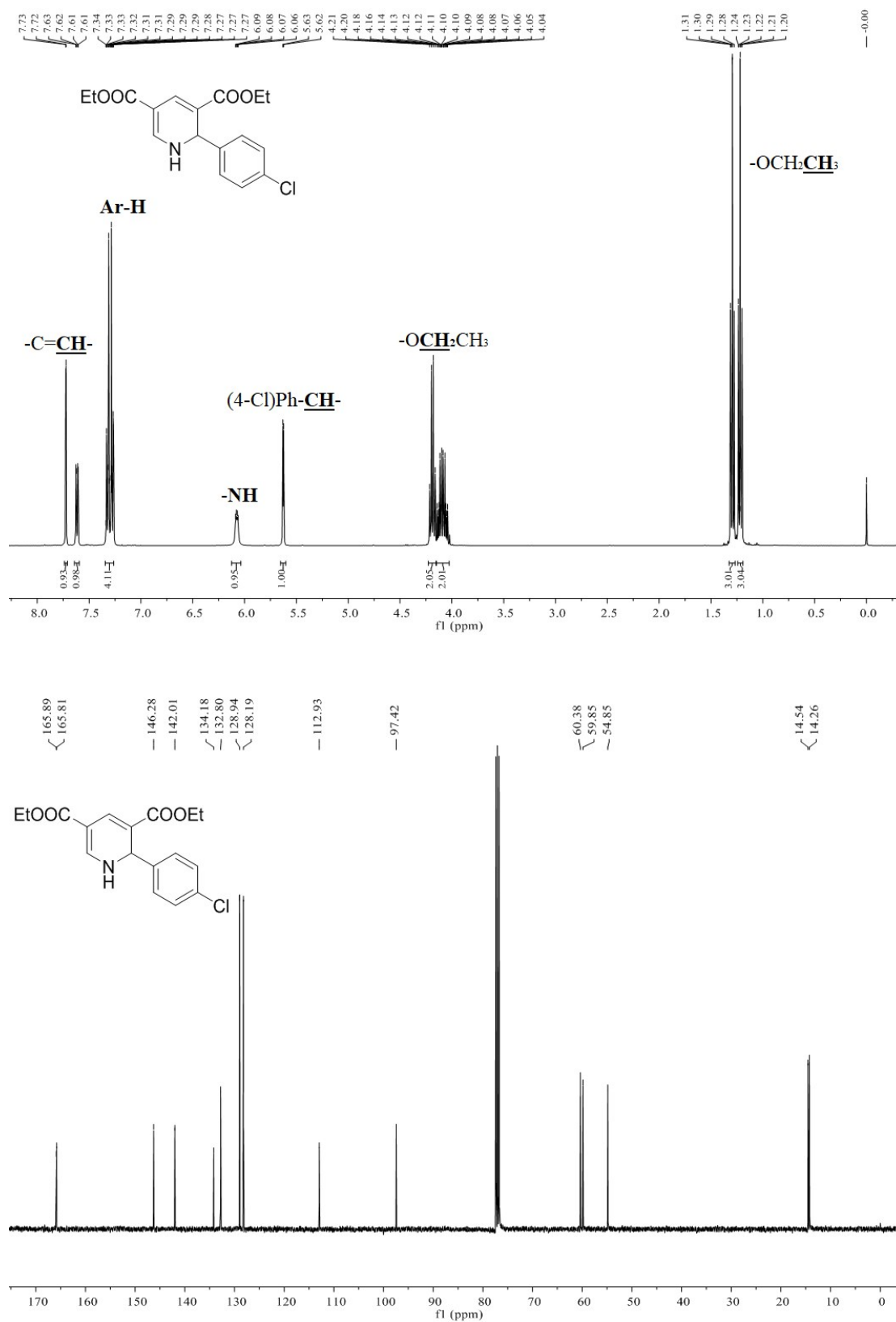


Figure S17 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of **5f**.

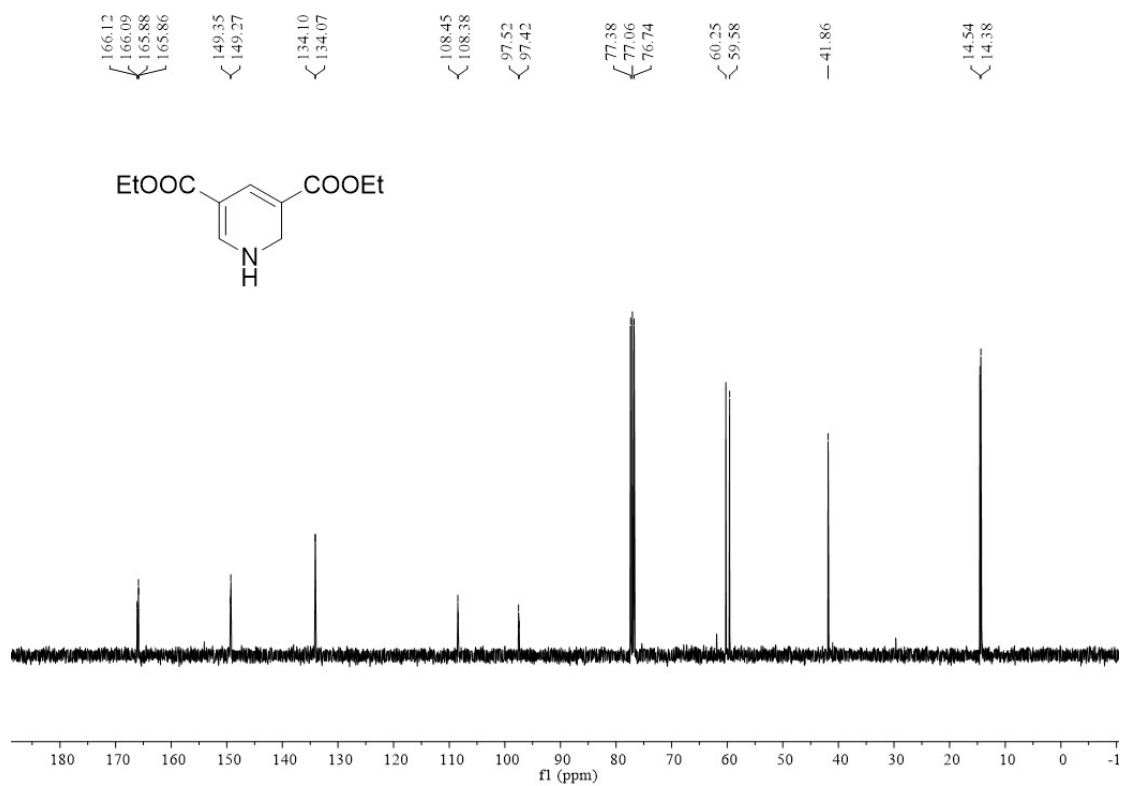
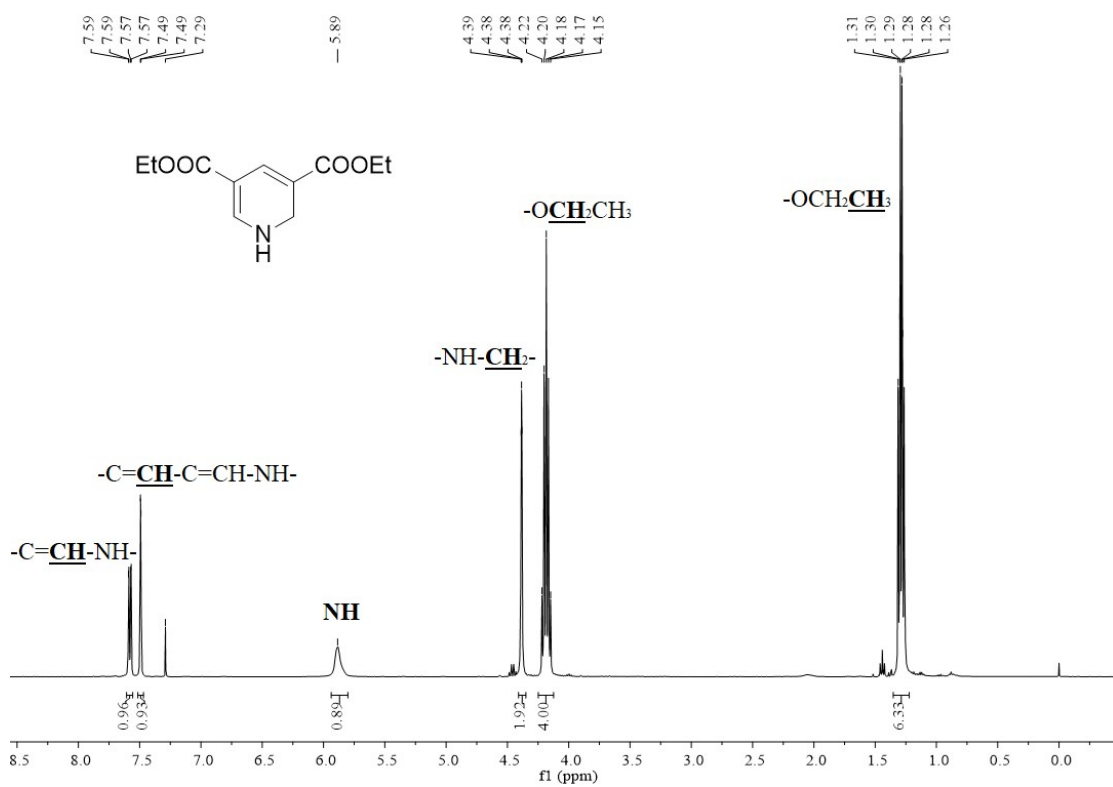


Figure S18  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra of **5g**.

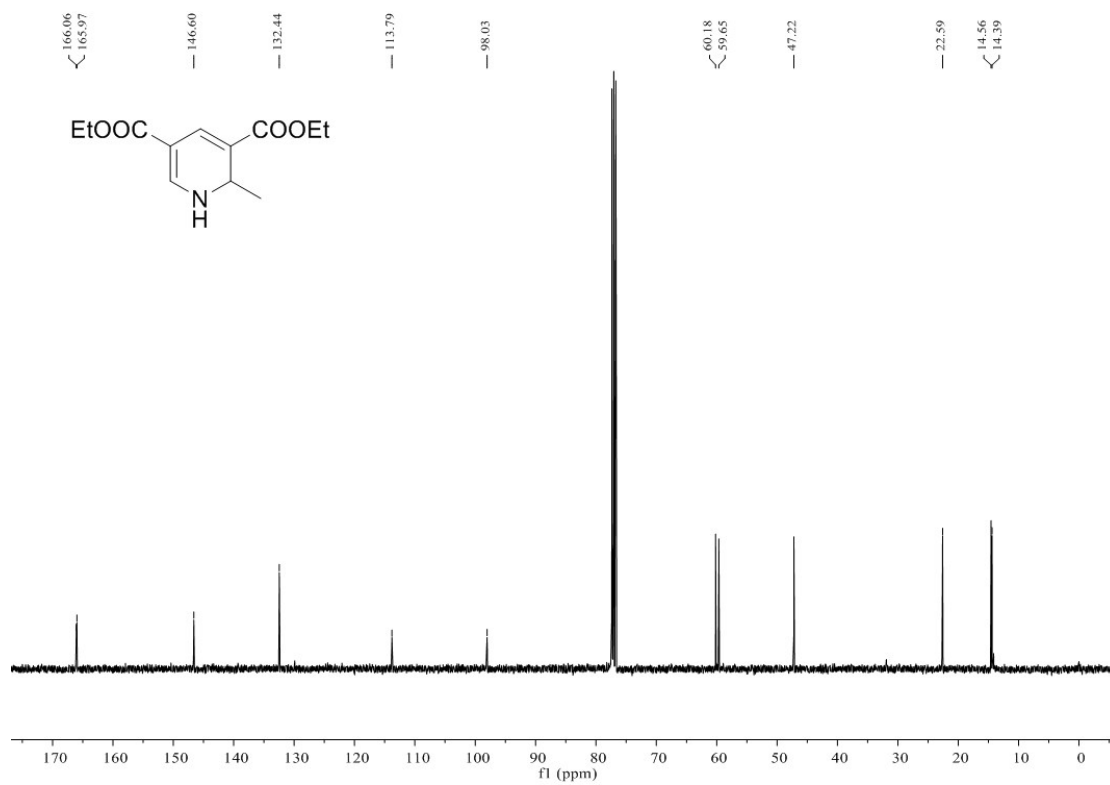
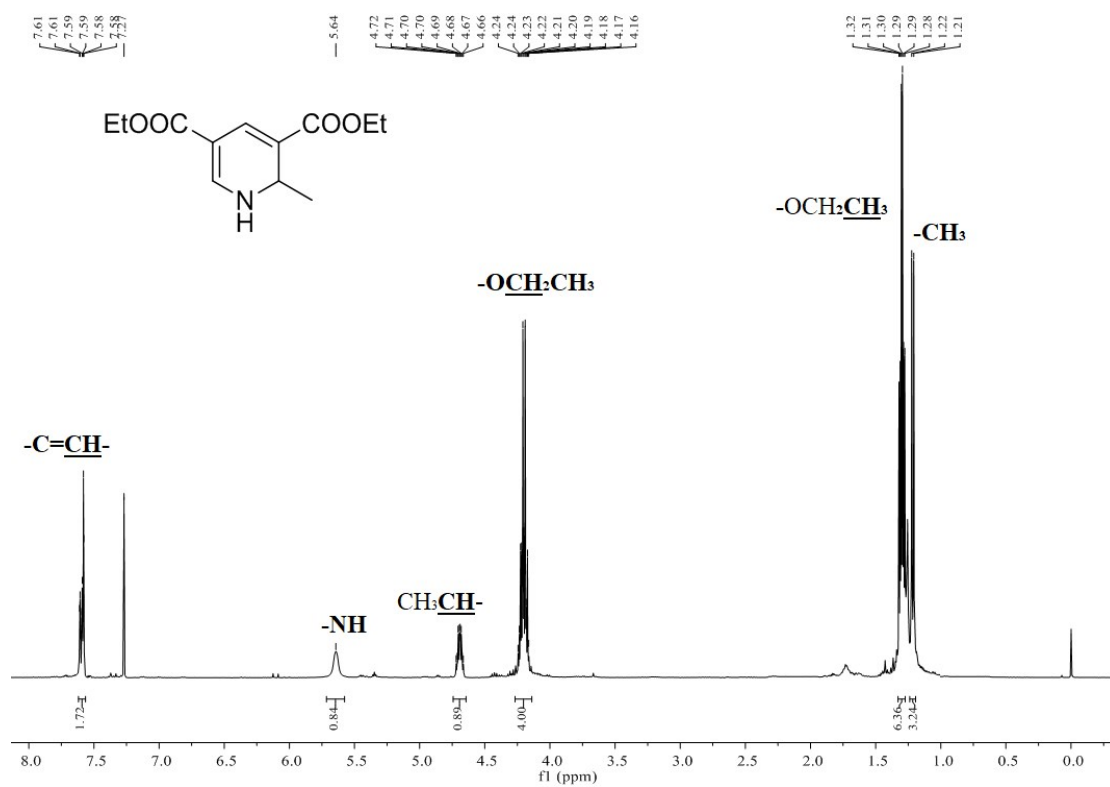


Figure S19  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra of 5h.

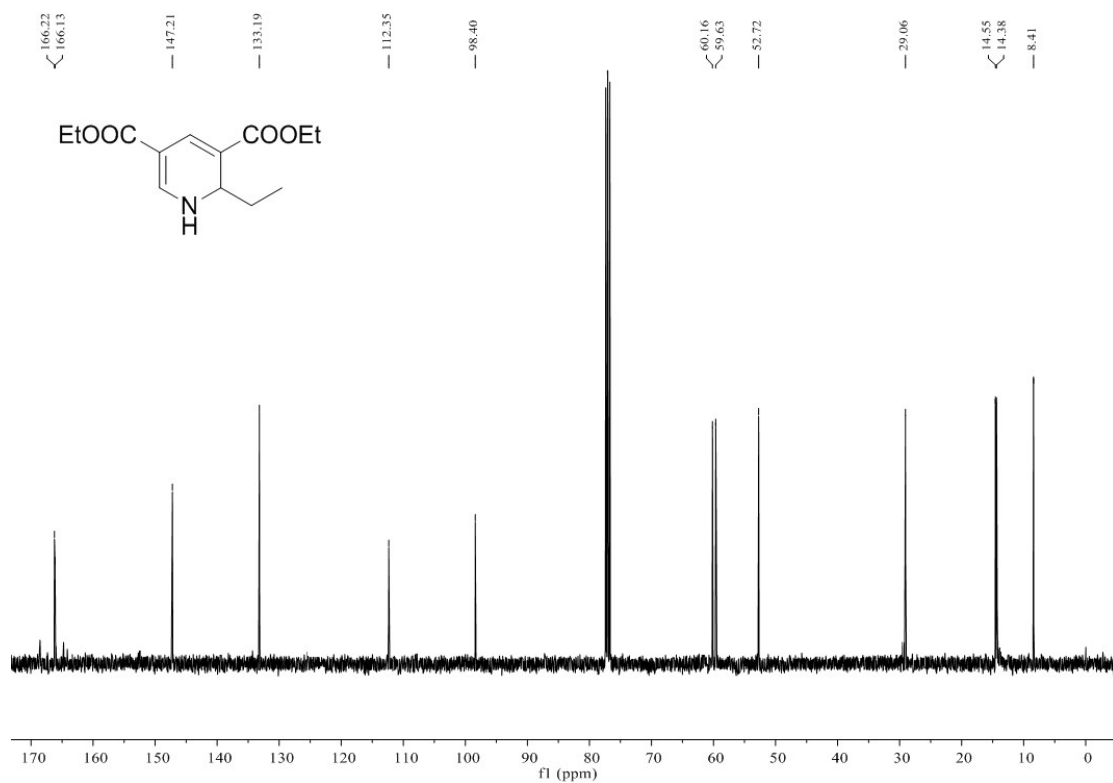
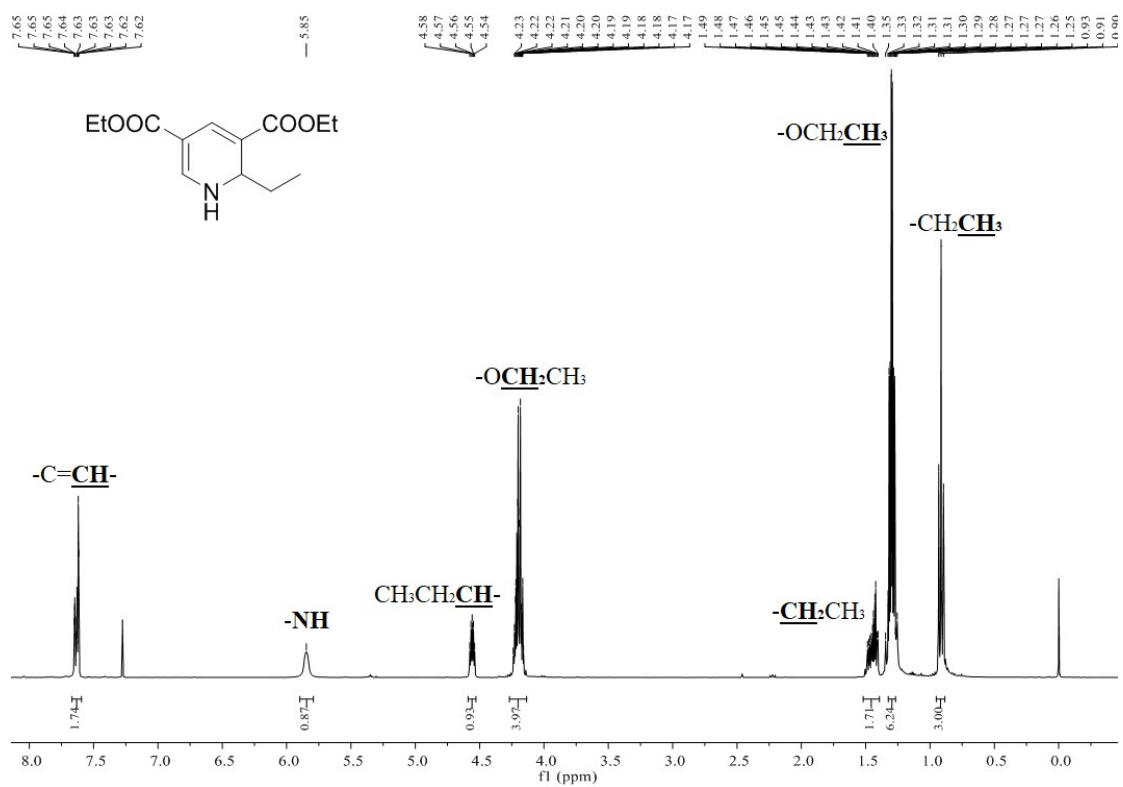


Figure S20 <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of **5i**.

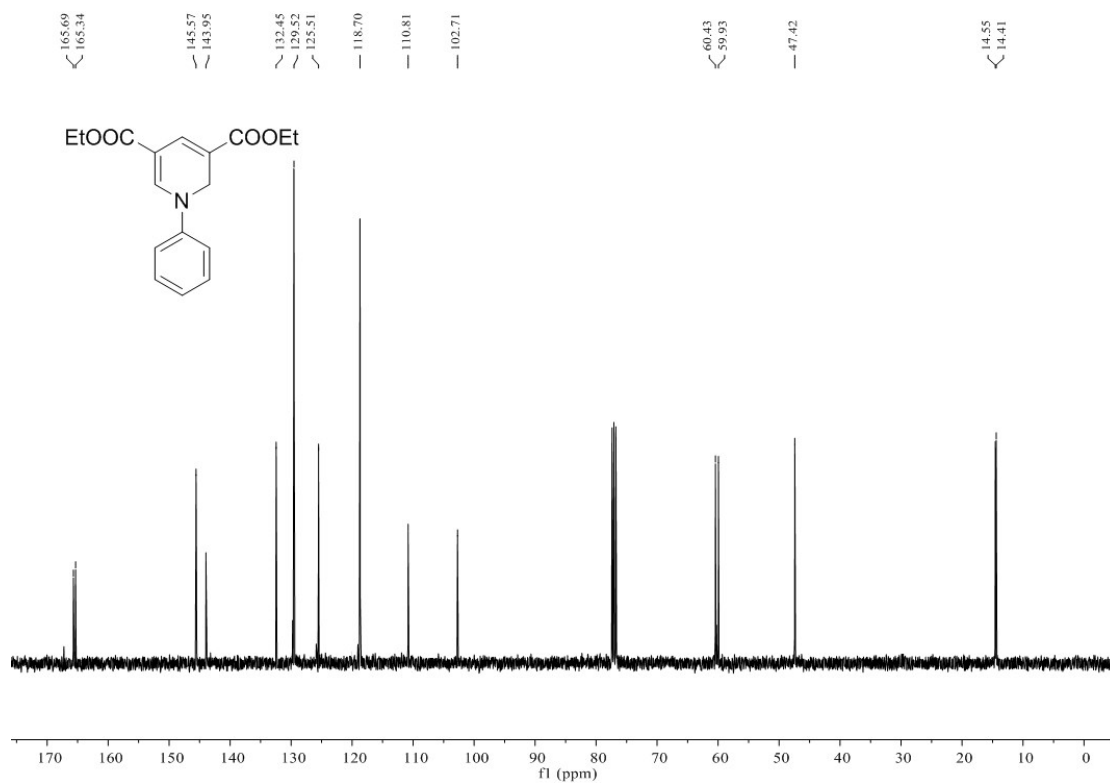
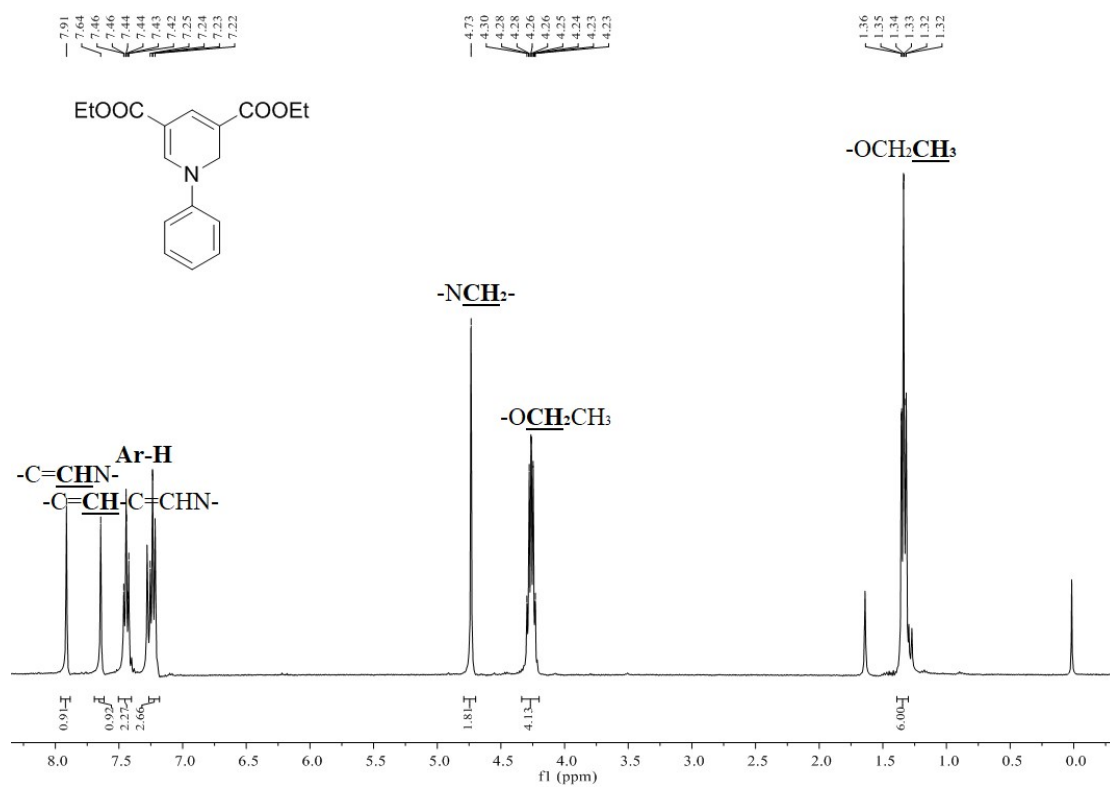
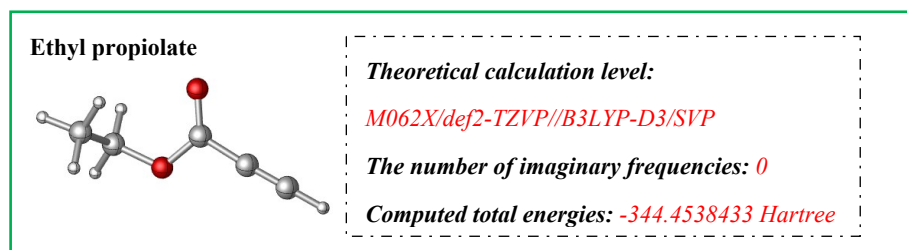
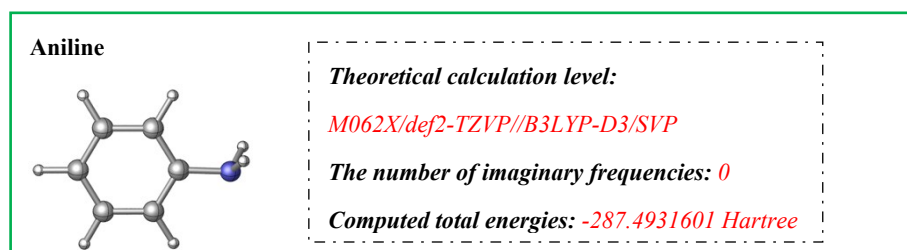


Figure S21  $^1\text{H NMR}$  and  $^{13}\text{C NMR}$  spectra of **5j**.

*Cartesian coordinates, the number of imaginary frequencies, computed total energies of every stationary points*

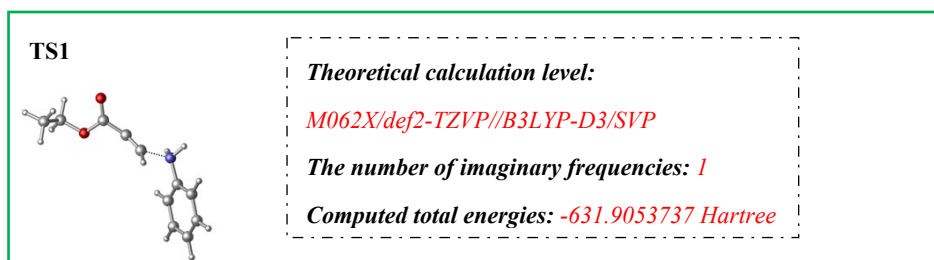


O	-3.71882800	-1.49846200	0.12836600
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H	-5.55645300	1.99175900	-0.75271000
H	-4.84327100	0.48523200	-1.39345500
H	-3.93961000	2.02541100	-1.51160100
C	-3.98643400	1.15894100	0.47734700
H	-3.77501300	2.09586100	1.01288100
H	-4.64781700	0.53762500	1.10042600
C	-2.69641400	-0.83315200	0.16506400
C	-1.27868625	-1.41546180	0.01485302
C	-0.17285861	-1.86966344	-0.10231154
H	0.81218599	-2.27425532	-0.20667891



C	-1.54087603	0.24465524	-1.31247764
C	-0.14571603	0.24465524	-1.31247764
C	0.55182197	1.45240624	-1.31247764
C	-0.14583203	2.66091524	-1.31367664
C	-1.54065703	2.66083724	-1.31415564
C	-2.23825803	1.45263124	-1.31315964
H	-2.09063503	-0.70766176	-1.31202764
H	0.40379197	-0.70785776	-1.31116264
H	0.40436797	3.61305824	-1.31373564
H	-2.09077903	3.61311824	-1.31510864
H	-3.33786203	1.45281424	-1.31333964

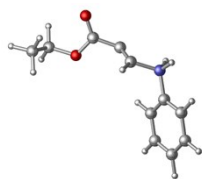
N	2.02182172	1.45251318	-1.31163014
H	2.35471812	0.98148338	-0.49473914
H	2.35565964	0.98078264	-2.12773218



O	3.50603000	-1.50208100	-0.09652900
O	3.02762300	0.70856900	-0.32877700
C	4.98497800	1.09672200	1.09134100
H	6.04178700	1.40717600	1.06866200
H	4.92093200	0.11536600	1.58493400
H	4.42010800	1.83064300	1.68865500
C	4.42995600	1.01184400	-0.32254400
H	4.51347500	1.97978700	-0.83873300
H	4.97403200	0.25442500	-0.90757600
C	2.67313300	-0.60691700	-0.19406100
C	1.26887400	-0.77965100	-0.24759100
C	0.15270500	-0.89784900	0.33736700
H	-0.35588300	-0.86888200	1.30162000
N	-1.29038800	-1.23015200	-0.71398400
H	-1.45146500	-2.23832100	-0.64774500
C	-2.44890100	-0.46531100	-0.36296400
C	-2.62898900	0.81185200	-0.91108400
C	-3.33495000	-0.95334100	0.60575000
C	-3.71247300	1.59085400	-0.50032900
H	-1.92567400	1.19033100	-1.65676200
C	-4.41480000	-0.16363500	1.01245200
H	-3.18676600	-1.94842600	1.03301800
C	-4.60787300	1.10724900	0.46148000
H	-3.85678200	2.58271900	-0.93516300
H	-5.10929800	-0.54839900	1.76297100
H	-5.45432200	1.72022800	0.77953500
H	-0.93661000	-1.02838200	-1.65199500



IM1



*Theoretical calculation level:*

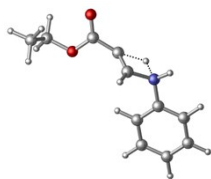
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*The number of imaginary frequencies: 0*

*Computed total energies: -631.9148571 Hartree*

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C	4.36977900	1.35087100	1.19300000
H	5.36850500	1.80382300	1.30177200
H	4.36395700	0.38652200	1.72184800
H	3.63250100	2.01829500	1.66694400
C	4.03879900	1.14305300	-0.27736000
H	4.07138000	2.09636400	-0.82691100
H	4.75620400	0.44679200	-0.73987900
C	2.50573400	-0.69855300	-0.31383300
C	1.15905100	-1.08302000	-0.64150300
C	0.19323000	-1.12983100	0.25671300
H	0.14944900	-0.88696500	1.32710800
N	-1.18472600	-1.57114200	-0.21082300
H	-1.47419200	-2.42594400	0.28159400
C	-2.24669300	-0.55793900	-0.09707300
C	-2.07403700	0.66486200	-0.74904900
C	-3.38295000	-0.82911700	0.66272400
C	-3.07583700	1.63158100	-0.64317800
H	-1.16242400	0.85227400	-1.31929000
C	-4.37799400	0.14961600	0.76664700
H	-3.49744700	-1.79160700	1.16751200
C	-4.22627500	1.37622600	0.11391400
H	-2.95473300	2.59053200	-1.15178200
H	-5.27203600	-0.05251400	1.36042000
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H	-1.04211900	-1.83926800	-1.19625900

TS2



*Theoretical calculation level:*

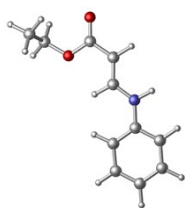
*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 1*

*Computed total energies: -631.8927475 Hartree*

O	3.34769900	-1.49536900	-0.38120300
O	2.76016600	0.68826600	-0.33078000
C	4.86311800	1.00457400	0.89519200
H	5.89527800	1.37551400	0.78694800
H	4.90281900	-0.03392400	1.25318000
H	4.35000900	1.62193400	1.64927500
C	4.14372100	1.07552200	-0.44122600
H	4.11527400	2.10545500	-0.82363500
H	4.64030300	0.43474500	-1.18609700
C	2.48243500	-0.63799400	-0.32693400
C	1.04890200	-0.90368700	-0.35396500
H	-0.30778300	-1.36581100	-0.91575100
C	0.18276500	-0.90458600	0.66319200
H	0.22891300	-0.69344100	1.73370400
N	-1.56914468	-1.50013799	-0.14707357
H	-1.83420368	-2.44966699	0.13929143
C	-2.71498368	-0.62081399	-0.14954757
C	-2.53210568	0.76159401	-0.28278257
C	-4.00588368	-1.16389299	-0.08612757
C	-3.65043368	1.59436401	-0.34689357
H	-1.52924168	1.17783501	-0.34023857
C	-5.11778468	-0.32212599	-0.15278557
H	-4.14238368	-2.24452799	0.01731643
C	-4.94343668	1.06024601	-0.28350357
H	-3.50839268	2.67348401	-0.45342357
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H	-5.81571968	1.72527301	-0.34424857

IM2



*Theoretical calculation level:*

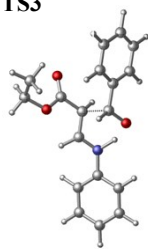
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*Computed total energies: -632.0057687 Hartree*

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O	2.89667100	0.52055400	-0.53398800
C	4.49898200	1.55431900	0.97977100
H	5.51670800	1.97041100	1.04901200
H	4.39874700	0.75413600	1.73011800
H	3.78071600	2.35448200	1.21789600
C	4.24111700	1.00556200	-0.41440800
H	4.33376300	1.79715800	-1.17485900
H	4.94668200	0.19836100	-0.65680300
C	2.64944000	-0.76347400	-0.12524900
C	1.19931494	-1.26827897	-0.00731150
H	1.00830680	-2.27147060	0.31209803
C	0.16429440	-0.44628391	-0.30668359
H	0.34904690	0.55791198	-0.62661660
N	-1.21696317	-0.93593387	-0.19148620
H	-1.25166291	-1.90039145	-0.45343563
C	-2.08938514	-0.15507575	-1.08032844
C	-2.71153713	1.00082309	-0.60778616
C	-2.29513668	-0.56963893	-2.39613686
C	-3.53977334	1.74155890	-1.45073158
H	-2.54973426	1.32696756	0.42985126
C	-3.12281298	0.17175175	-3.23976100
H	-1.80472062	-1.48054525	-2.76879055
C	-3.74522548	1.32712321	-2.76726074
H	-4.03069275	2.65231689	-1.07815338
H	-3.28452723	-0.15512944	-4.27729240
H	-4.39825643	1.91136121	-3.43172509

TS3



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

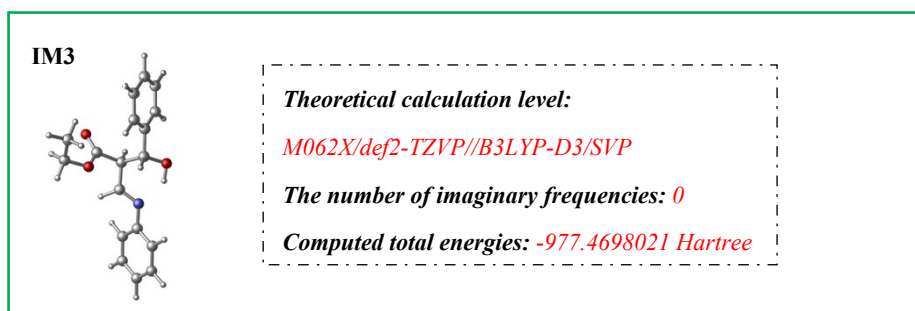
*The number of imaginary frequencies: 1*

*Computed total energies: -977.4359606 Hartree*

C	-0.60519900	-0.99034600	-0.54989700
O	-2.19978200	1.51186000	1.49604400
N	2.06022594	-0.51672190	0.50178918
H	1.35863100	-1.34167100	0.18666300
O	-0.87801200	2.32817700	-0.14673800
C	1.13808200	0.58557700	0.59227500
H	1.47021800	1.60686600	0.36115000
C	6.15552294	-0.28498590	-0.44376782
C	-0.25446200	0.29265400	0.82600300
C	-1.20993600	1.42373300	0.79890900
C	3.43211894	-0.40952390	0.19794018
C	-2.95549800	3.21756500	-1.10808800
H	-3.52557000	4.14928500	-1.25020200
H	-3.60118300	2.48841000	-0.59846000
H	-2.68544500	2.82346500	-2.10121700
C	4.21661094	0.65166510	0.67841218
H	3.77390394	1.41299410	1.32415218
C	5.57412994	0.70909510	0.35129018
H	6.18352494	1.53245710	0.73198418
C	-1.71188500	3.49942400	-0.28182000
H	-1.06669100	4.24214700	-0.77106200
H	-1.97840000	3.86457400	0.72191400
C	5.37145194	-1.34634890	-0.91184582
H	5.81806494	-2.12677190	-1.53264682
C	4.01541194	-1.41559790	-0.59070682
H	3.39265694	-2.23153890	-0.96164482
H	7.21765194	-0.23828190	-0.69026382
C	-2.05772600	-1.32314400	-0.33401300
C	-3.06395900	-0.54963900	-0.93088800
C	-2.41593900	-2.41650900	0.46842100
C	-4.41118900	-0.85485900	-0.71895600
H	-2.78931800	0.29769400	-1.56349200

s28

C	-3.76161200	-2.72259200	0.68171100
H	-1.62084100	-3.01962600	0.91027000
C	-4.76328000	-1.94113500	0.09047200
H	-5.18736800	-0.24401400	-1.18708900
H	-4.03310700	-3.57645400	1.30789800
H	-5.81632400	-2.18210300	0.25662800
O	0.27007200	-1.93761200	-0.37158300
H	-0.46794700	-0.32235100	-1.42931900
H	-0.45653300	-0.39052400	1.65524800

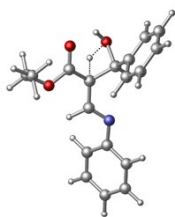


C	-0.53235633	-0.75507201	-0.29710174
O	-2.20966217	1.48828280	1.47358509
N	1.98711983	-0.41787320	0.51120309
H	1.47748732	-1.54273745	0.20200815
O	-0.83151517	2.36156380	-0.09027991
C	1.15333283	0.58249680	0.60174709
H	1.48607683	1.60492580	0.38030009
C	6.08351083	-0.18799820	-0.43078491
C	-0.24066617	0.29332580	0.83456909
C	-1.19463017	1.42510180	0.81134209
C	3.35894683	-0.31181220	0.20867009
C	-2.85651017	3.26441880	-1.13610291
H	-3.42798517	4.19443780	-1.28242591
H	-3.52389717	2.51201380	-0.69240491
H	-2.52055217	2.90588580	-2.12160591
C	4.13836983	0.76273280	0.66788309
H	3.69178283	1.53549980	1.29698809
C	5.49555983	0.81970580	0.34222209
H	6.09979583	1.65427180	0.70606409
C	-1.66984517	3.52873580	-0.22583491
H	-1.00668517	4.29904080	-0.64365091
H	-2.00152917	3.84811080	0.77365909
C	5.30529683	-1.26351520	-0.87623791

s29

H	5.75716383	-2.05568420	-1.47803891
C	3.94871083	-1.33229120	-0.55634991
H	3.33130183	-2.16167920	-0.90863891
H	7.14651683	-0.14004420	-0.67786891
C	-1.98456233	-1.08464001	-0.08464874
C	-2.98647533	-0.32587101	-0.70609974
C	-2.34820533	-2.16002001	0.73953026
C	-4.33541733	-0.62841401	-0.49870574
H	-2.70743333	0.50843299	-1.35476574
C	-3.69532833	-2.46201901	0.94983226
H	-1.55656633	-2.75387201	1.20121226
C	-4.69304733	-1.69574201	0.33250326
H	-5.10854433	-0.02995501	-0.98743174
H	-3.97157833	-3.30124901	1.59373526
H	-5.74724033	-1.93408501	0.49574026
O	0.50508022	-1.88657122	-0.08277734
H	-0.39043933	-0.08772201	-1.17597374
H	-0.44656117	-0.39544320	1.65801309

**TS4**



**Theoretical calculation level:**

*M062X/def2-TZVP//B3LYP-D3/SVP*

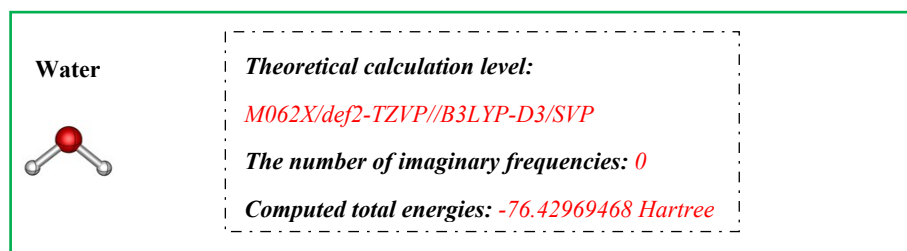
**The number of imaginary frequencies: 1**

**Computed total energies: -977.3934585 Hartree**

C	-0.98520100	-0.71791600	1.27694300
O	-2.39527600	1.63937700	0.80080100
N	1.79282100	-0.54703100	0.42288900
O	-0.63805800	2.62376100	-0.21893700
C	1.10042400	0.53857900	0.47121100
H	1.53210200	1.51594400	0.18987500
C	5.90481200	-0.54953500	-0.55328000
C	-0.28424700	0.56610800	0.89453500
C	-1.20175100	1.63192700	0.48253800
C	3.15803400	-0.50605000	0.11479000
C	-2.26392800	3.43917600	-1.85195000
H	-2.83487200	4.32914000	-2.16008400
H	-2.97093200	2.61712300	-1.66778100
H	-1.59393500	3.15327400	-2.67765200

C	4.03042800	0.50323800	0.57799800
H	3.64347500	1.29590300	1.22310600
C	5.38723800	0.47844300	0.24307100
H	6.04755100	1.26692500	0.61551000
C	-1.46708400	3.74481400	-0.59576300
H	-0.75940300	4.56987800	-0.75735600
H	-2.12954300	4.00099300	0.24426600
C	5.05040900	-1.56536800	-1.00342700
H	5.44446800	-2.37874900	-1.61905600
C	3.69661200	-1.55075000	-0.66528400
H	3.02425100	-2.34224500	-1.00590500
H	6.96664500	-0.56652800	-0.81107500
C	-2.00745200	-1.33991400	0.36369500
C	-1.82188700	-1.26574600	-1.02436600
C	-3.10487700	-2.04801400	0.87574300
C	-2.72732200	-1.88542500	-1.89030200
H	-0.96579900	-0.71816700	-1.42580800
C	-4.01533100	-2.65831800	0.00777300
H	-3.25276200	-2.11236000	1.95639800
C	-3.82827600	-2.57992800	-1.37662200
H	-2.57473700	-1.82014500	-2.97035100
H	-4.87359200	-3.19848600	0.41580300
H	-4.54000800	-3.05823300	-2.05397600
O	-1.69395945	-0.14508209	2.75921246
H	-0.24078600	-1.45865100	1.59892300
H	-0.81203457	0.53024509	2.39173225
H	-2.44053945	0.42224691	2.43088446

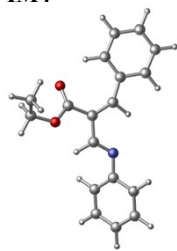
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O	1.30346234	0.66191445	0.00000000
H	2.26346234	0.66191445	0.00000000
H	0.98300775	1.56685028	0.00000000

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IM4



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 0*

*Computed total energies: -901.0384697 Hartree*

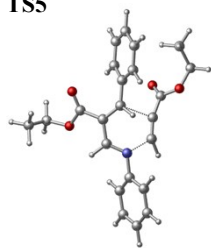
C	0.99055200	-0.52071200	-1.51305600
O	2.80542417	1.29423825	-0.68321721
N	-1.62424283	-0.27489075	-0.56514621
O	1.22692717	2.31001125	0.52848079
C	-0.85938883	0.74739925	-0.55515221
H	-1.18656483	1.74851325	-0.21993621
C	-5.70724483	-0.32907175	0.47460379
C	0.53748617	0.66626425	-1.08712321
C	1.63885717	1.41885525	-0.38357821
C	-2.98561483	-0.23547075	-0.19898821
C	3.18949117	2.80265825	2.00208679
H	3.96219717	3.57399725	2.16596779
H	3.72903317	1.91905625	1.66428679
H	2.68458517	2.57475825	2.96949079
C	-3.85371483	0.80319625	-0.59433421
H	-3.46748283	1.65318425	-1.16055221
C	-5.20705583	0.74923325	-0.26091921
H	-5.87252383	1.54660825	-0.58922321
C	2.21226317	3.30024925	0.95002379
H	1.60276417	4.12214825	1.31573979
H	2.75098117	3.64180325	0.04304779
C	-4.85485883	-1.37672475	0.84226779
H	-5.25526783	-2.23448975	1.38142679
C	-3.50769983	-1.34029575	0.49936179
H	-2.82807583	-2.15226475	0.77259679
H	-6.76352383	-0.37059475	0.74150379
C	1.63267300	-1.48792800	-0.54455600
C	0.78012000	-2.24293400	0.27144400
C	3.01710700	-1.69820900	-0.49489400
C	1.29707900	-3.20206400	1.14295500
H	-0.29482600	-2.04822200	0.22089300
C	3.53365100	-2.66480400	0.38485300

s32



H	3.67936200	-1.11252100	-1.12709600
C	2.67795400	-3.42183900	1.19662500
H	0.60230400	-3.78417000	1.77236100
H	4.62117800	-2.82754900	0.43296400
H	3.09030900	-4.17363300	1.87548000
H	0.13874800	-1.00615800	-2.00522300

**TS5**



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

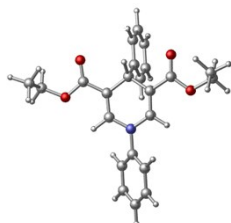
*The number of imaginary frequencies: 1*

*Computed total energies: -1245.446498 Hartree*

O	0.82859300	3.16714600	0.16291300
N	-2.05299400	-0.63452100	0.41098100
O	-1.17796800	3.00856500	-0.84083600
C	-1.75758500	0.63192500	0.24910200
H	-2.55248400	1.35973500	0.04554500
C	-6.05665800	-1.98307700	0.35685100
C	-0.40874800	1.10193800	0.29454600
C	-0.15038800	2.51032100	-0.12450200
C	-3.41083500	-1.04844200	0.37350400
C	-1.57406000	5.29496500	-0.05924100
H	-1.59128600	6.34587700	-0.38817200
H	-0.87939200	5.20870600	0.78913800
H	-2.58522300	5.02049300	0.27938400
C	-4.31278800	-0.59938600	-0.60648700
H	-3.97521100	0.10052600	-1.37450200
C	-5.63084400	-1.06344100	-0.60834300
H	-6.32605100	-0.71128600	-1.37451100
C	-1.12942500	4.40386000	-1.20621200
H	-1.80724000	4.48627500	-2.06715100
H	-0.10785700	4.65187700	-1.53076600
C	-5.15398200	-2.44686200	1.32121500
H	-5.47836100	-3.17077400	2.07281700
C	-3.83411400	-1.98978800	1.32520900
H	-3.11728600	-2.34632500	2.06810000
H	-7.08733700	-2.34578200	0.35098900
C	0.56821000	0.23983400	0.79145700

H	0.17093000	-0.57531800	1.40073500
C	2.01662000	0.41802900	0.87691400
C	2.68240000	-0.11599700	2.00089300
C	2.78141400	1.07184500	-0.11131000
C	4.05538300	0.06440500	2.17161600
H	2.10774200	-0.66011000	2.75503500
C	4.15512500	1.23429300	0.05179400
H	2.29478000	1.43587500	-1.01432400
C	4.79407500	0.74710100	1.19973800
H	4.55164700	-0.33785400	3.05791300
H	4.73596600	1.73958000	-0.72356700
H	5.87138000	0.88158400	1.32465200
O	2.08453800	-1.27734000	-2.18955400
O	2.17921700	-2.88648500	-0.59456700
C	1.56475000	-1.89915800	-1.27952900
C	4.58564500	-2.42335000	-0.47316400
H	5.57074800	-2.81165800	-0.77724800
H	4.53973500	-2.40531500	0.62571300
H	4.48607400	-1.39149300	-0.83547300
C	3.48741200	-3.29887100	-1.04591200
H	3.50681400	-3.28961800	-2.14636000
H	3.58080600	-4.33859700	-0.70057000
C	0.23402100	-1.67994400	-0.79151000
C	-1.00141100	-1.85194900	-0.70714100
H	-1.87827600	-2.40935200	-1.01481700

4a



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 0*

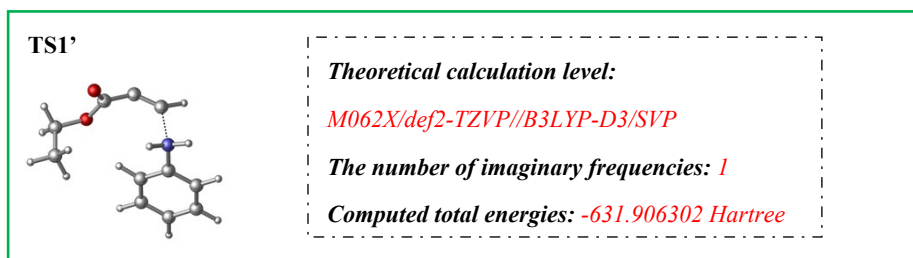
*Computed total energies: -1245.581386 Hartree*

O	0.82923800	3.16674900	0.15986500
N	-2.07550536	-0.73044610	0.42291338
O	-1.17905000	3.00947200	-0.84038500
C	-1.75777300	0.63213400	0.24820900
H	-2.55271200	1.35982800	0.04443000
C	-6.07893236	-2.07971110	0.36965338
C	-0.40891700	1.10222300	0.29345400

C	-0.15053600	2.51049100	-0.12589200
C	-3.43325536	-1.14461410	0.38565538
C	-1.57173400	5.29593800	-0.05729600
H	-1.58869300	6.34697900	-0.38581700
H	-0.87540400	5.20872400	0.78952400
H	-2.58237500	5.02227900	0.28330300
C	-4.33549036	-0.69583210	-0.59420462
H	-3.99820436	0.00404890	-1.36237262
C	-5.65347036	-1.16011210	-0.59572862
H	-6.34890636	-0.80816110	-1.36178462
C	-1.13033900	4.40483700	-1.20544600
H	-1.80998500	4.48803300	-2.06477800
H	-0.10937400	4.65219700	-1.53215800
C	-5.17597436	-2.54323710	1.33387938
H	-5.50007136	-3.26711710	2.08562938
C	-3.85618636	-2.08593510	1.33754538
H	-3.13913936	-2.44225510	2.08032638
H	-7.10955336	-2.44258810	0.36404538
C	0.56797400	0.24025400	0.79073100
H	0.17048900	-0.57470200	1.40014700
C	2.01638400	0.41825300	0.87658000
C	2.68158800	-0.11546500	2.00104300
C	2.78172400	1.07147700	-0.11160600
C	4.05453100	0.06471500	2.17227200
H	2.10649400	-0.65914800	2.75516500
C	4.15540600	1.23367900	0.05200300
H	2.29552700	1.43526900	-1.01493500
C	4.79377200	0.74684400	1.20041300
H	4.55032100	-0.33725800	3.05895500
H	4.73668900	1.73851300	-0.72332100
H	5.87104800	0.88116500	1.32572300
O	2.20712770	-0.57378259	-1.60942854
O	2.30153370	-2.18267359	-0.01419454
C	1.68726870	-1.19537759	-0.69932354
C	4.70787470	-1.71978259	0.10795746
H	5.69303670	-2.10806559	-0.19592654
H	4.66163170	-1.70198459	1.20682046
H	4.60845870	-0.68784259	-0.25415054
C	3.60976570	-2.59511259	-0.46530354

H	3.62943670	-2.58556659	-1.56574054
H	3.70296070	-3.63492659	-0.12019754
C	0.35659370	-0.97594859	-0.21140154
C	-0.87881930	-1.14798959	-0.12709154
H	-1.75562130	-1.70549859	-0.43458754

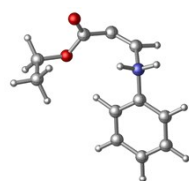
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O	3.31197500	-1.23760100	0.31344700
O	2.21672800	0.45540300	-0.73626000
C	3.09570400	1.90228200	1.03433100
H	3.89026700	2.63026000	1.26553300
H	3.15287600	1.08239200	1.76558300
H	2.12232600	2.40763500	1.14104600
C	3.27369500	1.36122200	-0.37480100
H	3.22571300	2.16962000	-1.11980300
H	4.24303700	0.84784100	-0.47324300
C	2.35796800	-0.85393400	-0.35271600
C	1.31485200	-1.67466800	-0.87708200
C	0.12030900	-2.02726600	-0.59574700
N	-0.71904200	-1.32622000	0.84537900
H	0.02981400	-0.85999900	1.36386000
C	-1.76651300	-0.41928700	0.46651000
C	-3.10099700	-0.83902600	0.48074700
C	-1.42088300	0.85619300	-0.00265900
C	-4.09999100	0.03420200	0.03746100
H	-3.35940000	-1.83898100	0.83997700
C	-2.42761900	1.72238100	-0.43322600
H	-0.36812000	1.14779800	-0.04641900
C	-3.76827900	1.31565500	-0.41478800
H	-5.14251700	-0.29207400	0.05052000
H	-2.16224300	2.72037600	-0.79077000
H	-4.55227600	1.99600000	-0.75610300
H	-1.06225300	-2.10004700	1.42088600
H	-0.68301900	-2.63622400	-1.00439400

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IMI'



*Theoretical calculation level:*

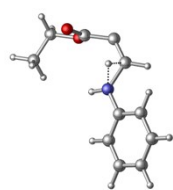
*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 0*

*Computed total energies: -631.9096556 Hartree*

O	3.24541500	-1.10723100	0.45004900
O	2.15731100	0.45841400	-0.78388000
C	2.63241400	2.00864200	1.04901200
H	3.30822500	2.81853100	1.36739200
H	2.66745000	1.21062900	1.80540700
H	1.60804700	2.41168400	1.00612000
C	3.06100200	1.46968400	-0.30662000
H	3.03637500	2.25765000	-1.07380200
H	4.07984500	1.05589700	-0.25811900
C	2.34250700	-0.81855700	-0.32369600
C	1.39785200	-1.72558900	-0.89488100
C	0.22095300	-2.14793900	-0.63652400
N	-0.49175480	-1.61021703	0.49330018
H	0.25335620	-1.19879003	1.06032518
C	-1.48850380	-0.64413503	0.12071018
C	-2.84835680	-0.96018403	0.20686618
C	-1.07273380	0.59078397	-0.39695582
C	-3.80029380	-0.02486403	-0.21273682
H	-3.16382880	-1.92715903	0.60715818
C	-2.03189180	1.51857397	-0.80584582
H	-0.00594580	0.80341797	-0.49832582
C	-3.39674480	1.21606697	-0.71482482
H	-4.86249780	-0.27023803	-0.14078482
H	-1.70961680	2.48315497	-1.20540282
H	-4.14287080	1.94559697	-1.03806182
H	-0.88706280	-2.39088403	1.02369318
H	-0.53686300	-2.81597300	-1.03886500

TS2'



*Theoretical calculation level:*

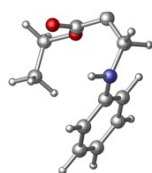
*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 1*

*Computed total energies: -631.8364921 Hartree*

O	2.73406600	-0.93680400	1.28862000
O	3.09773800	-0.09223300	-0.79024600
C	3.63768600	2.00963900	0.34790600
H	4.47670200	2.65724500	0.64921000
H	3.04128100	1.77384500	1.24229300
H	3.00657600	2.56743700	-0.36289300
C	4.16729100	0.73465600	-0.28878100
H	4.78677800	0.95520900	-1.17023900
H	4.76825100	0.15530800	0.42942700
C	2.45981200	-0.89477200	0.09532300
C	1.49139500	-1.75257400	-0.54671500
C	0.16423900	-1.49959700	-0.59029000
N	-0.45560900	-0.20950000	-0.00461700
H	0.15072800	0.60460700	-0.08995100
C	-1.84676600	0.03028700	0.01640000
C	-2.76722000	-1.01118700	0.22442400
C	-2.31322000	1.34363800	-0.16450400
C	-4.13691200	-0.73417700	0.23602800
H	-2.42309200	-2.03230100	0.39746800
C	-3.68399000	1.60770600	-0.13808900
H	-1.60019800	2.15578000	-0.32839300
C	-4.60432700	0.57157100	0.05606400
H	-4.84327100	-1.55197100	0.39880100
H	-4.03288400	2.63387400	-0.27764700
H	-5.67618900	0.78103200	0.07172100
H	-0.61074900	-2.12796900	-1.04027600
H	0.08298900	-1.30444200	0.63920000

IM2'



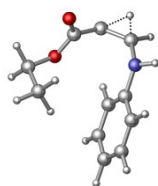
*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 0*

*Computed total energies: -631.8815589 Hartree*

O	3.32735977	-1.00020343	0.50171882
O	2.32988077	0.53983957	-0.84122718
C	2.62192677	2.09470957	1.02515182
H	3.24900777	2.92154457	1.39567582
H	2.61340077	1.29886857	1.78476882
H	1.59487277	2.47165857	0.89580782
C	3.17267577	1.56147557	-0.28886618
H	3.20544277	2.35156657	-1.05420618
H	4.18975277	1.16327457	-0.15074318
C	2.48089477	-0.74090443	-0.34945218
C	1.61555377	-1.66770843	-1.00862618
C	0.21248400	-2.08775000	-0.60198100
N	-0.52485400	-1.47916200	0.64646100
C	-1.58409700	-0.51578700	0.32307600
C	-2.91102700	-0.81543300	0.62878200
C	-1.22847700	0.67157100	-0.32280700
C	-3.90921100	0.10397600	0.28634900
H	-3.16883500	-1.75075000	1.13169100
C	-2.23342100	1.58327600	-0.65199900
H	-0.18230500	0.86428700	-0.57154400
C	-3.57206600	1.30191800	-0.35001100
H	-4.95165400	-0.12102900	0.52209200
H	-1.96819800	2.51724600	-1.15253000
H	-4.35349500	2.01814900	-0.61398800
H	-0.91032800	-2.24196300	1.21646300
H	-0.41771810	-1.90591720	-1.44736976
H	0.24205640	-3.14688105	-0.45276006

**TS3'**

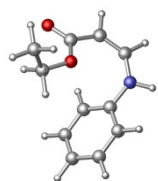
*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 1*

*Computed total energies: -631.8814766 Hartree*

O	2.86115500	-0.42970100	0.90181500
O	1.84749500	0.77678700	-0.73975500
C	1.06444100	2.37167700	0.93849300
H	1.26477400	3.36263500	1.37657400
H	1.05331400	1.62872800	1.75016000
H	0.07035300	2.38759500	0.46583900
C	2.13871400	2.03243700	-0.08068800
H	2.17409700	2.76985300	-0.89437500
H	3.13335300	1.96863500	0.38540400
C	2.20112000	-0.35691100	-0.12049500
C	1.80830300	-1.53774000	-0.88209200
C	0.72787100	-2.31522900	-0.38535500
N	-0.25786600	-1.83267400	0.53772200
H	1.65324300	-2.74906700	0.17550700
C	-1.22356500	-0.88187500	0.18342700
C	-2.31843000	-0.67150600	1.05076700
C	-1.14514000	-0.11313000	-0.99340500
C	-3.29139700	0.28207100	0.75286000
H	-2.39746500	-1.26350100	1.96717900
C	-2.12347200	0.84434300	-1.27810000
H	-0.31188600	-0.23694100	-1.68626700
C	-3.20308000	1.05315200	-0.41340000
H	-4.12963700	0.42209300	1.44178500
H	-2.03478200	1.43235900	-2.19576900
H	-3.96423800	1.80214800	-0.64382300
H	-0.59976800	-2.54597700	1.17495000
H	0.41230400	-3.17027500	-1.00977300

**IM3'**

*Theoretical calculation level:*

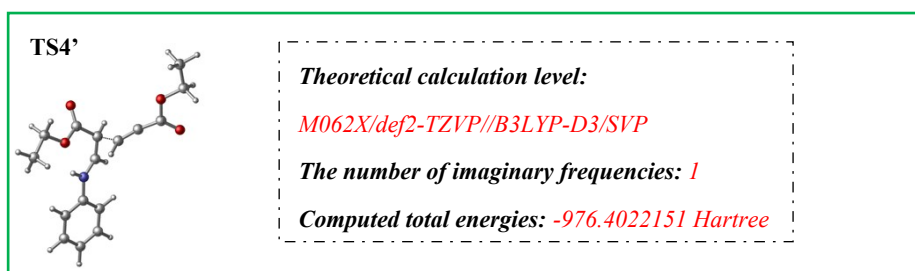
*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 0*

*Computed total energies: -631.9942037 Hartree*



O	-2.87917066	-0.07076830	-0.88991677
O	-1.71153966	0.92490270	0.78981823
C	-0.63972866	2.36733570	-0.86662877
H	-0.65641866	3.38096870	-1.29694577
H	-0.75781166	1.64087570	-1.68431077
H	0.33770834	2.19975770	-0.38987877
C	-1.76431766	2.21921470	0.14365923
H	-1.66914666	2.94143070	0.96595323
H	-2.75065866	2.34337870	-0.32735377
C	-2.22422766	-0.12484030	0.13659823
C	-2.00268066	-1.37540730	0.85681023
C	-0.98512600	-2.28292300	0.30735800
N	0.05326700	-1.86224600	-0.58524300
H	-1.98612205	-2.13166850	0.14309124
C	1.07458900	-0.98381800	-0.20443800
C	2.09235900	-0.68187600	-1.13404500
C	1.12101800	-0.37140000	1.06197900
C	3.10983700	0.21456900	-0.80911700
H	2.06890600	-1.14887400	-2.12250800
C	2.14174400	0.53064200	1.37400800
H	0.35081400	-0.57664400	1.80680400
C	3.14250400	0.83520200	0.44632000
H	3.88324000	0.43483900	-1.54999300
H	2.14984500	0.99904600	2.36181300
H	3.93612400	1.54286000	0.69643700
H	0.32725300	-2.55891400	-1.27127800
H	-0.77105600	-3.19326700	0.89541500

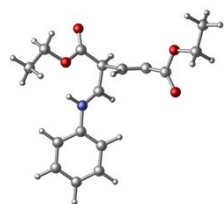


O	1.17911400	2.49501100	0.88534100
N	-2.14173893	-0.07770074	0.03846092

H	-2.21354493	0.91505826	-0.20817808
O	-0.84722500	2.28657600	-0.06859000
C	-0.84997300	-0.49458400	0.45553300
H	-0.74399000	-1.53615200	0.77053100
C	-5.74434193	-2.24656174	-0.24407708
C	0.35611300	0.28818400	0.40622000
C	0.29440500	1.79158300	0.46074300
C	-3.32796093	-0.84514674	-0.05577808
C	-2.38554400	4.02242600	-0.64924600
H	-2.53541500	5.11118400	-0.70550700
H	-3.16682600	3.60096100	0.00251100
H	-2.50542600	3.60374200	-1.66031000
C	-3.33185893	-2.24511674	0.04429592
H	-2.40474793	-2.80409074	0.17638692
C	-4.54172193	-2.93519874	-0.04610008
H	-4.54044893	-4.02486974	0.03044892
C	-1.00717800	3.72551000	-0.10137500
H	-0.20824200	4.14660500	-0.73150400
H	-0.86998700	4.11650700	0.91850500
C	-5.73227893	-0.85227974	-0.35509308
H	-6.66351793	-0.30403574	-0.51422808
C	-4.53002793	-0.14968974	-0.26145508
H	-4.52141493	0.94010026	-0.34289408
H	-6.68542693	-2.79594474	-0.31739608
O	4.21946334	-2.75916551	0.09008858
O	5.08759634	-0.67885051	-0.04455142
C	1.98337634	-0.52309351	1.13795958
C	2.76356634	-0.87109351	0.10439958
C	4.04957834	-1.54751951	0.08941158
C	7.38310234	-0.11192351	-0.35286242
H	8.40420134	-0.50869751	-0.46358642
H	7.36242134	0.55338549	0.52453158
H	7.14412434	0.48667149	-1.24583942
C	6.39631434	-1.24968251	-0.18821842
H	6.40612534	-1.92800651	-1.05829842
H	6.62898334	-1.86460051	0.69787758
H	2.16542634	-0.62117351	2.21895958
H	0.87017819	0.03271760	-0.49676056

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IM4'



*Theoretical calculation level:*

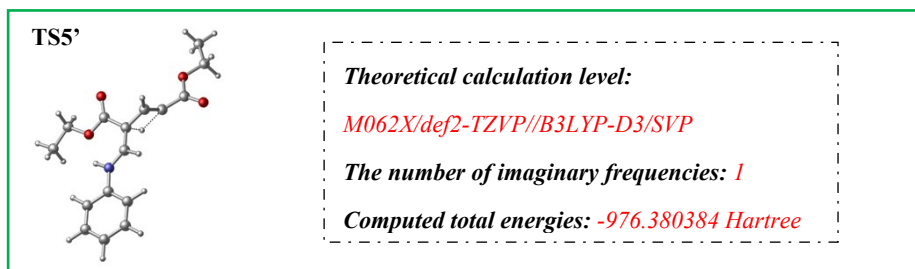
*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 0*

*Computed total energies: -976.409133 Hartree*

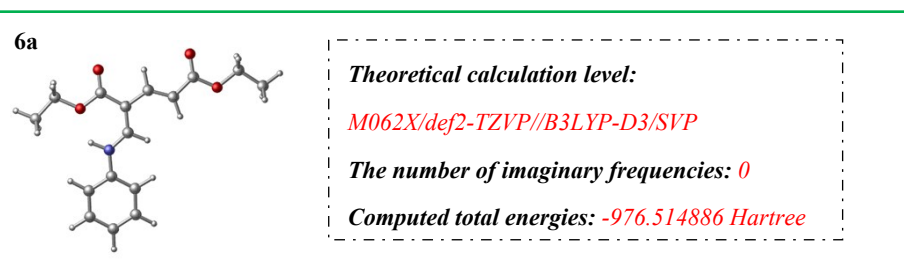
O	0.98789062	2.64589742	-1.55320098
N	-1.91309438	-0.08988258	-0.24939298
H	-1.83617638	0.80359842	0.24718702
O	-0.53784738	2.24880542	0.05760002
C	-0.92108038	-0.35854458	-1.07510698
H	-0.99416738	-1.26796258	-1.67493298
C	-5.46218238	-2.23381858	0.49765302
C	0.32683262	0.37581842	-1.09939098
C	0.30182962	1.87440942	-0.92897598
C	-3.08684138	-0.84439058	-0.01204398
C	-1.65374538	3.82346942	1.46945402
H	-1.72038538	4.88262542	1.76051002
H	-1.38880738	3.23452342	2.36082902
H	-2.64522538	3.50121942	1.11472302
C	-3.21525838	-2.17996458	-0.42431998
H	-2.39417238	-2.69712058	-0.92230898
C	-4.40537038	-2.86349958	-0.17041298
H	-4.50134538	-3.90359458	-0.49015298
C	-0.61159238	3.65876342	0.38629202
H	-0.86539138	4.21678642	-0.52794798
H	0.38733862	3.98559342	0.71417602
C	-5.32269038	-0.90658058	0.91756102
H	-6.13889138	-0.40659058	1.44377802
C	-4.14054538	-0.20963458	0.66489402
H	-4.03401038	0.82951142	0.98597002
H	-6.38792338	-2.77848058	0.69563102
O	3.56685100	-2.69774100	0.35746300
O	4.53609600	-0.63664400	0.28802600
C	1.12943700	-0.17323000	0.14590900
C	2.25471400	-0.77938300	0.02100400
C	3.44289800	-1.47428400	0.24223000
C	6.86468500	-0.17582300	0.45172400

H	7.86644800	-0.61577000	0.57639600
H	6.69202800	0.53399800	1.27608900
H	6.84742600	0.38637400	-0.49529000
C	5.80933400	-1.26456300	0.45004100
H	5.97820900	-1.98757400	-0.36726600
H	5.82700000	-1.84284900	1.39033400
H	0.53242400	0.08461800	1.03658200
H	0.91437462	0.13189442	-1.98678898



O	0.77858764	3.34687365	0.13900964
N	-1.78318736	-0.07891735	-0.00007336
H	-2.19637636	0.85292665	-0.07008736
O	-1.33625736	2.56935465	0.09049064
C	-0.46014836	-0.10711635	0.11992864
H	0.02588964	-1.08538735	0.18367764
C	-4.56318736	-3.24797935	-0.06789036
C	0.40414164	0.99062665	0.15701164
C	0.00417064	2.41238965	0.12782064
C	-2.67669936	-1.17046535	-0.01467936
C	-3.36897936	3.81692265	0.04338164
H	-3.80893536	4.82542865	0.02669664
H	-3.73951536	3.29168465	0.93722664
H	-3.71333836	3.27464065	-0.85102836
C	-2.25489936	-2.50461035	0.10816864
H	-1.20017336	-2.75392935	0.22885064
C	-3.20035636	-3.53143735	0.07897764
H	-2.86374736	-4.56644835	0.17484364
C	-1.85949936	3.91740065	0.06559064
H	-1.46182636	4.43110465	-0.82361536
H	-1.48993336	4.45246765	0.95409564
C	-4.97925736	-1.91767035	-0.18657336
H	-6.03953236	-1.68020735	-0.30063736
C	-4.04438436	-0.88191835	-0.16094936
H	-4.37113336	0.15711865	-0.25539936

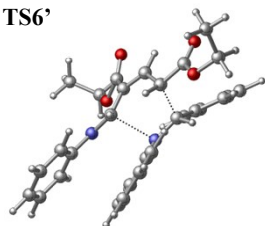
H	-5.29486736	-4.05859535	-0.08797736
O	4.04948008	-1.18097623	1.75782466
O	4.61664708	-0.49494023	-0.32453234
C	1.80532908	0.75382877	0.38982166
C	2.35828508	-0.48198923	0.26336366
C	3.71959908	-0.72498023	0.67000366
C	6.78875808	-0.54318223	-1.30718234
H	7.84732708	-0.80022523	-1.14704334
H	6.72540508	0.52731277	-1.55783334
H	6.41656608	-1.12234023	-2.16670634
C	5.98361908	-0.85163023	-0.06165434
H	6.03772508	-1.92063823	0.20489566
H	6.35034008	-0.28412723	0.81001566
H	2.29596008	1.68948677	0.68800966
H	1.26052195	-0.20420182	-0.92989566



O	1.24919287	2.50994632	0.73274146
N	-2.05599986	-0.05260171	-0.11477892
H	-2.12780586	0.94015729	-0.36141792
O	-0.77714613	2.30151132	-0.22118954
C	-0.76423392	-0.46948497	0.30229316
H	-0.65825092	-1.51105297	0.61729116
C	-5.65860286	-2.22146271	-0.39731692
C	0.42619187	0.30311932	0.25362046
C	0.36448387	1.80651832	0.30814346
C	-3.24222186	-0.82004771	-0.20901792
C	-2.31546513	4.03736132	-0.80184554
H	-2.46533613	5.12611932	-0.85810654
H	-3.09674713	3.61589632	-0.15008854
H	-2.43534713	3.61867732	-1.81290954
C	-3.24611986	-2.22001771	-0.10894392
H	-2.31900886	-2.77899171	0.02314708
C	-4.45598286	-2.91009971	-0.19933992

H	-4.45470986	-3.99977071	-0.12279092
C	-0.93709913	3.74044532	-0.25397454
H	-0.13816313	4.16154032	-0.88410354
H	-0.79990813	4.13144232	0.76590546
C	-5.64653986	-0.82718071	-0.50833292
H	-6.57777886	-0.27893671	-0.66746792
C	-4.44428886	-0.12459071	-0.41469492
H	-4.43567586	0.96519929	-0.49613392
H	-6.59968786	-2.77084571	-0.47063592
O	3.91581987	-2.55790968	-0.23056454
O	4.78395287	-0.47759468	-0.36520454
C	1.67973287	-0.32183768	0.81730646
C	2.45992287	-0.66983768	-0.21625354
C	3.74593487	-1.34626368	-0.23124154
C	7.07945887	0.08933232	-0.67351554
H	8.10055787	-0.30744168	-0.78423954
H	7.05877787	0.75464132	0.20387846
H	6.84048087	0.68792732	-1.56649254
C	6.09267087	-1.04842668	-0.50887154
H	6.10248187	-1.72675068	-1.37895154
H	6.32533987	-1.66334468	0.37722446
H	1.86178287	-0.41991768	1.89830646
H	2.64598533	-0.45563848	-1.23757595

TS6'



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

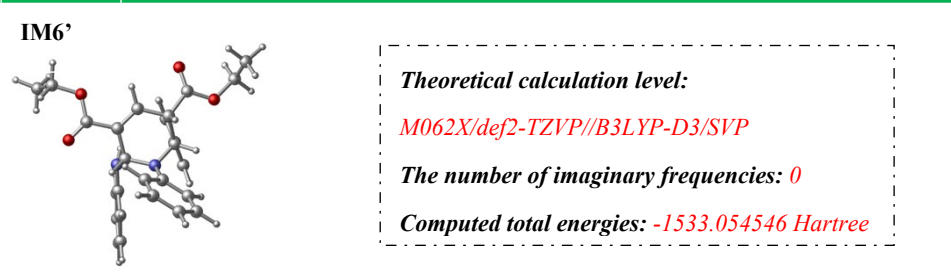
*The number of imaginary frequencies: 1*

*Computed total energies: -1533.000695 Hartree*

O	-0.74973019	3.41848534	-1.73329930
N	2.17141029	0.78188142	-0.29902941
H	2.23460029	1.74085342	0.03416059
O	1.01483681	3.19445034	-0.35384130
C	0.92527329	0.33485042	-0.58808341
H	0.91333129	-0.63526958	-1.08994841
C	5.82875029	-1.33245758	-0.43503941
C	-0.10638419	1.22210834	-1.02780630

C	0.01026681	2.71042734	-1.11118630
C	3.38015629	0.06336942	-0.38327741
C	2.00246381	5.10681134	-1.52486630
H	2.19602581	6.18771934	-1.42914830
H	1.44079081	4.93150234	-2.45495930
H	2.96751081	4.58159034	-1.59380330
C	3.53214029	-1.07533658	-1.19612341
H	2.70760829	-1.44083258	-1.81097141
C	4.74488829	-1.76522158	-1.20893741
H	4.84304329	-2.65800258	-1.83084141
C	1.21416381	4.63009134	-0.31865930
H	1.75973681	4.80468934	0.61786870
H	0.23165081	5.12010534	-0.25367030
C	5.69037129	-0.17768758	0.34321559
H	6.52726529	0.17609242	0.95575459
C	4.47918929	0.51809642	0.36611559
H	4.37186929	1.40782842	0.99231659
H	6.76862429	-1.89124558	-0.43848141
O	-4.01586834	-0.35191358	-1.47904339
O	-3.23115534	-2.39796258	-0.94047339
C	-1.38173005	0.69202184	-1.25693779
C	-1.69652434	-0.63563458	-0.82899739
C	-3.10615234	-1.07610358	-1.13956539
C	-4.80664334	-3.28482558	-2.59333939
H	-5.77549634	-3.79712958	-2.69985139
H	-4.02243134	-3.93574458	-3.00989539
H	-4.84408834	-2.35323258	-3.17622039
C	-4.53650934	-2.99234258	-1.12853939
H	-5.29265234	-2.31323158	-0.70761039
H	-4.50880034	-3.91196158	-0.52820539
H	-2.19712805	1.35136584	-1.55812479
H	-1.01477434	-1.40473958	-1.22370539
C	-1.31588777	-0.61996531	0.79446360
H	-1.74333577	-1.58352731	1.12105860
C	-2.08993377	0.49750169	1.48232960
C	-3.46623177	0.35614269	1.72509560
C	-1.46853777	1.70467069	1.83883860
C	-4.21252277	1.40675269	2.27055860
H	-3.96374777	-0.58685031	1.48291160

C	-2.20999477	2.75769769	2.38334760
H	-0.39402677	1.80995469	1.68409760
C	-3.58684177	2.61650769	2.59372560
H	-5.28506177	1.27979769	2.44259860
H	-1.70675377	3.69374069	2.64234660
H	-4.16808377	3.44068069	3.01476960
N	0.03379600	-0.55741300	1.02104900
C	0.71164100	-1.77788700	1.10630900
C	0.25482300	-3.01858600	0.58808000
C	1.98941800	-1.76289900	1.71589500
C	1.06645600	-4.15767500	0.63592000
H	-0.73645900	-3.10506900	0.13891000
C	2.79427400	-2.89783700	1.75293900
H	2.33616700	-0.82182900	2.14492700
C	2.34429100	-4.10610400	1.20225800
H	0.69338000	-5.09557600	0.21250500
H	3.78619800	-2.83818200	2.20896500
H	2.97874000	-4.99588300	1.22226500



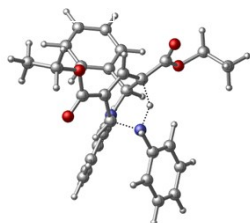
O	1.07913400	3.65595000	-0.94832400
N	1.33380500	0.96431500	0.63353000
H	0.67293200	0.77105600	1.37773800
O	-1.09396000	4.05862200	-0.50132500
C	0.73025000	0.84343500	-0.69448100
H	1.48249400	1.17151400	-1.42316800
C	5.21301000	-0.40735900	1.59956200
C	-0.42621900	1.81371900	-0.80189200
C	-0.05130000	3.25543600	-0.75468100
C	2.61776800	0.50086000	0.91988300
C	-0.31491300	5.93313800	0.86368400
H	-0.21497500	7.02982900	0.87741300
H	0.67540100	5.49185100	1.04879500
H	-0.99435500	5.63577900	1.67738600



C	3.68924700	0.63557000	0.01289900
H	3.52858200	1.09648900	-0.96261200
C	4.96406300	0.17936200	0.35269200
H	5.77599100	0.28995000	-0.37151000
C	-0.85816000	5.48305200	-0.48126300
H	-1.84078200	5.92881900	-0.68905400
H	-0.16769900	5.74421200	-1.29719200
C	4.15633600	-0.53143700	2.50918700
H	4.32610000	-0.98788900	3.48839000
C	2.87509000	-0.09088900	2.17532600
H	2.05192100	-0.21156400	2.88560000
H	6.21402700	-0.76071800	1.85764900
O	-4.20119700	0.48109900	-0.09955000
O	-3.72191900	-1.64370600	-0.67779900
C	-1.69043300	1.40393000	-0.98364600
C	-2.06113700	-0.04298200	-1.12668700
C	-3.44722000	-0.34052000	-0.56976800
C	-6.10509100	-1.90953800	-1.17538900
H	-7.04024400	-2.34553900	-0.79049100
H	-5.86246500	-2.39768100	-2.13187700
H	-6.27014800	-0.83706100	-1.35455100
C	-4.98960900	-2.11782400	-0.16724300
H	-5.20364200	-1.60275100	0.78112000
H	-4.82065100	-3.18394000	0.03657100
H	-2.49622900	2.13595000	-1.05789400
H	-2.13259300	-0.25561300	-2.21048100
C	-0.97239500	-1.00282400	-0.56895100
H	-1.12519600	-1.97307600	-1.05680700
C	-1.11461900	-1.25675100	0.94189800
C	-0.98874900	-2.56798000	1.42740000
C	-1.40135600	-0.23859000	1.86843800
C	-1.08807400	-2.85083300	2.79291300
H	-0.81997300	-3.38735500	0.72402500
C	-1.49983400	-0.51492800	3.23645300
H	-1.56401000	0.78574500	1.52971000
C	-1.33191100	-1.82089400	3.70667800
H	-0.98095900	-3.88106100	3.14172900
H	-1.71542700	0.29725700	3.93514800
H	-1.40688800	-2.03660900	4.77525300

N	0.31846000	-0.50622100	-1.05090200
C	1.31043500	-1.39809900	-1.52854600
C	1.95467700	-1.11472700	-2.74907200
C	1.68391400	-2.55737100	-0.82718700
C	2.94602600	-1.96168500	-3.24648300
H	1.66071400	-0.22488300	-3.31097700
C	2.65758500	-3.41926200	-1.34269300
H	1.24001100	-2.75881700	0.14595600
C	3.29779200	-3.12509000	-2.55043400
H	3.43424800	-1.72138400	-4.19469500
H	2.93396300	-4.31483700	-0.77943200
H	4.06649200	-3.79356300	-2.94571900

**TS7'**



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 1*

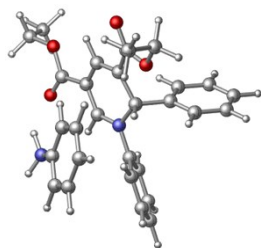
*Computed total energies: -1533.010888 Hartree*

O	2.27581500	-3.15332900	-1.26981600
O	3.72635500	-1.47032200	-1.69014800
C	0.13860500	-1.30094800	-0.66783500
C	1.53837500	-0.90687800	-1.08214700
C	2.51889900	-1.95888200	-1.34838400
C	5.43579400	-2.88958600	-0.66889500
H	6.28528800	-3.55119800	-0.90090700
H	4.71550500	-3.45099100	-0.05585400
H	5.81003400	-2.03538300	-0.08347300
C	4.78234500	-2.41376900	-1.95542500
H	5.49444600	-1.86452900	-2.58741900
H	4.37632100	-3.25998000	-2.53009400
O	1.22435700	3.13503600	-2.16172300
O	-0.51055000	3.31497300	-0.72055900
C	1.70509100	0.43375000	-1.26763000
C	0.56222100	1.23659700	-0.88241500
C	0.50445200	2.63132900	-1.31529700
C	-1.61720000	4.66741200	-2.42688700
H	-1.85380800	5.70366500	-2.71604100
H	-2.56331500	4.12740900	-2.26497500

H	-1.07509100	4.19086400	-3.25704200
C	-0.76847600	4.65777300	-1.16649100
H	0.18838900	5.17564600	-1.33062200
H	-1.29126000	5.13792300	-0.32678900
H	2.59560300	0.86191600	-1.73350700
C	-0.00112600	0.84175800	0.51106000
H	-0.94285900	1.39104500	0.65205000
C	0.96141700	1.25294500	1.62552900
C	0.94828500	2.57420200	2.10109200
C	1.89096200	0.35043900	2.16155600
C	1.85432000	2.98731900	3.08223600
H	0.22356000	3.28129300	1.69170800
C	2.79982000	0.76318400	3.14166200
H	1.89156900	-0.68387800	1.81356800
C	2.78679900	2.08324300	3.60449700
H	1.82943900	4.01888500	3.44357900
H	3.51813900	0.04699700	3.54973100
H	3.49422400	2.40440100	4.37338800
N	-0.28927200	-0.60310300	0.51332900
C	-1.16634500	-1.15993000	1.45307500
C	-1.63635800	-0.38767000	2.54106200
C	-1.61187700	-2.49930000	1.36700400
C	-2.50912500	-0.93320100	3.48555900
H	-1.31346200	0.64384000	2.66729100
C	-2.48221800	-3.03066800	2.31876800
H	-1.29941800	-3.14016000	0.54435900
C	-2.94383400	-2.25741500	3.38924400
H	-2.84942600	-0.30289900	4.31179800
H	-2.80745800	-4.06903200	2.21141300
H	-3.62699800	-2.67851000	4.13017400
N	-0.76136600	-0.81674600	-1.82562300
H	-0.45357800	-1.24953500	-2.69896400
C	-2.18990800	-0.91689900	-1.65082100
C	-2.90514800	0.19645200	-1.19701100
C	-2.84706700	-2.12530300	-1.90829500
C	-4.28115700	0.08944000	-0.97534800
H	-2.39049300	1.14373700	-1.02473300
C	-4.22437300	-2.22245600	-1.69715200
H	-2.27751500	-2.98799700	-2.26215000

C	-4.94166500	-1.11869600	-1.22100500
H	-4.83816700	0.95691200	-0.61380300
H	-4.73711200	-3.16623700	-1.89695100
H	-6.01710500	-1.19975300	-1.04635600
H	-0.32361000	0.40325800	-1.67885600
H	0.05576300	-2.38509500	-0.56433900

**5a+aniline**



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

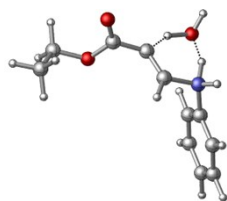
*The number of imaginary frequencies: 0*

*Computed total energies: -1533.080653 Hartree*

O	2.27581500	-3.15332900	-1.26981600
O	3.72635500	-1.47032200	-1.69014800
C	0.13860500	-1.30094800	-0.66783500
C	1.53837500	-0.90687800	-1.08214700
C	2.51889900	-1.95888200	-1.34838400
C	5.43579400	-2.88958600	-0.66889500
H	6.28528800	-3.55119800	-0.90090700
H	4.71550500	-3.45099100	-0.05585400
H	5.81003400	-2.03538300	-0.08347300
C	4.78234500	-2.41376900	-1.95542500
H	5.49444600	-1.86452900	-2.58741900
H	4.37632100	-3.25998000	-2.53009400
O	1.22435700	3.13503600	-2.16172300
O	-0.51055000	3.31497300	-0.72055900
C	1.70509100	0.43375000	-1.26763000
C	0.56222100	1.23659700	-0.88241500
C	0.50445200	2.63132900	-1.31529700
C	-1.61720000	4.66741200	-2.42688700
H	-1.85380800	5.70366500	-2.71604100
H	-2.56331500	4.12740900	-2.26497500
H	-1.07509100	4.19086400	-3.25704200
C	-0.76847600	4.65777300	-1.16649100
H	0.18838900	5.17564600	-1.33062200
H	-1.29126000	5.13792300	-0.32678900
H	2.59560300	0.86191600	-1.73350700
C	-0.00112600	0.84175800	0.51106000

H	-0.94285900	1.39104500	0.65205000
C	0.96141700	1.25294500	1.62552900
C	0.94828500	2.57420200	2.10109200
C	1.89096200	0.35043900	2.16155600
C	1.85432000	2.98731900	3.08223600
H	0.22356000	3.28129300	1.69170800
C	2.79982000	0.76318400	3.14166200
H	1.89156900	-0.68387800	1.81356800
C	2.78679900	2.08324300	3.60449700
H	1.82943900	4.01888500	3.44357900
H	3.51813900	0.04699700	3.54973100
H	3.49422400	2.40440100	4.37338800
N	-0.28927200	-0.60310300	0.51332900
C	-1.16634500	-1.15993000	1.45307500
C	-1.63635800	-0.38767000	2.54106200
C	-1.61187700	-2.49930000	1.36700400
C	-2.50912500	-0.93320100	3.48555900
H	-1.31346200	0.64384000	2.66729100
C	-2.48221800	-3.03066800	2.31876800
H	-1.29941800	-3.14016000	0.54435900
C	-2.94383400	-2.25741500	3.38924400
H	-2.84942600	-0.30289900	4.31179800
H	-2.80745800	-4.06903200	2.21141300
H	-3.62699800	-2.67851000	4.13017400
N	-0.72389212	-0.83690768	-1.77741388
C	-2.15243412	-0.93706068	-1.60261188
C	-2.86767412	0.17629032	-1.14880188
C	-2.80959312	-2.14546468	-1.86008588
C	-4.24368312	0.06927832	-0.92713888
H	-2.35301912	1.12357532	-0.97652388
C	-4.18689912	-2.24261768	-1.64894288
H	-2.24004112	-3.00815868	-2.21394088
C	-4.90419112	-1.13885768	-1.17279588
H	-4.80069312	0.93675032	-0.56559388
H	-4.69963812	-3.18639868	-1.84874188
H	-5.97963112	-1.21991468	-0.99814688
H	0.05576300	-2.38509500	-0.56433900
H	-0.52159519	0.13385301	-1.90664099
H	-0.49503350	-1.40240875	-2.56977256

TS2\_W



*Theoretical calculation level:*

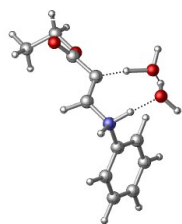
*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 1*

*Computed total energies: -708.343382 Hartree*

O	-3.53694100	-1.05184800	-0.53928700
O	-2.52808900	0.58850700	0.65176100
C	-3.77873700	2.24078600	-0.62630200
H	-4.63367300	2.93549500	-0.59191000
H	-3.88640600	1.60284100	-1.51621000
H	-2.85655700	2.83292200	-0.73002000
C	-3.72329000	1.39279500	0.63649700
H	-3.65531500	2.02637500	1.53576000
H	-4.61064400	0.74506900	0.72512500
C	-2.53199400	-0.58216300	-0.03476800
C	-1.20206300	-1.19130600	-0.02450300
C	-0.27332000	-0.74233800	-0.86634900
H	-0.34398100	0.05581900	-1.61477200
N	1.10521900	-1.30537100	-0.76587900
H	1.39403200	-1.72429800	-1.65619600
C	2.08895000	-0.30774800	-0.34989900
C	1.99755000	0.20760600	0.94814900
C	3.07734800	0.13176700	-1.23287500
C	2.91687100	1.17601200	1.36176300
H	1.20880300	-0.14837500	1.61571000
C	3.99496700	1.10070000	-0.80780800
H	3.12803800	-0.27137800	-2.24789600
C	3.91683600	1.62194400	0.48723800
H	2.85205100	1.58224000	2.37270700
H	4.77111300	1.45024500	-1.49747700
H	4.63274100	2.38134200	0.81337200
O	0.40346200	-2.85073100	1.08829600
H	-0.53994100	-2.21797000	0.77415200
H	0.99138100	-2.13139900	0.02507300
H	0.20566200	-3.75707900	0.80070700

TS2\_2W



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

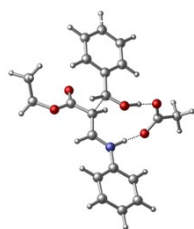
*The number of imaginary frequencies: 1*

*Computed total energies: -784.7674898 Hartree*

O	3.29858400	0.56594500	-1.26004500
O	2.80915000	-0.38961900	0.72767200
C	4.37305800	-2.15838700	0.07300500
H	5.38951400	-2.54405200	0.25038300
H	4.25212100	-1.98120600	-1.00582500
H	3.65047200	-2.92703500	0.38879700
C	4.16091100	-0.86936500	0.85051700
H	4.30550500	-1.02757300	1.92908100
H	4.85672200	-0.08663000	0.51118700
C	2.48548900	0.30277100	-0.39154600
C	1.08514100	0.74422600	-0.35101100
C	0.24823800	0.27684000	-1.27201600
H	0.45386600	-0.46463000	-2.05326600
N	-1.18049800	0.70590600	-1.29511800
H	-1.49234800	0.76489000	-2.27011900
C	-2.09544600	-0.16921800	-0.55038100
C	-2.10995200	-0.07788400	0.84511400
C	-2.91689000	-1.06596300	-1.23363100
C	-2.97538600	-0.90906700	1.56142500
H	-1.45049600	0.62766700	1.35654300
C	-3.77723900	-1.89282800	-0.50311200
H	-2.88998700	-1.12140200	-2.32472700
C	-3.80754300	-1.81504200	0.89248200
H	-2.99833100	-0.84608300	2.65190700
H	-4.42280200	-2.59808700	-1.02996500
H	-4.48050500	-2.46126000	1.46064600
O	0.10066800	2.18894800	1.59778400
H	0.63988300	1.55146700	0.72621300
H	0.77915800	2.77098000	1.96838400
O	-1.44824200	3.07193200	-0.18369100
H	-1.28244300	1.72010100	-0.88873500
H	-0.81805200	2.86349100	0.60821900

H -2.33236200 3.12387300 0.20826300

TS3\_HOAc



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 1*

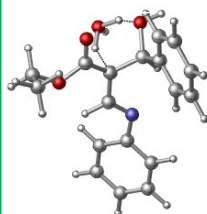
*Computed total energies: -1206.503825 Hartree*

C	-0.77388800	0.22447900	1.14724800
O	-2.36638700	-1.15812400	-1.87214700
N	1.95141600	-0.39653000	-0.35651800
O	-1.46100800	-2.68320100	-0.47790800
C	0.88288900	-1.15318700	-0.38038800
H	0.95002100	-2.19231200	-0.04317400
C	5.86328400	-1.27028200	0.93448600
C	-0.38791300	-0.59502500	-0.68321900
C	-1.49895200	-1.48334700	-1.09004300
C	3.25504200	-0.73183300	0.06999900
C	-3.78832300	-3.48975100	-0.29392000
H	-4.45799200	-4.29322200	-0.64024900
H	-4.21655600	-2.52414700	-0.59698900
H	-3.74157600	-3.53337400	0.80504300
C	3.72335500	-2.05073700	0.12681100
H	3.08124900	-2.88535100	-0.17637900
C	5.02456800	-2.31062700	0.56030200
H	5.38877800	-3.33666600	0.59030300
C	-2.41452900	-3.68165500	-0.91035200
H	-1.96823500	-4.63680000	-0.60267500
H	-2.47145900	-3.65416200	-2.00873800
C	5.40013300	0.06407400	0.85994500
H	6.04374500	0.87875300	1.15032900
C	4.09904500	0.32808000	0.43141200
H	3.72418100	1.35781100	0.37958600
H	6.88310100	-1.47865000	1.26547800
C	-2.17093900	0.71944300	1.00065400
C	-3.22539700	-0.19518400	1.20307500
C	-2.46698600	2.06427500	0.71547700
C	-4.55226500	0.22905600	1.12984800



H	-2.99934500	-1.25186900	1.41404100
C	-3.79763600	2.48446700	0.65001300
H	-1.66047900	2.77521100	0.55082100
C	-4.84142100	1.57536900	0.85836800
H	-5.36228600	-0.49538100	1.28700100
H	-4.02170100	3.52707000	0.43513000
H	-5.88021900	1.91081600	0.80920600
O	0.23033400	1.02565300	1.37709400
H	-0.71467800	-0.71741100	1.71310300
H	-0.38016700	0.34227400	-1.24172900
C	1.10317100	3.02504200	-0.98149700
O	1.58104800	1.96528100	-1.45412000
O	0.50332900	3.11401100	0.14114400
H	0.31005200	1.95878500	0.80647200
C	1.26371700	4.31287100	-1.77419100
H	0.32672400	4.88724400	-1.77779700
H	2.03133500	4.93555500	-1.28219700
H	1.58474700	4.09863200	-2.80097300
H	1.81058700	0.60077300	-0.69667400

TS4\_W



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

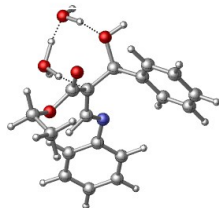
*The number of imaginary frequencies: 1*

*Computed total energies: -1053.838342 Hartree*

C	-1.07422500	-0.46696200	1.30281700
O	-2.54402400	1.67112900	0.29434100
N	1.70799900	-0.42619100	0.43247400
O	-0.80753900	2.51071400	-0.88051200
C	0.95629700	0.59445800	0.16293600
H	1.33995300	1.44789800	-0.42571300
C	5.81490000	-0.51289600	-0.56919700
C	-0.40524900	0.71351000	0.60452400
C	-1.33957600	1.63973500	-0.00193800
C	3.06332900	-0.41025200	0.09908900
C	-2.44791600	2.92030700	-2.64832700
H	-3.04893200	3.70981300	-3.12681300

H	-3.12532600	2.12278300	-2.30980400
H	-1.75880800	2.50499700	-3.40024700
C	3.88292100	0.73596000	0.21383000
H	3.45364100	1.66752000	0.59108300
C	5.23920700	0.68098500	-0.11991900
H	5.85436600	1.57968800	-0.01825600
C	-1.67667600	3.49507900	-1.47218600
H	-1.00386400	4.30366500	-1.79196900
H	-2.36054400	3.88563100	-0.70358200
C	5.01640000	-1.66037900	-0.67136900
H	5.45462700	-2.60194300	-1.01421800
C	3.66348100	-1.61325900	-0.33385600
H	3.03596100	-2.50510300	-0.40649000
H	6.87645100	-0.55295000	-0.82565700
C	-1.78730000	-1.45611100	0.38869700
C	-1.32256600	-1.68983000	-0.91479600
C	-2.89399400	-2.18547700	0.85150000
C	-1.95283700	-2.62840900	-1.73788700
H	-0.46045700	-1.13601800	-1.28871800
C	-3.52848900	-3.11946500	0.02632600
H	-3.26440100	-2.00972900	1.86281600
C	-3.06005200	-3.34547800	-1.27222700
H	-1.57818200	-2.79588700	-2.75113700
H	-4.39412500	-3.67231700	0.40090000
H	-3.55567200	-4.07481200	-1.91810300
O	-2.11121703	0.08421506	2.41872532
H	-0.30016900	-1.01319000	1.86416700
H	-2.24010727	-0.71250756	2.99603966
O	-0.42577100	1.71776300	3.06492200
H	0.28713700	1.37959500	3.63618900
H	-0.14267000	1.55057900	2.03357000
H	-1.21293700	0.98234500	3.00778800

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**TS4\_2W**

*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

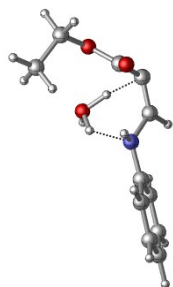
*The number of imaginary frequencies: 1*

*Computed total energies: -1130.266497 Hartree*

C	-0.89180118	0.45937950	-1.21562191
O	-2.48278300	-1.31730200	0.33923700
N	1.89925050	0.49913812	-0.43649041
O	-0.67508500	-1.95429100	1.53722600
C	1.07287650	-0.36483488	0.08221859
H	1.41877950	-1.06834088	0.86003859
C	6.04659950	0.43072312	0.39734659
C	-0.34126800	-0.50149300	-0.29516700
C	-1.27181800	-1.24753600	0.53097800
C	3.25817350	0.43388312	-0.14367941
C	-2.19599100	-1.95952300	3.45261800
H	-2.77498000	-2.62152400	4.11642500
H	-2.88183400	-1.22424800	3.00715000
H	-1.44997400	-1.42418600	4.06100900
C	3.96642350	-0.77783888	0.04566459
H	3.43659050	-1.72906788	-0.04840541
C	5.33764850	-0.77348388	0.31616259
H	5.86043850	-1.72465988	0.45357059
C	-1.51582100	-2.77212400	2.36182300
H	-0.84222100	-3.52806500	2.79244500
H	-2.26249800	-3.28226100	1.73362600
C	5.36280050	1.63749812	0.19328259
H	5.90359050	2.58692212	0.24524059
C	3.99486350	1.63965512	-0.07988441
H	3.46047450	2.57892312	-0.24446341
H	7.11975250	0.42949912	0.60391359
C	-1.67855418	1.56190950	-0.52229991
C	-0.97166418	2.59797650	0.11198709
C	-3.07877418	1.56151350	-0.46414291
C	-1.65196718	3.61133850	0.79155709
H	0.12109482	2.59271650	0.07438609

C	-3.76099718	2.57934650	0.21265009
H	-3.62945818	0.75092750	-0.94190991
C	-3.05202018	3.60675550	0.84333409
H	-1.08860818	4.41135750	1.27968209
H	-4.85382518	2.56605950	0.25046409
H	-3.58605418	4.40102050	1.37159409
H	-0.02456618	0.92411450	-1.70982591
O	-0.43583043	-2.74712156	-1.84132425
H	-0.69990264	-2.31175672	-2.92120045
H	0.39581206	-3.24832172	-1.88628829
O	-2.18607422	-2.57462897	-2.96907741
H	-2.37717327	-2.67662179	-3.91603138
O	-1.75262756	-0.26550325	-2.32464082
H	-2.10377356	0.39493275	-2.93998582
H	-0.07391188	-1.62398142	-1.05209530
H	-2.13390400	-1.39268297	-2.76837388

TS3'\_W



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 1*

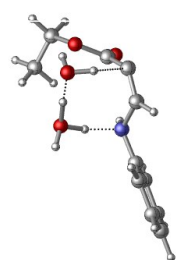
*Computed total energies: -708.2979502 Hartree*

O	2.73406600	-0.93680400	1.28862000
O	3.09773800	-0.09223300	-0.79024600
C	3.63768600	2.00963900	0.34790600
H	4.47670200	2.65724500	0.64921000
H	3.04128100	1.77384500	1.24229300
H	3.00657600	2.56743700	-0.36289300
C	4.16729100	0.73465600	-0.28878100
H	4.78677800	0.95520900	-1.17023900
H	4.76825100	0.15530800	0.42942700
C	2.45981200	-0.89477200	0.09532300
C	1.49139500	-1.75257400	-0.54671500
C	0.16423900	-1.49959700	-0.59029000
N	-0.45560900	-0.20950000	-0.00461700

s60

C	-1.84676600	0.03028700	0.01640000
C	-2.76722000	-1.01118700	0.22442400
C	-2.31322000	1.34363800	-0.16450400
C	-4.13691200	-0.73417700	0.23602800
H	-2.42309200	-2.03230100	0.39746800
C	-3.68399000	1.60770600	-0.13808900
H	-1.60019800	2.15578000	-0.32839300
C	-4.60432700	0.57157100	0.05606400
H	-4.84327100	-1.55197100	0.39880100
H	-4.03288400	2.63387400	-0.27764700
H	-5.67618900	0.78103200	0.07172100
H	-0.61074900	-2.12796900	-1.04027600
H	-0.18697050	-0.21621761	0.95860064
O	1.15592470	0.36031740	-1.01491117
H	1.76647785	-0.67070270	-1.18320378
H	1.41375036	1.27589486	-1.14469506
H	0.03438923	0.43022071	-0.92340234

TS3'\_2W



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 1*

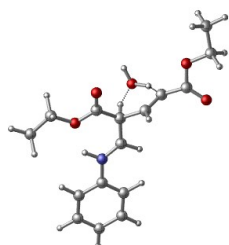
*Computed total energies: -784.7469786 Hartree*

O	2.83247500	-0.49204500	-2.27966900
N	-0.58071000	-0.15997000	-0.22476900
H	-0.12390300	0.54681700	-0.80587500
O	2.37787800	0.29498700	-0.18323400
C	0.05170300	-1.47602400	-0.42304200
H	-0.55133100	-2.26586100	0.03880700
C	-4.77435700	0.52582000	-0.07924800
C	1.30075800	-1.66589300	-0.83206700
C	2.19780400	-0.60205500	-1.22847600
C	-2.00981800	0.02728900	-0.22371800
C	3.08365100	2.45287900	0.55316600
H	3.94020300	3.13667900	0.64473700
H	2.73686200	2.18870100	1.56482700
H	2.26667100	2.98366200	0.04073700

s61

C	-2.91496500	-1.04081000	-0.12483800
H	-2.56685100	-2.07355200	-0.10831200
C	-4.28931500	-0.78455500	-0.05073500
H	-4.98460800	-1.62626200	0.02821000
C	3.47957800	1.20866100	-0.22032000
H	3.73662600	1.43812100	-1.26626600
H	4.35732200	0.71745600	0.24075300
C	-3.86841100	1.59036300	-0.18853800
H	-4.23119100	2.62123200	-0.21790500
C	-2.49581400	1.34529400	-0.25661100
H	-1.79206600	2.18109600	-0.33254800
H	-5.84863100	0.71690900	-0.01991100
O	0.49279900	0.15570800	2.02435700
H	-0.06092900	0.09598700	1.00086500
H	-0.12916100	-0.07317300	2.73190300
O	2.11603400	-1.80413100	1.89446400
H	1.92259300	-2.05284500	0.93882700
H	3.05034000	-1.54304600	1.88933500
H	1.22464300	-0.59408900	2.00440300

TS5\*\_W



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 1*

*Computed total energies: -1052.8242 Hartree*

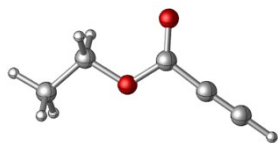
O	-0.98821700	2.66723700	-0.46167700
N	2.12568200	-0.13483500	-0.04514800
H	2.30924500	0.87688100	-0.07668200
O	1.18948000	2.35566200	-0.01027100
C	0.86543200	-0.45147800	0.03995600
H	0.61439800	-1.51578400	0.08072600
C	5.58299900	-2.54036500	-0.20506500
C	-0.26643400	0.46180000	0.16249000
C	-0.08515100	1.92927400	-0.15364700
C	3.26409800	-0.98638200	-0.08977900
C	2.94602800	3.98141200	-0.05195500
H	3.18142700	5.04781400	-0.18758600

s62

H	3.52975200	3.40695500	-0.78801300
H	3.25945200	3.68265600	0.96021600
C	3.16931000	-2.38149700	0.01686500
H	2.20700300	-2.87726000	0.14963800
C	4.33227900	-3.14975800	-0.04289800
H	4.25815500	-4.23648800	0.04059200
C	1.46177800	3.76119300	-0.24296500
H	0.85798800	4.34783800	0.46639600
H	1.12804700	4.01696100	-1.26043800
C	5.66933800	-1.14832500	-0.30458400
H	6.63902300	-0.66279100	-0.42662200
C	4.51321700	-0.36797200	-0.24651100
H	4.58021100	0.72002100	-0.32237900
H	6.48686600	-3.15117800	-0.25102800
O	-3.80040700	-2.47163600	-0.46883300
O	-4.75959900	-0.46609000	-0.09235700
C	-1.55922400	-0.12399300	-0.41552200
C	-2.47825200	-0.67480000	0.38856600
C	-3.68809000	-1.30491300	-0.12222200
C	-7.05891100	0.09224200	-0.39390100
H	-8.05153200	-0.28937100	-0.68386900
H	-6.79534300	0.92151500	-1.07032400
H	-7.12465600	0.48956400	0.63122200
C	-6.02830500	-1.01575200	-0.47678700
H	-6.28041100	-1.85788700	0.19072700
H	-5.95799000	-1.42787000	-1.49760200
H	-1.64468700	-0.05539200	-1.51101600
O	-1.33954000	-0.04409100	2.62102300
H	-2.01922100	-0.45567100	1.76198200
H	-0.50263600	0.39663700	1.32748100
H	-1.80927000	0.75392600	2.90729000

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**Ethyl propiolate other conformation**



*Theoretical calculation level:*

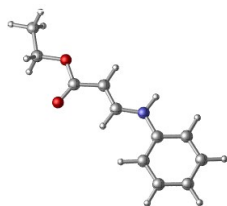
*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 0*

*Computed total energies: -344.4551684 Hartree*

O	-0.29800100	-0.68049000	-0.35542300
C	-1.69495700	-0.35964000	-0.57539263
H	-2.17374008	-1.17529099	-1.07577271
H	-2.17398717	-0.18800146	0.36586732
C	-1.79997365	0.90799551	-1.44353530
H	-2.70155076	0.87270266	-2.01869886
H	-1.81290911	1.77220748	-0.81276566
H	-0.95842712	0.95983575	-2.10233120
C	0.05856734	-1.82244946	0.42795917
O	-0.78371209	-2.55856850	0.93293553
C	1.56970006	-2.06721004	0.59579890
C	2.74838357	-2.25812329	0.72671390
H	3.79832643	-2.42818422	0.84332982

**IM2 other conformation**



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

*The number of imaginary frequencies: 0*

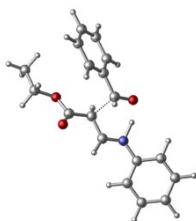
*Computed total energies: -632.00793 Hartree*

O	-2.93754726	0.35180690	0.32950753
O	-3.67505522	-1.77223712	0.09283566
C	-5.03550886	-1.33540996	0.24555619
H	-5.16927810	-0.40194601	-0.26006308
C	-2.69641400	-0.83315200	0.16506400
C	-1.35404100	-1.38451100	0.02283700
H	-1.30873500	-2.46682500	-0.11935800
C	-0.22539200	-0.62333200	0.05993600
H	-0.32390100	0.45413400	0.19976800
N	1.03994000	-1.09726800	-0.06609400



H	1.14167500	-2.10004600	-0.19579500
C	2.23737300	-0.36814000	-0.03924900
C	2.28023800	1.02684000	0.14604400
C	3.44729400	-1.07021200	-0.20507700
C	3.50882900	1.69137800	0.16379800
H	1.36411600	1.60313400	0.27802900
C	4.66743500	-0.39412200	-0.18498600
H	3.42572300	-2.15383900	-0.35047000
C	4.70955400	0.99251500	-0.00033500
H	3.52197000	2.77461900	0.30930100
H	5.59340500	-0.95990300	-0.31552500
H	5.66509200	1.52130600	0.01548500
H	-5.25610142	-1.21264455	1.28534827
C	-5.98345747	-2.38745361	-0.35958643
H	-5.81577438	-3.33258207	0.11318685
H	-6.99795262	-2.08540760	-0.20316461
H	-5.79528472	-2.47533624	-1.40923764

### TS3 other conformation



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

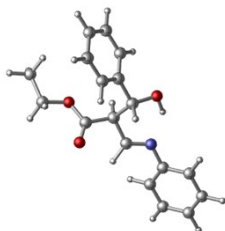
*The number of imaginary frequencies: 1*

*Computed total energies: -977.4384375 Hartree*

C	0.33020300	-1.07274100	0.47558000
O	0.82319800	2.31298400	1.15114400
N	-2.14008900	-0.06770800	-0.47869600
H	-1.55721800	-1.07110300	-0.48360800
O	2.19542600	1.65463100	-0.51825700
C	-1.28823300	0.86513800	-0.15023100
H	-1.61536100	1.75568300	0.40414700
C	-6.29559400	-0.07383200	0.18557000
C	0.11343400	0.61677100	-0.37698700
C	1.04496800	1.62907800	0.16853200
C	-3.52987200	-0.03535900	-0.25100700
C	-4.27602400	1.14796500	-0.38558300

H	-3.78420600	2.07550500	-0.68915600
C	-5.65540000	1.12150200	-0.16457100
H	-6.23536900	2.04168000	-0.27974700
C	3.26309000	2.48721000	-0.02723700
H	3.35250700	2.34978400	1.06395500
C	-5.54778800	-1.25267300	0.31207400
H	-6.03995500	-2.19000400	0.58554200
C	-4.17025600	-1.23978800	0.09062600
H	-3.57573600	-2.15124700	0.19668500
H	-7.37538100	-0.08914800	0.35016700
C	1.80186000	-1.34613600	0.31874800
C	2.71192100	-0.93168000	1.30185400
C	2.27533300	-2.01203300	-0.82112100
C	4.07972400	-1.17525300	1.14674300
H	2.34583700	-0.40970700	2.19114700
C	3.64223000	-2.24943600	-0.98126400
H	1.55279800	-2.34135400	-1.57101400
C	4.54842100	-1.83206400	0.00269700
H	4.78182100	-0.84867400	1.91796800
H	4.00518200	-2.76584800	-1.87421400
H	5.61788100	-2.02066800	-0.12173700
O	-0.50878200	-1.86808300	-0.12801200
H	0.08616700	-0.76662700	1.51753000
H	0.37553900	0.25440700	-1.37447800
H	2.99931500	3.54594900	-0.20911100
C	4.52473900	2.08122700	-0.75886000
H	4.39515800	2.18221300	-1.84966100
H	5.36397000	2.72226100	-0.44794200
H	4.77240900	1.03723800	-0.52797400

### IM3 other conformation



**Theoretical calculation level:**

*M062X/def2-TZVP//B3LYP-D3/SVP*

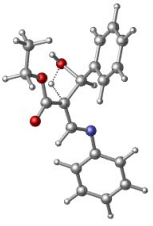
**The number of imaginary frequencies:** *0*

**Computed total energies:** *-977.4711834 Hartree*

C	0.78346700	-0.96973700	0.40314600
O	0.53947957	2.35146784	-0.81172371
N	-2.01526100	-0.61537800	-0.05422200
H	-0.81813700	-2.00767500	0.36118000
O	2.34045418	1.00080696	-0.96350861
C	-1.23727900	0.21029800	-0.63416200
H	-1.61364000	1.14768100	-1.08223100
C	-6.18959700	-0.08273100	0.24075600
C	0.24835000	-0.05533800	-0.75466500
C	1.02758900	1.24636100	-0.83696400
C	-3.40892700	-0.41363500	0.00795800
C	-4.15118700	0.12311000	-1.06074300
H	-3.64925300	0.38683800	-1.99436200
C	-5.53384200	0.28480200	-0.93960800
H	-6.10329100	0.69417300	-1.77789000
C	3.24038051	2.13213960	-1.04767490
H	2.89576856	2.91097004	-0.39993596
C	-5.45508500	-0.63016500	1.30006000
H	-5.96144000	-0.92841900	2.22149700
C	-4.07578600	-0.80841700	1.18124500
H	-3.49300900	-1.24399400	1.99596400
H	-7.27110400	0.04446600	0.33020800
C	2.28185300	-1.16510000	0.29376000
C	3.16396500	-0.37831900	1.04617000
C	2.80467000	-2.10941600	-0.60266500
C	4.54792300	-0.51954800	0.89683100
H	2.76528900	0.35267900	1.75340200
C	4.18640800	-2.25675800	-0.74922100
H	2.11601500	-2.73347500	-1.17606900
C	5.06236900	-1.45857400	-0.00285800
H	5.22432200	0.10262100	1.48849700
H	4.58323600	-2.99686300	-1.44911500
H	6.14318700	-1.57249000	-0.11943300
O	0.14010900	-2.21979800	0.36043200
H	0.56321000	-0.43469900	1.34770600
H	0.43057500	-0.58862200	-1.70269900
H	3.26770656	2.49198110	-2.05498189
C	4.65410224	1.69647006	-0.61967617
H	4.68242251	1.57118677	0.44258654

H	4.90097145	0.77006365	-1.09478326
H	5.36117359	2.44545448	-0.90945619

**TS4 other conformation**



*Theoretical calculation level:*  
*M062X/def2-TZVP//B3LYP-D3/SVP*

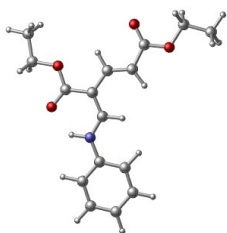
*The number of imaginary frequencies: 1*

*Computed total energies: -977.3936819 Hartree*

C	0.70750400	0.41162300	1.03659100
O	0.49009300	-2.55206400	-1.18043600
N	-2.11649500	0.31600100	0.33813400
O	2.16808600	-1.67047900	0.05047900
C	-1.36690300	-0.68597600	0.03220400
H	-1.76227600	-1.56717800	-0.50604000
C	-6.28871500	0.31292400	-0.33742000
C	0.04163400	-0.76187200	0.36324300
C	0.86889300	-1.73593300	-0.36118200
C	-3.49609000	0.27113400	0.10851500
C	-4.27921200	-0.88573100	0.31566800
H	-3.80298900	-1.79980900	0.67855300
C	-5.65866700	-0.86052600	0.09215400
H	-6.24775600	-1.76560800	0.26475700
C	3.14053900	-2.48814400	-0.62067800
H	2.99328200	-2.39778700	-1.70854400
C	-5.52295700	1.47032800	-0.53165800
H	-6.00462000	2.39563500	-0.85956700
C	-4.14660800	1.45380100	-0.30190500
H	-3.54366300	2.35411000	-0.44323500
H	-7.36807600	0.32966400	-0.50738700
C	1.82753800	1.17452500	0.38229300
C	1.83423100	1.33889600	-1.01025600
C	2.84485800	1.76175600	1.14876900
C	2.85324600	2.06732100	-1.62913500
H	1.04322100	0.88464200	-1.61149500
C	3.87066400	2.48053300	0.52702400
H	2.84358200	1.64808900	2.23545100

C	3.87832600	2.63433700	-0.86319000
H	2.85123100	2.18478700	-2.71557000
H	4.66524300	2.92283700	1.13293300
H	4.68058400	3.19506300	-1.34901900
O	1.18888400	-0.32416700	2.30481200
H	-0.07029200	1.08677500	1.41930600
H	0.43397900	-1.11118800	1.80236900
H	2.05443300	-0.72385800	2.07098900
H	2.97087300	-3.54380800	-0.35096700
C	4.51144900	-2.00544400	-0.19403900
H	4.65689100	-0.95152400	-0.48044900
H	4.63428600	-2.08899800	0.89778500
H	5.29266100	-2.61148100	-0.67763000

#### 6a other conformation



*Theoretical calculation level:*

*M062X/def2-TZVP//B3LYP-D3/SVP*

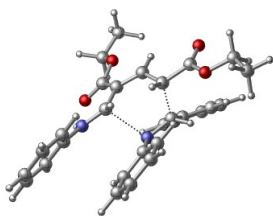
*The number of imaginary frequencies:0*

*Computed total energies: -976.5170728 Hartree*

O	-1.65887454	2.64233246	-0.00998548
N	-1.89551600	-0.26717800	0.00584700
H	-2.43190400	0.60050700	0.02873300
O	0.44529775	3.42979739	-0.01620737
C	-0.56535300	-0.11117900	-0.01003400
H	0.00794400	-1.03952100	-0.02080000
C	-4.21969000	-3.78796700	-0.00479300
C	0.15462400	1.07754600	-0.01292800
C	-0.46299800	2.42132300	-0.01274400
C	-2.62808500	-1.46737000	-0.00198300
C	1.14583457	5.70984425	-0.01177058
H	0.80815472	6.75727281	-0.01082044
H	1.76879194	5.54783086	-0.90529282
H	1.76666903	5.54537630	0.88273532
C	-2.02829900	-2.73583100	-0.09116000
H	-0.94554000	-2.84344300	-0.16476900

C	-2.82614800	-3.88201600	-0.09049100
H	-2.34714600	-4.86173100	-0.16056900
C	-0.05168376	4.78382722	-0.01426818
H	-0.68791484	4.92581132	0.87360890
H	-0.68668143	4.92866889	-0.90260995
C	-4.81529500	-2.52464500	0.08068700
H	-5.90203000	-2.43196500	0.14732400
C	-4.02948000	-1.37184900	0.08276400
H	-4.49922900	-0.38701400	0.15215600
H	-4.83486600	-4.69044300	-0.00606500
O	4.47906500	1.31920400	-0.04618600
O	4.58717300	-0.93143700	0.02337500
C	1.60618200	1.06621000	-0.01966800
C	2.46204700	0.01495700	0.00568600
C	3.91324300	0.23980300	-0.00975000
C	6.55665900	-2.27682200	0.06329400
H	7.65738800	-2.26396800	0.05876200
H	6.21250300	-2.85469900	-0.80854900
H	6.21911100	-2.79150400	0.97631600
C	6.02208000	-0.86073300	0.01542900
H	6.35904400	-0.26512500	0.88018900
H	6.35246500	-0.32736500	-0.89151300
H	2.06356000	2.05969100	-0.04705300
H	2.13746000	-1.02743100	0.04105800

**TS6' other conformation**



**Theoretical calculation level:**

*M062X/def2-TZVP//B3LYP-D3/SVP*

**The number of imaginary frequencies: 1**

**Computed total energies: -1533.524136 Hartree**

O	-0.11645800	-3.56579900	-0.07604700
N	-1.99552800	-1.61177300	-0.22890700
H	-1.72646600	-2.51207300	0.17458700
O	1.78989100	-3.21165600	-1.20444300
C	-0.97672700	-0.84828700	-0.63852100

H	-1.25028800	0.07430700	-1.14486400
C	-6.13543100	-0.83708200	-0.47001500
C	0.33900000	-1.37495900	-0.91966400
C	0.62352900	-2.81796600	-0.69877700
C	-3.37210200	-1.32814200	-0.33335700
C	-3.87926800	-0.40051400	-1.25826800
H	-3.20958800	0.13760300	-1.93039600
C	-5.25112800	-0.15564700	-1.31480400
H	-5.63265400	0.57422300	-2.03301500
C	2.21463700	-4.56514500	-0.92867400
H	1.43430700	-5.25903900	-1.27941100
C	-5.63030500	-1.77758000	0.43449200
H	-6.30783700	-2.32160700	1.09724700
C	-4.25809300	-2.02486900	0.50488600
H	-3.86343700	-2.74728600	1.22386300
H	-7.20873700	-0.64072000	-0.52076900
O	3.53779500	1.28599400	-1.62035800
O	2.17372400	3.03893800	-1.25350600
C	1.36361000	-0.50818500	-1.20073200
C	1.23574800	0.91738900	-0.96252100
C	2.44641500	1.72809400	-1.33430300
C	3.25338600	3.96347300	-1.50620600
H	2.36289000	-0.90351400	-1.38508500
H	0.34034100	1.39475400	-1.38384500
C	0.90252500	1.06307800	0.72881800
H	1.04642200	2.14758500	0.86641600
C	1.98033400	0.31134600	1.48336500
C	3.24855000	0.88586100	1.66313600
C	1.74791900	-0.97816900	1.98632900
C	4.27049600	0.17881000	2.30394900
H	3.43950000	1.90085200	1.30416500
C	2.77005500	-1.69103700	2.61998400
H	0.75204700	-1.40870100	1.87932300
C	4.03718300	-1.11731200	2.77689900
H	5.25117600	0.64314900	2.43665800
H	2.57404200	-2.69821400	2.99785600
H	4.83597700	-1.67313000	3.27471300
N	-0.39136200	0.62440600	1.01847000
C	-1.43041200	1.53628800	0.91264500

C	-1.37904500	2.78404400	0.23362100
C	-2.66500700	1.17595700	1.51223800
C	-2.51361200	3.59740800	0.14485000
H	-0.45172500	3.12951200	-0.22718400
C	-3.78829500	1.98968000	1.41616300
H	-2.70899100	0.22604200	2.04776900
C	-3.72601400	3.20866900	0.72380200
H	-2.44566900	4.55004900	-0.38880700
H	-4.72571600	1.67062600	1.87987500
H	-4.60816700	3.84890300	0.64575500
H	2.30204000	-4.68599800	0.16367900
C	3.53506900	-4.78329500	-1.63458100
H	4.29704300	-4.07739700	-1.26852100
H	3.89131800	-5.80760200	-1.44673800
H	3.42379500	-4.64742400	-2.72185900
H	3.56914700	3.85559400	-2.55693700
C	2.74781300	5.35710800	-1.20242100
H	3.54437500	6.09231100	-1.39272000
H	1.88383800	5.60884400	-1.83713200
H	2.44299700	5.44014100	-0.14745900
H	4.11166000	3.68587200	-0.87328000

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