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# Supplementary Materials

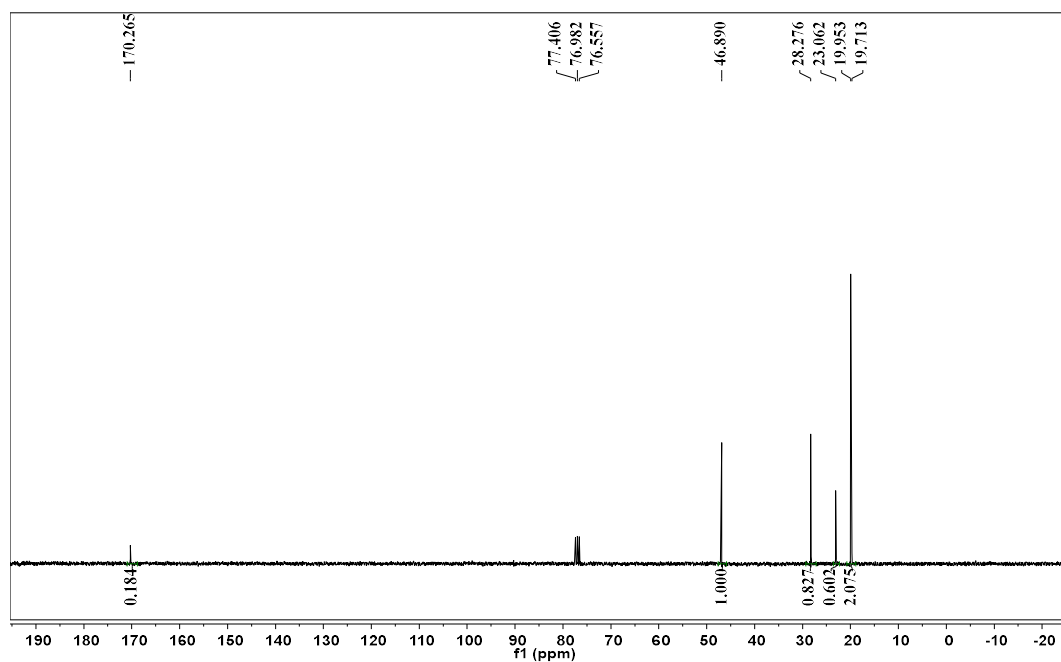
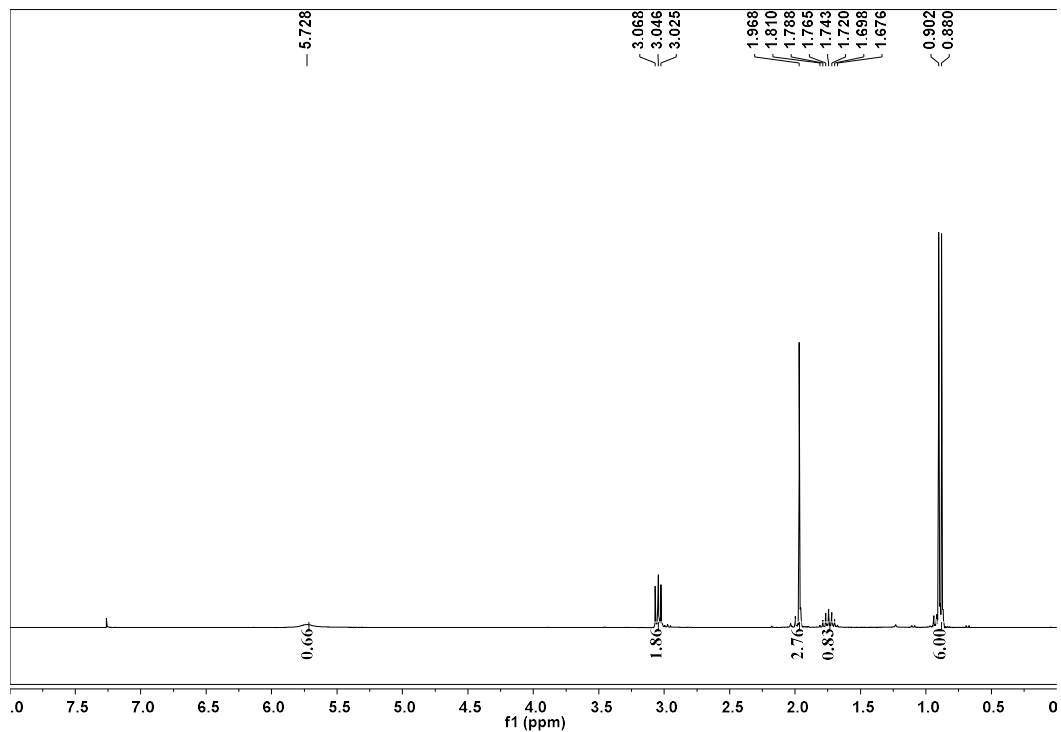
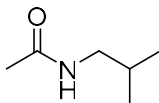
## New Lead Discovery of Herbicide Safener for metolachlor Based on a Scaffold-hopping Strategy

Xile Deng, Wenna Zheng, Qingcai Zhan, Yanan Deng, Yong Zhou, Lianyang Bai \*

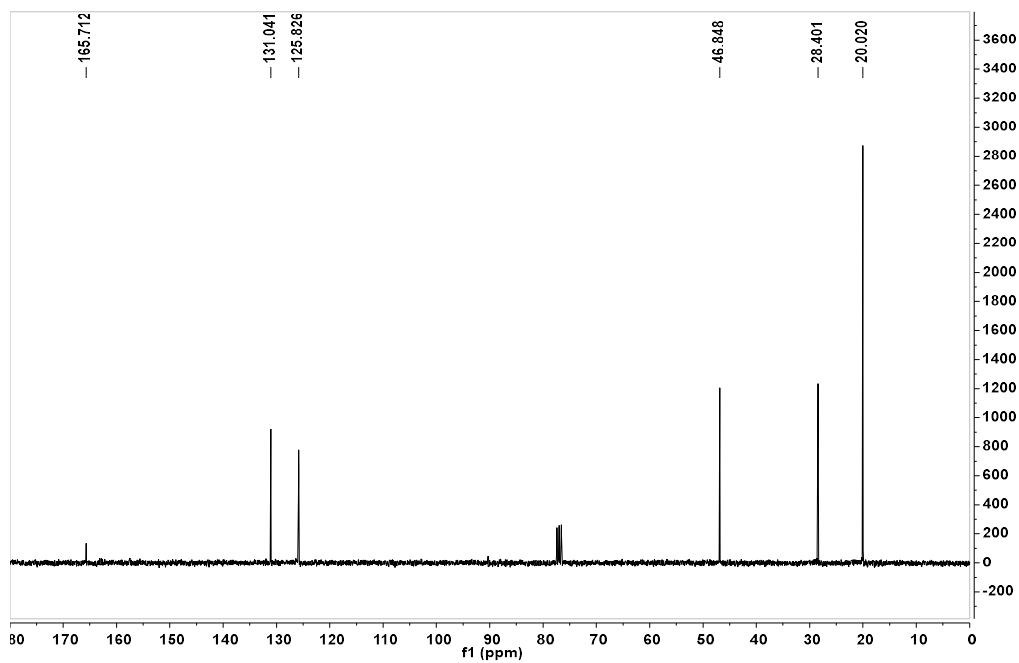
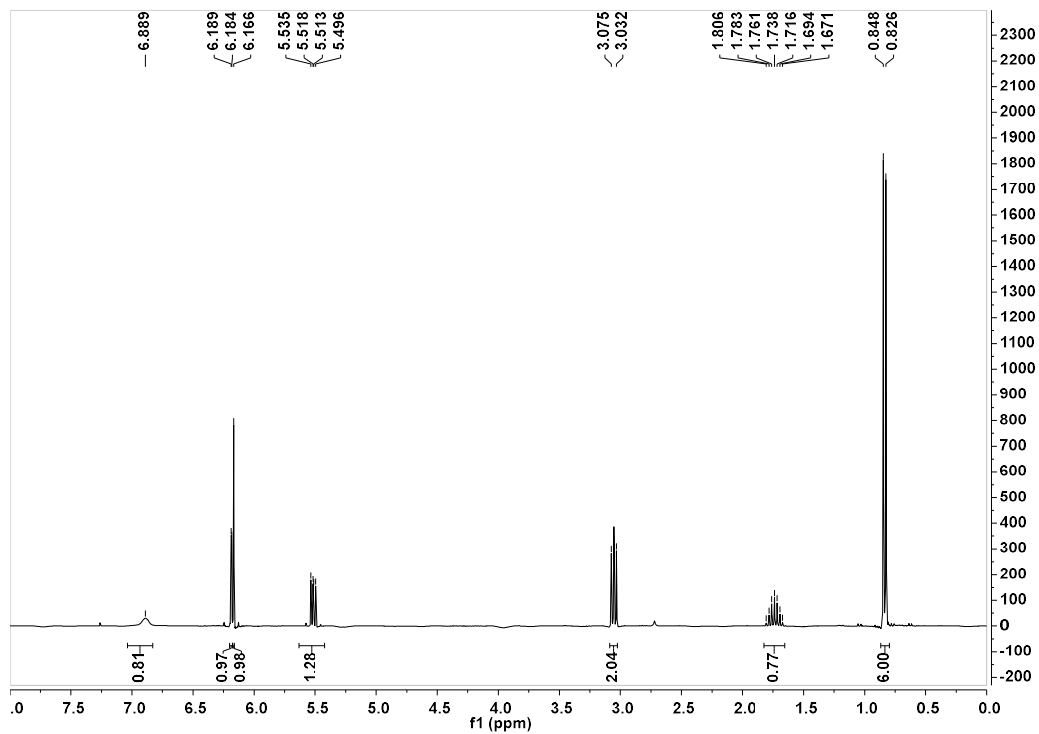
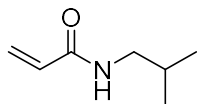
Biotechnology Research Institute, Hunan Academy of Agricultural Sciences, Changsha 410125, China;  
dengxile@hunaas.cn (X.D.); zhengwenna1994@163.com (W.Z.); zhanqc@hotmail.com (Q.Z.);  
[dengyanan007@hunaas.cn](mailto:dengyanan007@hunaas.cn) (Y.D.); [qimiaobuchugan@126.com](mailto:qimiaobuchugan@126.com) (Y.Z.); lybai@hunaas.cn (L.B.)

\* Correspondence: lybai@hunaas.cn (L.B.); Tel.: +86-0731-8469-2799 (L.B.)

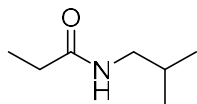
*N*-isobutylacetamide (**2a**)



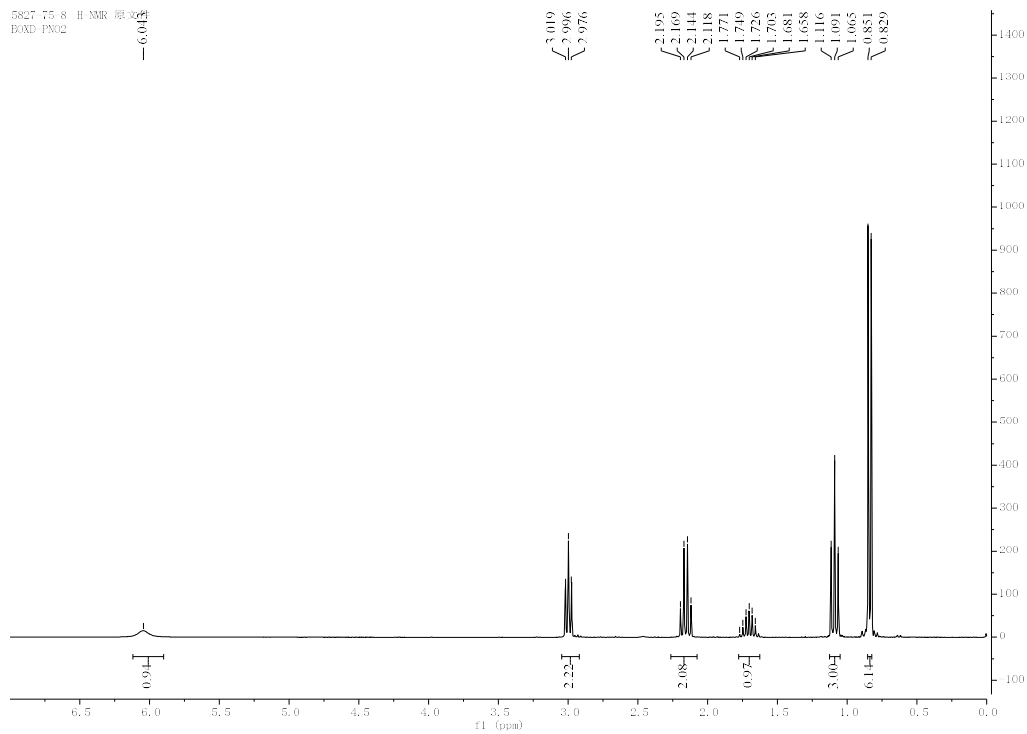
*N*-isobutylacrylamide (**2b**)



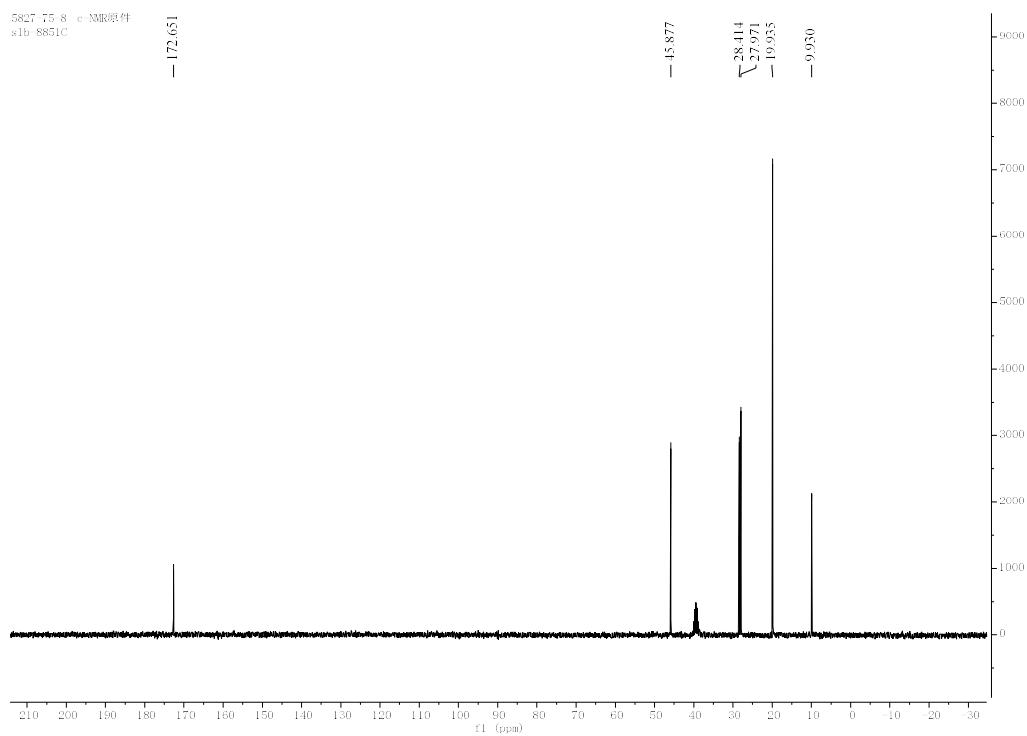
# *N*-isobutylpropionamide (2c)



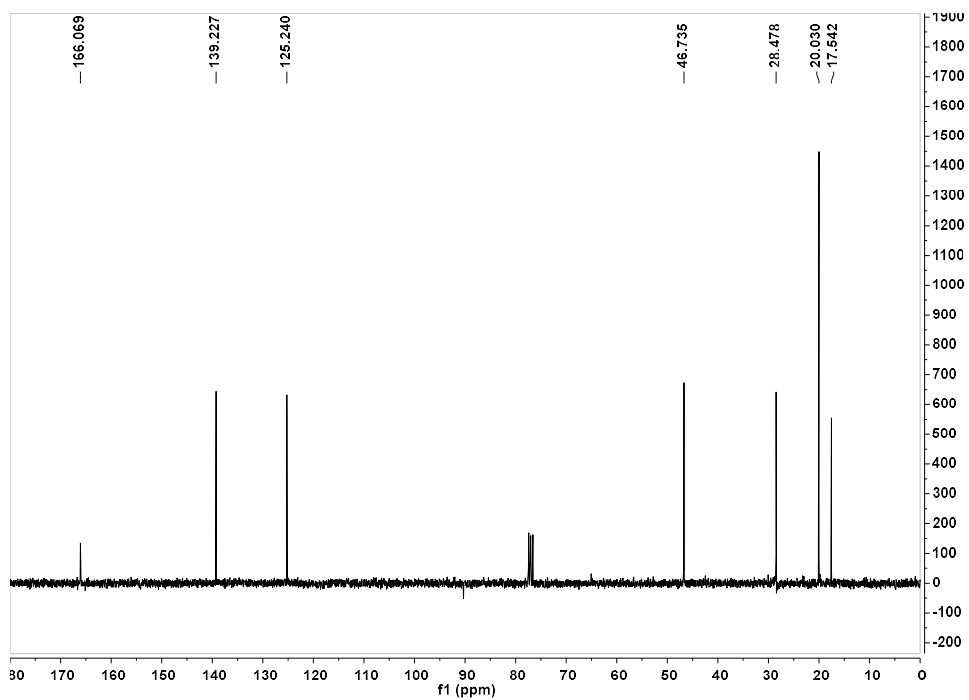
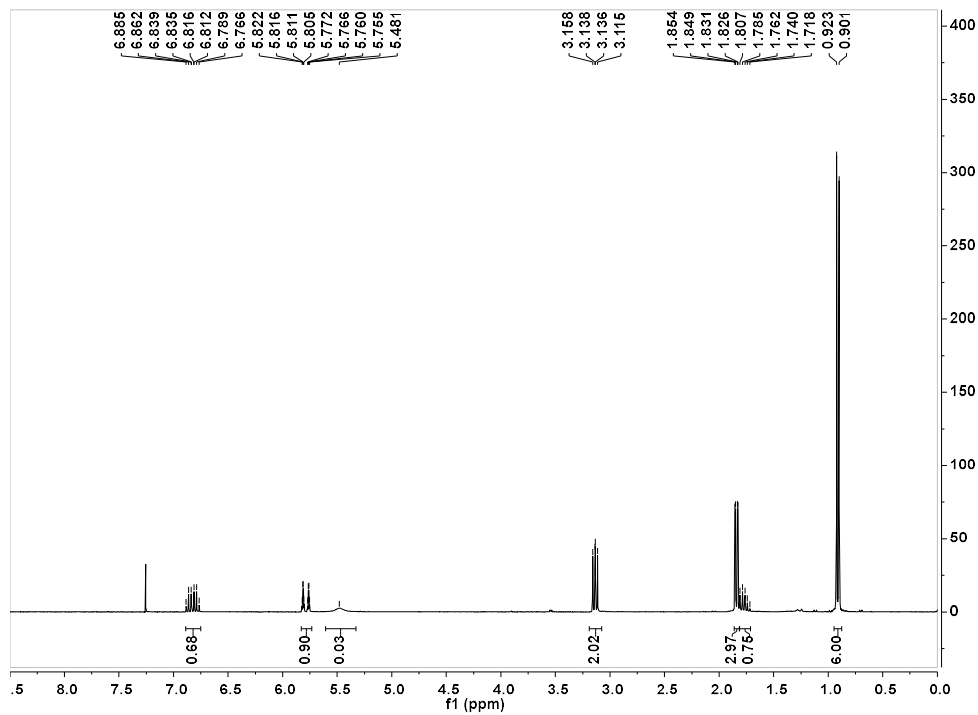
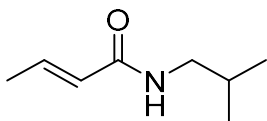
582T 75.8 H NMR 原液  
BXND P802



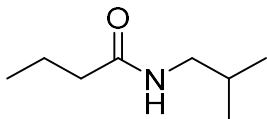
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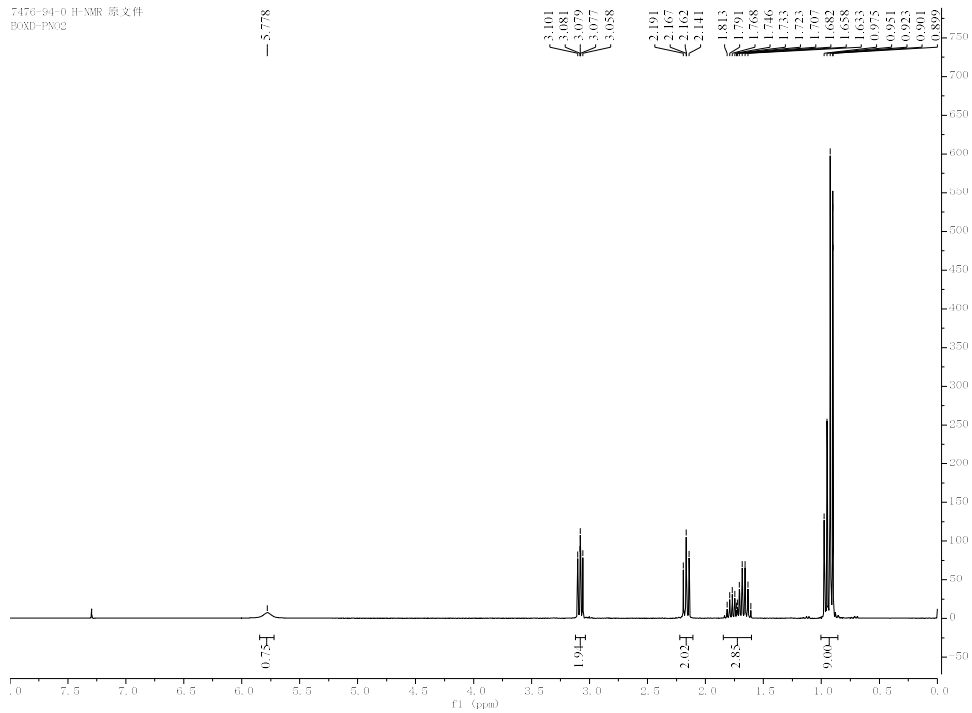
(E)-N-isobutylbut-2-enamide (2d)



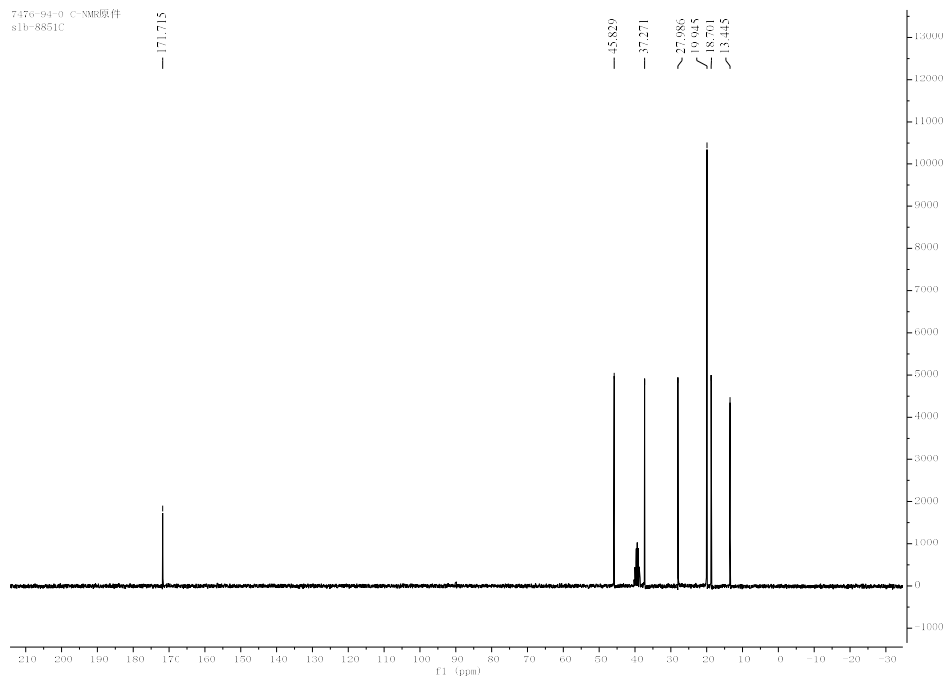
## *N*-isobutylbutamide (2e)



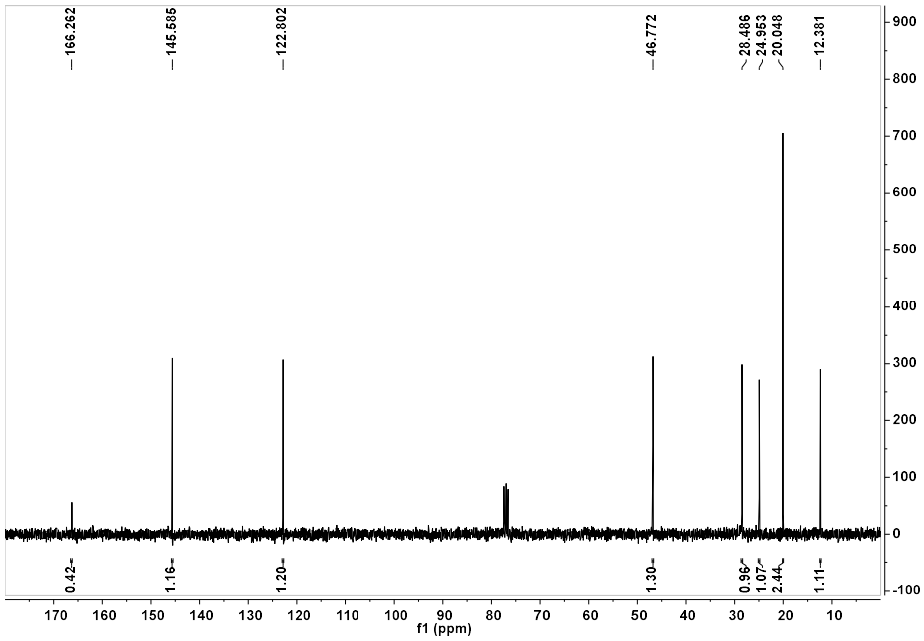
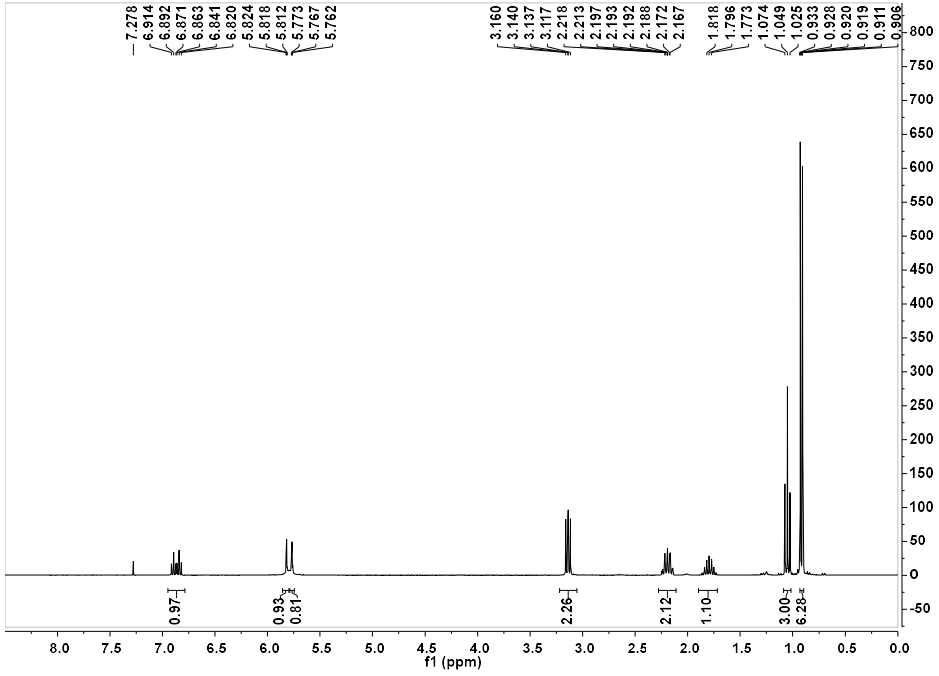
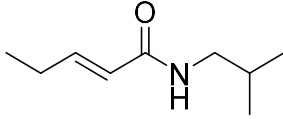
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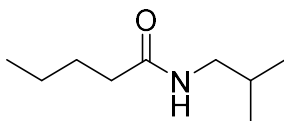
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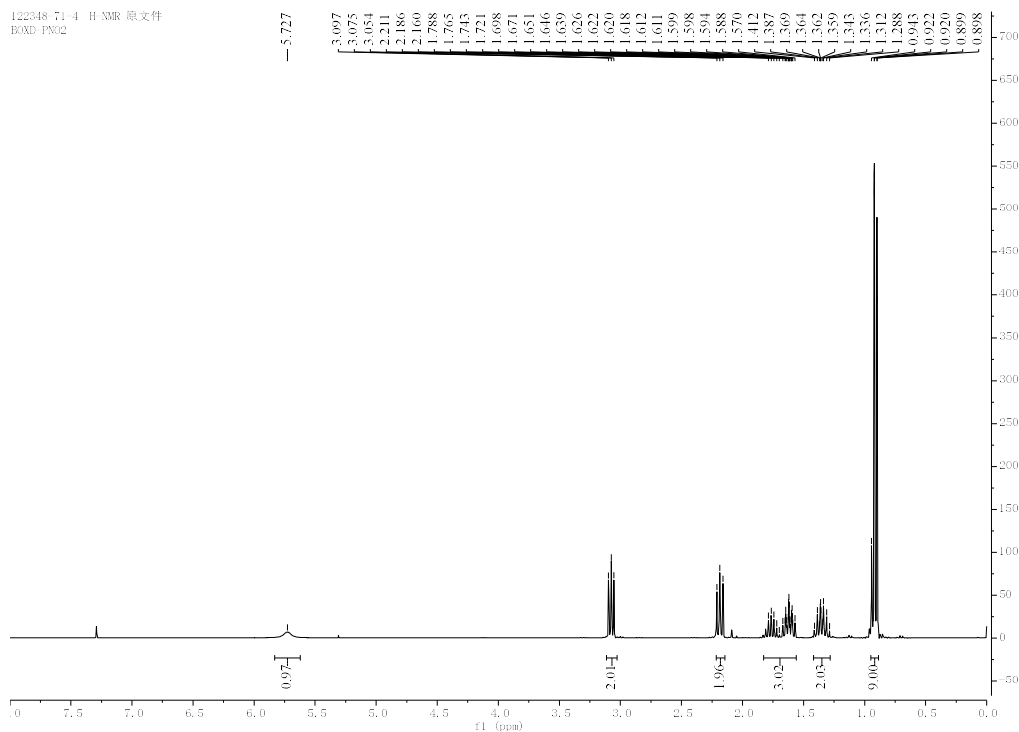
## (*E*)-*N*-isobutylpent-2-enamide (2f)



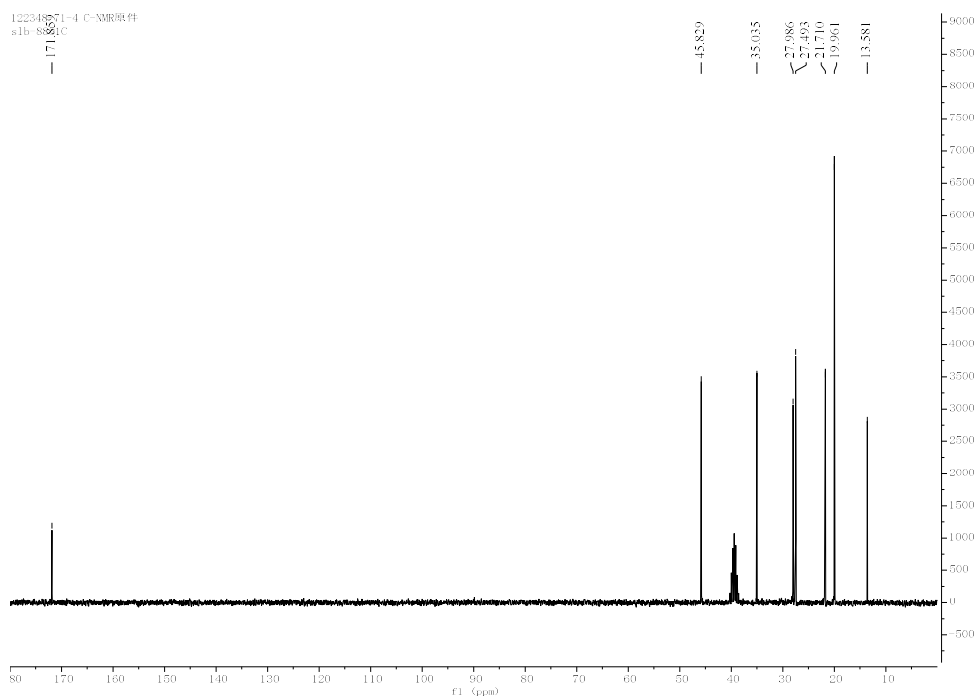
# N-isobutylpentanamide (2g)



122348 71-4 H-NMR 原文件  
BOXD-F302

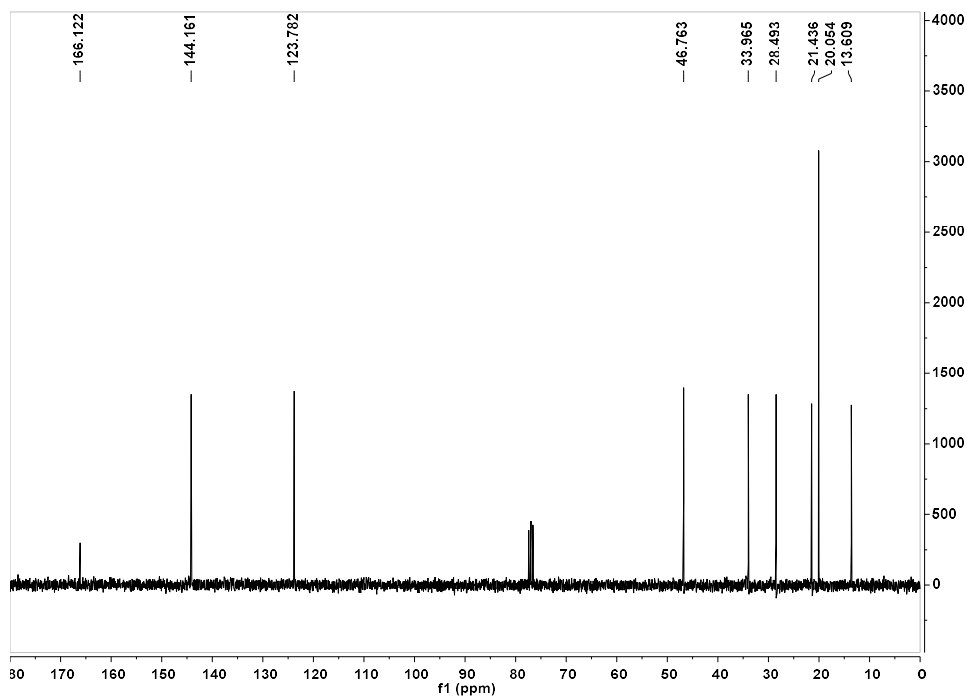
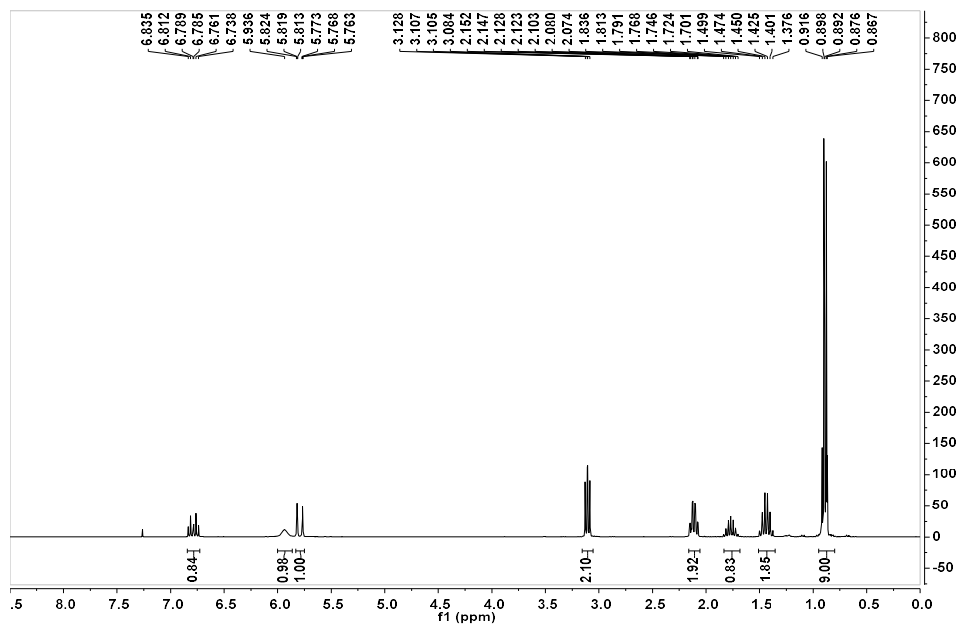
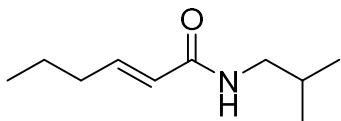


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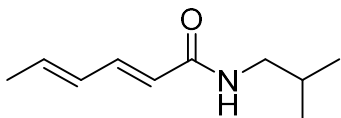


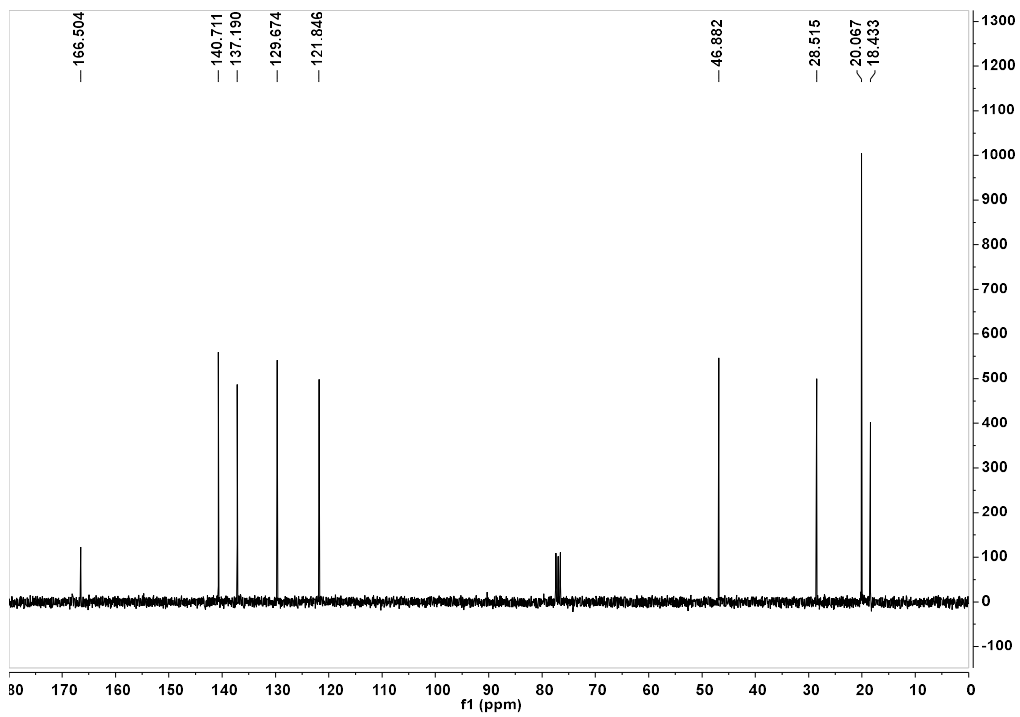
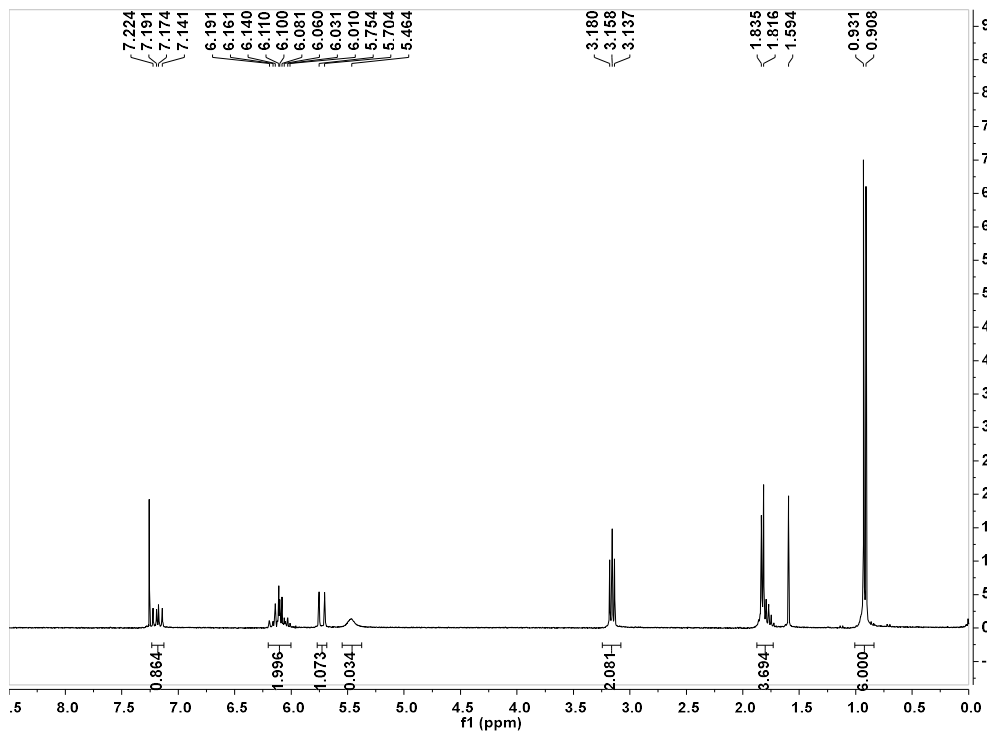


(*E*)-*N*-isobutylhex-2-enamide (**2h**)

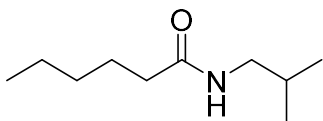


(*2E, 4E*)-*N*-isobutylhexa-2,4-dienamide (**2i**)

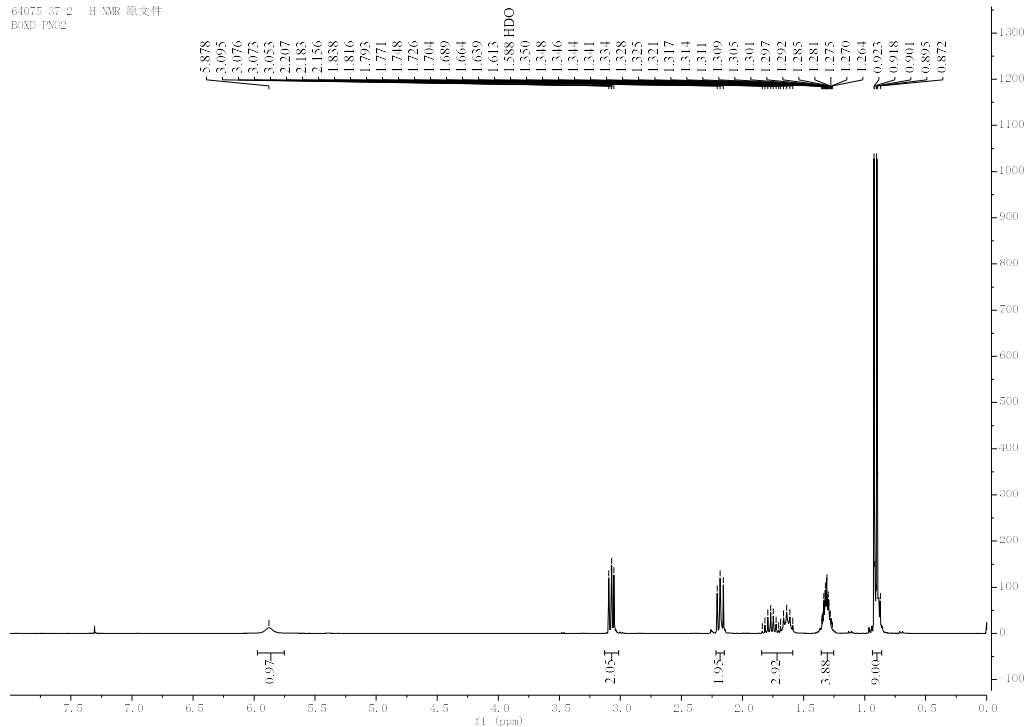




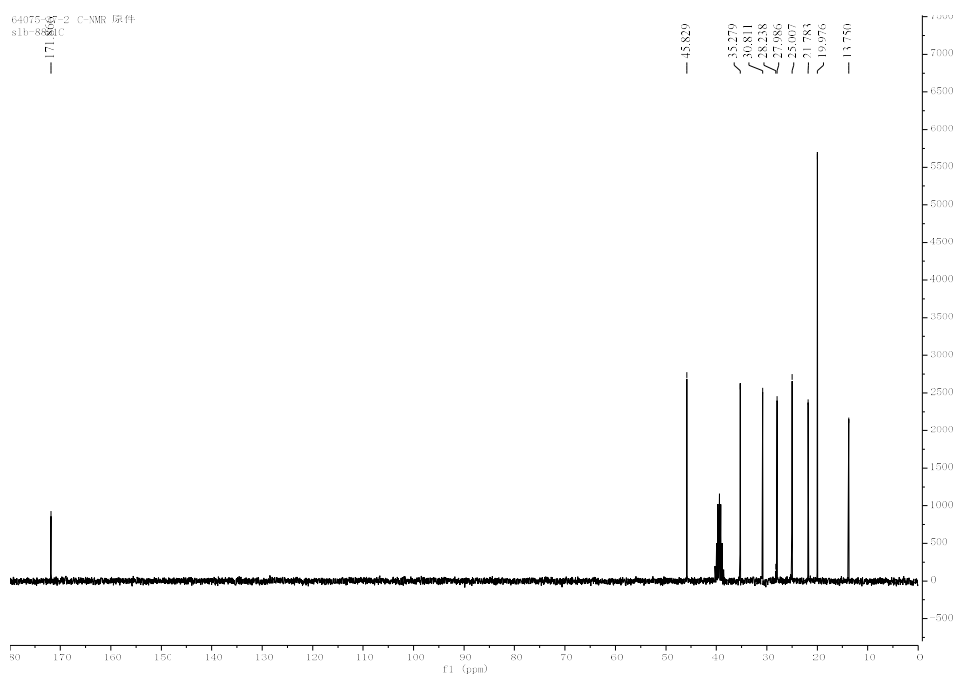
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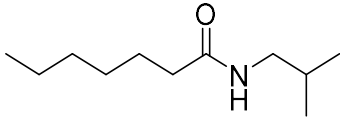
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BOXD-F3032



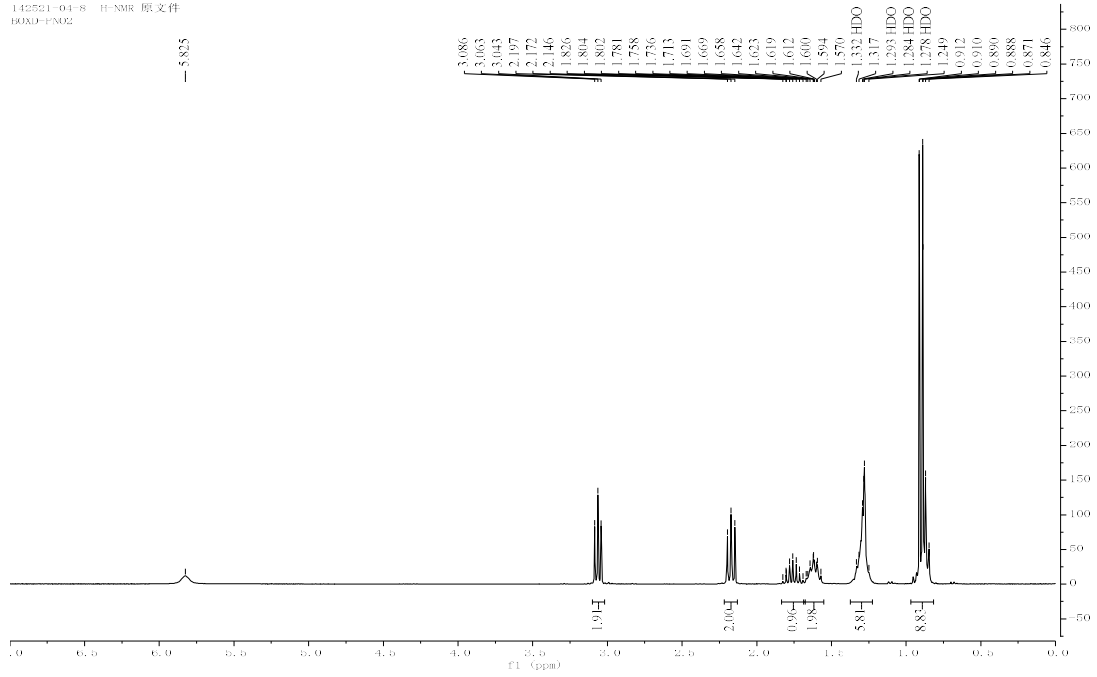
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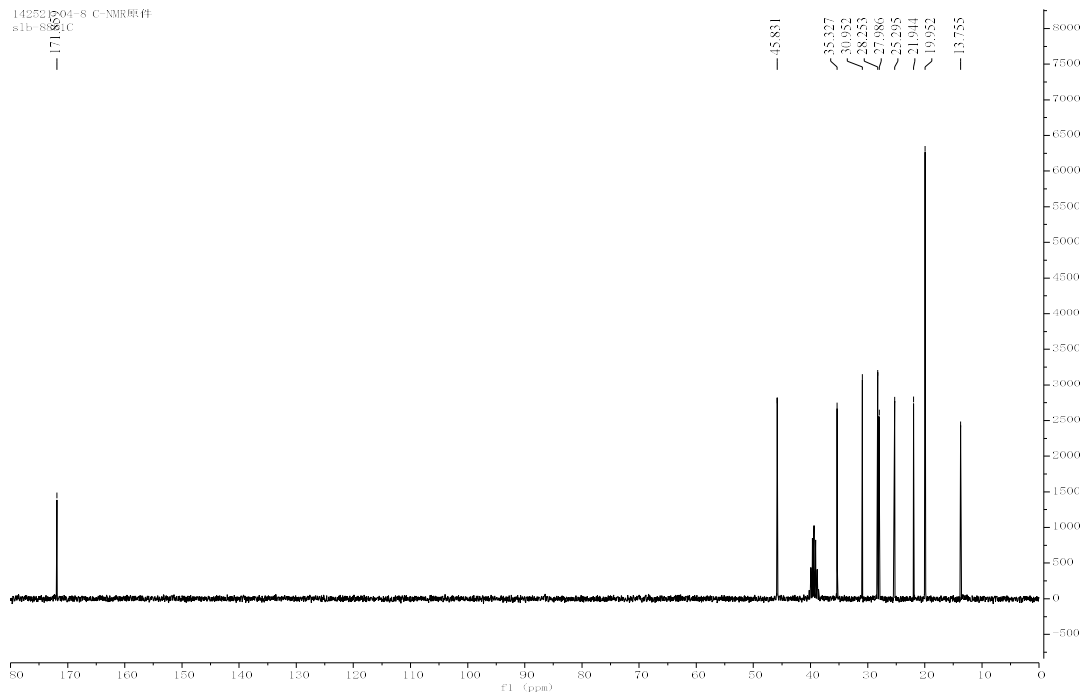
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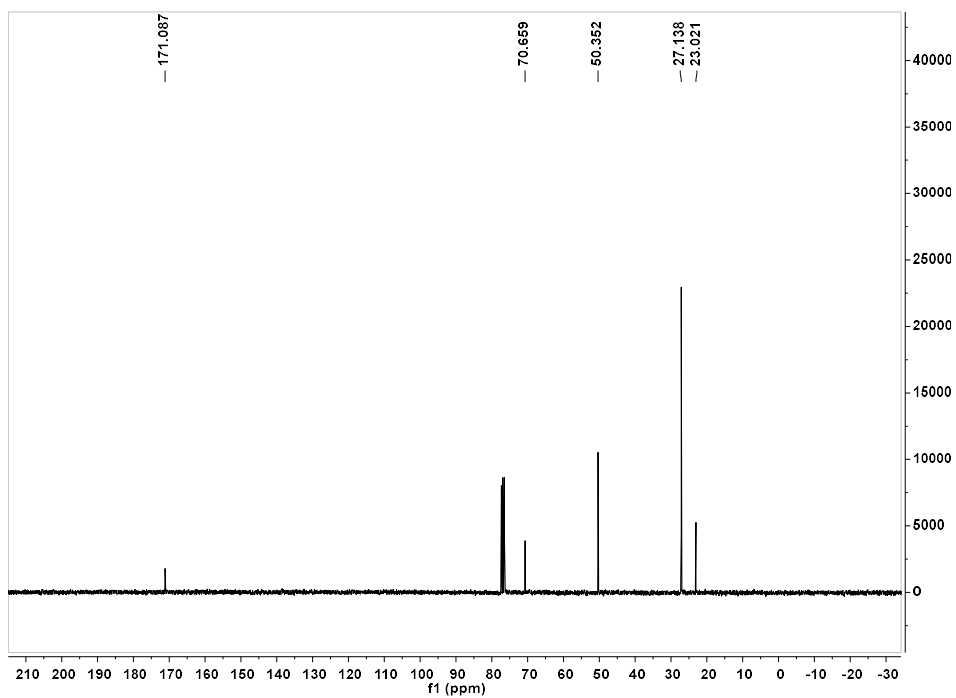
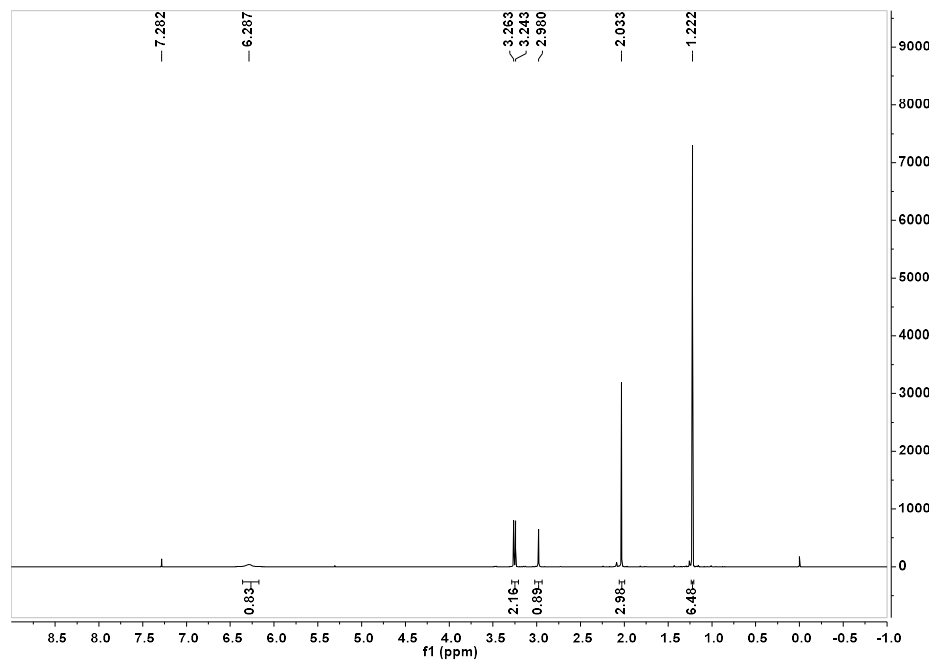
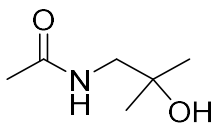
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H2O-DMSO



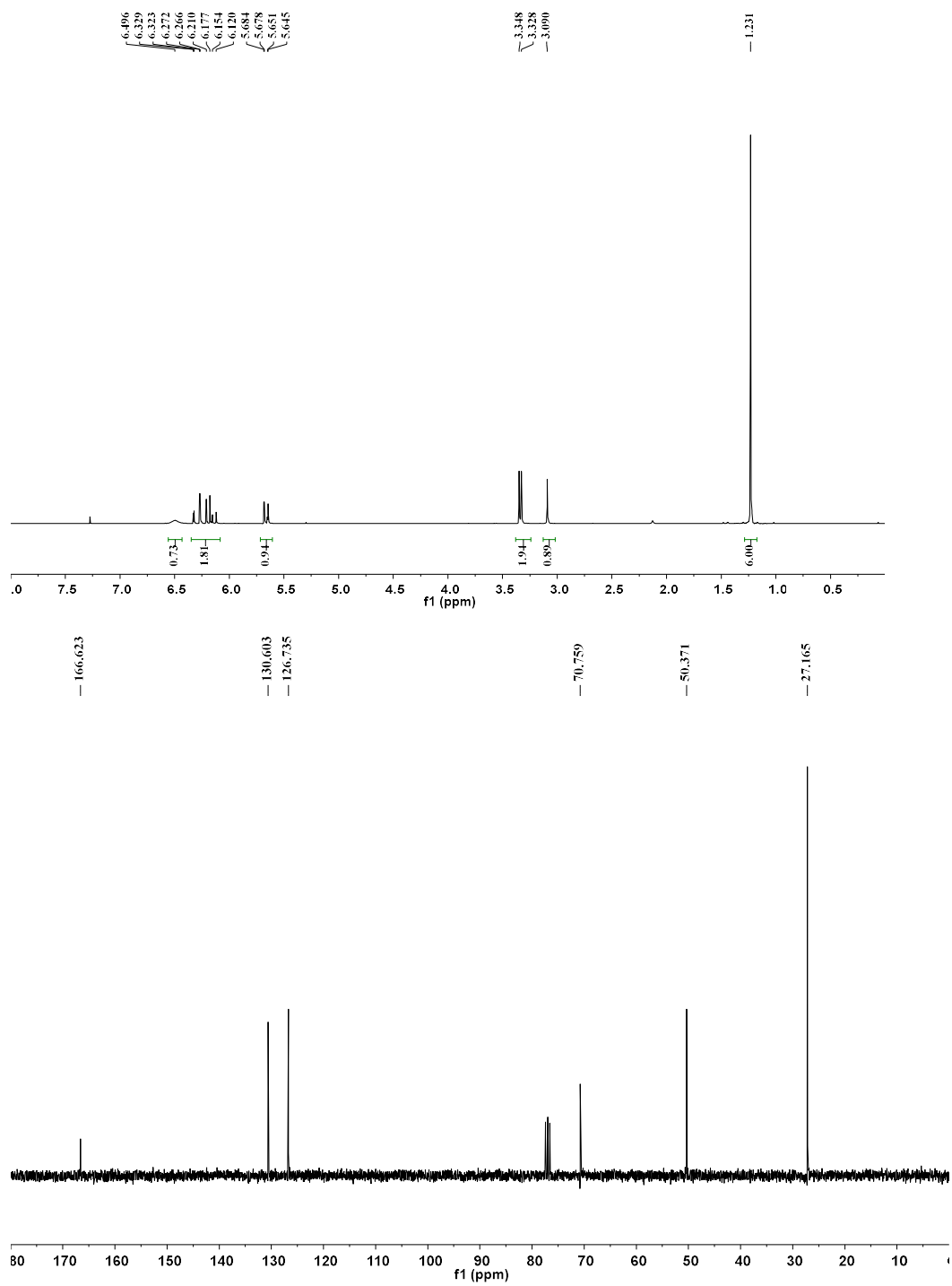
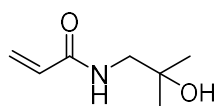
142521-04-S C-NMR原文件  
s1b-S11C



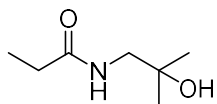
*N*-(2-hydroxy-2-methylpropyl)acetamide (**3a**)



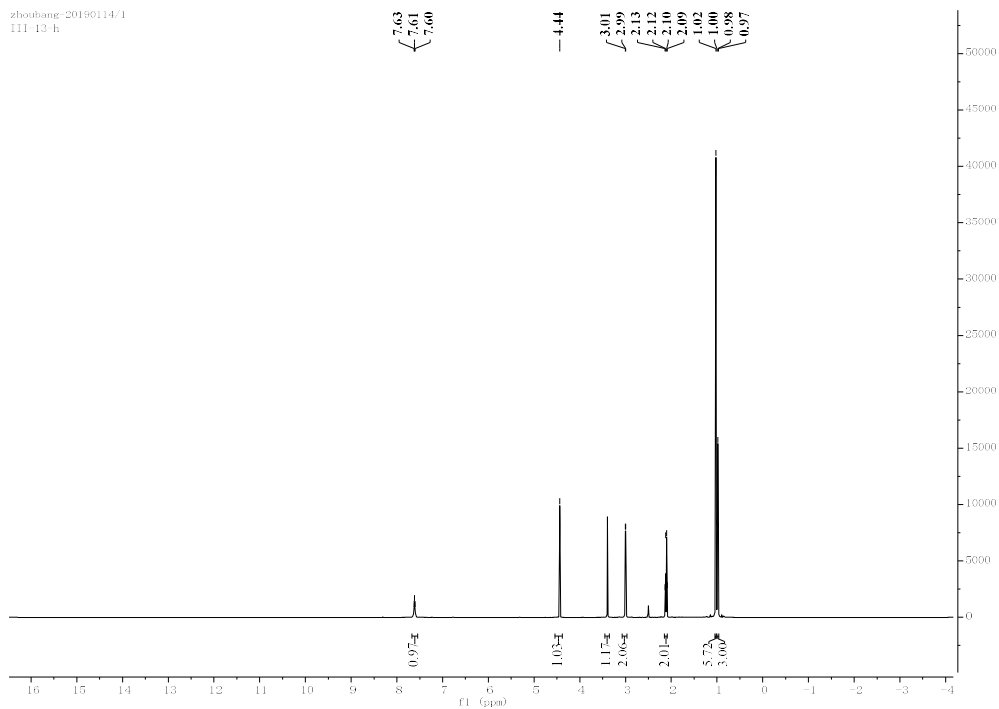
*N*-(2-hydroxy-2-methylpropyl)acrylamide (**3b**)



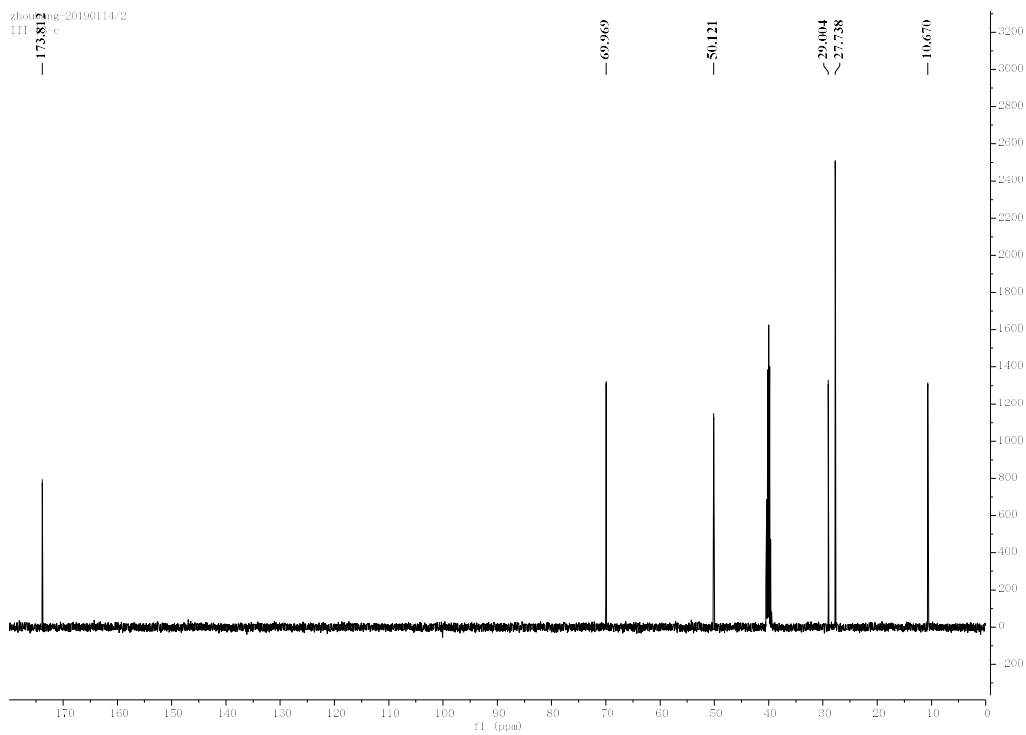
*N*-(2-hydroxy-2-methylpropyl)propionamide (**3c**)



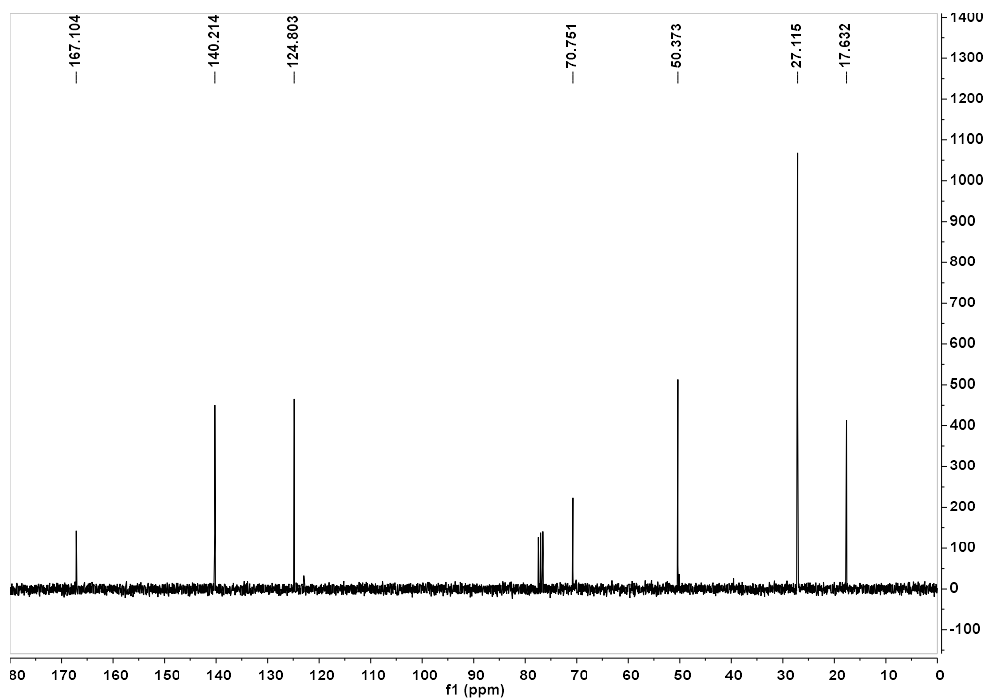
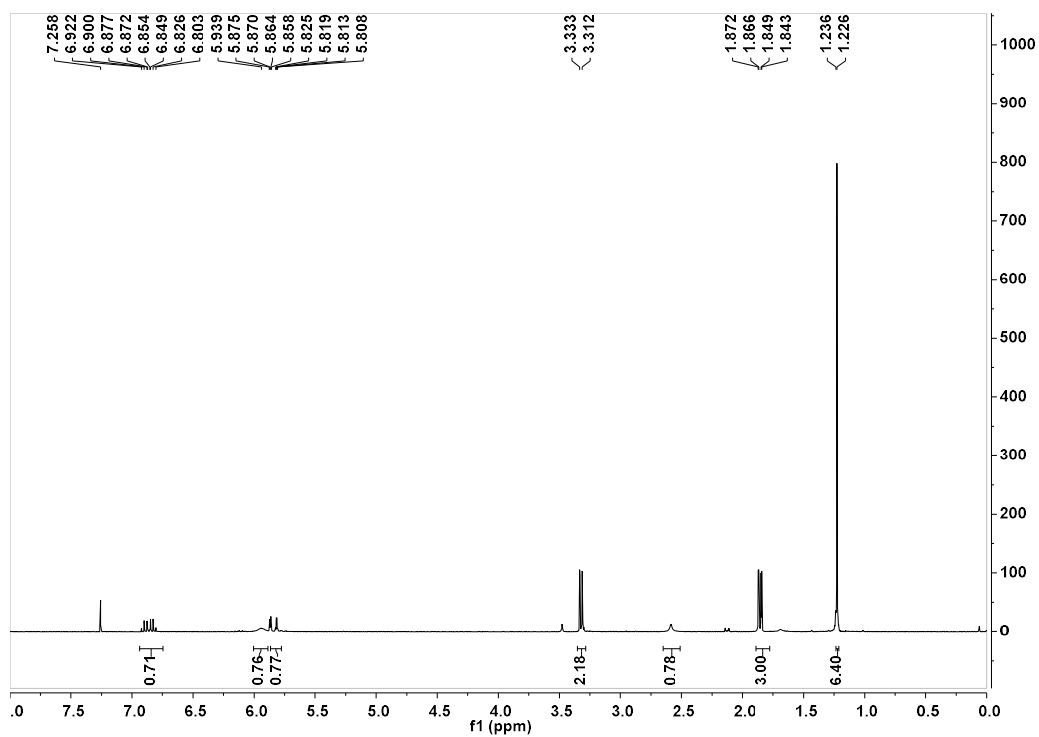
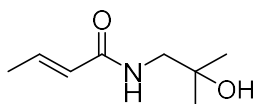
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111 13 h



zhoudang-20190114/2  
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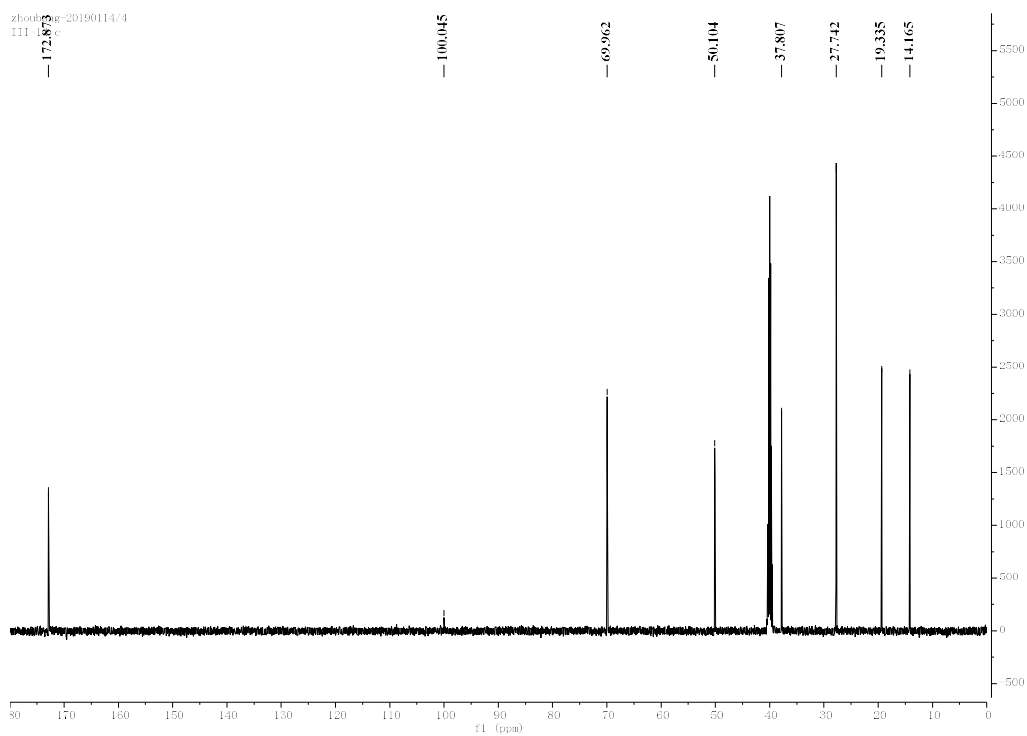
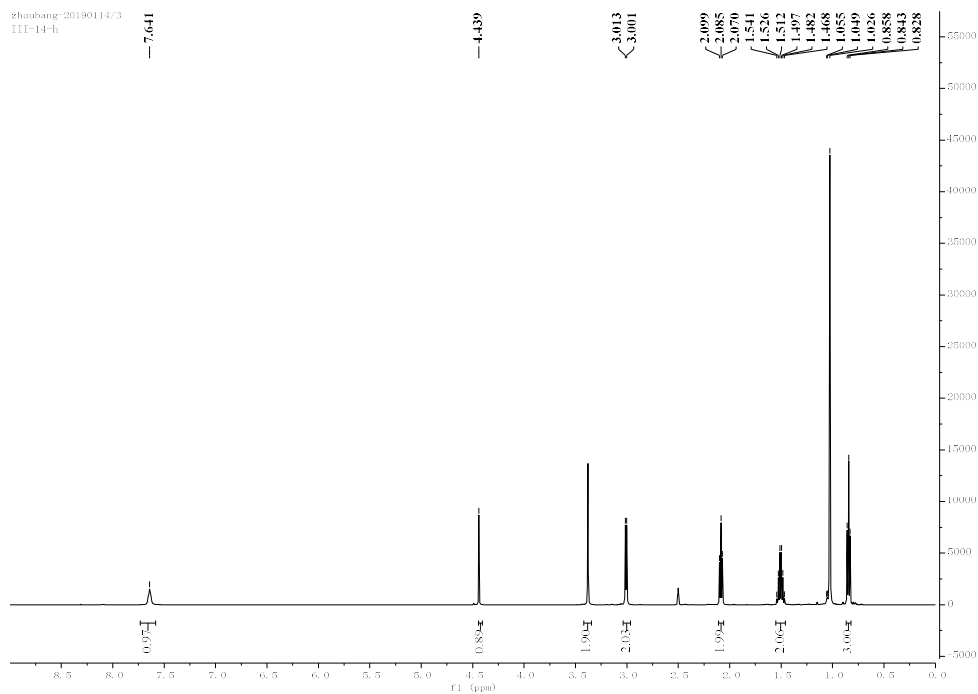
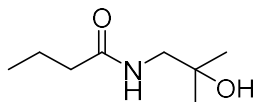


(*E*)-*N*-(2-hydroxy-2-methylpropyl)but-2-enamide (**3d**)

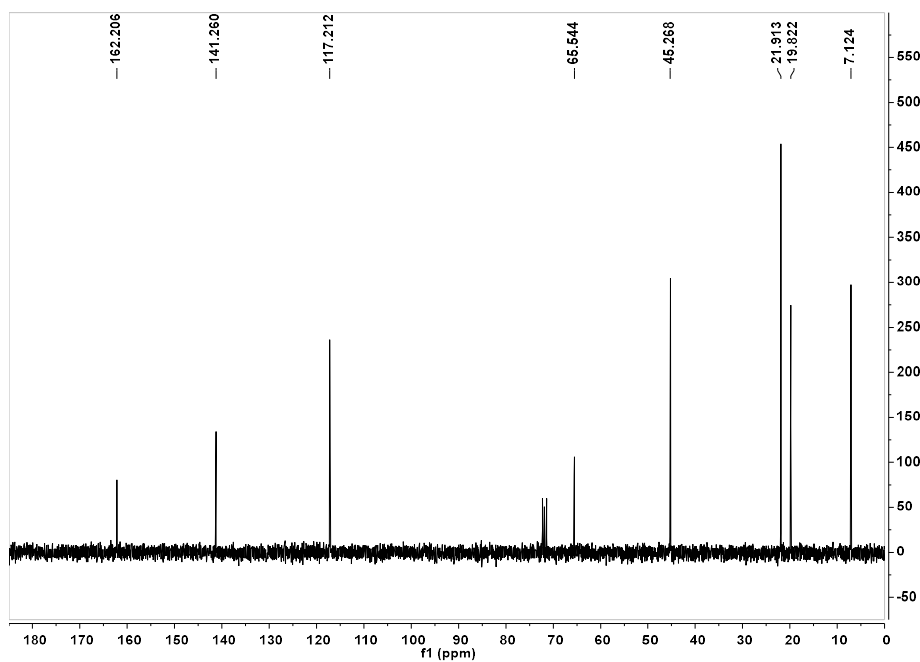
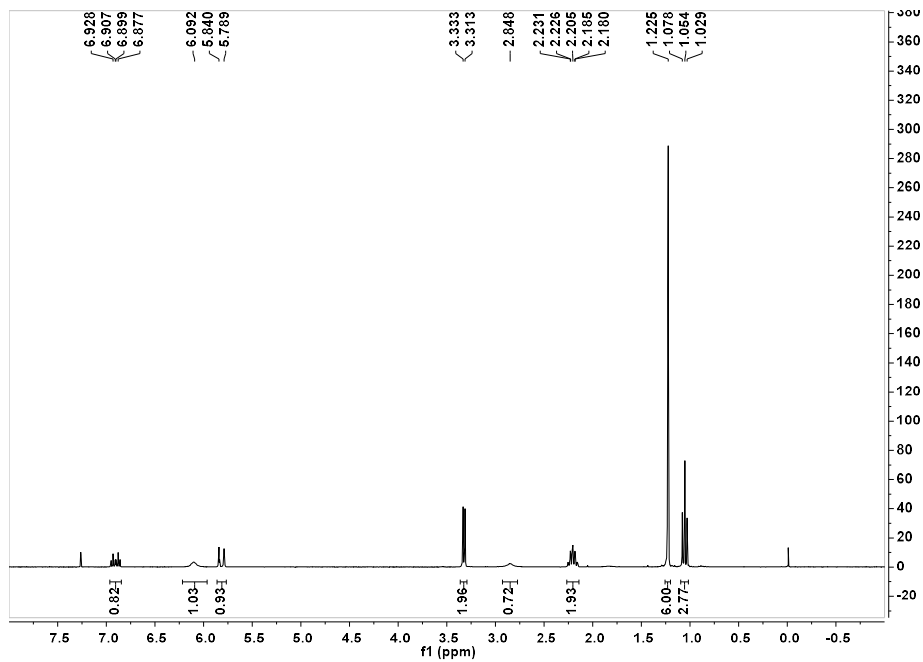
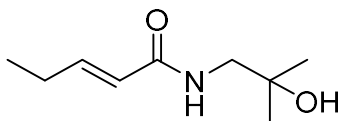




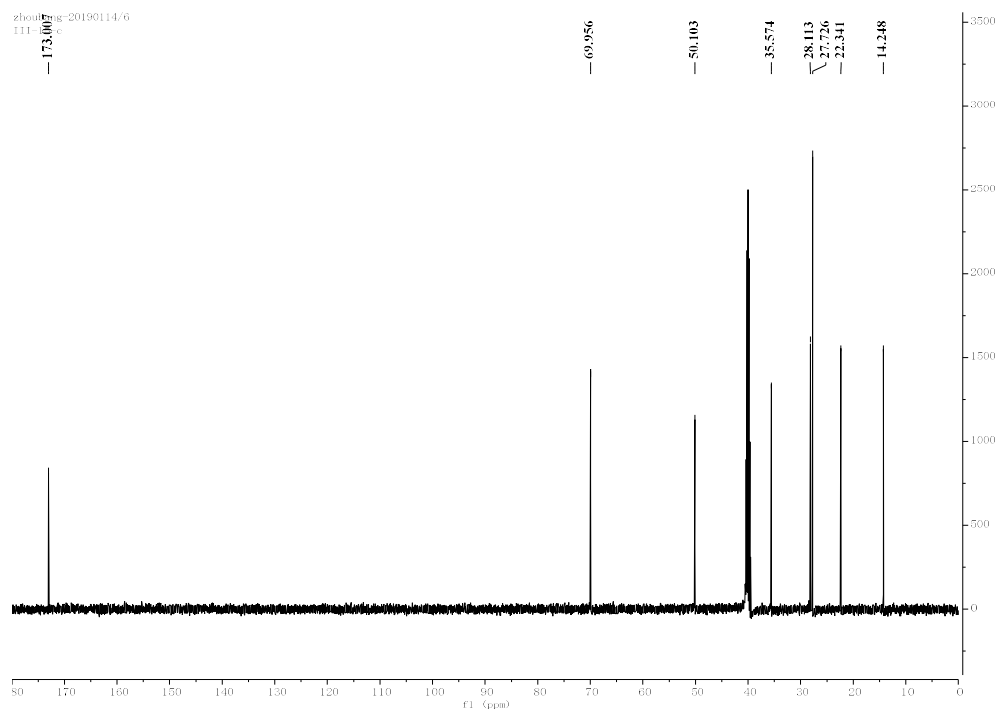
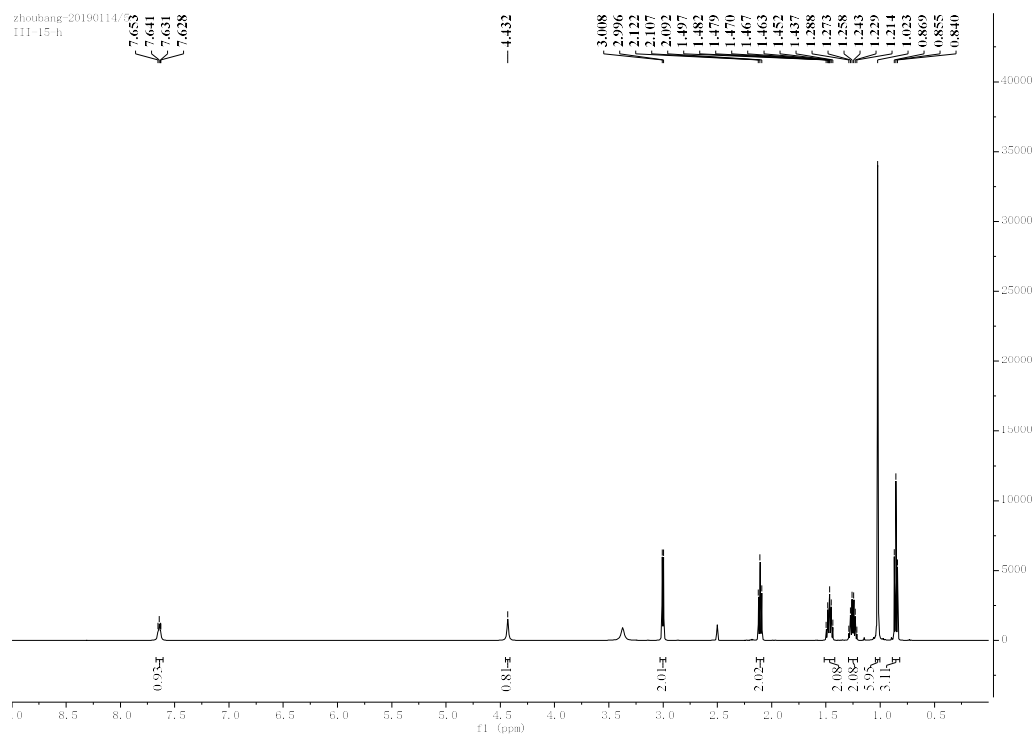
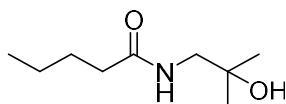
# N-(2-hydroxy-2-methylpropyl)butyramide (3e)



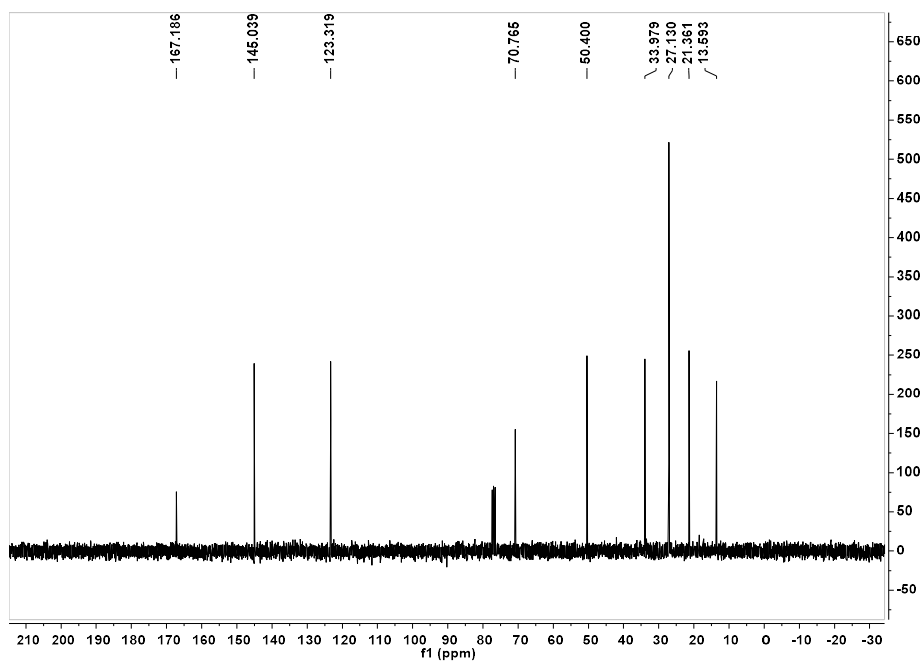
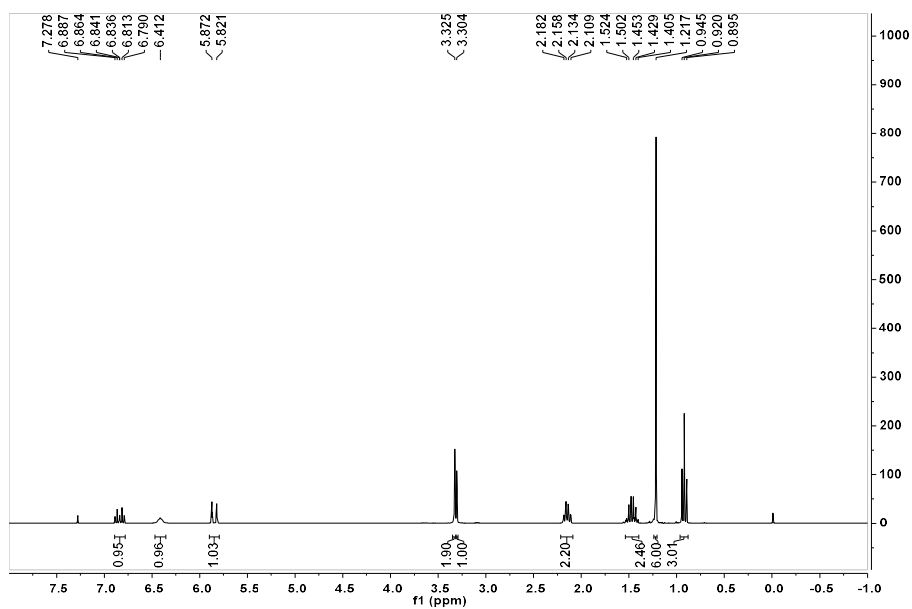
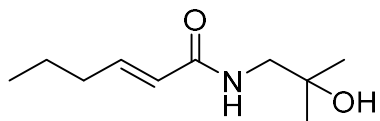
(*E*)-*N*-(2-hydroxy-2-methylpropyl)pent-2-enamide (**3f**)



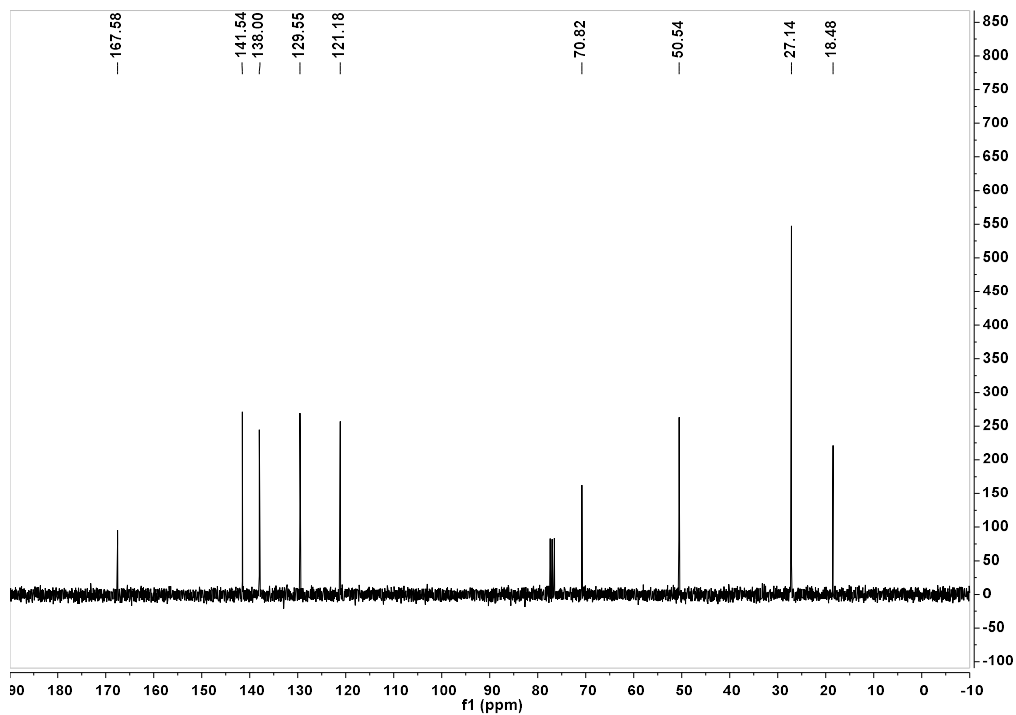
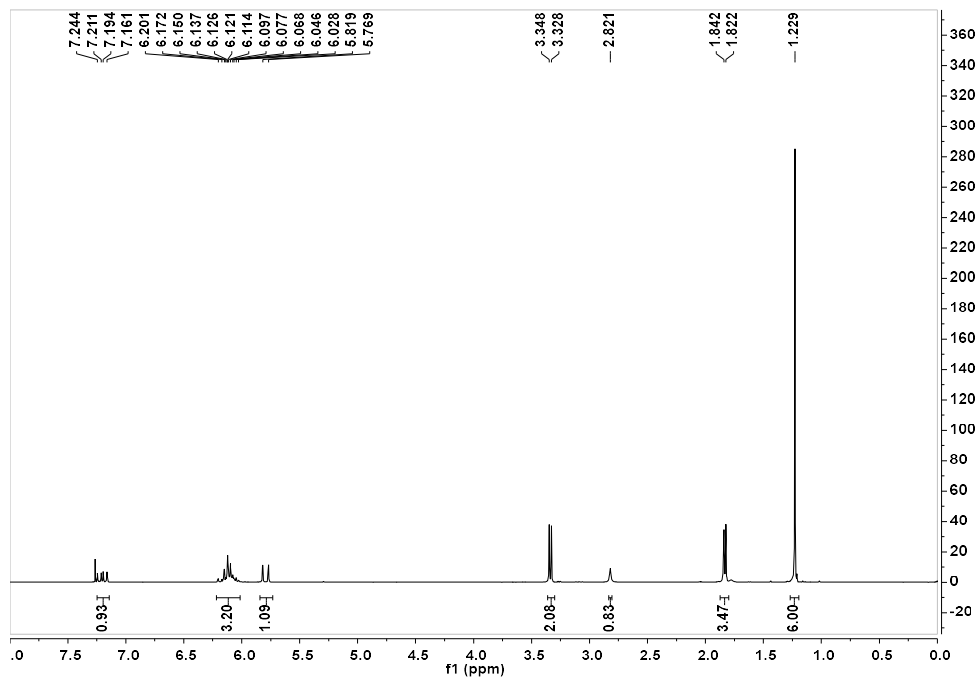
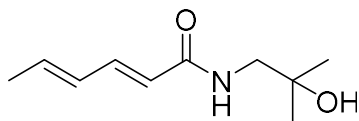
# *N*-(2-hydroxy-2-methylpropyl)pentanamide (**3g**)



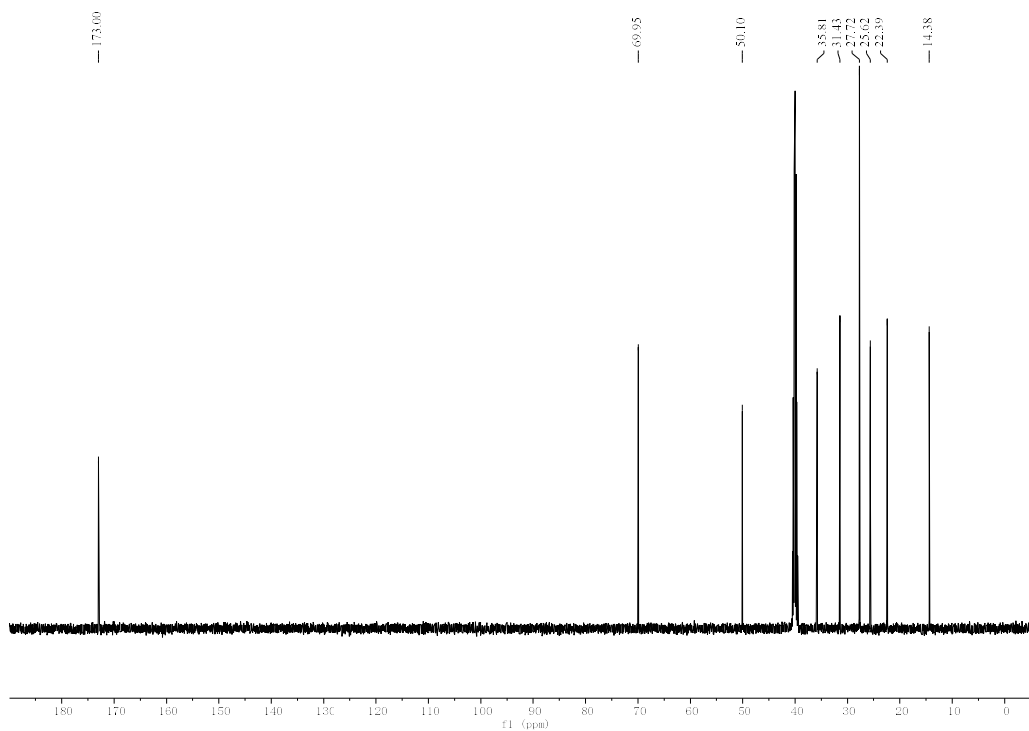
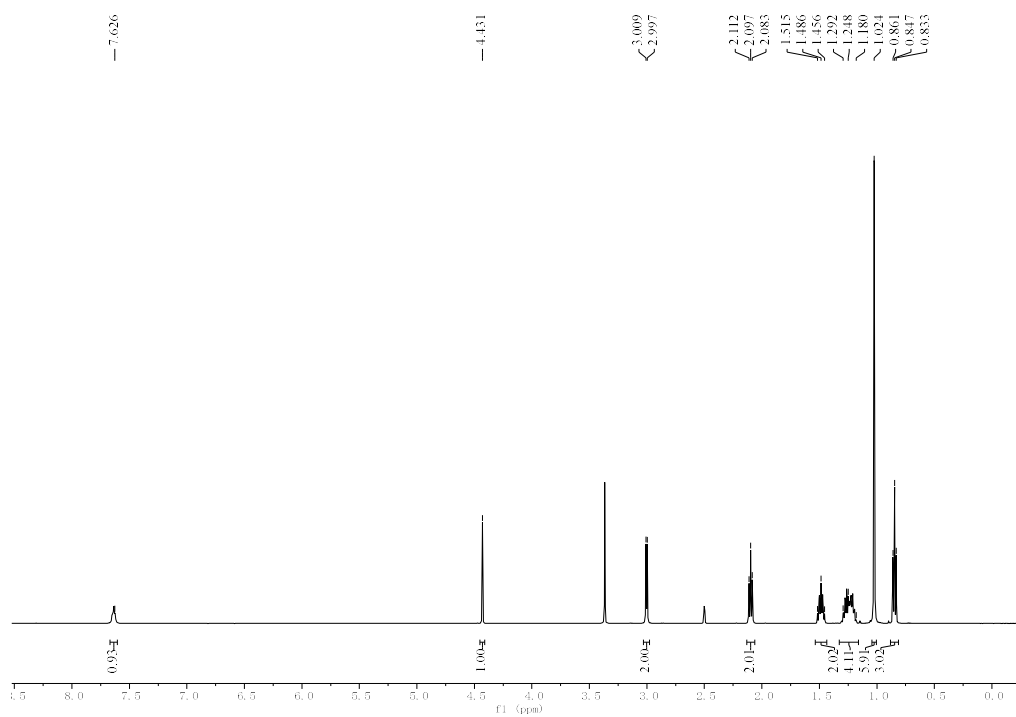
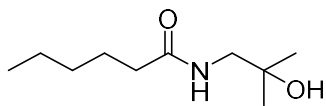
(*E*)-*N*-(2-hydroxy-2-methylpropyl)hex-2-enamide (**3h**)



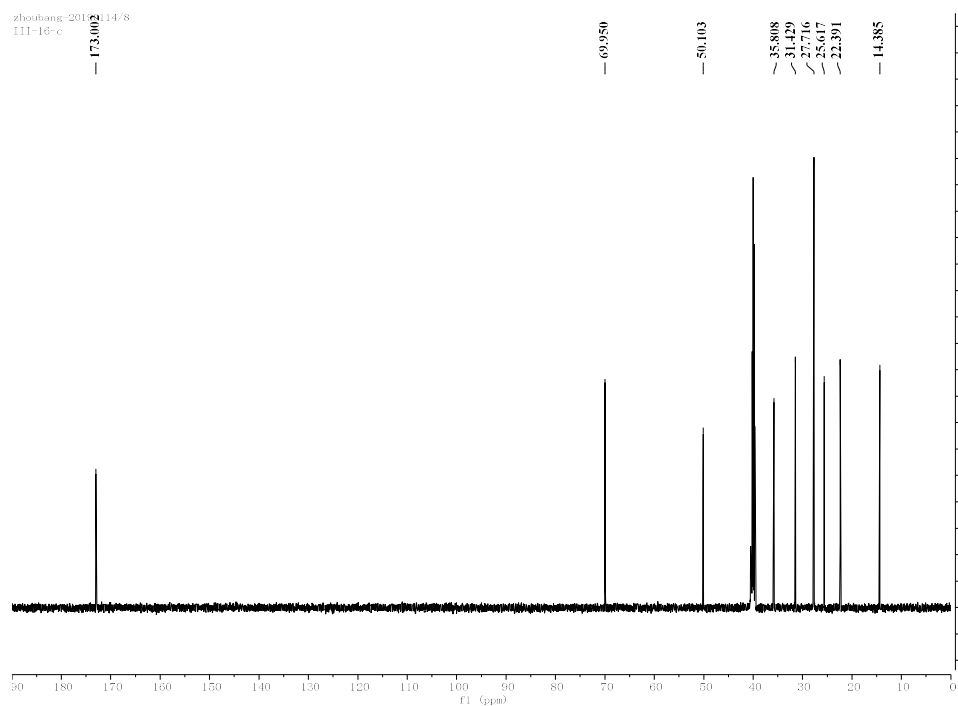
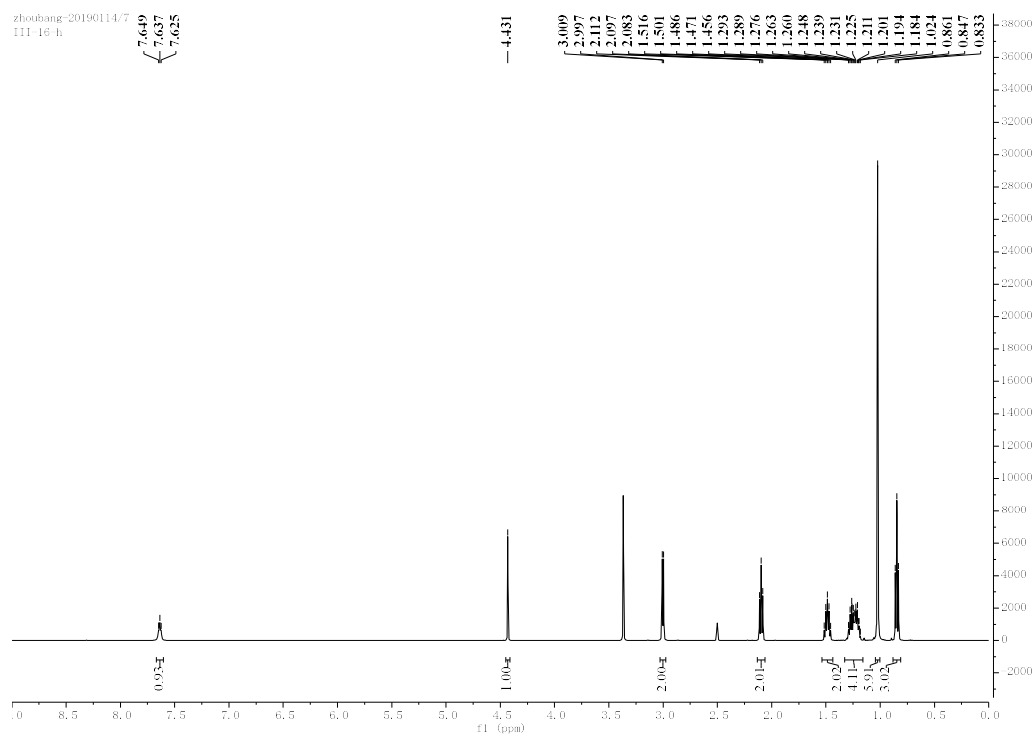
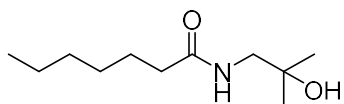
(2*E*,4*E*)-*N*-(2-hydroxy-2-methylpropyl)hexa-2,4-dienamide (**3i**)



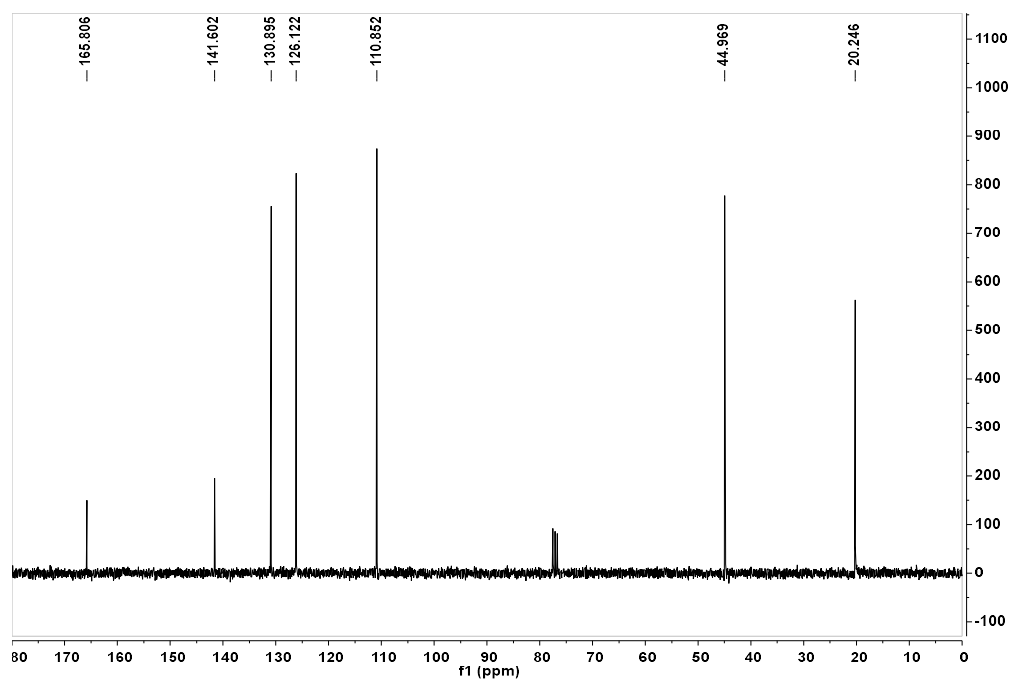
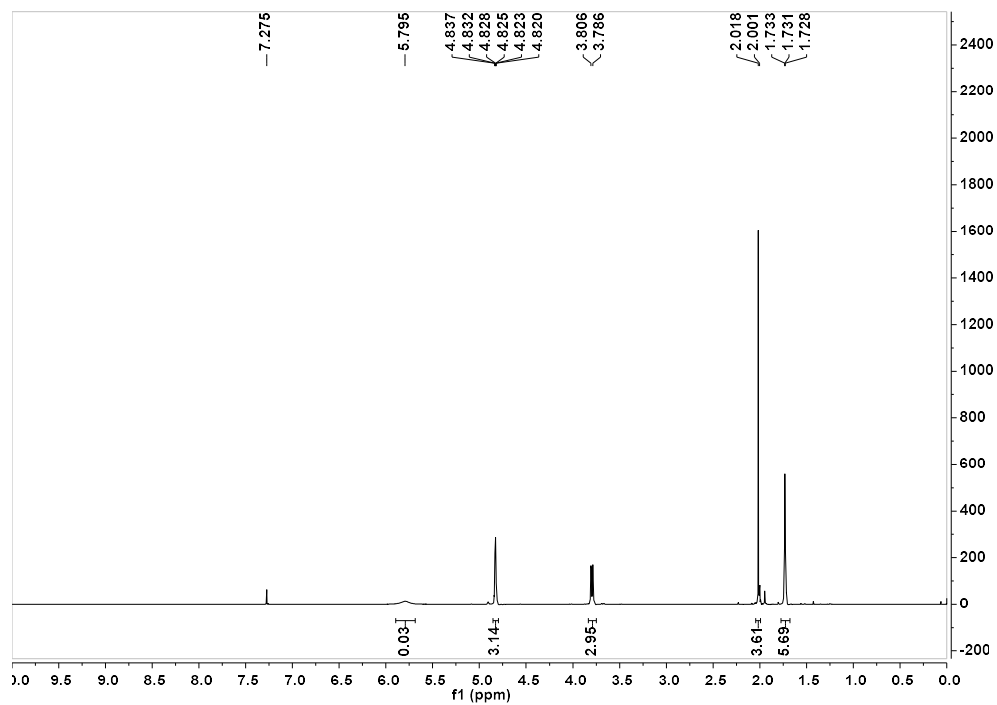
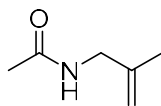
*N*-(2-hydroxy-2-methylpropyl)hexanamide (**3j**)



*N*-(2-hydroxy-2-methylpropyl)heptanamide (**3k**)

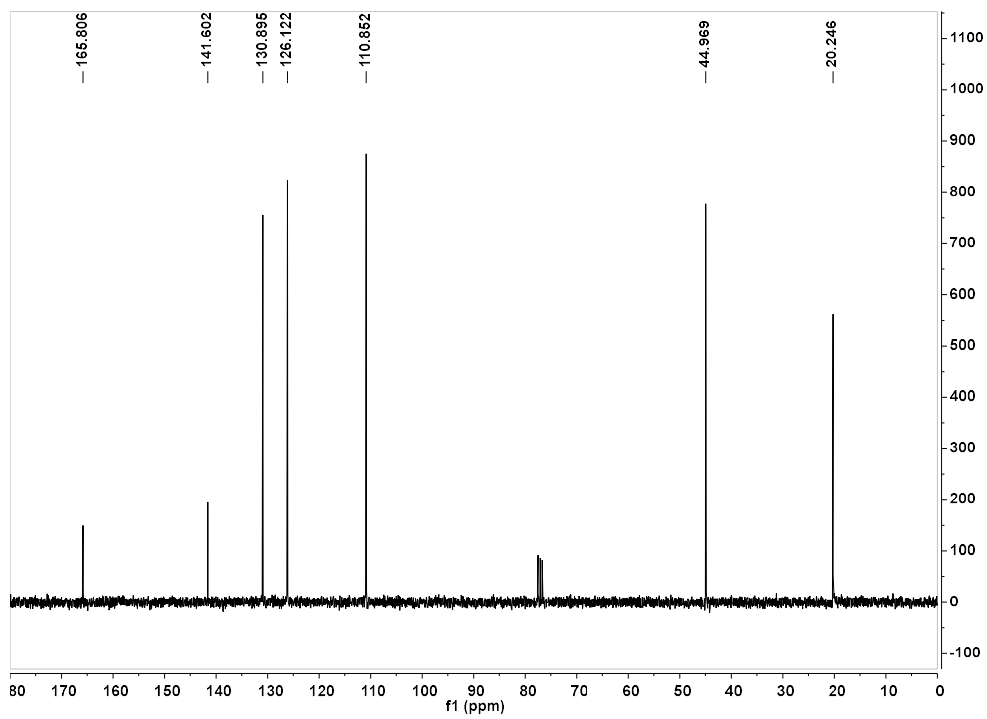
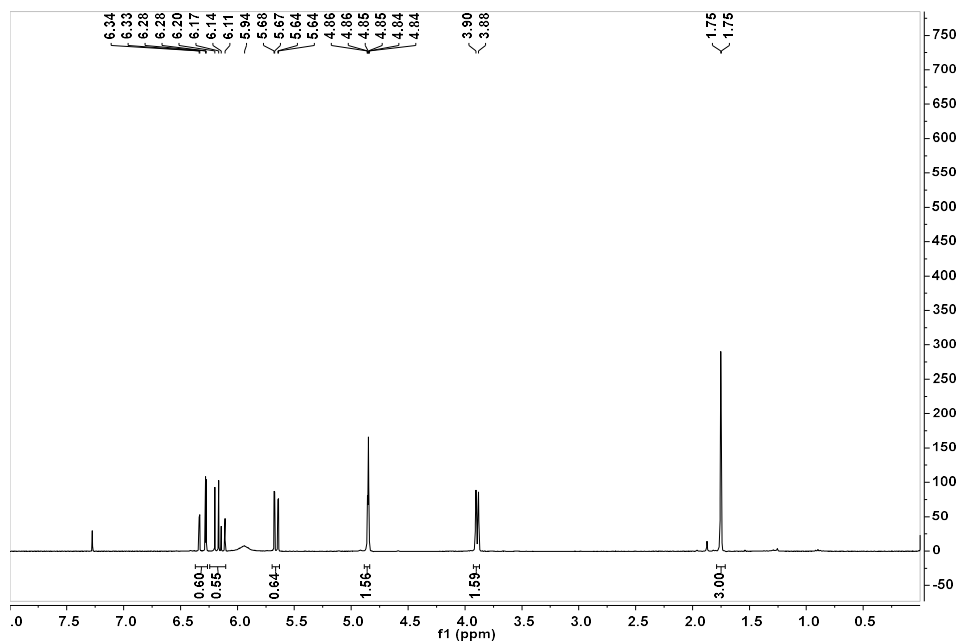
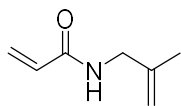


*N*-(2-methylallyl)acetamide (**4a**)

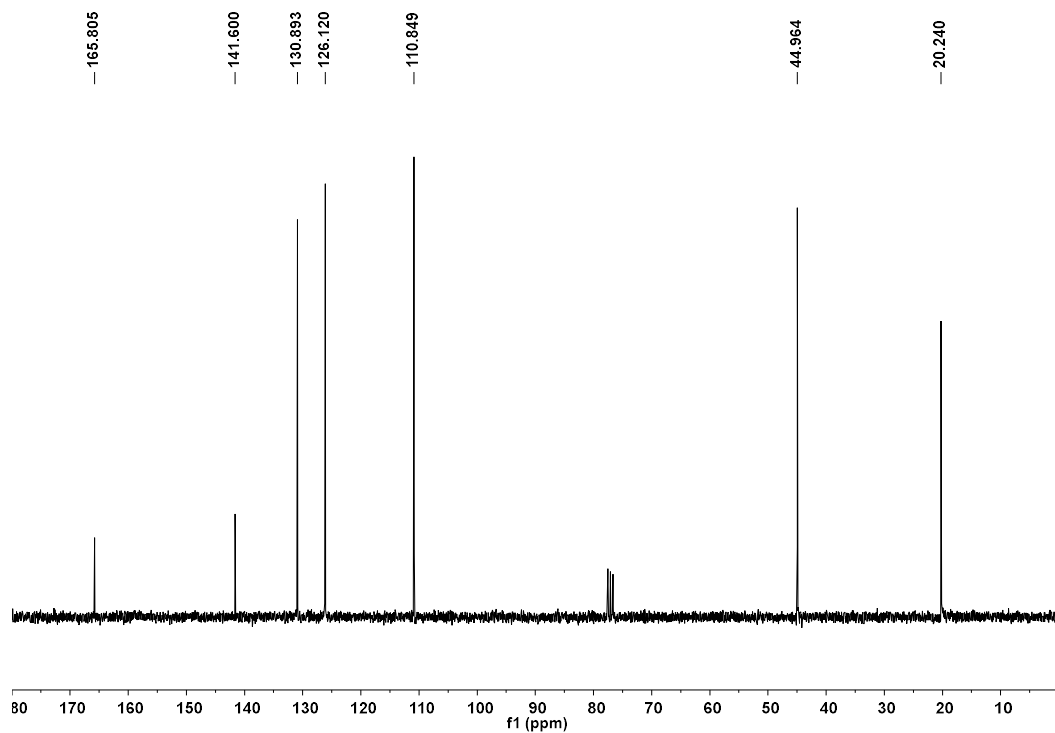
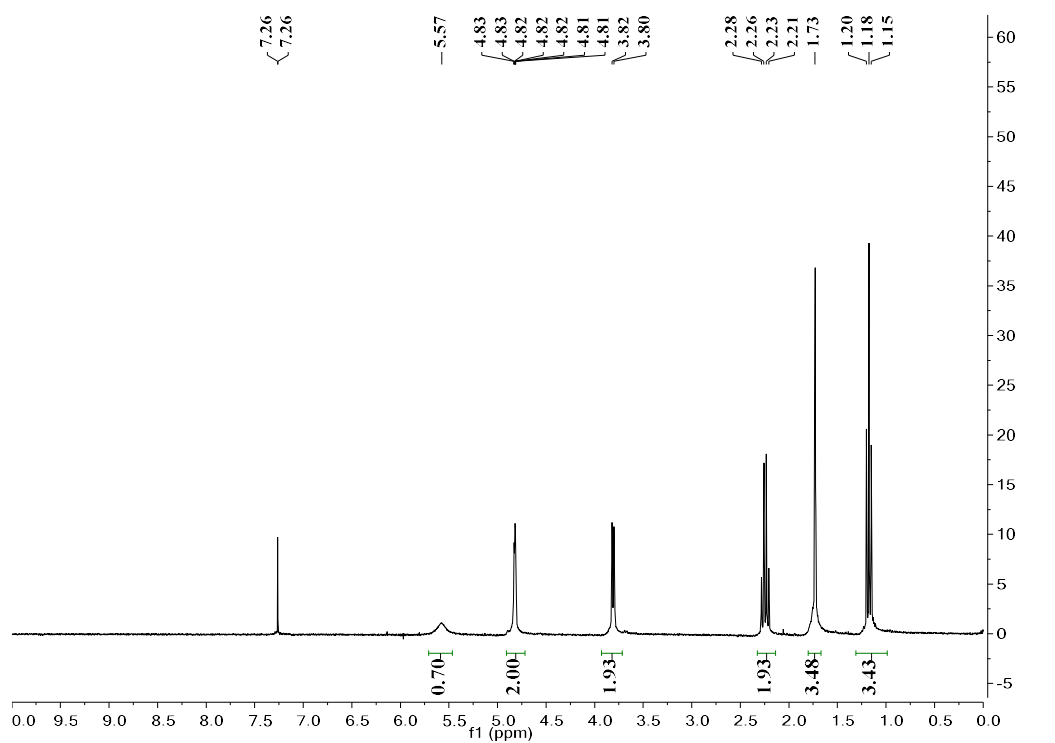
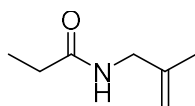


*N*-(2-methylallyl)acrylamide (**4b**)

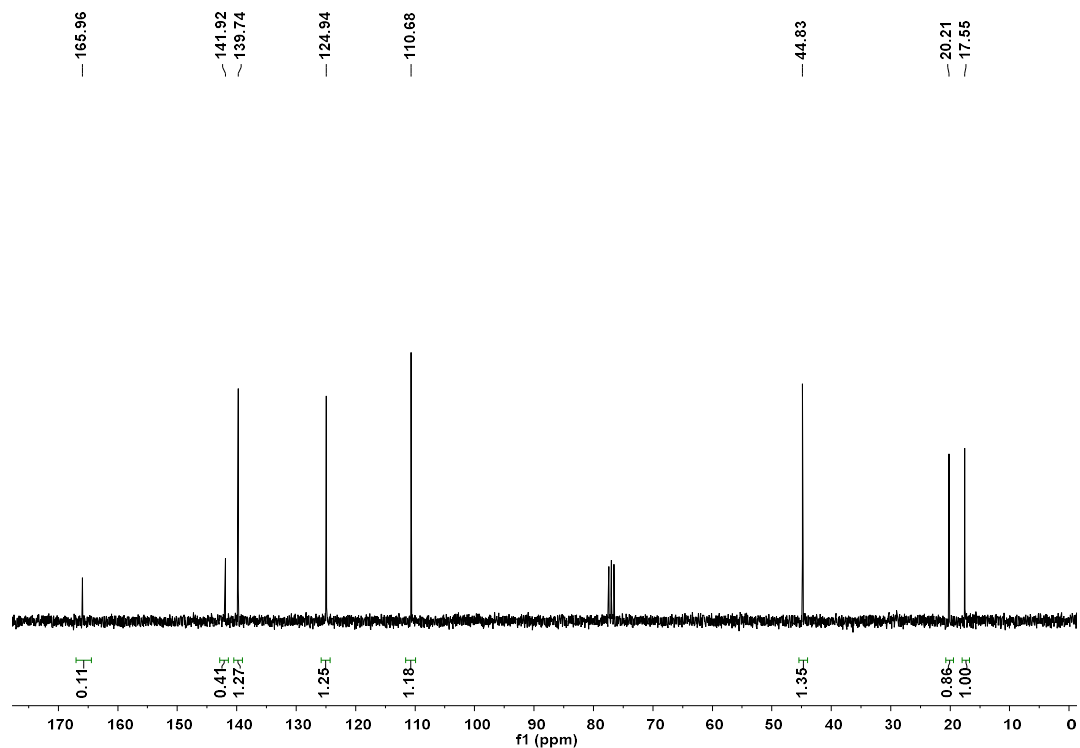
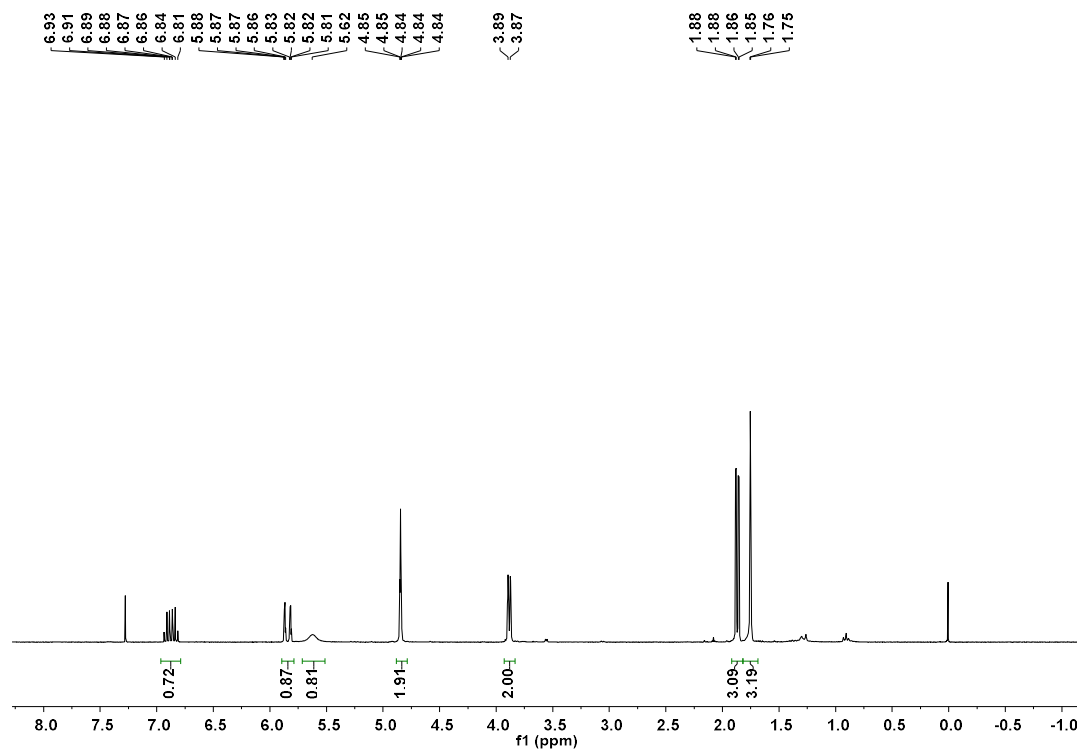
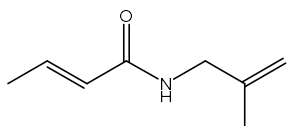




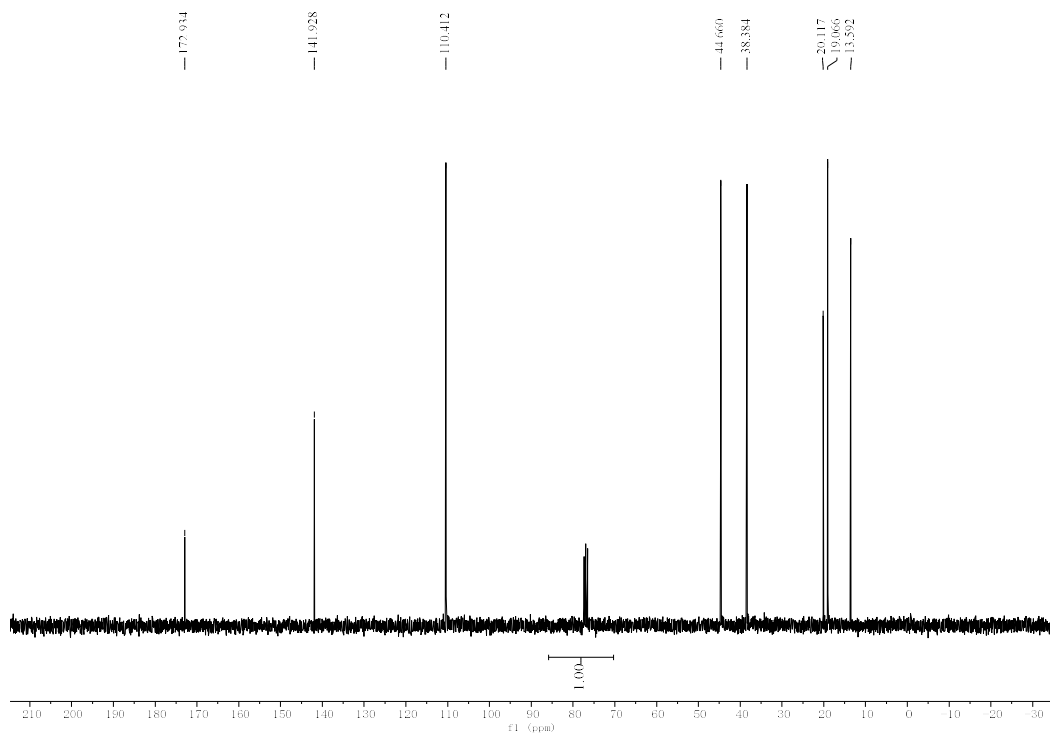
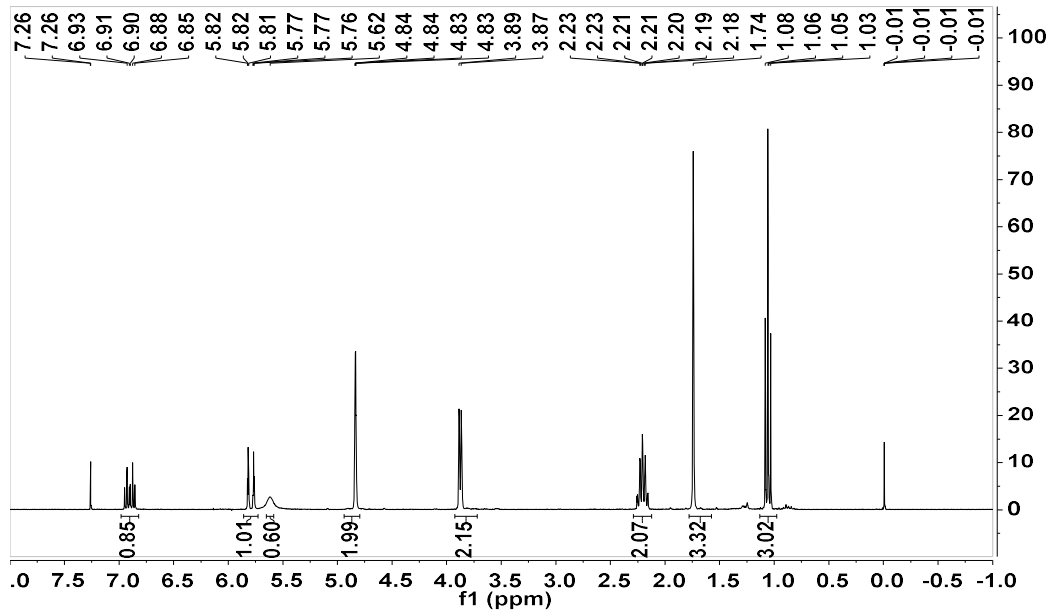
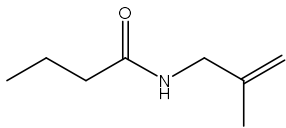
*N*-(2-methylallyl)propionamide (**4c**)



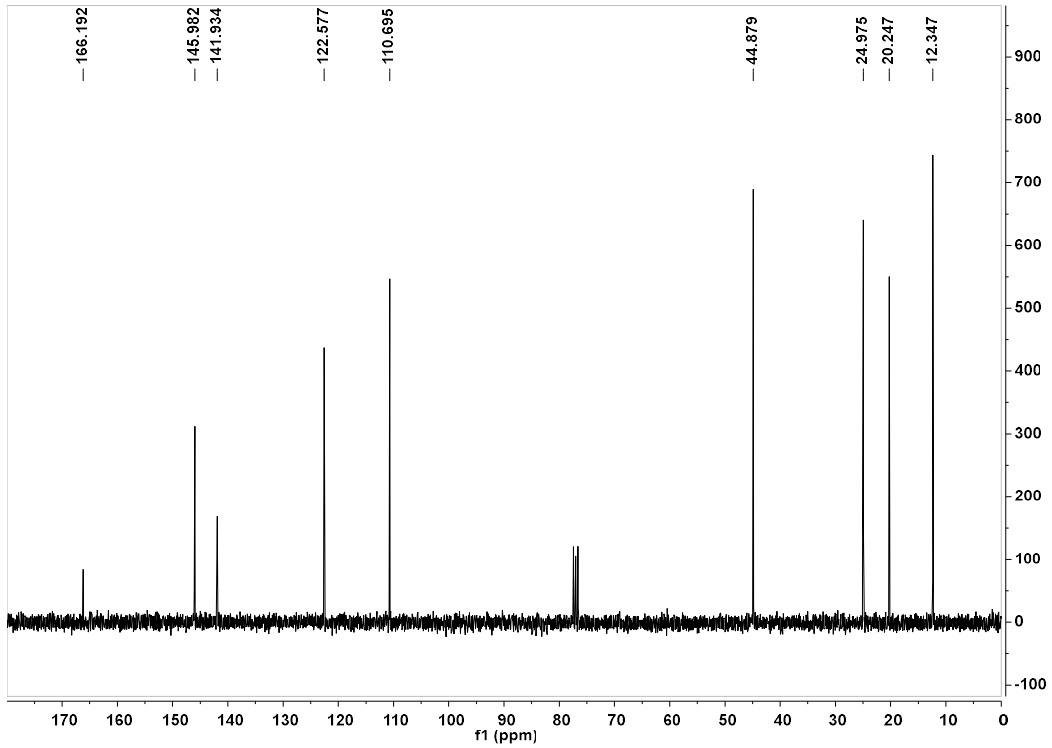
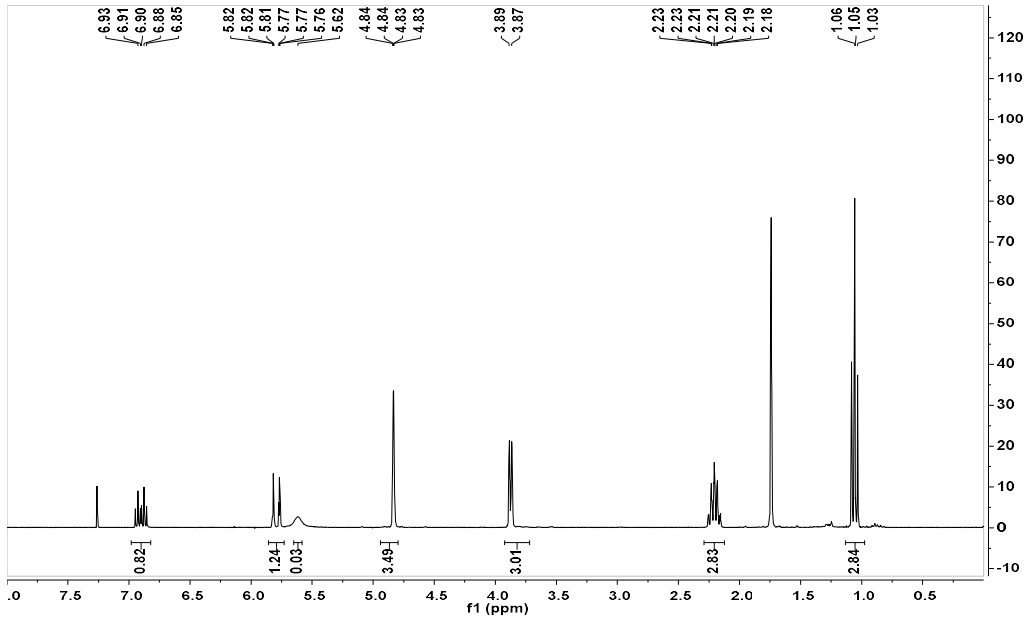
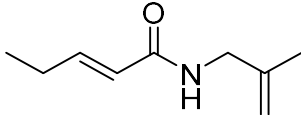
*N*-(2-methylallyl)butyramide (**4d**)



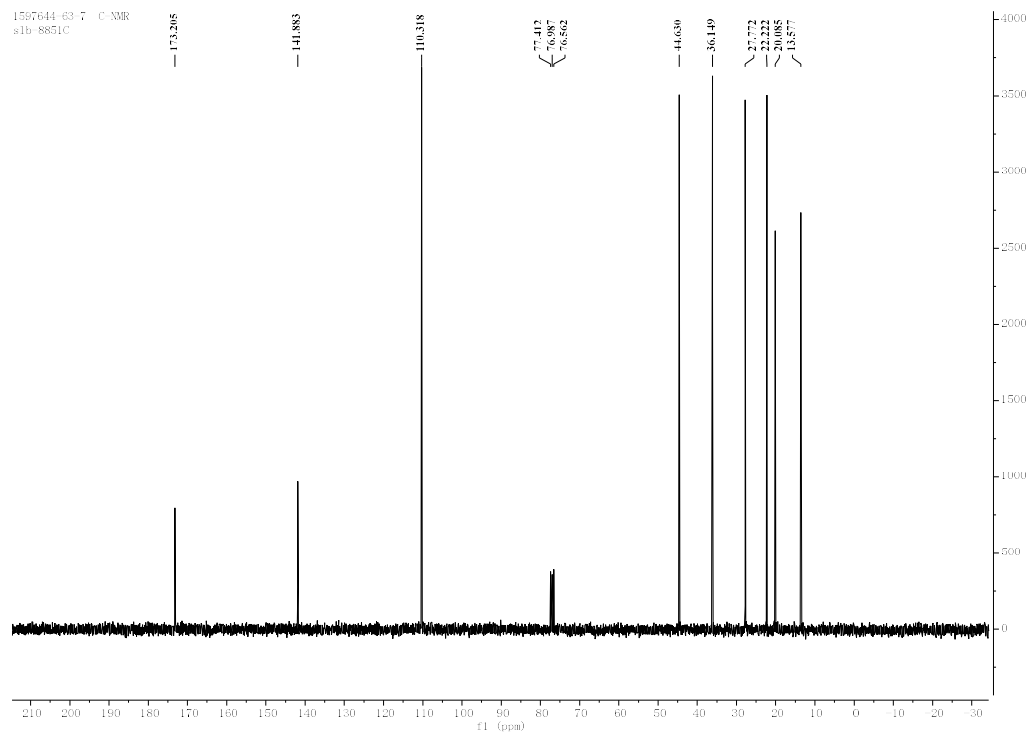
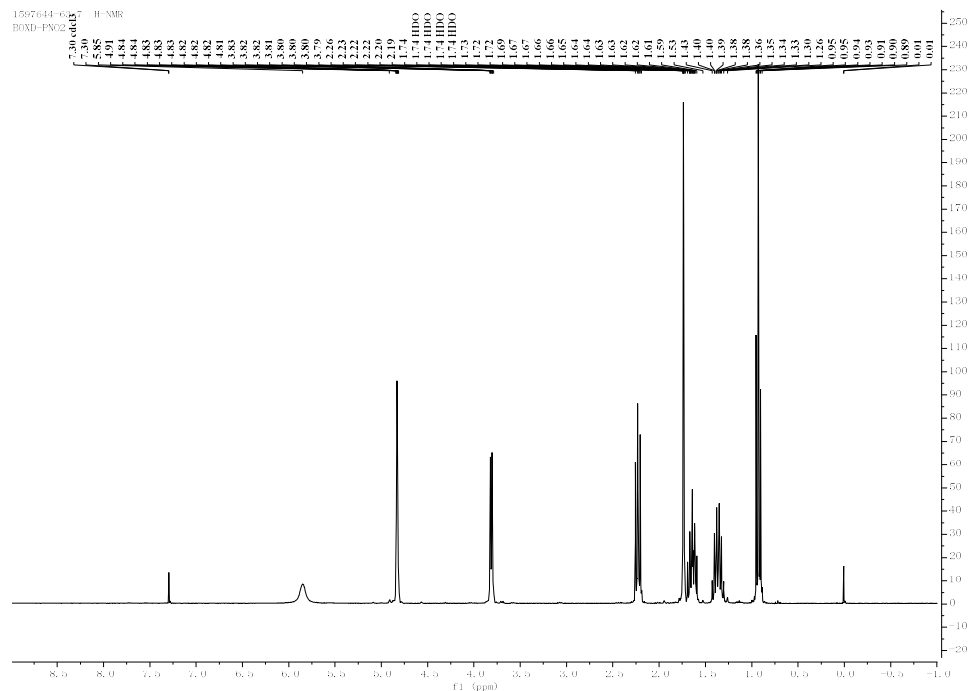
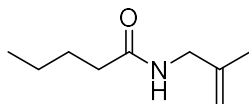
*N*-(2-methylallyl)butyramide (**4e**)



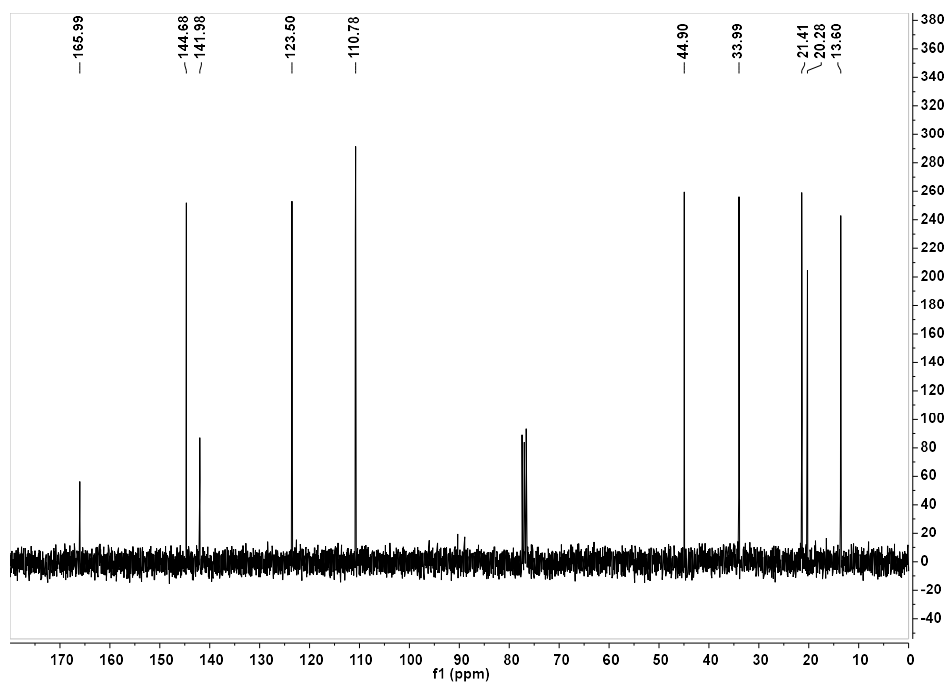
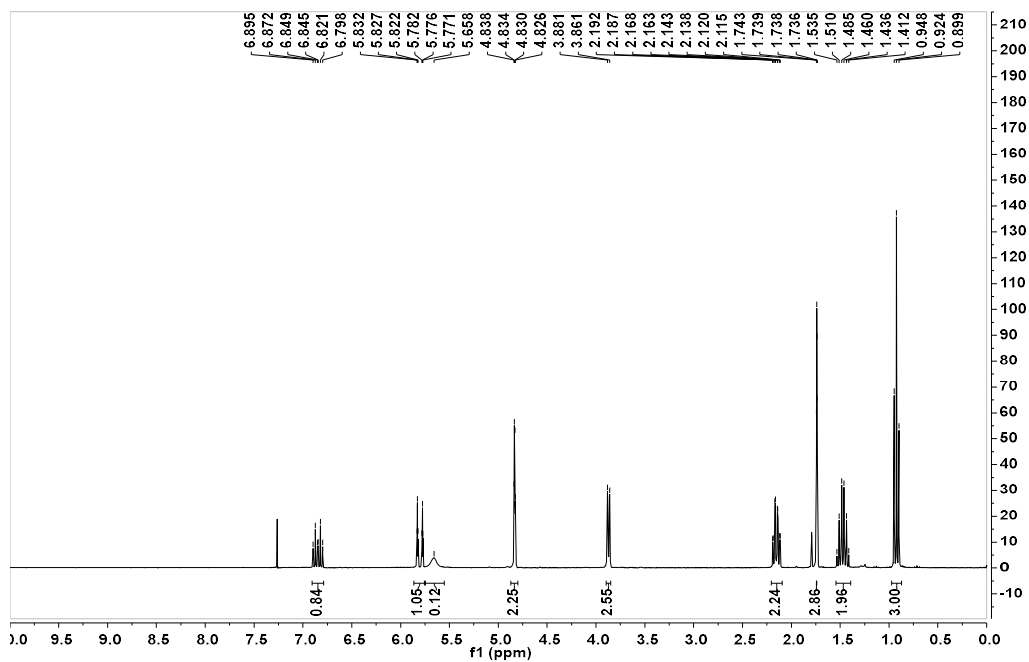
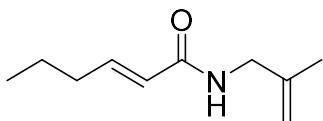
*(E)*-*N*-(2-methylallyl)pent-2-enamide (**4f**)



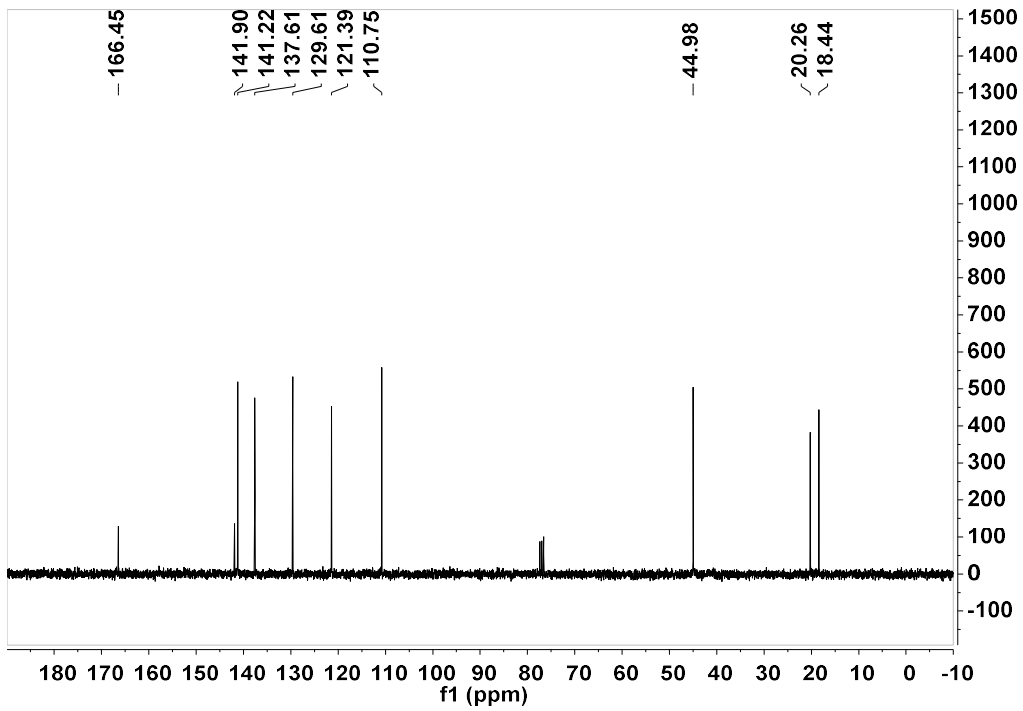
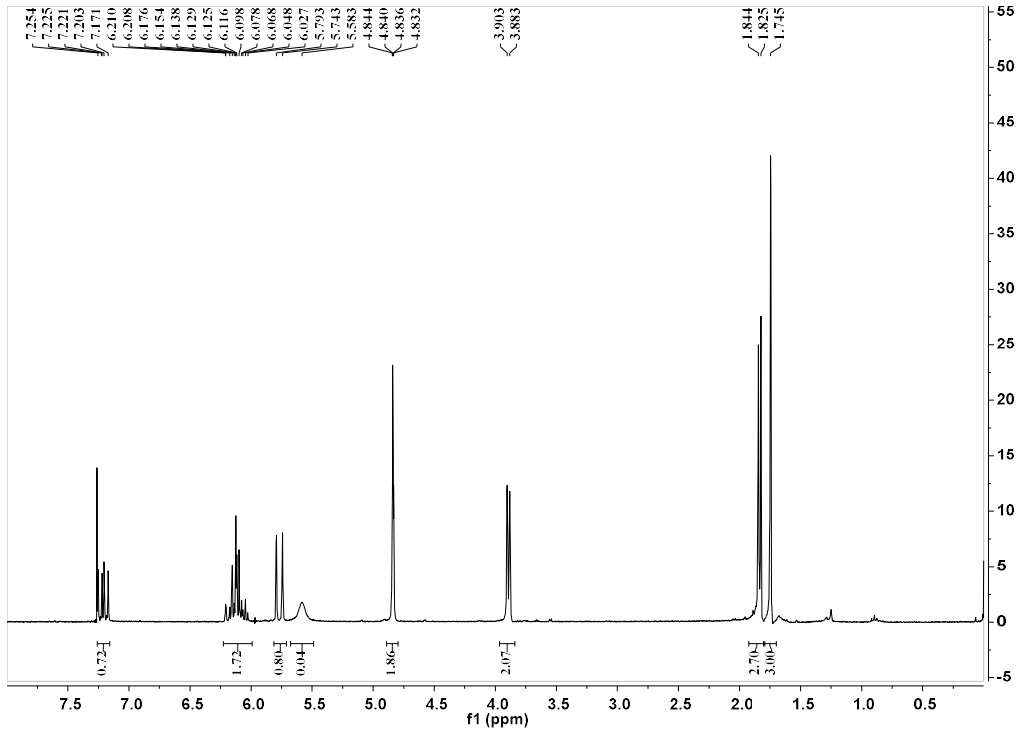
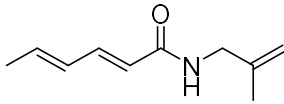
# *N*-(2-methylallyl)pentanamide (**4g**)



(*E*)-*N*-(2-methylallyl)hex-2-enamide (**4h**)

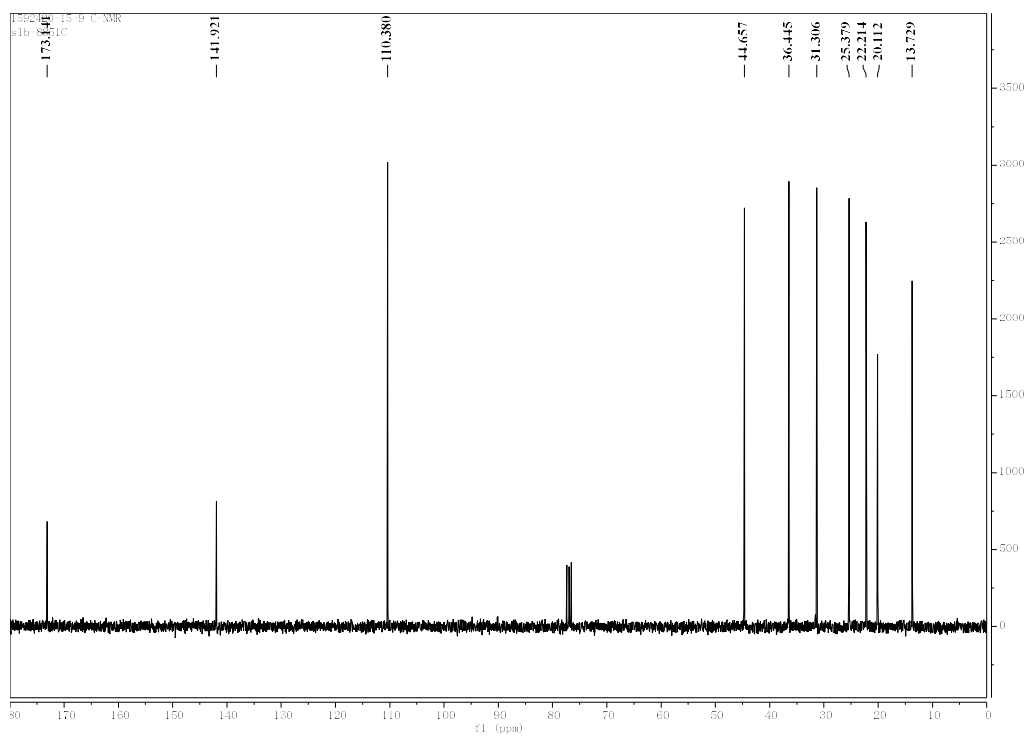
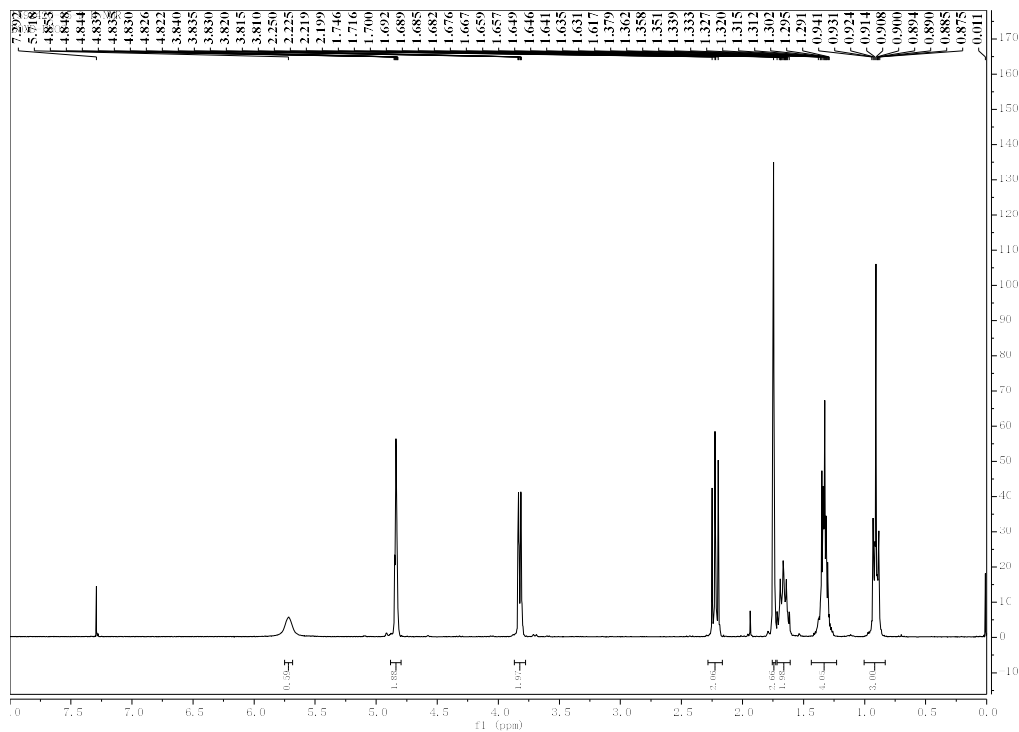
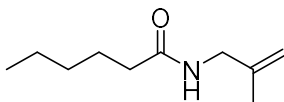


(*2E,4E*)-*N*-(2-methylallyl)hexa-2,4-dienamide (**4i**)

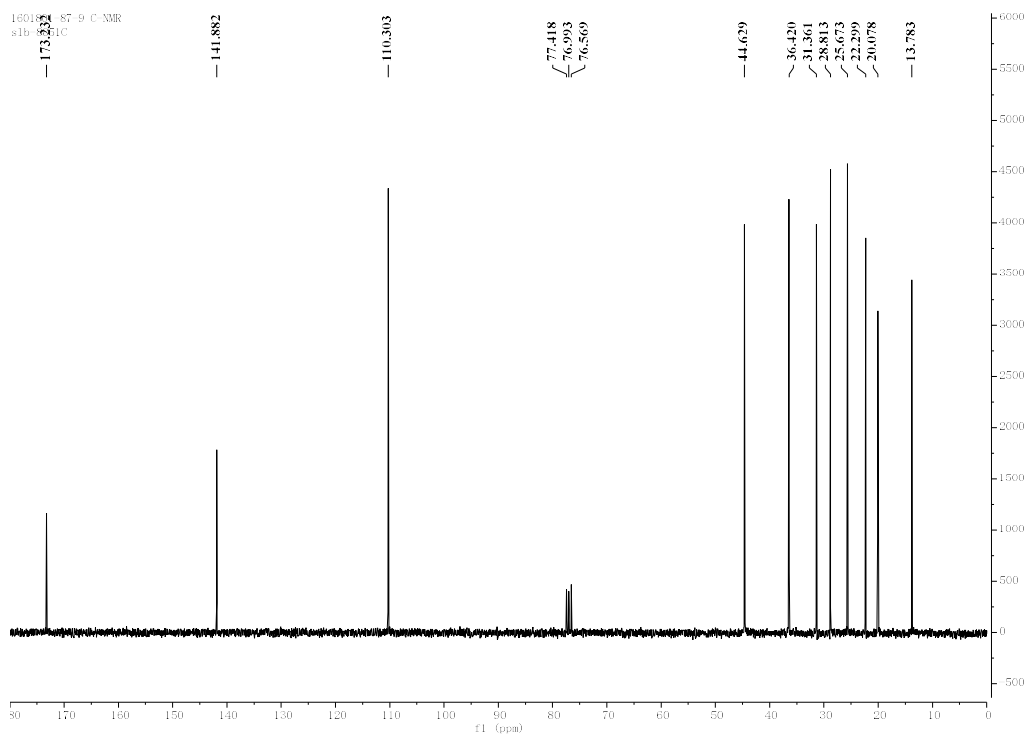
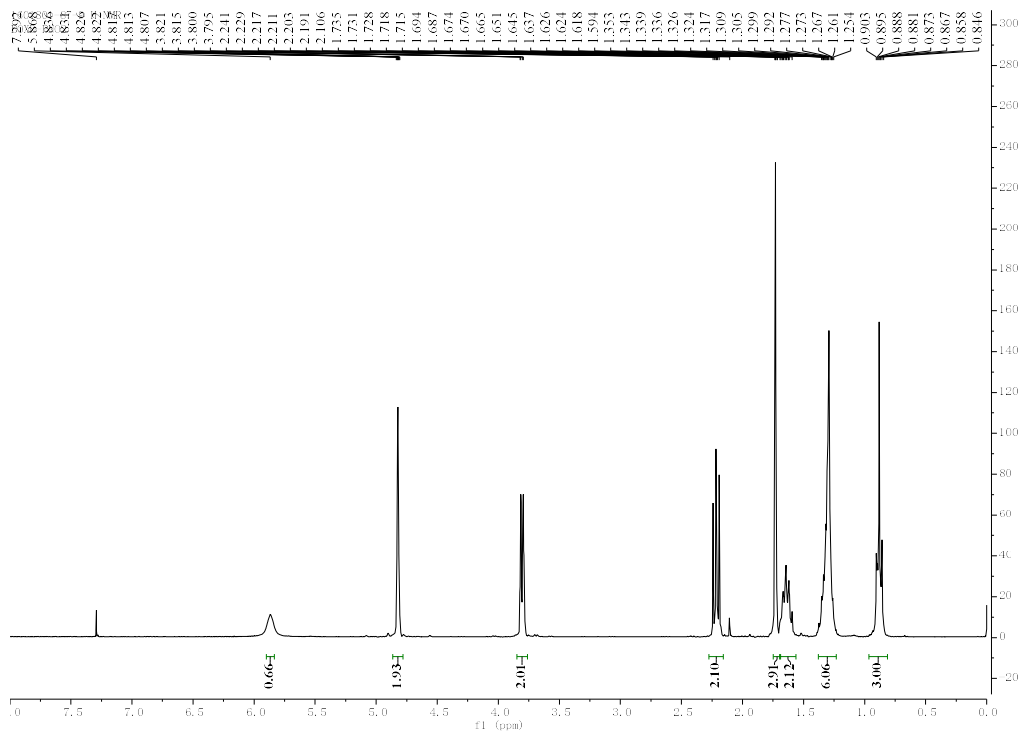
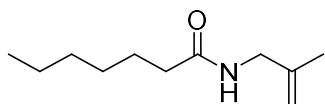




# *N*-(2-methylallyl)hexanamide (**4j**)



*N*-(2-methylallyl)heptanamide (**4k**)



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