

Supporting Information

A four-component domino reaction for the synthesis of novel bridgehead nitrogen-containing pyrido[1,2-*d*][1,4]diazepines

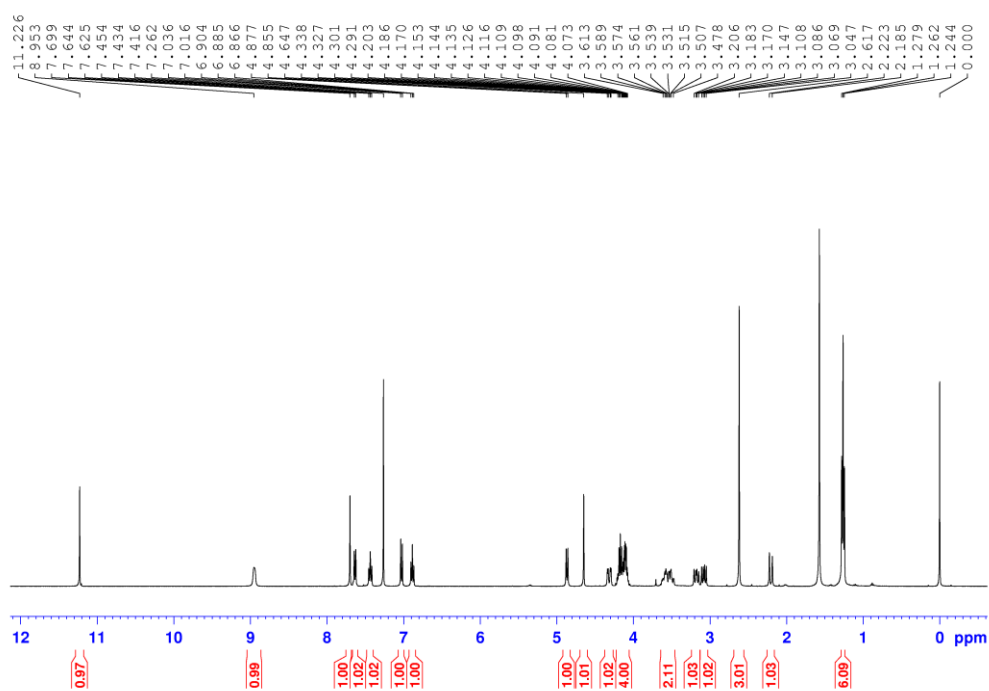
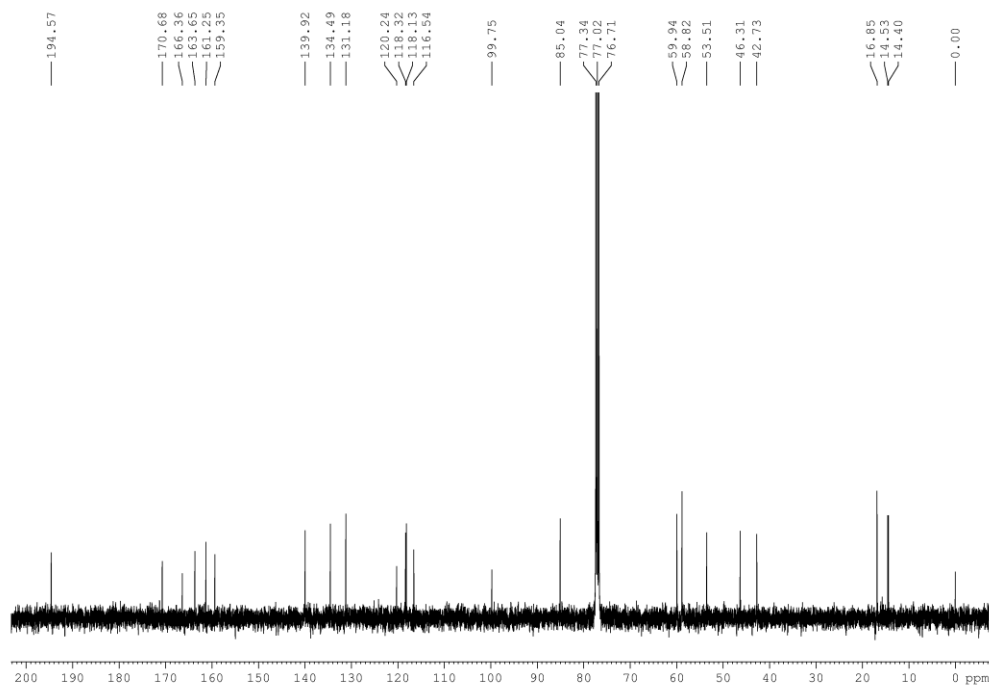
Rui Wang[#], Wei Zhang[#], Ying Tang, Ze-Hui Qi, Yuan-Hui Yu, and Hong-Bo Tan*,
Dian-Yong Tang, Zhi-Gang Xu, Zhong-Zhu Chen*

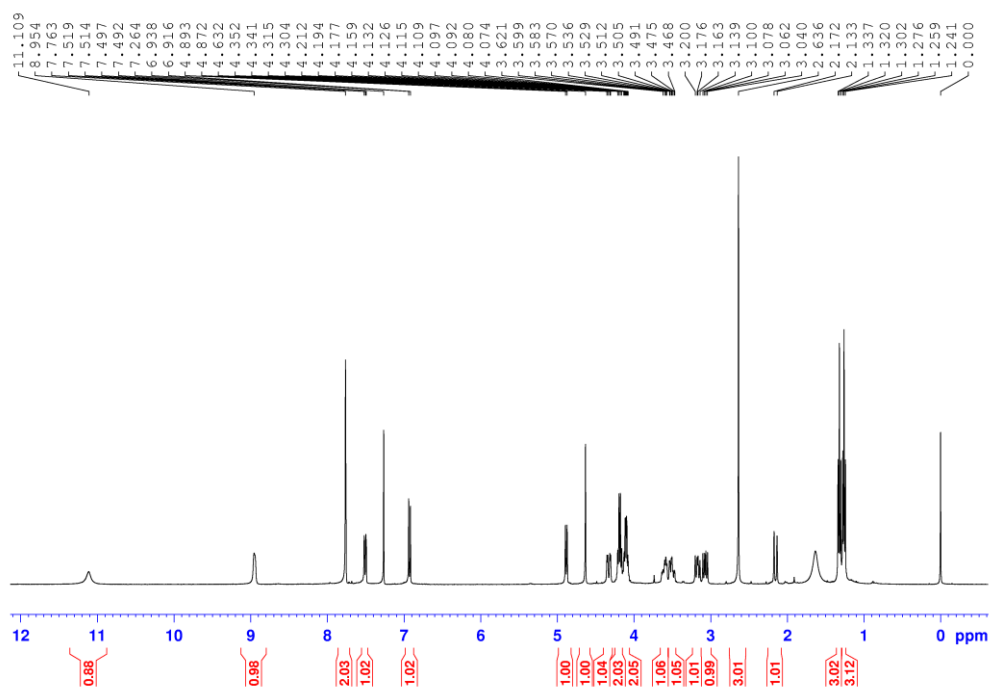
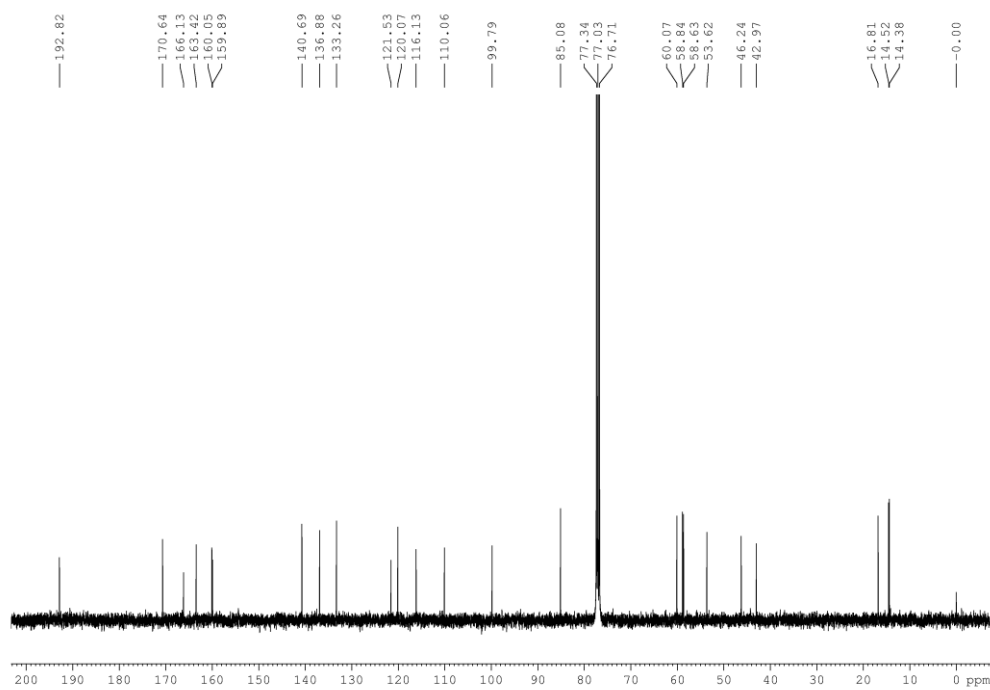
National & Local Joint Engineering Research Center of Targeted and Innovative Therapeutics,
Chongqing Engineering Laboratory of Targeted and Innovative Therapeutics, Chongqing Key
Laboratory of Kinase Modulators as Innovative Medicine, Chongqing Collaborative Innovation
Center of Targeted and Innovative Therapeutics, College of Pharmacy & IATTI, Chongqing
University of Arts and Sciences, Chongqing 402160, China.

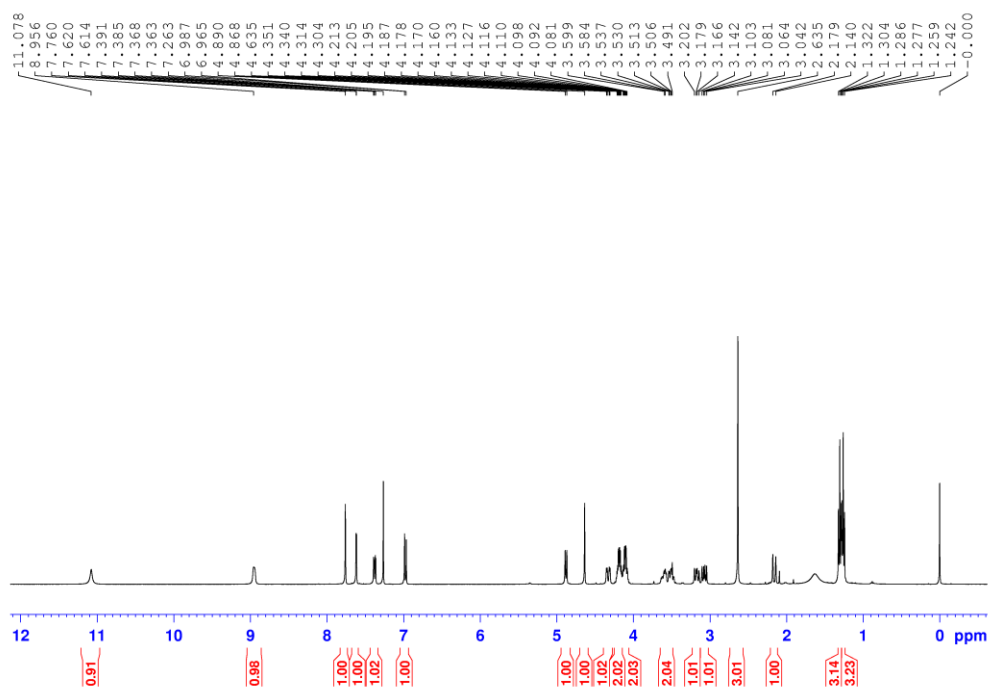
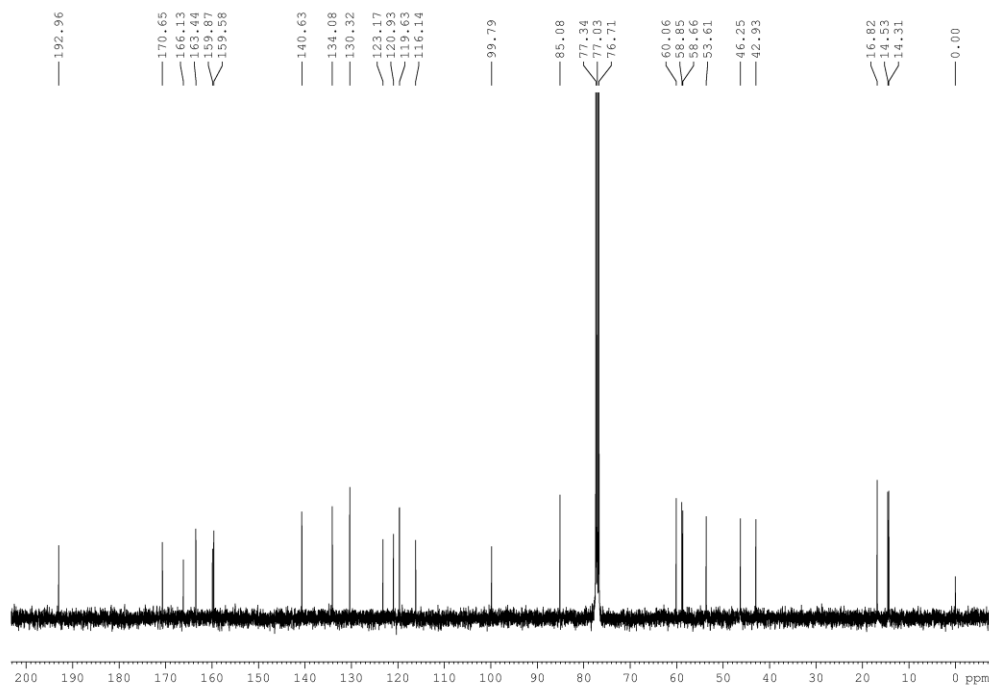
[#]These authors contributed equally to this work.

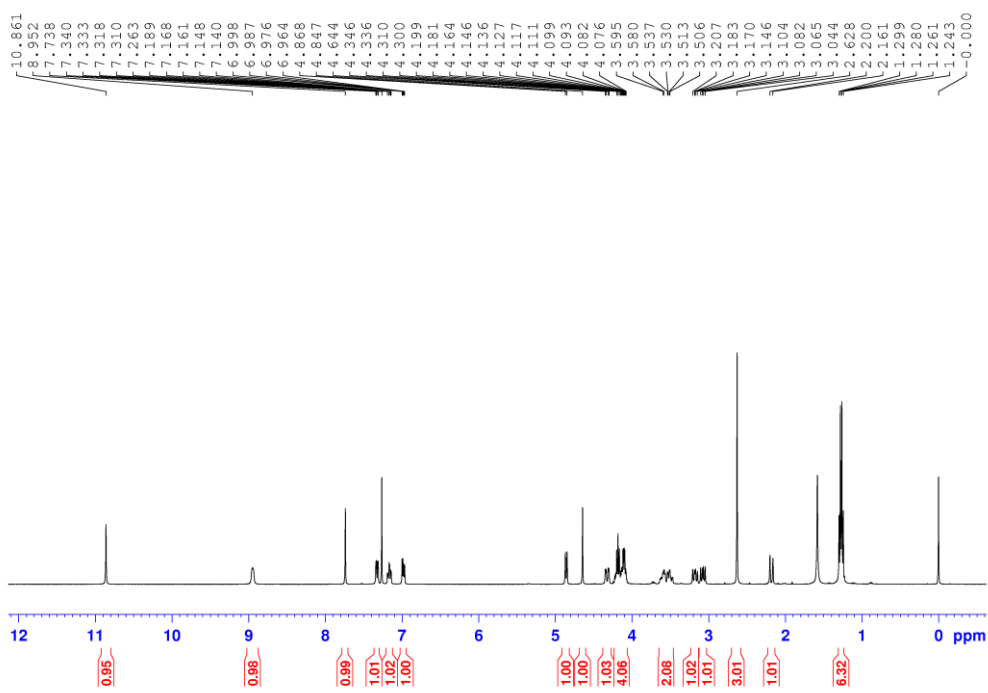
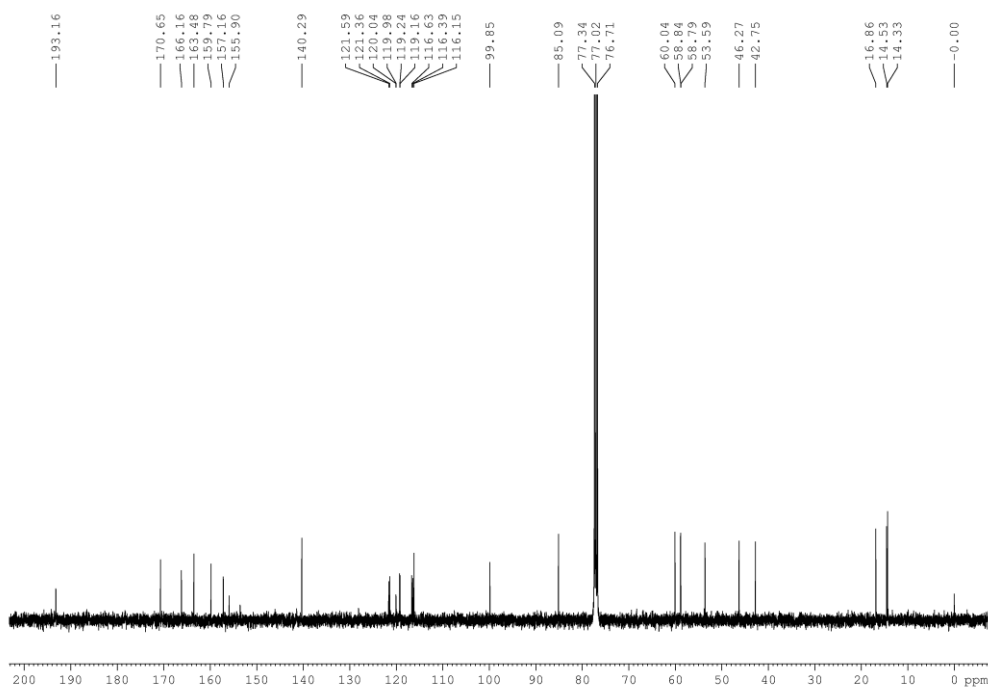
*Corresponding author: 13167859296@163.com (Hong-Bo Tan); 18883138277@163.com
(Zhong-Zhu Chen)

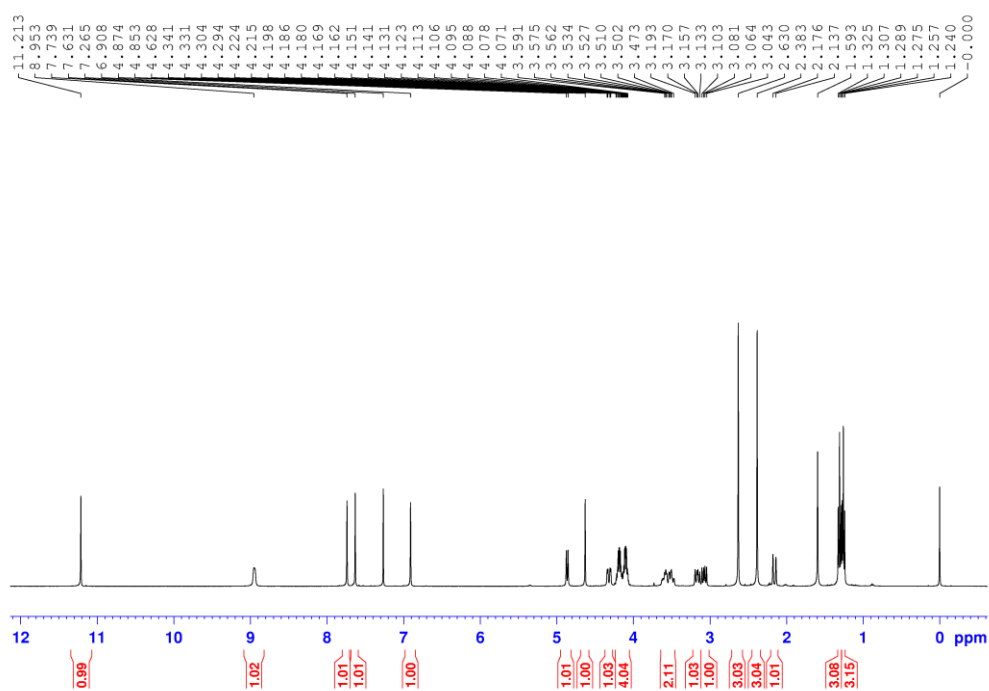
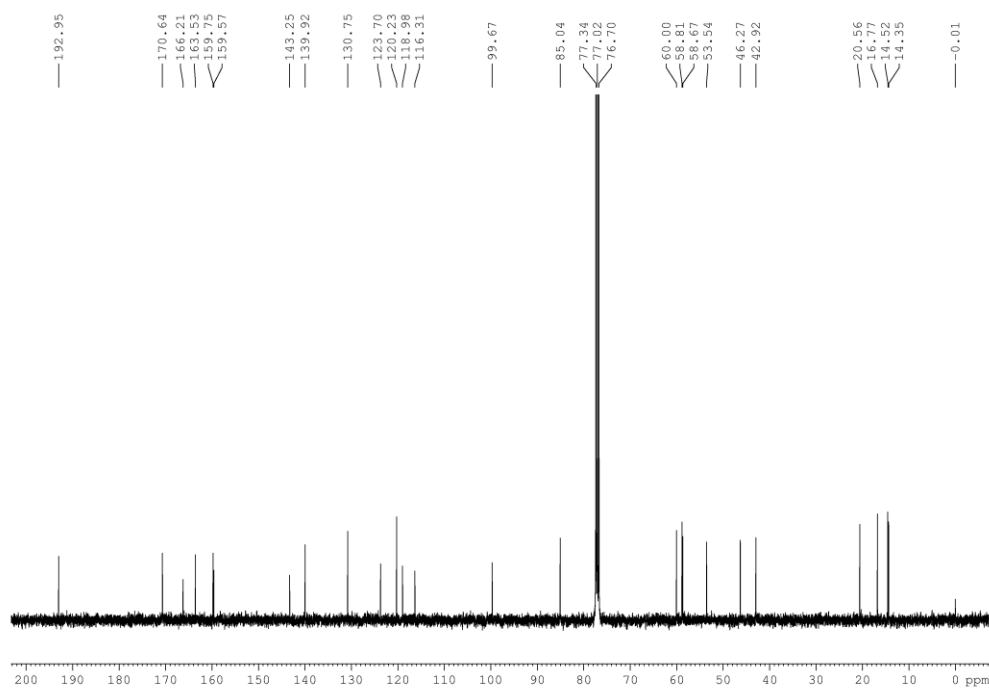
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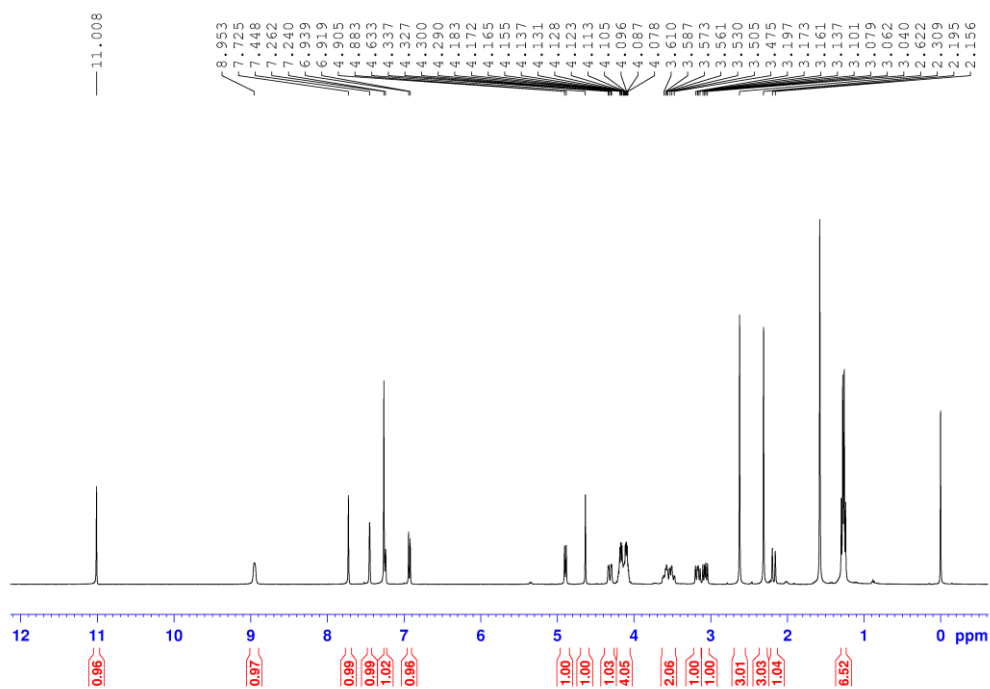
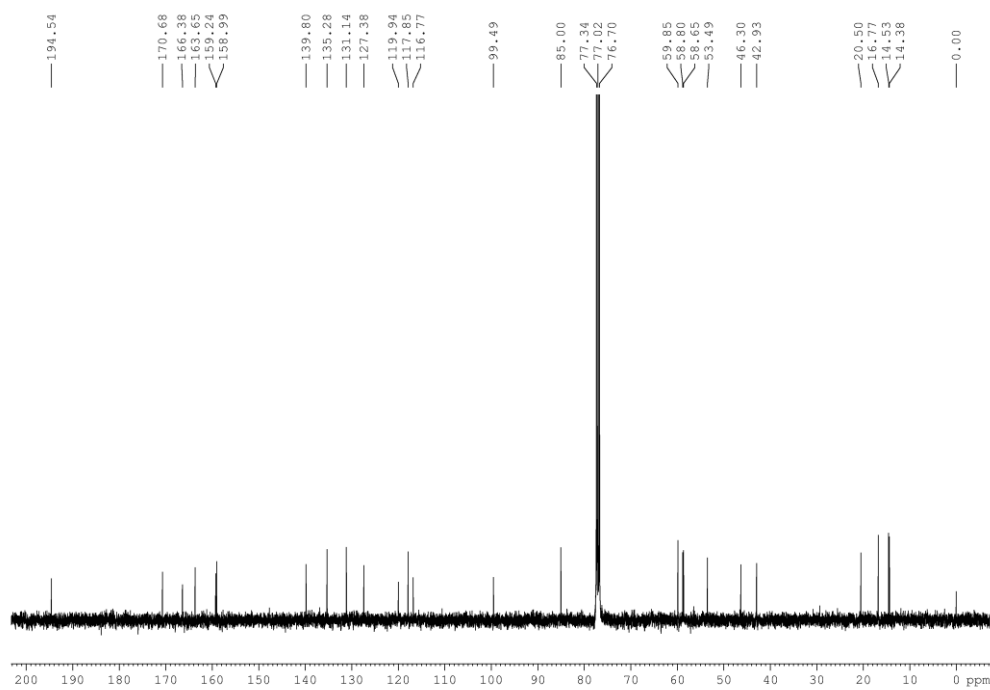
SI-Fig. 1. ¹H NMR spectrum of compound 4a.SI-Fig. 2. ¹³C NMR spectrum of compound 4a.

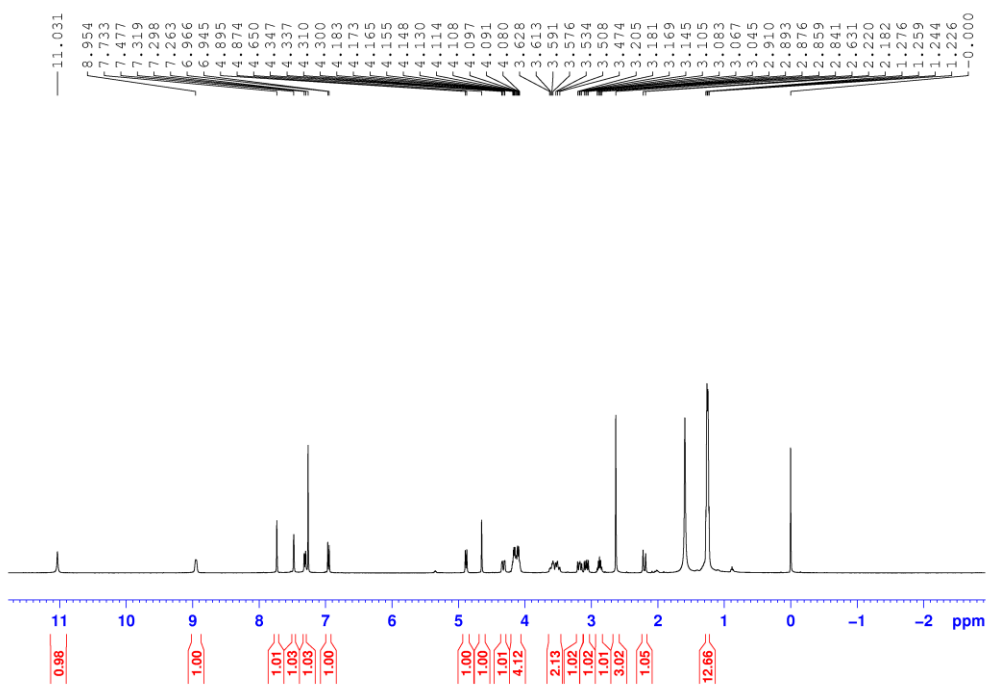
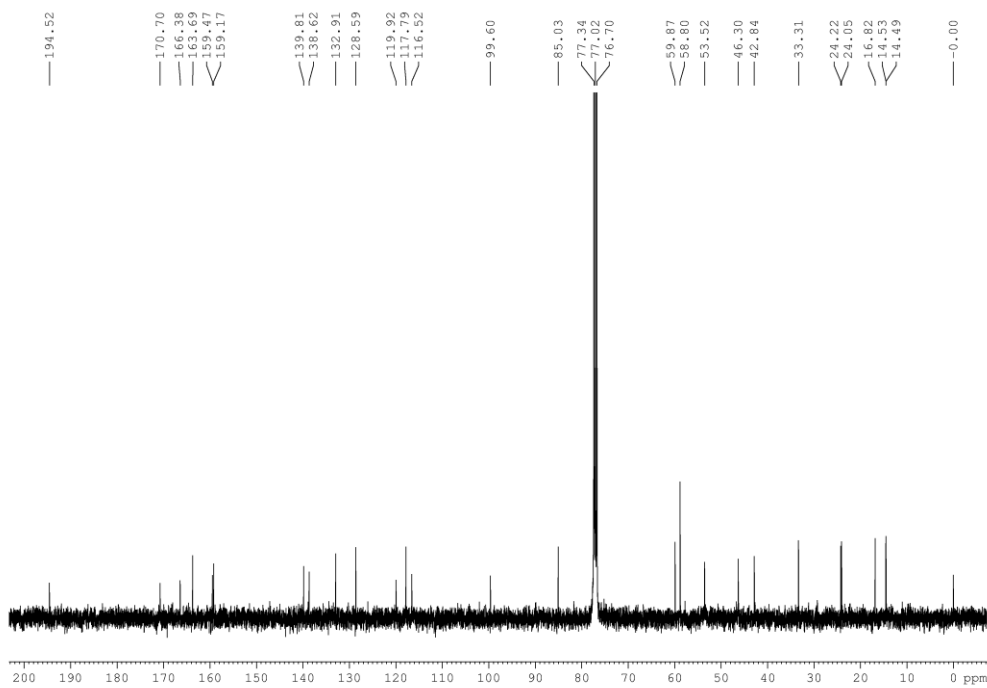
SI-Fig. 3. ¹H NMR spectrum of compound 4b.SI-Fig. 4. ¹³C NMR spectrum of compound 4b.

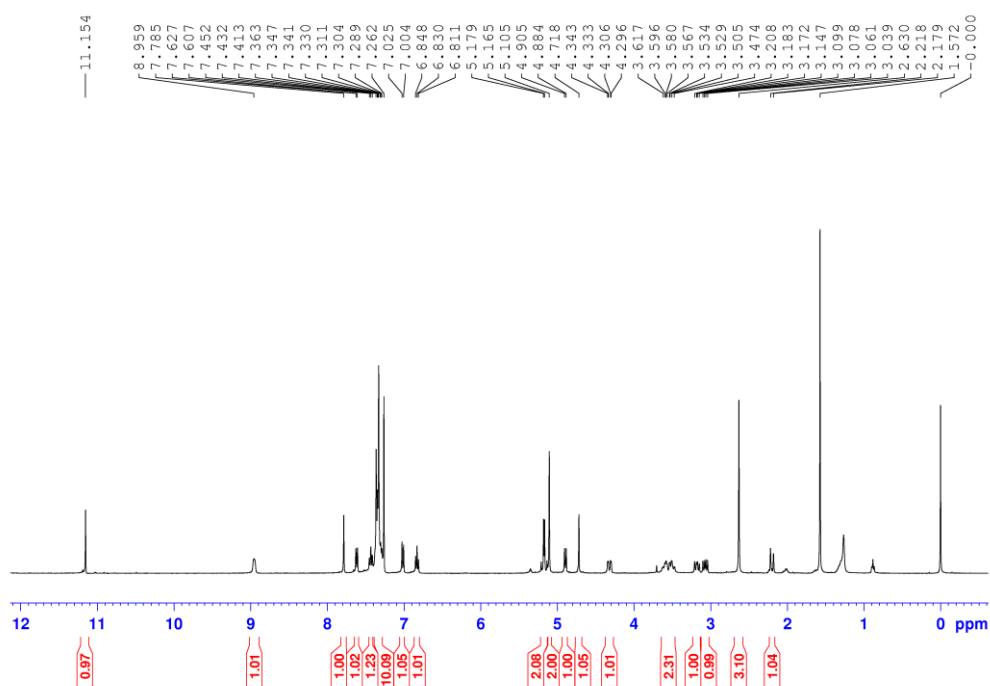
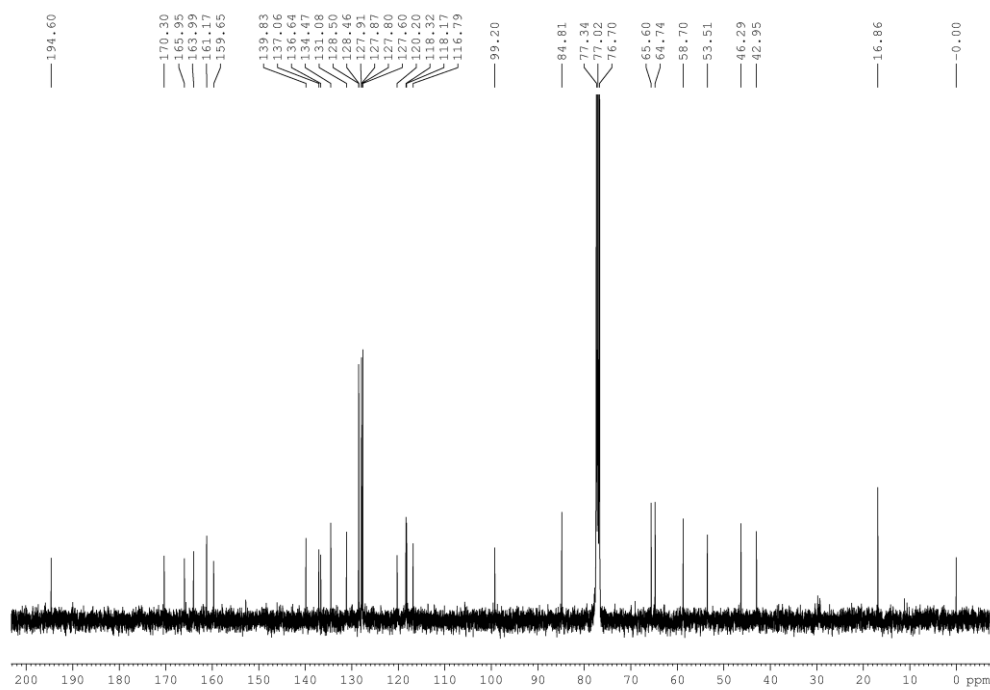
SI-Fig. 5. ^1H NMR spectrum of compound **4c**.SI-Fig. 6. ^{13}C NMR spectrum of compound **4c**.

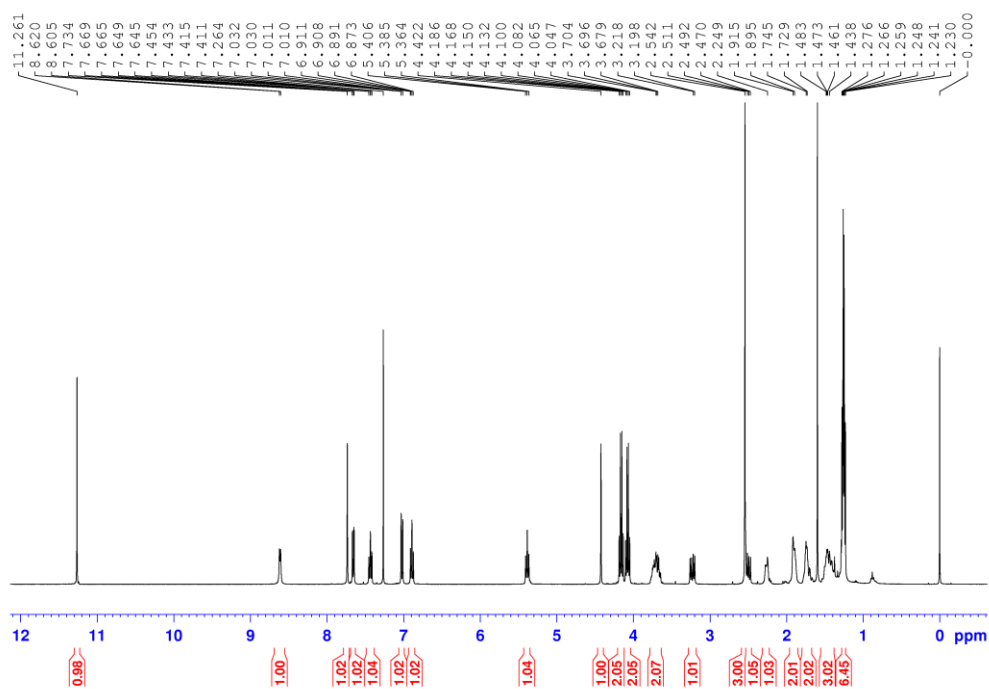
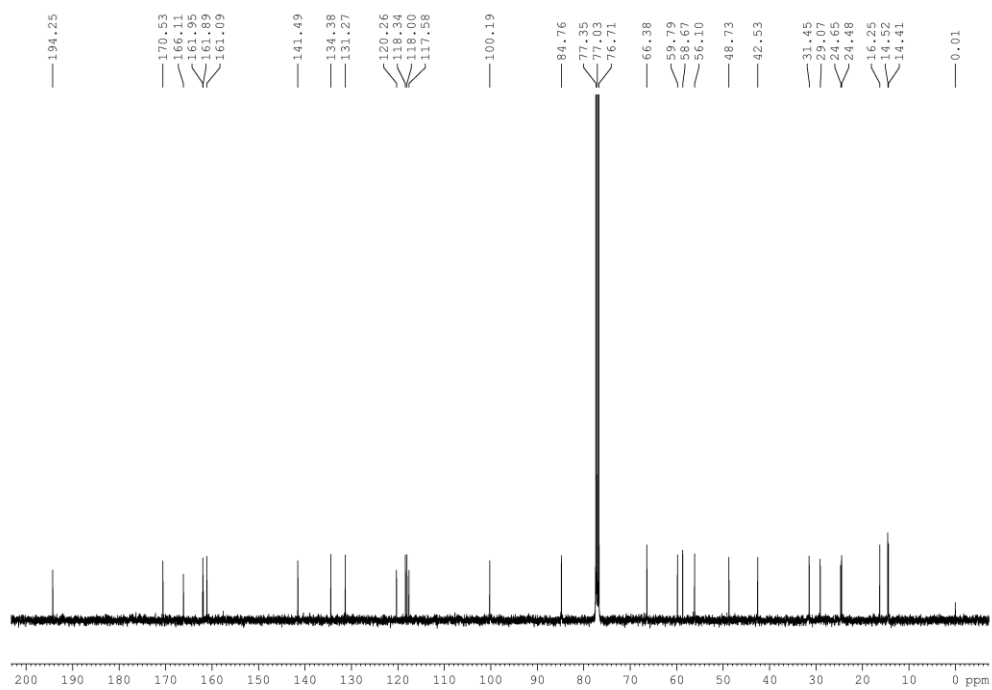
SI-Fig. 7. ¹H NMR spectrum of compound **4d**.SI-Fig. 8. ¹³C NMR spectrum of compound **4d**.

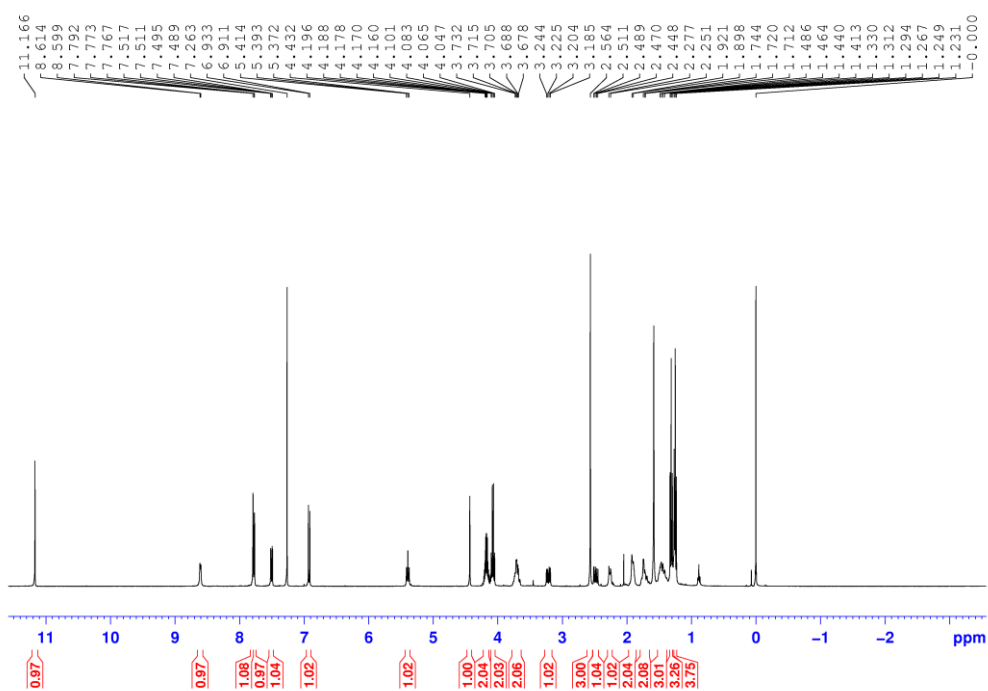
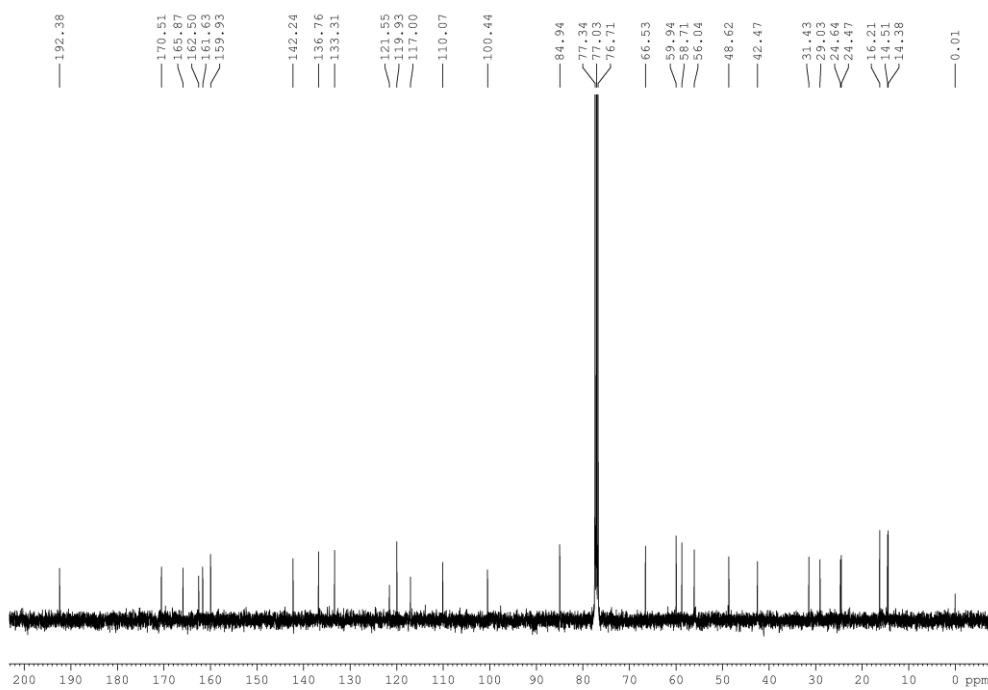
SI-Fig. 9. ¹H NMR spectrum of compound 4e.SI-Fig. 10. ¹³C NMR spectrum of compound 4e.

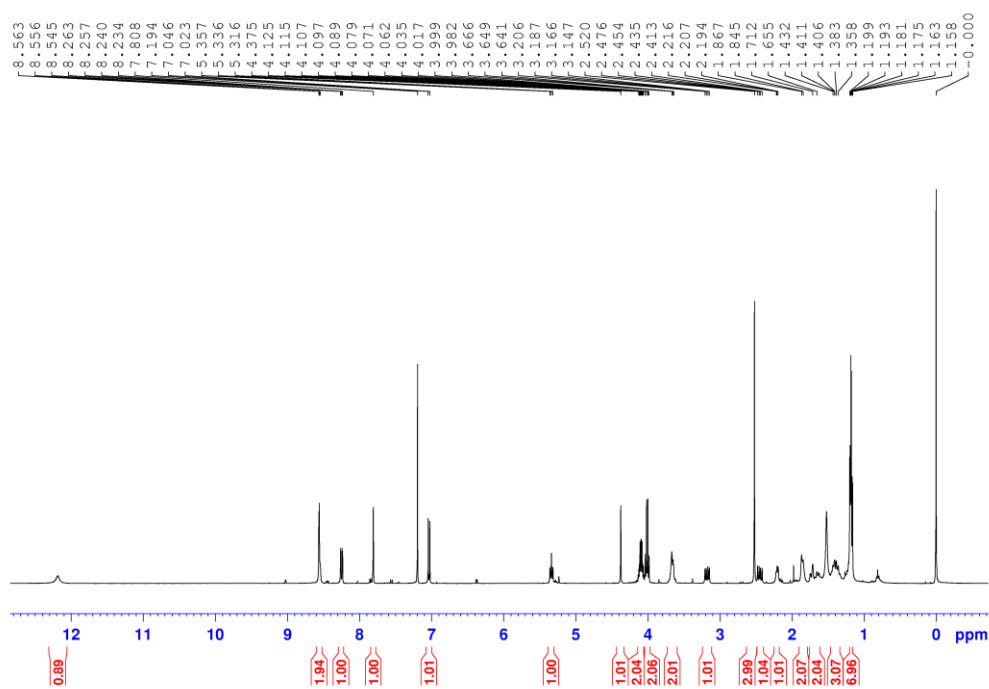
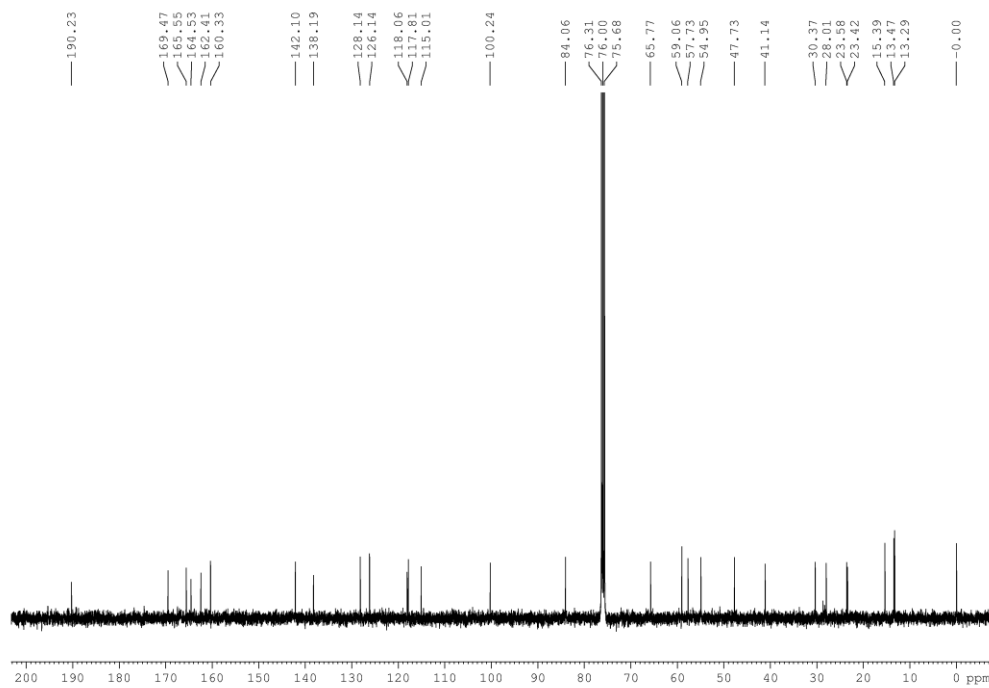
SI-Fig. 11. ^1H NMR spectrum of compound **4f**.SI-Fig. 12. ^{13}C NMR spectrum of compound **4f**.

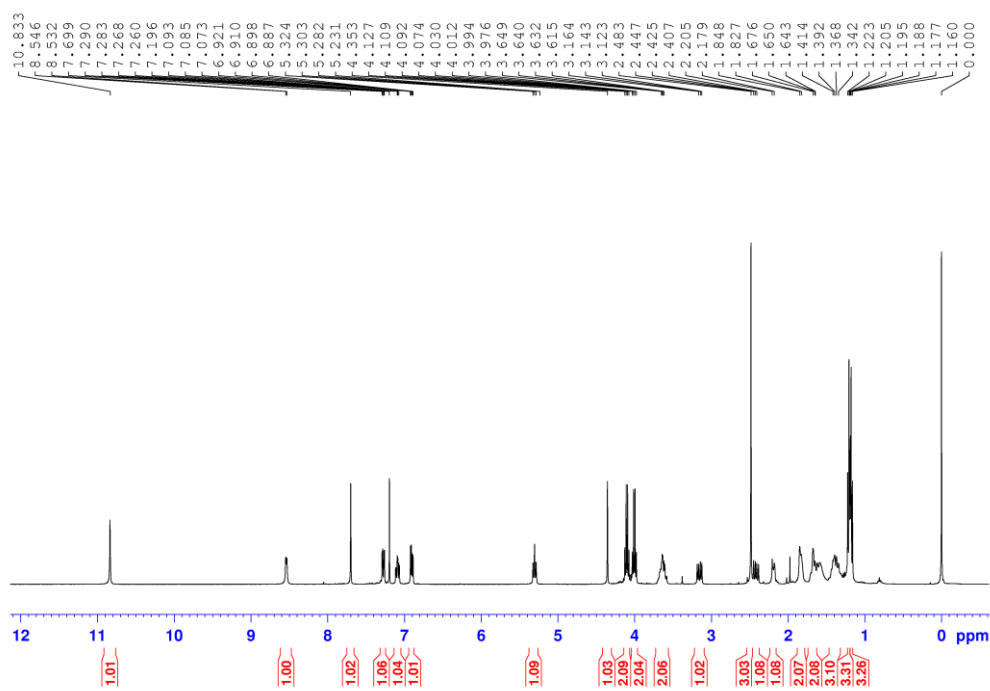
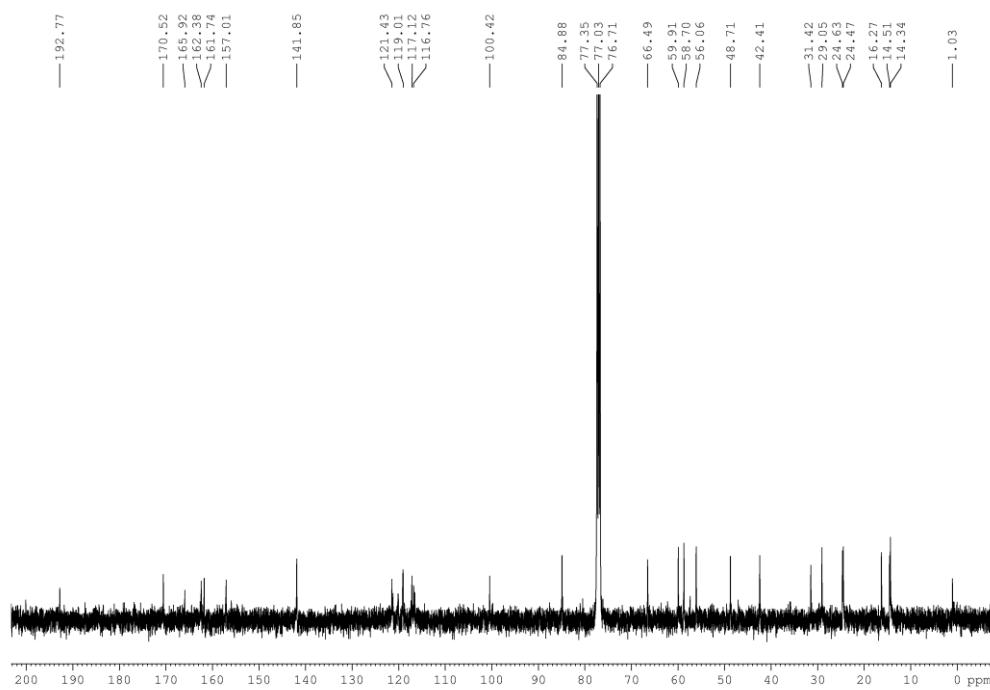
SI-Fig. 13. ¹H NMR spectrum of compound **4g**.SI-Fig. 14. ¹³C NMR spectrum of compound **4g**.

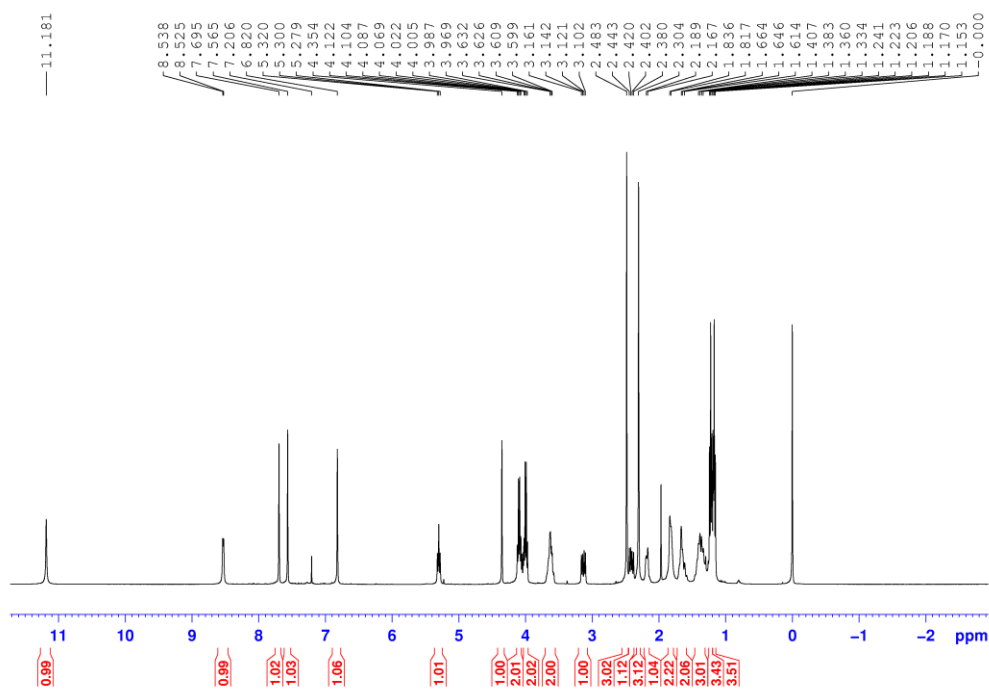
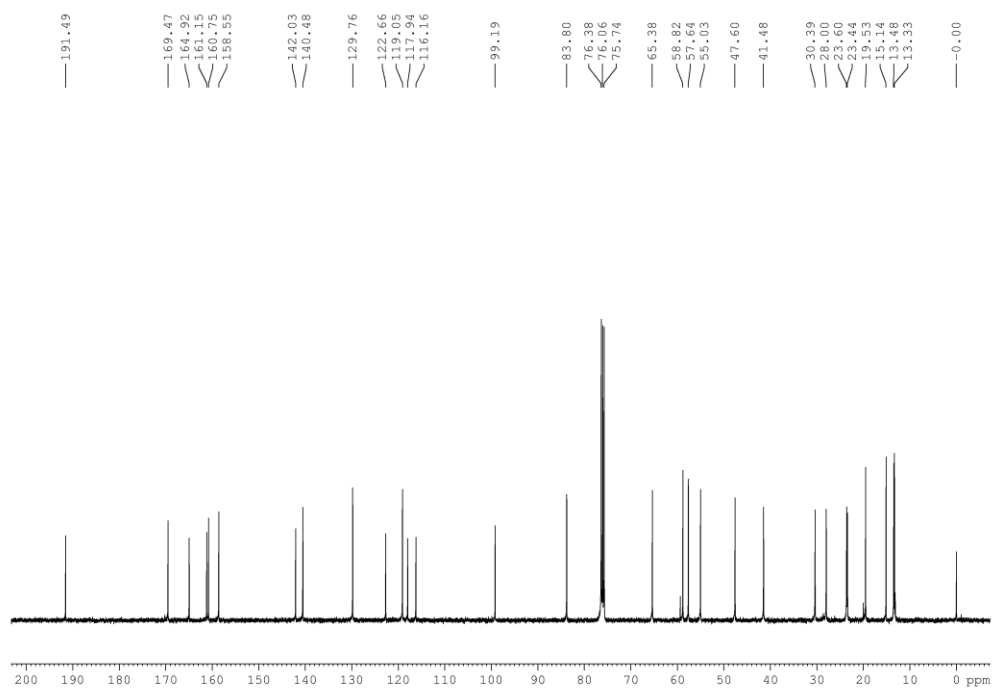
SI-Fig. 15. ¹H NMR spectrum of compound **4h**.SI-Fig. 16. ¹³C NMR spectrum of compound **4h**.

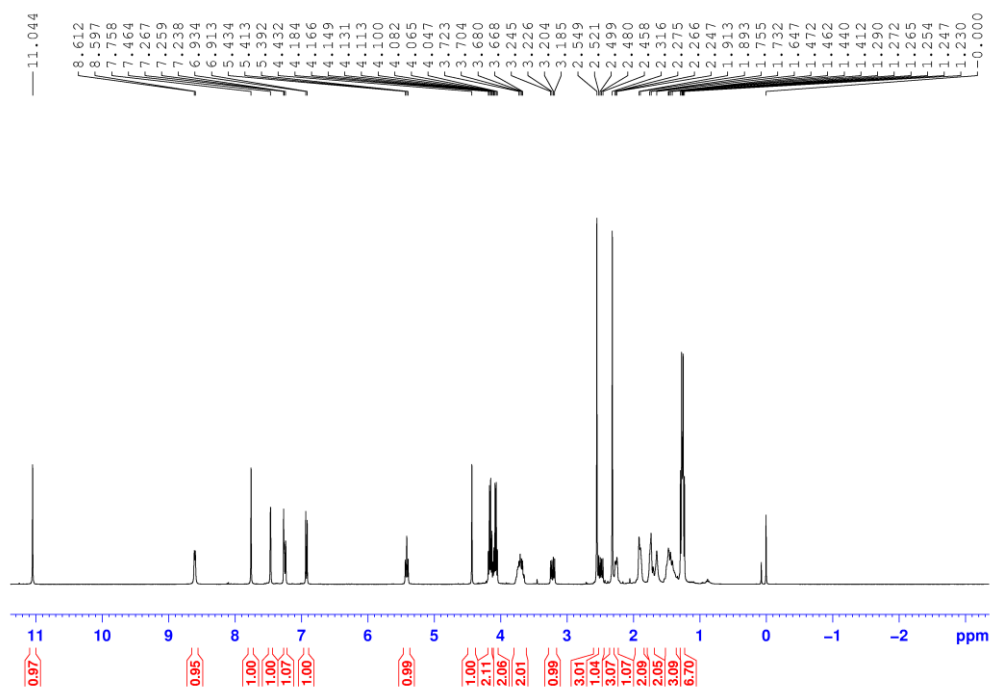
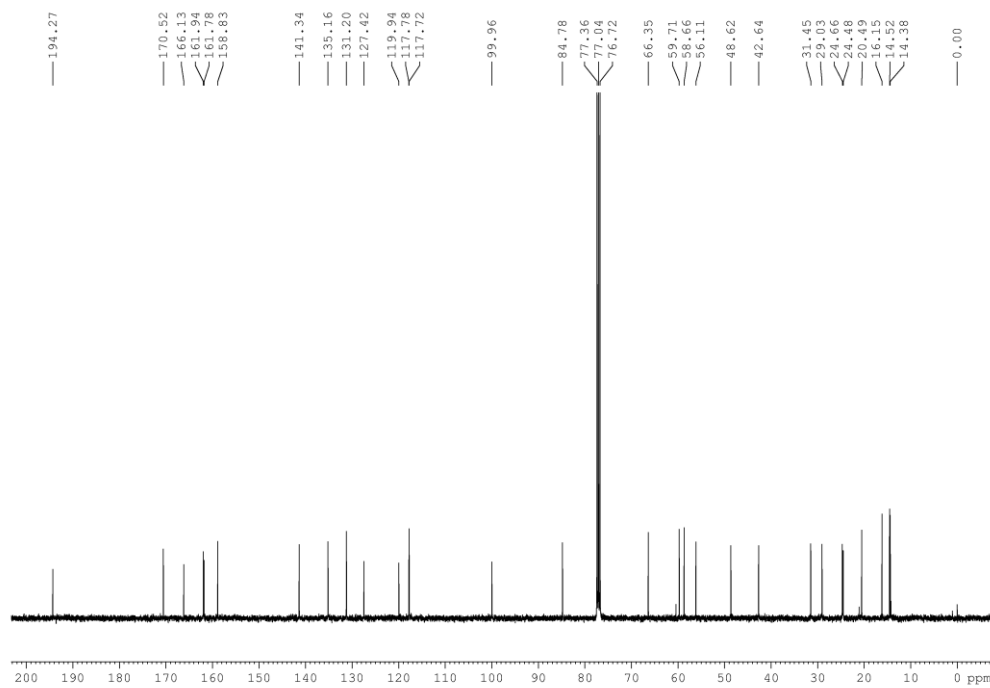
SI-Fig. 17. ^1H NMR spectrum of compound **4i**.SI-Fig. 18. ^{13}C NMR spectrum of compound **4i**.

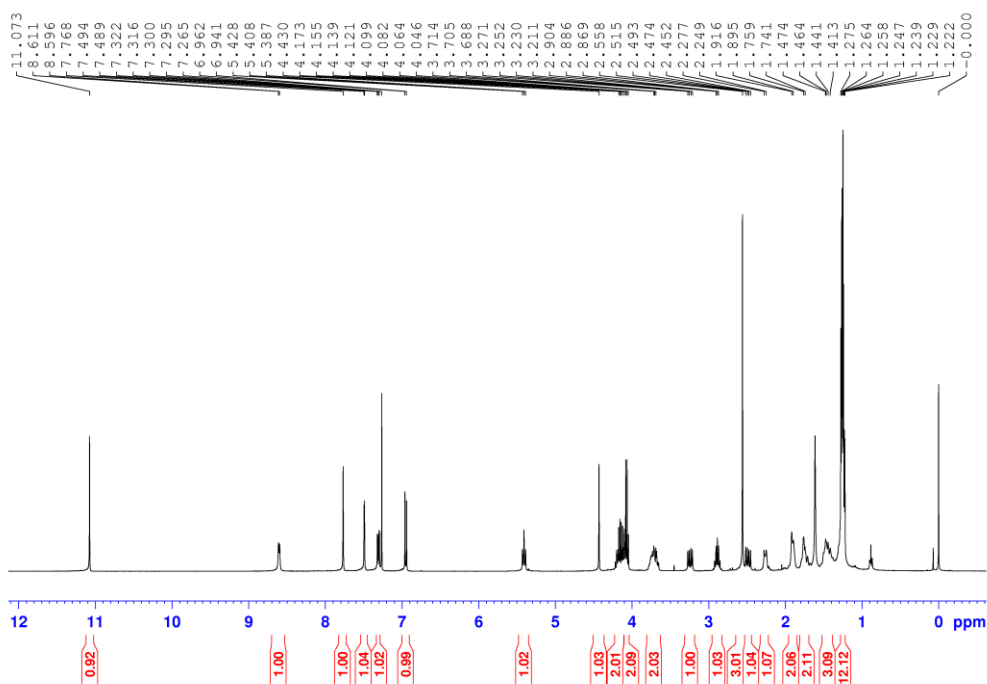
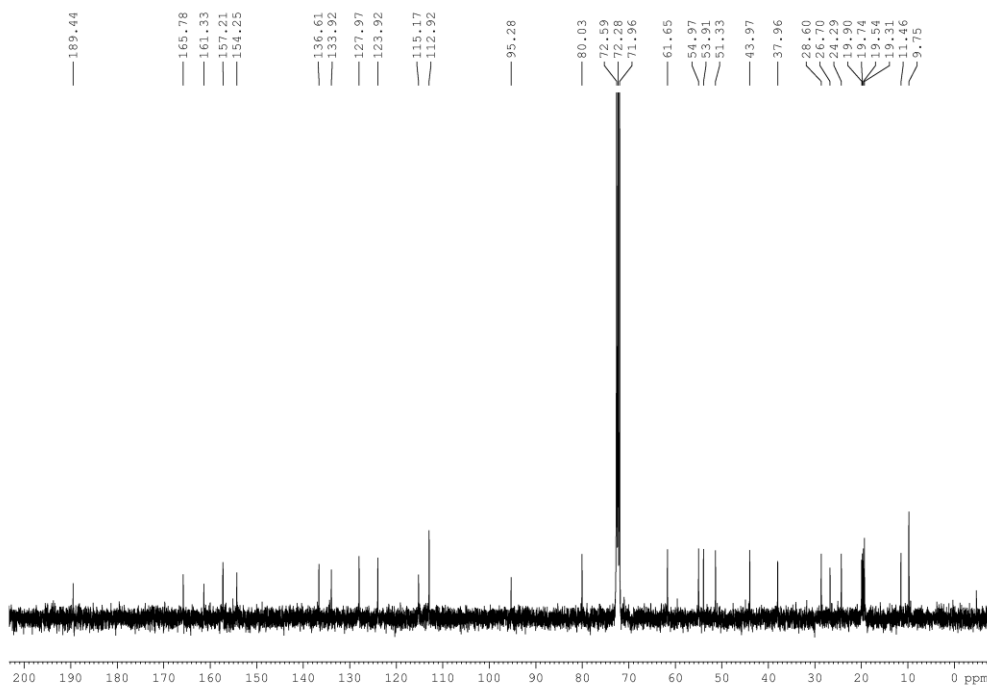
SI-Fig. 19. ¹H NMR spectrum of compound 4j.SI-Fig. 20. ¹³C NMR spectrum of compound 4j.

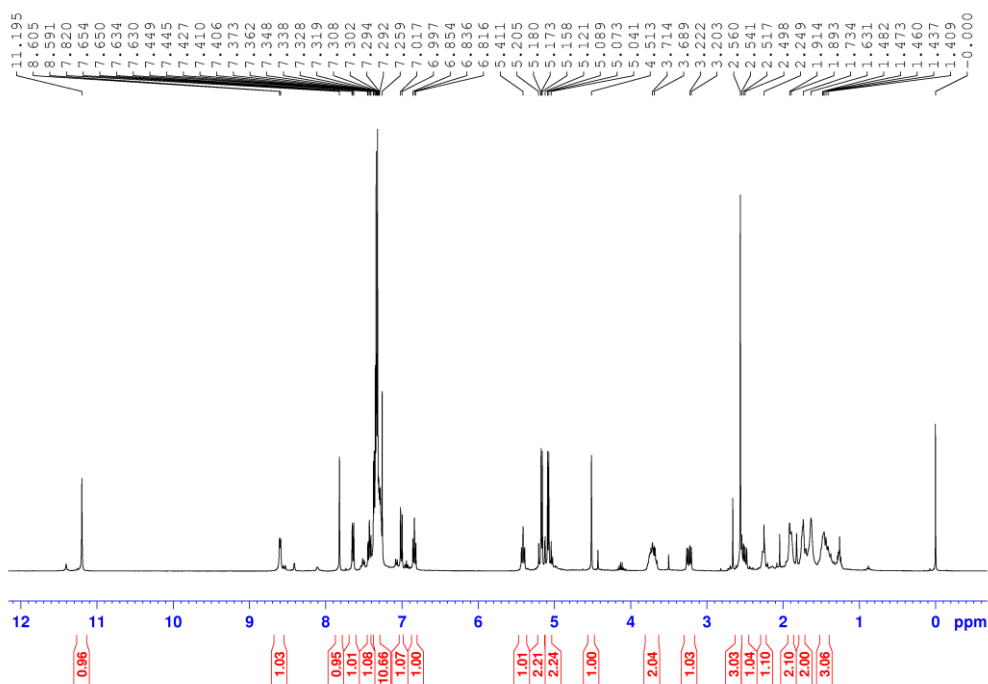
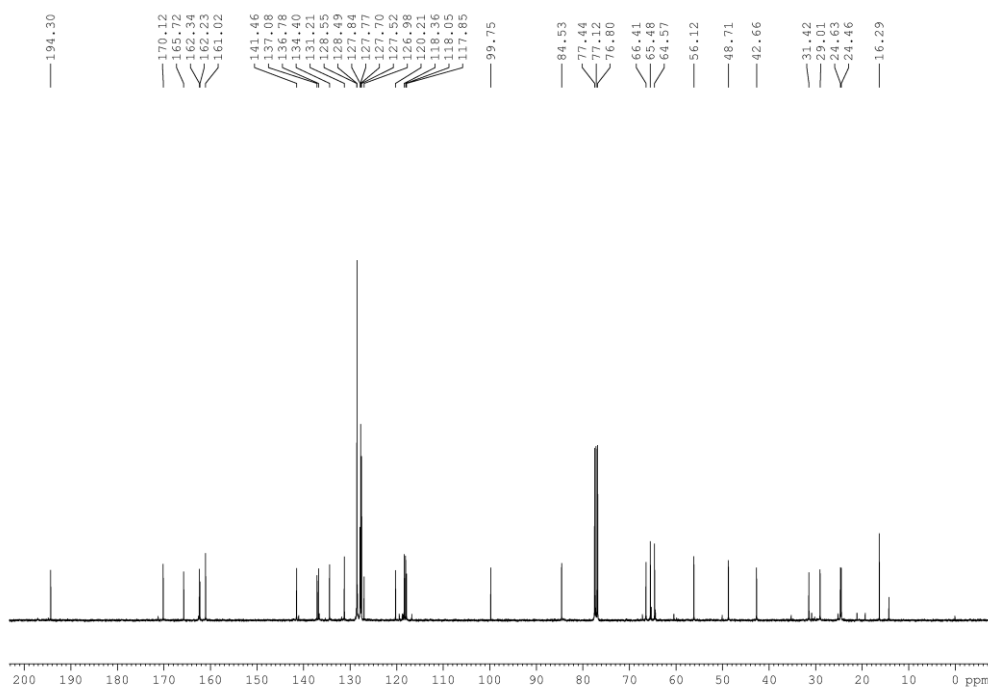
SI-Fig. 21. ¹H NMR spectrum of compound 4k.SI-Fig. 22. ¹³C NMR spectrum of compound 4k.

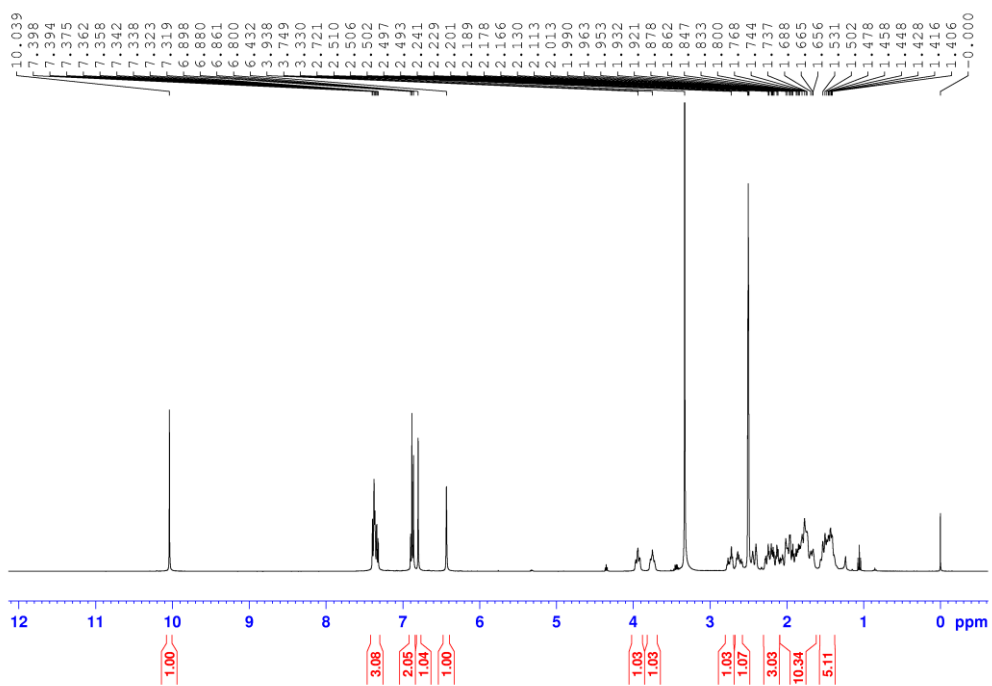
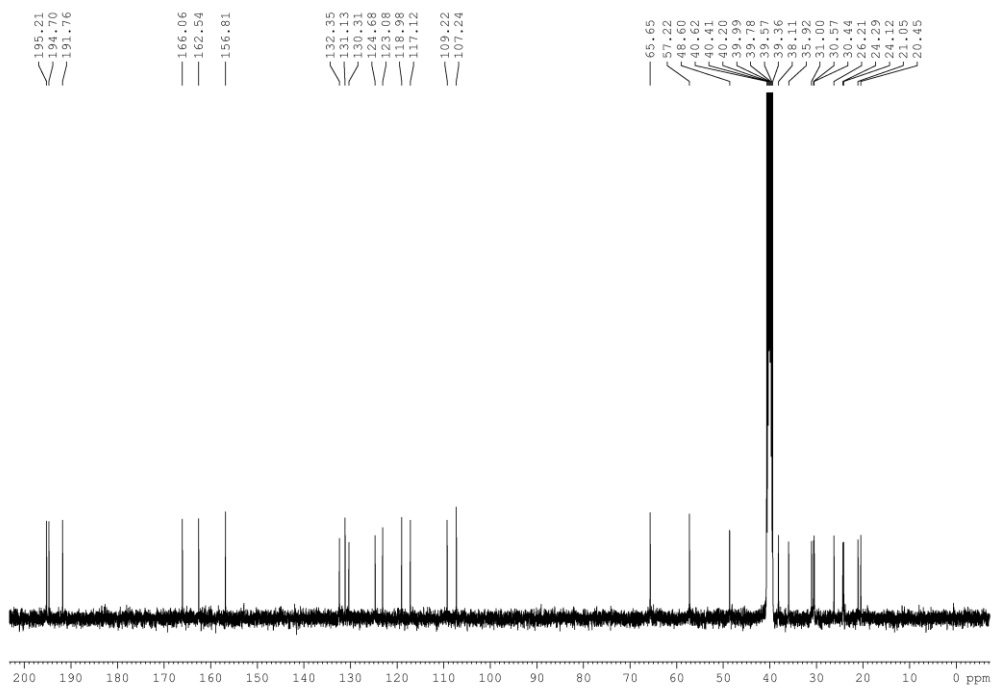
SI-Fig. 23. ^1H NMR spectrum of compound 4l.SI-Fig. 24. ^{13}C NMR spectrum of compound 4l.

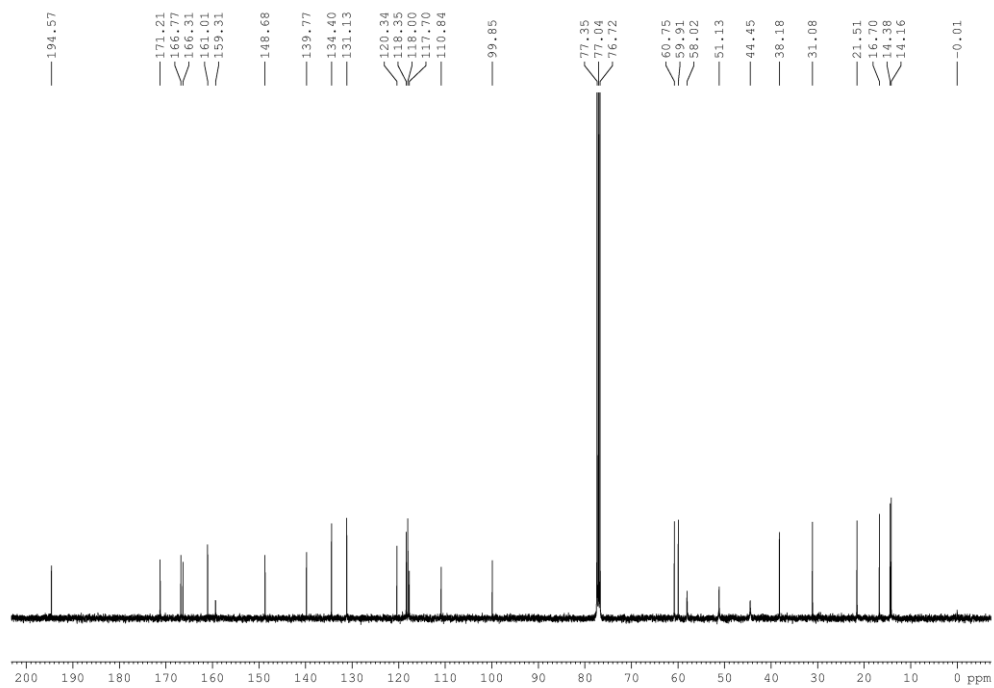
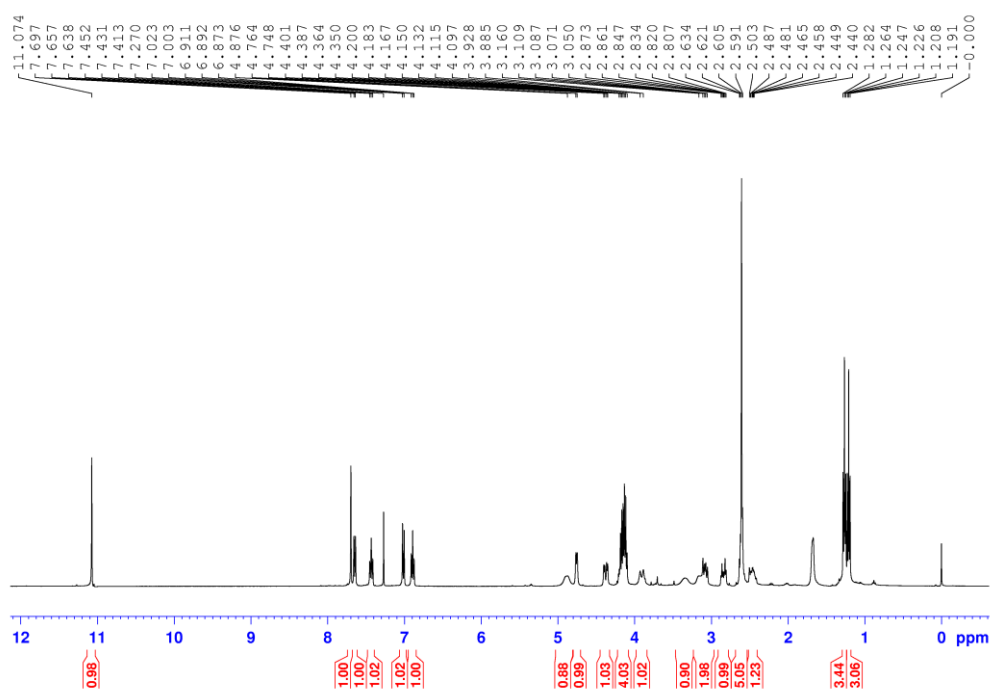
SI-Fig. 25. ^1H NMR spectrum of compound **4m**.SI-Fig. 26. ^{13}C NMR spectrum of compound **4m**.

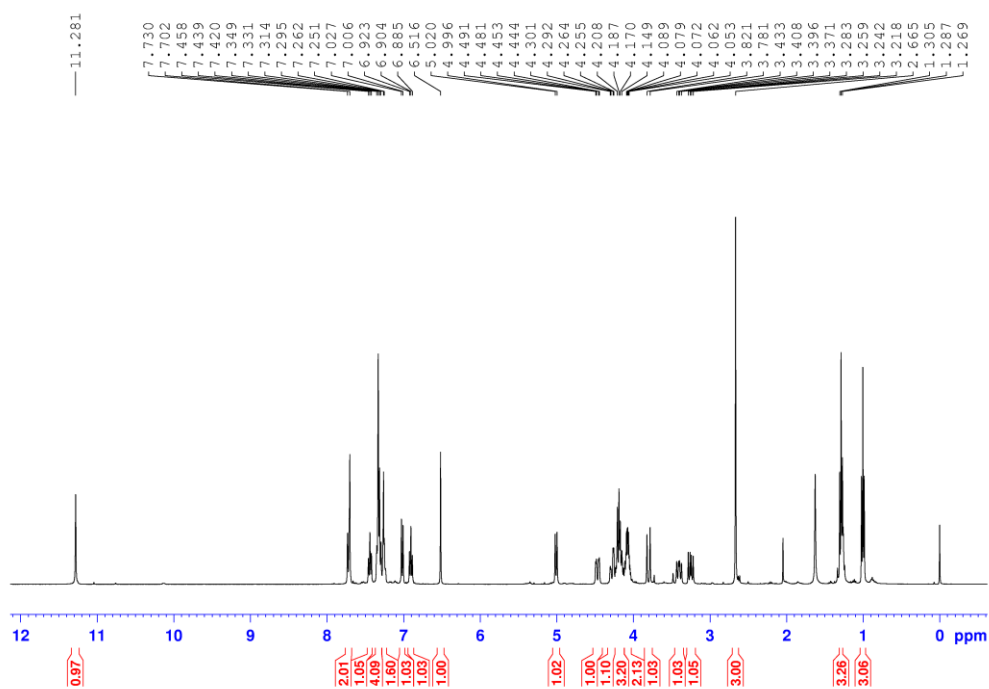
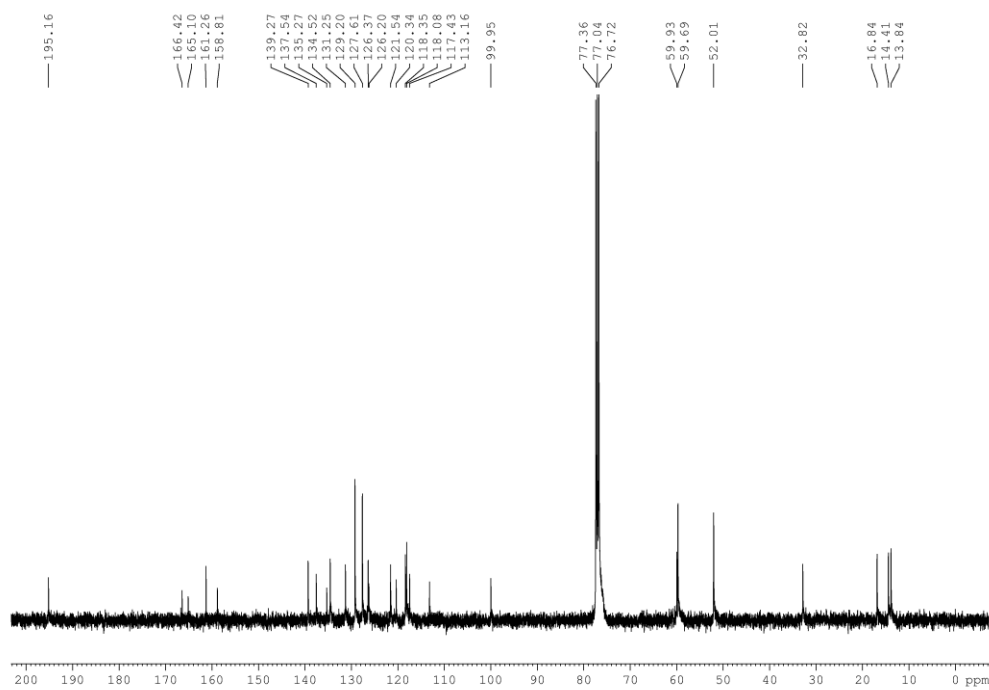
SI-Fig. 27. ^1H NMR spectrum of compound **4n**.SI-Fig. 28. ^{13}C NMR spectrum of compound **4n**.

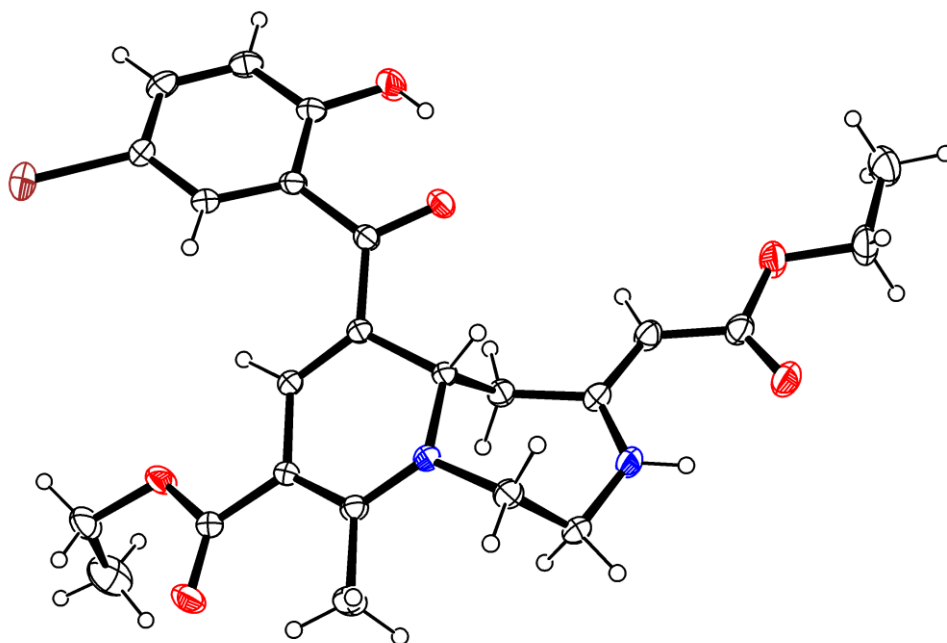
SI-Fig. 29. ¹H NMR spectrum of compound 4o.SI-Fig. 30. ¹³C NMR spectrum of compound 4o.

SI-Fig. 31. ¹H NMR spectrum of compound 4p.SI-Fig. 32. ¹³C NMR spectrum of compound 4p.

SI-Fig. 33. ¹H NMR spectrum of compound **4u**.SI-Fig. 34. ¹³C NMR spectrum of compound **4u**.

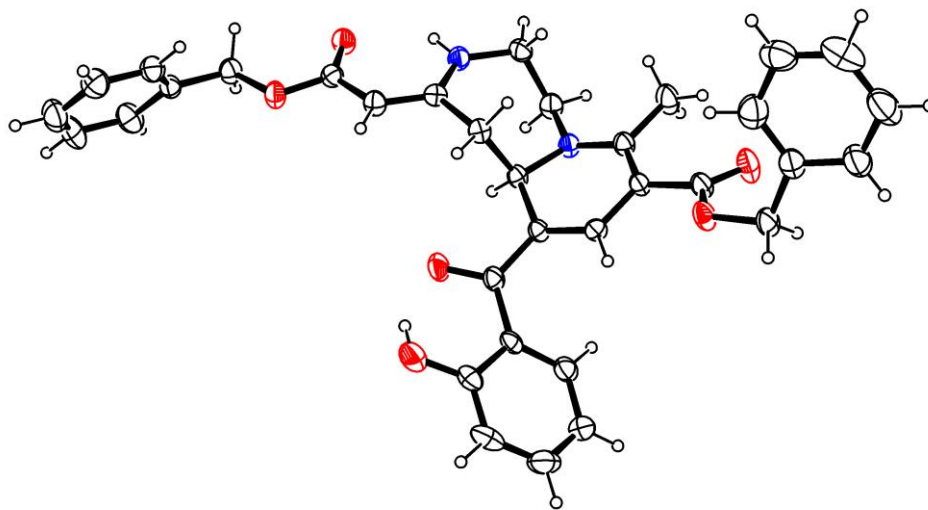


SI-Fig. 37. ¹H NMR spectrum of compound **8a**.SI-Fig. 38. ¹³C NMR spectrum of compound **8a**.



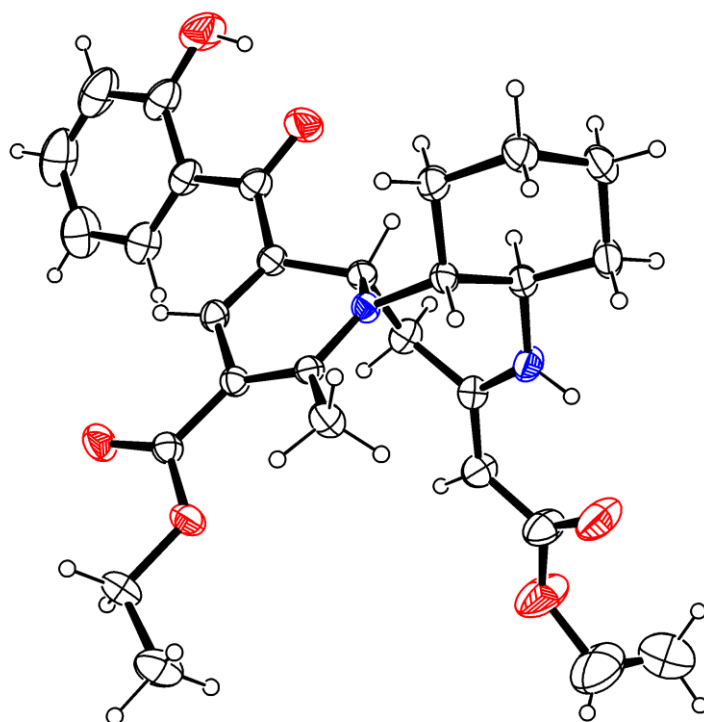
SI-Fig. 39. ORTEP diagram of crystal structures of **4b**.

(CCDC-2099263)



SI-Fig. 40. ORTEP diagram of crystal structures of **4h**.

(CCDC-2099269)



SI-Fig. 41. ORTEP diagram of crystal structures of **4i**.

(CCDC-2099272)

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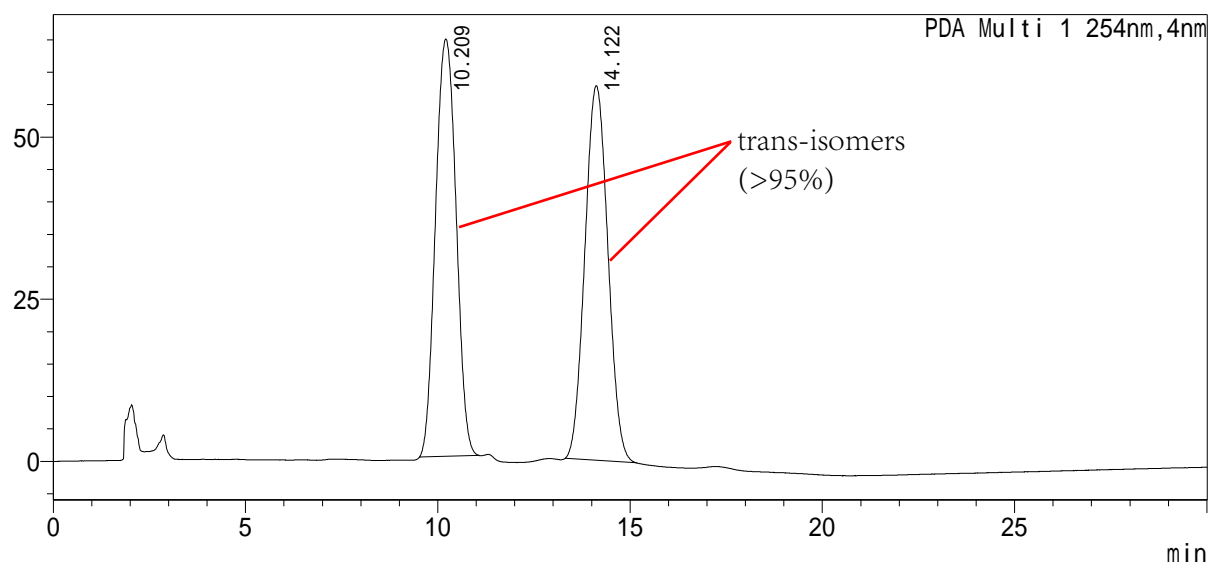
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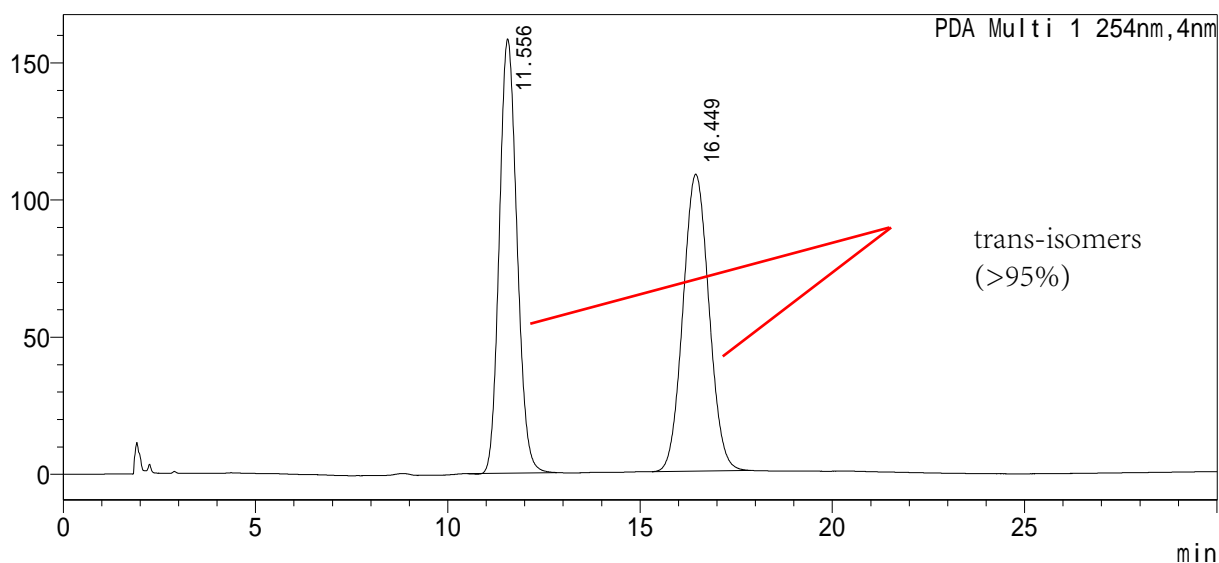
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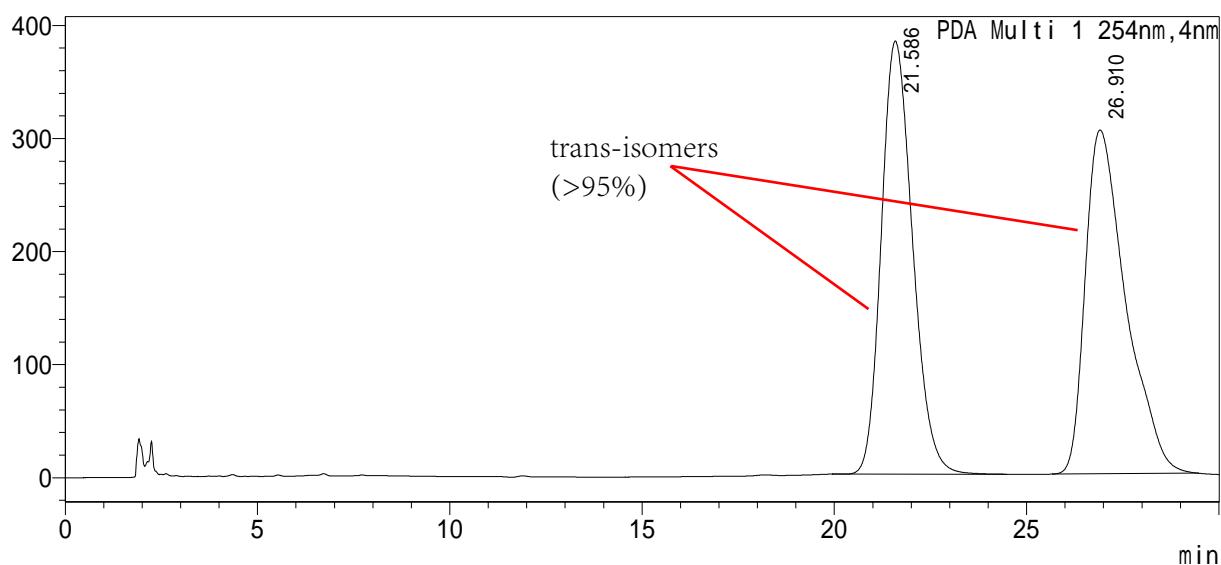
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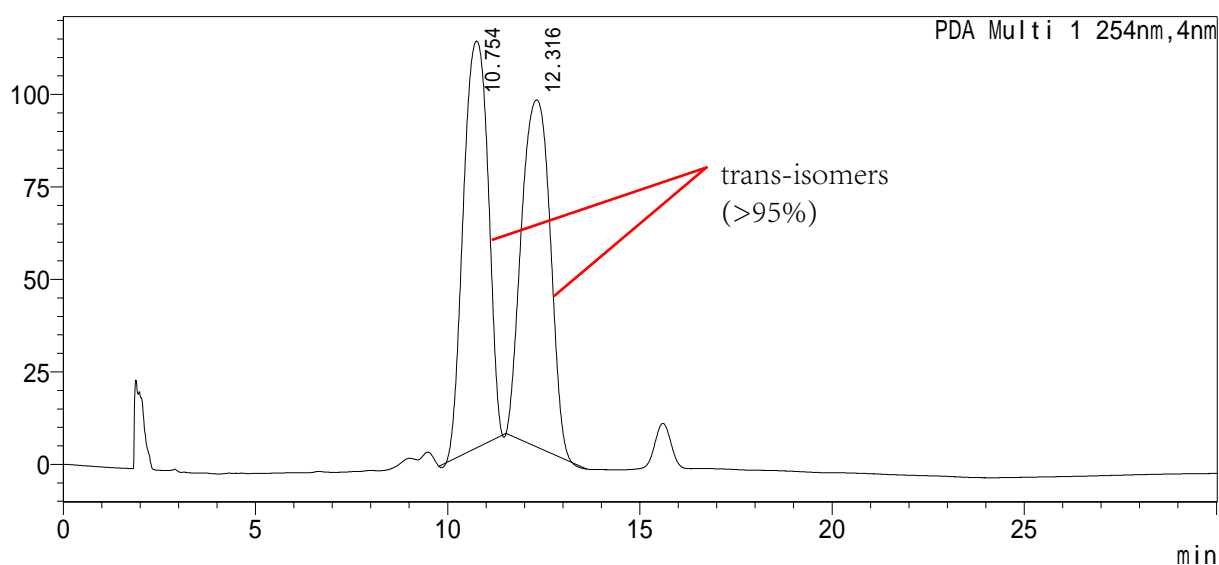
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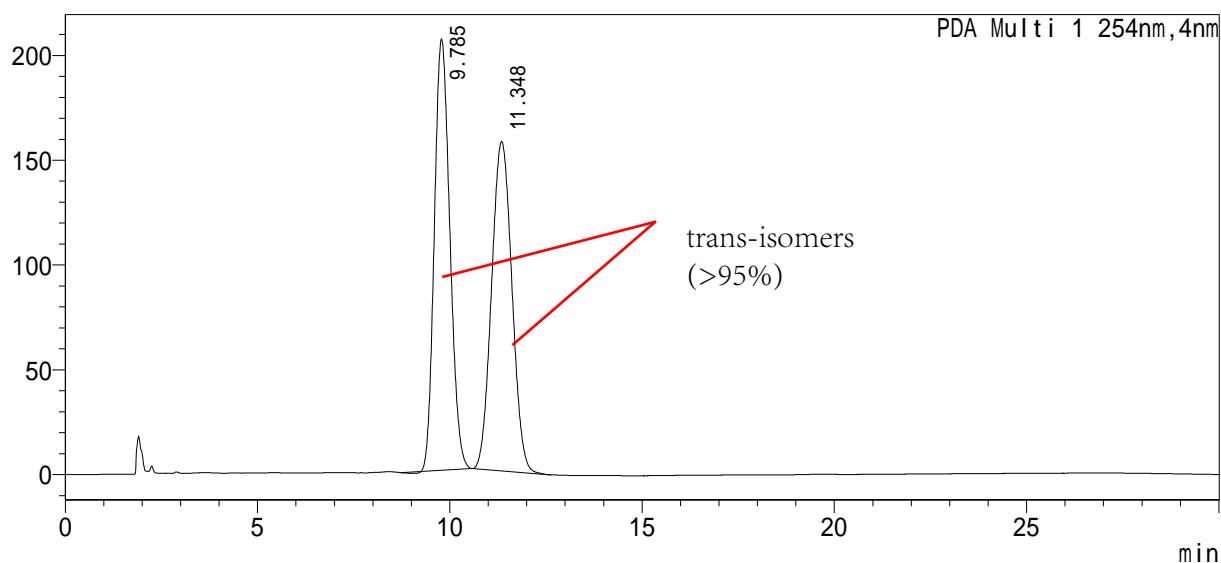
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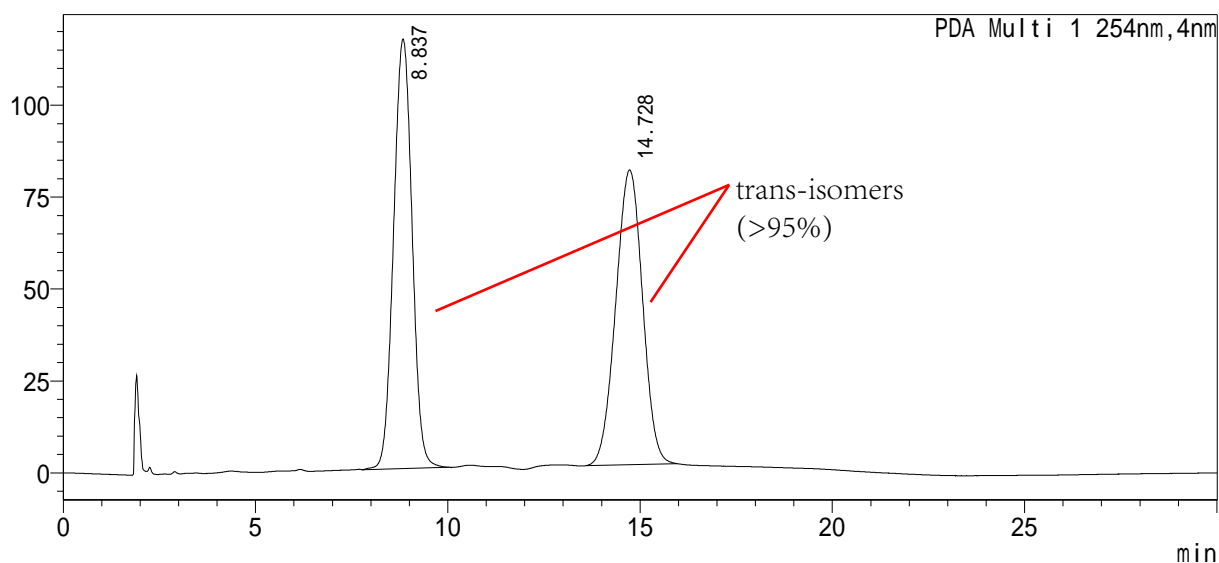
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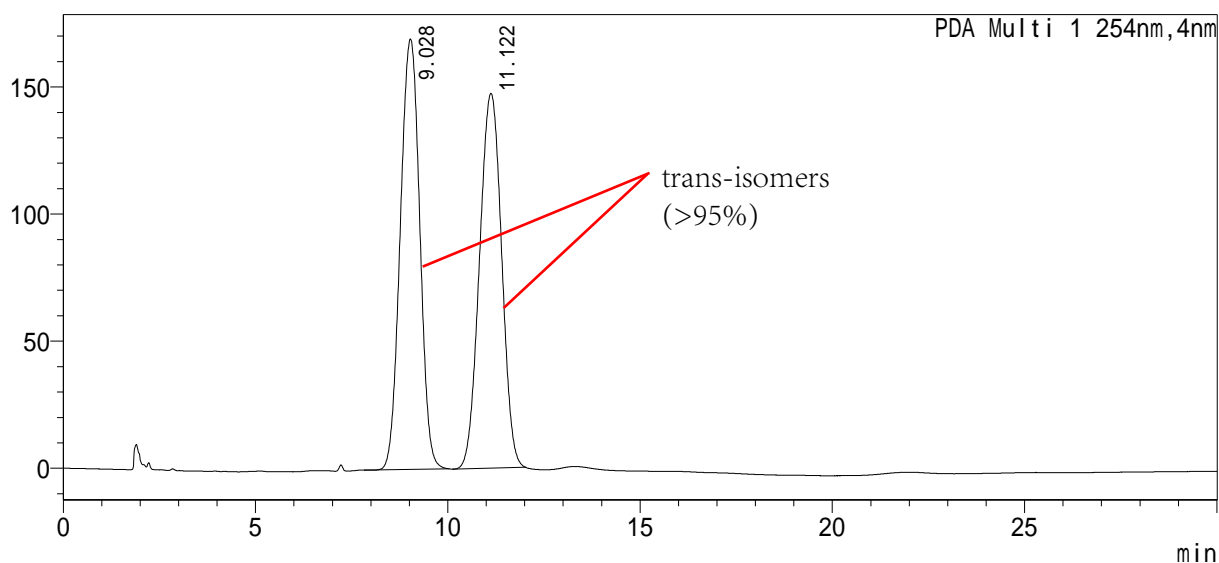
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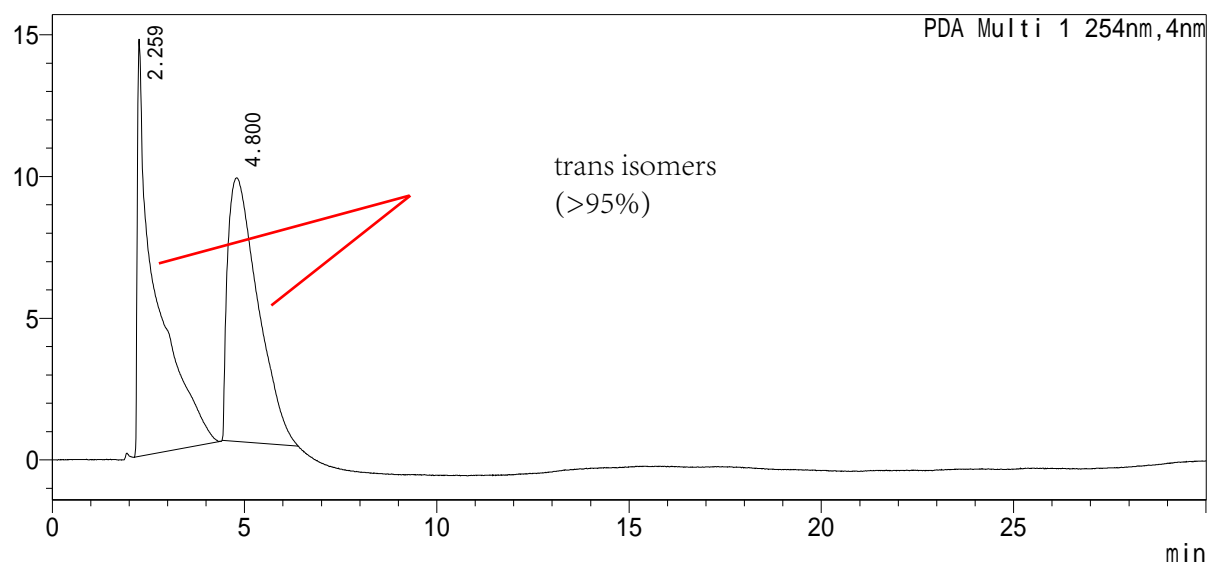
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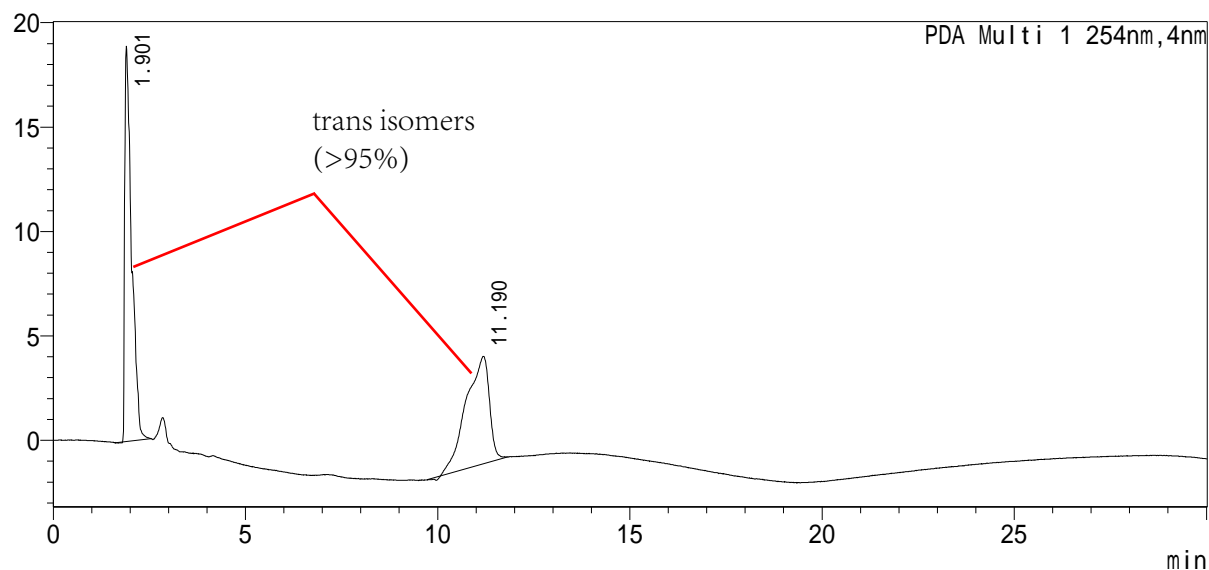
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 样品ID : THB-13-fan-solid-5IPA-30MIN-4
 数据文件名 : THB-13-fan-solid-5IPA-30MIN-4.lcd
 方法文件名 : Chiral-IPA-95Hex-30min.lcm
 批处理文件名 : 20201218-FB.lcb
 样品瓶号 : 1-98
 进样体积 : 20 uL
 分析日期 : 2021/11/6 15:52:46
 处理日期 : 2021/11/22 20:29:53

样品类型 : 未知
 分析者 : System Administrator
 处理者 : System Administrator

<色谱图>

mAU



<峰表>

PDA Ch1 254nm

峰号	保留时间	峰开始	峰结束	面积	面积%
1	1.901	1.600	2.539	235152	51.855
2	11.190	9.728	11.819	218330	48.145
总计				453482	100.000