

Supporting Information

UNCOMMON REACTIVITY OF A *SECO*-OXACASSANE DITERPENOID AND ANTIPROLIFERATIVE ACTIVITY OF SOME DERIVATIVES

Alexia Hernández-Jiménez^a, Ledy De-la-Cruz-Martínez^a, Raúl Velasco-Azorsa^a, Reyna Zeferino-Díaz^a, José G. Alvarado-Rodríguez^a, Luis H. Mendoza-Huizar^a, J. Jesús Manríquez-Torres^b, Horacio Almanza-Reyes^b, Carlos M. Cerda-García-Rojas^c, Pedro Joseph-Nathan^c, J. Martín Torres-Valencia^{a,*}

^aÁrea Académica de Química, Universidad Autónoma del Estado de Hidalgo, km 4.5 Carretera Pachuca-Tulancingo, Mineral de la Reforma, Hidalgo 42184, Mexico

^bEscuela de Medicina y Psicología, Universidad Autónoma de Baja California, Tijuana, Baja California 22390, Mexico

^cDepartamento de Química, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Apartado 14-740, Mexico City 07000, Mexico

List of Supporting Information

Figure S1. Oxime 2 , ^1H (400 MHz), CDCl_3	3
Figure S2. Oxime 2 , ^{13}C (100 MHz), CDCl_3	4
Figure S3. Oxime 2 , COSY EXPERIMENT (400 MHz), CDCl_3	5
Figure S4. Oxime 2 , HSQC EXPERIMENT (400 MHz), CDCl_3	6
Figure S5. β -Hydroxyketone 3 , ^1H (400 MHz), CDCl_3	7
Figure S6. β -Hydroxyketone 3 , ^{13}C (100 MHz), CDCl_3	8
Figure S7. β -Hydroxyketone 3 , COSY EXPERIMENT (400 MHz), CDCl_3	9
Figure S8. β -Hydroxyketone 3 , HSQC EXPERIMENT (400 MHz), CDCl_3	10
Figure S9. β -Hydroxyketone 3 , HMBC EXPERIMENT (400 MHz), CDCl_3	11
Figure S10. Aldo- ϵ -lactone 4 , ^1H (400 MHz), CDCl_3	12
Figure S11. Aldo- ϵ -Lactone 4 , ^{13}C (100 MHz), CDCl_3	13
Figure S12. Aldo- ϵ -lactone 4 , COSY EXPERIMENT (400 MHz), CDCl_3	14
Figure S13. Aldo- ϵ -lactone 4 , HSQC EXPERIMENT (400 MHz), CDCl_3	15
Figure S14. Aldo- ϵ -lactone 4 , HMBC EXPERIMENT (400 MHz), CDCl_3	16
Figure S15. Epoxyformate 5 , ^1H (400 MHz), CDCl_3	17
Figure S16. Epoxyformate 5 , ^{13}C (100 MHz), CDCl_3	18
Figure S17. Epoxyformate 5 , COSY EXPERIMENT (400 MHz), CDCl_3	19
Figure S18. Epoxyformate 5 , HSQC EXPERIMENT (400 MHz), CDCl_3	20
Figure S19. Epoxyformate 5 , HMBC EXPERIMENT (400 MHz), CDCl_3	21
Figure S20. 17- <i>nor</i> -Ketone 6 , ^1H (400 MHz), CDCl_3	22
Figure S21. 17- <i>nor</i> -Ketone 6 , ^{13}C (100 MHz), CDCl_3	23
Figure S22. 17- <i>nor</i> -Ketone 6 , COSY EXPERIMENT (400 MHz), CDCl_3	24
Figure S23. 17- <i>nor</i> -Ketone 6 , HSQC EXPERIMENT (400 MHz), CDCl_3	25
Figure S24. 17- <i>nor</i> -Ketone 6 , HMBC EXPERIMENT (400 MHz), CDCl_3	26

Figure S1. Oxime 2, ^1H (400 MHz), CDCl_3

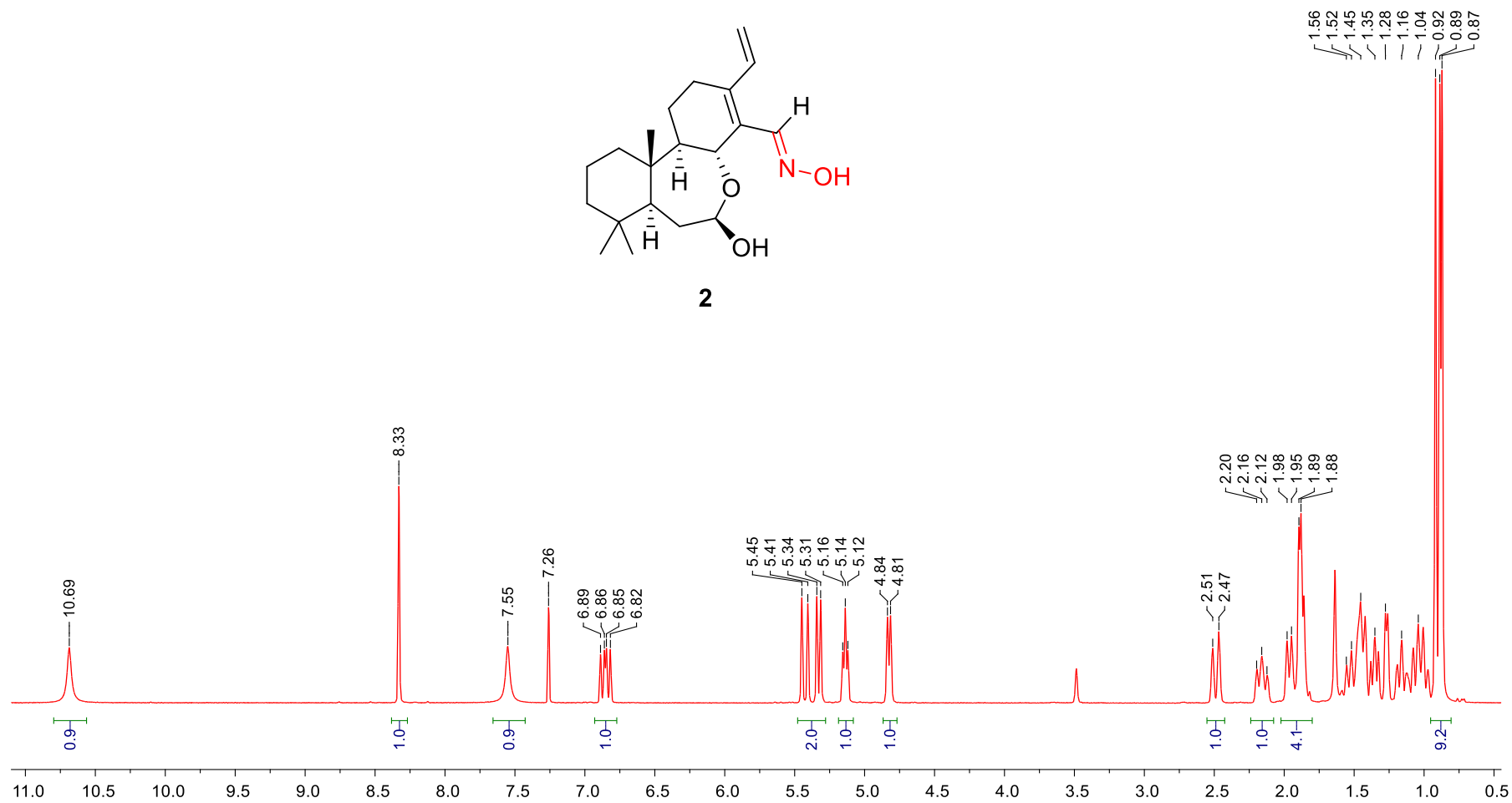


Figure S2. Oxime **2**, ^{13}C (100 MHz), CDCl_3

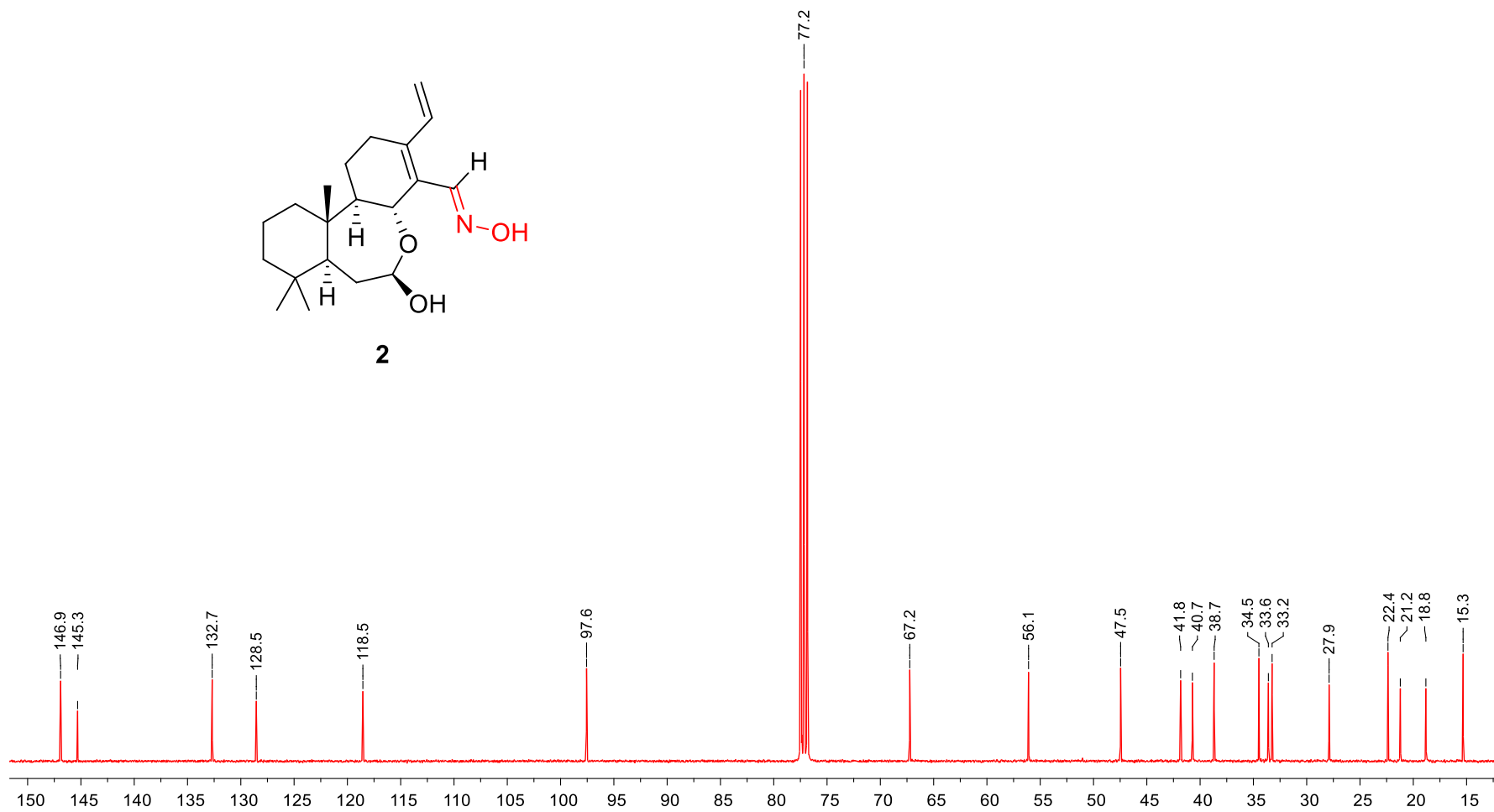
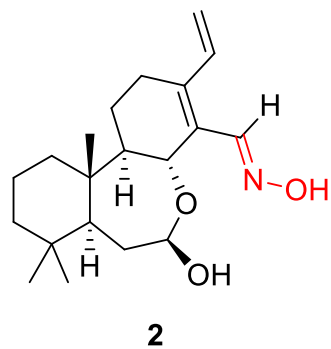


Figure S3. Oxime 2, COSY EXPERIMENT (400 MHz), CDCl₃

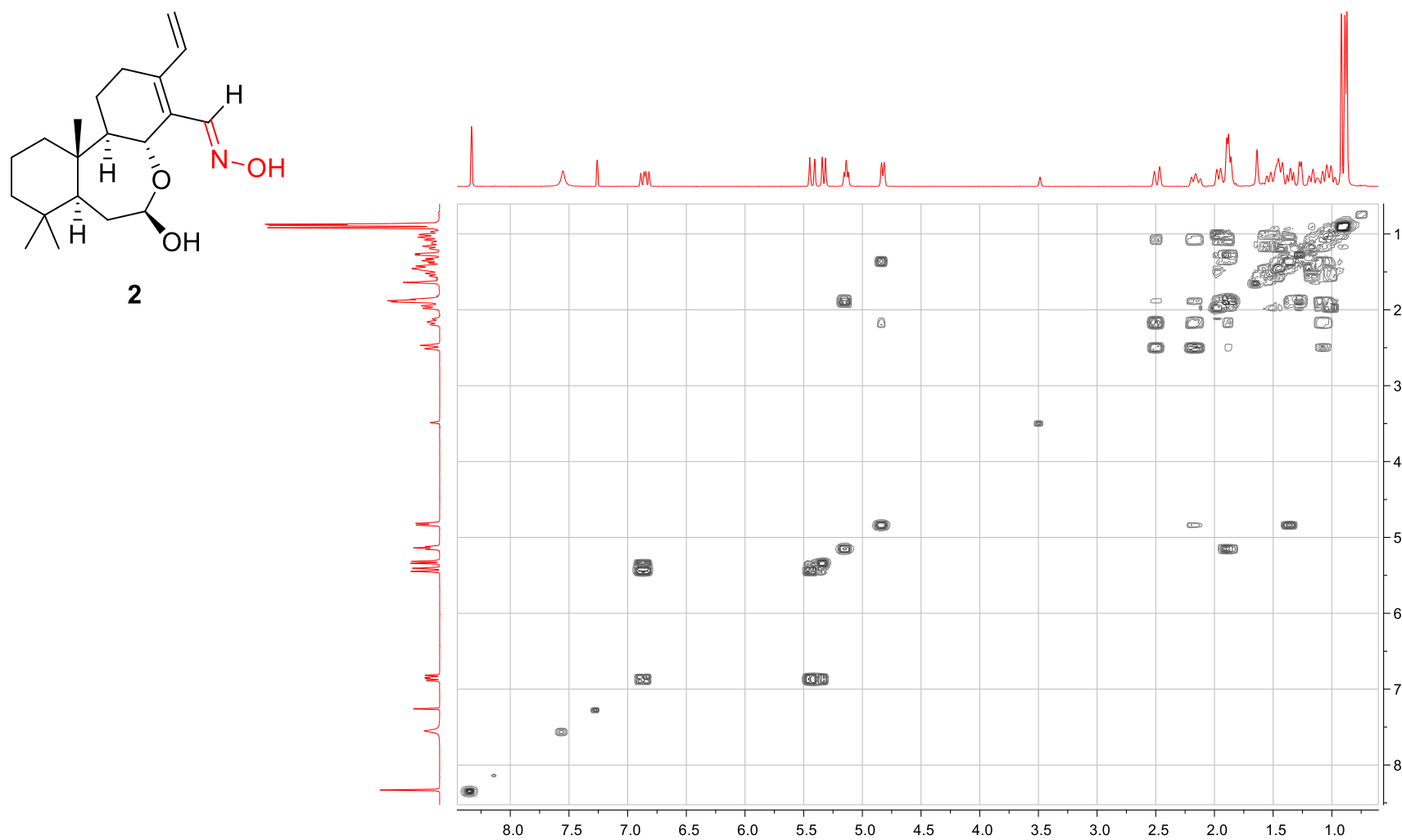


Figure S4. Oxime 2, HSQC EXPERIMENT (400 MHz), CDCl₃

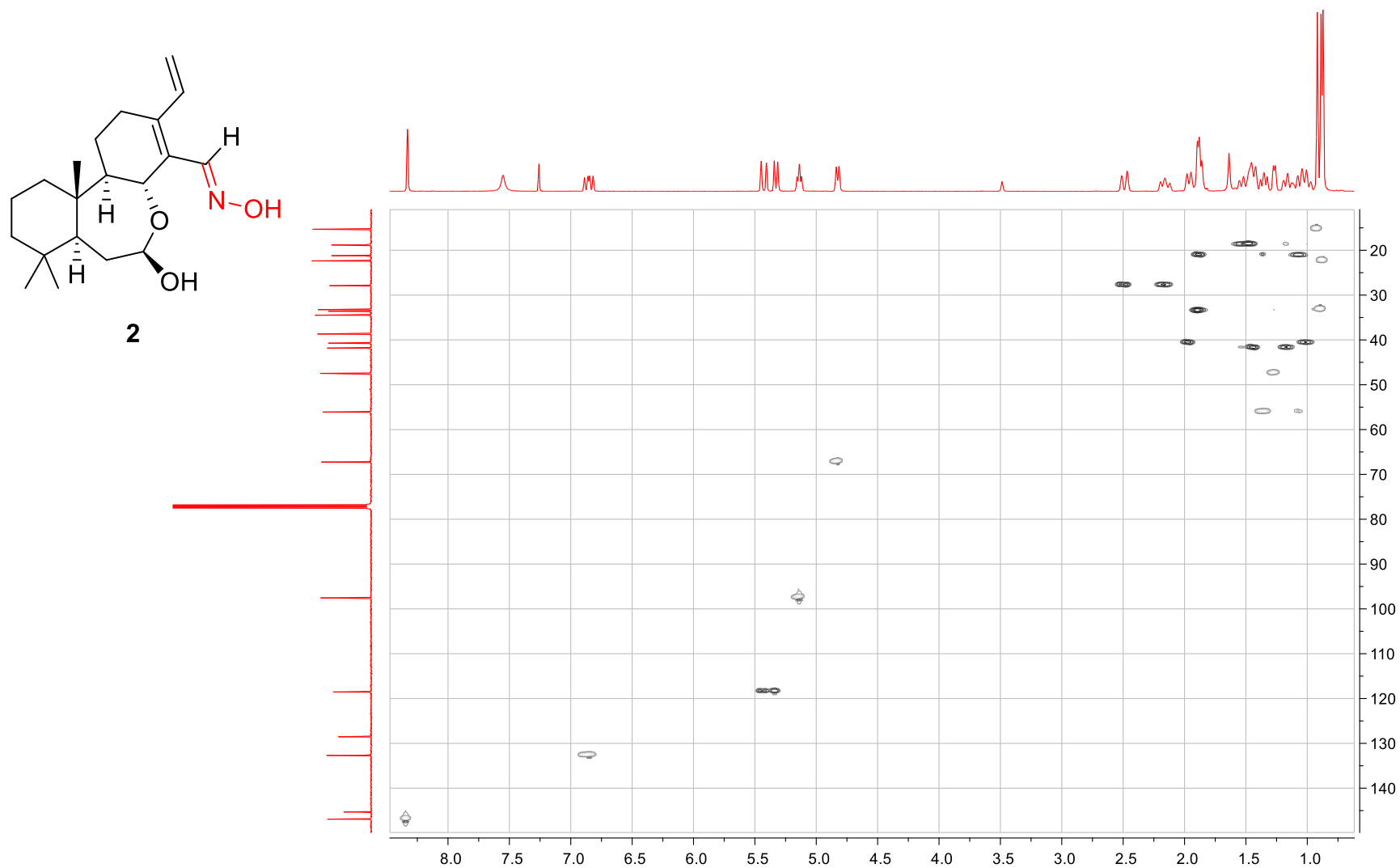


Figure S5. β -Hydroxyketone **3**, ^1H (400 MHz), CDCl_3

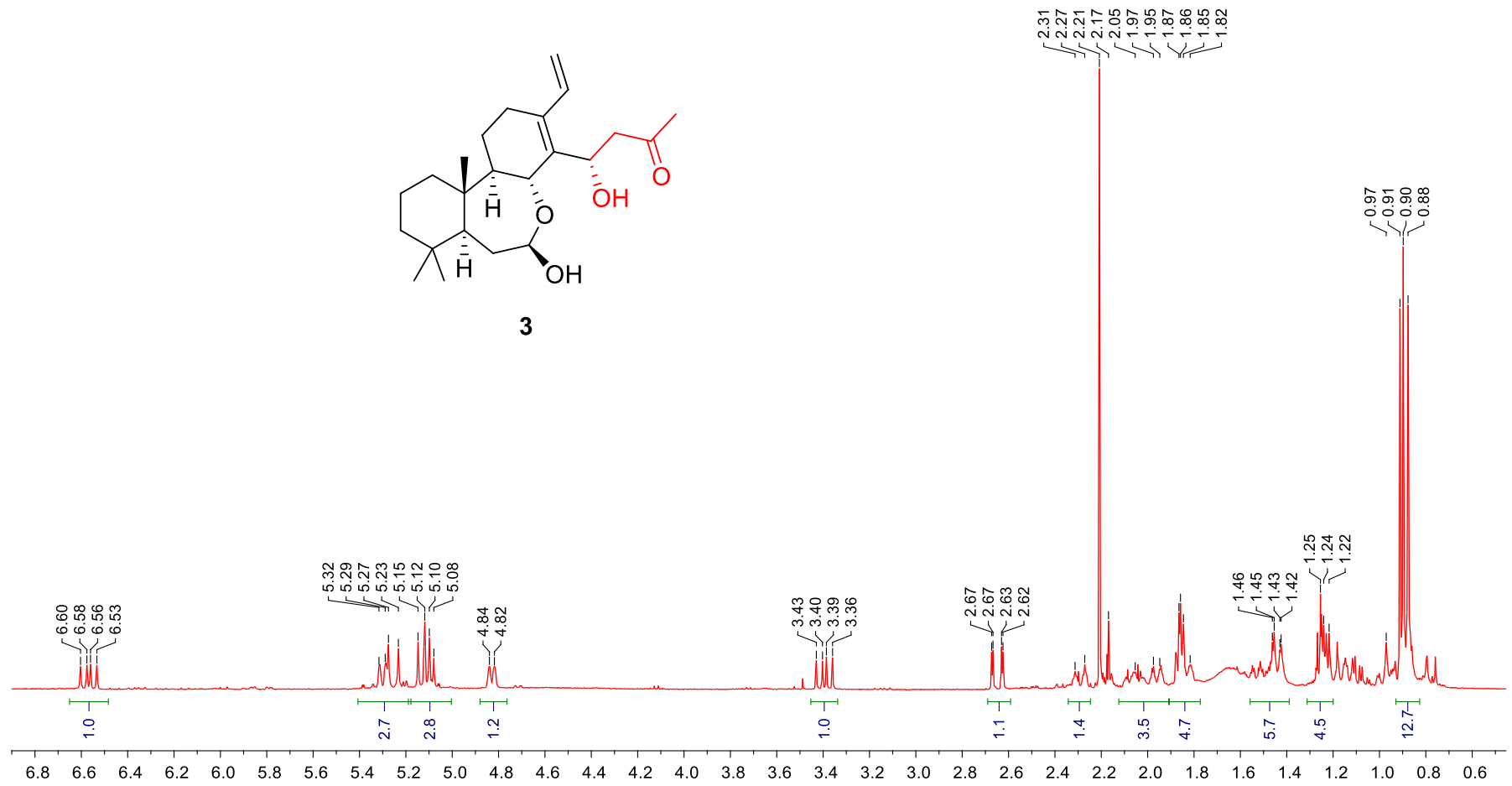


Figure S6. β -Hydroxyketone **3**, ^{13}C (100 MHz), CDCl_3

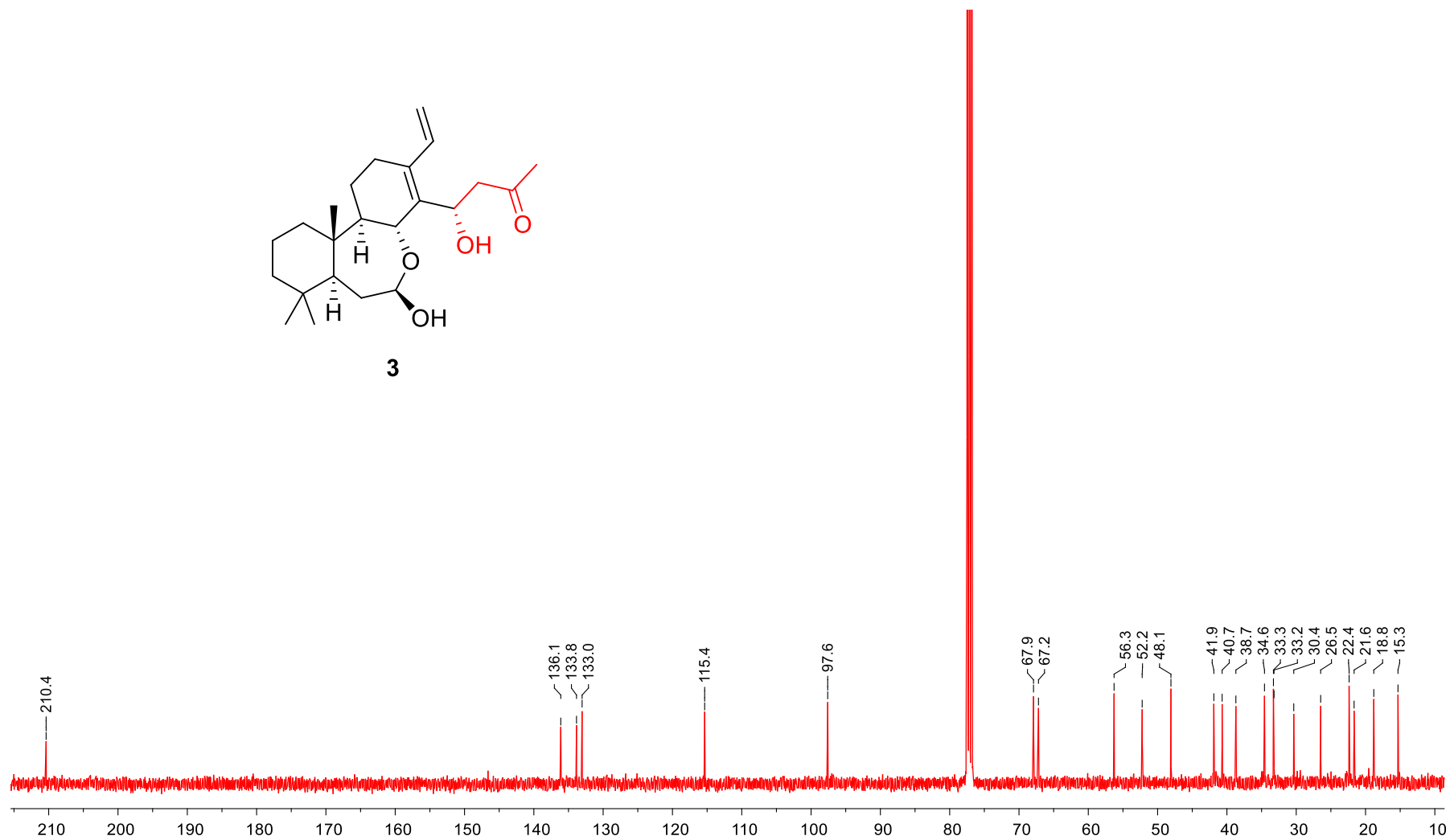
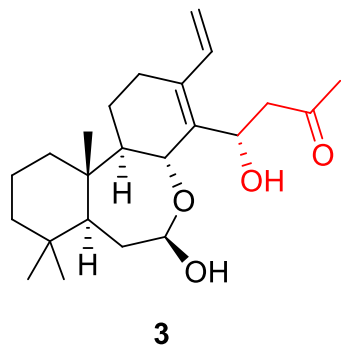


Figure S7. β -Hydroxyketone **3**, COSY EXPERIMENT (400 MHz), CDCl_3

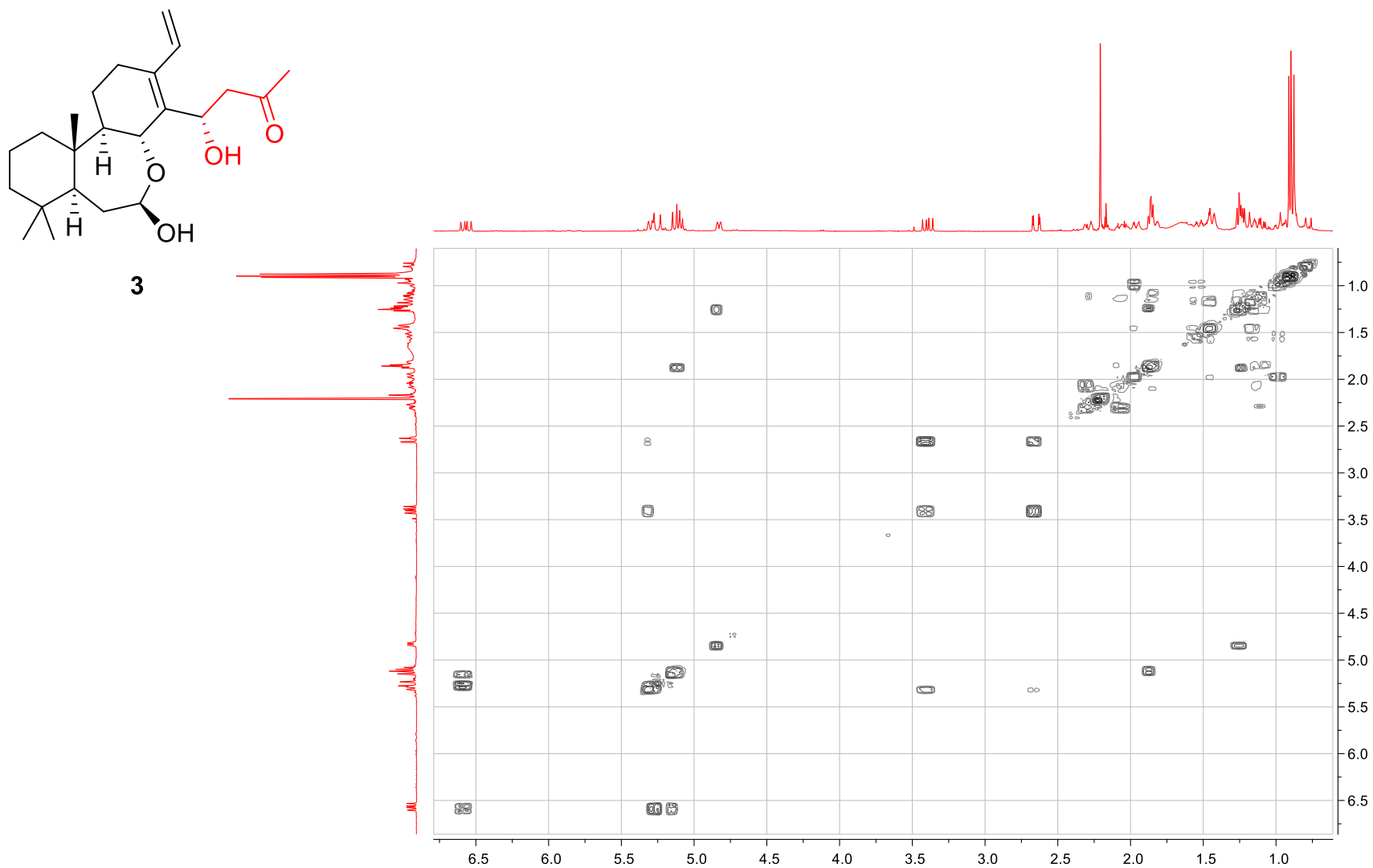


Figure S8. β -Hydroxyketone **3**, HSQC EXPERIMENT (400 MHz), CDCl_3

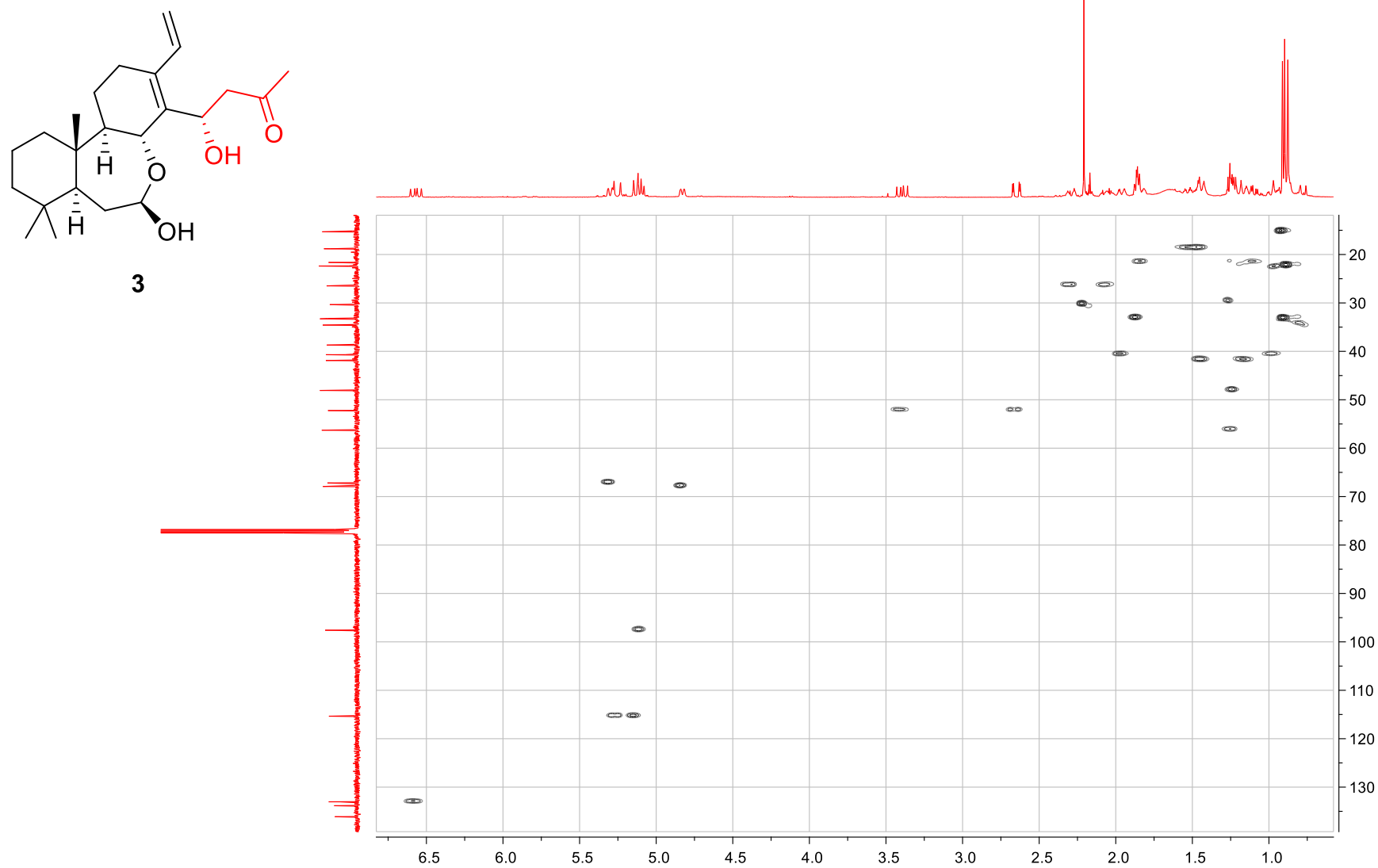


Figure S9. β -Hydroxyketone **3**, HMBC EXPERIMENT (400 MHz), CDCl_3

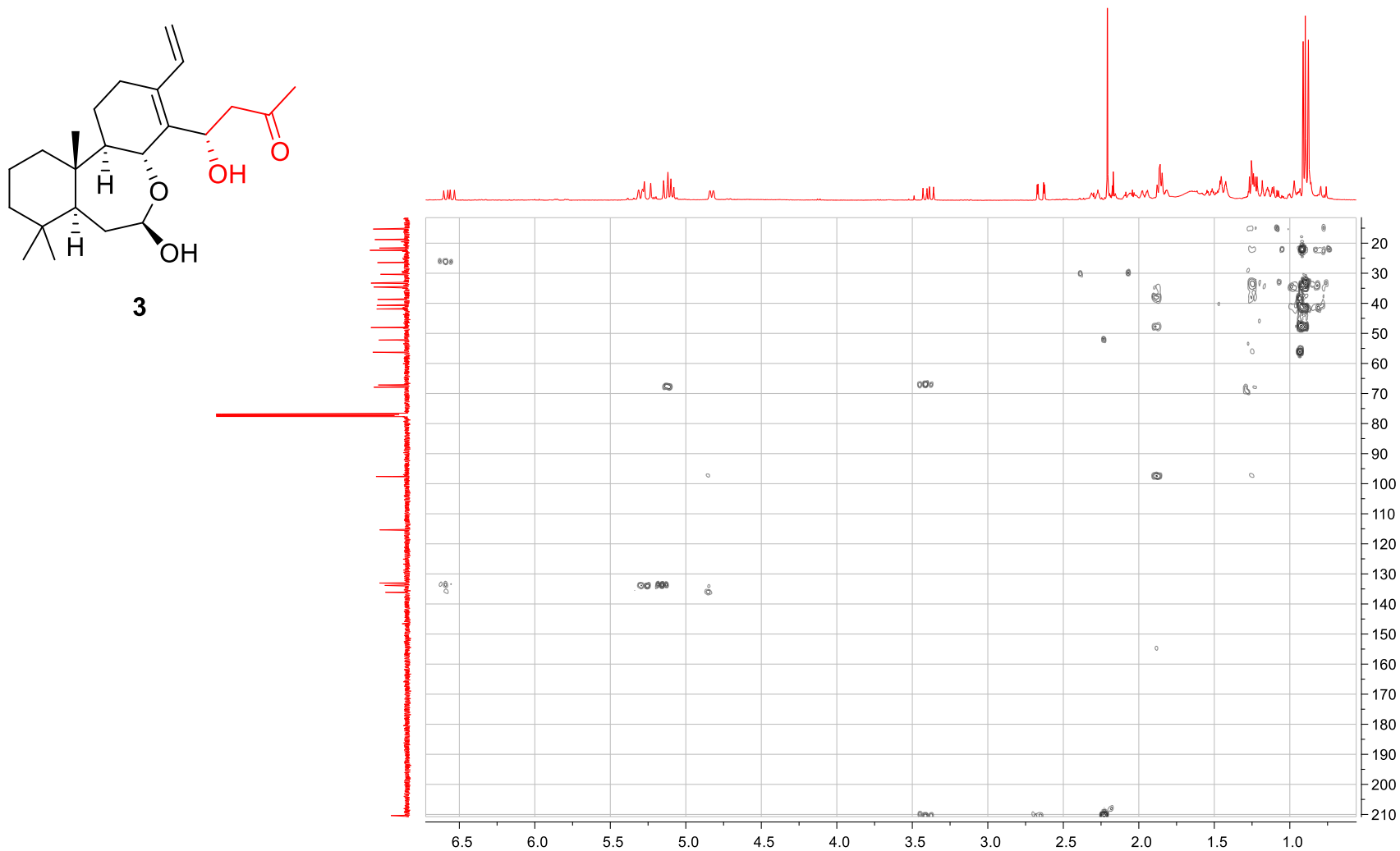


Figure S10. Aldo- ϵ -lactone **4**, ^1H (400 MHz), CDCl_3

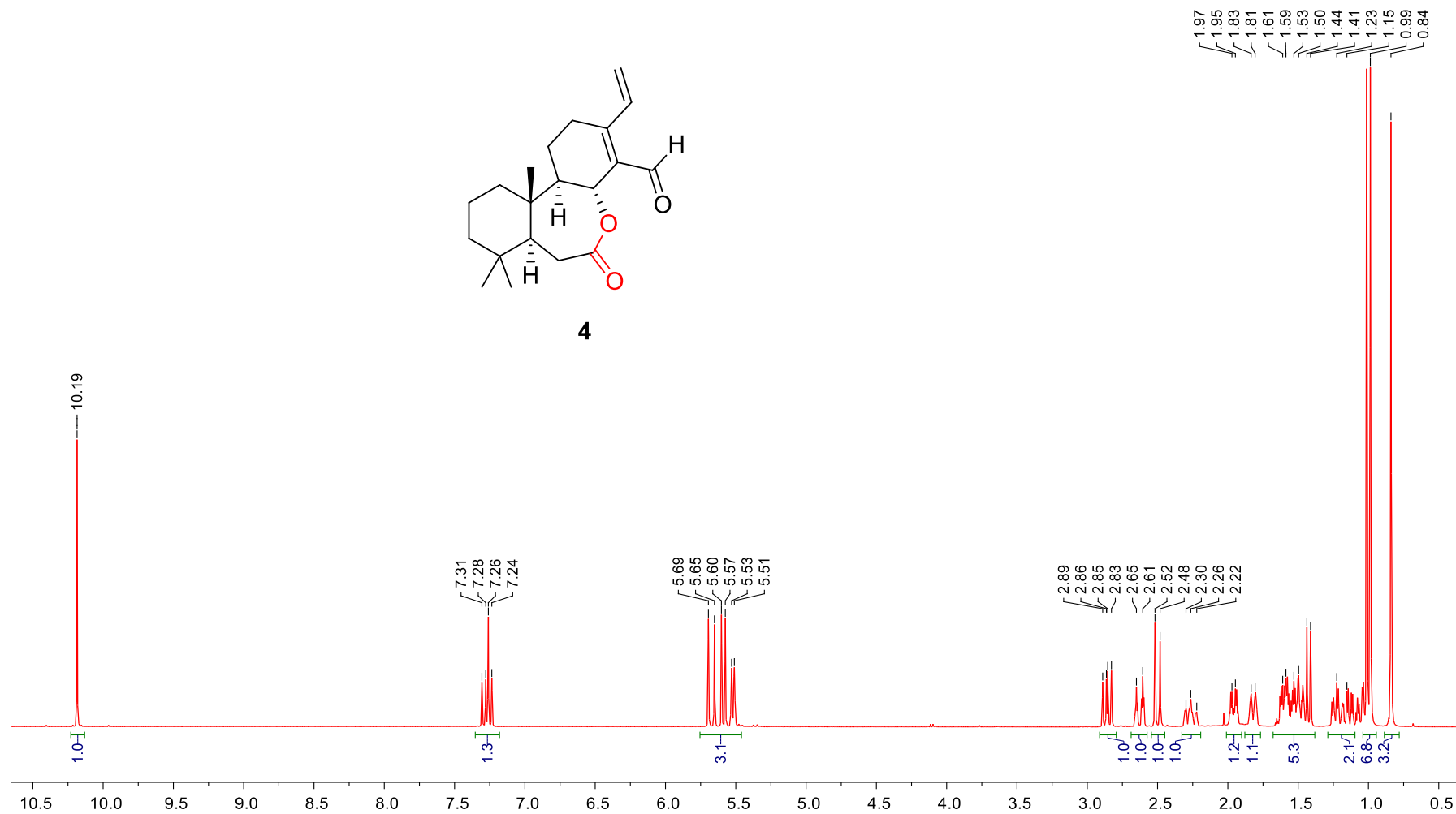


Figure S11. Aldo- ϵ -Lactone **4**, ^{13}C (100 MHz), CDCl_3

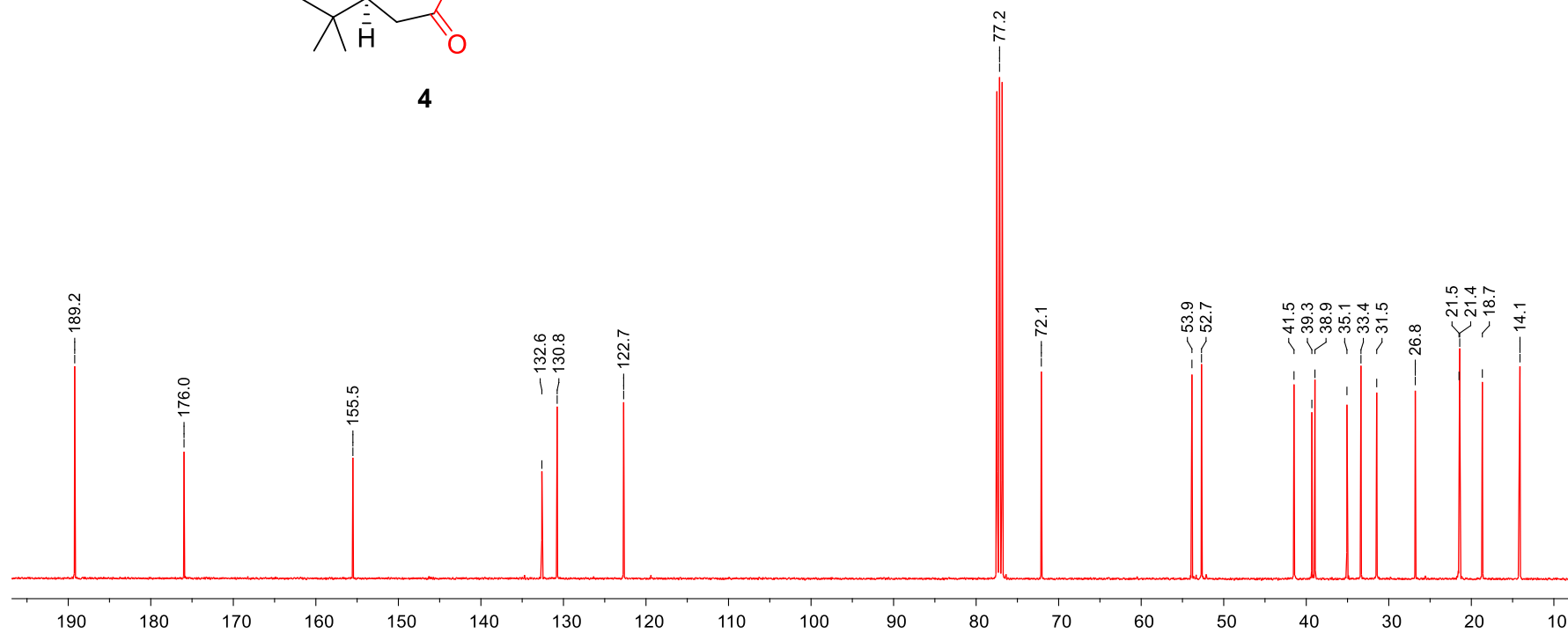
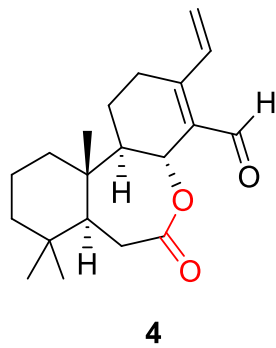


Figure S12. Aldo- ϵ -lactone **4**, COSY EXPERIMENT (400 MHz), CDCl_3

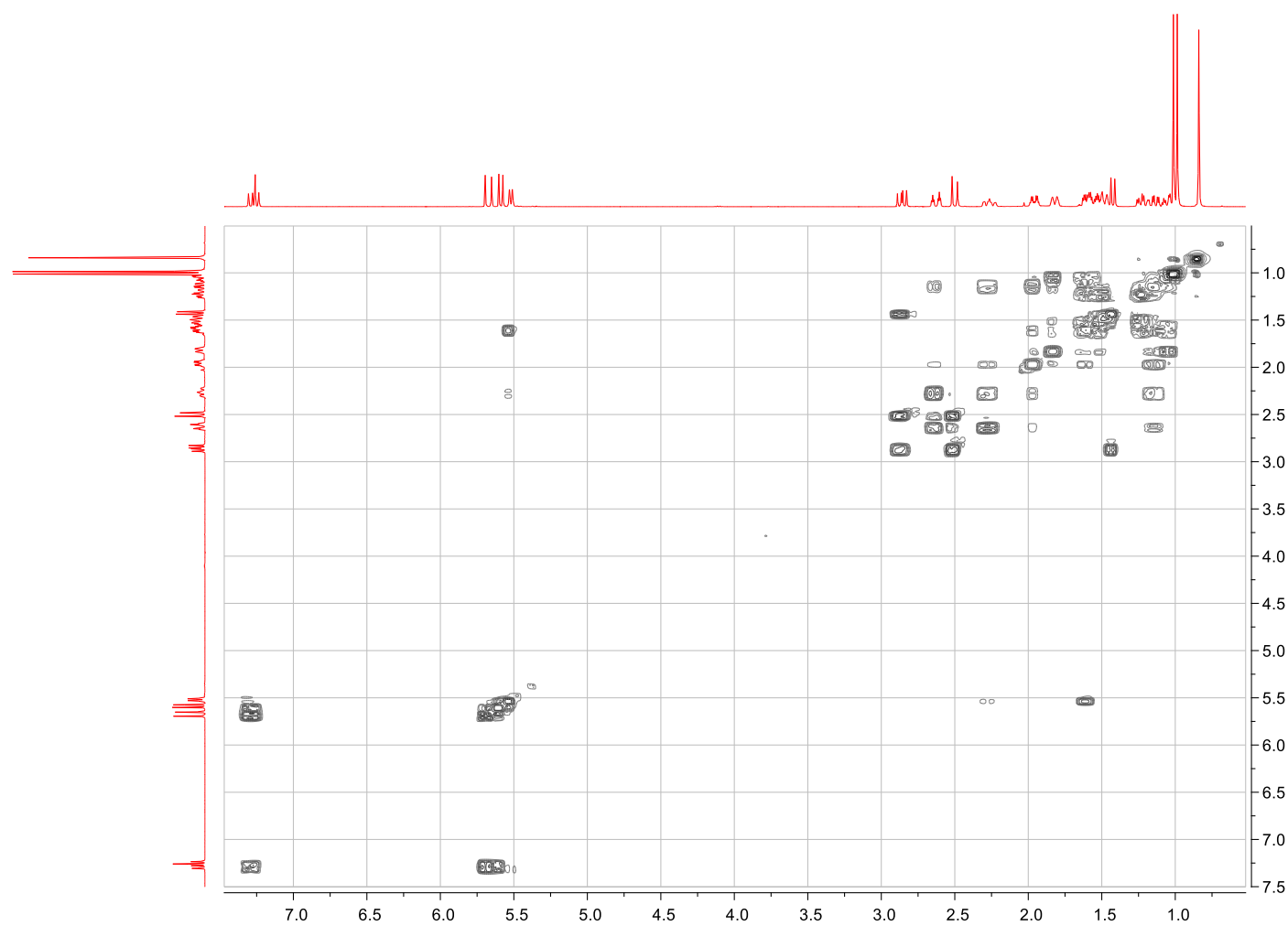
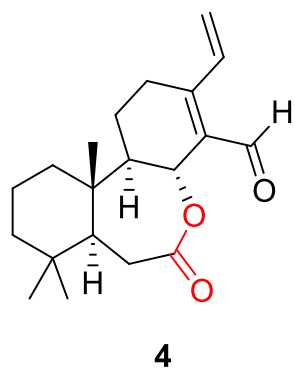


Figure S13. Aldo- ϵ -lactone **4**, HSQC EXPERIMENT (400 MHz), CDCl₃

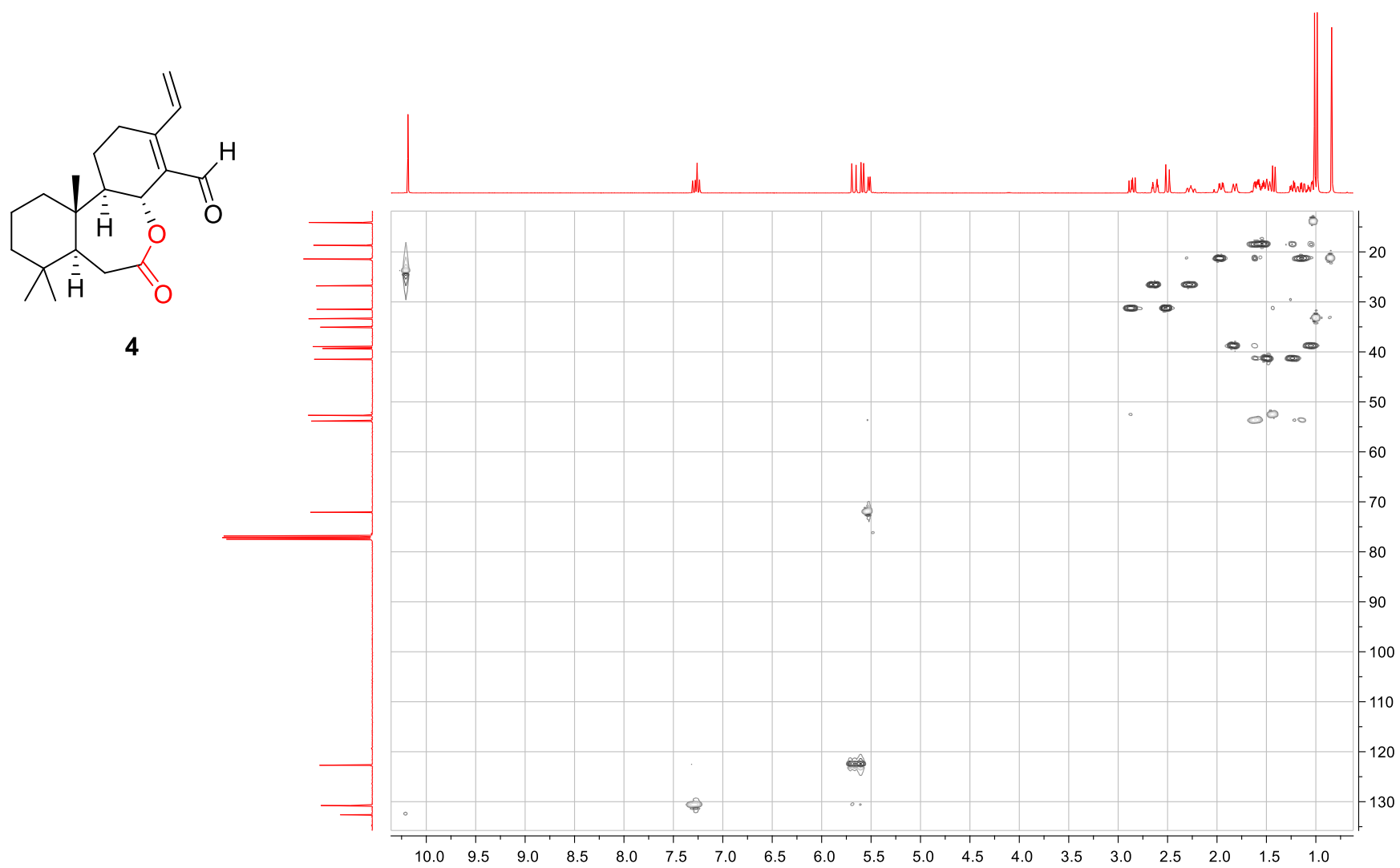


Figure S14. Aldo- ϵ -lactone **4**, HMBC EXPERIMENT (400 MHz), CDCl₃

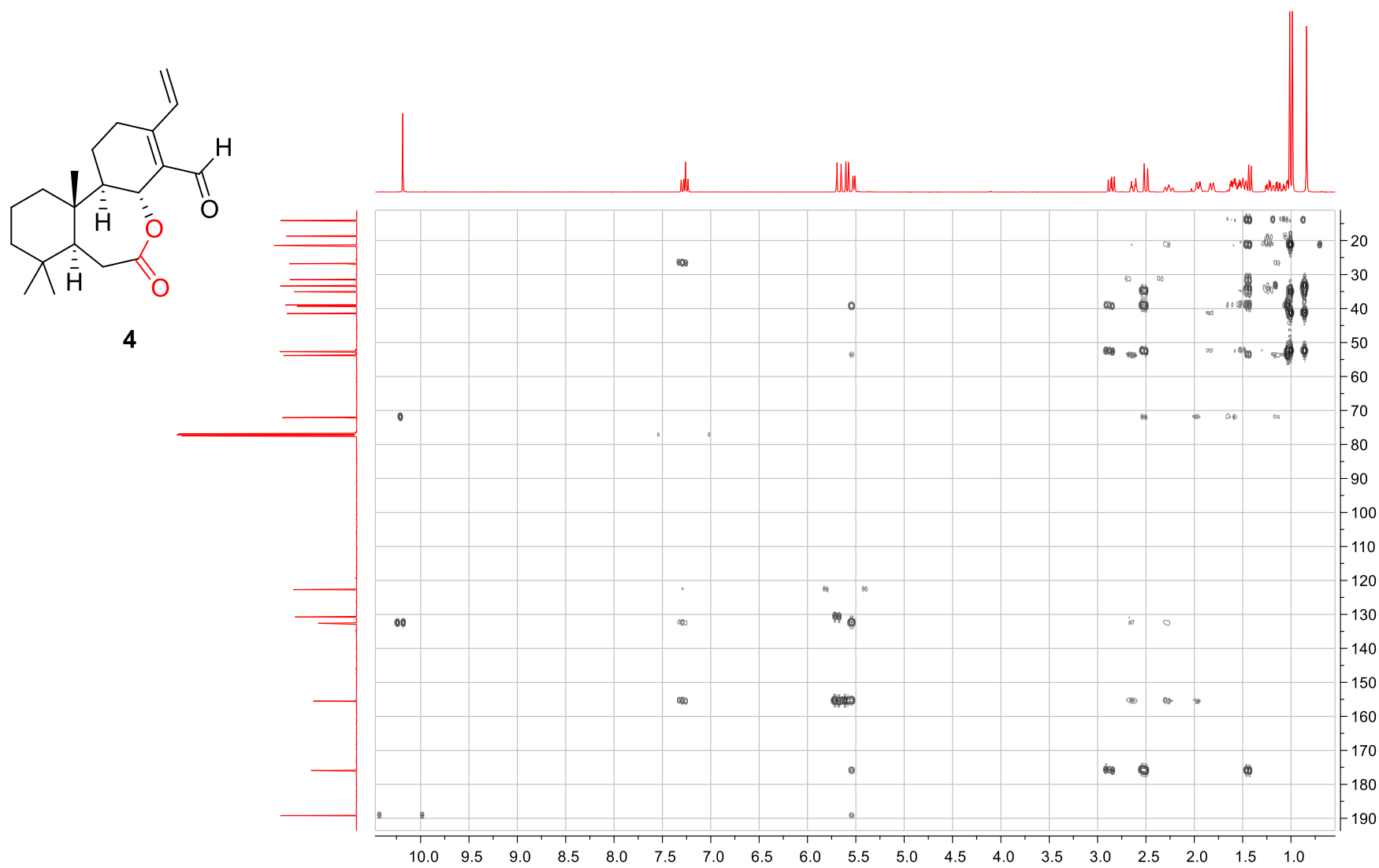


Figure S15. Epoxyformate **5**, ^1H (400 MHz), CDCl_3

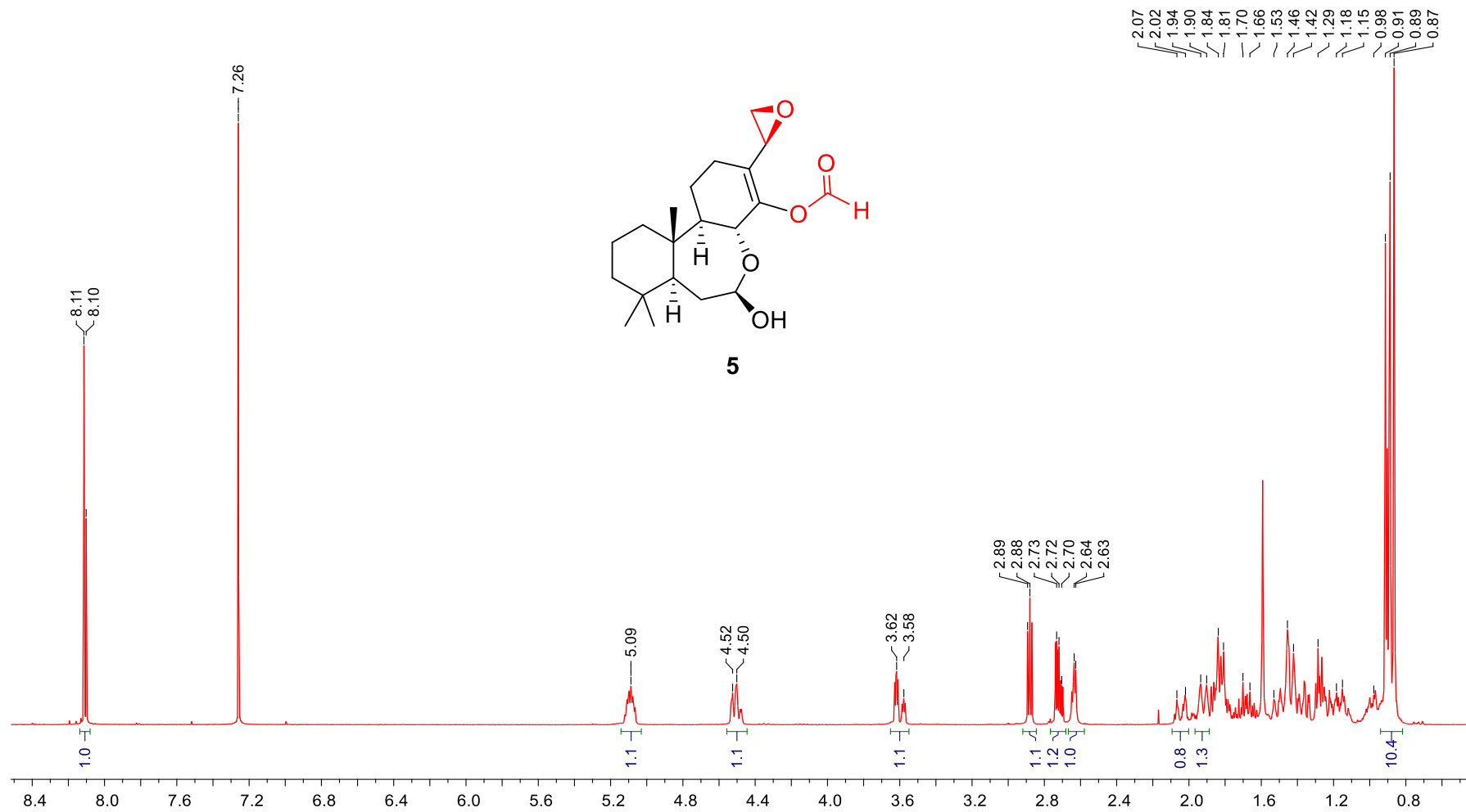


Figure S16. Epoxyformate **5**, ^{13}C (100 MHz), CDCl_3

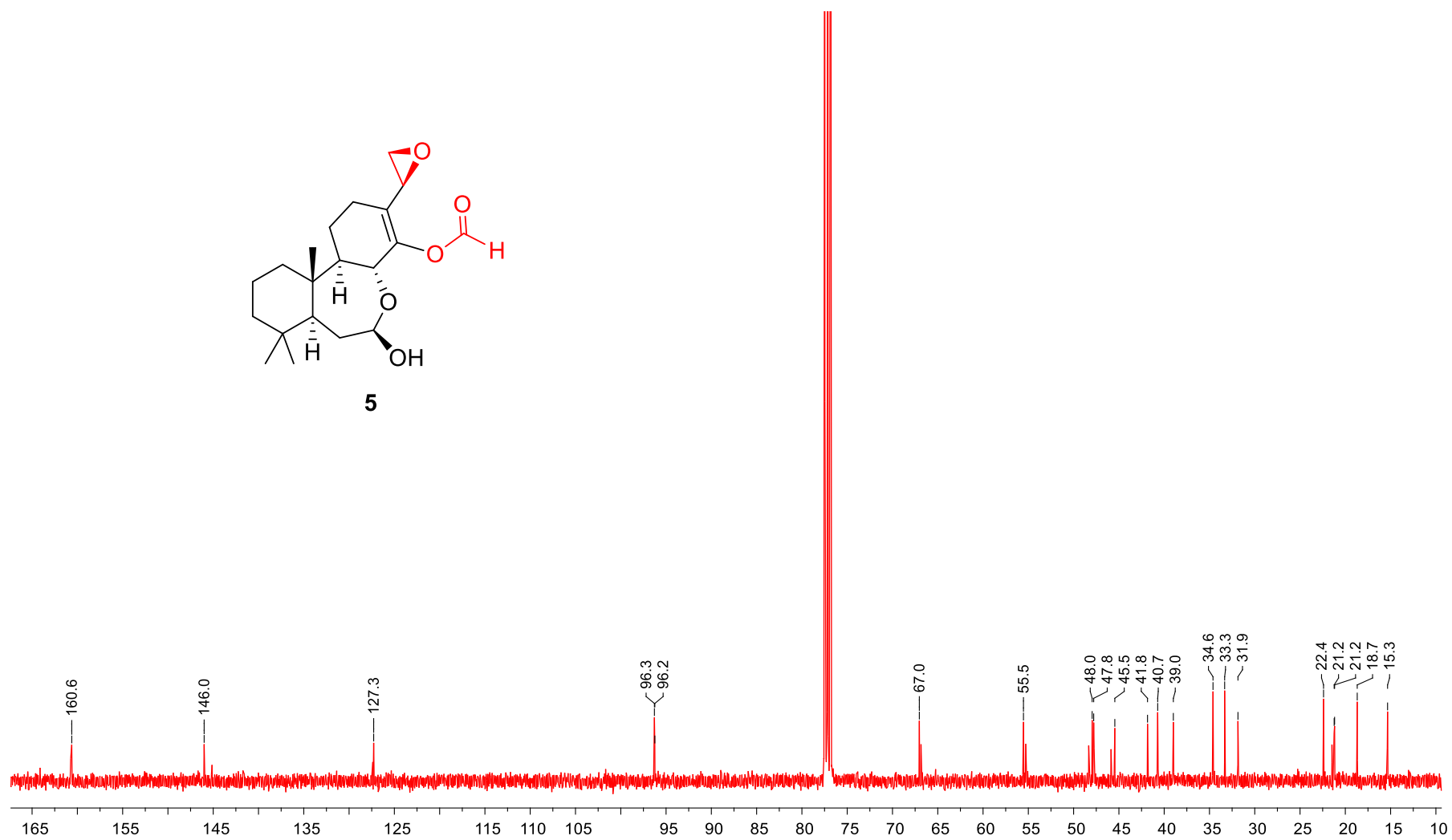


Figure S17. Epoxyformate **5**, COSY EXPERIMENT (400 MHz), CDCl₃

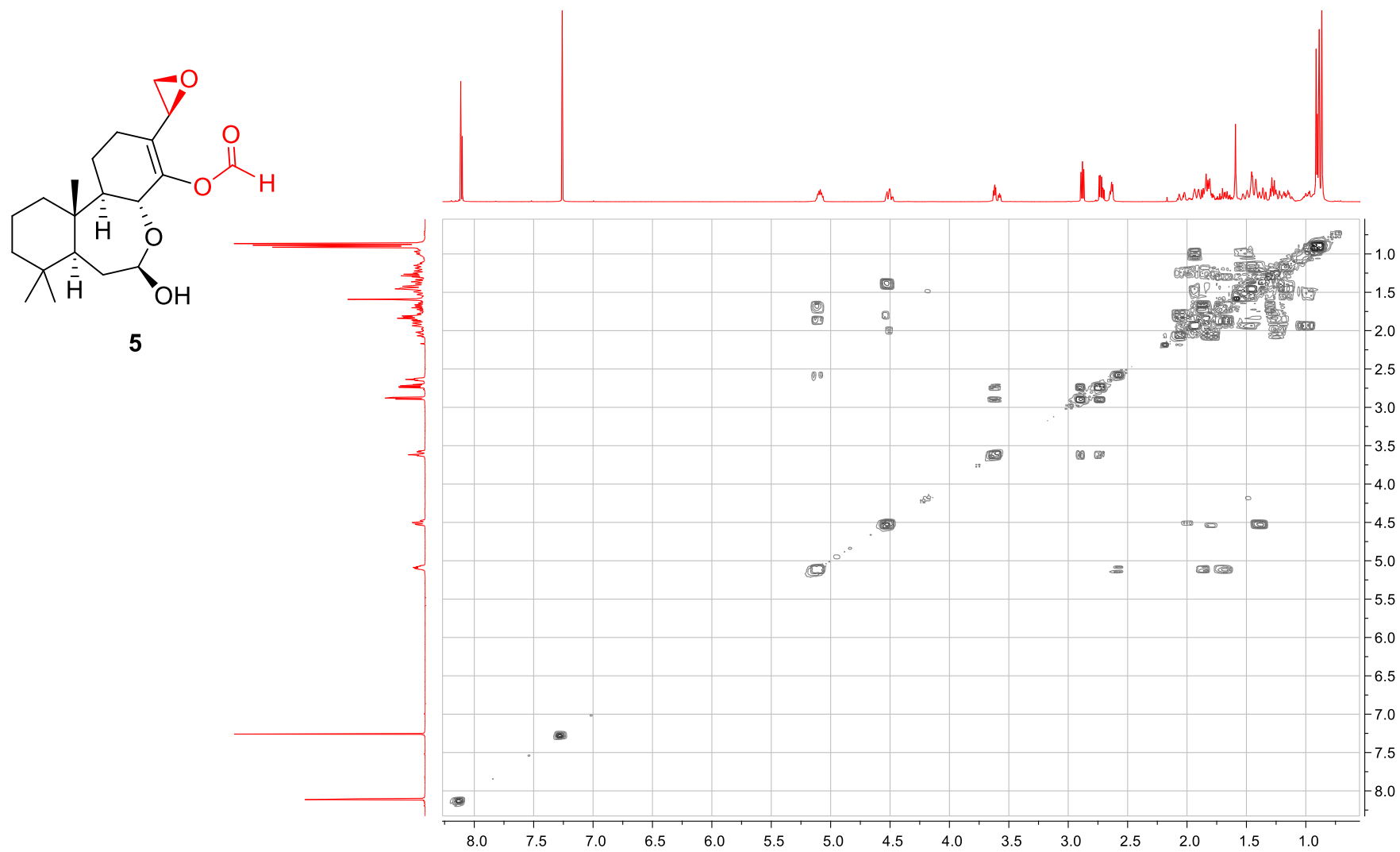


Figure S18. Epoxyformate **5**, HSQC EXPERIMENT (400 MHz), CDCl₃

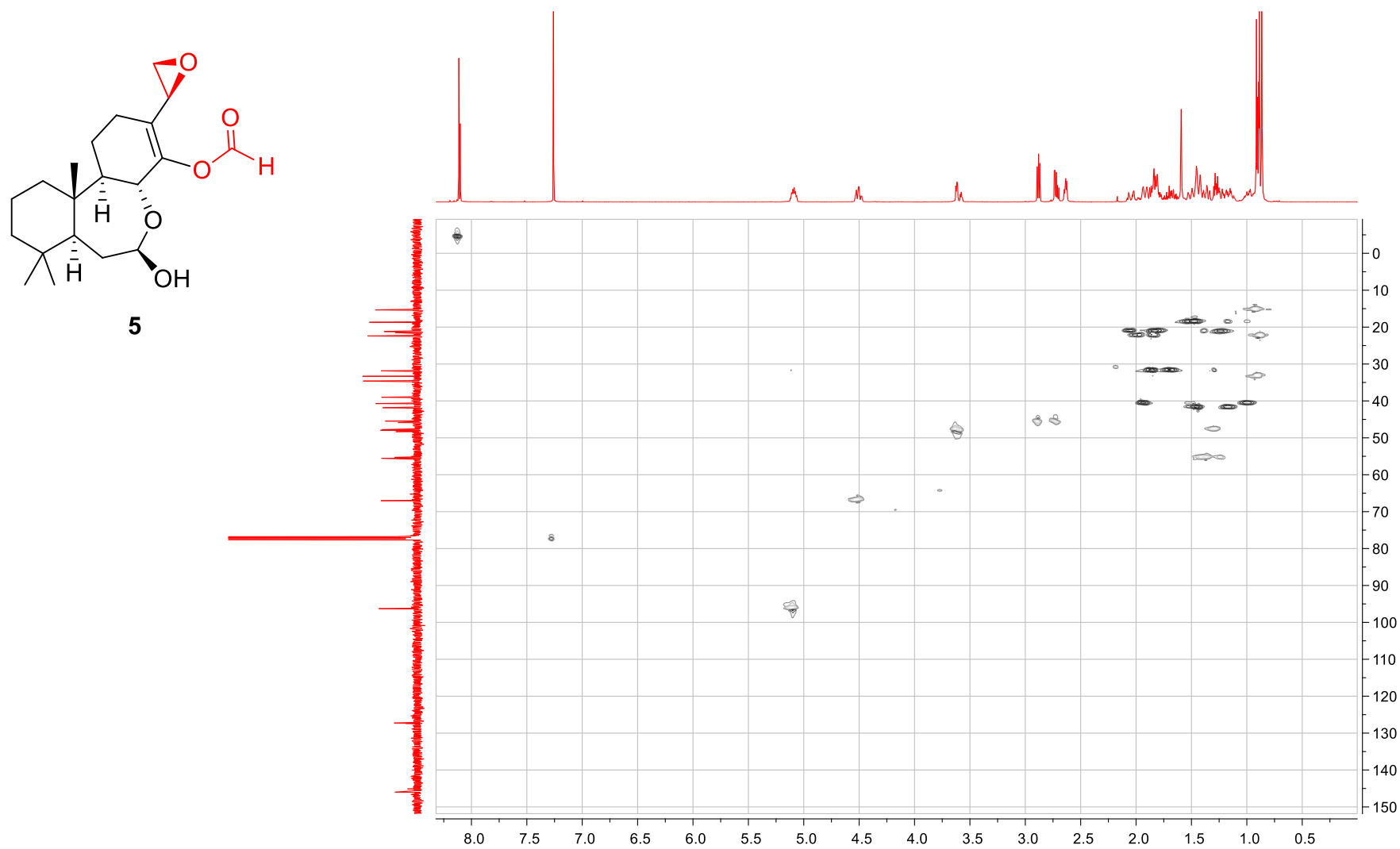


Figure S19. Epoxyformate **5**, HMBC EXPERIMENT (400 MHz), CDCl₃

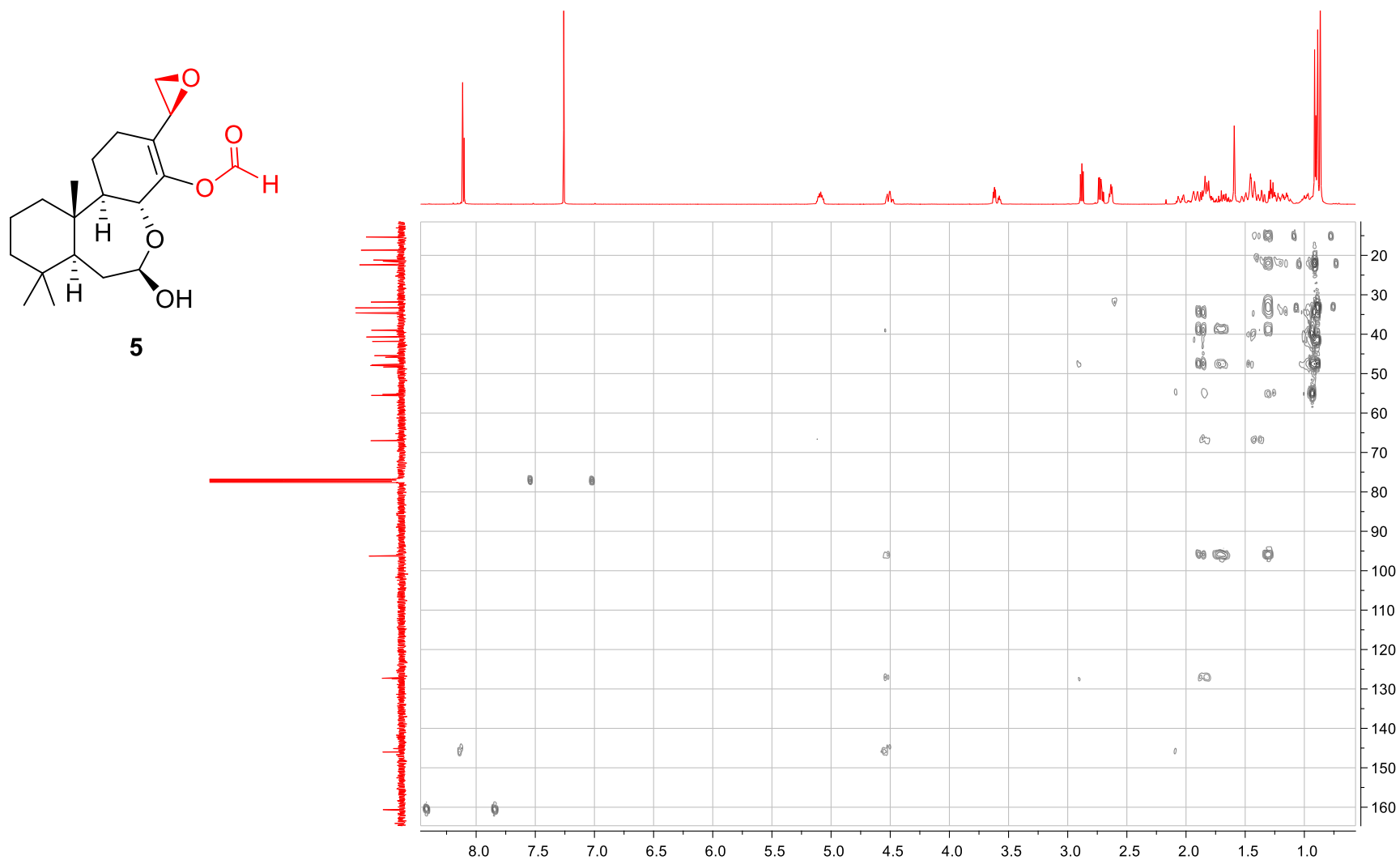


Figure S20. 17-nor-Ketone **6**, ^1H (400 MHz), CDCl_3

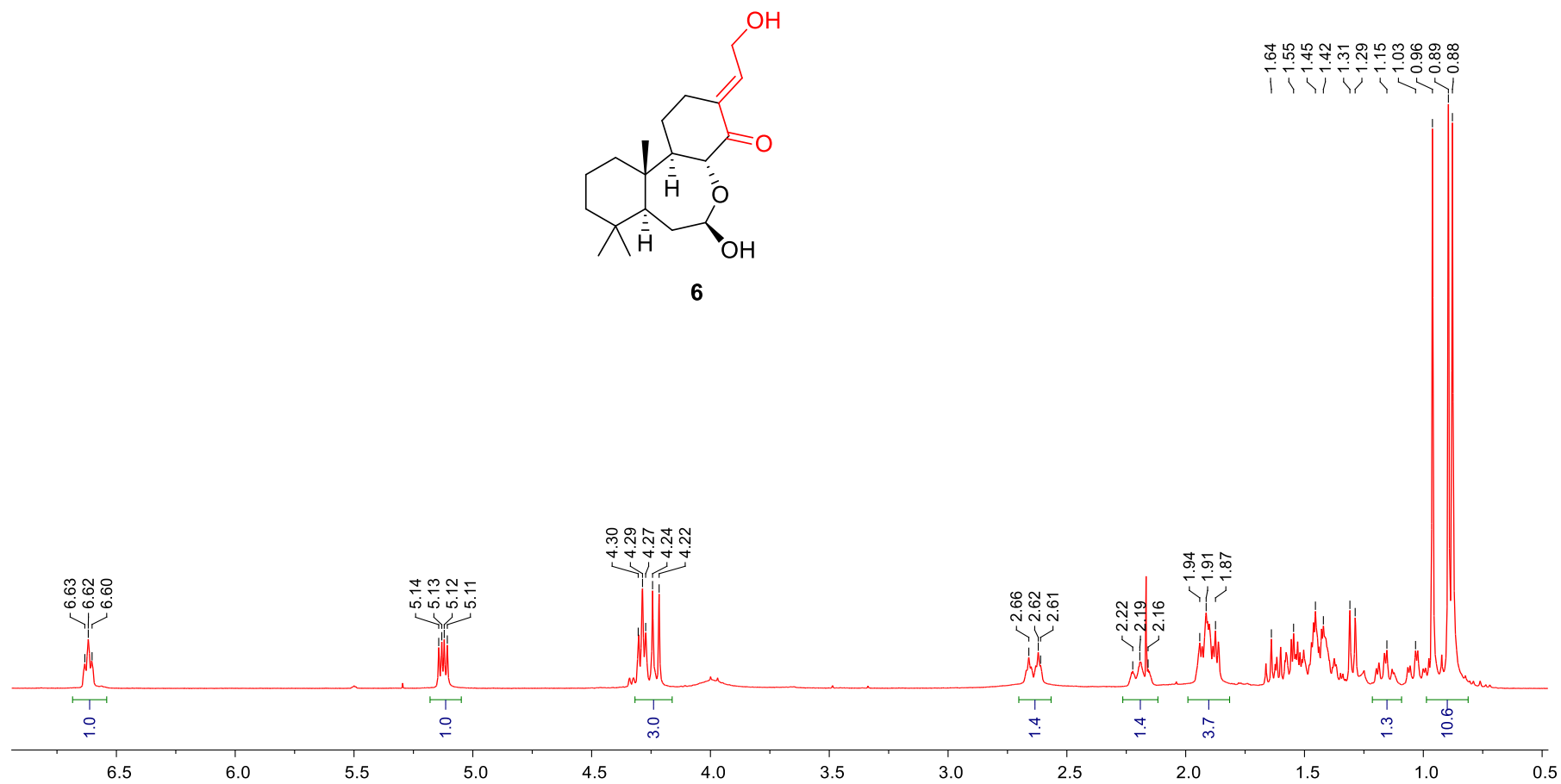


Figure S21. 17-nor-Ketone **6**, ^{13}C (100 MHz), CDCl_3

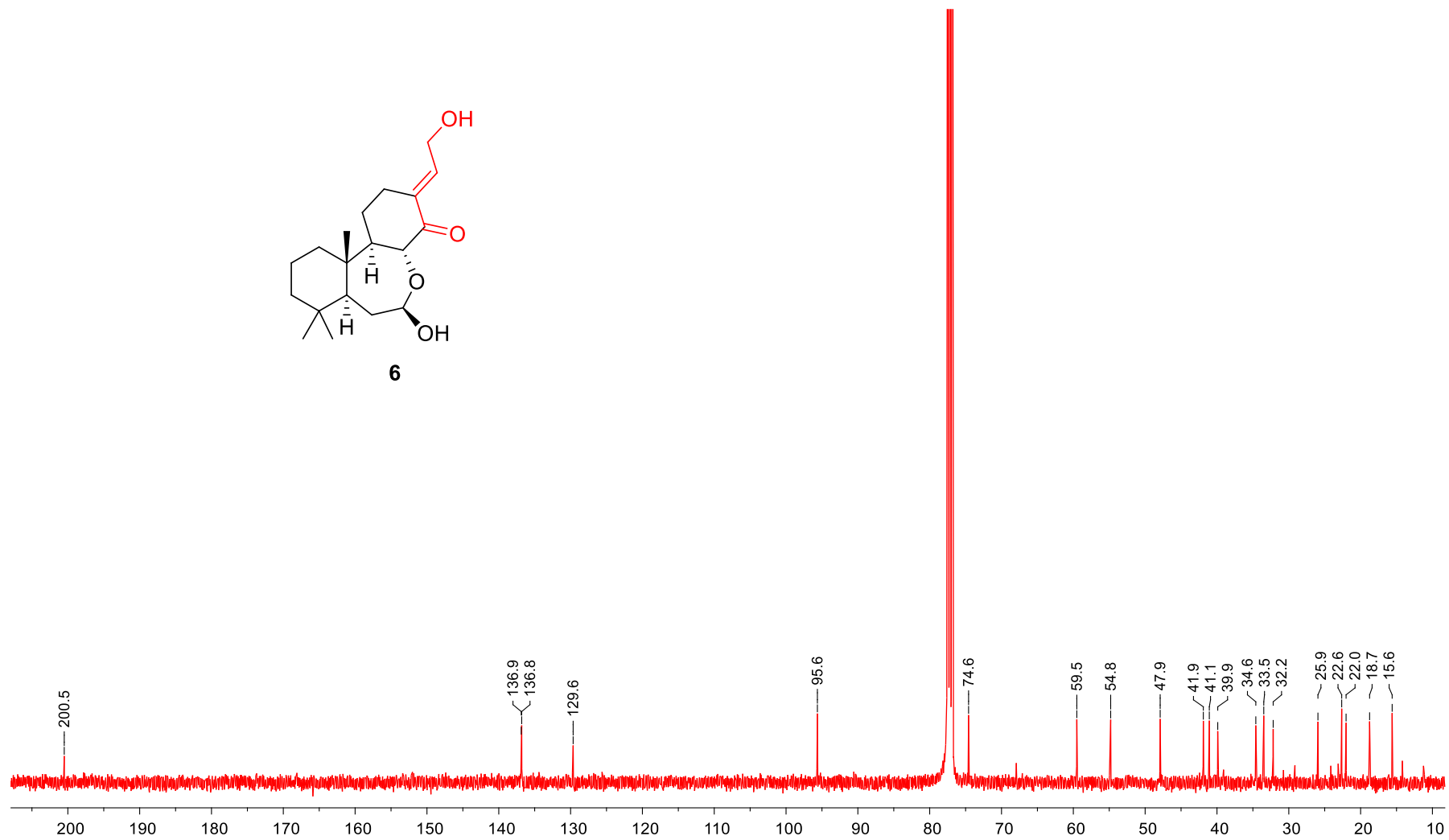
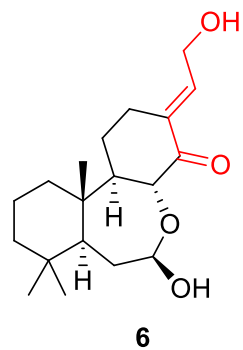


Figure S22. 17-nor-Ketone **6**, COSY EXPERIMENT (400 MHz), CDCl₃

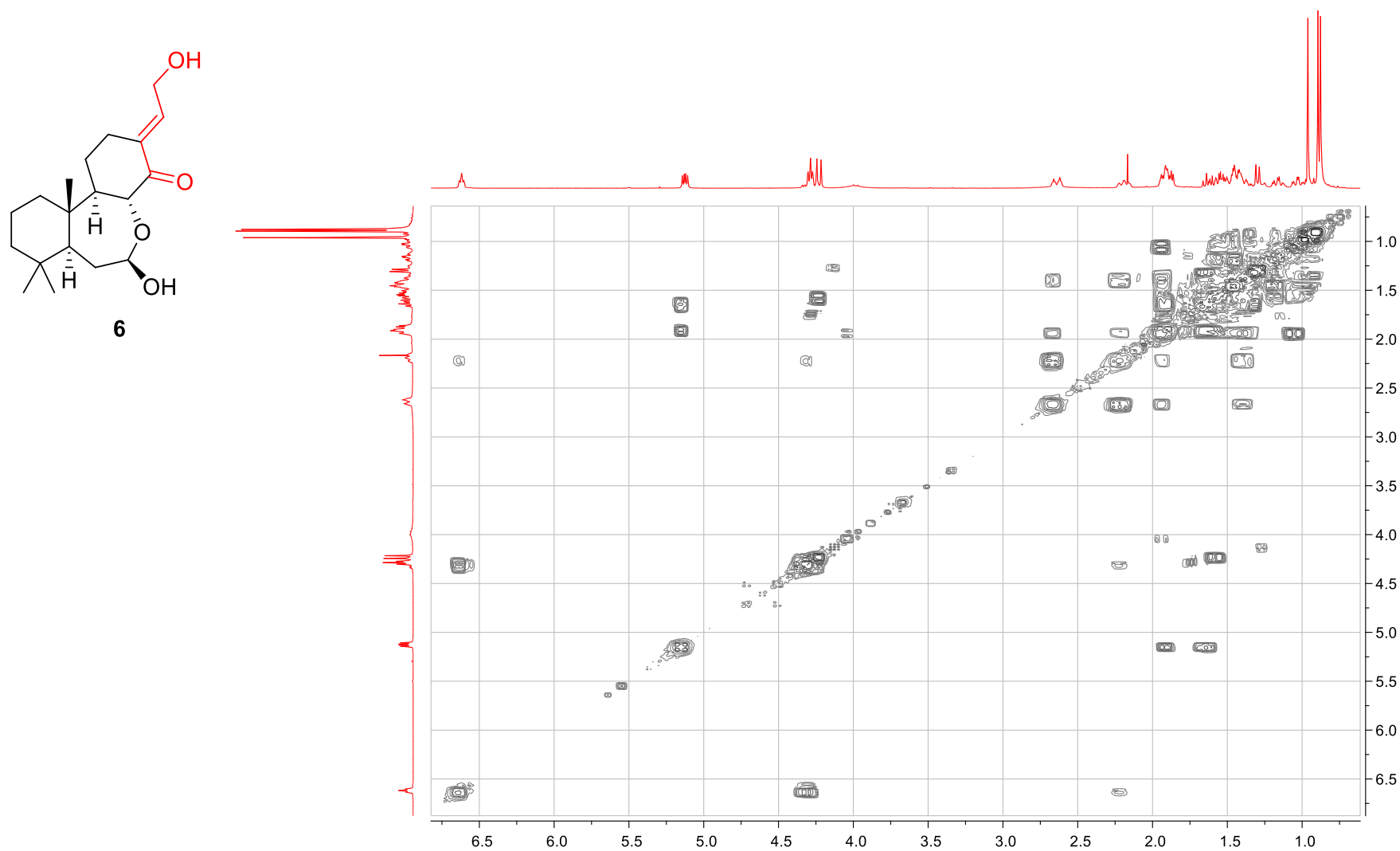


Figure S23. 17-*nor*-Ketone **6**, HSQC EXPERIMENT (400 MHz), CDCl₃

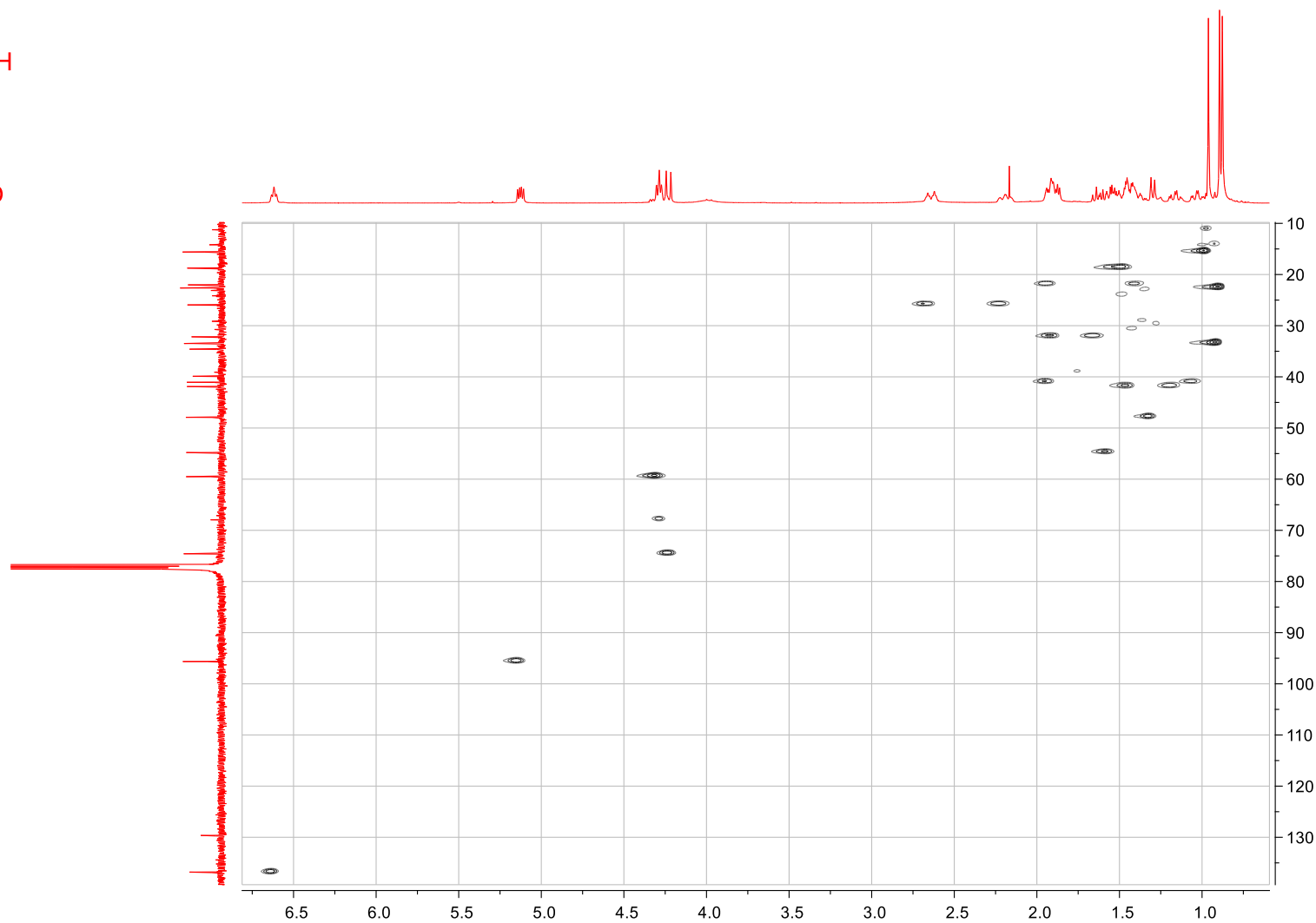
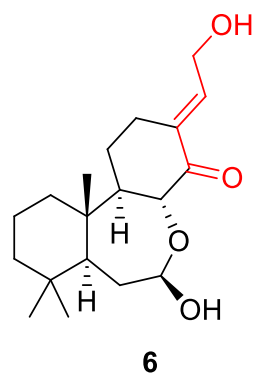


Figure S24. 17-*nor*-Ketone **6**, HMBC EXPERIMENT (400 MHz), CDCl₃

