# Supporting Information

## Quinazoline Containing Indole Alkaloids from the Marine-Derived Fungus *Aspergillus* sp. HNMF114

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**The ITS gene sequences for *Aspergillus* sp. HNMF114**

CTTCCCGCTTAGGG-GGTGCCTGCGGAAGGATCAGTACCGAGCGC-

GGGCCCTCTGGGTCCAACCTCCCACCCGTGTCTATTGTACCTTGTTGCTTC

GGCGGGCCCGCCGTCTTCGGACGGCCGCCGGGGAGGCCTCCGCGCCCCCG

GGCCCGCGCCCGCCGAAGACCACAACATGAACTCTGTTCTGAAGTTTTGC

AGTCTGAGTTGATTATCATAATCAGTTAAAACTTTCAACAACGGATCTCTT

GGTTCCGGCATCGATGAAGAACGCAGCGAAATGCGATAACTAATGTGAAT

TGCAGAATTCAGTGAATCATCGAGTCTTTGAACGCACATTGCGCCCCCTG

GTATTCCGGGGGGCATGCCTGTCCGAGCGTCATTGCTGCCCTCAAGCACG

GCTTGTGTGTTGGGCCCCCGTCCCCGCCTCACCGCGGGGACGGGCCCGAA

AGGCAGCGGCGGCACCGCGTCCGGTCCTCGAGCGTATGGGGCTTTGTCAC

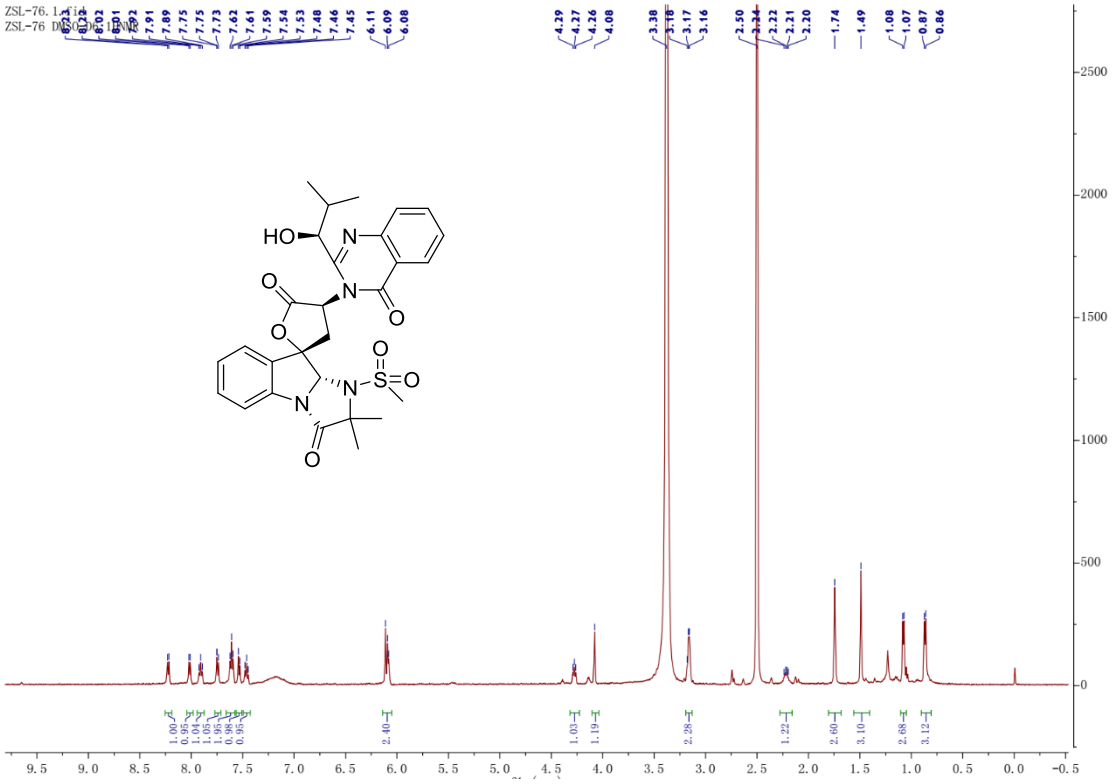
CCGCTCTTGTAGGCCCGGCCGGCGCCTGTCGACACCAACCCCAATTTTTCT

AAGGTTGACCTCGGATCAGGTAGAGATAACCGCTGAACTTAAGCATATCA

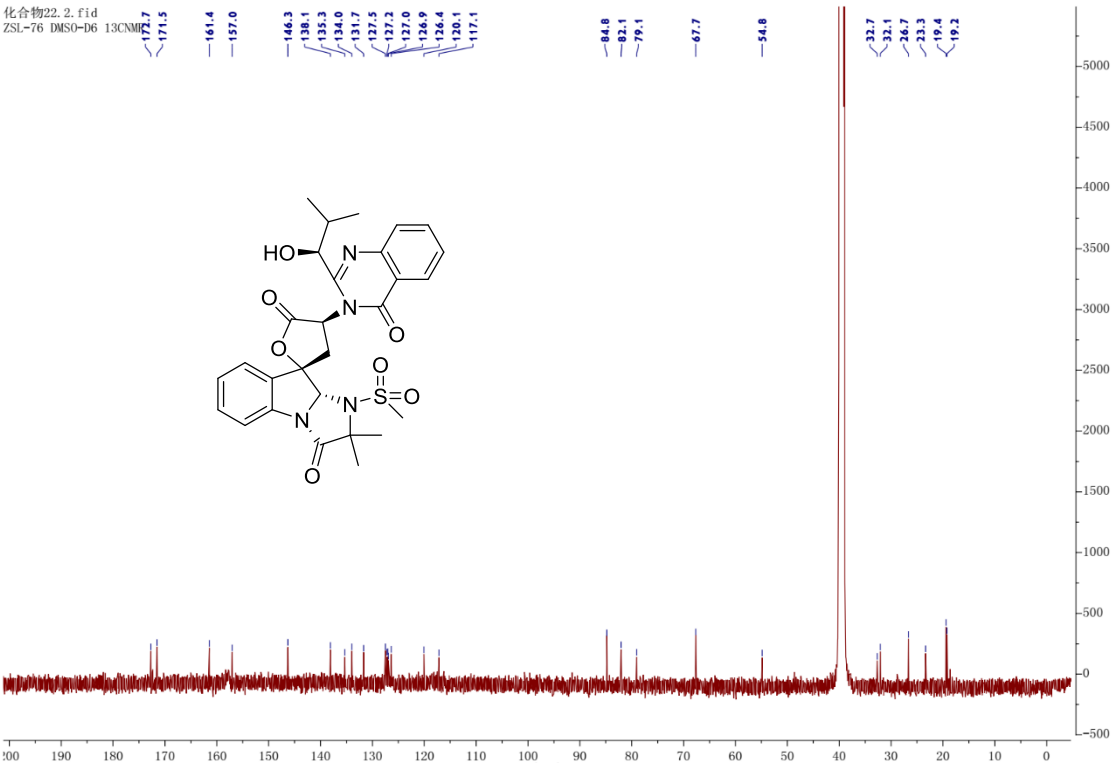
AAAGGCGGGAGGAATTA

# NMR, HRESIMS, and IR spectra of compound 1

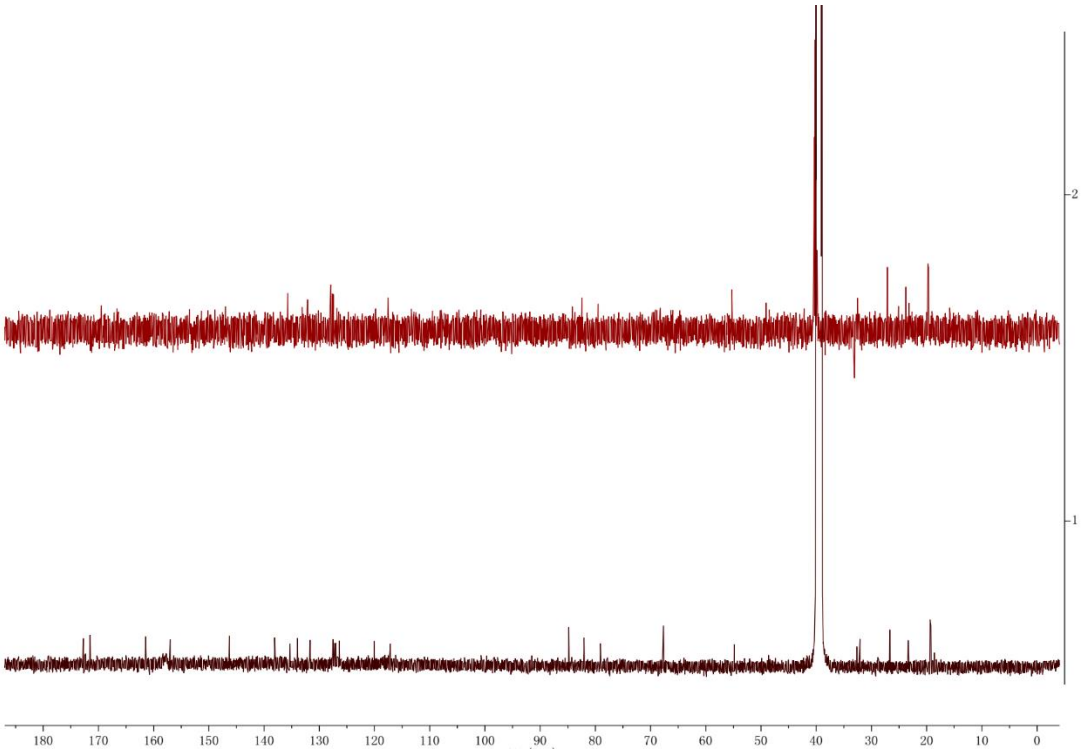
## $^{1}$H-NMR spectrum of 1



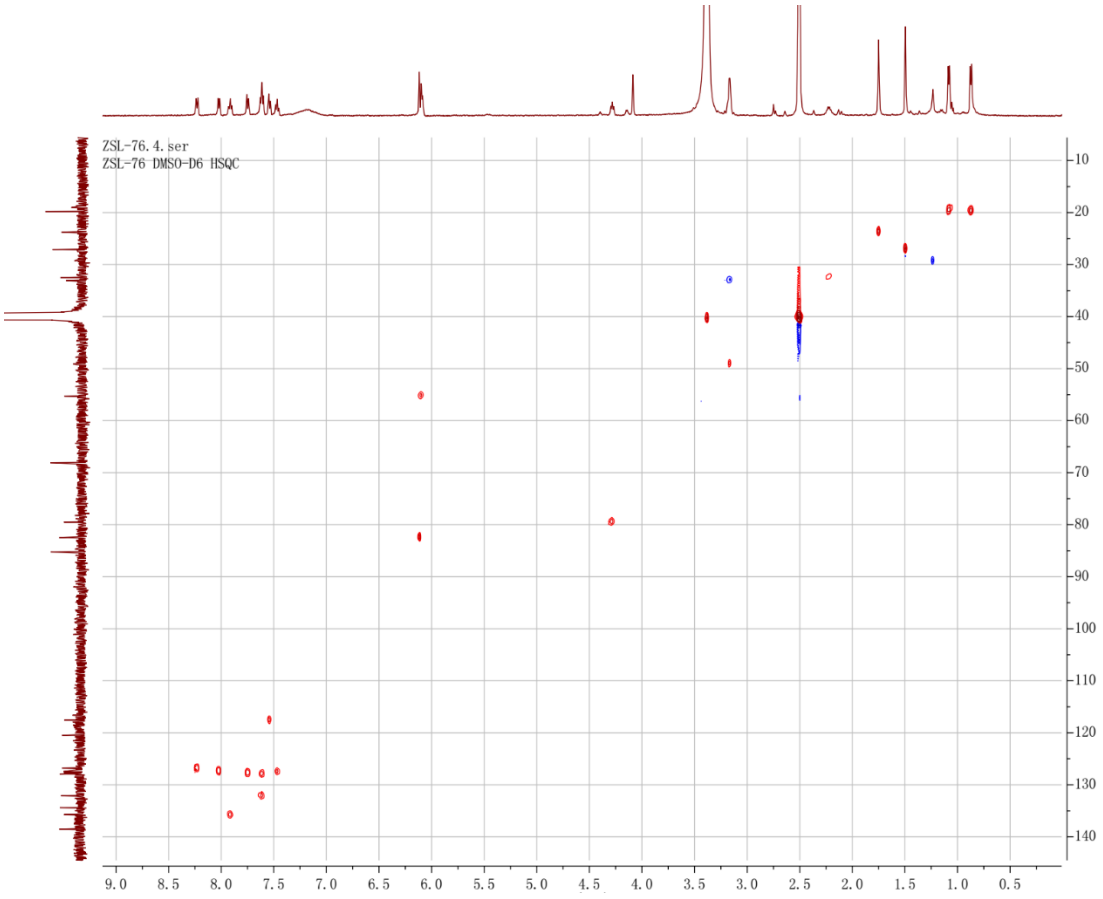

## $^{13}$C-NMR spectrum of 1



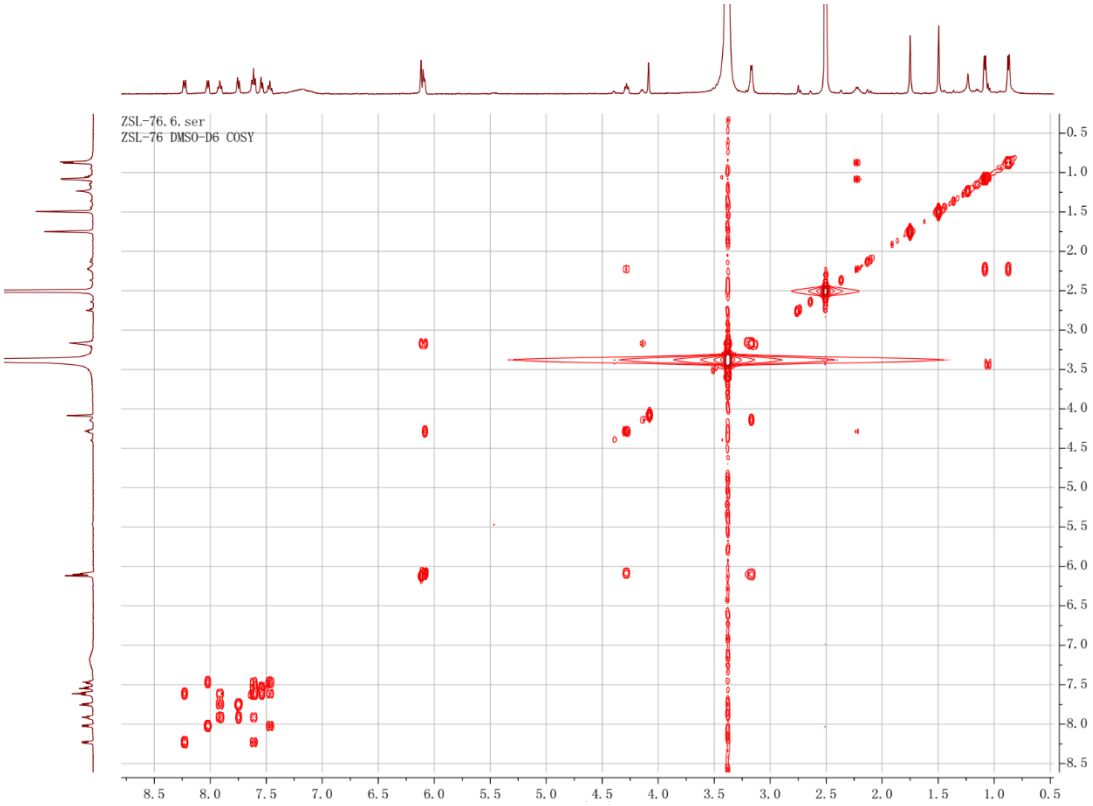
## DEPT spectrum of 1



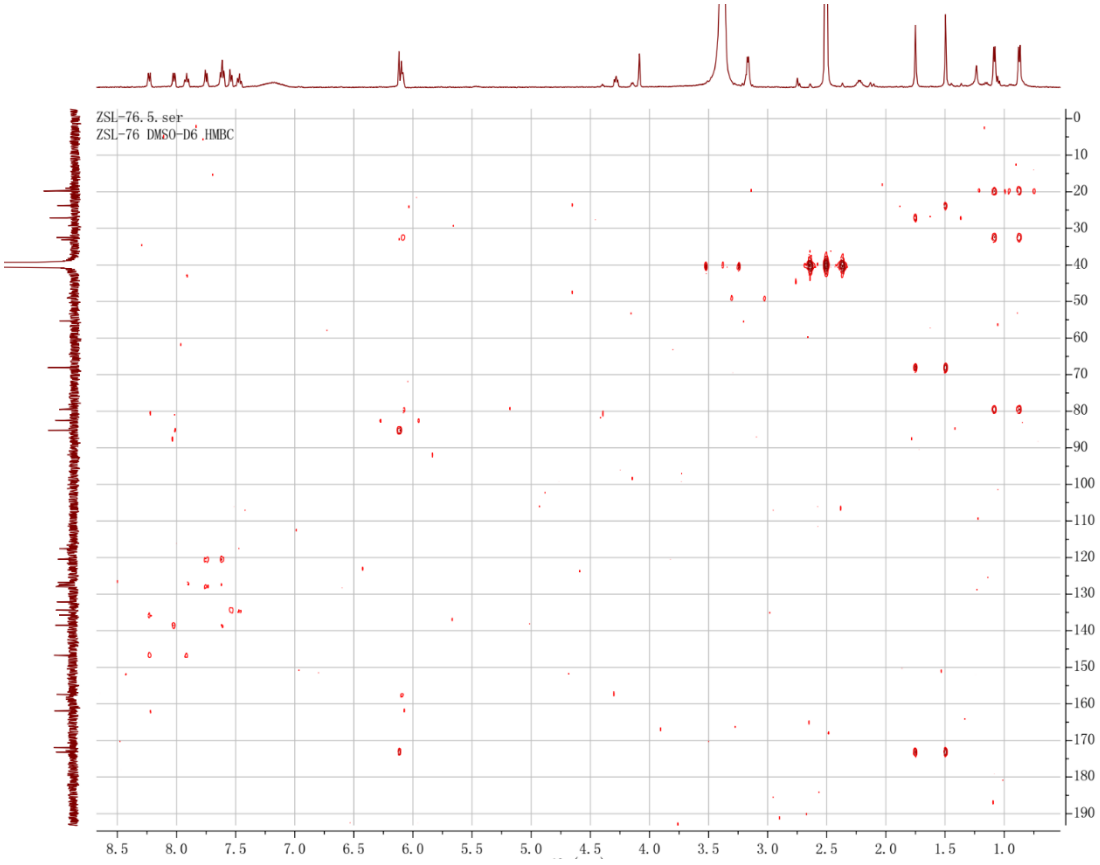

## HSQC spectrum of 1



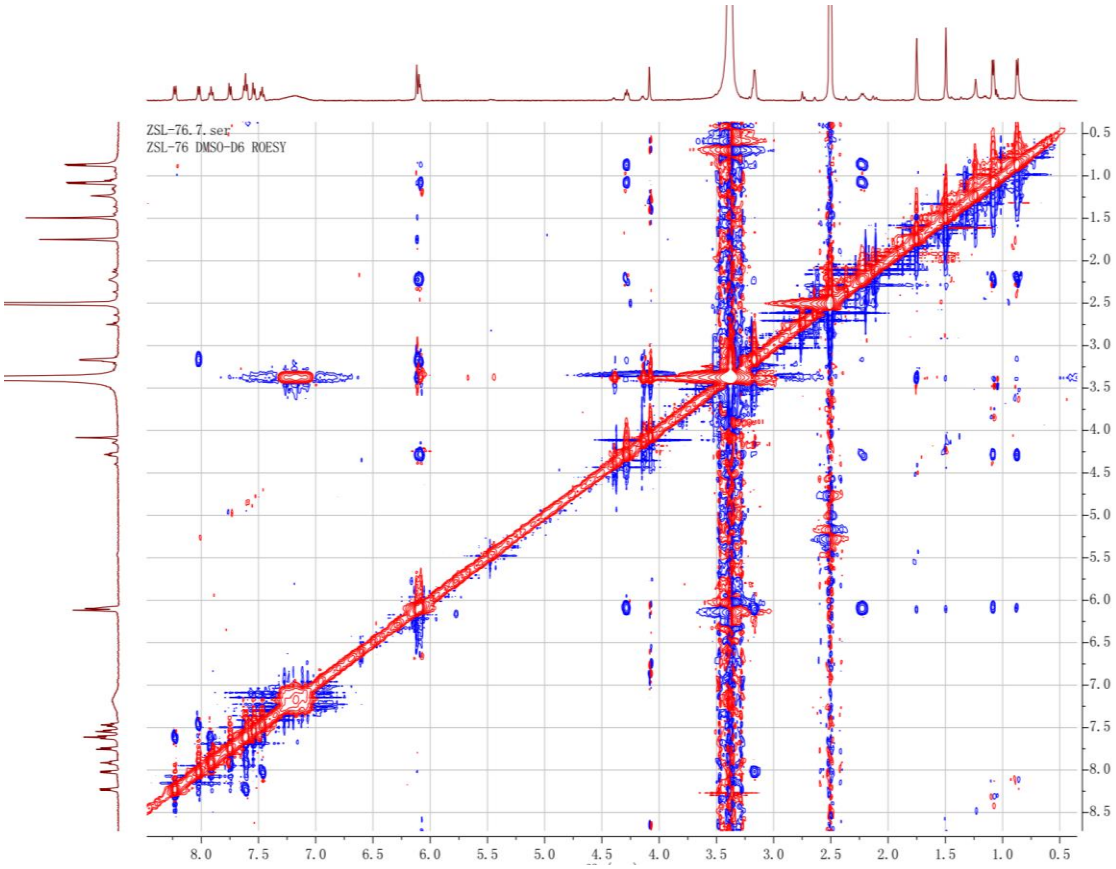
## $^{1}H$-$^{1}H$ COSY spectrum of 1



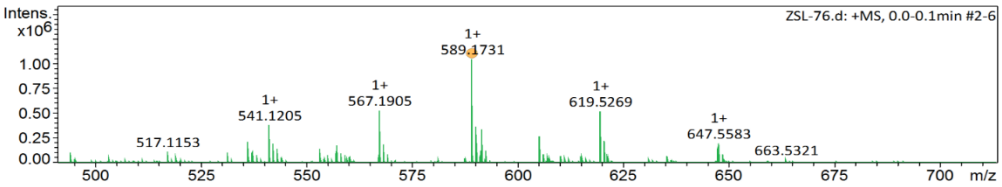

## HMBC spectrum of 1



## ROESY spectrum of 1

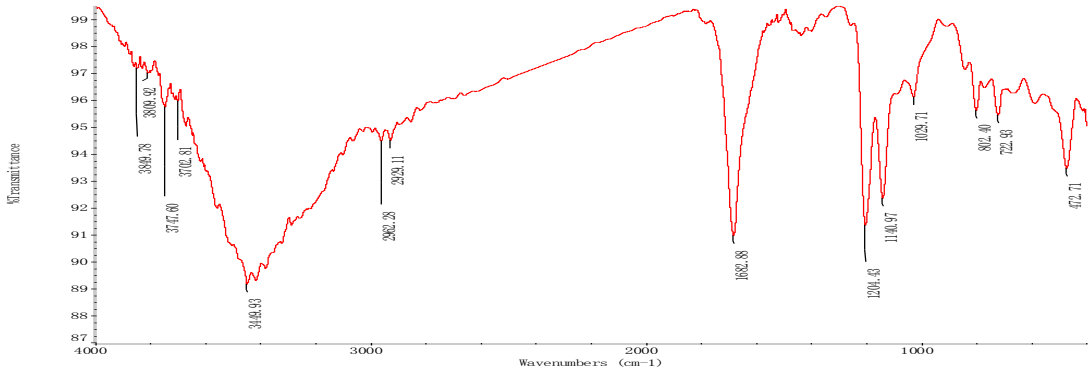



## HRESIMS spectrum of 1



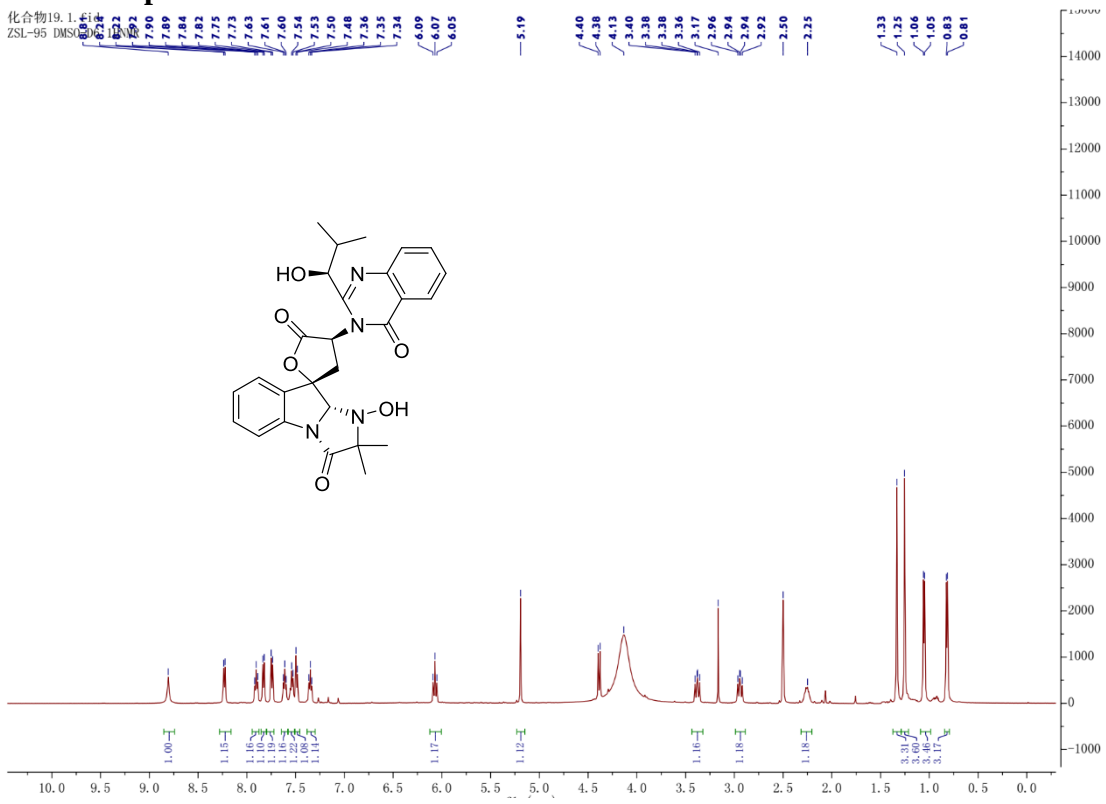

| Meas. m/z | # | Ion Formula | m/z | err [ppm] | Mean err [ppm] | rdb | N-Rule | e⁻ Conf | mSigma | Std I | Std Mean m/z | Std I Var Norm | Std m/z Diff | Std Comb Dev | Adduct |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 589.173103 | 1 | C28H30N4NaO7S | 589.172741 | -0.6 | -1.8 | 16.0 | ok | even | 7.0 | 10.6 | n.a. | n.a. | n.a. | n.a. | M+Na |

## IR spectrum of 1

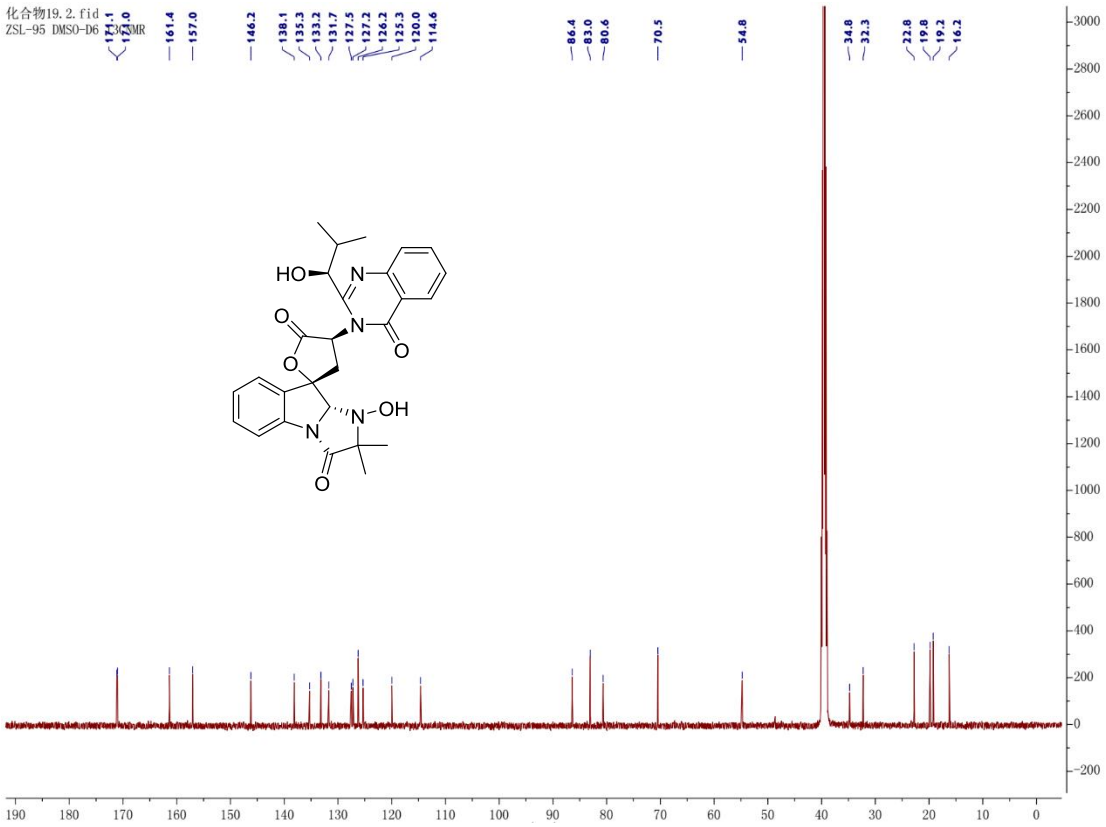


# NMR, HRESIMS, and IR spectra of compound 2

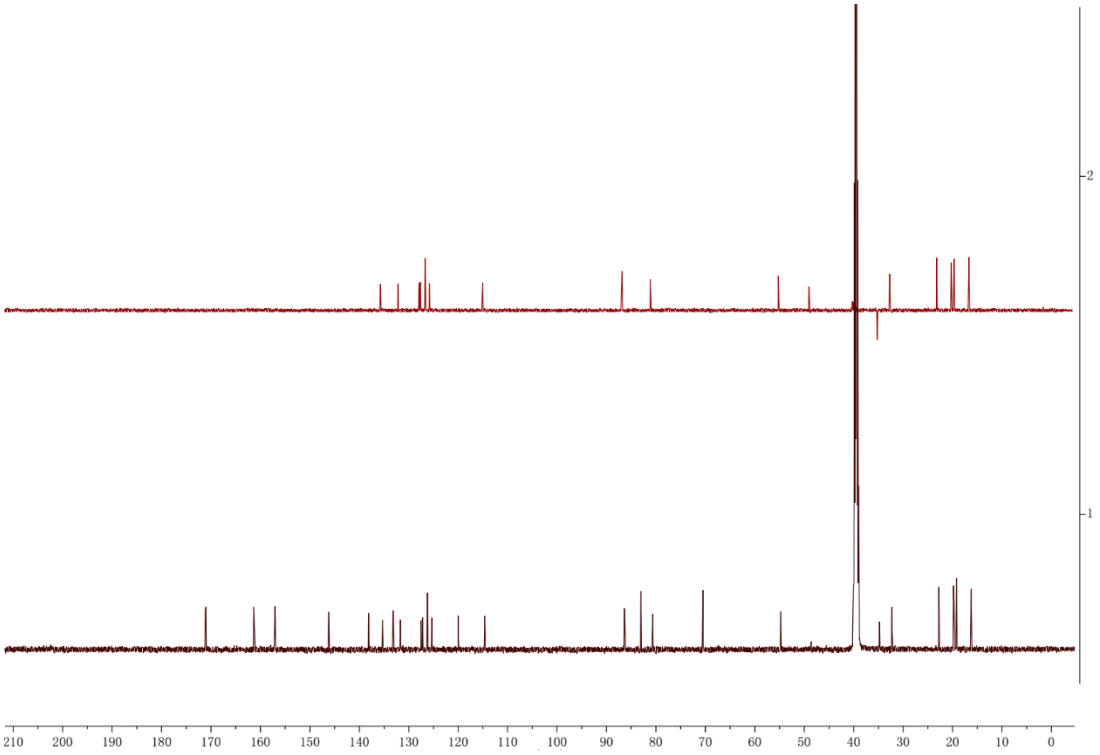
## $^{1}$H-NMR spectrum of 2



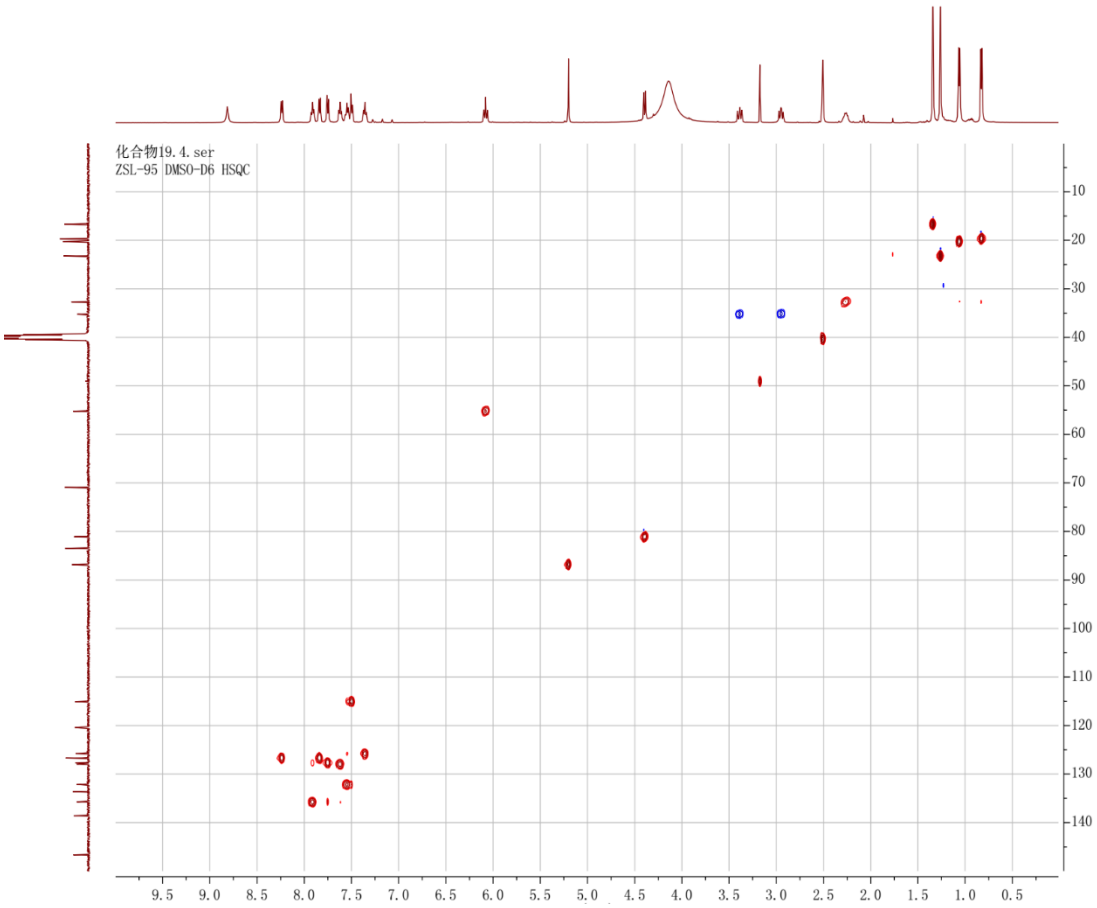

## $^{13}$C-NMR spectrum of 2



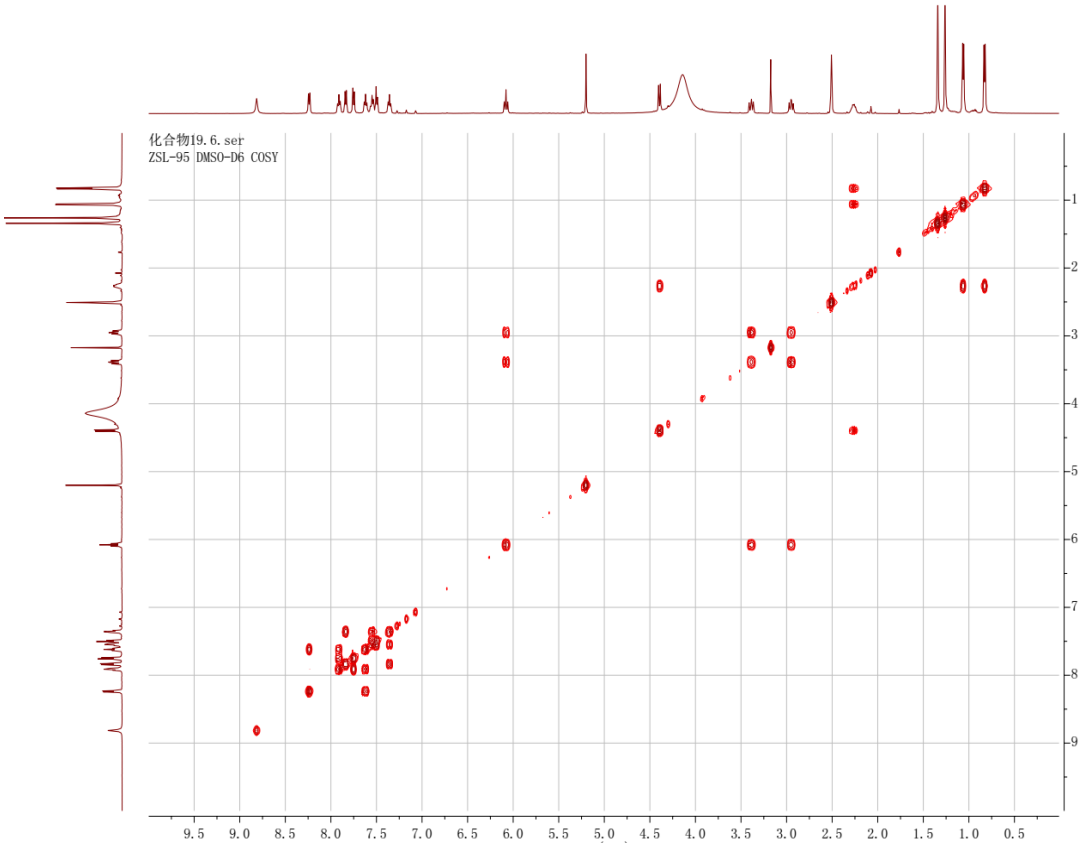
## DEPT spectrum of 2



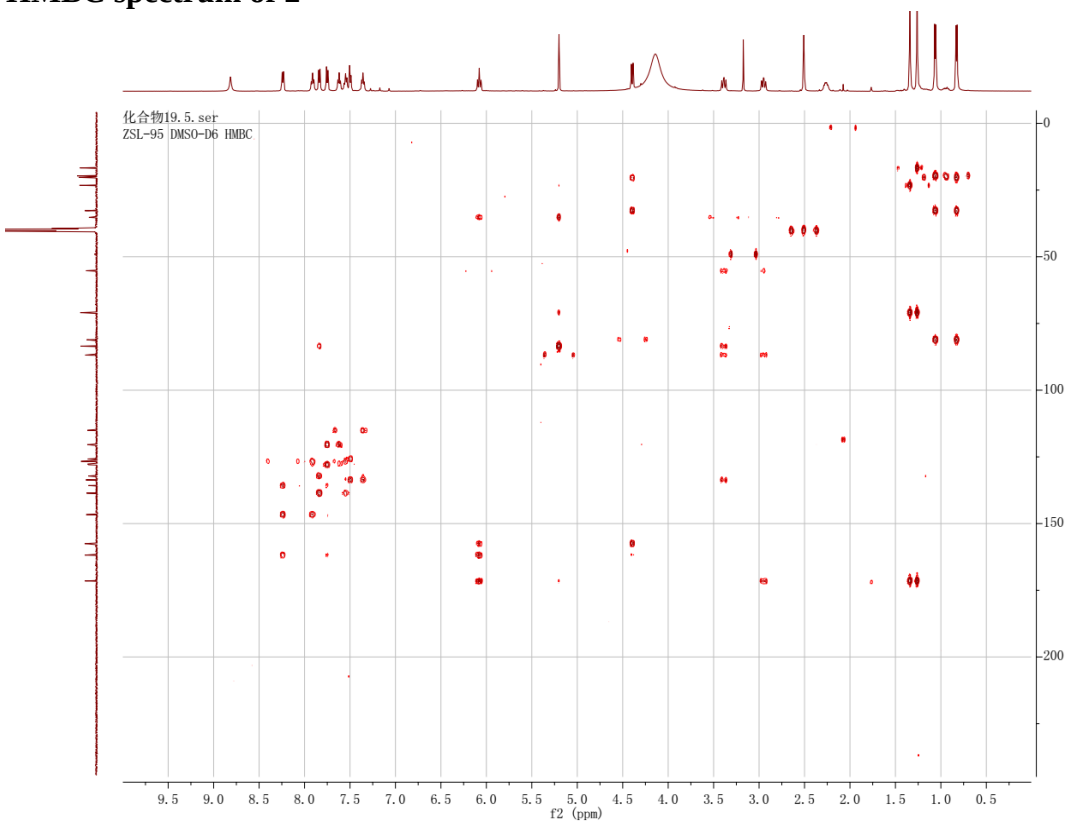

## HSQC spectrum of 2



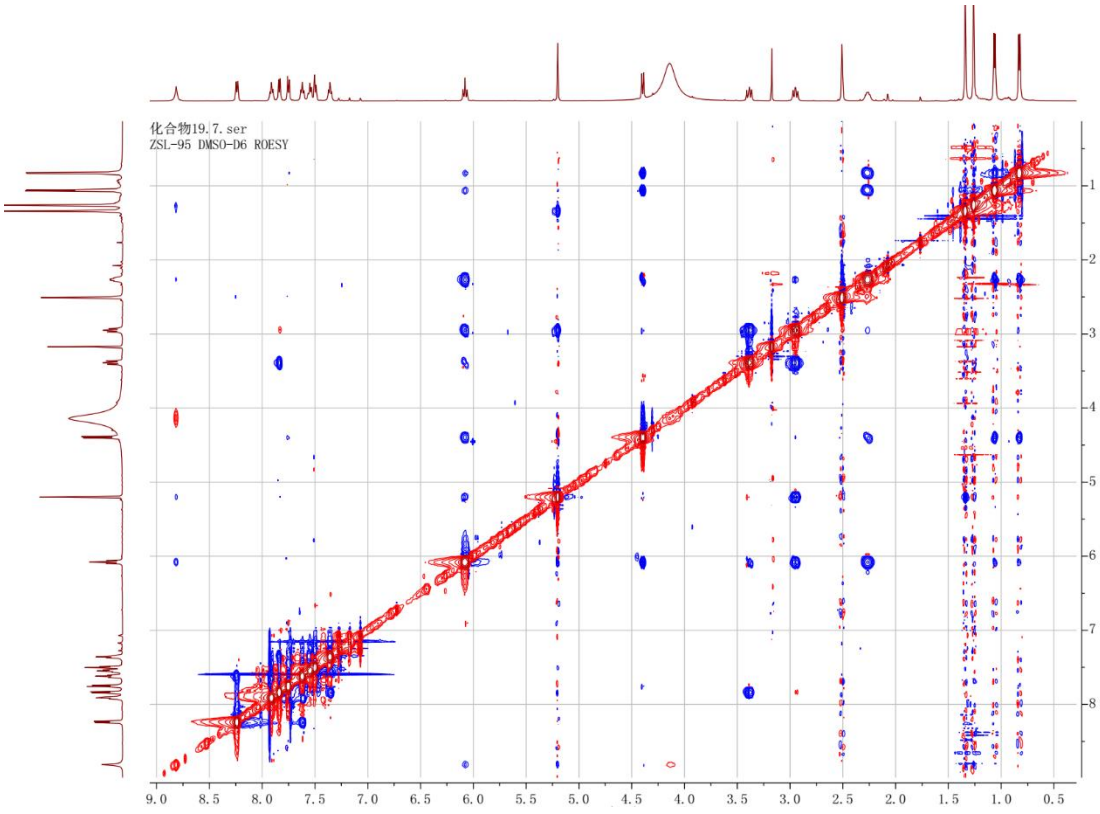
## $^{1}H$-$^{1}H$ COSY spectrum of 2



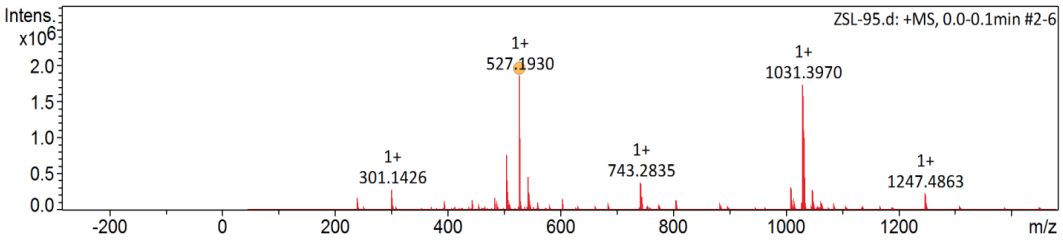

## HMBC spectrum of 2



## ROESY spectrum of 2

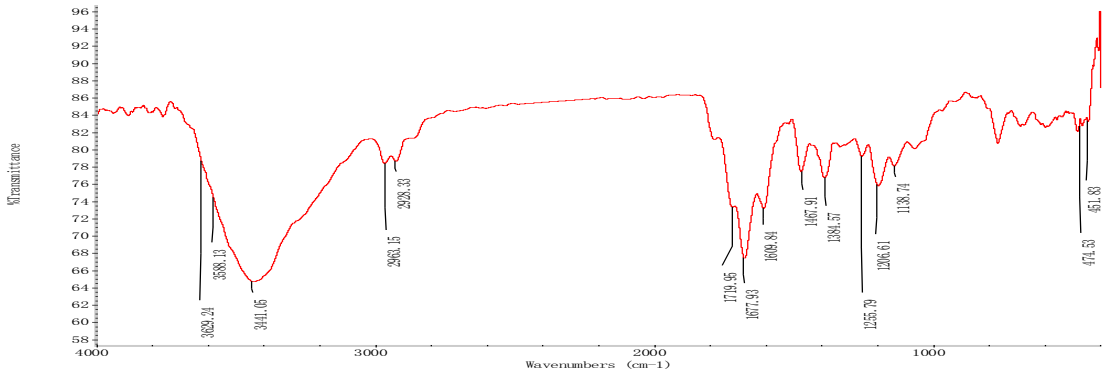



## HRESIMS spectrum of 2



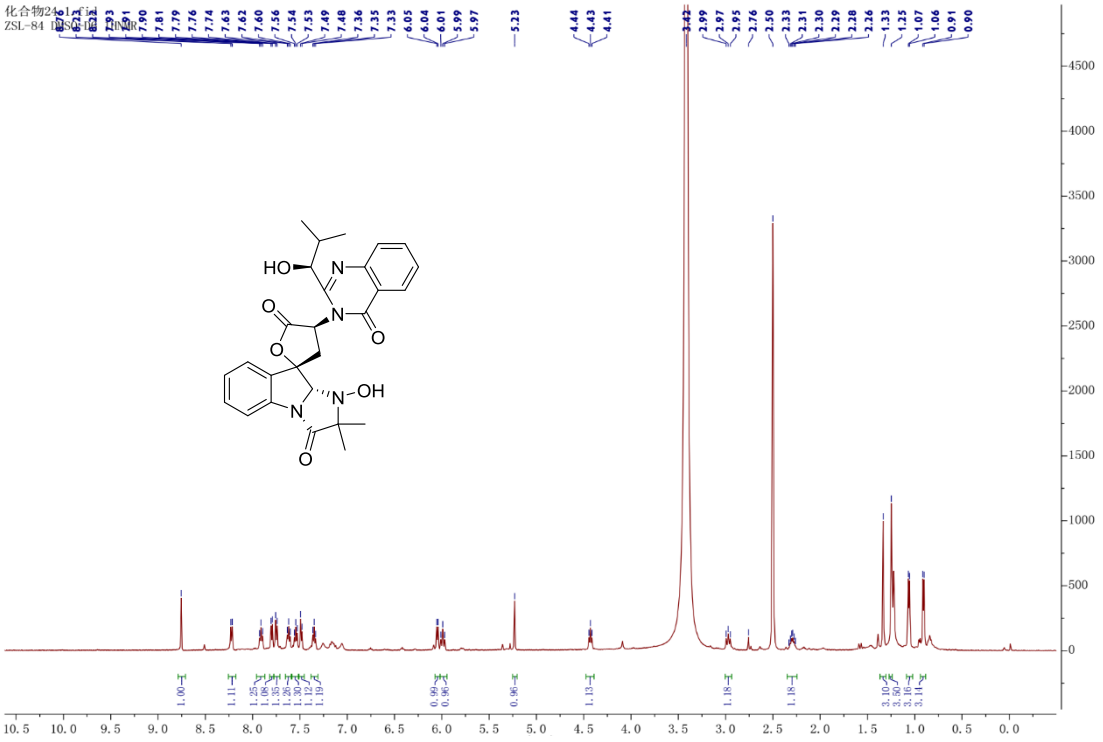

| Meas. m/z | # | Ion Formula | m/z | err [ppm] | Mean err [ppm] | rdb | N-Rule | e¯ Conf | mSigma | Adduct |
|---|---|---|---|---|---|---|---|---|---|---|
| 527.192962 | 1 | C27H28N4NaO6 | 527.190105 | -5.4 | -6.2 | 16.0 | ok | even | 6.3 | M+Na |

## IR spectrum of 2

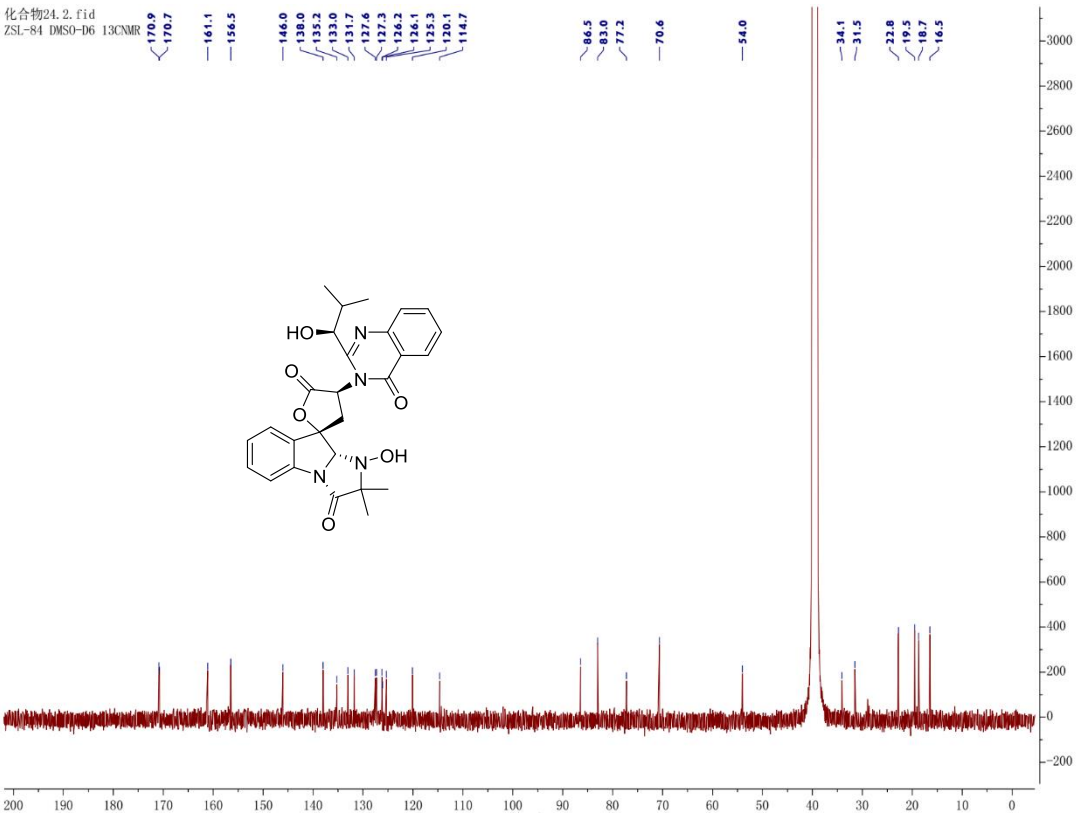


# NMR, HRESIMS, and IR spectra of compound 3

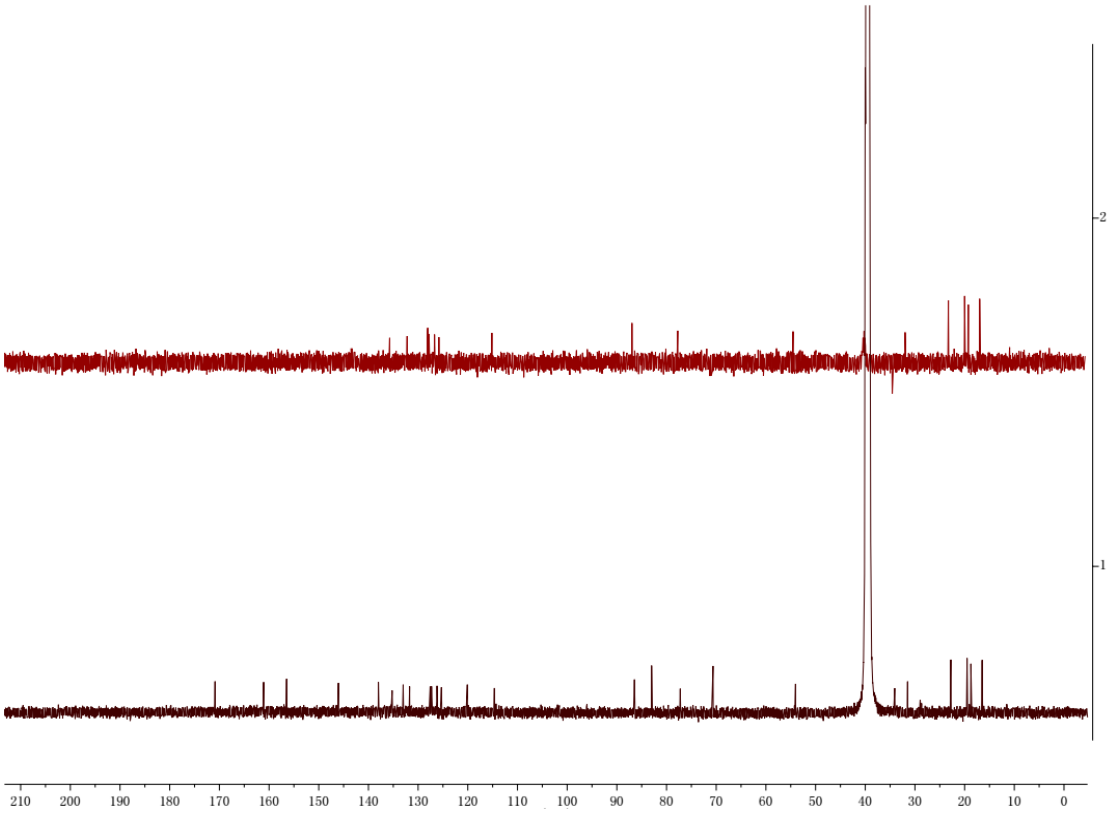
## $^{1}$H-NMR spectrum of 3



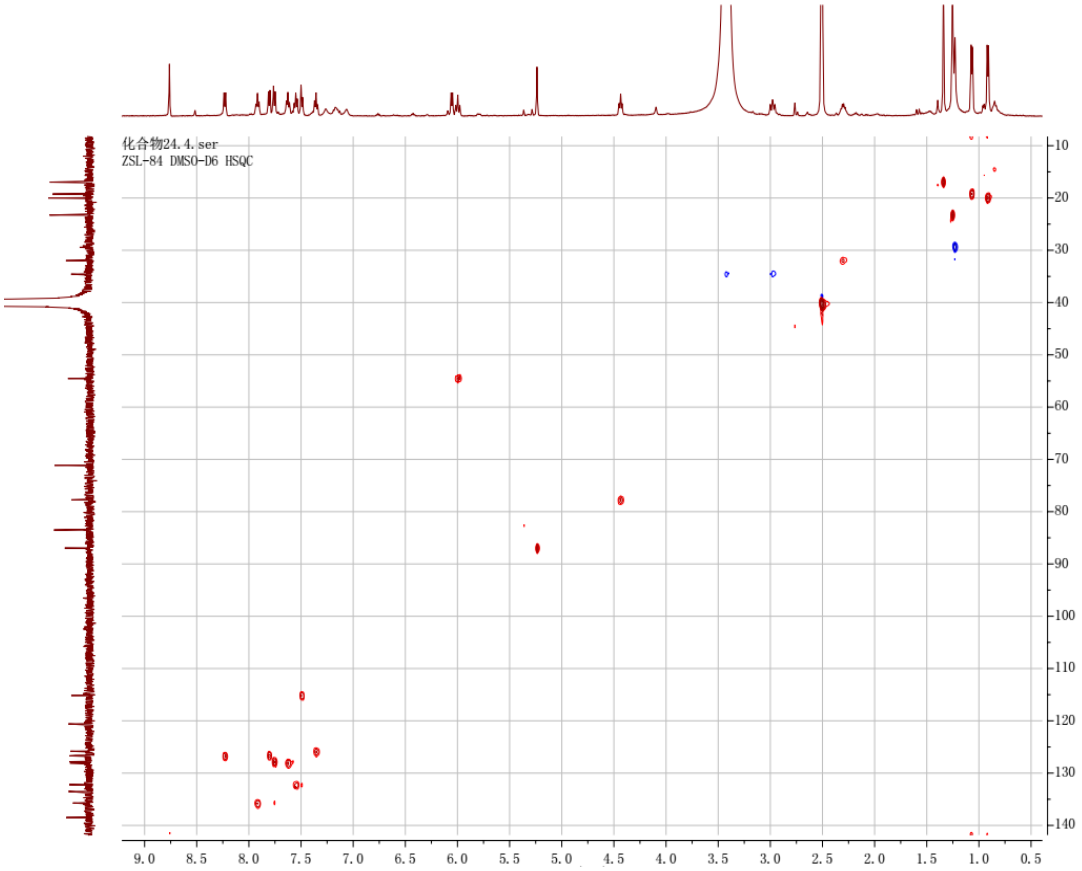

## $^{13}$C-NMR spectrum of 3



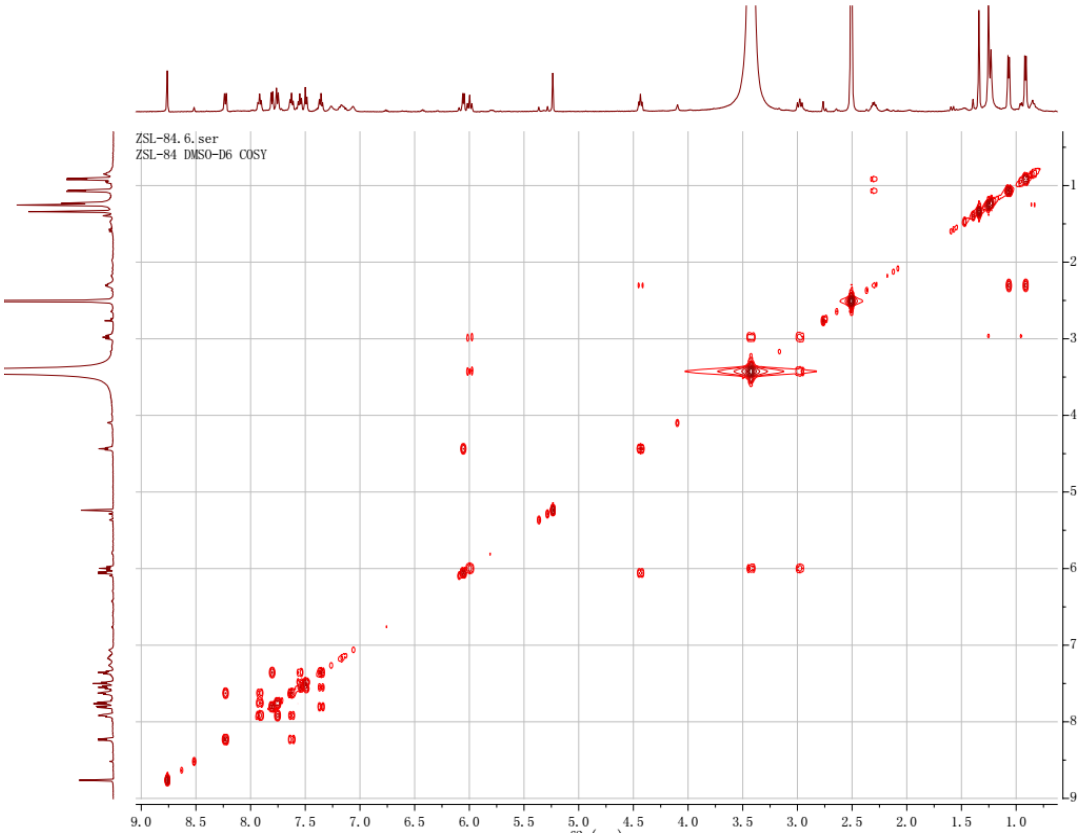
## DEPT spectrum of 3



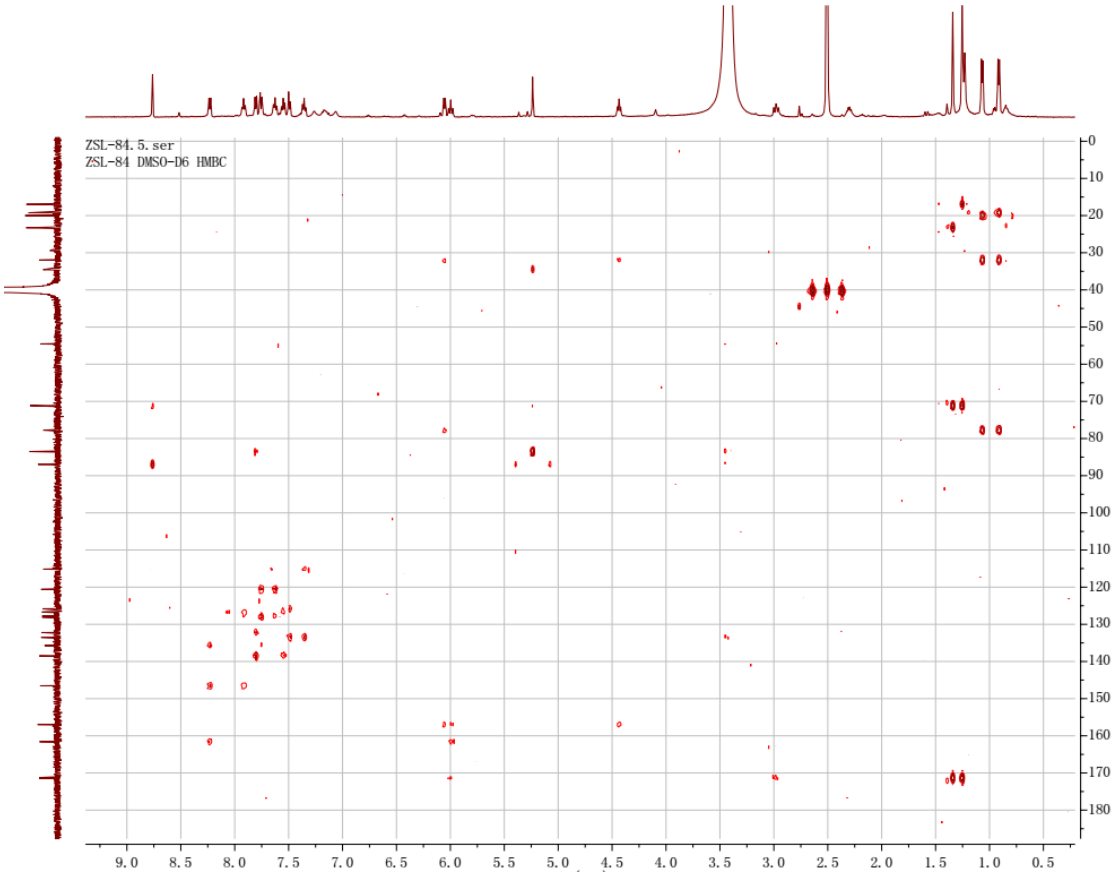

## HSQC spectrum of 3



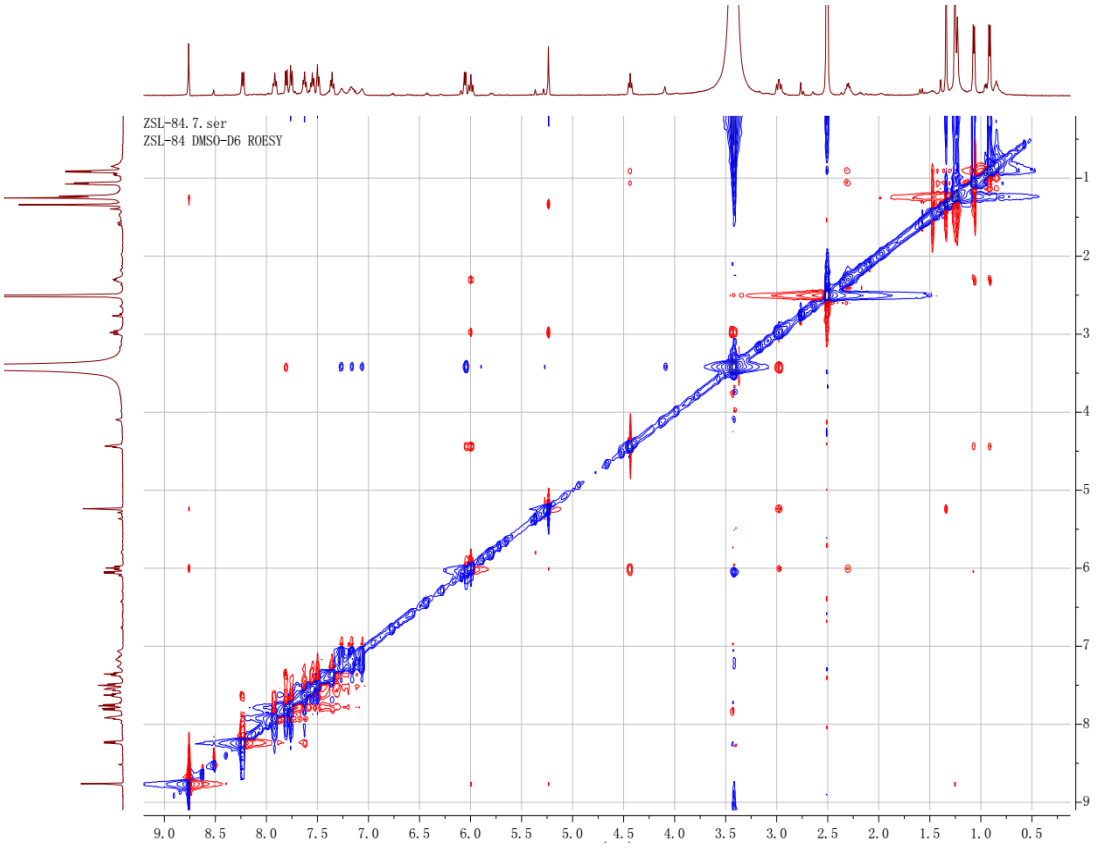
**$^{1}$H-$^{1}$H COSY spectrum of 3**



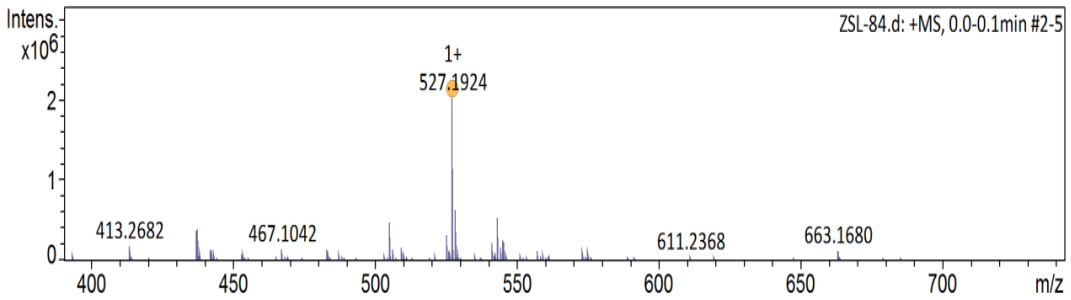

**HMBC spectrum of 3**



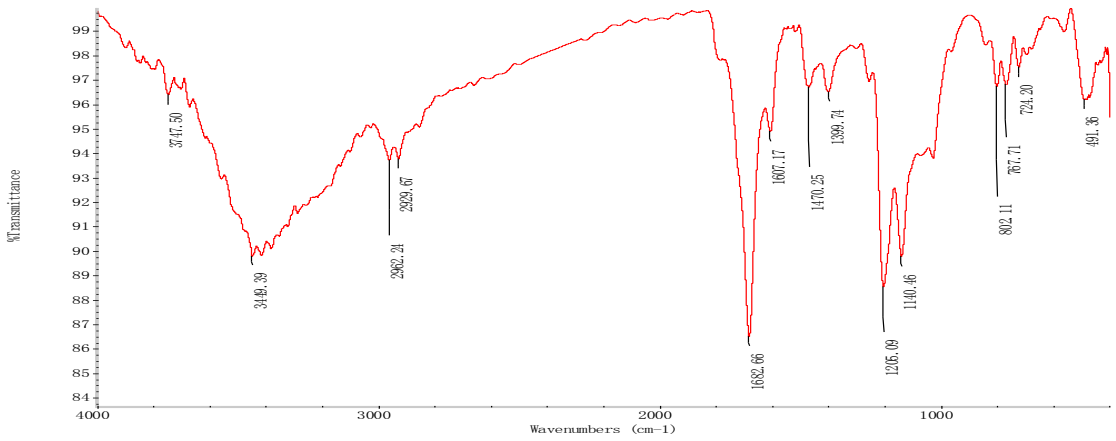
## ROESY spectrum of 3




## HRESIMS spectrum of 3

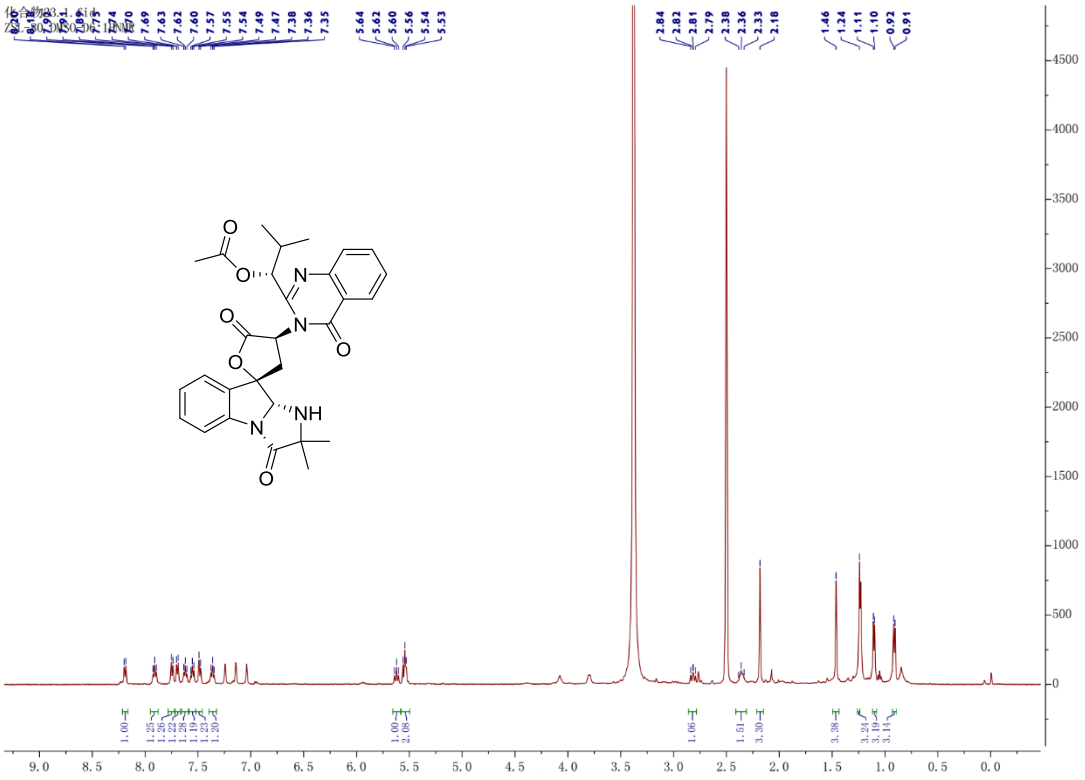



## IR spectrum of 3

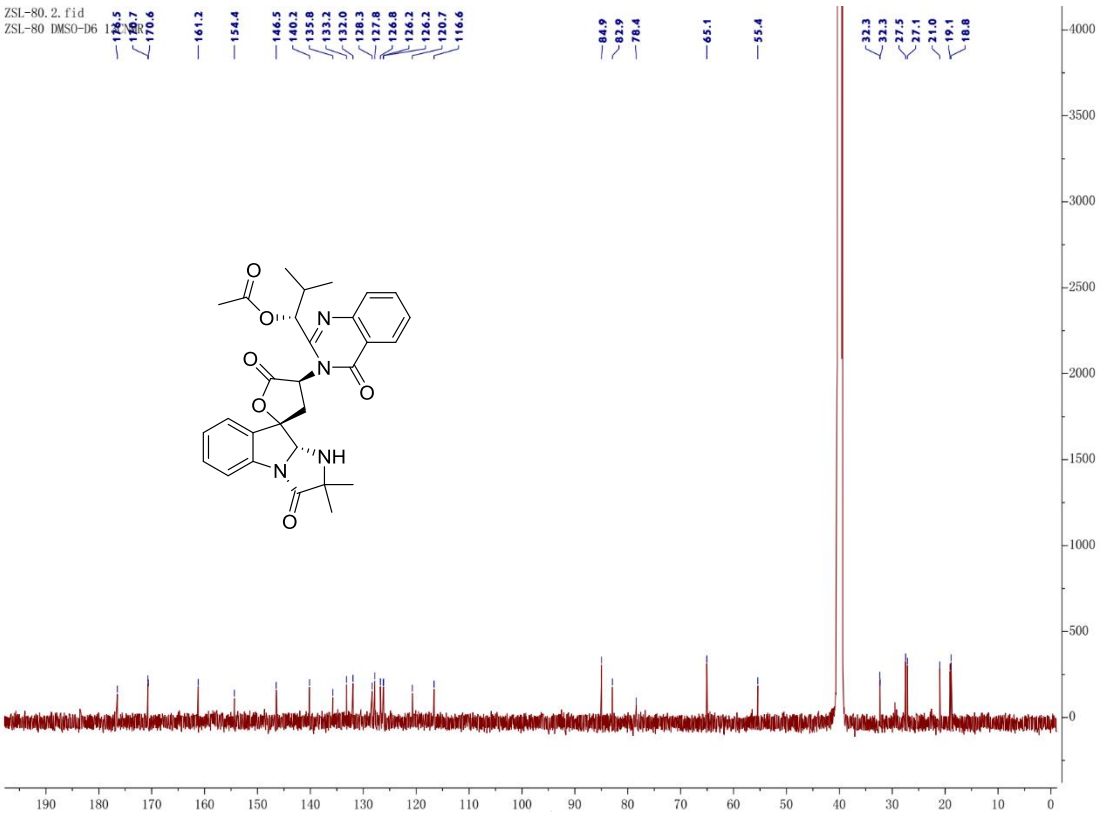


# NMR, HRESIMS, and IR spectra of compound 4

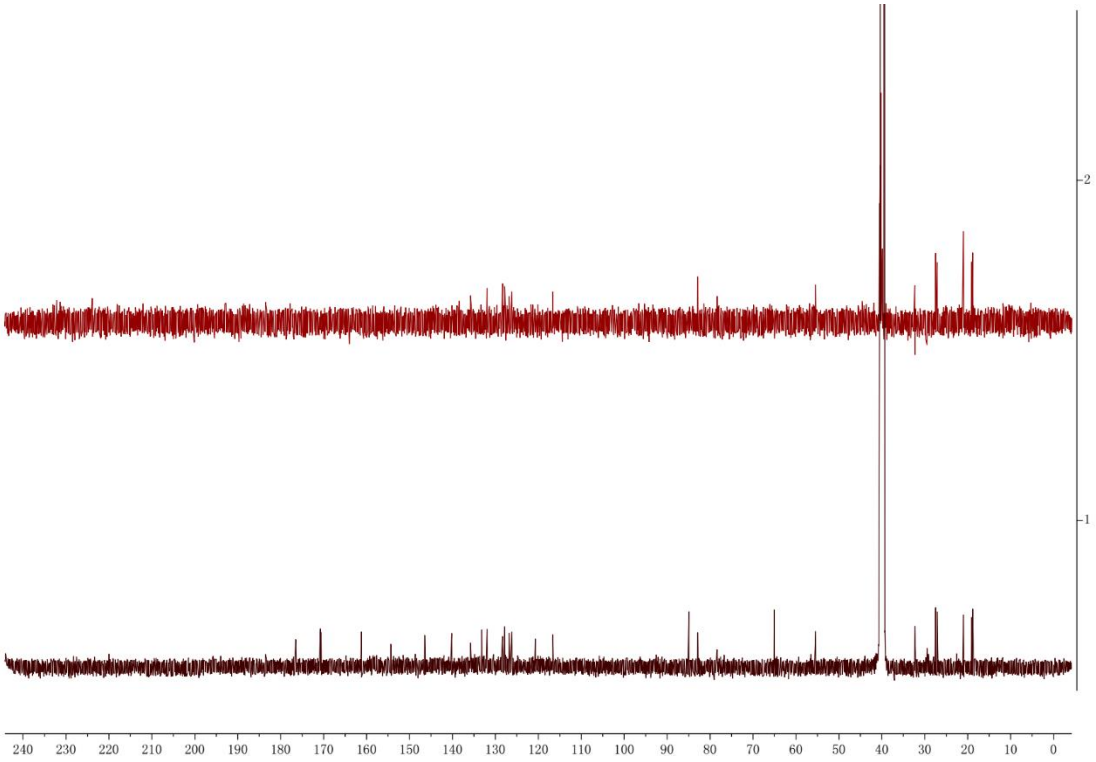
## $^{1}$H-NMR spectrum of 4



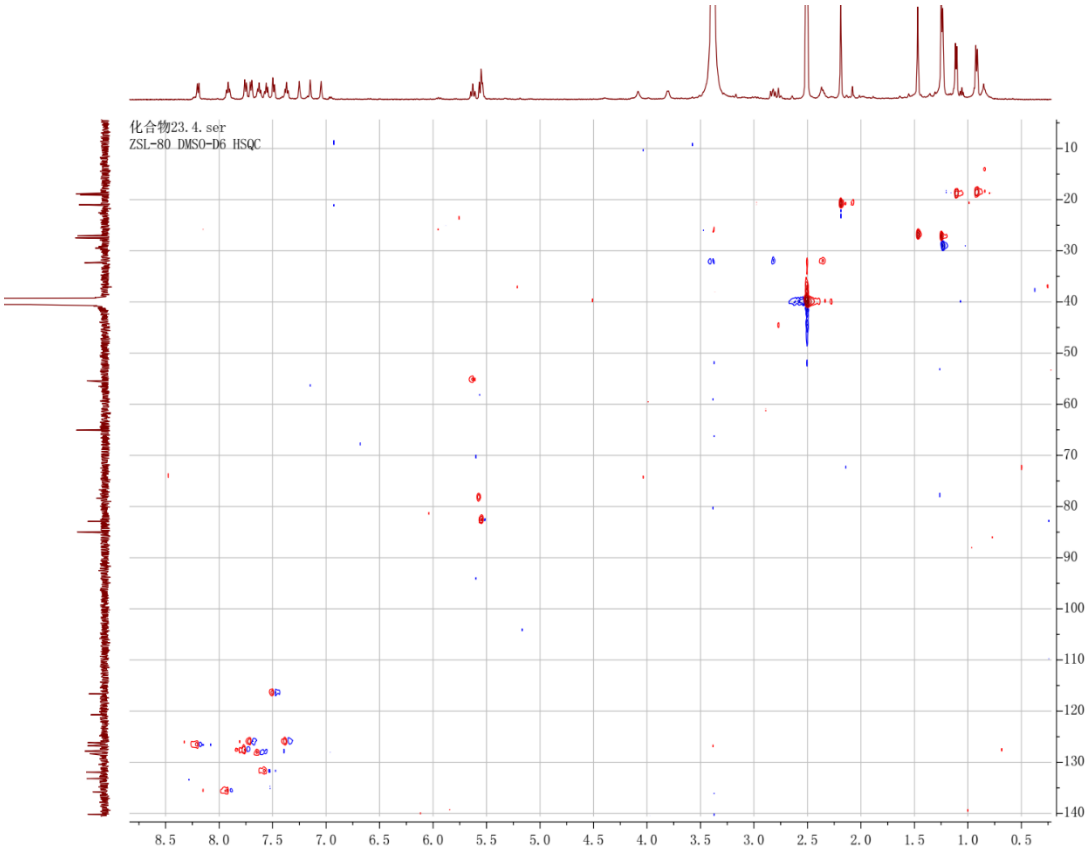

## $^{13}$C-NMR spectrum of 4



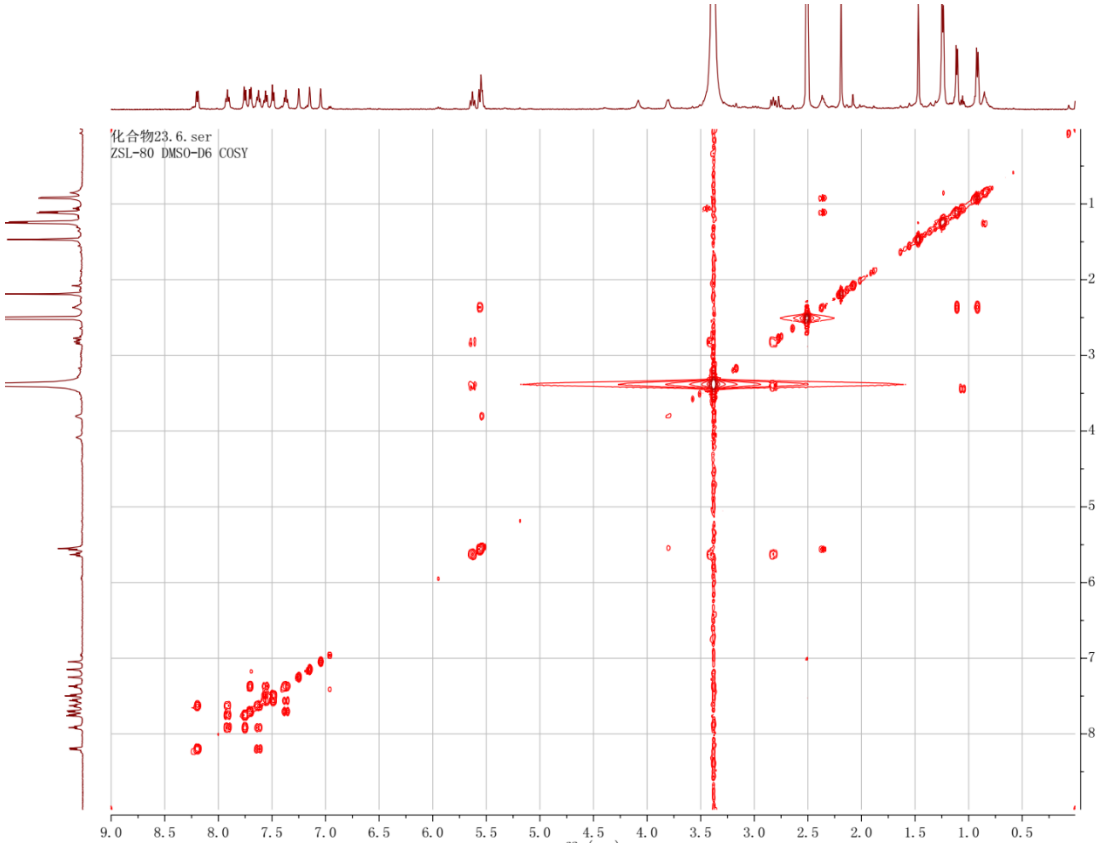
## DEPT spectrum of 4



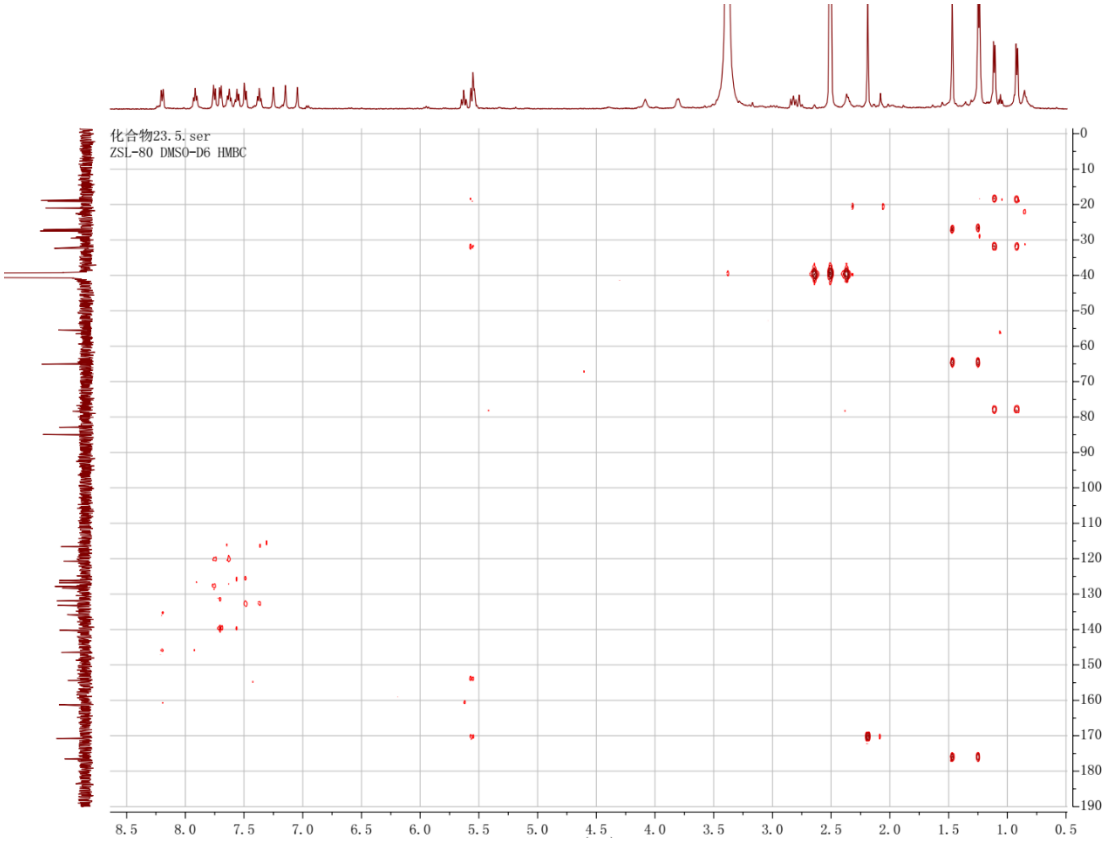

## HSQC spectrum of 4



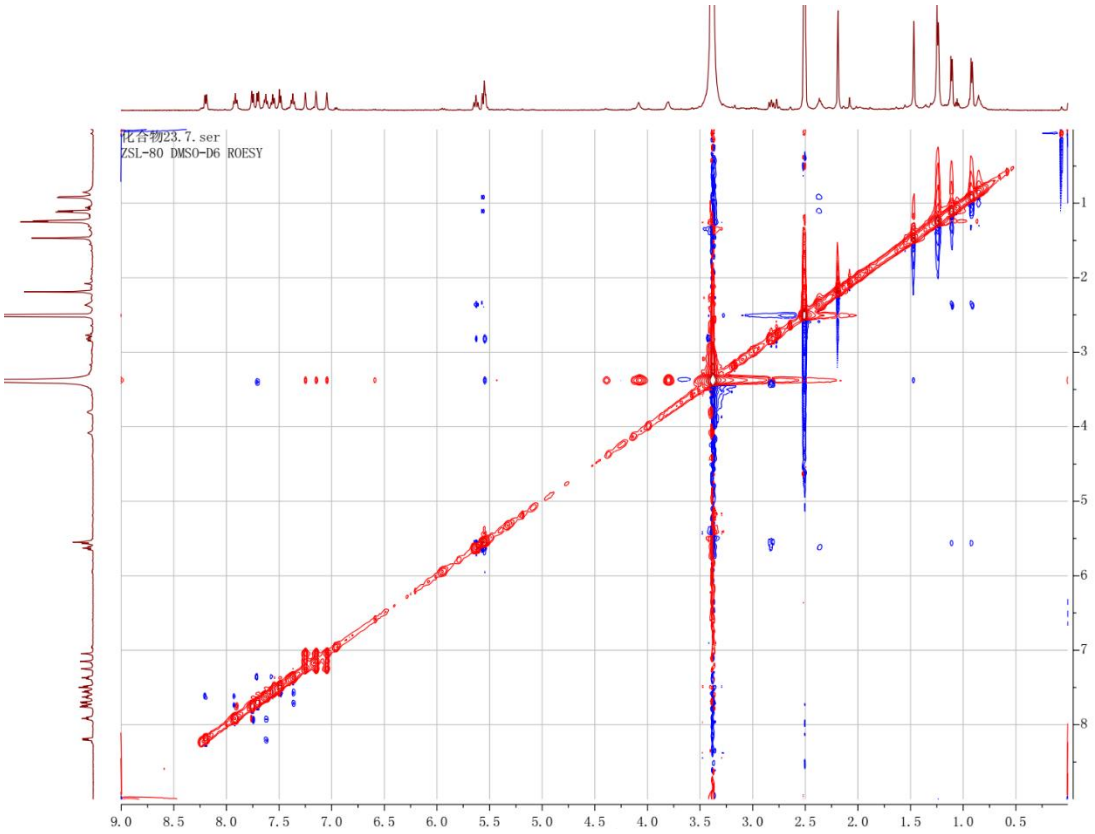
## $^{1}H$-$^{1}H$ COSY spectrum of 4



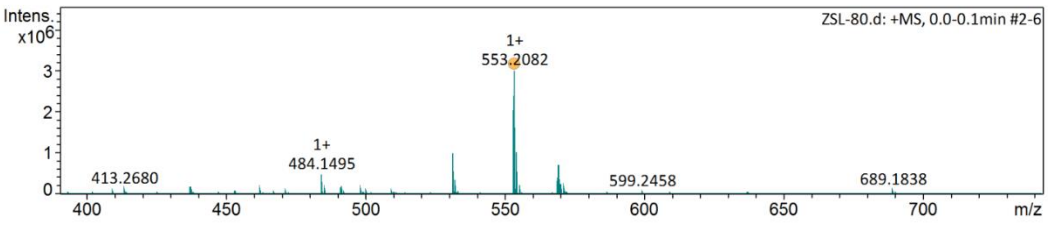

## HMBC spectrum of 4



## ROESY spectrum of 4

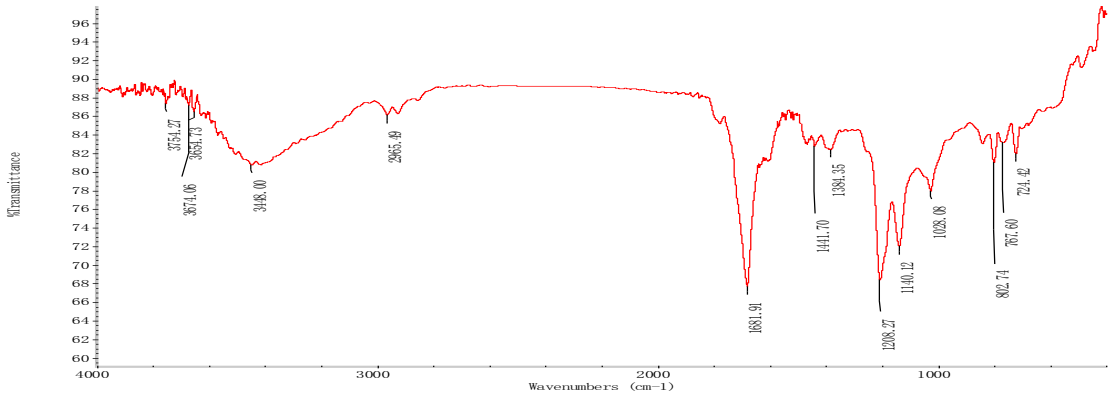



## HRESIMS spectrum of 4



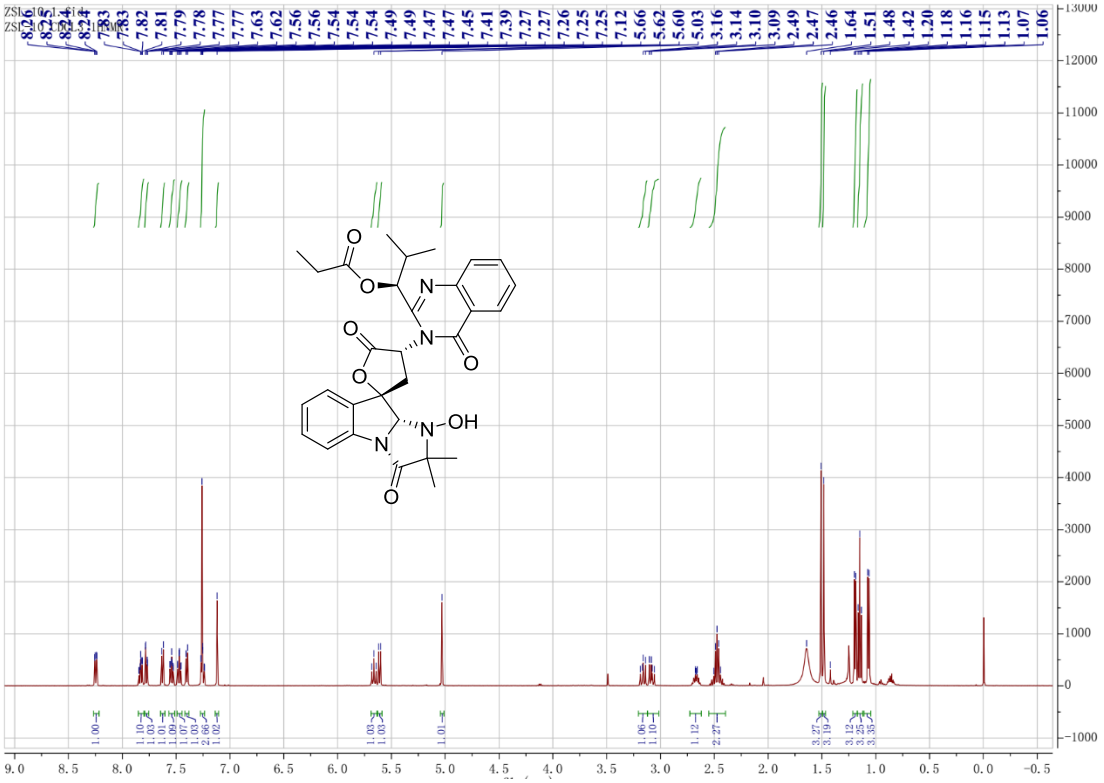

| Meas. m/z | # | Ion Formula | m/z | err [ppm] | Mean err [ppm] | rdb | N-Rule | e⁻ Conf | mSigma | Adduct |
|---|---|---|---|---|---|---|---|---|---|---|
| 553.208202 | 1 | C29H30N4NaO6 | 553.205755 | -4.4 | -4.0 | 17.0 | ok | even | 2.3 | M+Na |

## IR spectrum of 4

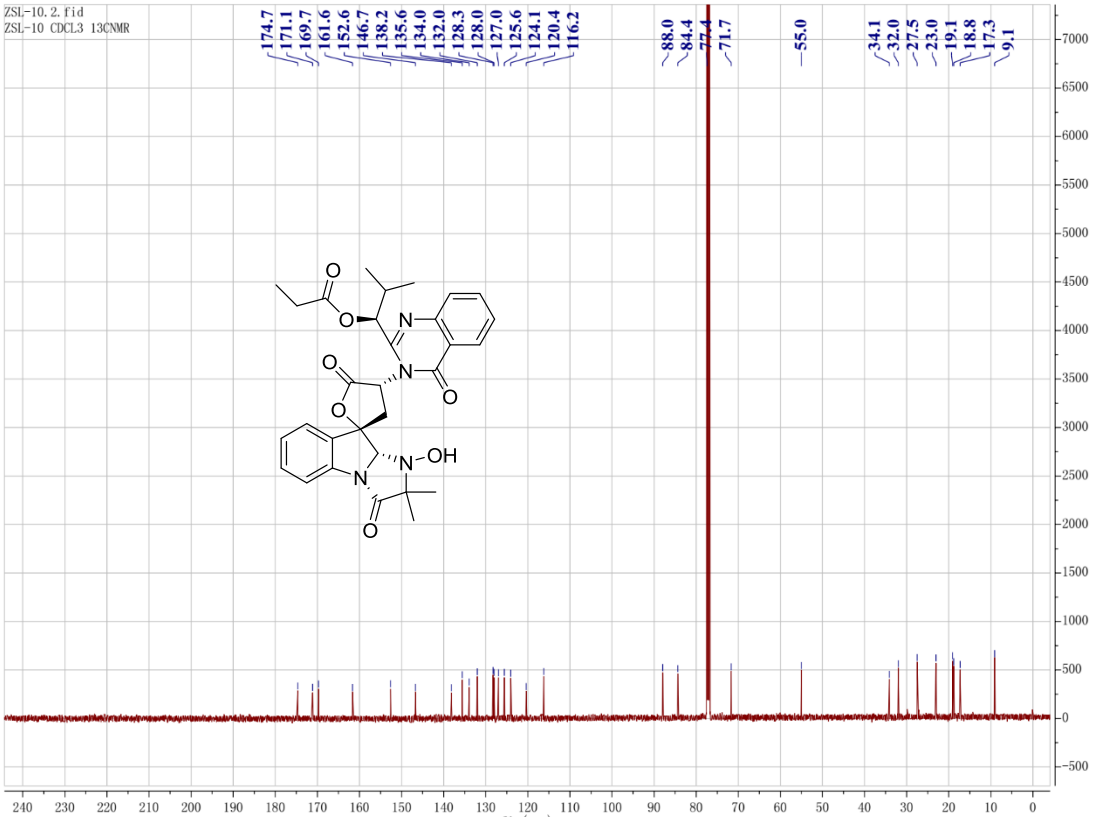


# NMR, HRESIMS, and IR spectra of compound 5

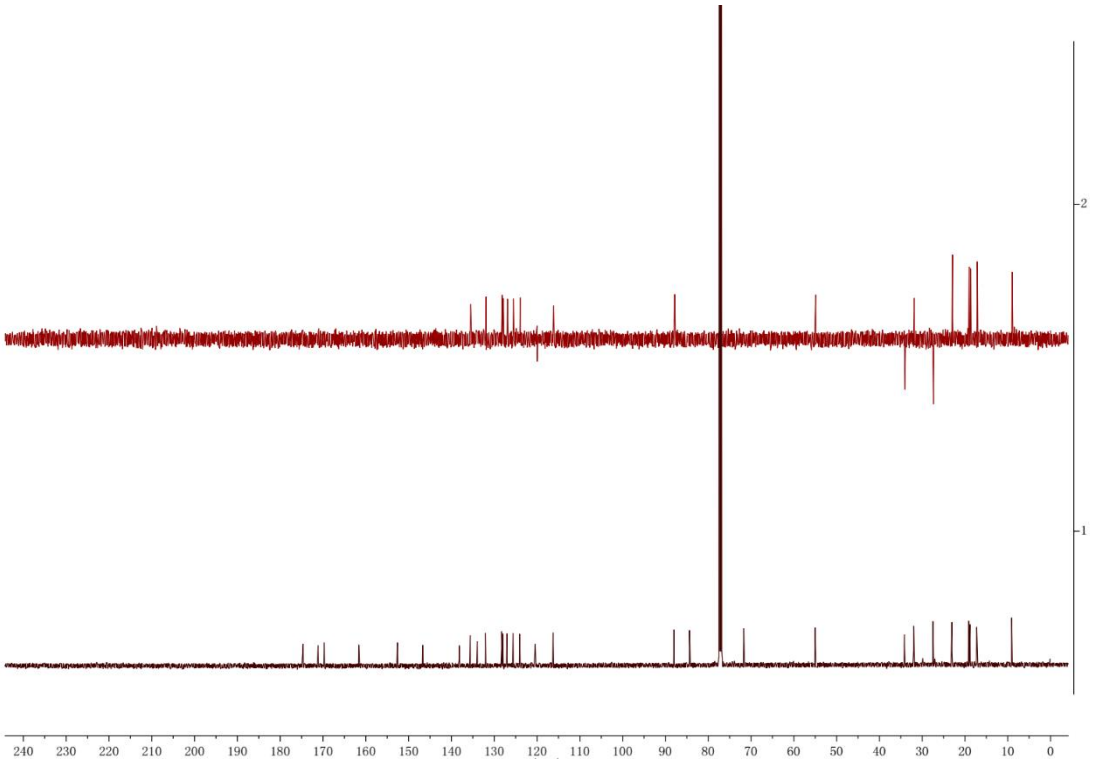
## $^{1}$H-NMR spectrum of 5



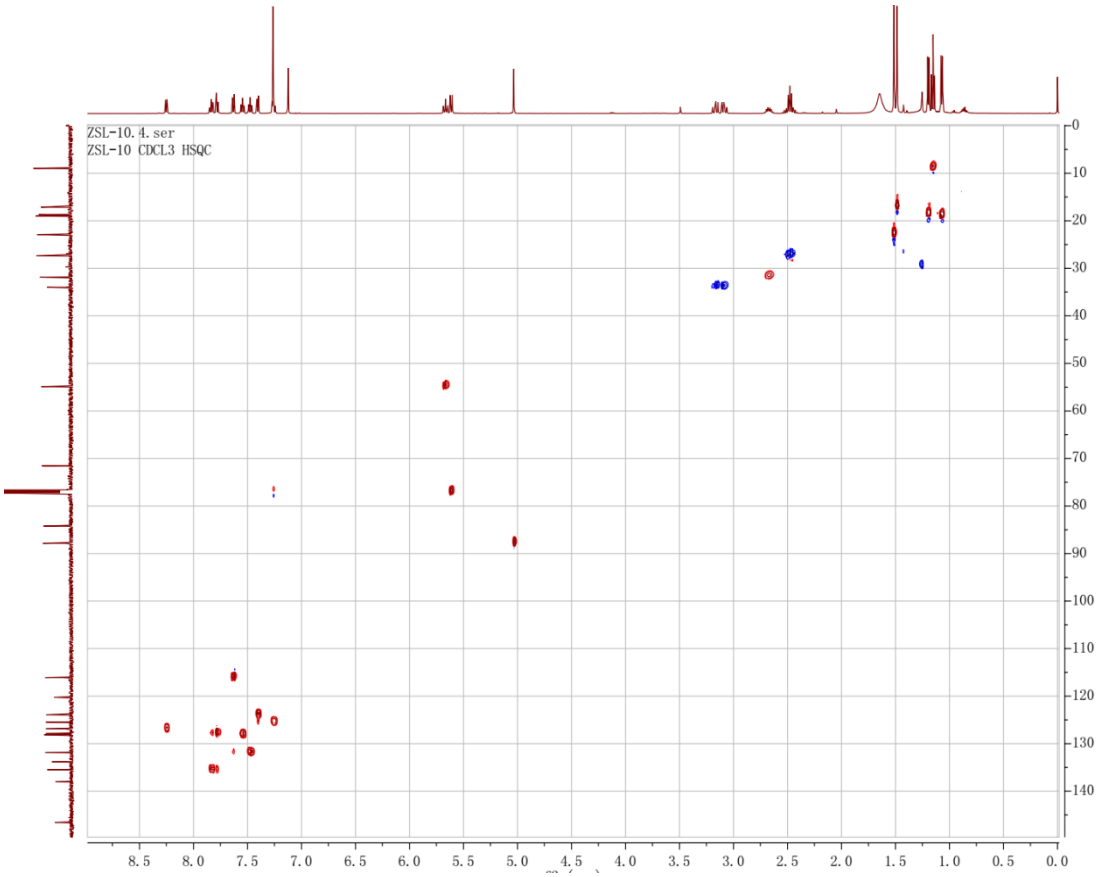
## $^{13}$C-NMR spectrum of 5



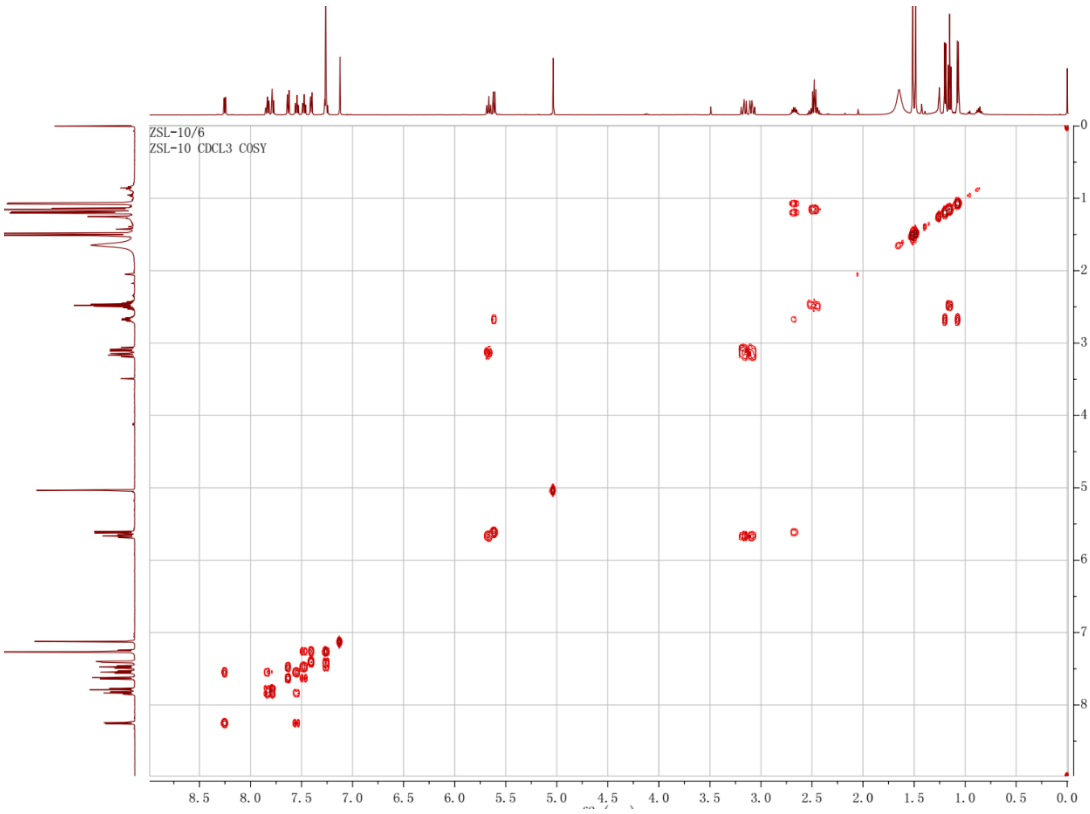
## DEPT spectrum of 5



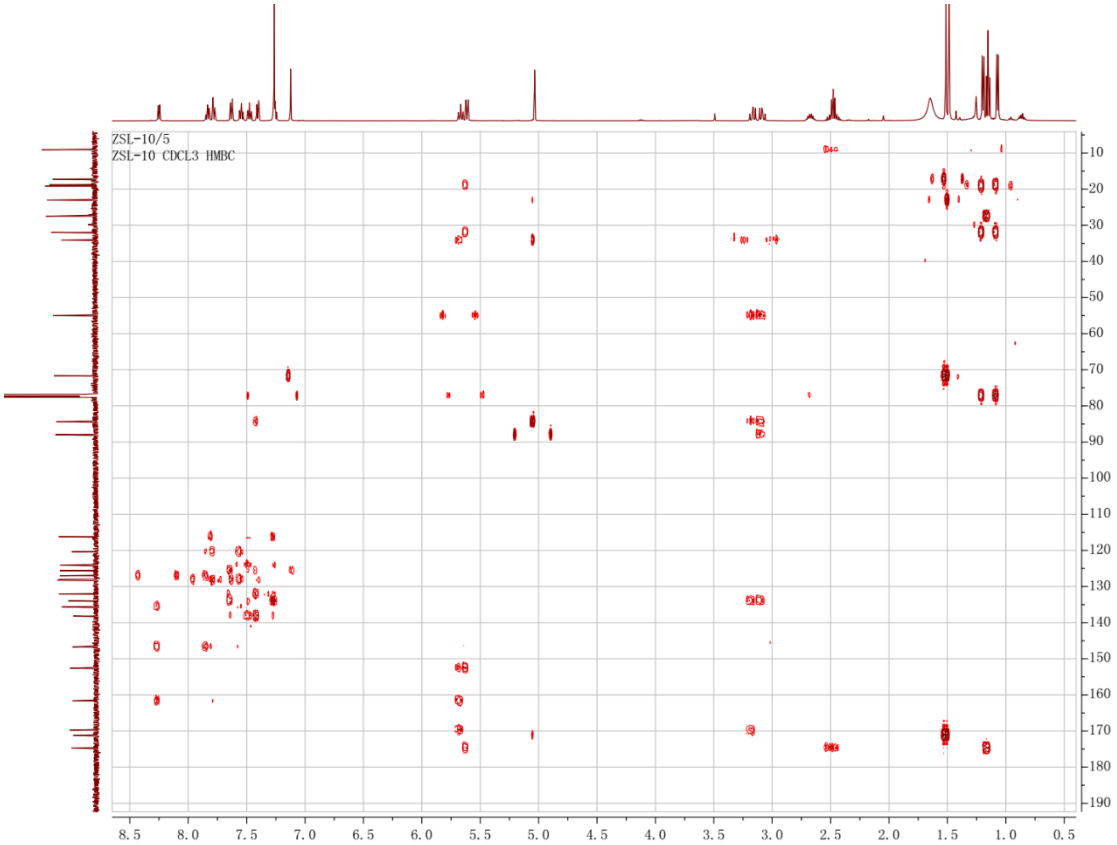

## HSQC spectrum of 5



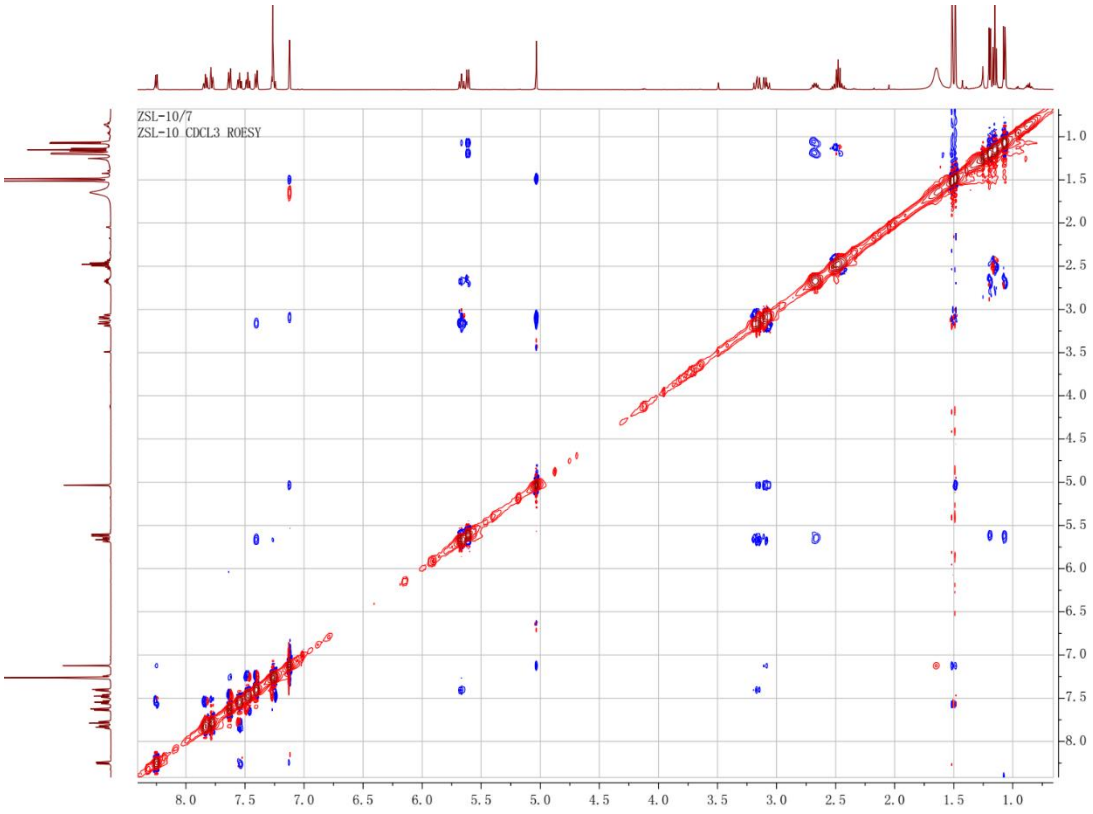
## $^{1}H$-$^{1}H$ COSY spectrum of 5



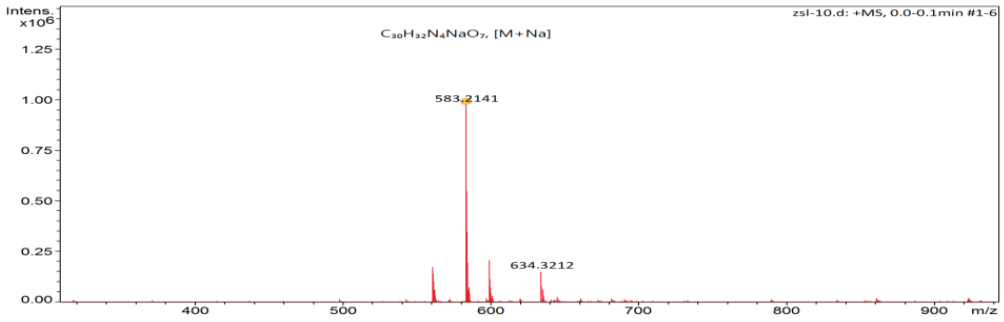

## HMBC spectrum of 5



## ROESY spectrum of 5

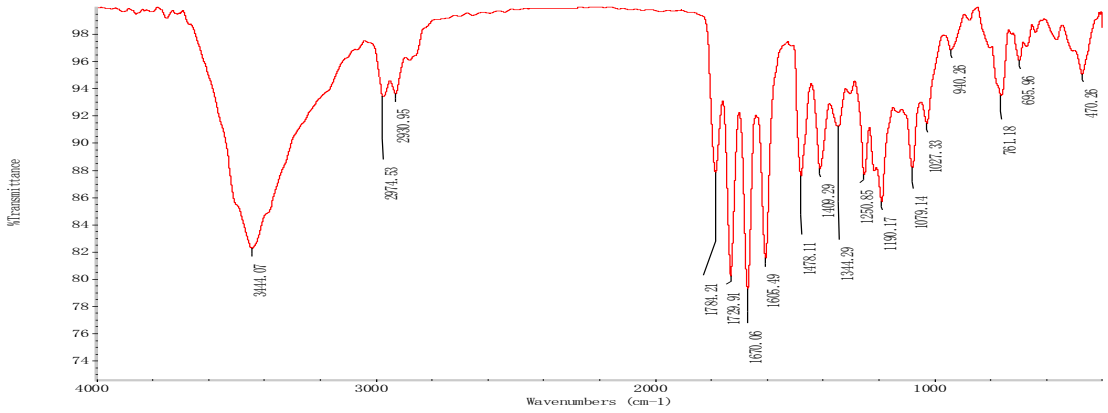



## HRESIMS spectrum of 5



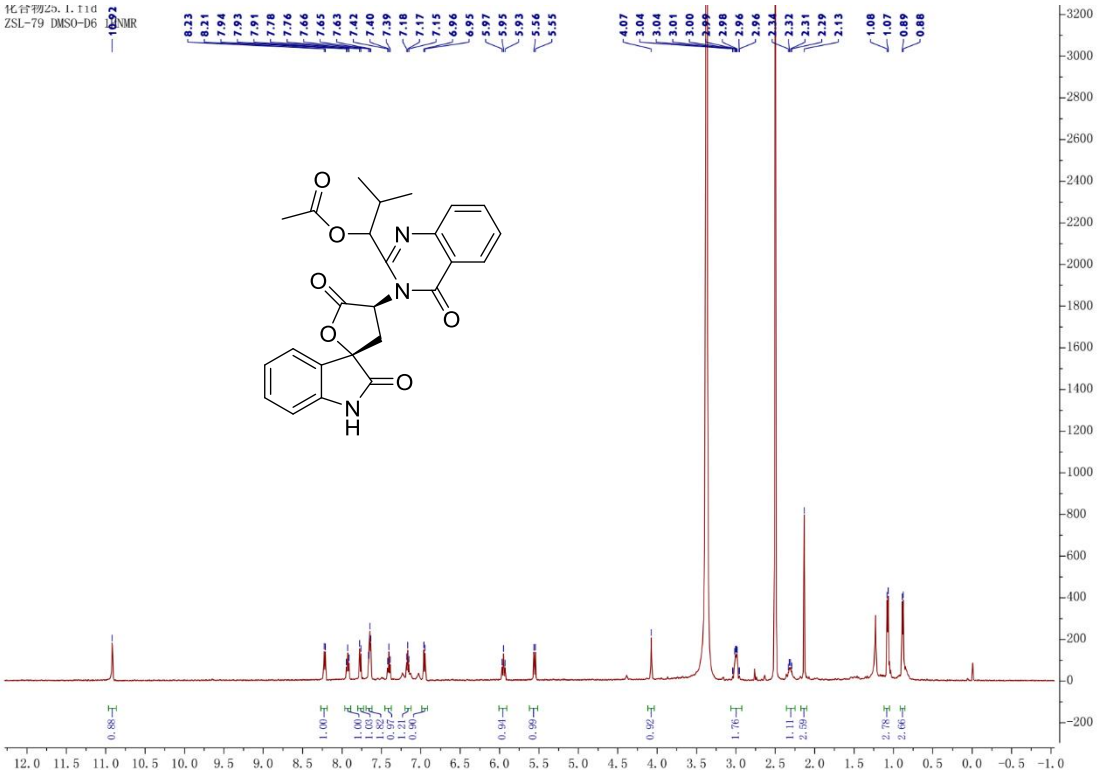

| Sum Formula | Ion Formula | Meas. m/z | m/z | err [mDa] | err [ppm] |
|---|---|---|---|---|---|
| C30H32N4O7 | C30H32N4NaO7 | 583.2141 | 583.2163 | 2.2 | 3.9 |

## IR spectrum of 5

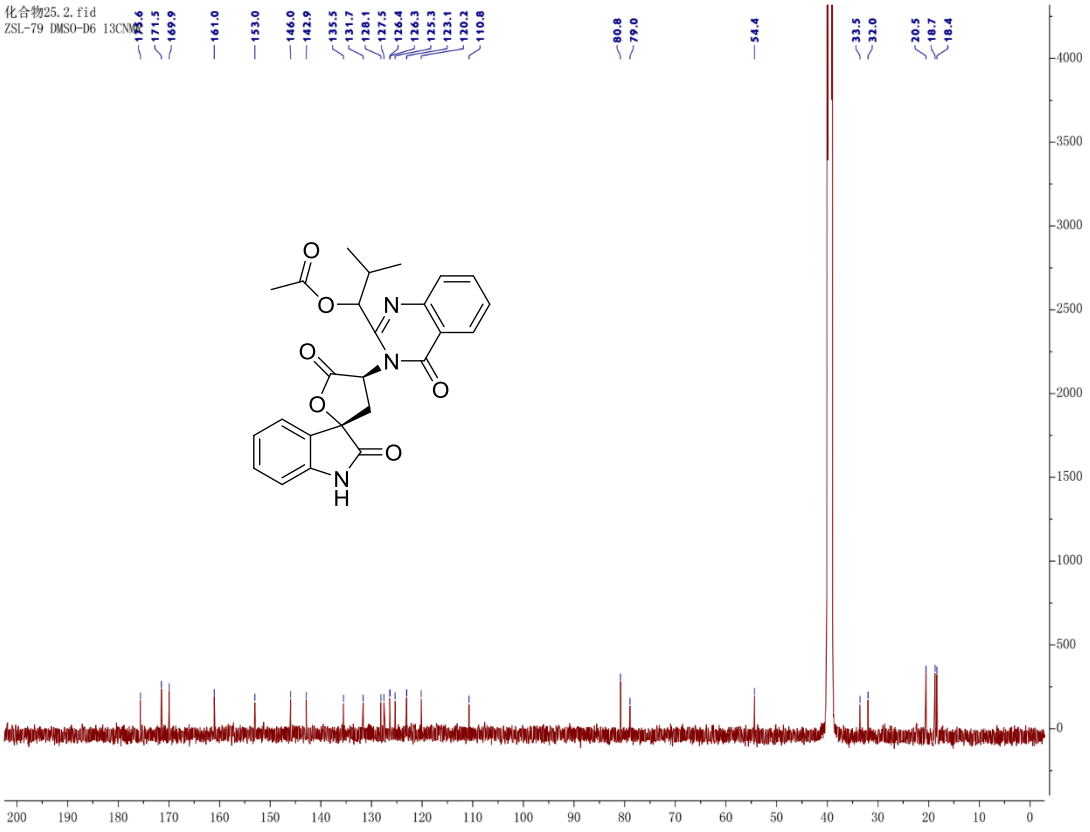


# NMR, HRESIMS, and IR spectra of compound 6

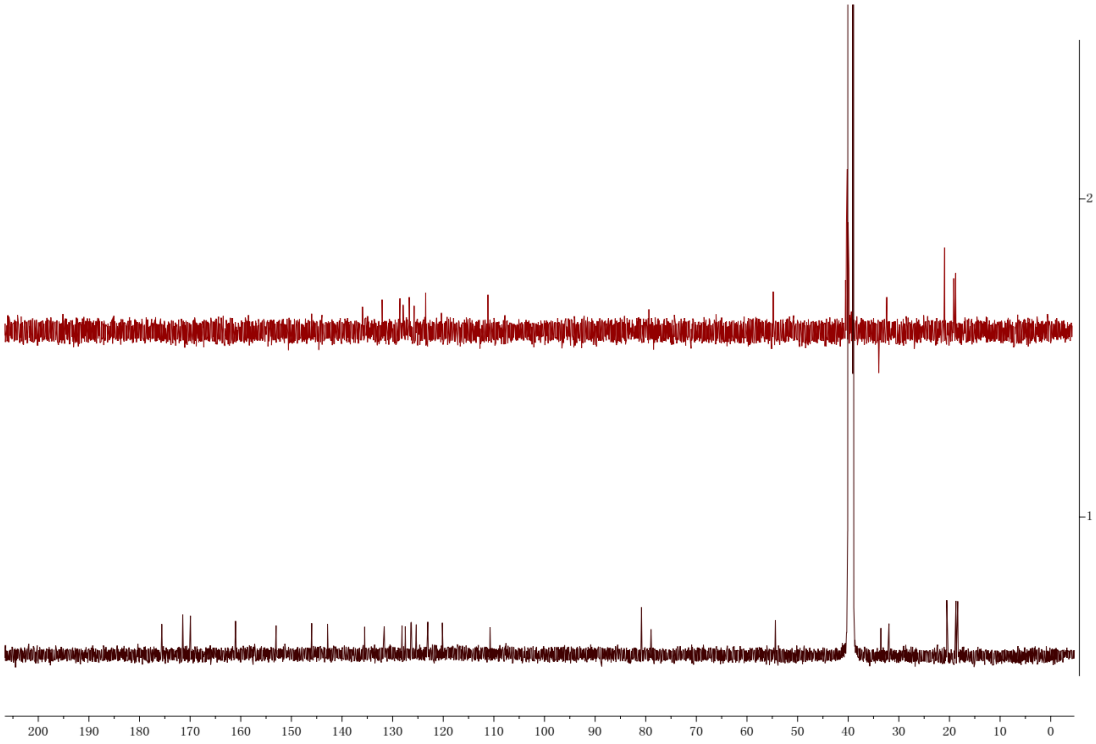
## $^{1}$H-NMR spectrum of 6



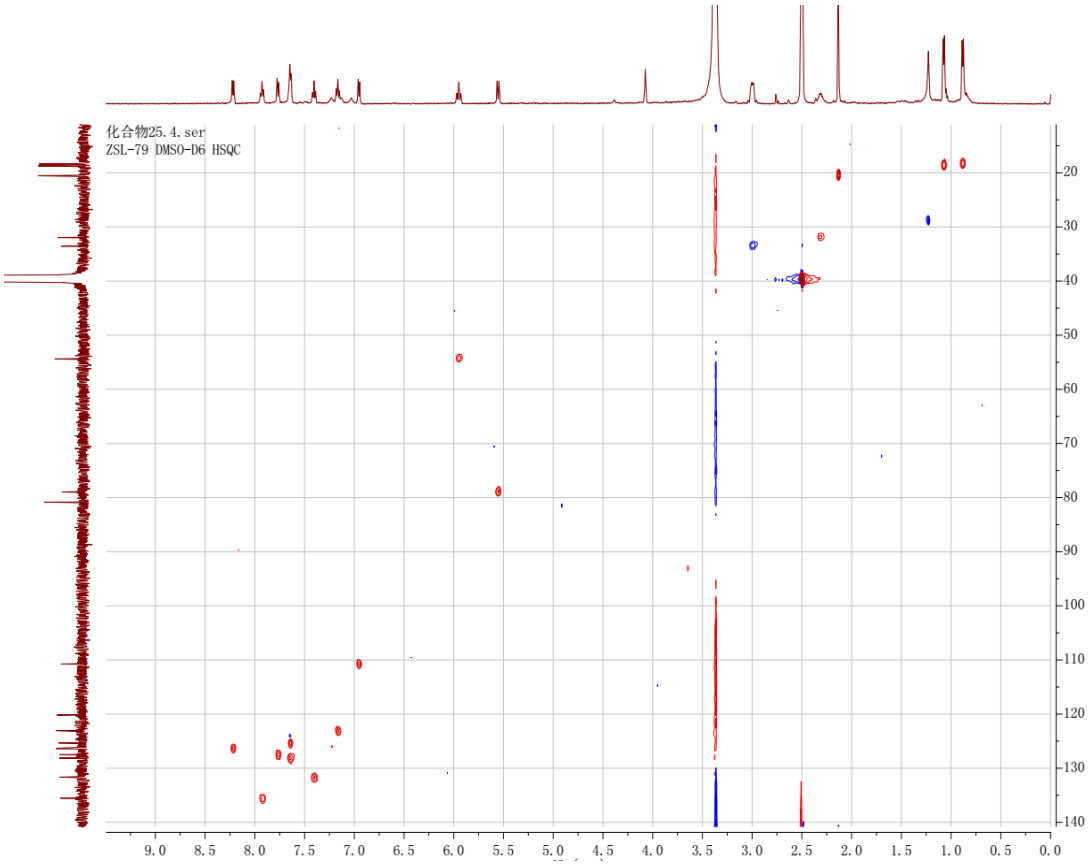

## $^{13}$C-NMR spectrum of 6



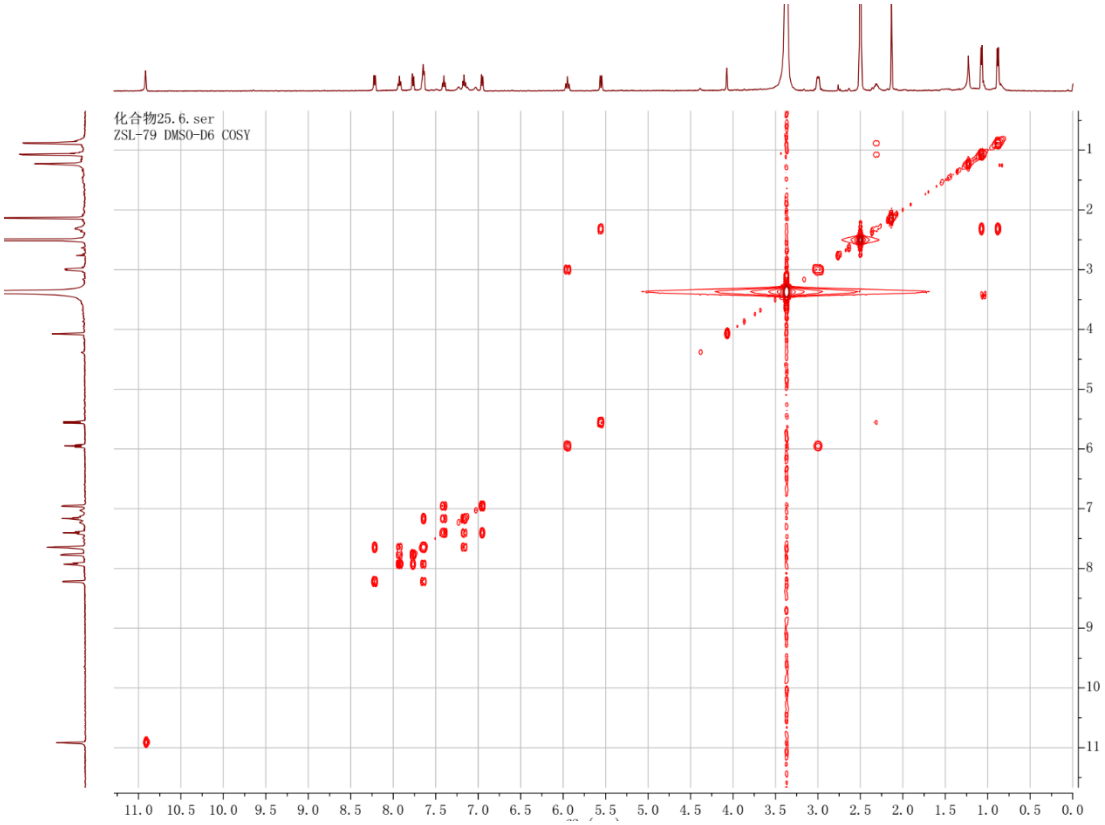
## DEPT spectrum of 6



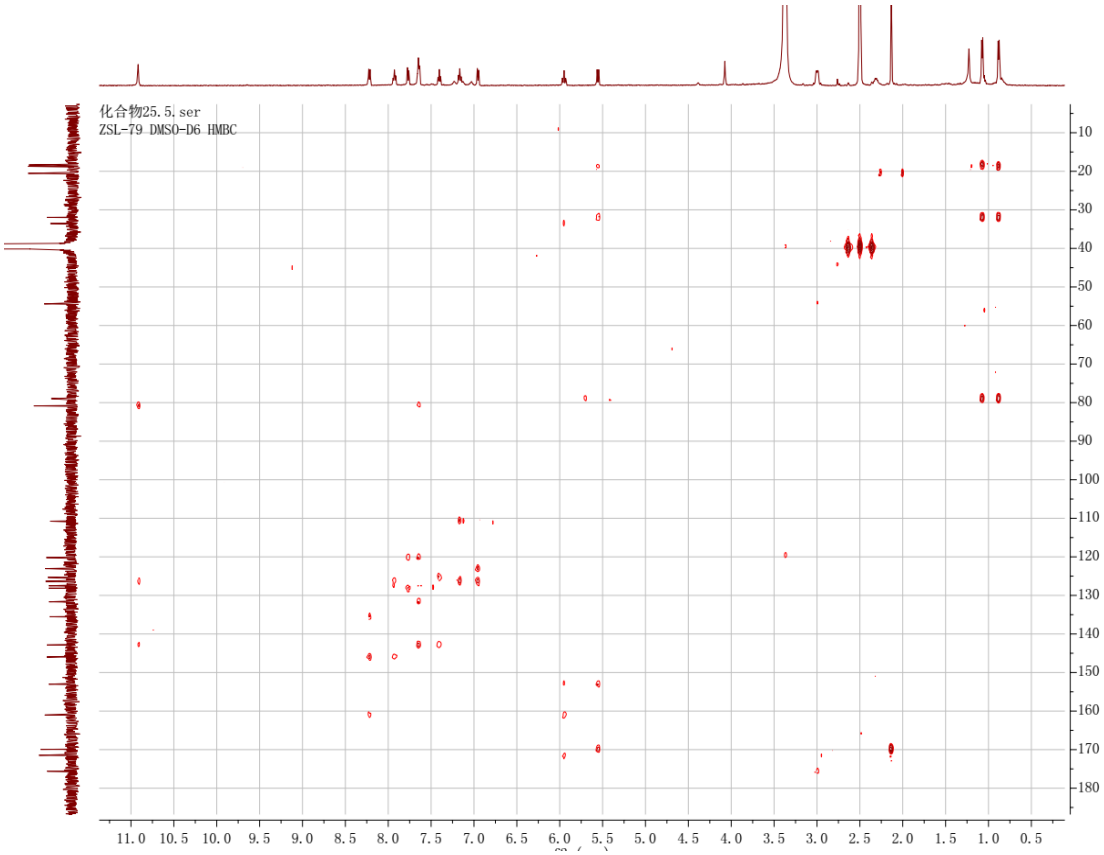

## HSQC spectrum of 6



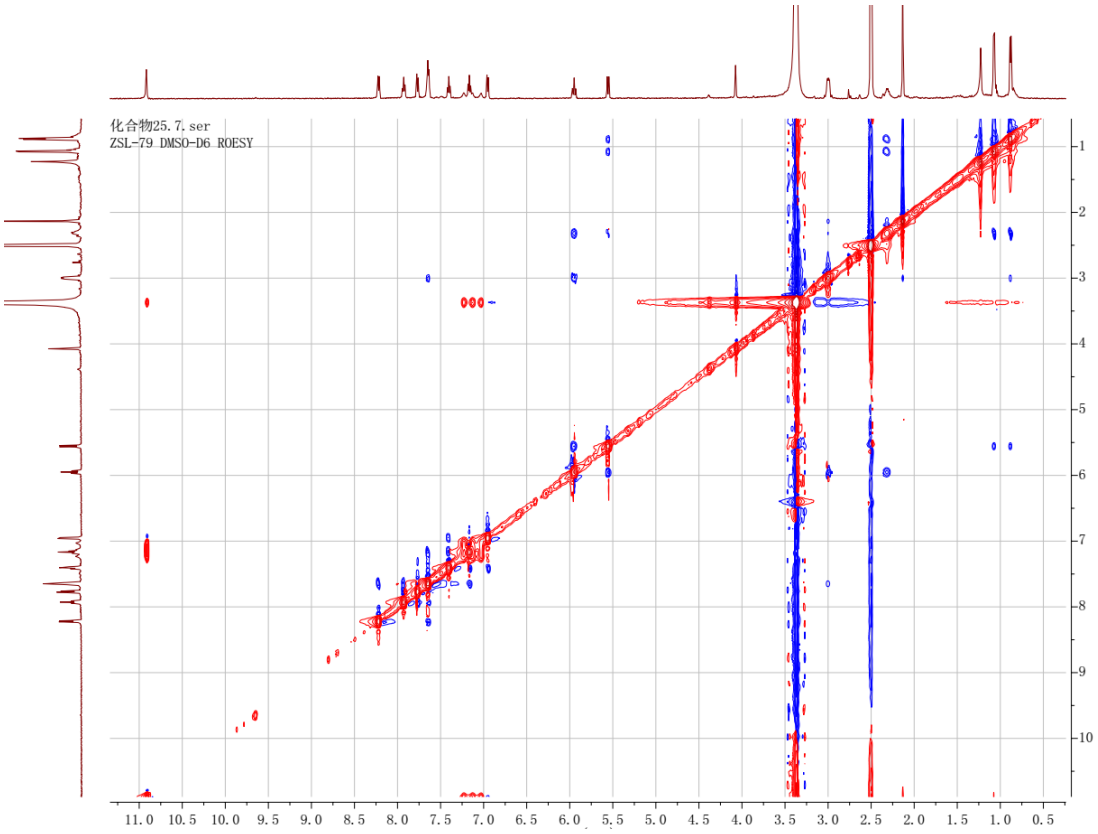
## $^{1}H$-$^{1}H$ COSY spectrum of 6



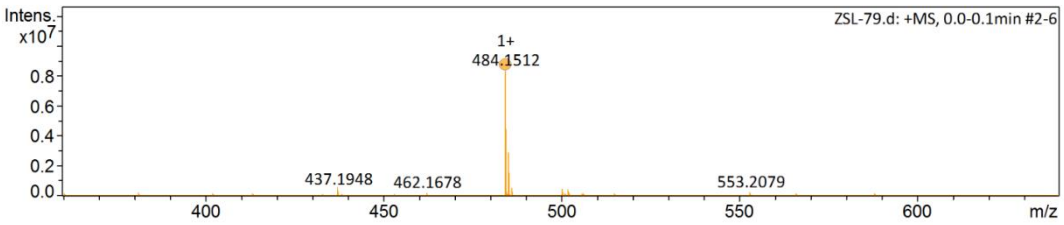

## HMBC spectrum of 6



## ROESY spectrum of 6

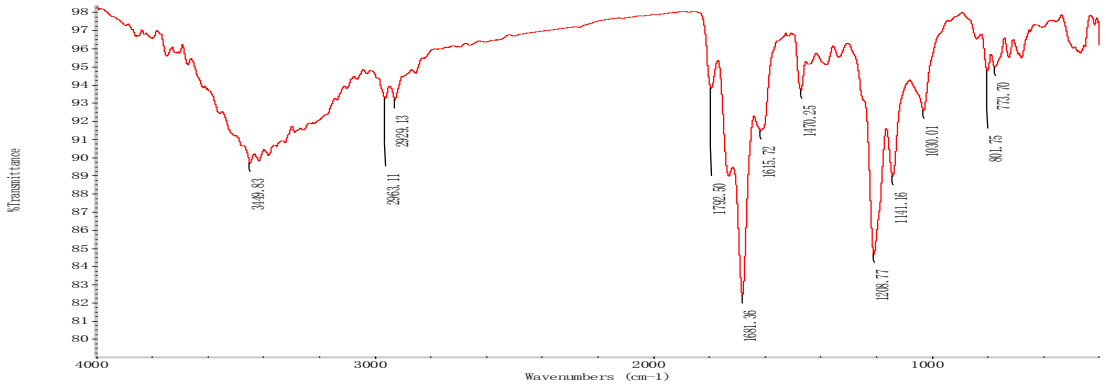



## HRESIMS spectrum of 6



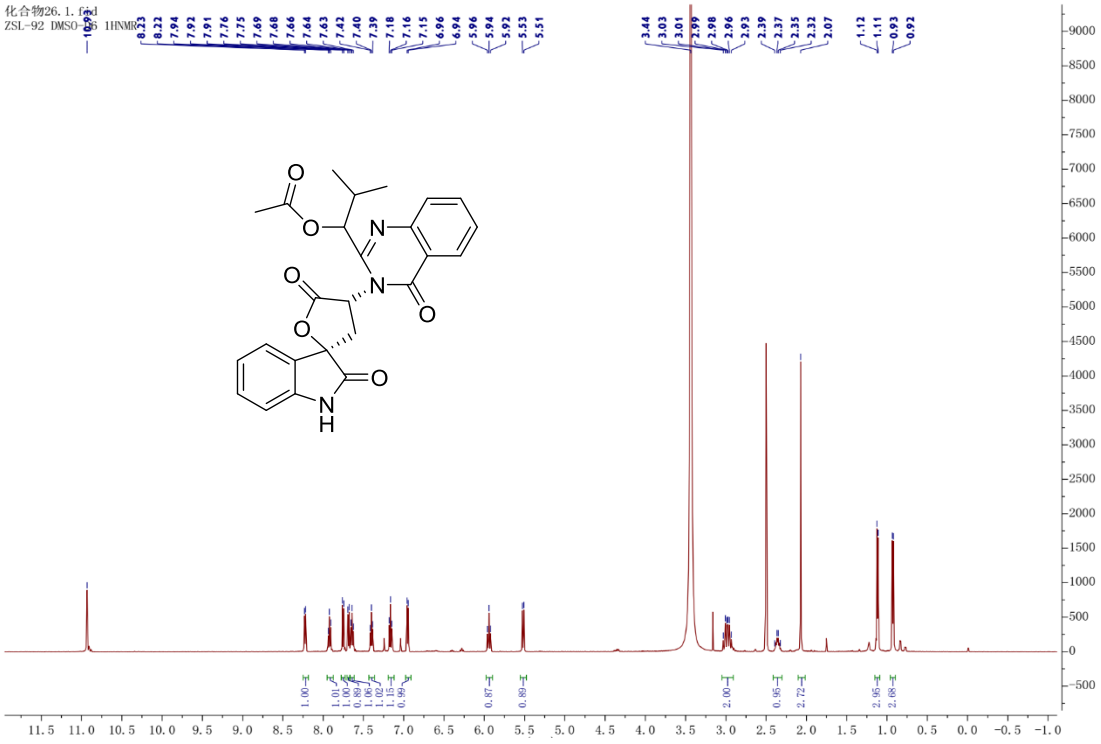

| Meas. m/z | # | Ion Formula | m/z | err [ppm] | Mean err [ppm] | rdb | N-Rule | e⁻ Conf | mSigma | Adduct |
|---|---|---|---|---|---|---|---|---|---|---|
| 484.151235 | 1 | C25H23N3NaO6 | 484.147906 | -6.9 | -5.8 | 16.0 | ok | even | 33.0 | M+Na |

## IR spectrum of 6

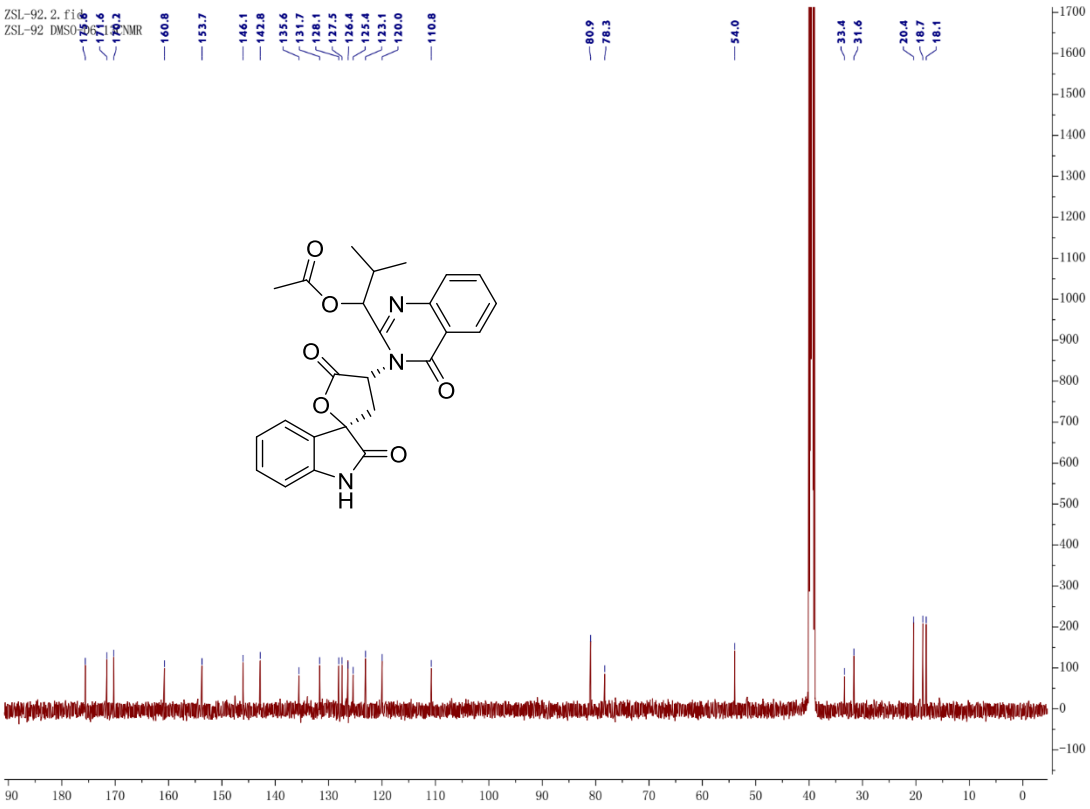


# NMR, HRESIMS, and IR spectra of compound 7

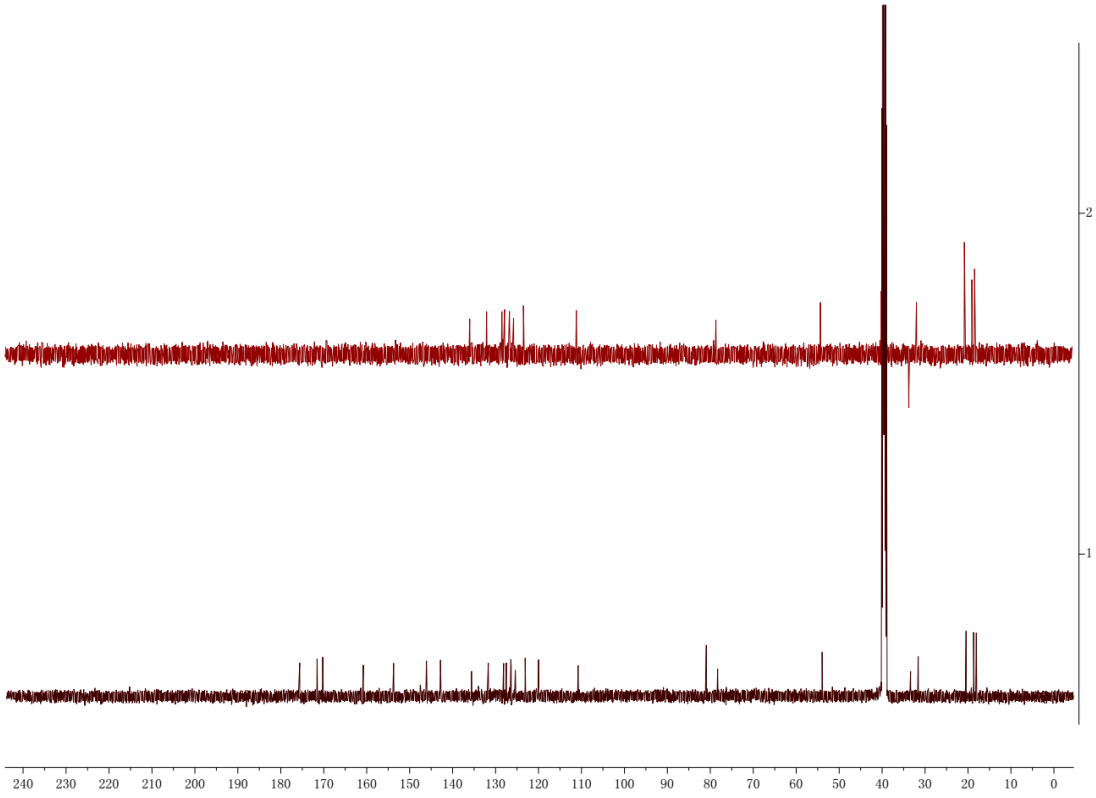
## $^{1}$H-NMR spectrum of 7



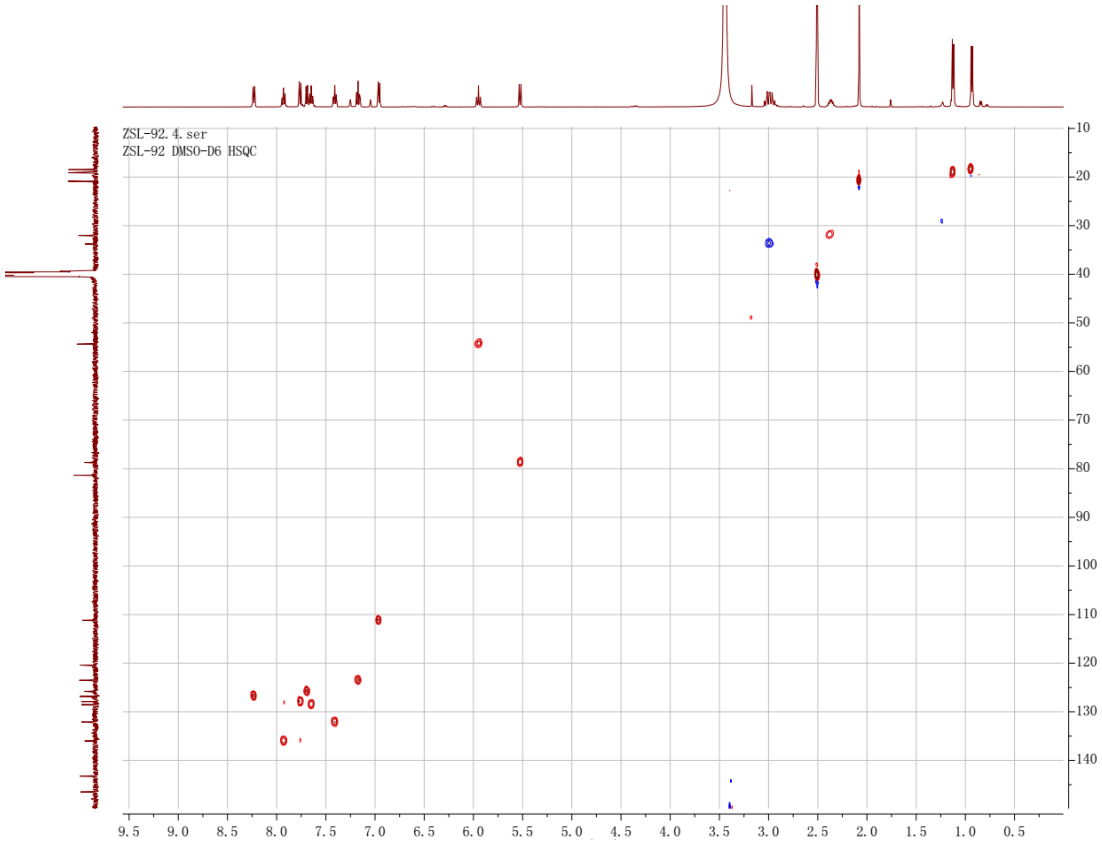
## $^{13}$C-NMR spectrum of 7



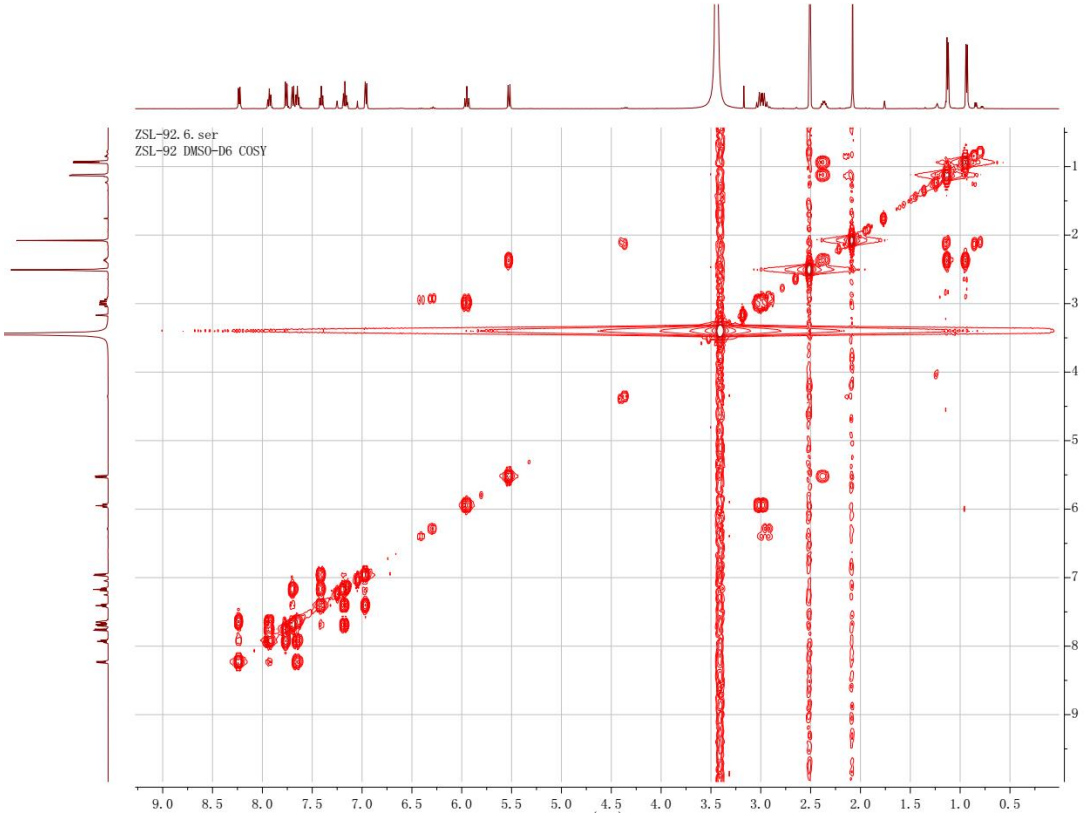
## DEPT spectrum of 7



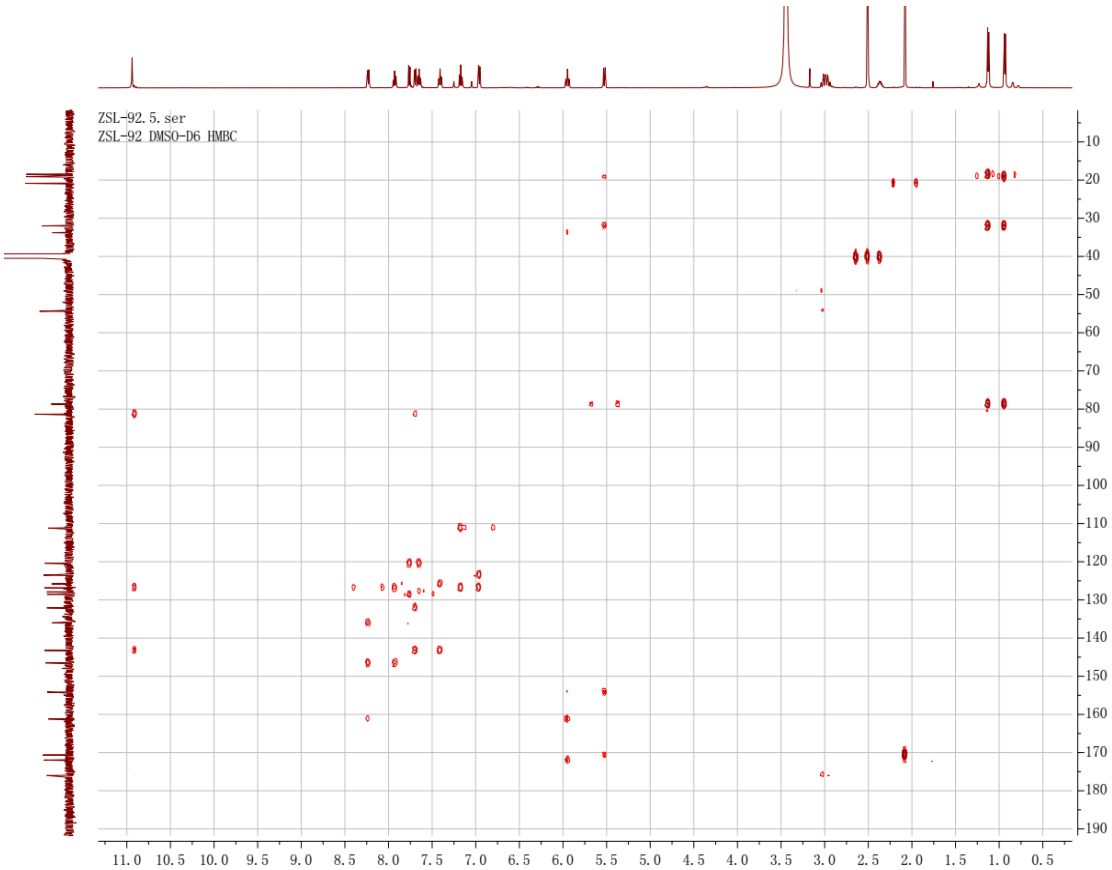

## HSQC spectrum of 7



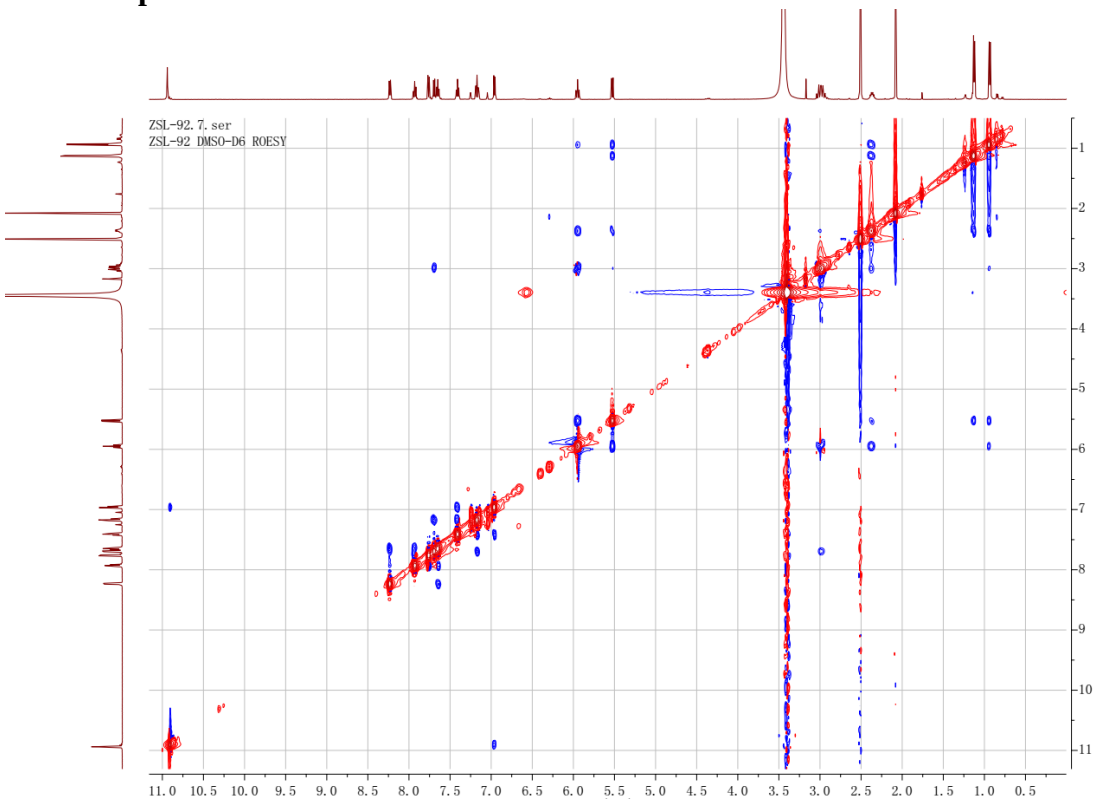
## $^{1}H$-$^{1}H$ COSY spectrum of 7



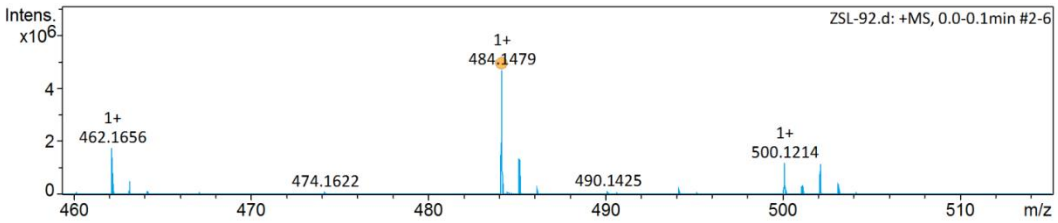

## HMBC spectrum of 7



## ROESY spectrum of 7

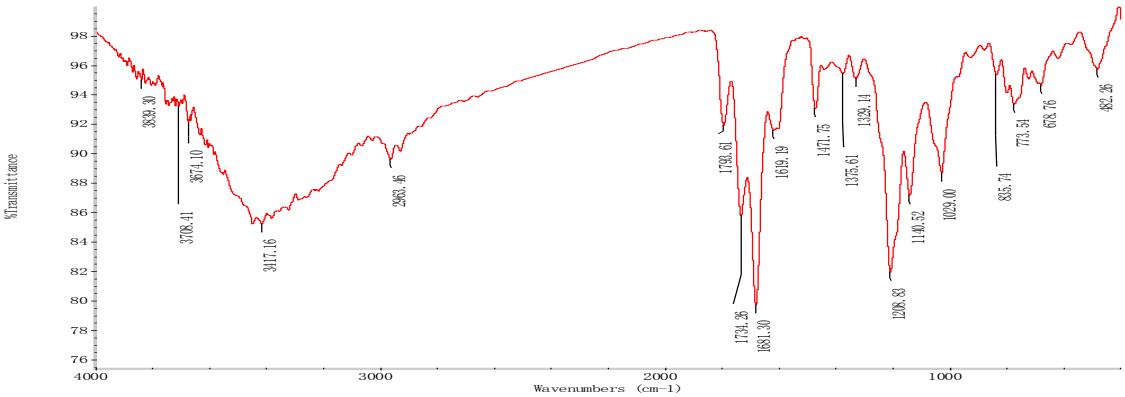



## HRESIMS spectrum of 7

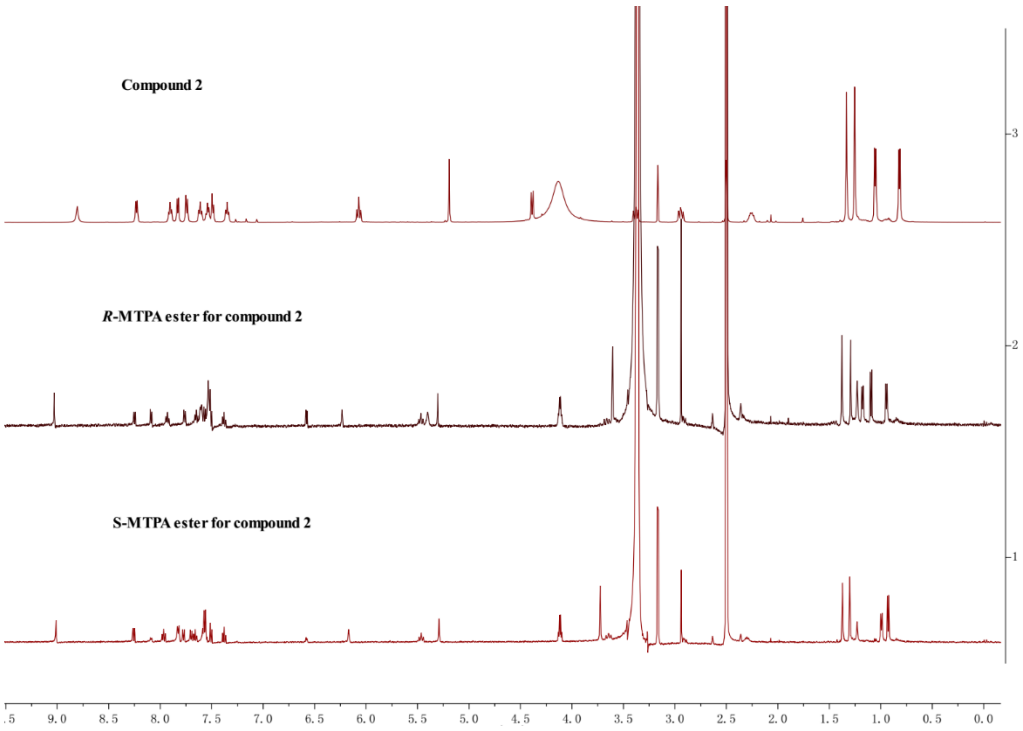



| Meas. m/z | # | Ion Formula | m/z | err [ppm] | Mean err [ppm] | rdb | N-Rule | e⁻ Conf | mSigma | Std I | Adduct |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 484.147921 | 1 | C25H23N3NaO6 | 484.147906 | -0.0 | -0.6 | 16.0 | ok | even | 1.5 | 2.4 | M+Na |

## IR spectrum of 7



**$^1$H NMR spectra for (*R*)- and (*S*)-MTPA esters of compound 2**



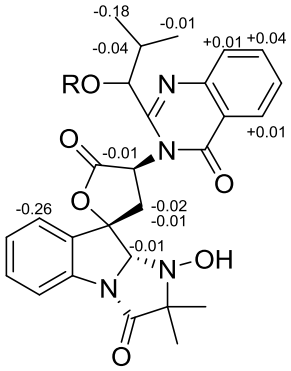




**Figure S1. $\Delta\delta$ (= $\delta_S - \delta_R$) values for (*S*)- and (*R*)-MTPA esters of 2.**

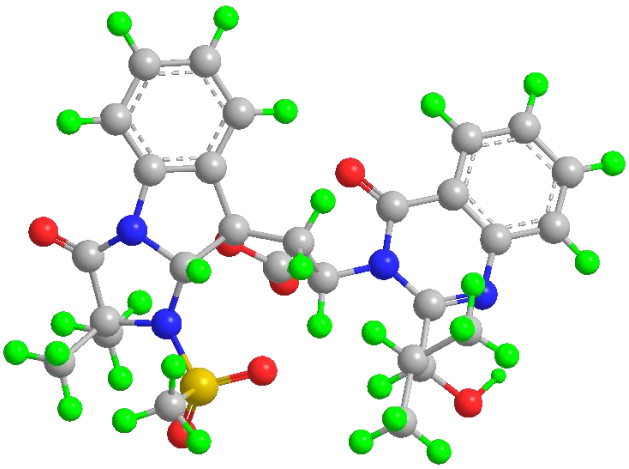
**Theory and Calculation Details.**

The geometry determined from the X-ray analysis of **1** was used as the input for the structural optimization by the density functional theory method at the B3PW91/TZVP level in Gaussian 03 programpackage.[S1,S2] The ECD of the lowest energy conformers were then calculated by the TDDFT method at the B3LYP/6-31levels with the CPCM model in methanol solution. [S3]

(S1) Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J.C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D.J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

(S2) Sai, C.; Li, D.; Xue, C.; Wang, K.; Hu, P.; Pei, Y.; Bai, J.; Jing Y.; Li, Z.; Hua H. *Org. Lett.* **2015**, *17*, 4102-5.

(S3) (a) Miertus, S.; Tomasi, *J. Chem. Phys.* **1982**, *65*, 239–245. (b) Tomasi, J.; Persico, M. *Chem.Rev.* **1994**, *94*, 2027–2094. (c) Cammi, R.; Tomasi, J. J. *Comp.Chem.* **1995**, *16*, 1449–1458.



B3PW91/TZVP optimized lowest energy 3D conformer of **1**