SupplementaryMaterials: Inhibitors of BRD4 Protein from a Marine-derived Fungus *Alternaria* sp. NH-F6

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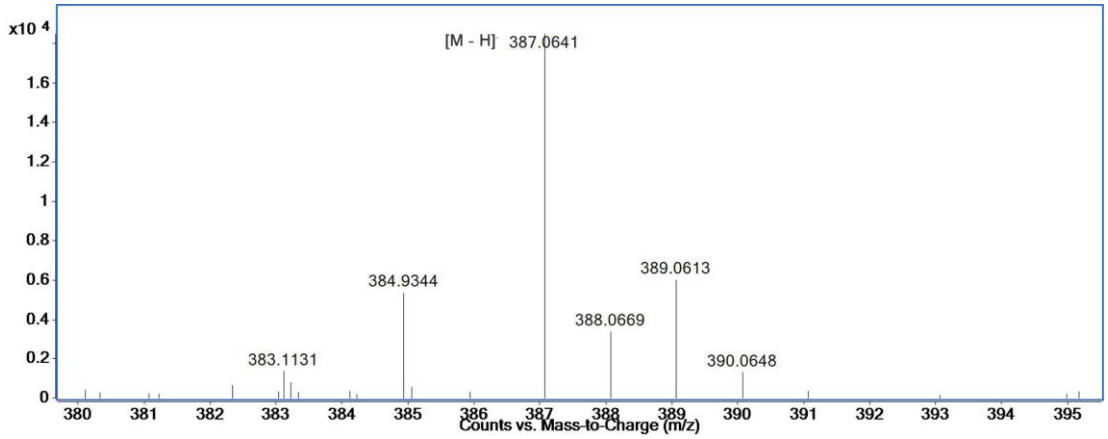

Figure S1. HR-ESI-MS spectrum of the new compound **1**

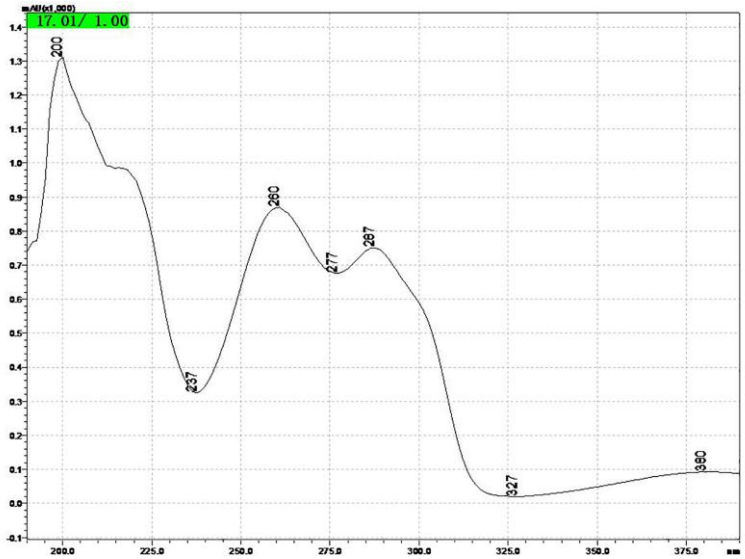

Figure S2. UV spectrum of the new compound **1**

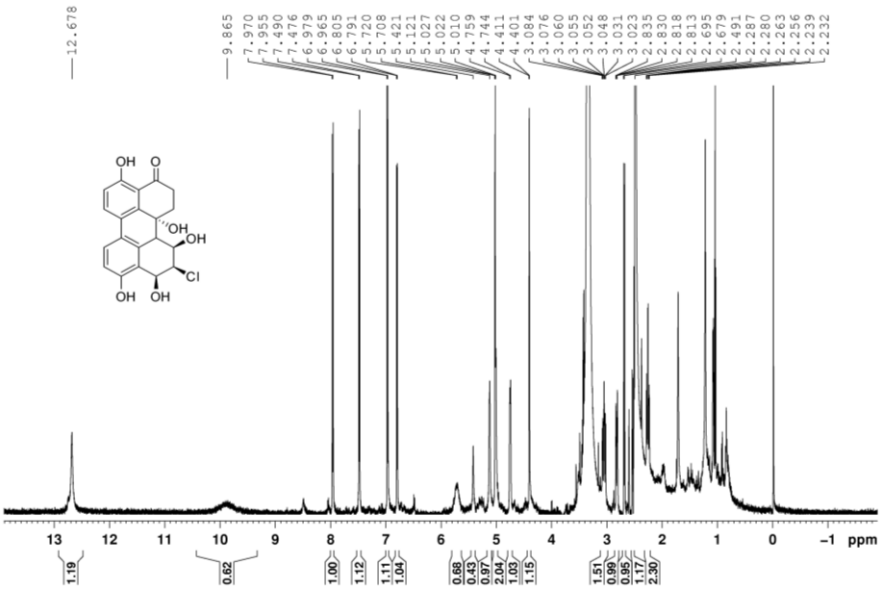

Figure S3. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of the new compound **1**

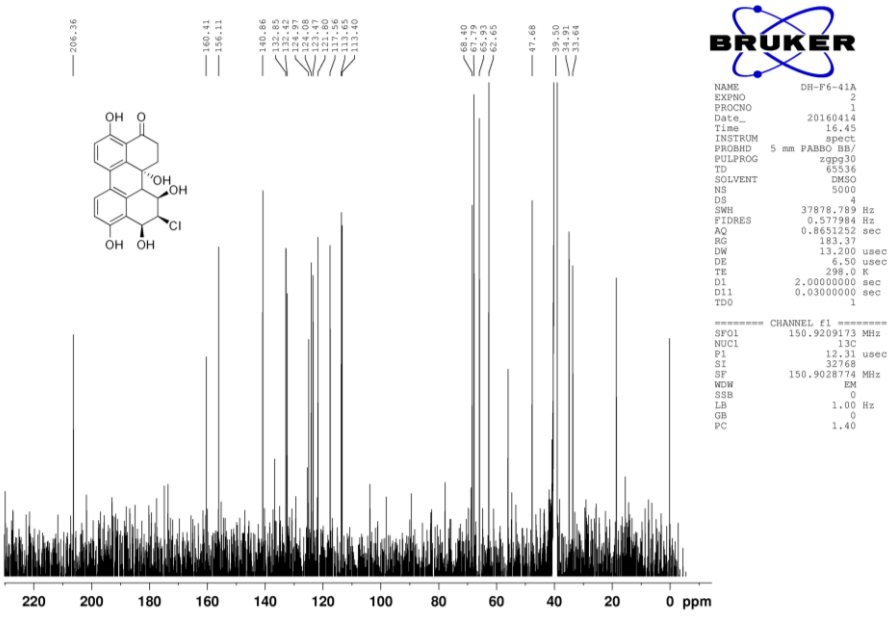

Figure S4. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of the new compound **1**

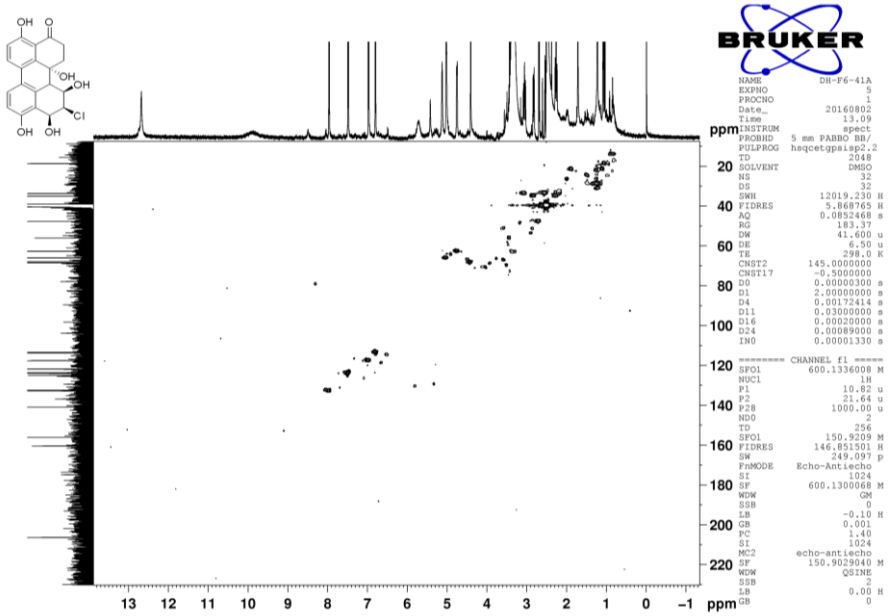

Figure S5. HSQC spectrum of the new compound **1**

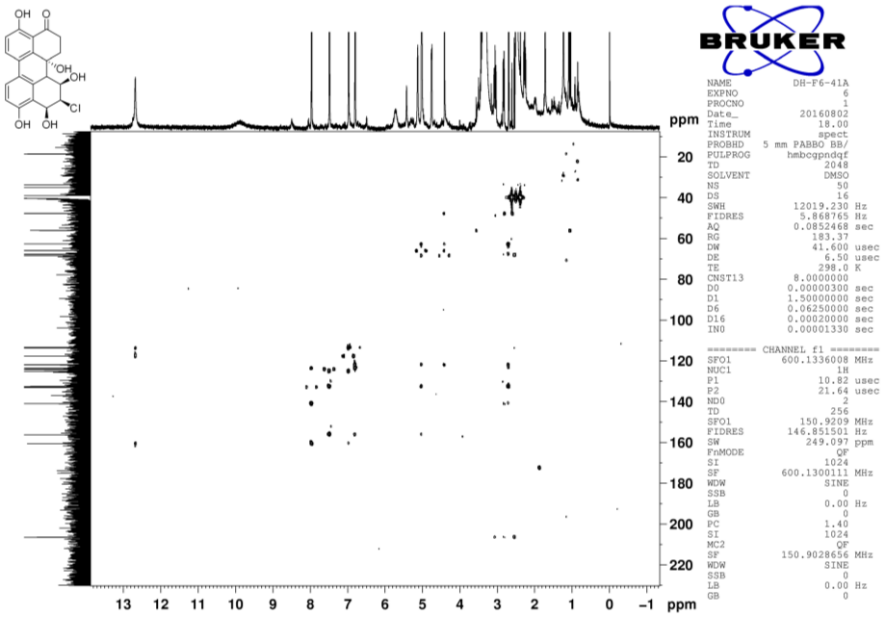

Figure S6. HMBC spectrum of the new compound **1**

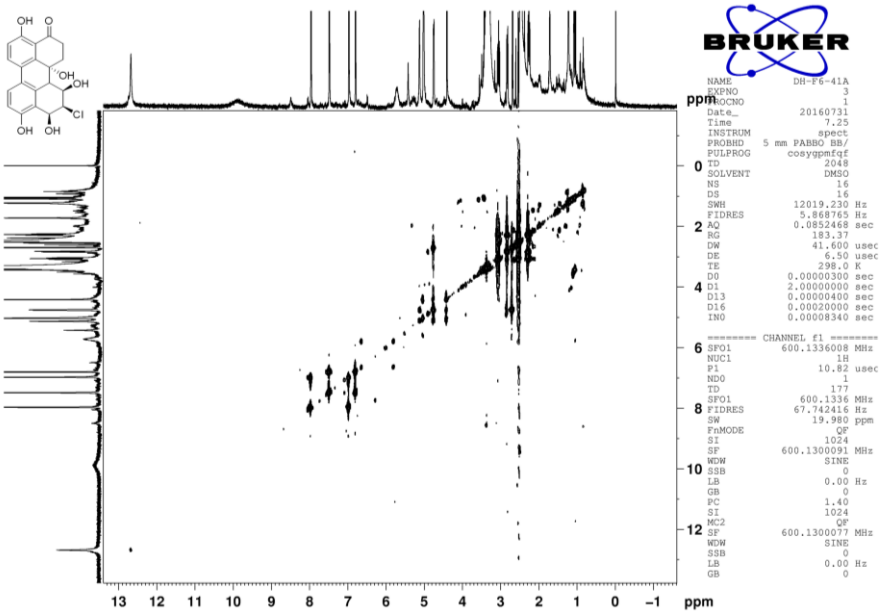

Figure S7. ^{1}H-^{1}H COSY spectrum of the new compound **1**

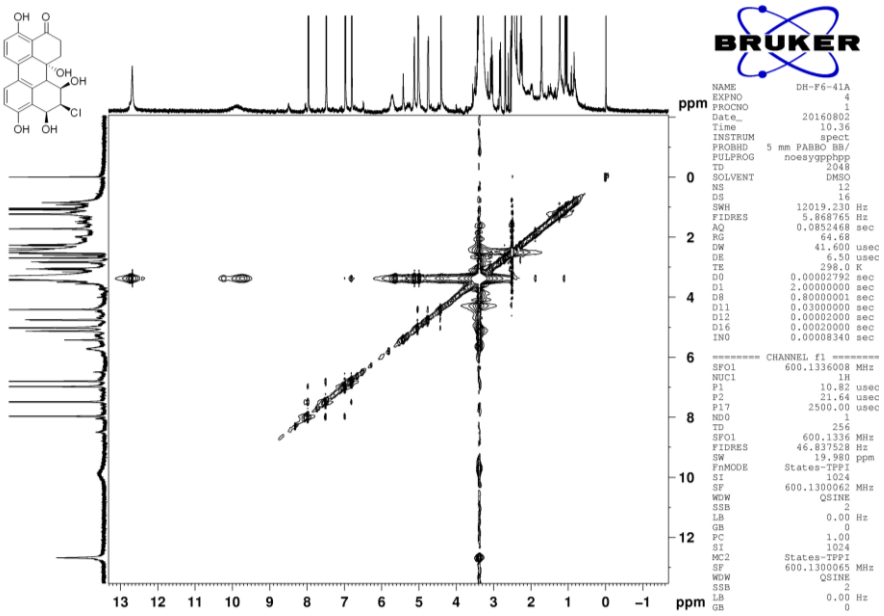

Figure S8. NOESY spectrum of the new compound **1**

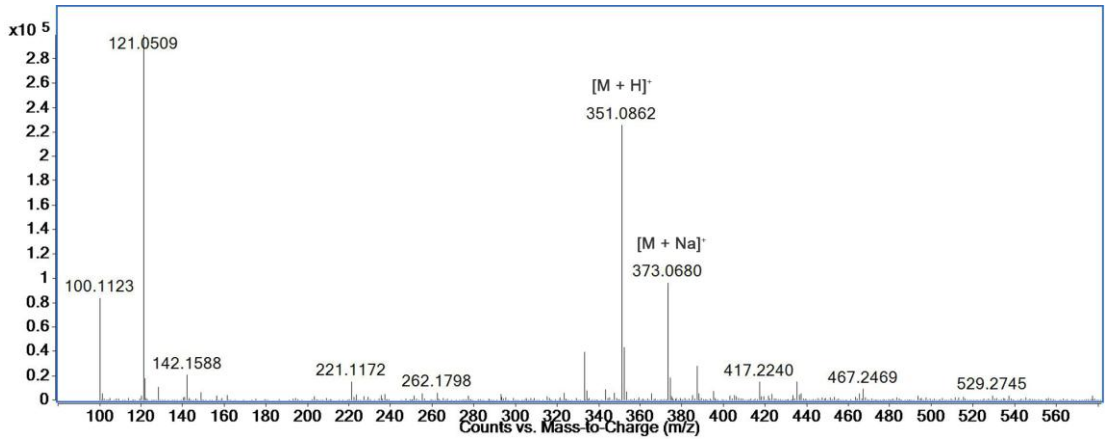

Figure S9. HR-ESI-MS spectrum of the new compound **2**

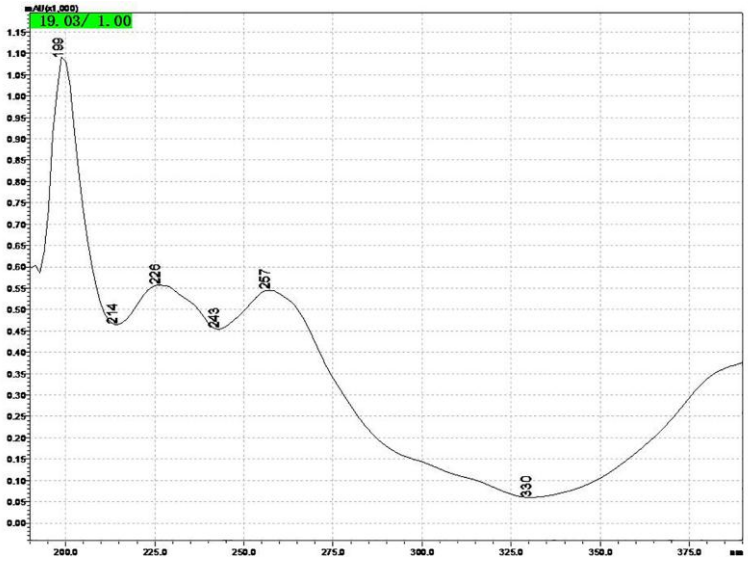

Figure S10. UV spectrum of the new compound **2**

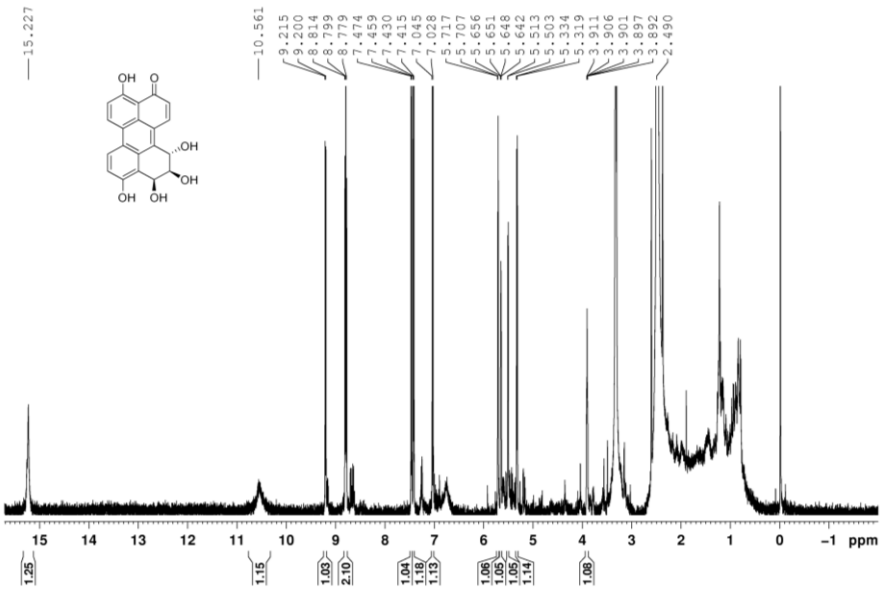

Figure S11. [1]H NMR (600 MHz, DMSO-d_6) spectrum of the new compound **2**

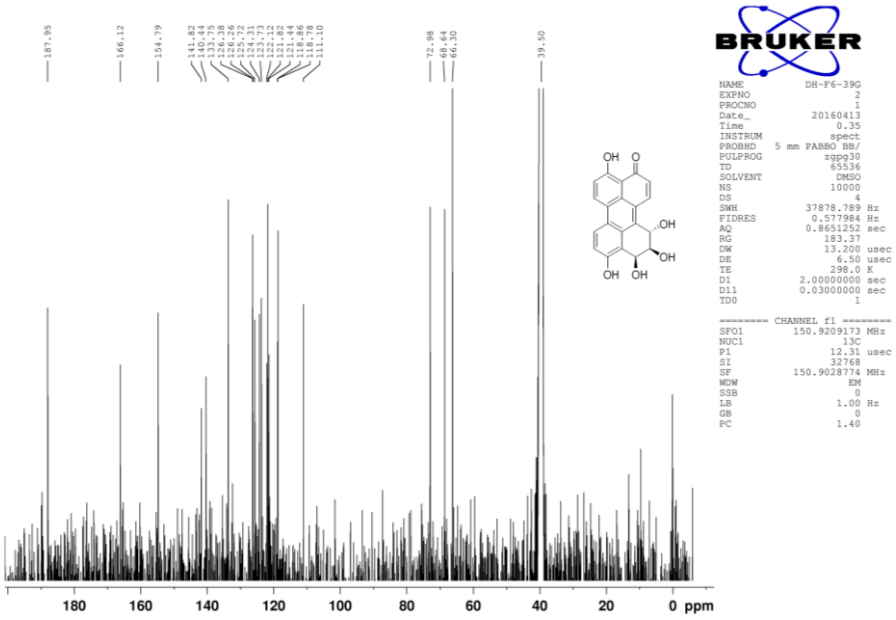

Figure S12. [13]C NMR (150 MHz, DMSO-d_6) spectrum of the new compound **2**

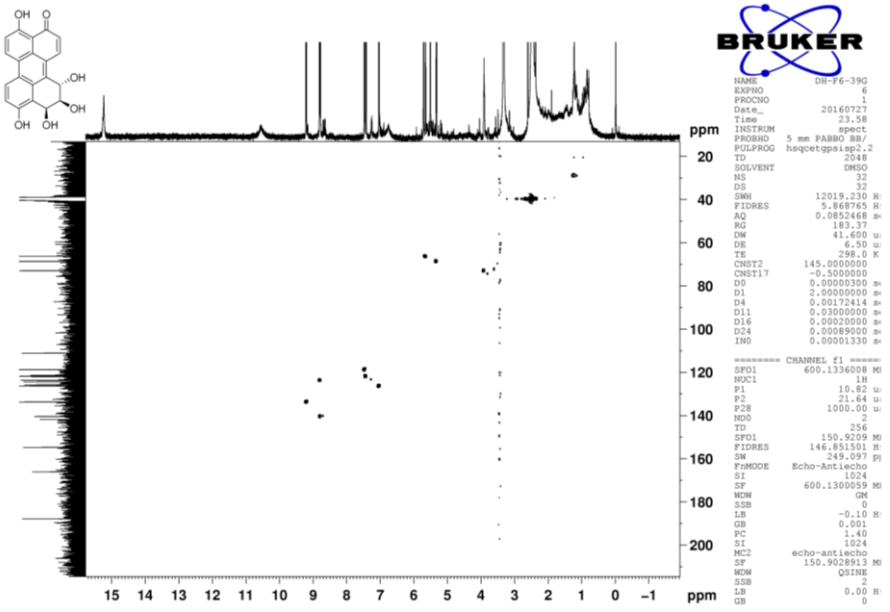

Figure S13. HSQC spectrum of the new compound **2**

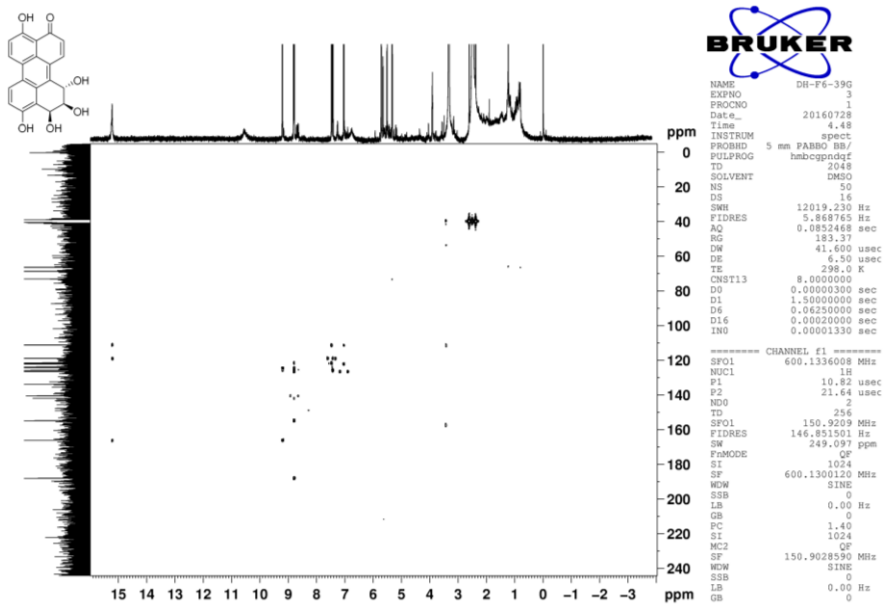

Figure S14. HMBC spectrum of the new compound **2**

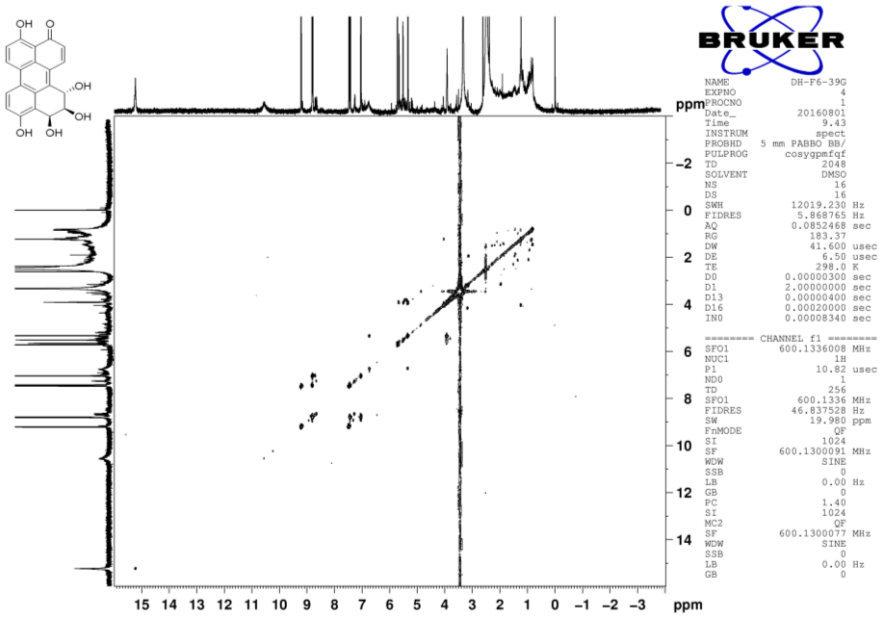

Figure S15. ^{1}H-^{1}H COSY spectrum of the new compound **2**

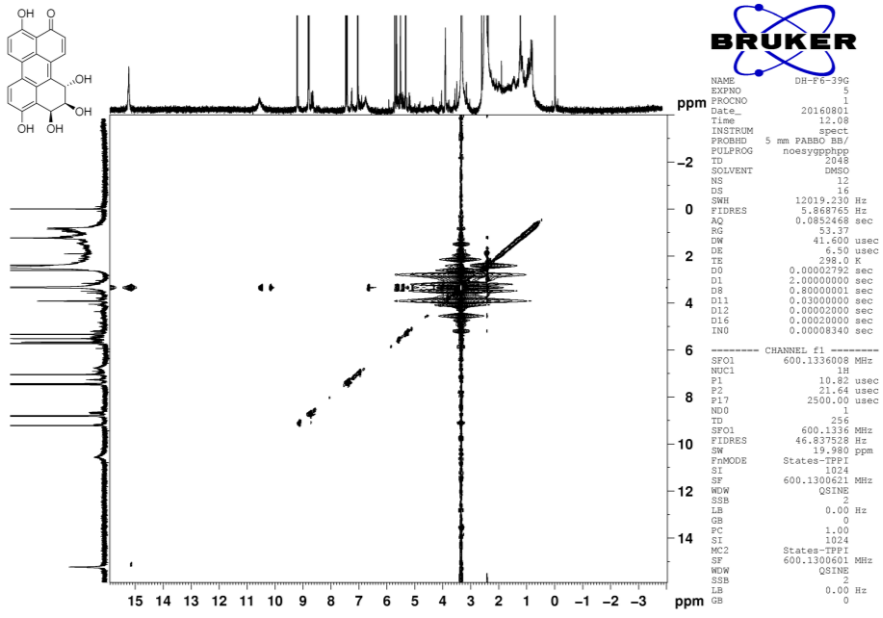

Figure S16. NOESY spectrum of the new compound **2**

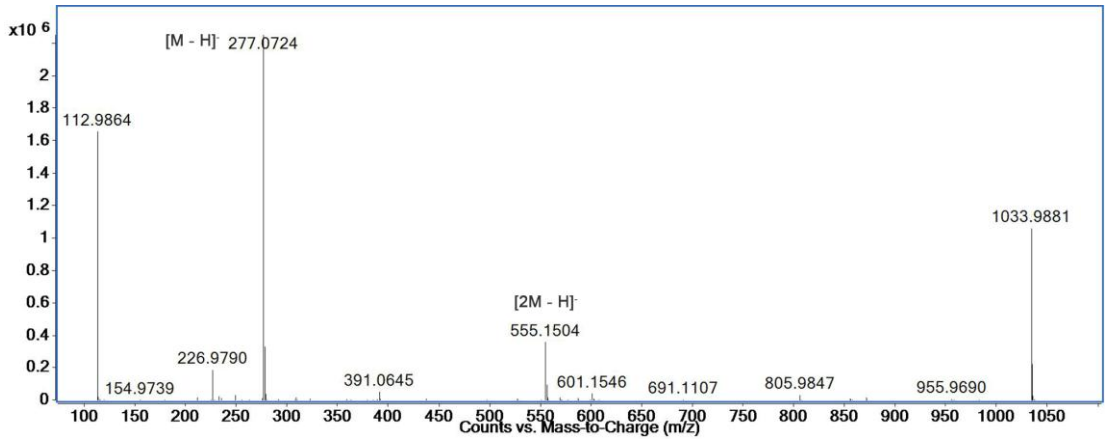

Figure S17. HR-ESI-MS spectrum of the new compound **3**

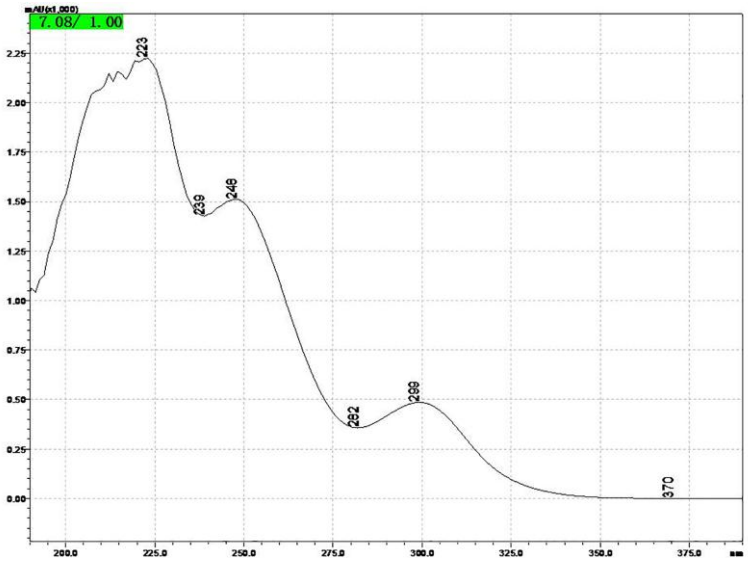

Figure S18. UV spectrum of the new compound **3**

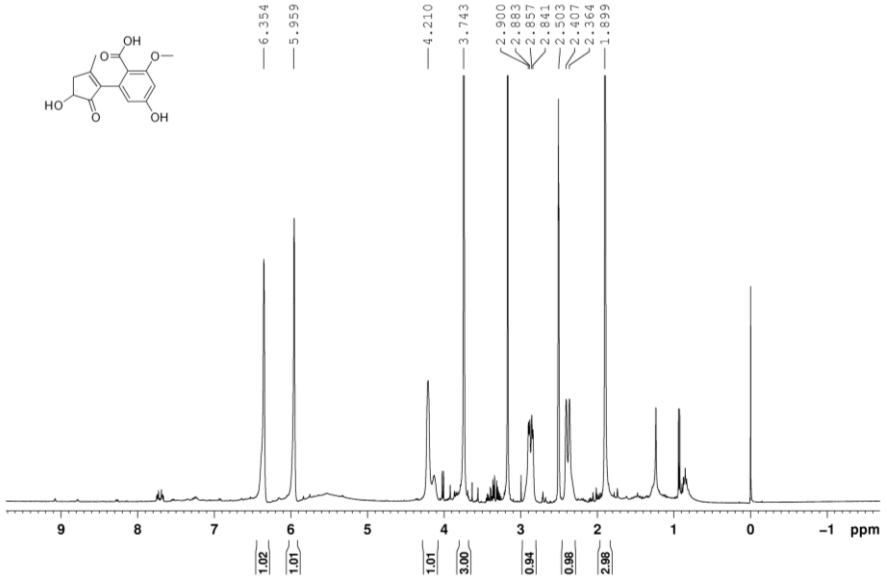

Figure S19. [1]H NMR (400 MHz, DMSO-d_6) spectrum of the new compound **3**

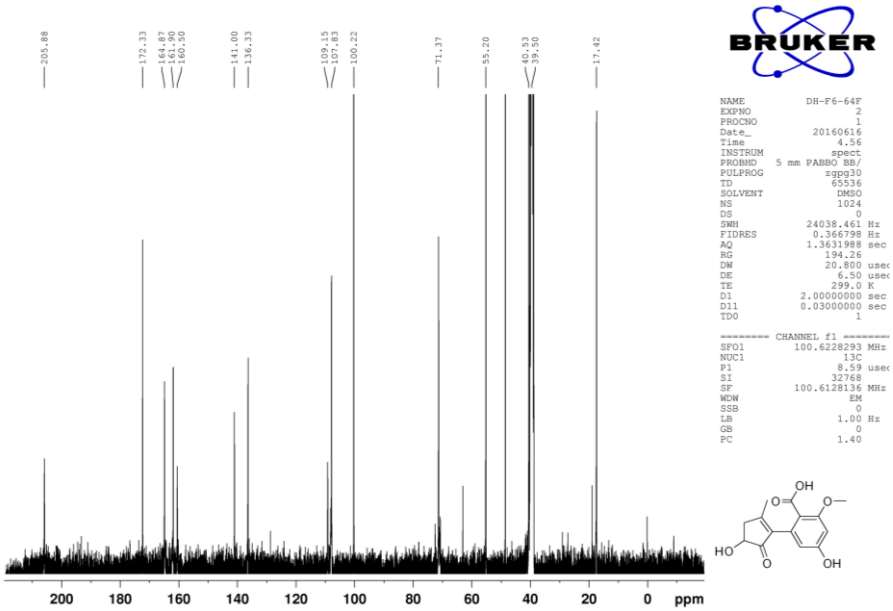

Figure S20. [13]C NMR (100 MHz, DMSO-d_6) spectrum of the new compound **3**

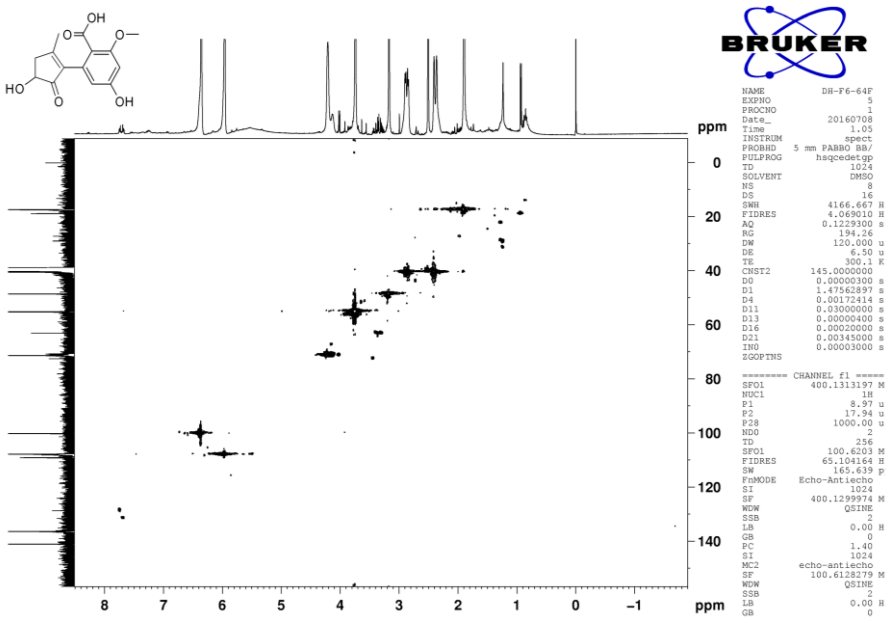

Figure S21. HSQC spectrum of the new compound **3**

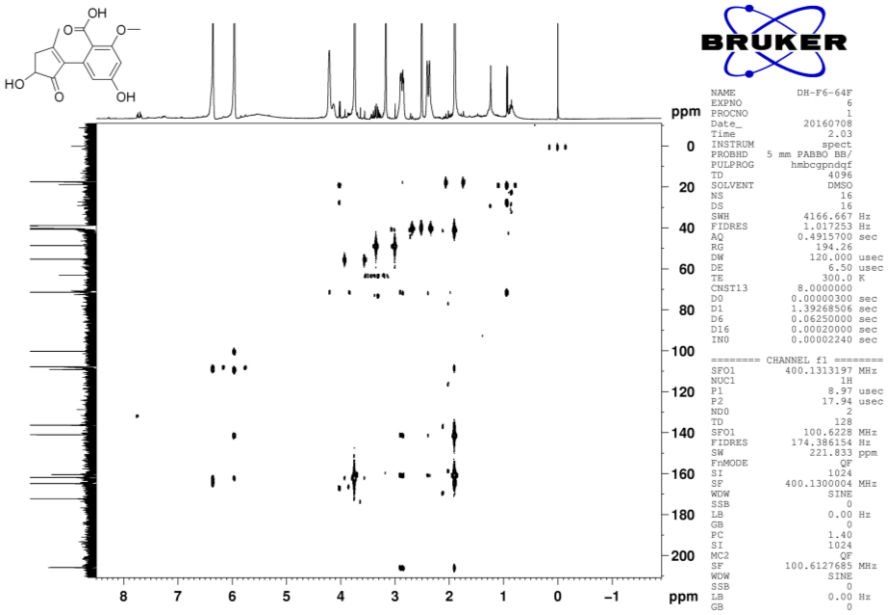

Figure S22. HMBC spectrum of the new compound **3**

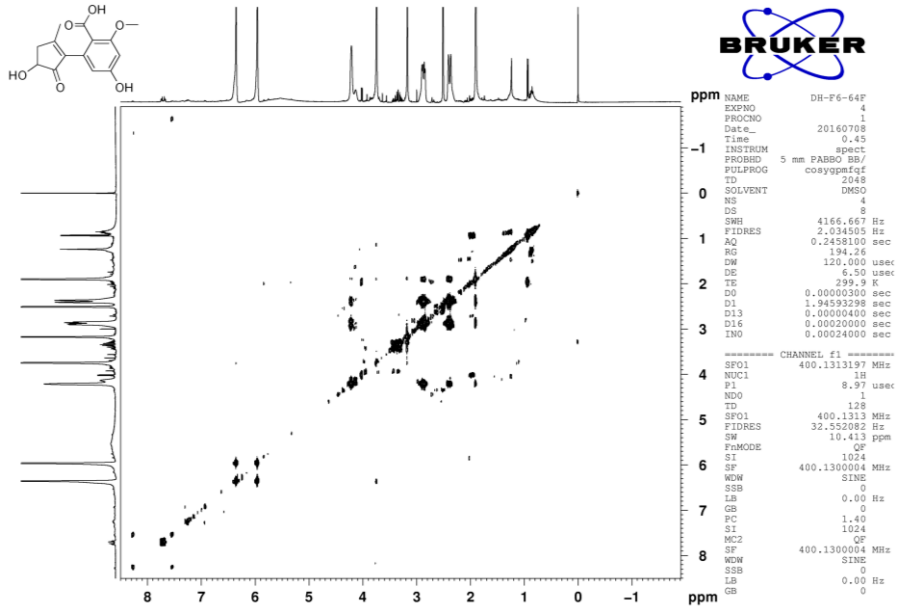

Figure S23. ^{1}H-^{1}H COSY spectrum of the new compound **3**

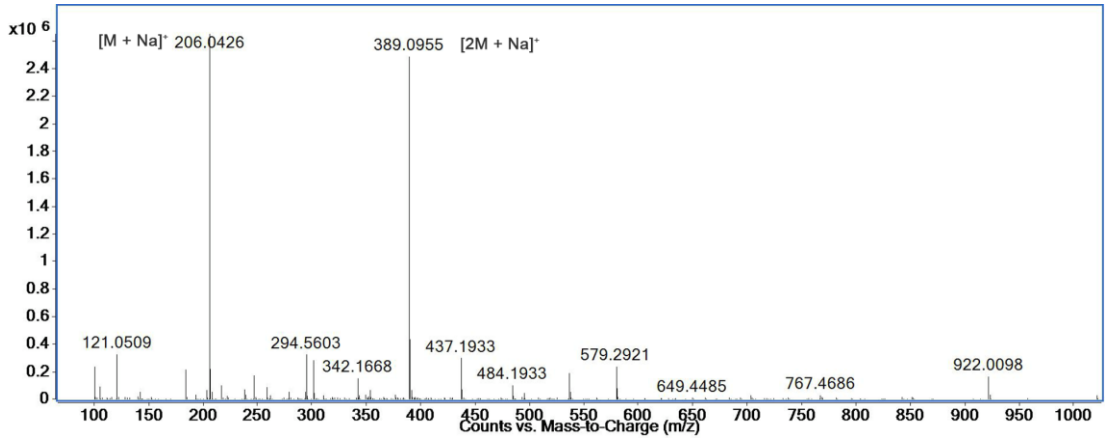

Figure S24. HR-ESI-MS spectrum of the new compound **4**

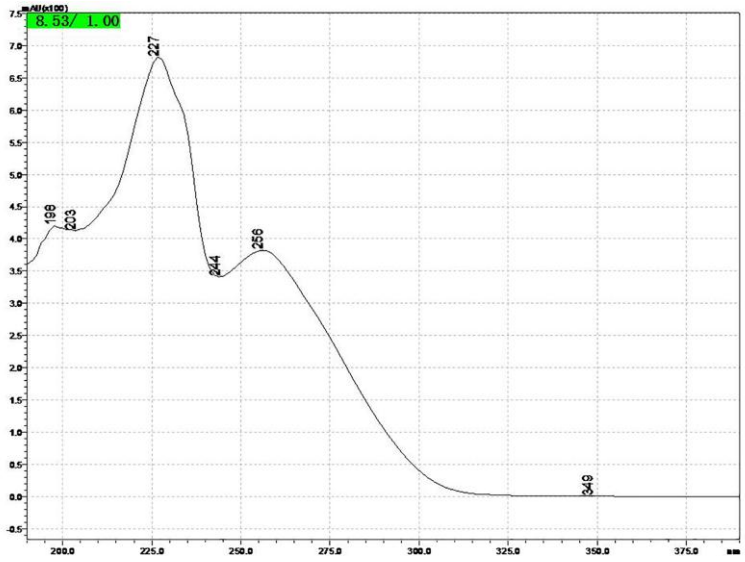

Figure S25. UV spectrum of the new compound **4**

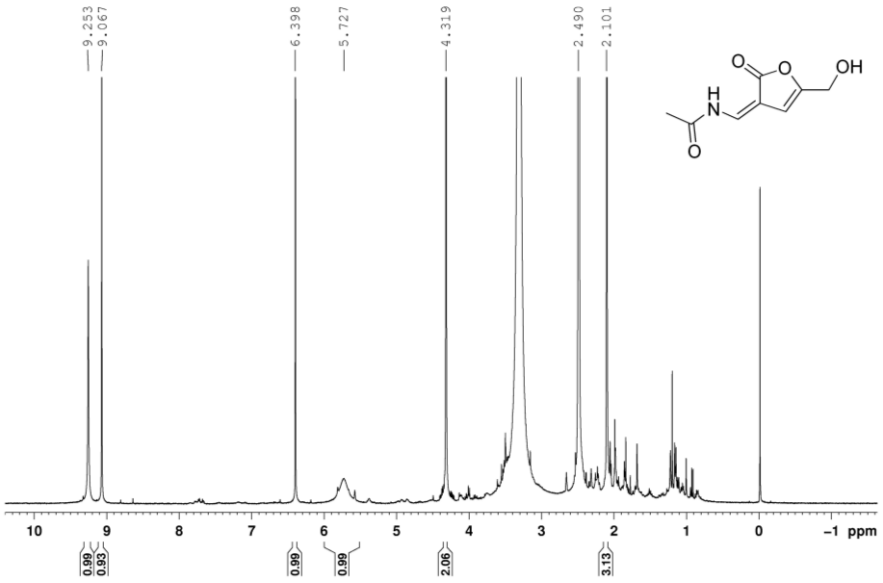

Figure S26. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of the new compound **4**

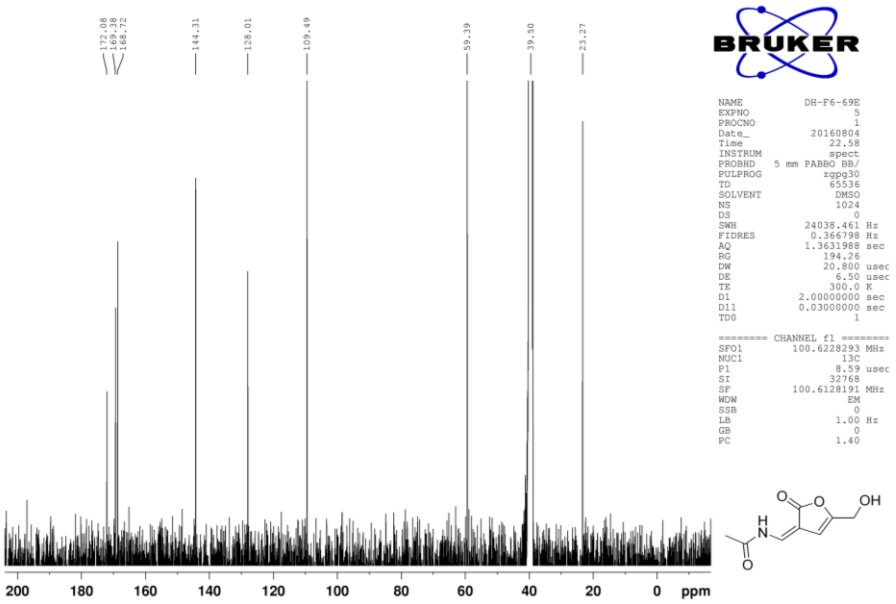

Figure S27. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of the new compound **4**

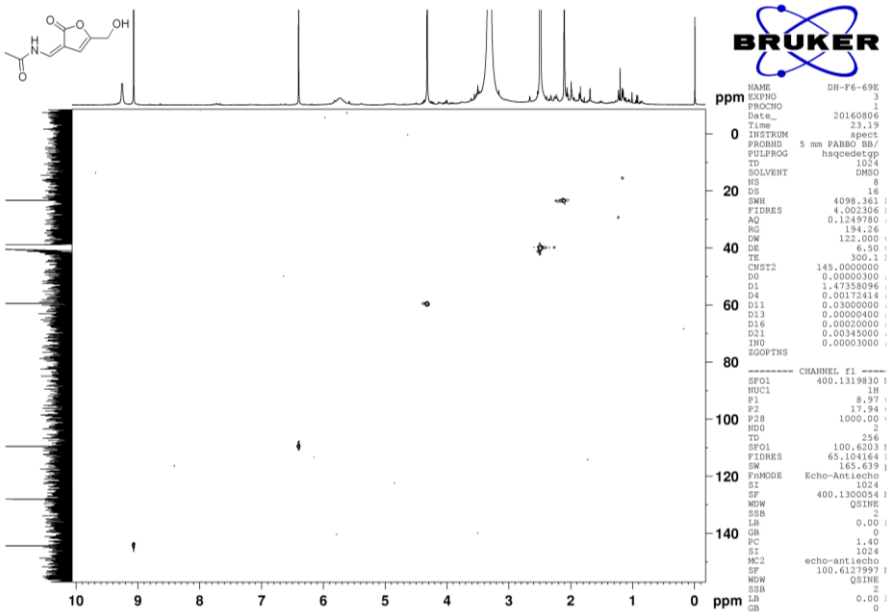

Figure S28. HSQC spectrum of the new compound **4**

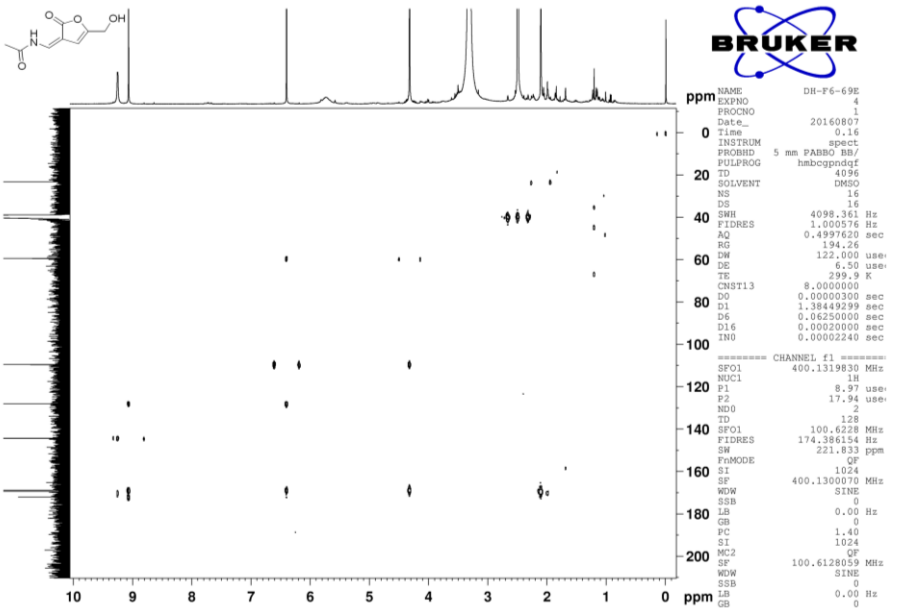

Figure S29. HMBC spectrum of the new compound **4**

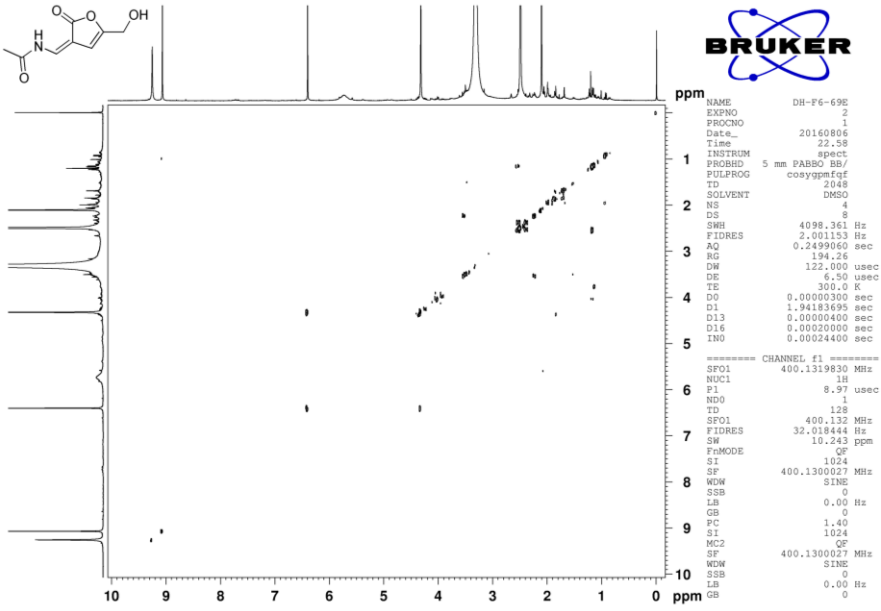

Figure S30. ^{1}H-^{1}H COSY spectrum of the new compound **4**

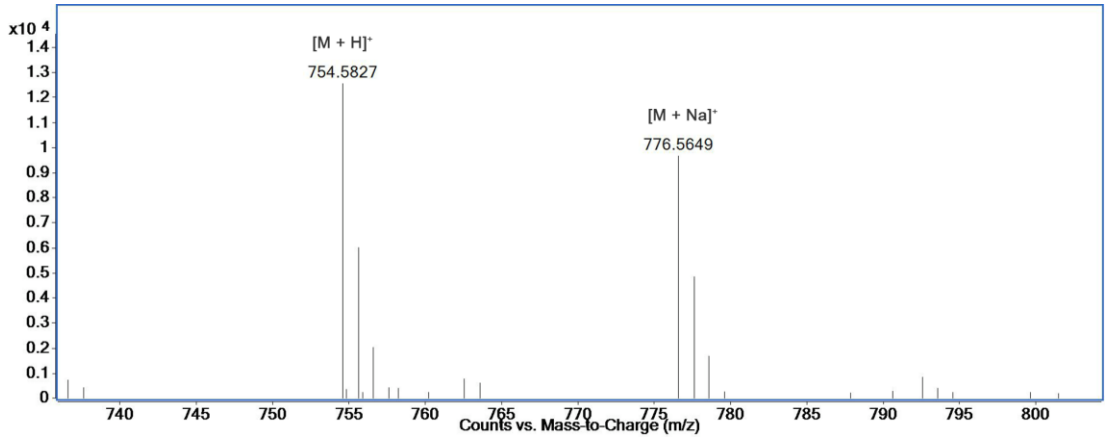

Figure S31. HR-ESI-MS spectrum of the new compound **5**

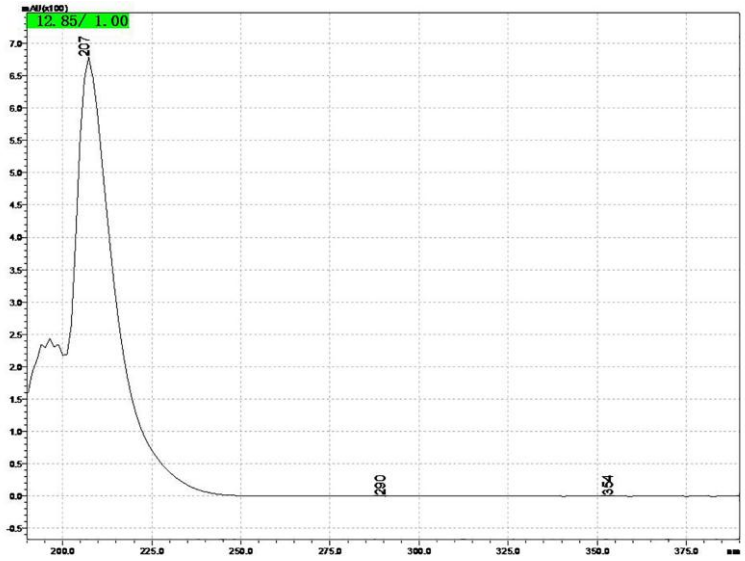

Figure S32. UV spectrum of the new compound **5**

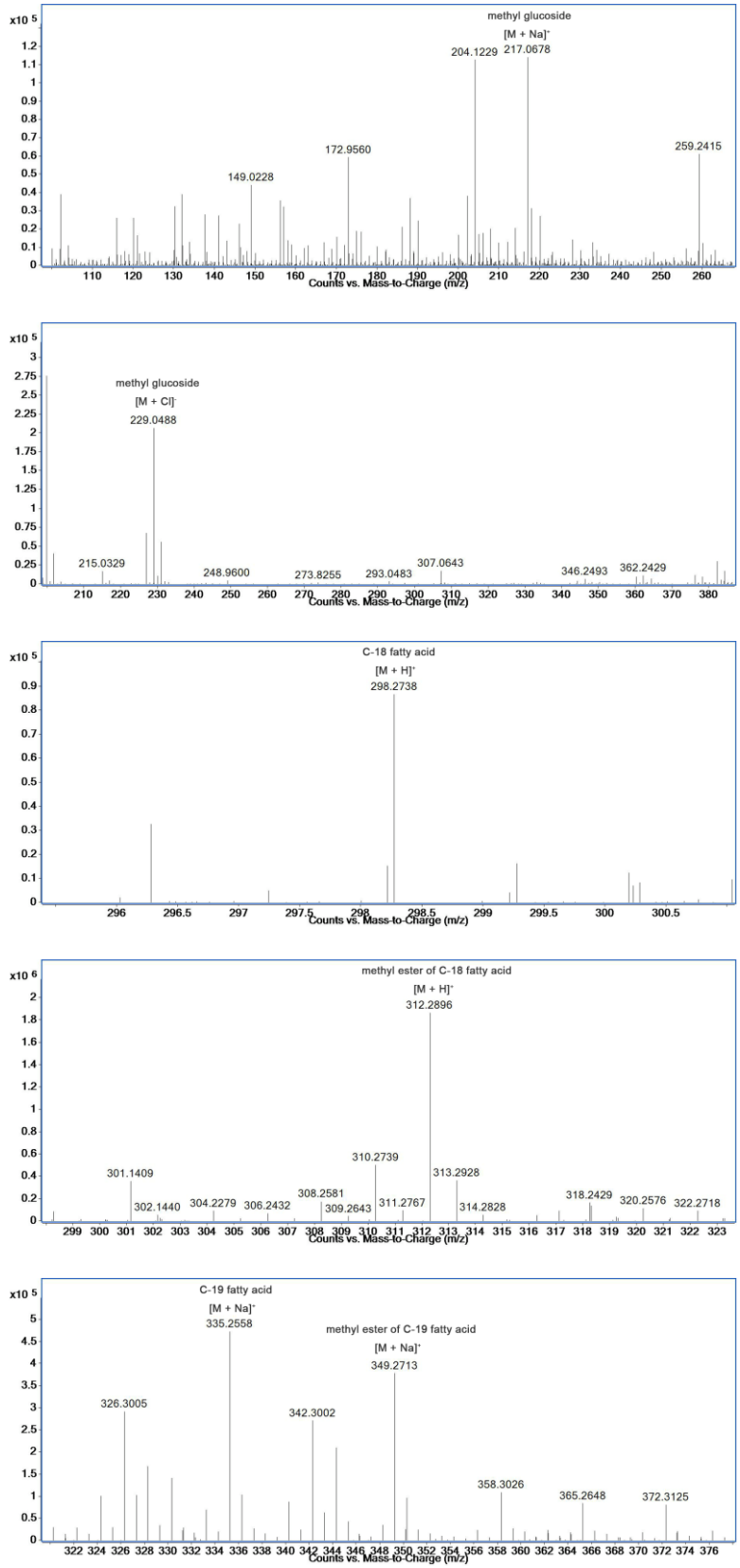

Figure S33. The methanolysis products' HR-ESI-MS spectra of the new compound **5**

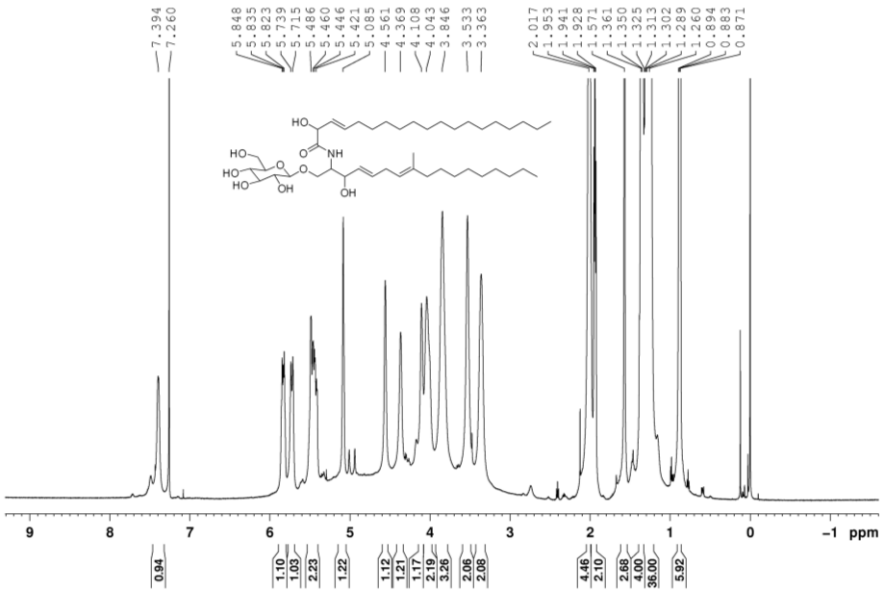

Figure S34. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of the new compound **5**

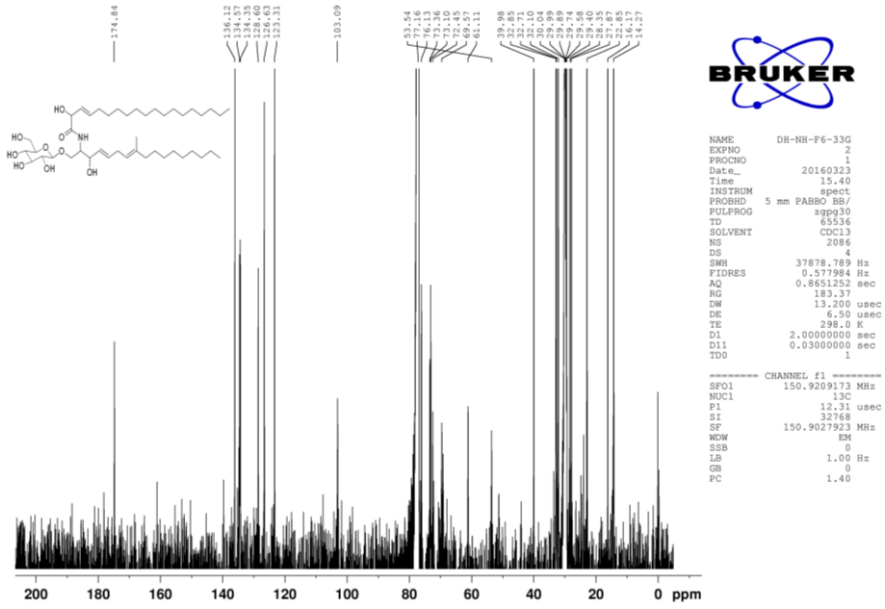

Figure S35. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of the new compound **5**

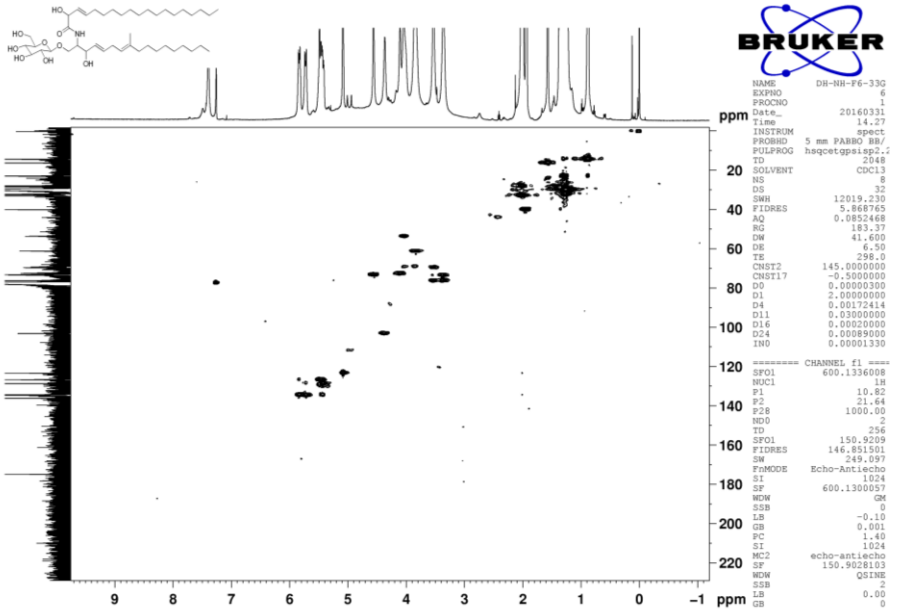

Figure S36. HSQC spectrum of the new compound **5**

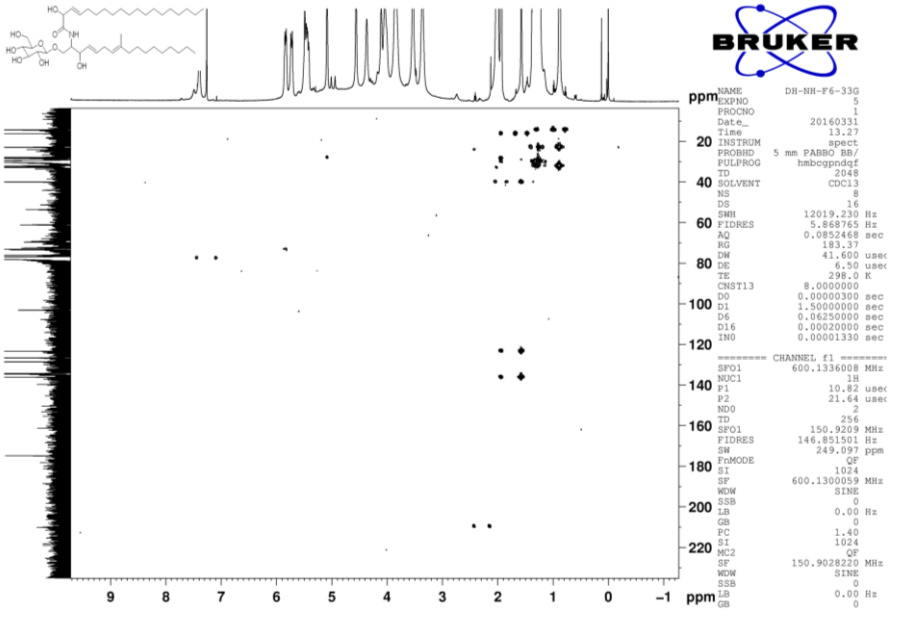

Figure S37. HMBC spectrum of the new compound **5**

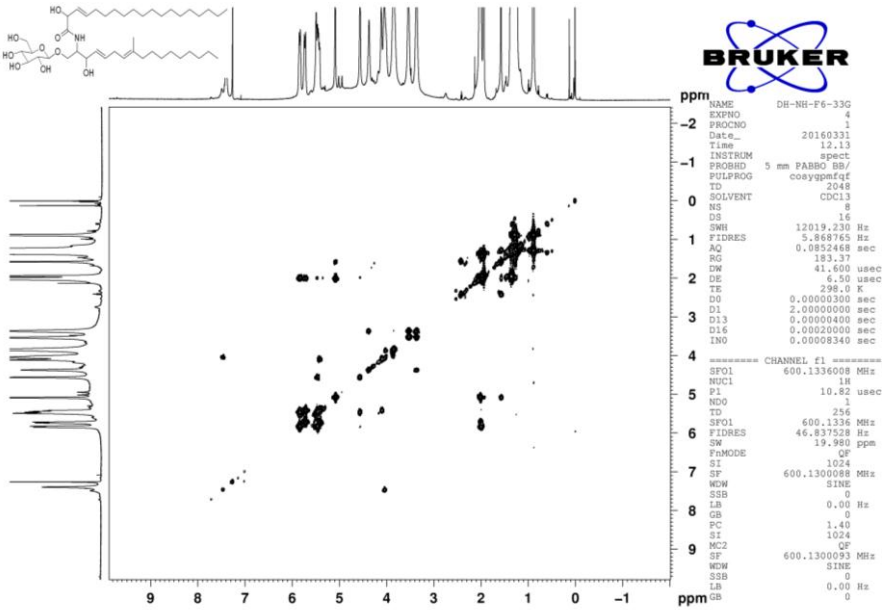

Figure S38. ^{1}H-^{1}H COSY spectrum of the new compound **5**

Table S1. ^{1}H NMR (600 MHz) and ^{13}C NMR (150 MHz) data of compound **6** in MeOH-d_4.

position	compound **6**	
	δ_C, type	δ_H (J in Hz)
1	165.4, C	
2	109.3, C	
3	137.1, C	
4	109.9, CH	6.07, 1H, d (2.3)
5	163.8, CH	6.40, 1H, d (2.3)
6	101.4, C	
7	168.5, C	
1'	142.6, C	
2'	165.3, C	
3'a	41.8, CH_2	3.04, 1H, dd (17.0, 6.5)
3'b		2.53, 1H, d (17.0)
4'	73.4, CH	4.33, 1H, dd (6.5, 2.8)
5'	209.7, C	
5-OCH_3	55.8, CH_3	3.78, 3H, s
2'-CH_3	17.9, CH_3	1.99, 3H, s

Table S2. Abbreviations

full name	abbreviation
nuclear magnetic resonance	NMR
high resolution electrospray ionization mass spectrometry	HR-ESI-MS
bromodomain-containing protein 4	BRD4
human immunodeficiency virus	HIV
bromodomain	BRD
bromodomain and extra-terminal domain	BET
heteronuclear singular quantum correlation	HSQC
heteronuclear multiple bond correlation	HMBC
homonuclear chemical shift correlation spectroscopy	^{1}H-^{1}H COSY
nuclear overhauser effect spectroscopy	NOESY
infrared ray	IR
high performance liquid chromatography	HPLC
medium performance liquid chromatography	MPLC
time-resolved fluorescence resonance energy transfer	TR-FRET
bromodomain 1	BD1
ribosomal deoxyribose nucleic acid	rDNA
potato dextrose agar	PDA
potato dextrose broth	PDB
*chemical formula	$C_{20}H_{17}ClO_6$, $C_{20}H_{14}O_6$, et al.

*1. Confirm whether a heteroatom is in the structure according to the isotopic peak in HR-ESI-MS spectrum. For example, if the isotopic peak is 3:1, there is a chlorine atoms in the structure.

2. Count the number of carbon and hydrogen atoms in NMR spectrum.

3. Calculate the sum of all atoms' atomic mass using ChemDraw software.

molecular formula (calculated) = (carbon atom's atomic mass) × (the number of carbon atoms) + (hydrogen atom's atomic mass) × (the number of hydrogen atoms) + (oxygen atom's atomic mass) × (the number of oxygen atoms) + (nitrogen atom's atomic mass) × (the number of nitrogen atoms) + (chlorine atom's atomic mass) × (the number of chlorine atoms)

Atomic mass (calculated): C, 12.0000, H, 1.0078, O, 15.9949, N, 14.0031, Cl, 34.9689

4. Compare the calculated value with the result of HR-ESI-MS until they are almost the same (± 0.0006).