

## Supplementary information

# NOVEL BENZOFURANOID NORLIGANA FROM THE AERIAL PARTS OF *ASPARAGUS* *COCHINCHINENSIS* AND THEIR BIOLOGICAL ACTIVITY

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## Contents of supplemental material

**Figure S1-1-1-6.** NMR spectra of compound 1.

**Figure S2.** (-)-HRESIMS of compound 1.

**Figure S3.** UV of compound 1.

**Figure S4.** IR of compound 1.

**Figure S5-1-5-6.** NMR spectra of compound 2.

**Figure S6.** (-)-HRESIMS of compound 2.

**Figure S7.** UV of compound 2.

**Figure S8.** IR of compound 2.

**Figure S9-1-9-6.** NMR spectra of compound 3.

**Figure S10.** (-)-HRESIMS of compound 3.

**Figure S11.** UV of compound 3.

**Figure S12.** IR of compound 3.

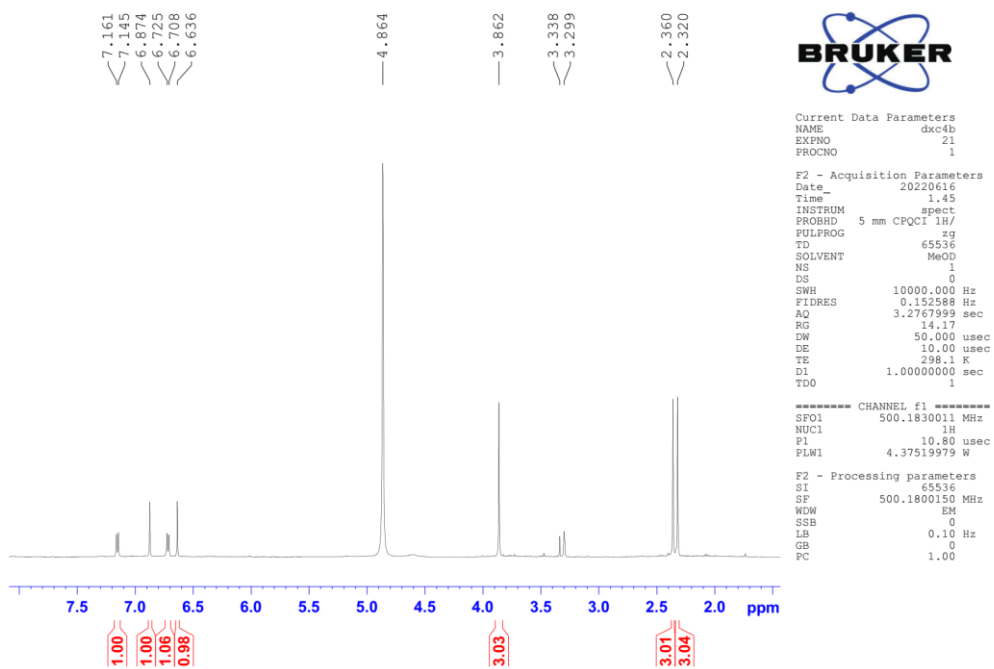


Figure S1-1.  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **1**.

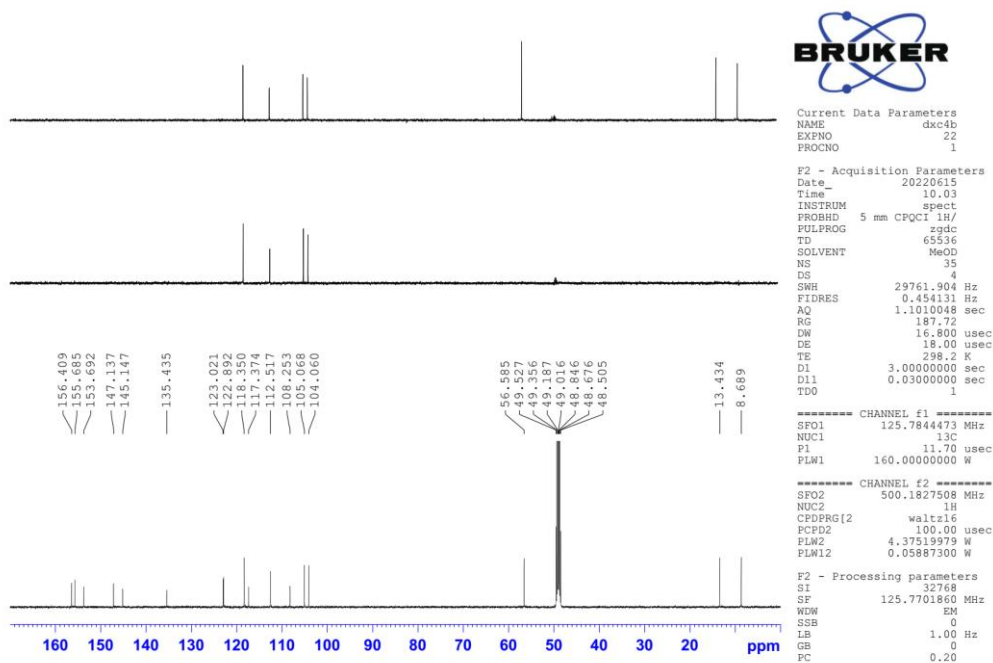


Figure S1-2.  $^{13}\text{C}$  NMR and DEPT (125MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **1**.

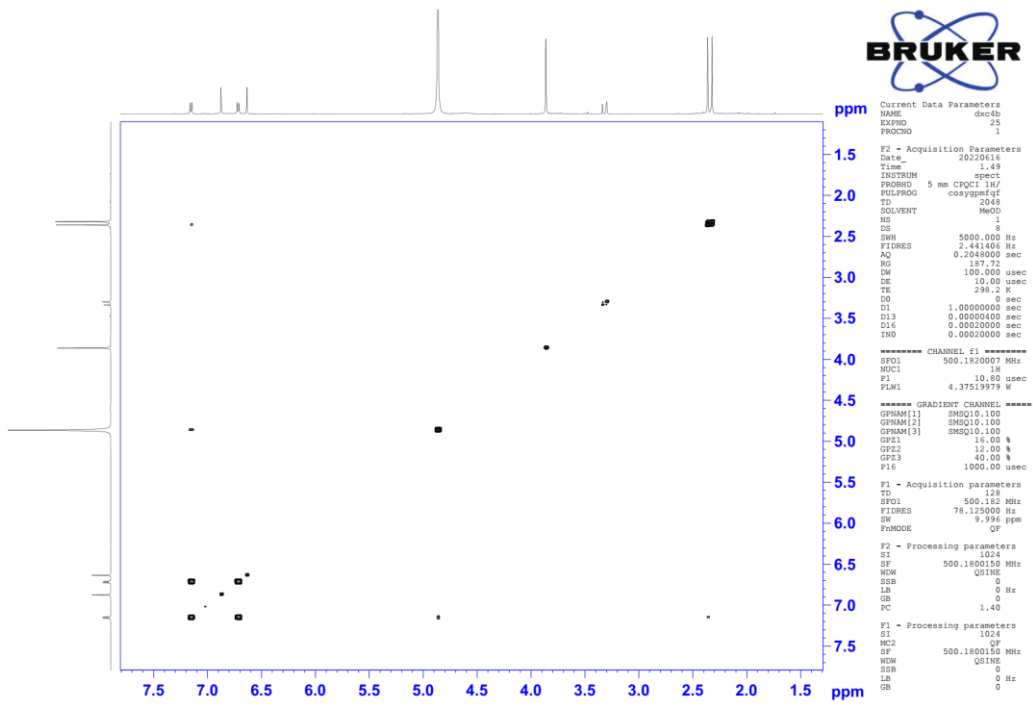


Figure S1-3. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 1.

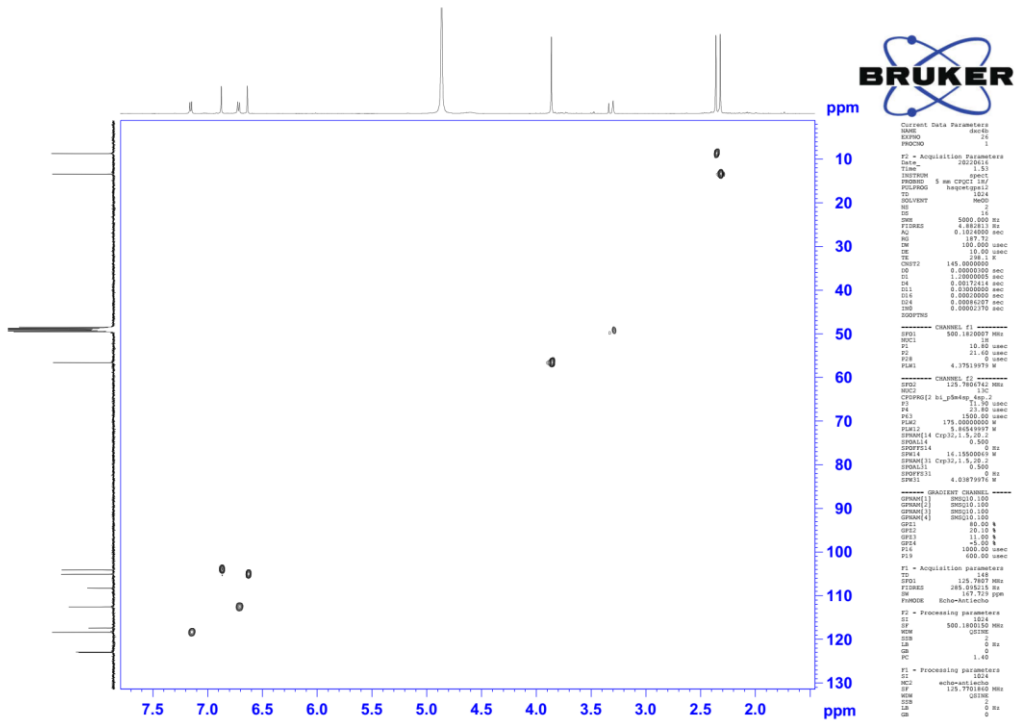


Figure S1-4. HSQC spectrum of compound 1.

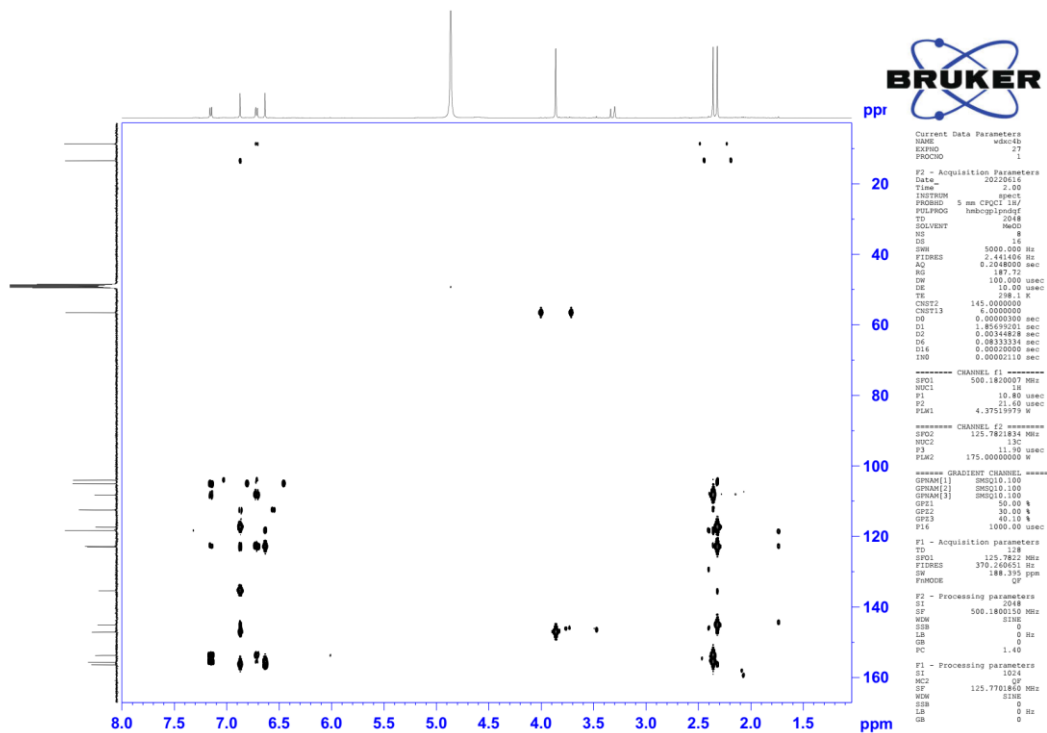


Figure S1-5. HMBC spectrum of compound 1.

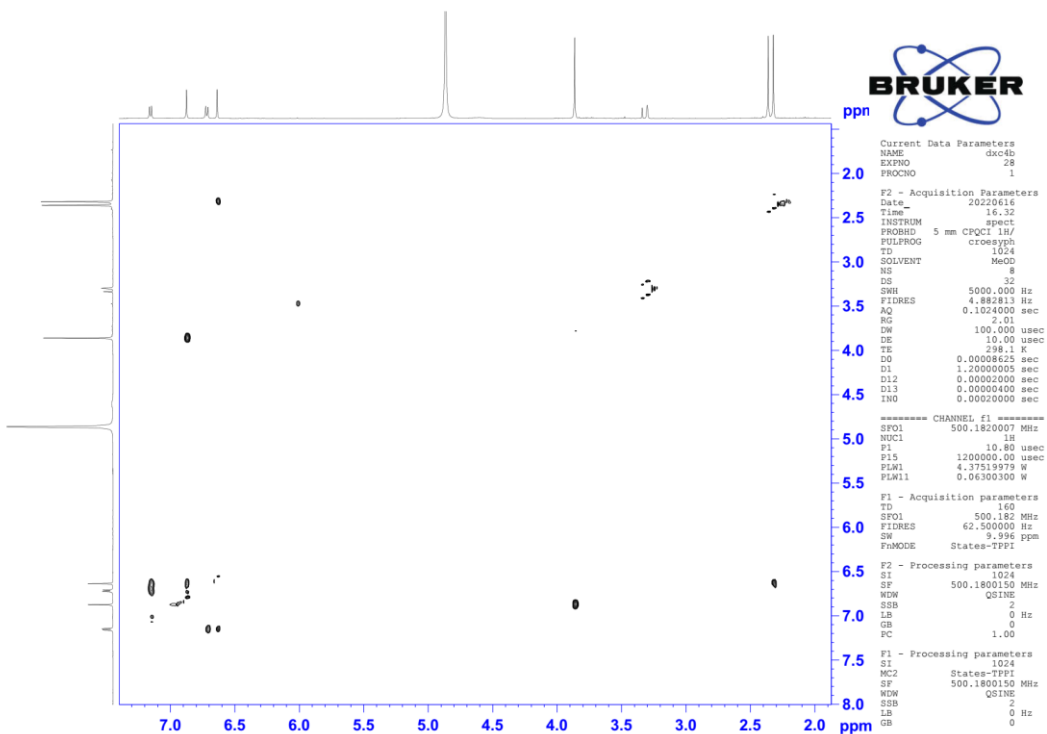


Figure S1-6. ROESY spectrum of compound 1.

Data File: E:\DATA\2022\0615\wdx-4b.lcd

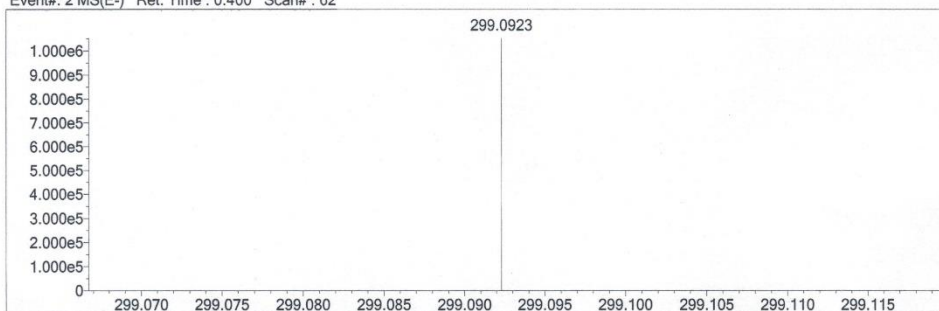
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2H	1	0	0	Na	1	0	0	Co	2	0	0	I	3	0	0	
B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	50	Si	4	0	0	Se	2	0	0					
N	3	0	10	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

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 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

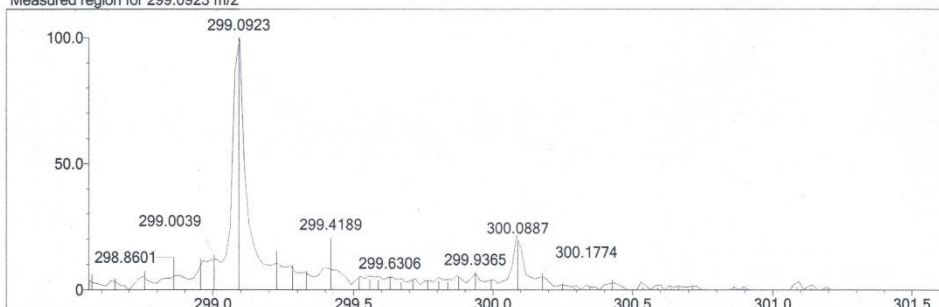
DBE Range: not fixed  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: OR

Electron Ions: both  
 Use MSn Info: yes  
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 Max Results: 30

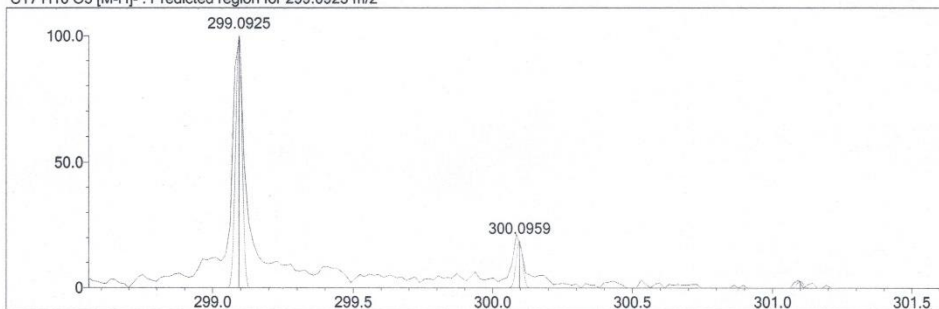
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Measured region for 299.0923 m/z

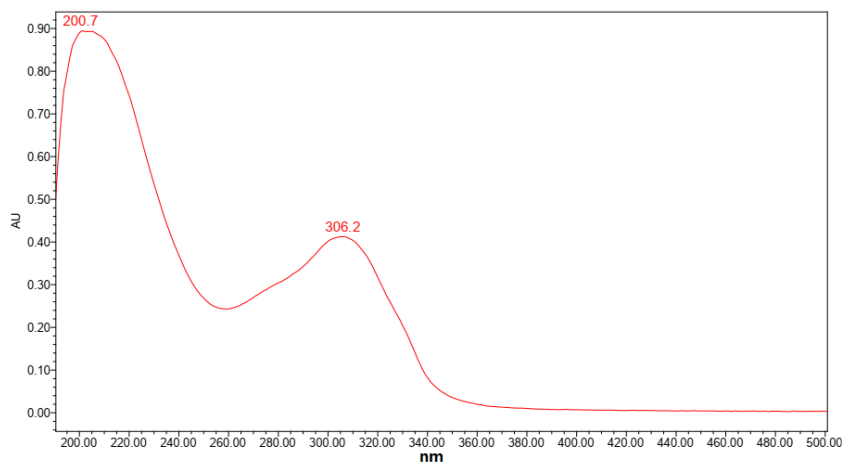


C17 H16 O5 [M-H]- : Predicted region for 299.0925 m/z

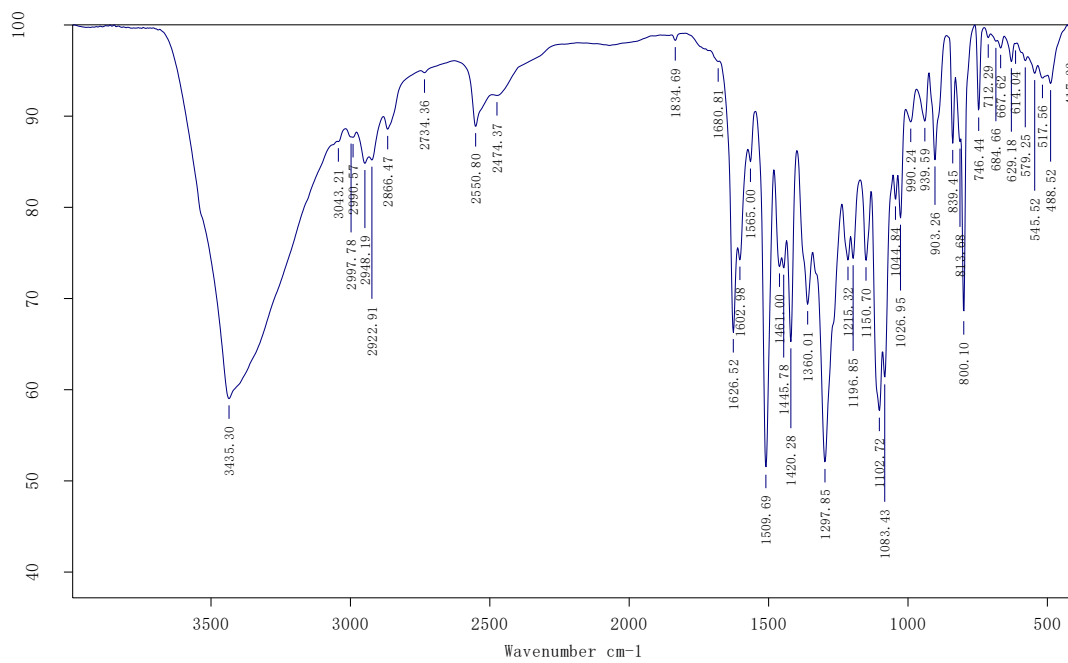


Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C17 H16 O5	[M-H]-	299.0923	299.0925	-0.2	-0.67	10.0

Figure S2. (-)-HRESIMS of compound 1.



**Figure S3.** UV spectra of compound 1.



**Figure S4.** IR spectra of compound 1.

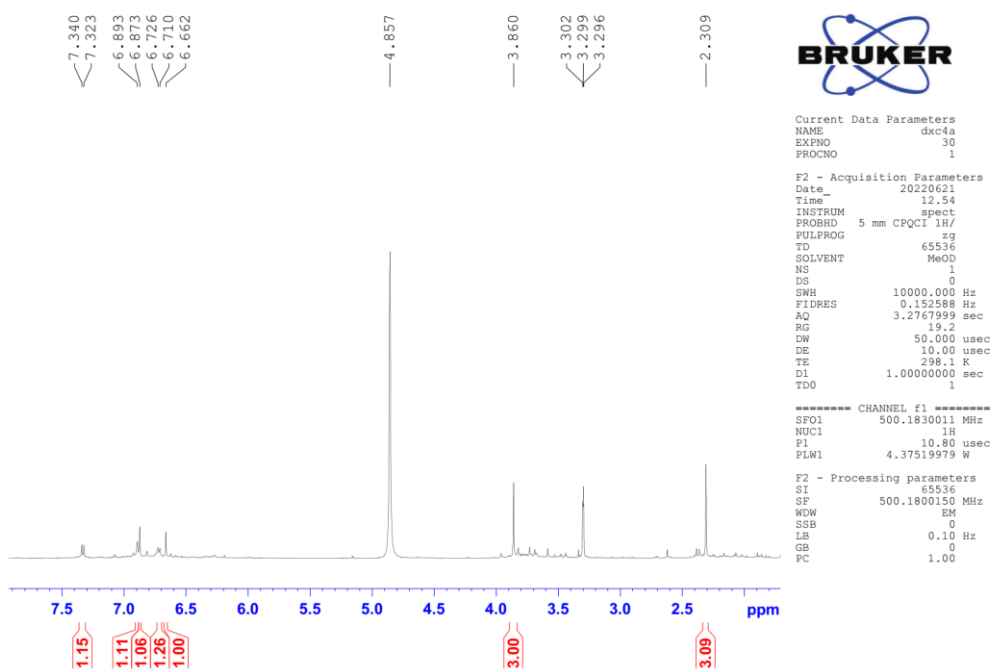


Figure S5-1.  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 2.

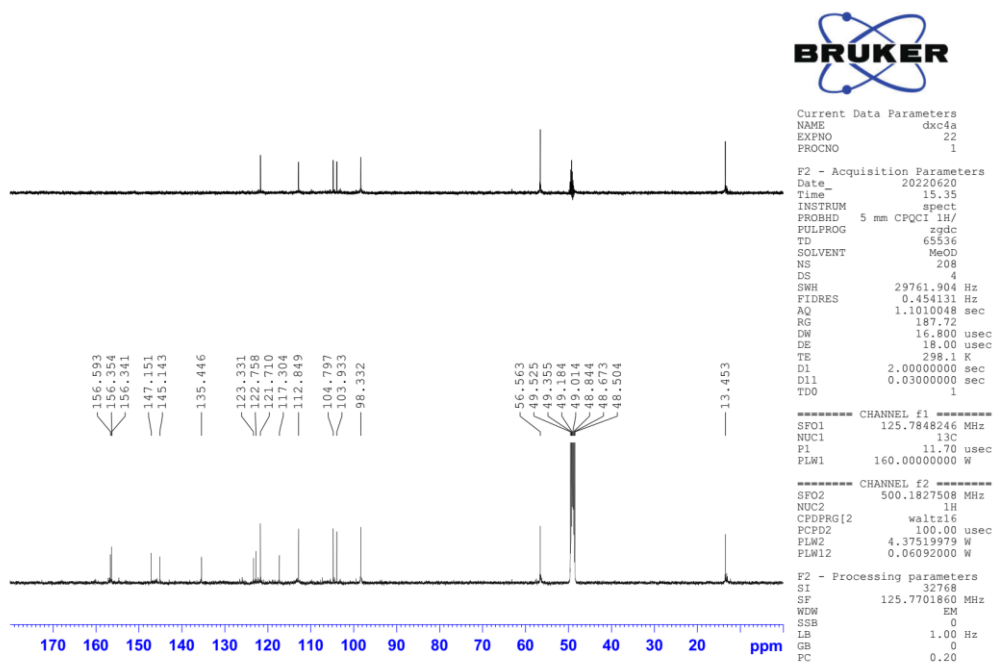


Figure S5-2.  $^{13}\text{C}$  NMR and DEPT (125 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 2.



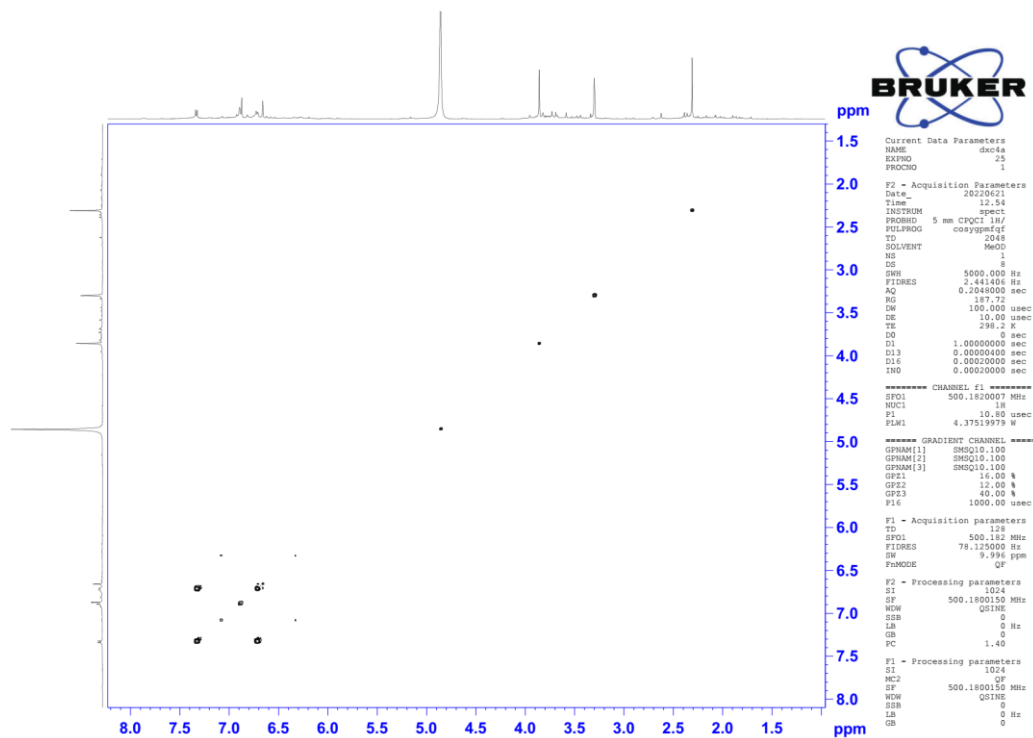


Figure S5-3.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 2.

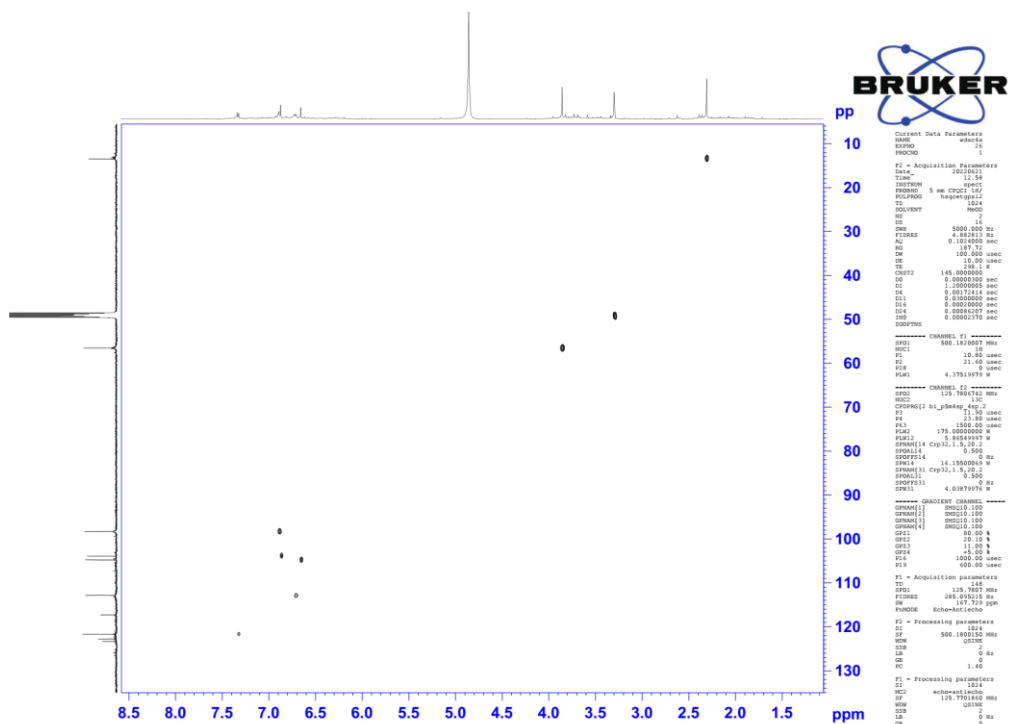


Figure S5-4. HSQC spectrum of compound 2.

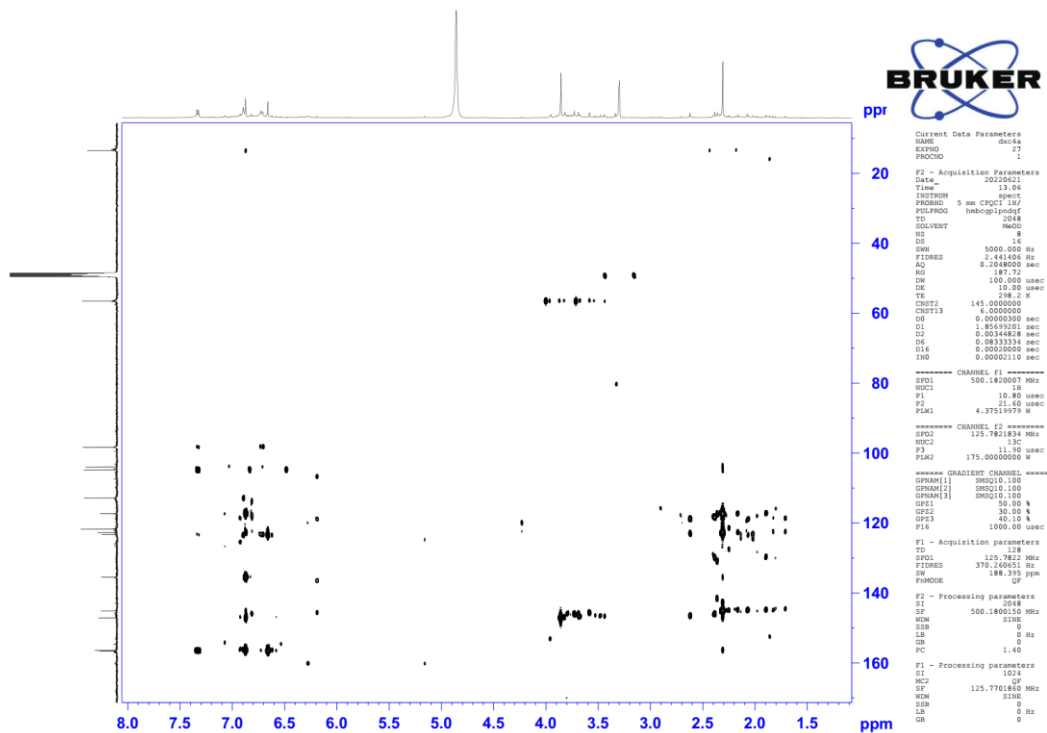


Figure S5-5. HMBC spectrum of compound 2.

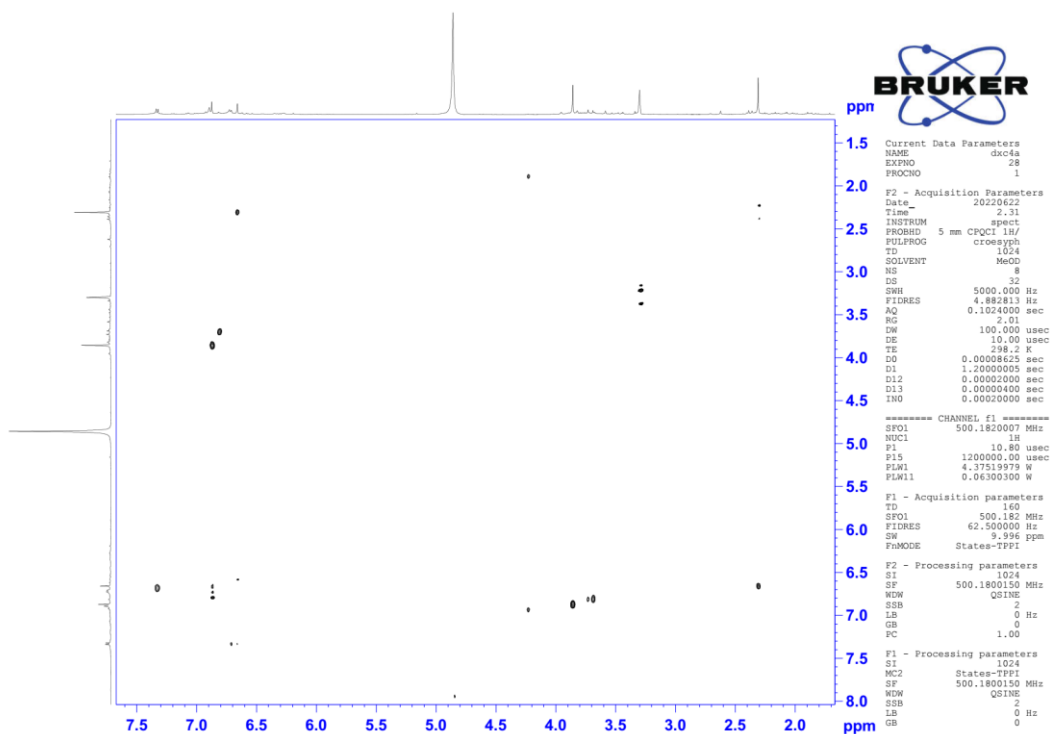


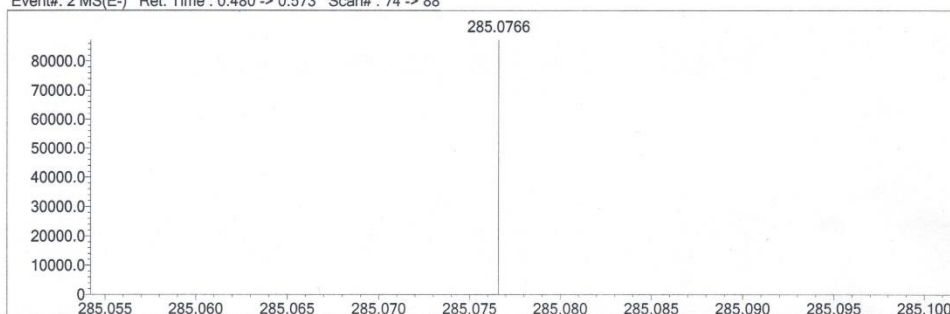
Figure S5-6. ROESY spectrum of compound 2.

Data File: E:\DATA\2022\0621\wdx-4a.lcd

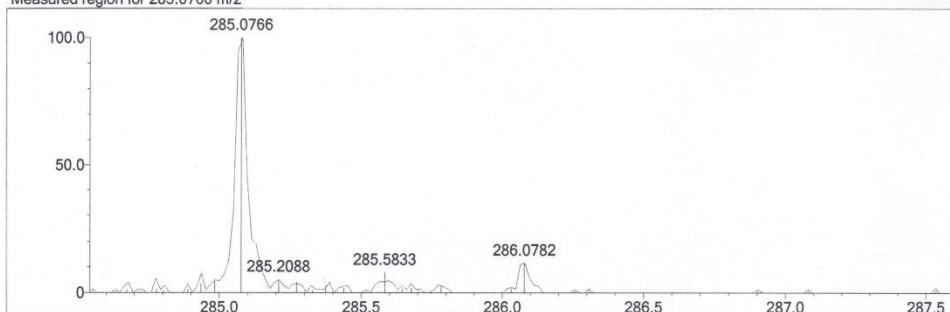
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2H	1	0	0	Na	1	0	0	Co	2	0	0	I	3	0	0	
B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	50	Si	4	0	0	Se	2	0	0					
N	3	0	10	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 5  
 DBE Range: not fixed  
 Electron Ions: both  
 HC Ratio: unlimited  
 Apply N Rule: no  
 Use MSn Info: yes  
 Max Isotopes: all  
 Isotope RI (%): 1.00  
 Isotope Res: 10000  
 MSn Iso RI (%): 75.00  
 MSn Logic Mode: OR  
 Max Results: 30

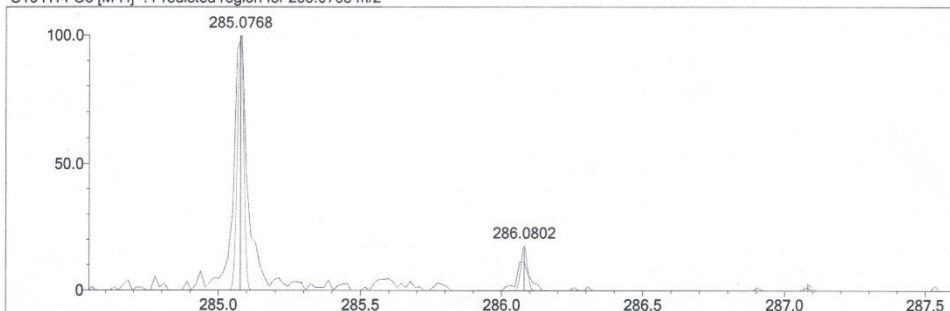
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Measured region for 285.0766 m/z

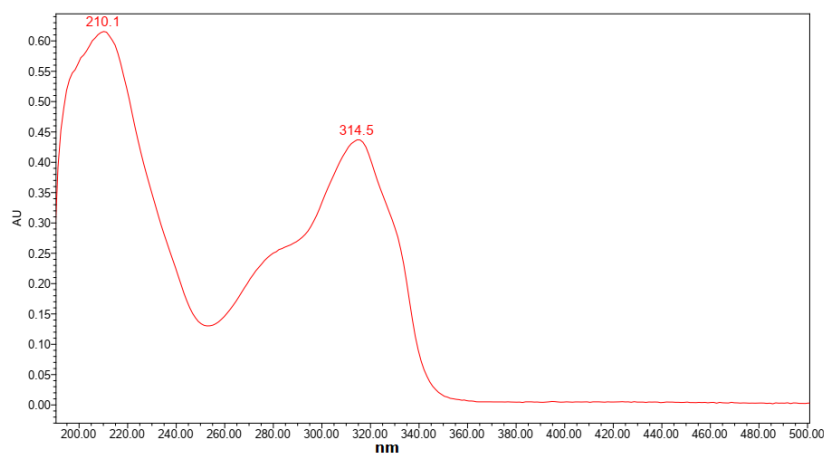


C16 H14 O5 [M-H]- : Predicted region for 285.0768 m/z

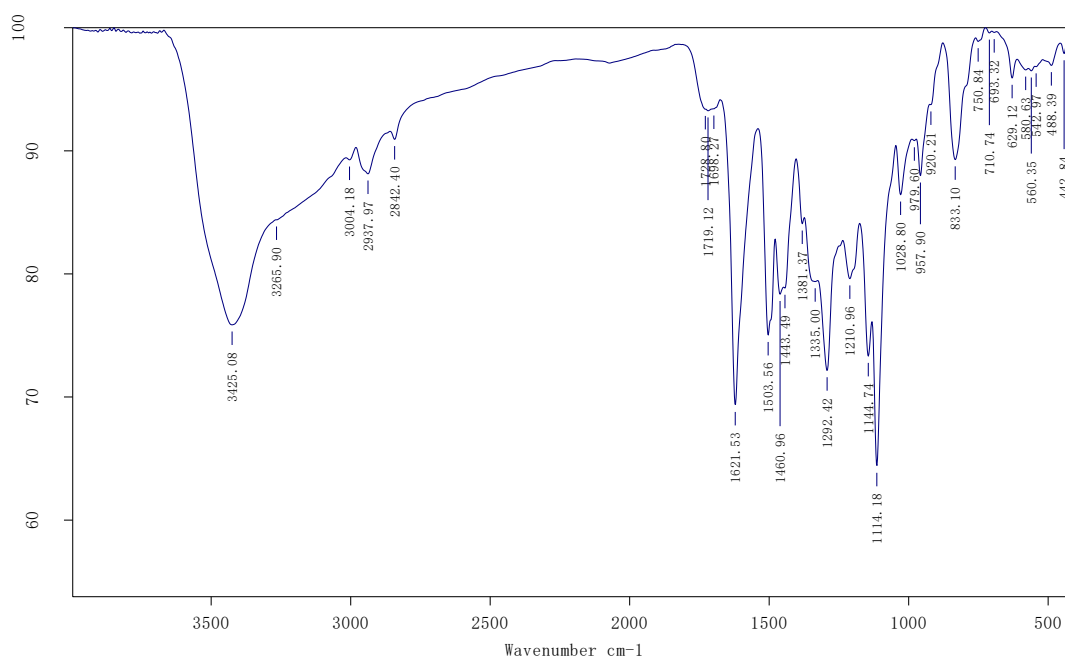


Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C16 H14 O5	[M-H]-	285.0766	285.0768	-0.2	-0.70	10.0

Figure S6. (-)-HRESIMS of compound 2.



**Figure S7.** UV spectra of compound **2**.



**Figure S8.** IR spectra of compound **2**.

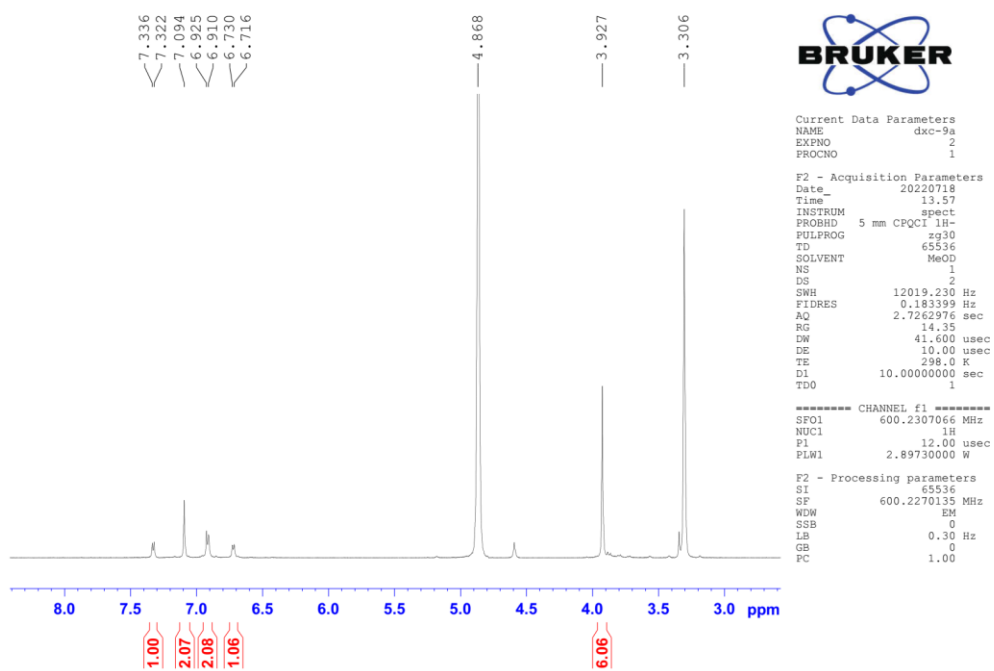


Figure S9-1.  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **3**.

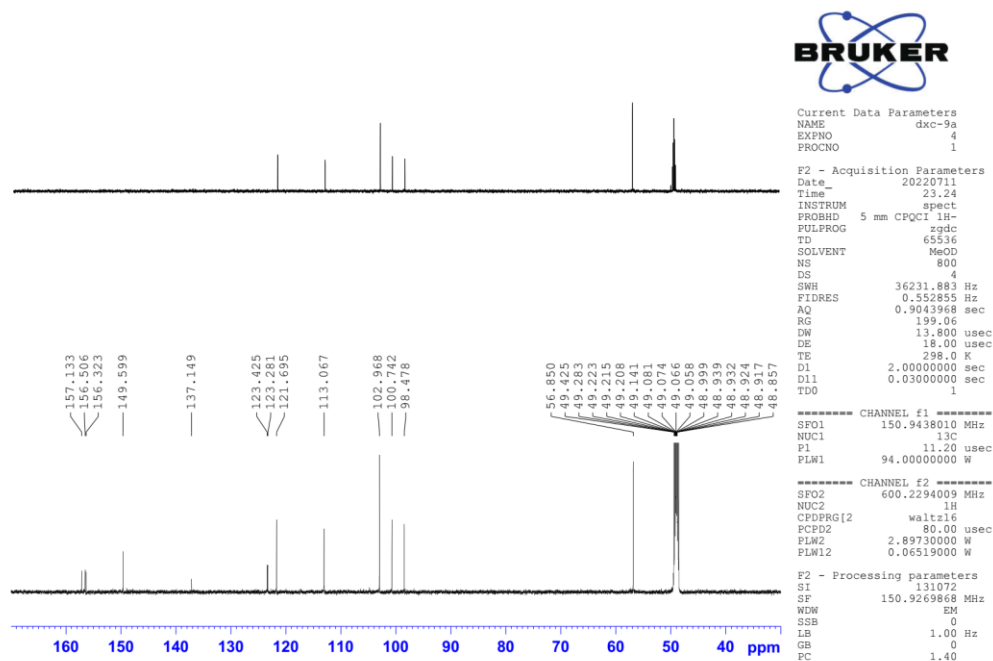


Figure S9-2.  $^{13}\text{C}$  NMR and DEPT (150 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **3**.

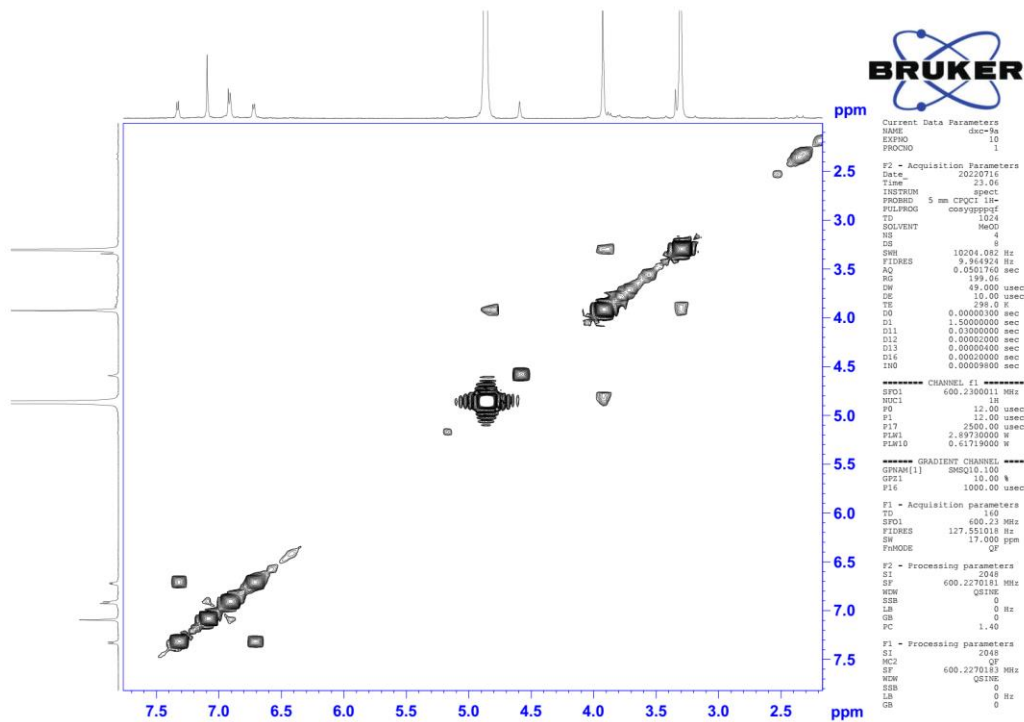


Figure S9-3.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 3.

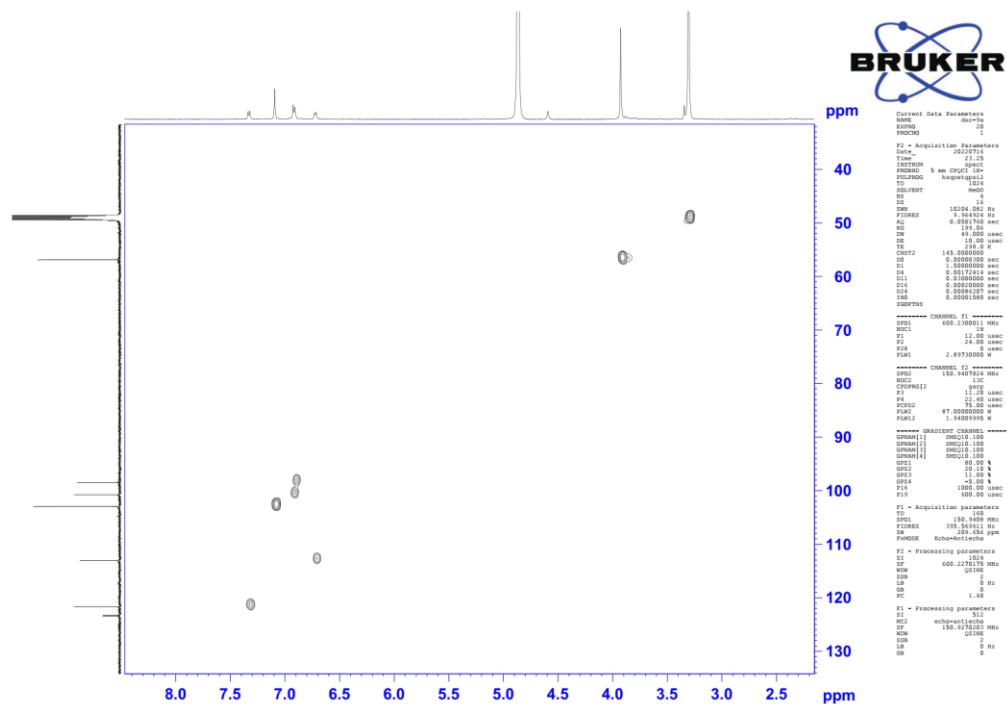


Figure S9-4. HSQC spectrum of compound 3.

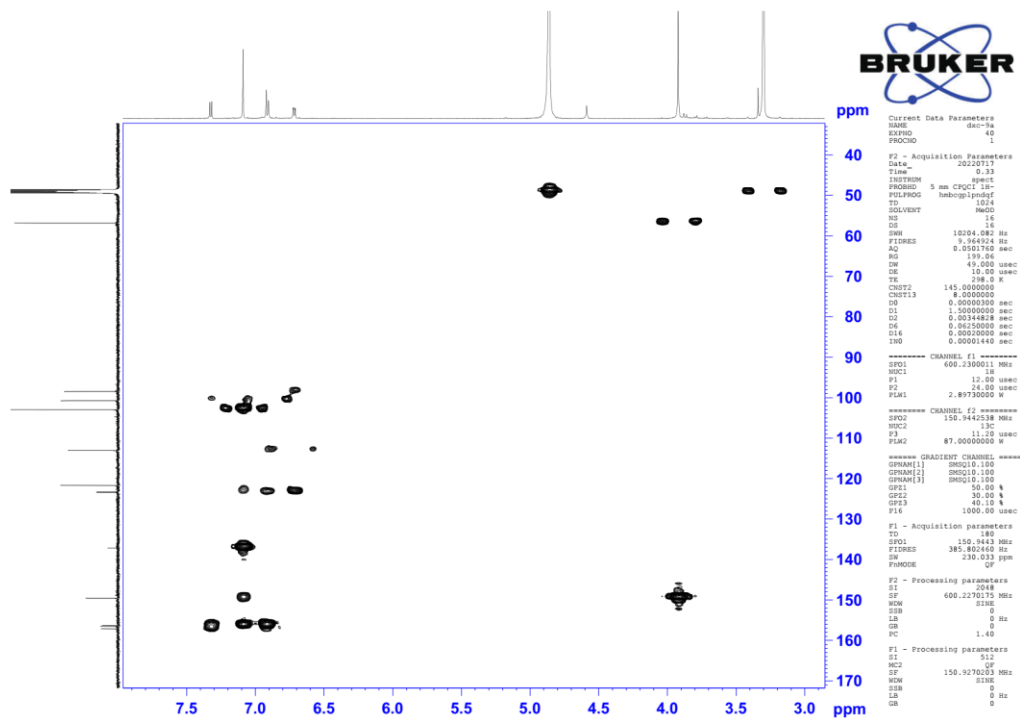


Figure S9-5. HMBC spectrum of compound 3.

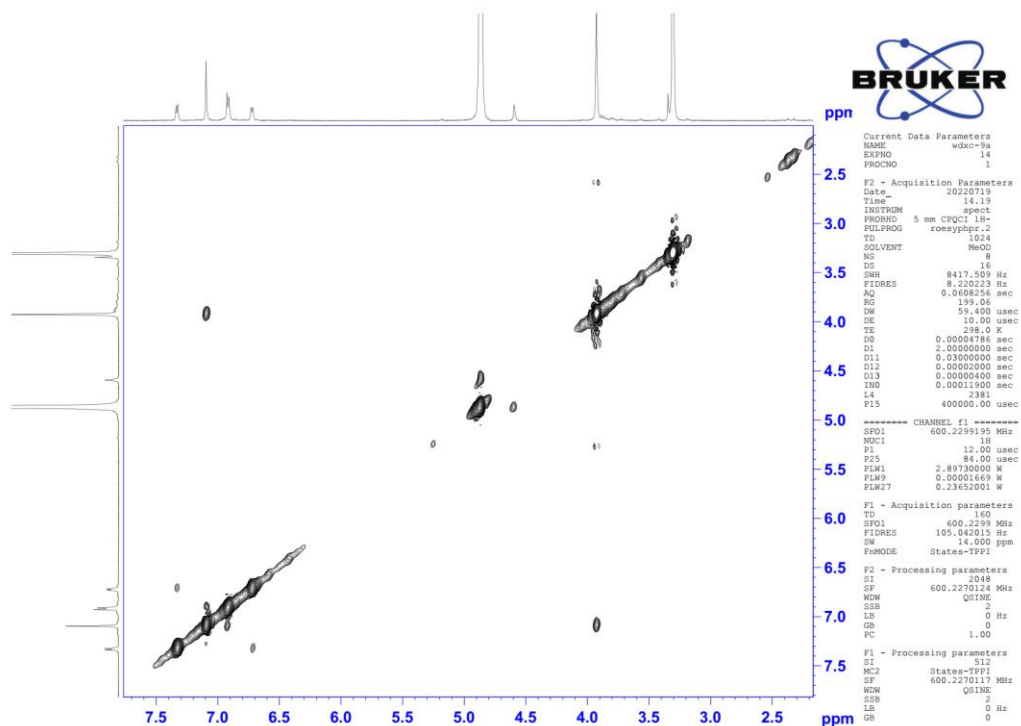


Figure S9-6. ROESY spectrum of compound 3.

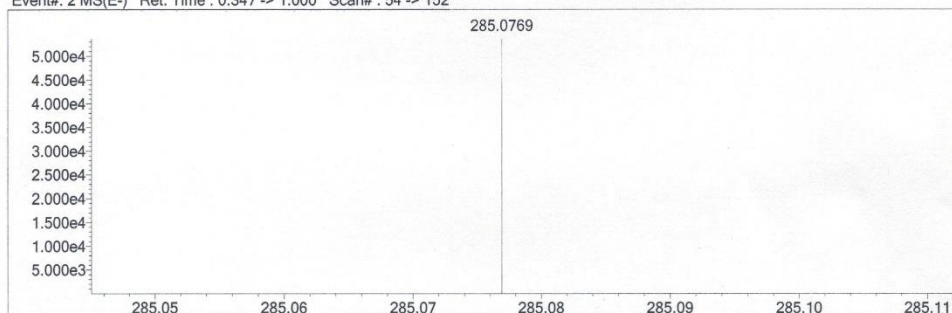
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H	1	5	100	F	1	0	0	Cl	1	0	0	Ag	1	0	0	H
2H	1	0	0	Na	1	0	0	Co	2	0	0	I	3	0	0	
B	3	0	0	Mg	2	0	0	Cu	2	0	0	Ir	3	0	0	
C	4	5	50	Si	4	0	0	Se	2	0	0					
N	3	0	0	P	3	0	0	Br	1	0	0					
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 5  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

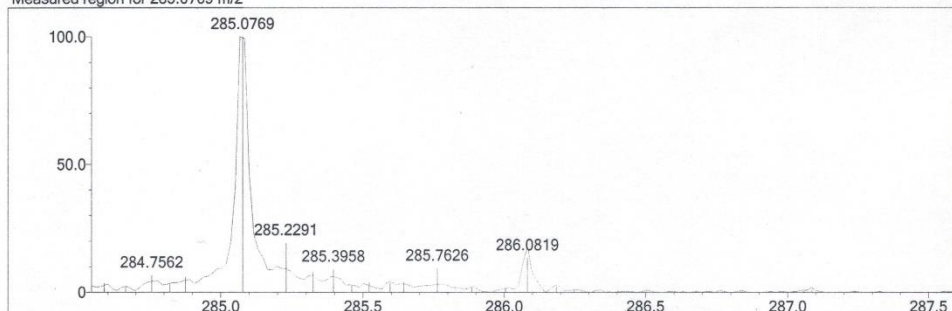
DBE Range: not fixed  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: OR

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 30

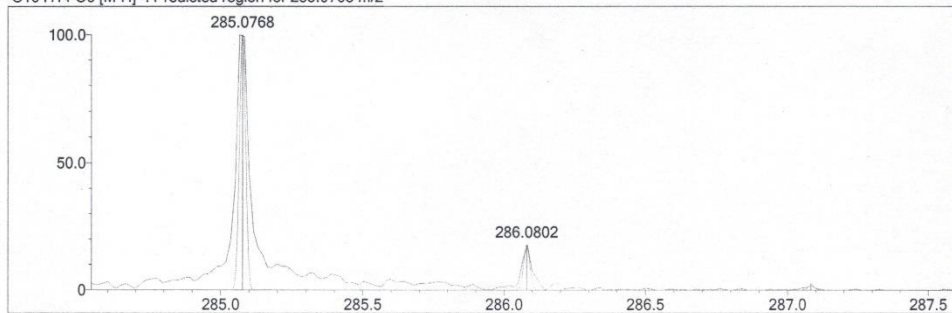
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Measured region for 285.0769 m/z



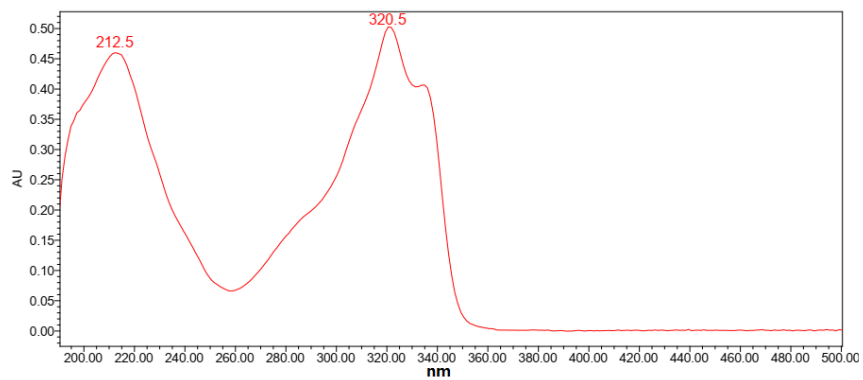
C16 H14 O5 [M-H]- : Predicted region for 285.0768 m/z



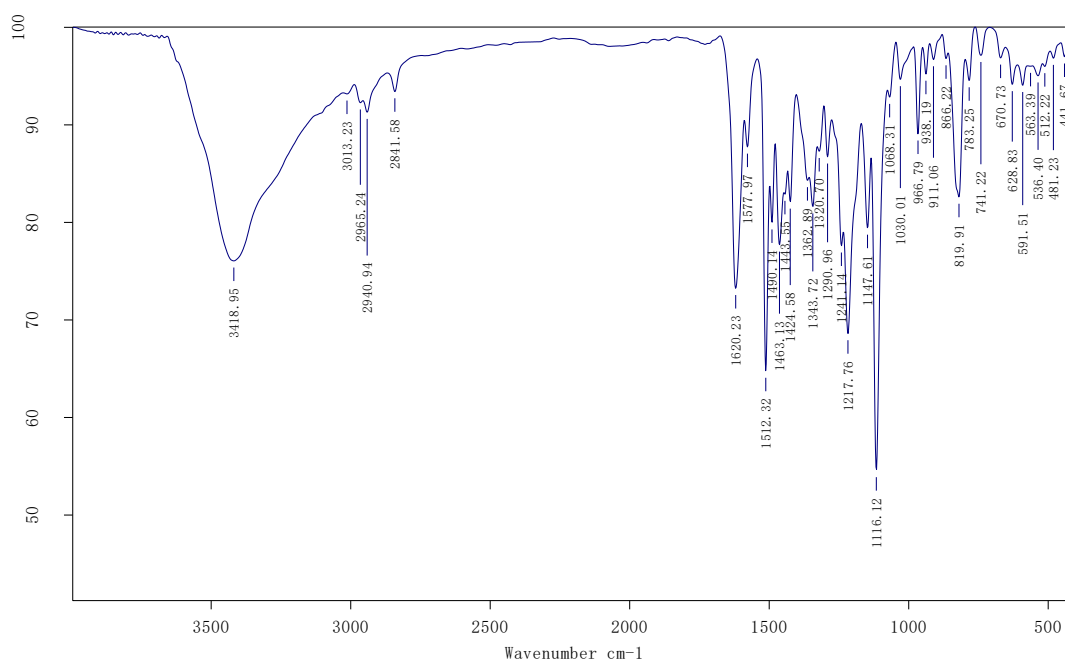
Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C16 H14 O5	[M-H]-	285.0769	285.0768	0.1	0.35	10.0

Figure S10. (-)-HRESIMS of compound 3.





**Figure S11.** UV spectra of compound 3.



**Figure S12.** IR spectra of compound 3.