

## **Meirols A–C: Bioactive Catecholic Compounds from the Marine-Derived Fungus *Meira* sp. 1210CH-42**

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# Contents

Figure S1. $^1\text{H}$ NMR spectrum of 1 in $\text{CD}_3\text{OD}$ (600 MHz).	3
Figure S2. $^{13}\text{C}$ NMR spectrum of 1 in $\text{CD}_3\text{OD}$ (150 MHz).	3
Figure S3. HSQC spectrum of 1 in $\text{CD}_3\text{OD}$ .	4
Figure S4. COSY spectrum of 1 in $\text{CD}_3\text{OD}$ .	4
Figure S5. HMBC spectrum of 1 in $\text{CD}_3\text{OD}$ .	5
Figure S6. HR-ESIMS spectrum of 1.	6
Figure S7. $^1\text{H}$ NMR spectrum of 2 in $\text{CD}_3\text{OD}$ (600 MHz).	7
Figure S8. $^{13}\text{C}$ NMR spectrum of 2 in $\text{CD}_3\text{OD}$ (150 MHz).	7
Figure S9. HSQC spectrum of 2 in $\text{CD}_3\text{OD}$ .	8
Figure S10. COSY spectrum of 2 in $\text{CD}_3\text{OD}$ .	8
Figure S11. HMBC spectrum of 2 in $\text{CD}_3\text{OD}$ .	9
Figure S12. HR-ESIMS spectrum of 2.	10
Figure S13. UV spectrum of 2.	11
Figure S14. IR spectrum of 2.	12
Figure S15. $^1\text{H}$ NMR spectrum of 3 in $\text{CD}_3\text{OD}$ (600 MHz).	13
Figure S16. $^{13}\text{C}$ NMR spectrum of 3 in $\text{CD}_3\text{OD}$ (150 MHz).	13
Figure S17. HSQC spectrum of 3 in $\text{CD}_3\text{OD}$ .	14
Figure S18. COSY spectrum of 3 in $\text{CD}_3\text{OD}$ .	14
Figure S19. HMBC spectrum of 3 in $\text{CD}_3\text{OD}$ .	15
Figure S20. HR-ESIMS spectrum of 3.	16
Figure S21. UV spectrum of 3.	17
Figure S22. IR spectrum of 3.	18
Figure S23. $^1\text{H}$ NMR spectrum of 4 in $\text{CD}_3\text{OD}$ (600 MHz).	19
Figure S24. $^{13}\text{C}$ NMR spectrum of 4 in $\text{CD}_3\text{OD}$ (150 MHz).	19
Figure S25. HSQC spectrum of 4 in $\text{CD}_3\text{OD}$ .	20
Figure S26. COSY spectrum of 4 in $\text{CD}_3\text{OD}$ .	20
Figure S27. HMBC spectrum of 4 in $\text{CD}_3\text{OD}$ .	21
Figure S28. HR-ESIMS spectrum of 4.	22
Figure S29. UV spectrum of 4.	23
Figure S30. IR spectrum of 4.	24
Figure S31. Initial geometry optimized conformers of 3.	25
Figure S32. Initial geometry optimized conformers of 4.	26
Table S1. Total Gibbs Free Energy and Boltzmann population of initial geometry optimized conformers of 3.	25
Table S2. The cartesian coordinates of conformers of 3.	25
Table S3. Total Gibbs Free Energy and Boltzmann population of initial geometry optimized conformers of 4.	26
Table S4. The cartesian coordinates of conformers of 4.	27

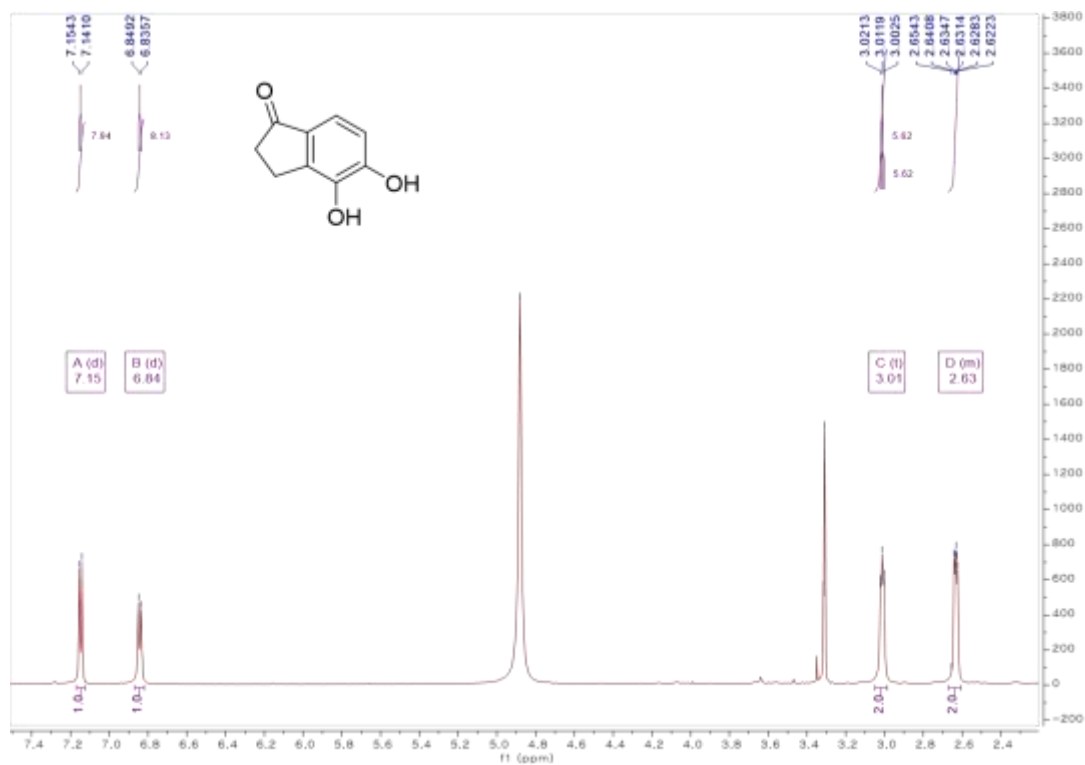


Figure S1. <sup>1</sup>H NMR spectrum of **1** in CD<sub>3</sub>OD (600 MHz).

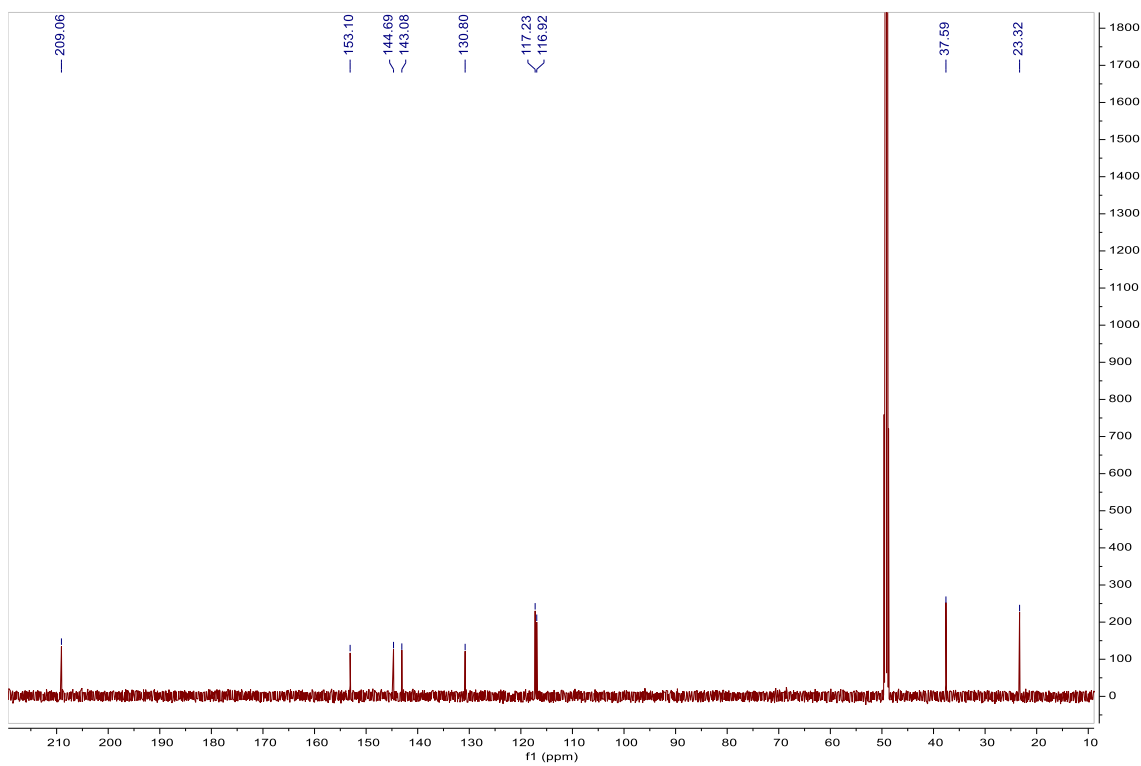


Figure S2. <sup>13</sup>C NMR spectrum of **1** in CD<sub>3</sub>OD (150 MHz).

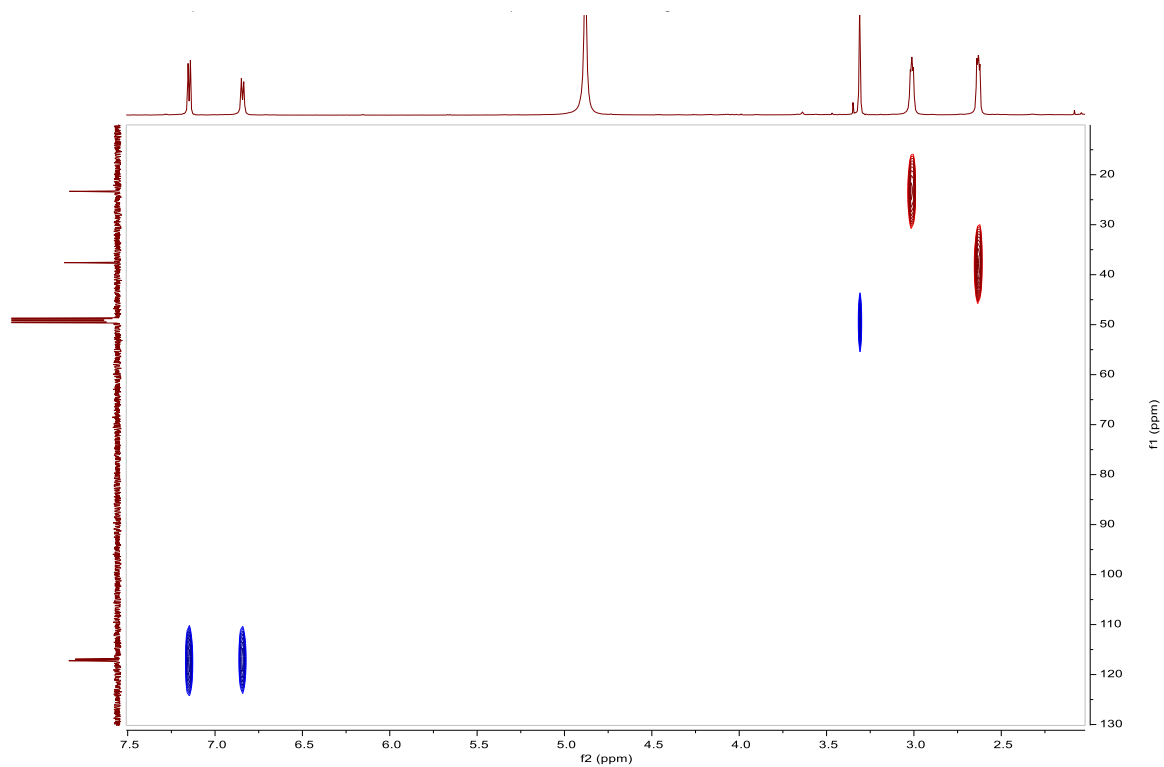


Figure S3. HSQC spectrum of **1** in CD<sub>3</sub>OD.

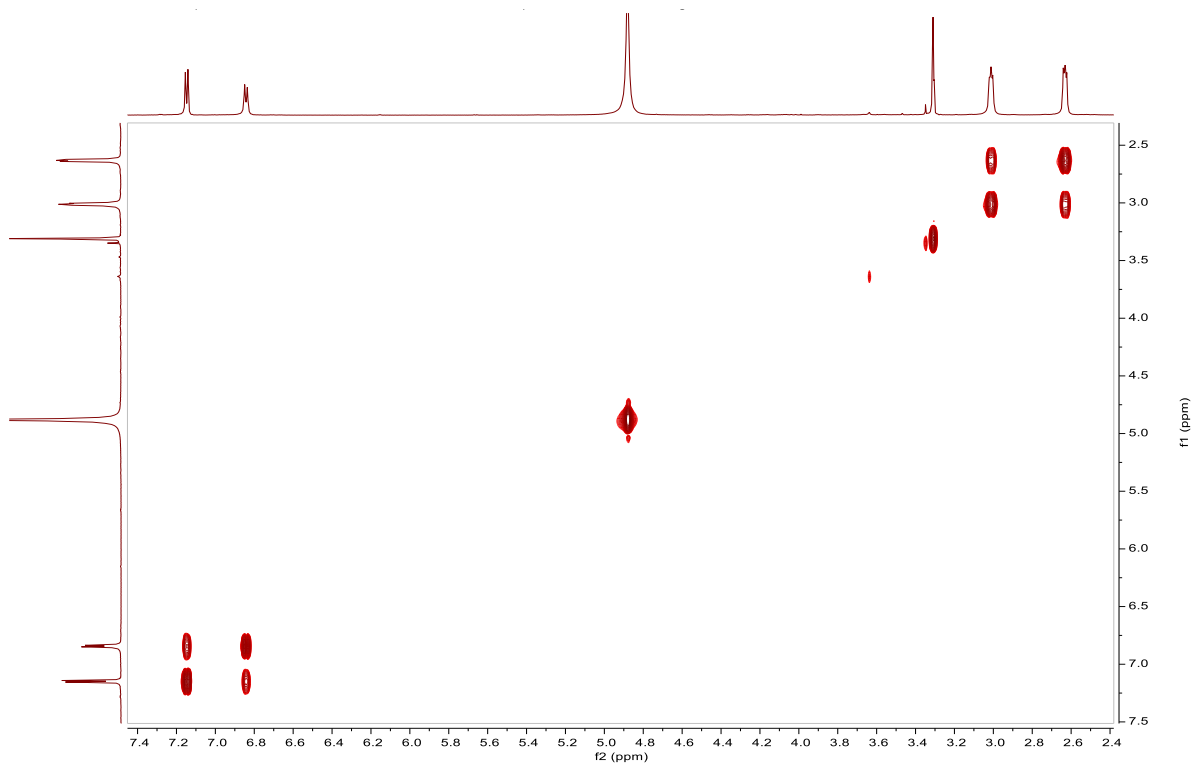


Figure S4. COSY spectrum of **1** in CD<sub>3</sub>OD.

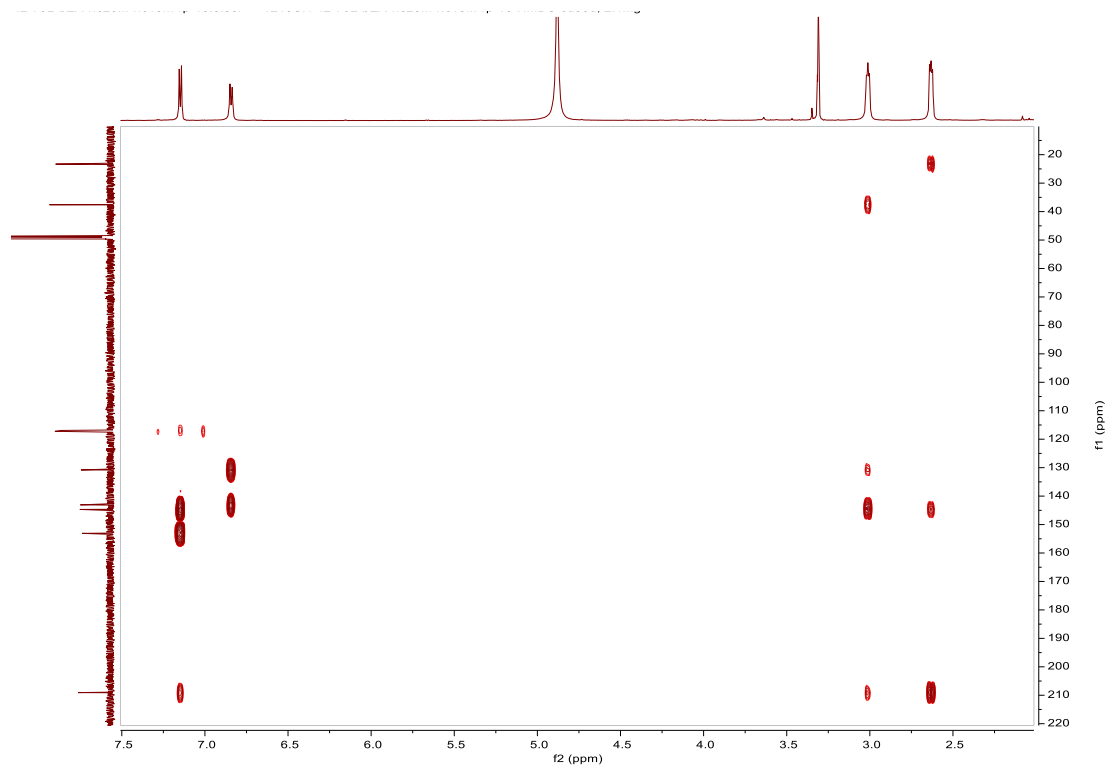
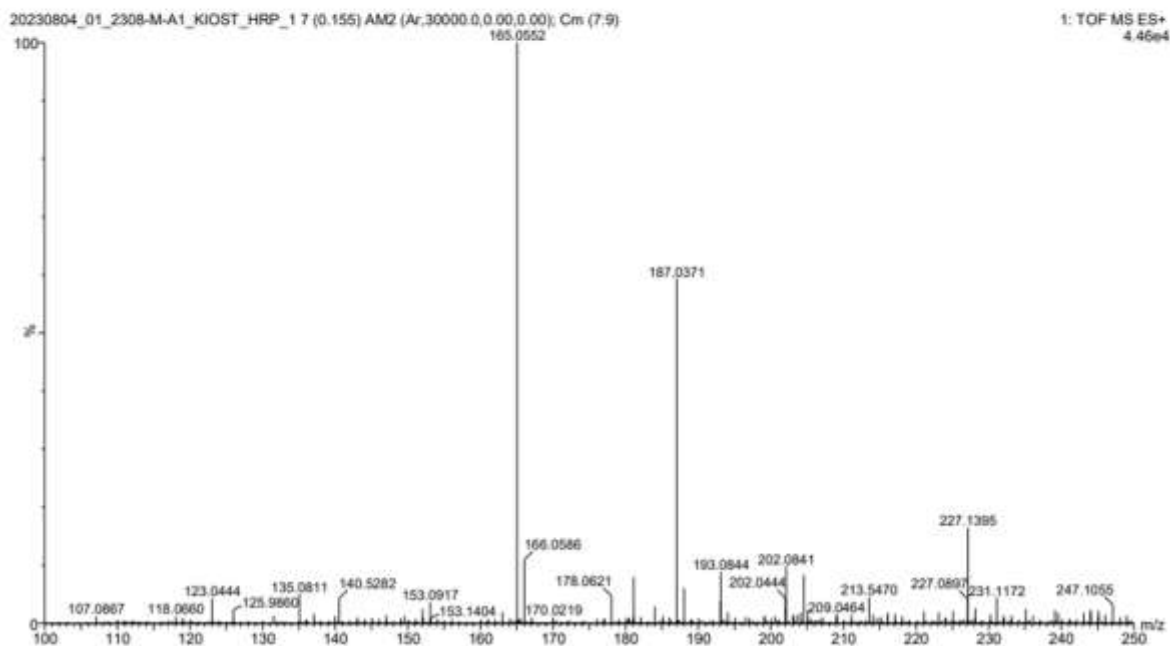


Figure S5. HMBC spectrum of **1** in CD<sub>3</sub>OD.

Sample : 01. 2308-M-A1

(+) ESI-MS

Range : 100-250 m/z



#### Elemental Composition Report

##### Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

##### Monoisotopic Mass, Even Electron Ions

Elements Used:

C: 0-10 H: 0-300 O: 0-5 Na: 0-1 Pt: 0-1

Minimum: -1.5

Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
165.0552	165.0552	0.0	0.0	5.5	990.7	n/a	n/a	C9 H9 O3
187.0371	187.0371	0.0	0.0	5.5	811.3	n/a	n/a	C9 H8 O3 Na

Figure S6. HR-ESIMS spectrum of **1**.

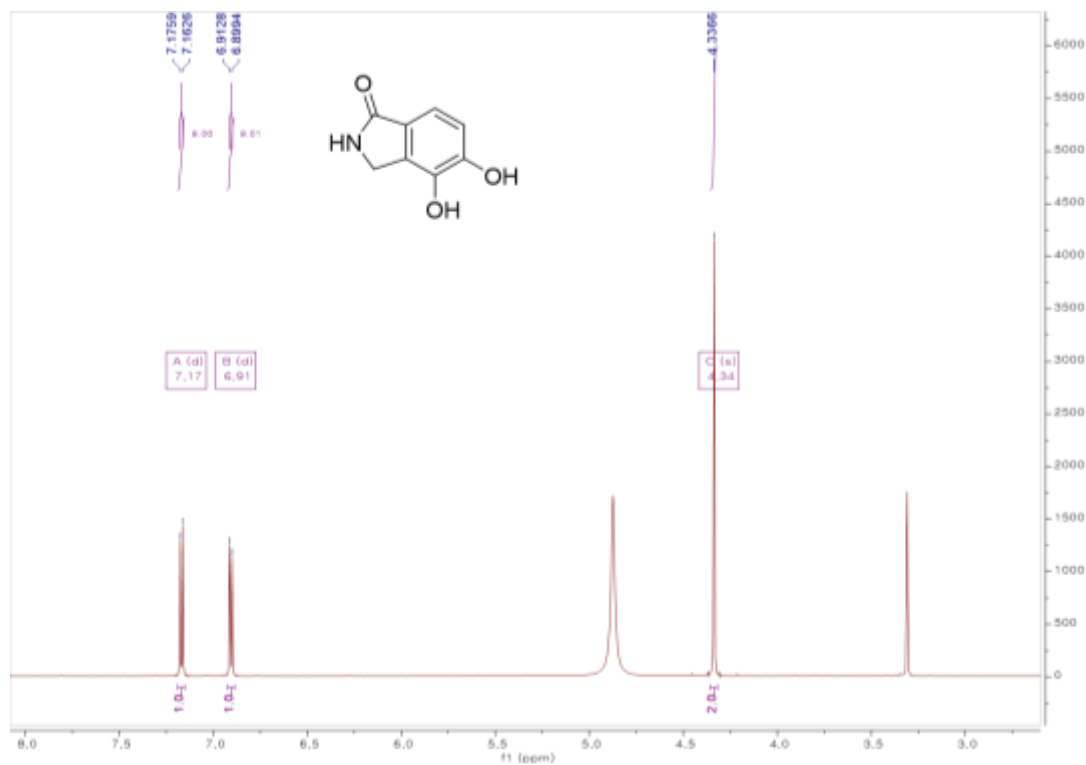


Figure S7. <sup>1</sup>H NMR spectrum of **2** in CD<sub>3</sub>OD (600 MHz).

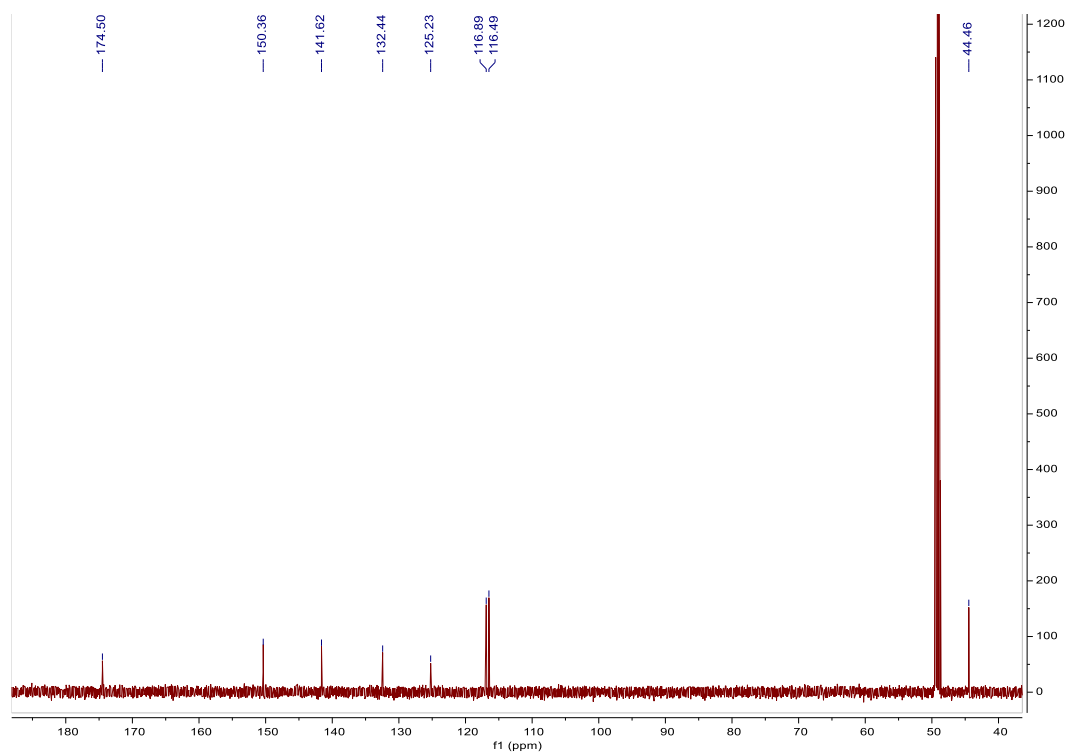


Figure S8. <sup>13</sup>C NMR spectrum of **2** in CD<sub>3</sub>OD (150 MHz).

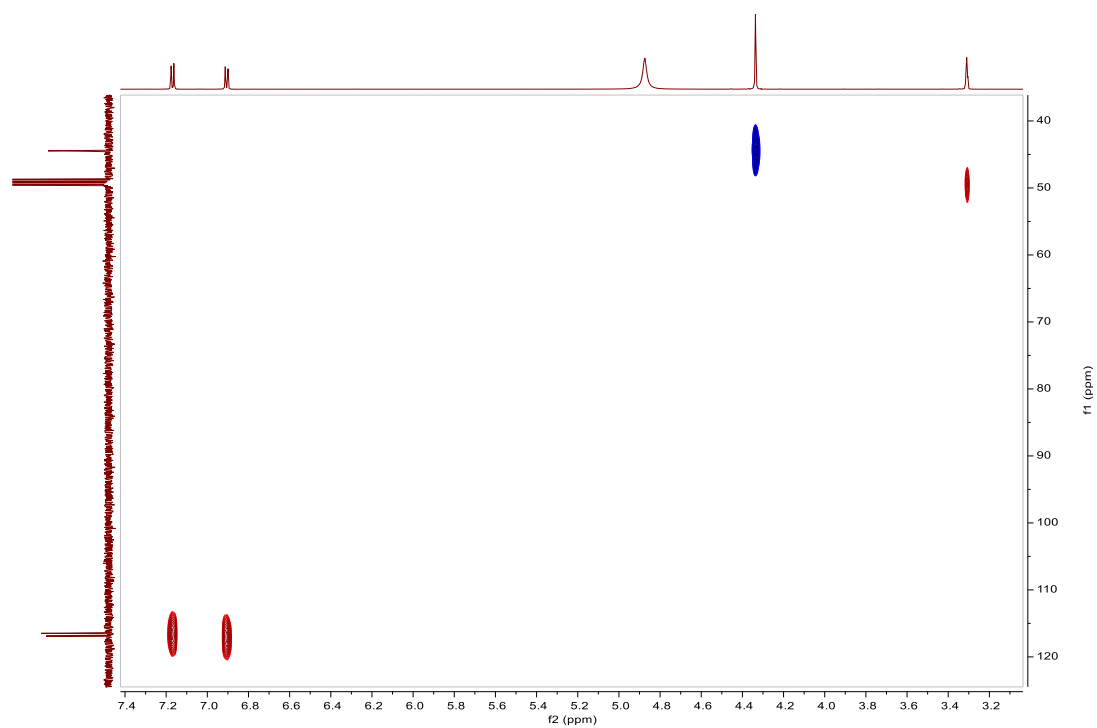


Figure S9. HSQC spectrum of **2** in  $\text{CD}_3\text{OD}$ .

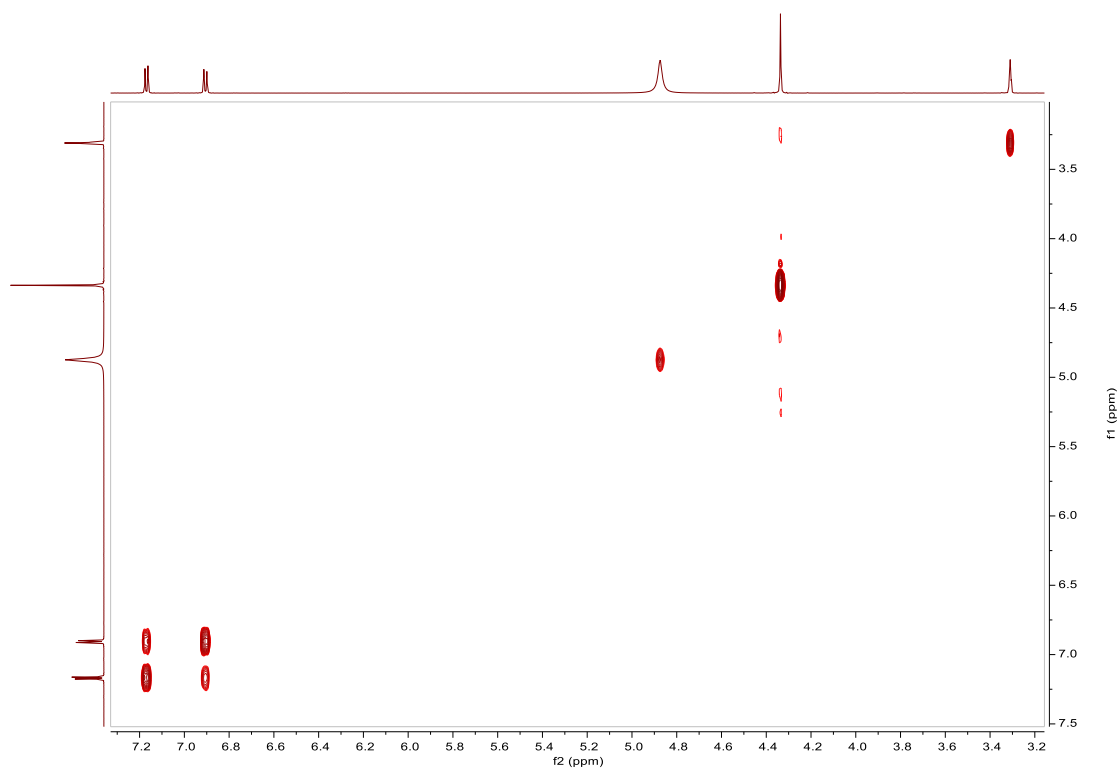


Figure S10. COSY spectrum of **2** in  $\text{CD}_3\text{OD}$ .



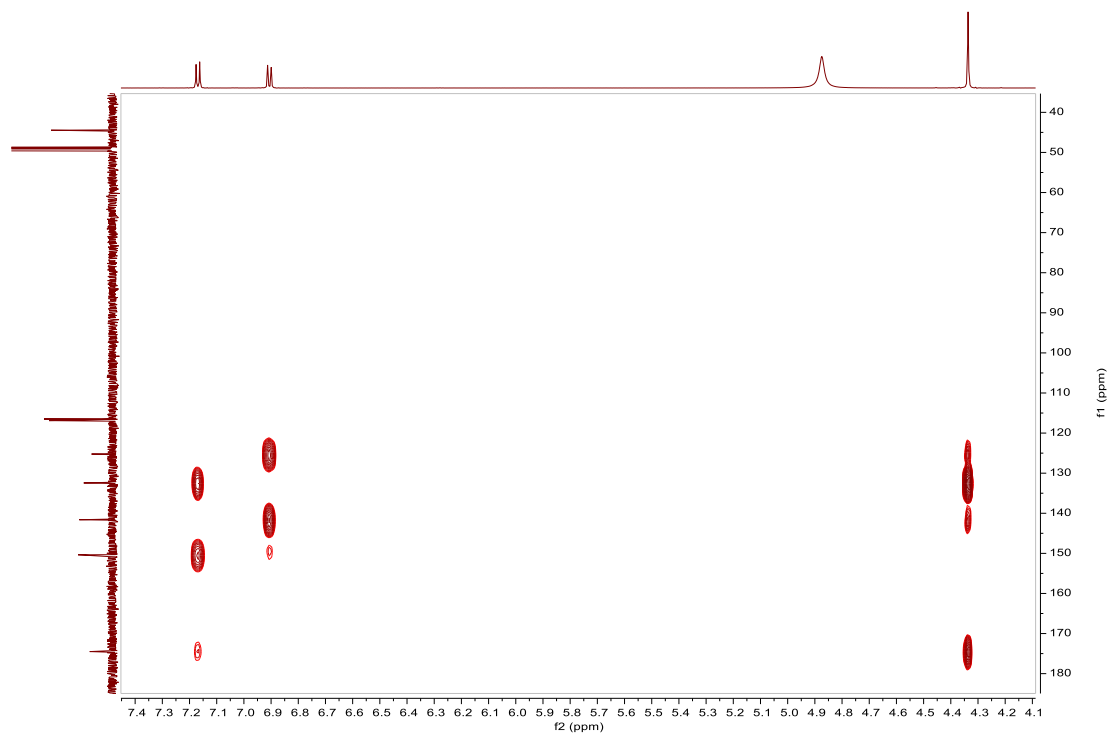
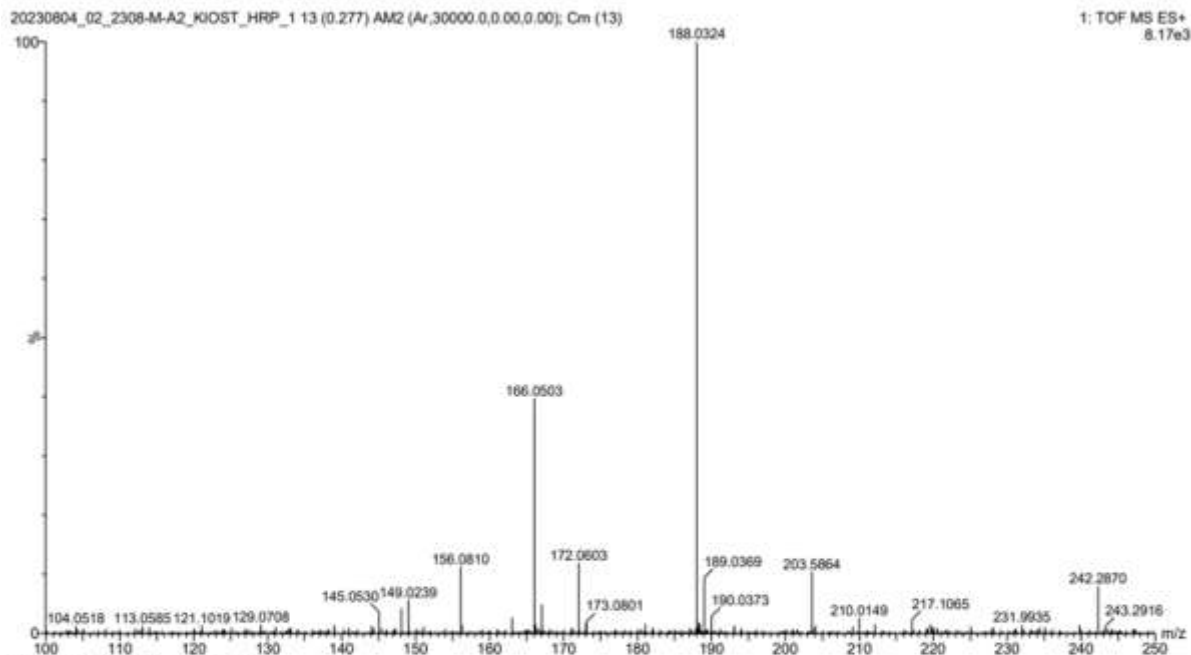


Figure S11. HMBC spectrum of **2** in CD<sub>3</sub>OD.

Sample : 02. 2308-M-A2

(+) ESI-MS

Range : 100-250 m/z



#### Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

Elements Used:

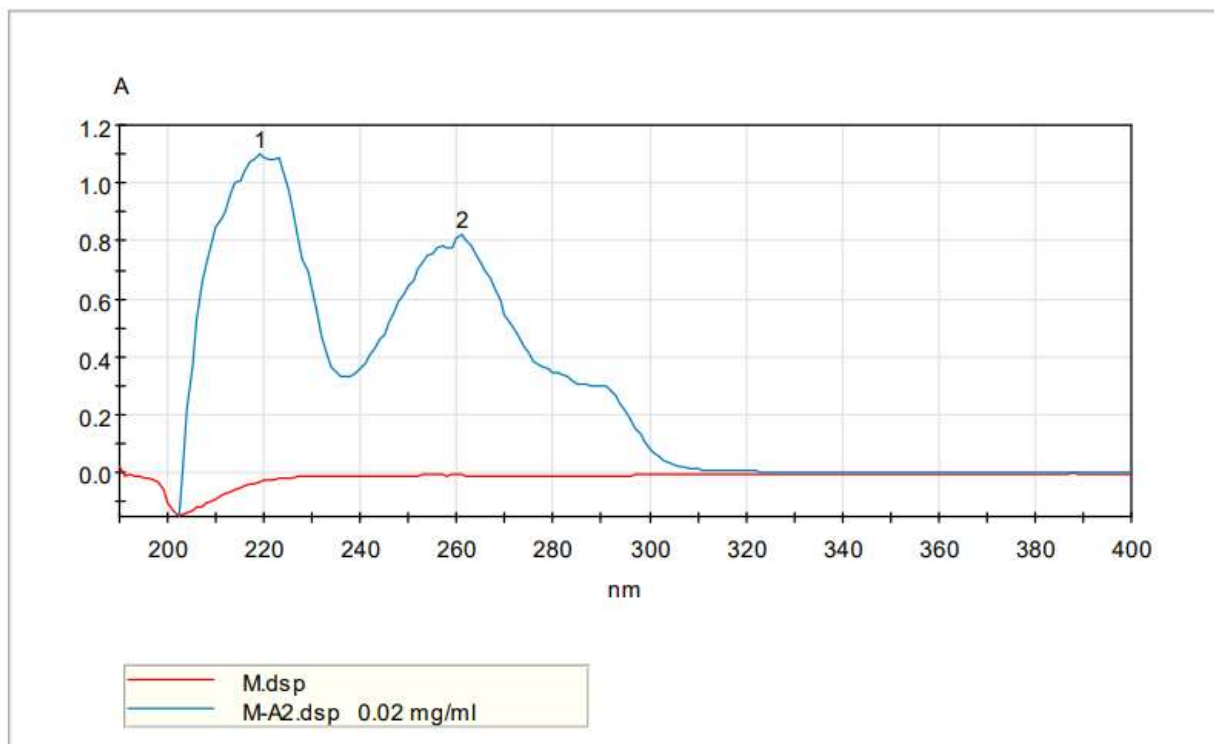
C: 0-10 H: 0-300 N: 0-2 O: 0-5 Na: 0-1 Pt: 0-1

Minimum:

Maximum: 5.0 10.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
166.0503	166.0504	-0.1	-0.6	5.5	227.9	n/a	n/a	C8 H8 N O3
188.0324	188.0324	0.0	0.0	5.5	337.1	n/a	n/a	C8 H7 N O3 Na

Figure S12. HR-ESIMS spectrum of **2**.



M-A2.dsp 0.02 mg/ml

Maxima Threshold: 0.1 A  
 1 219 nm; 1.100 A 2 261 nm; 0.824 A

M-A2.dsp 0.02 mg/ml  
 290 nm 0.301 A

Figure S13. UV spectrum of **2**.

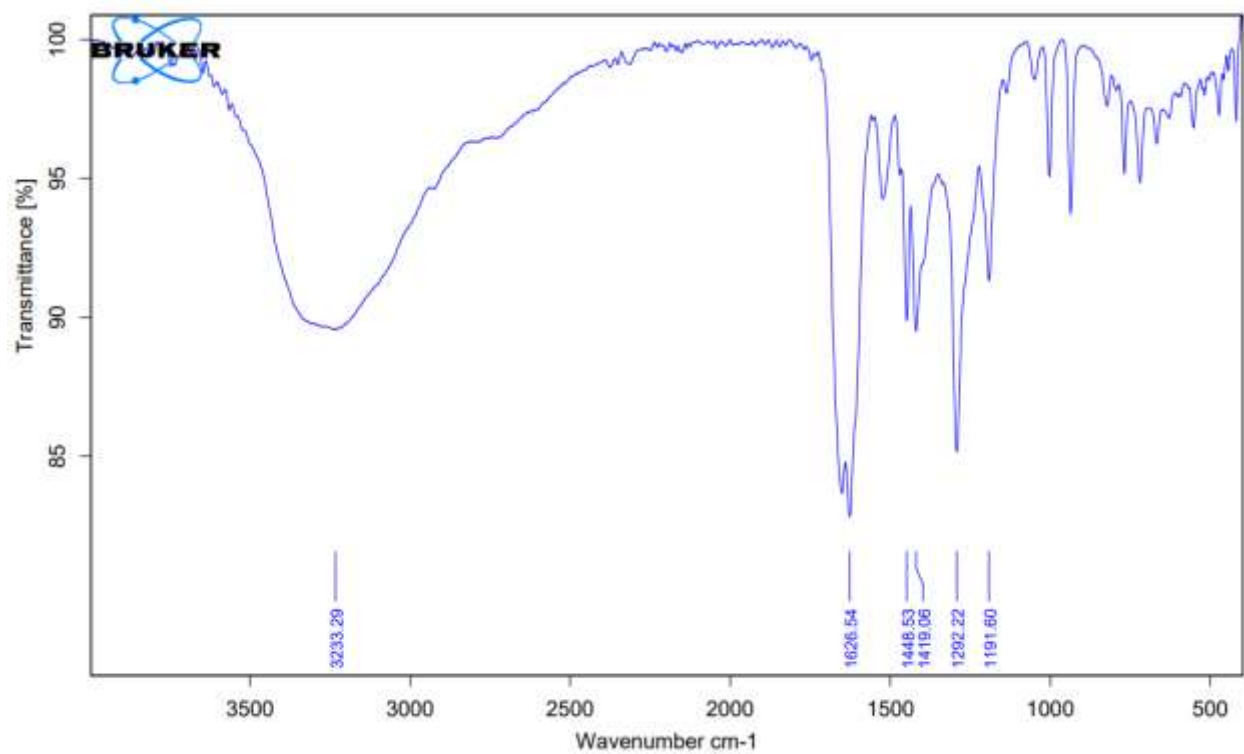


Figure S14. IR spectrum of **2**.

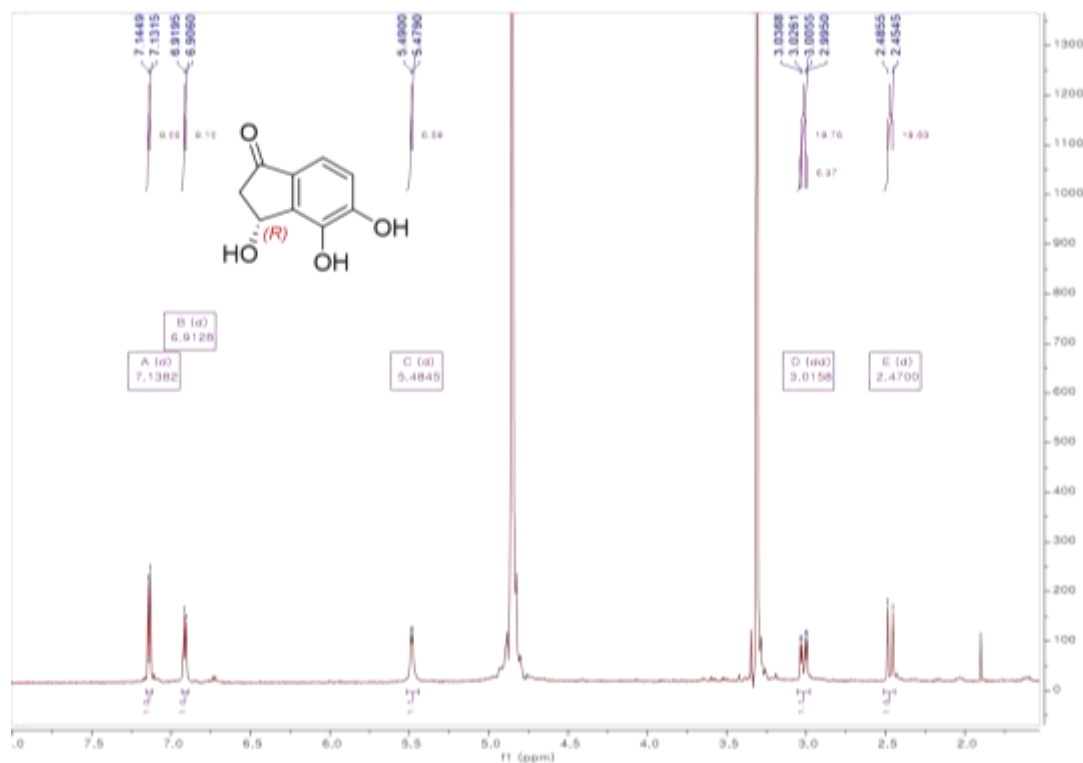


Figure S15. <sup>1</sup>H NMR spectrum of **3** in CD<sub>3</sub>OD (600 MHz).

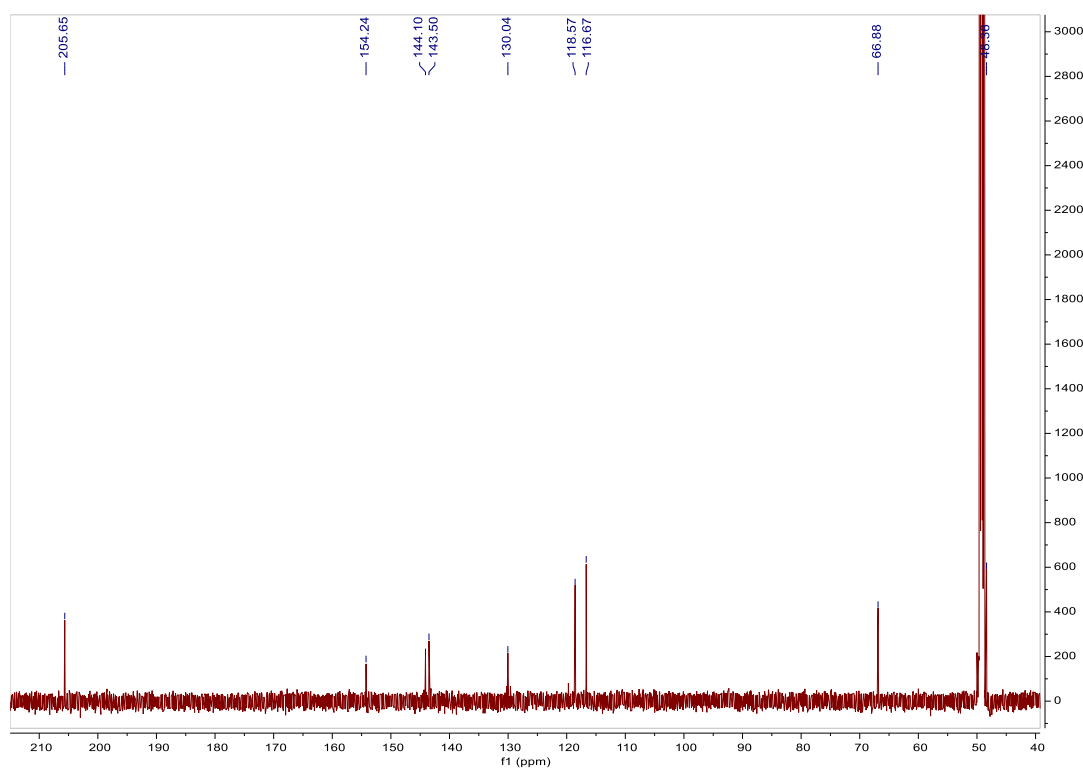


Figure S16. <sup>13</sup>C NMR spectrum of **3** in CD<sub>3</sub>OD (150 MHz).

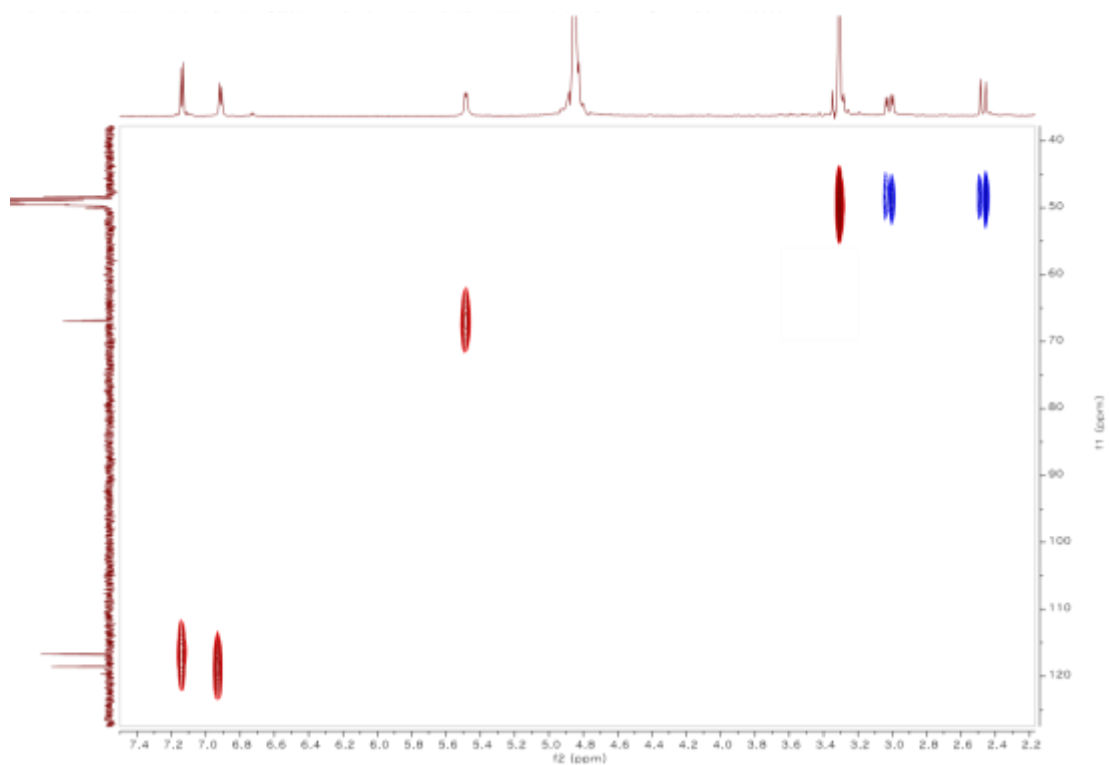


Figure S17. HSQC spectrum of **3** in CD<sub>3</sub>OD.

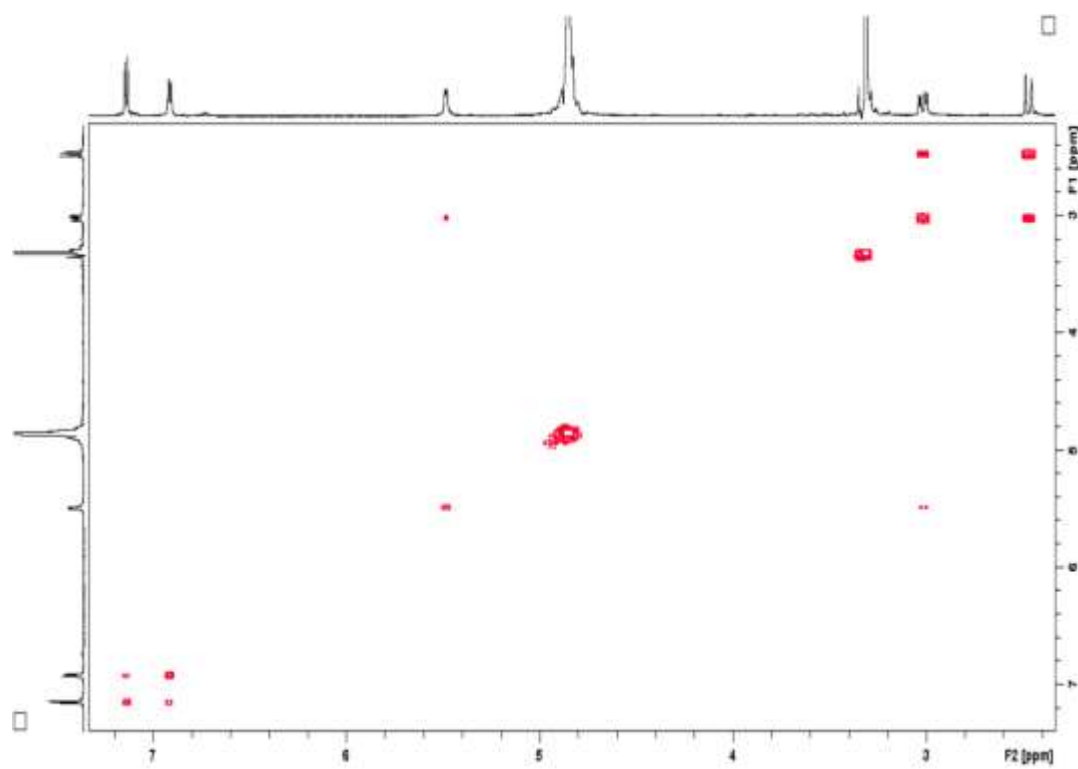


Figure S18. COSY spectrum of **3** in CD<sub>3</sub>OD.

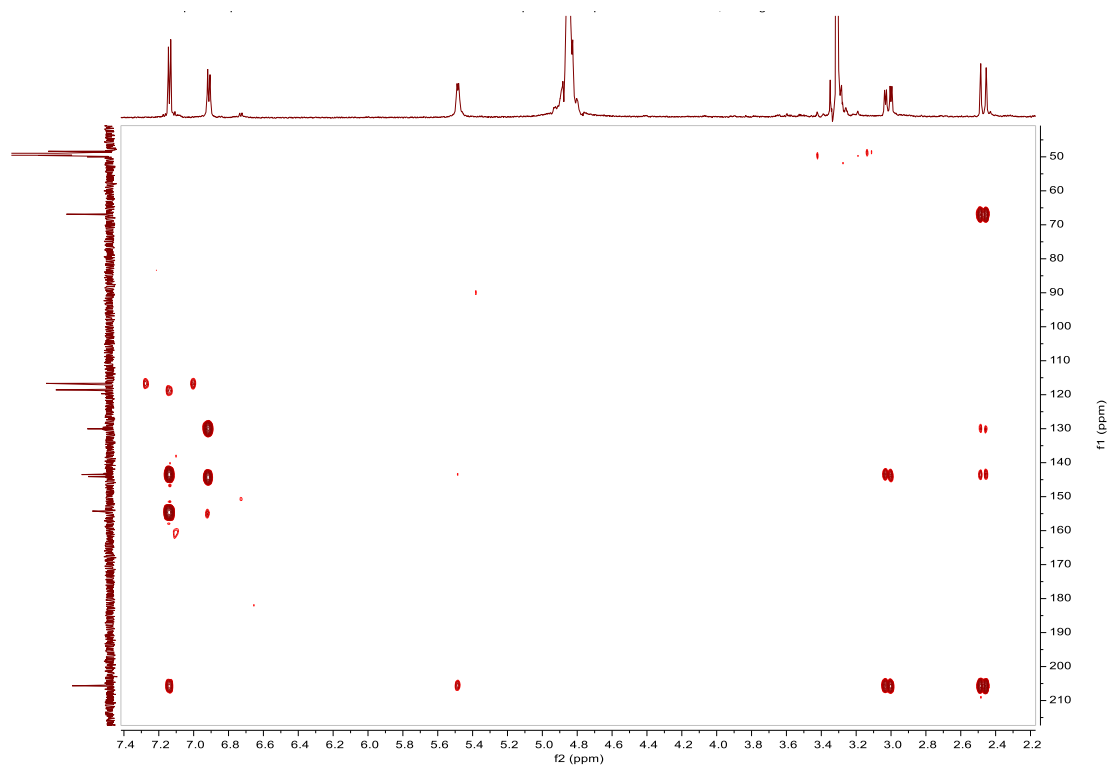
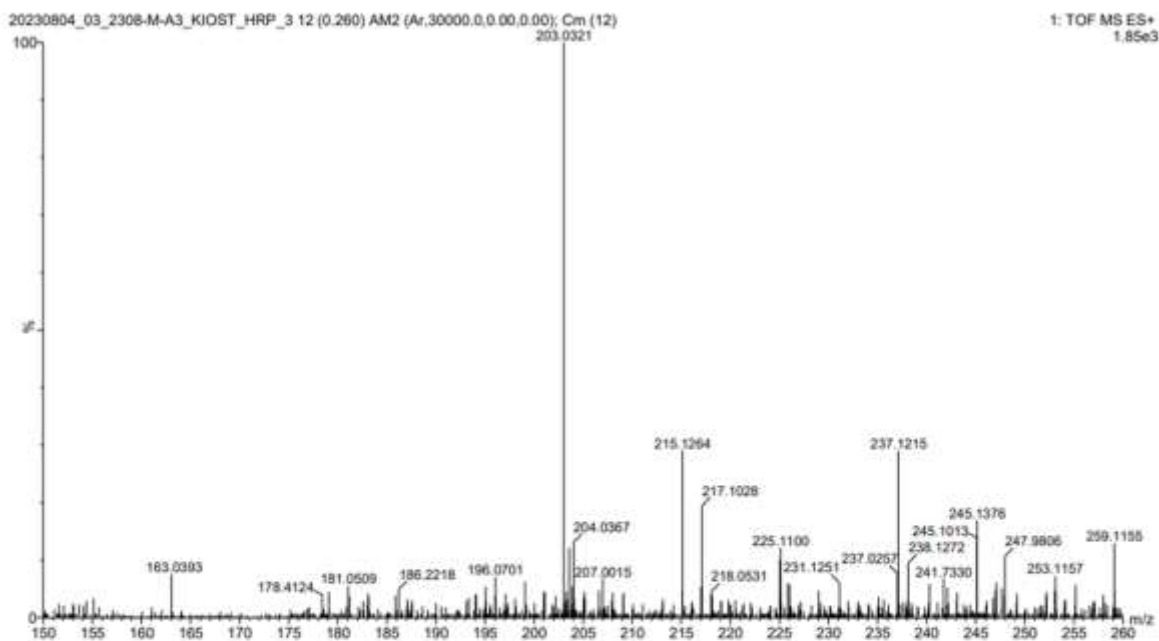


Figure S19. HMBC spectrum of **3** in CD<sub>3</sub>OD.

Sample : 03. 2308-M-A3  
 (+) ESI-MS  
 Range : 150-250 m/z



#### Elemental Composition Report

##### Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

61 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-10 H: 0-300 N: 0-2 O: 0-5 Na: 0-1 Pt: 0-1

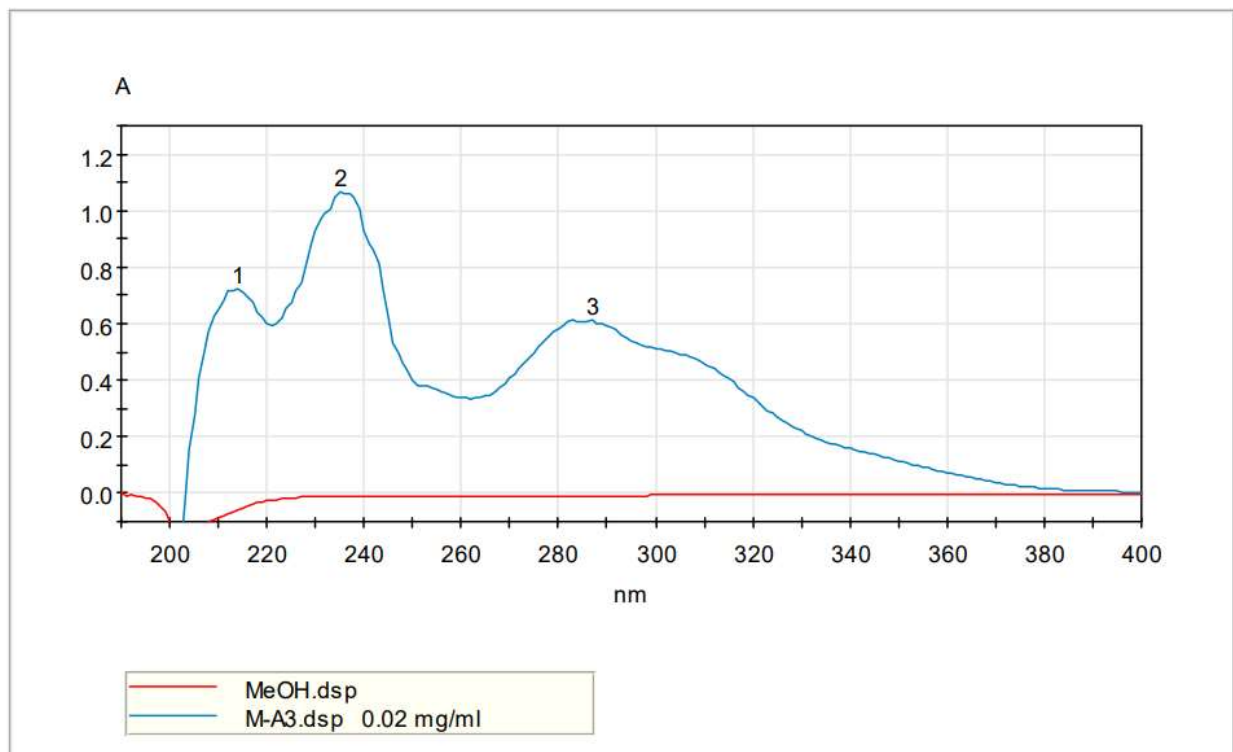
Minimum:

Maximum: 5.0 10.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
203.0321	203.0320	0.1	0.5	5.5	231.7	n/a	n/a	C9 H8 O4 Na

Figure S20. HR-ESIMS spectrum of **3**.





M-A3.dsp 0.02 mg/ml

Maxima		Threshold: 0.1 A	
1	214 nm;	0.725 A	2 235 nm; 1.068 A
3	287 nm;	0.613 A	

Figure S21. UV spectrum of **3**.

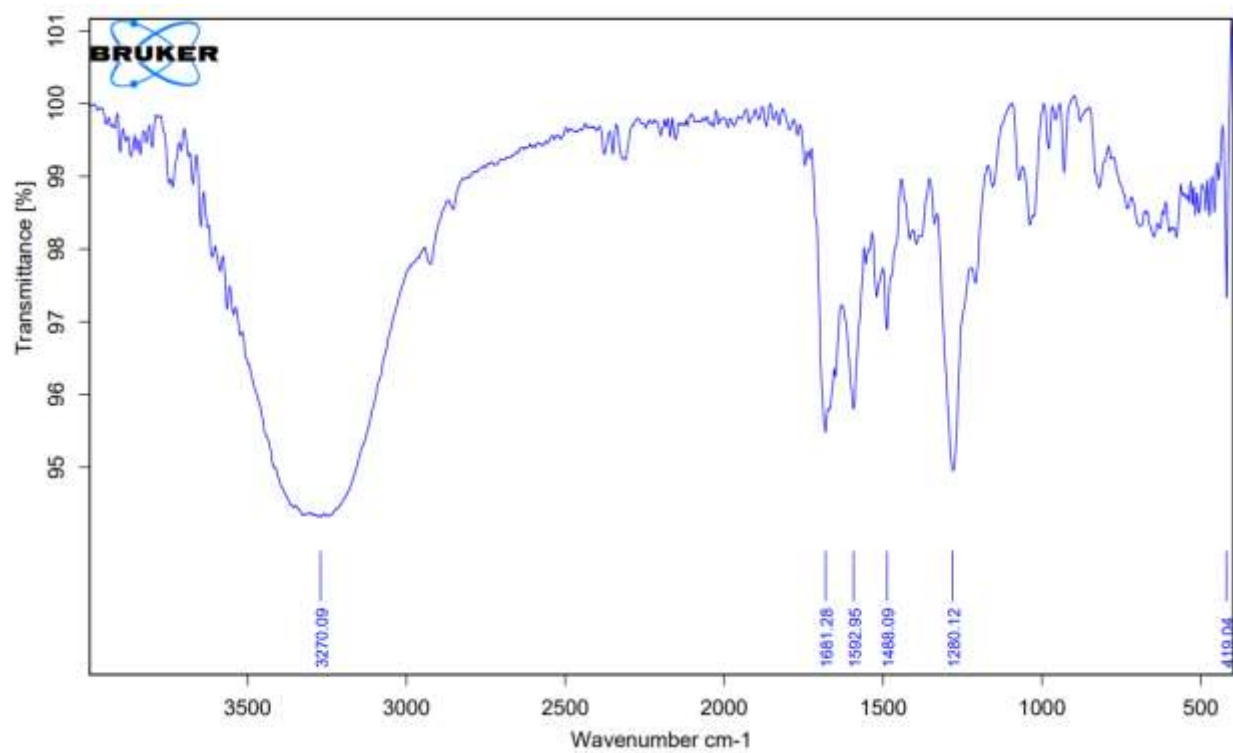


Figure S22. IR spectrum of **3**.

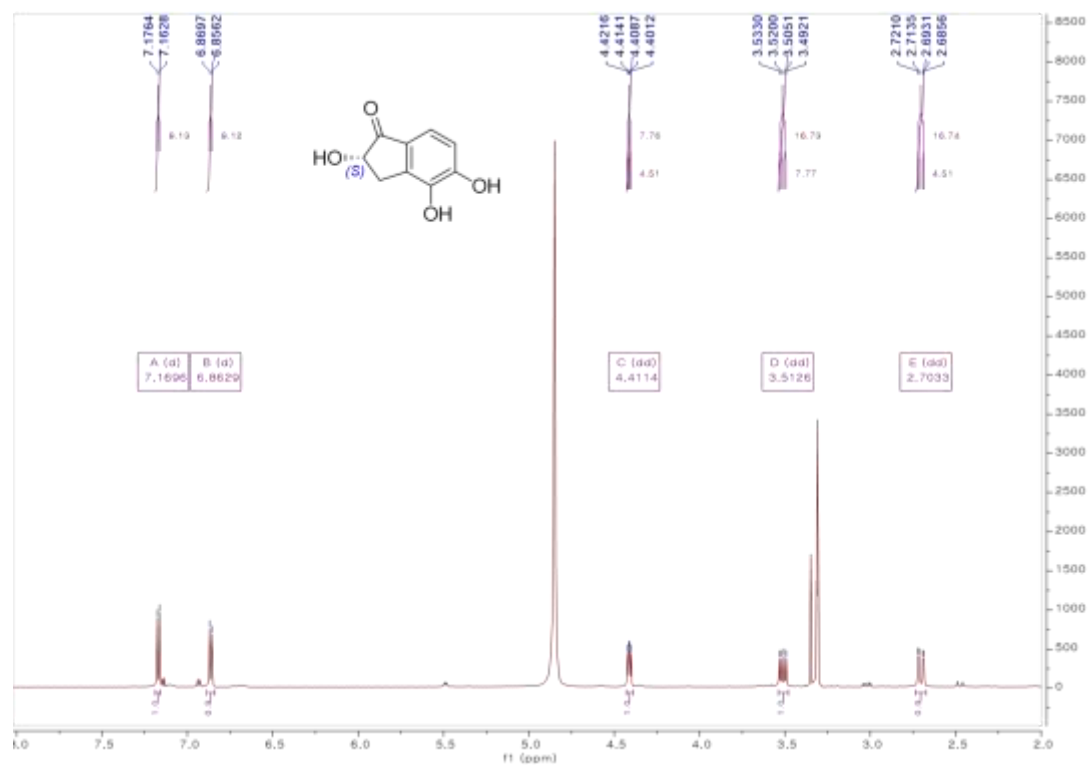


Figure S23. <sup>1</sup>H NMR spectrum of **4** in CD<sub>3</sub>OD (600 MHz).

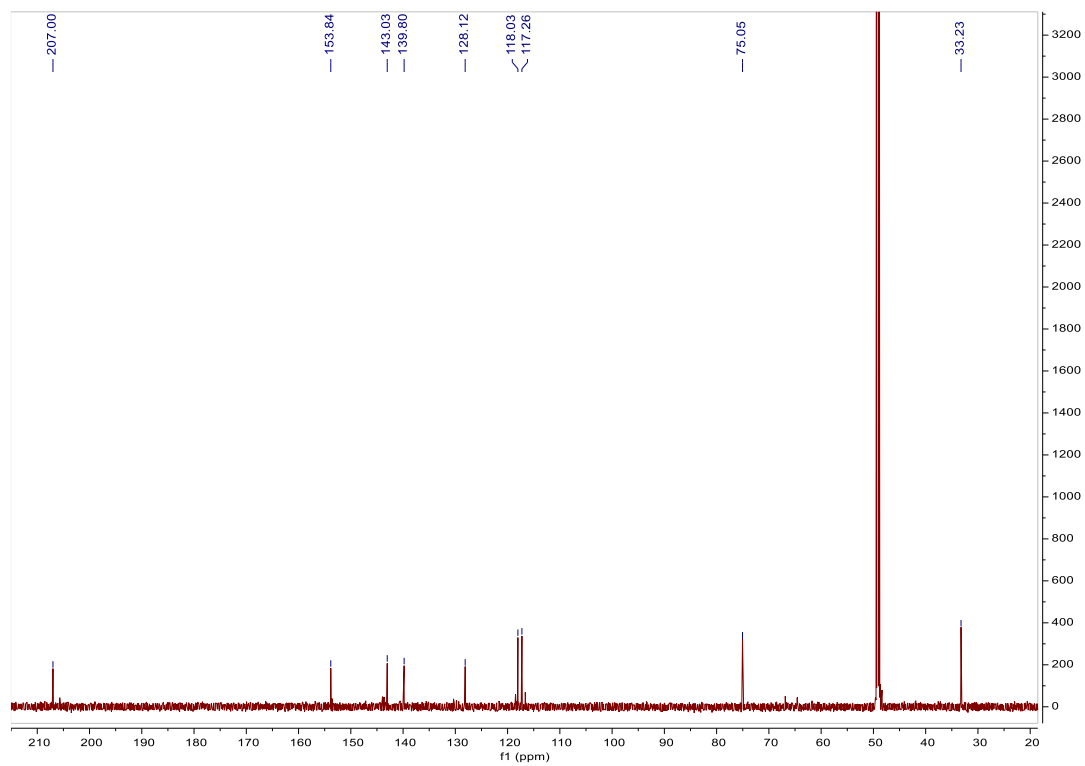


Figure S24. <sup>13</sup>C NMR spectrum of **4** in CD<sub>3</sub>OD (150 MHz).

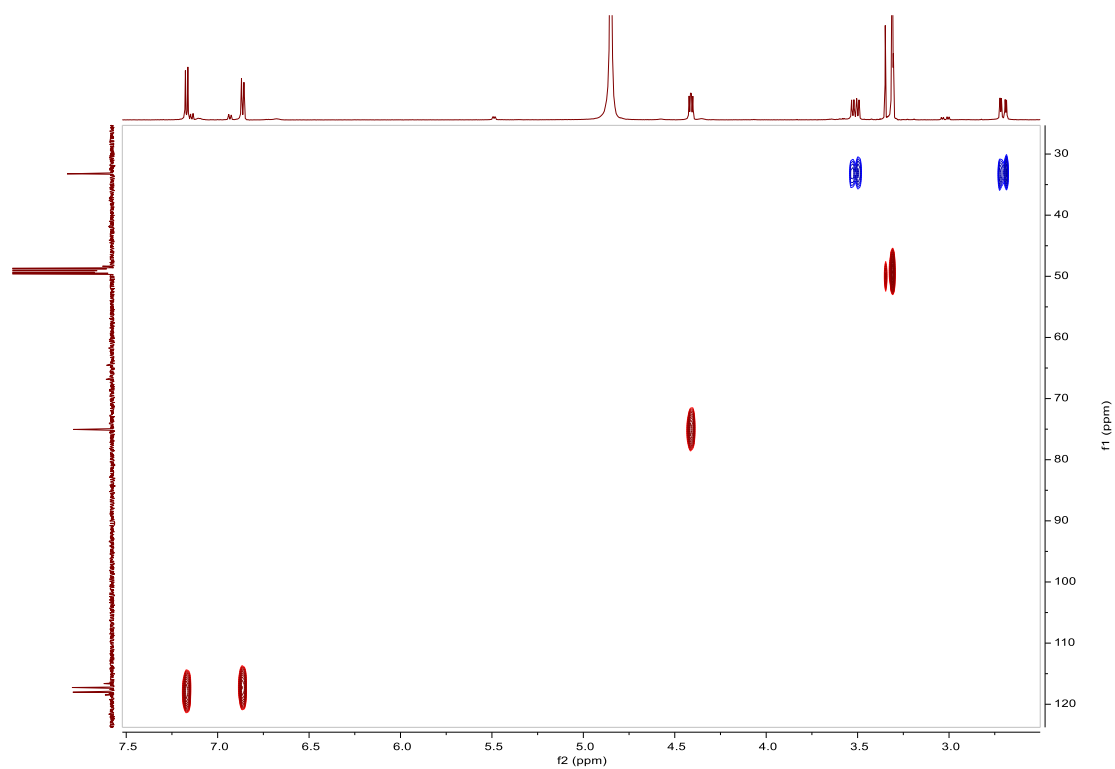


Figure S25. HSQC spectrum of **4** in  $\text{CD}_3\text{OD}$ .

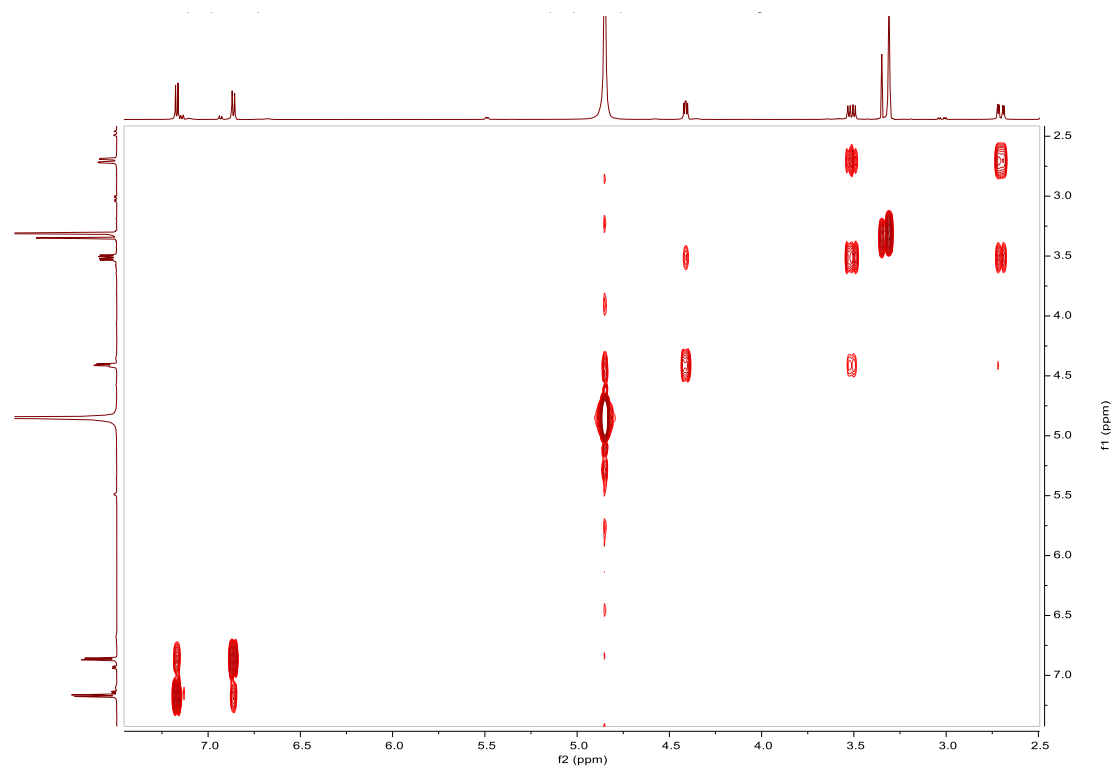


Figure S26. COSY spectrum of **4** in  $\text{CD}_3\text{OD}$ .

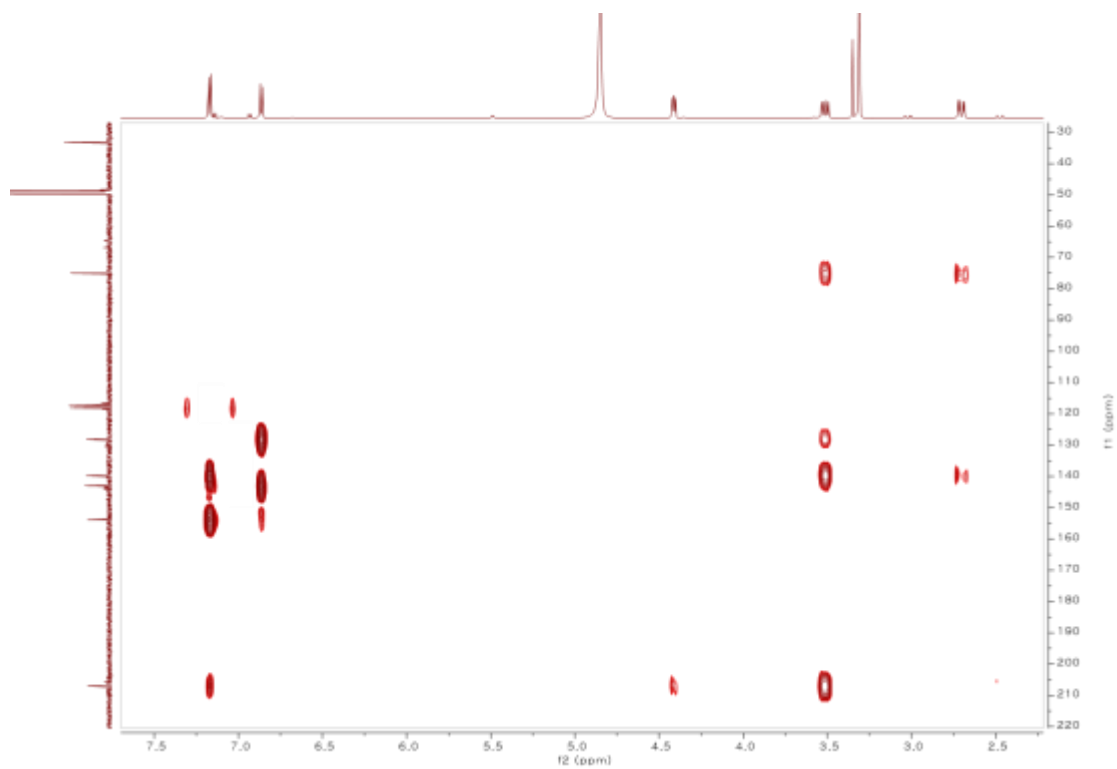
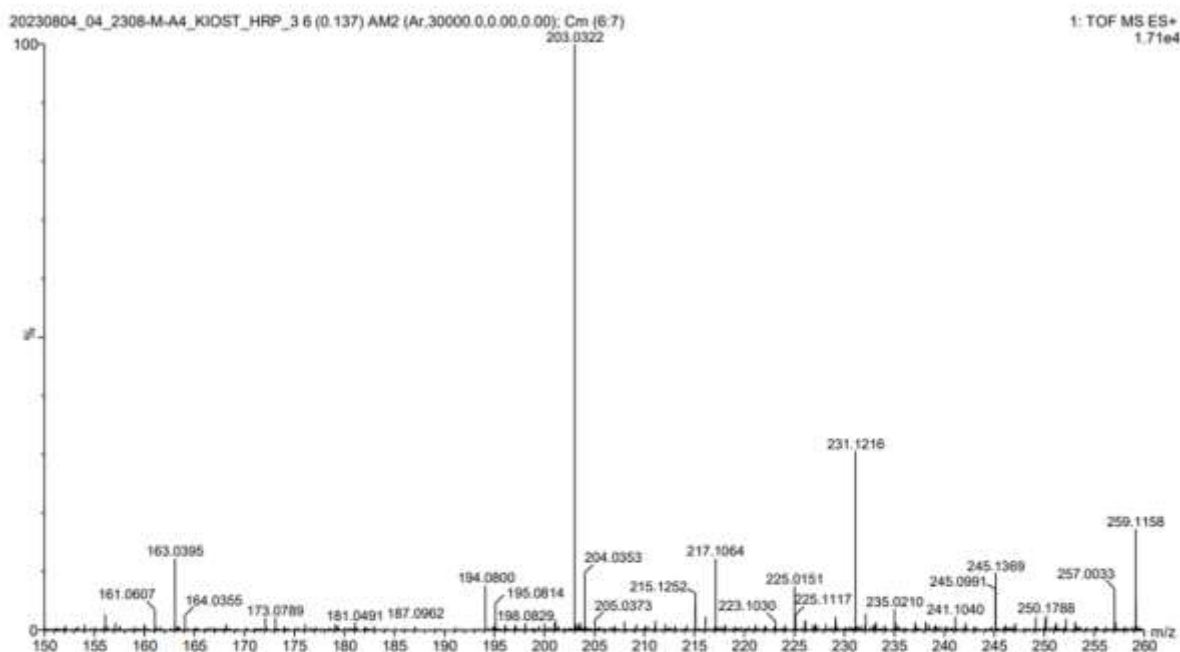


Figure S27. HMBC spectrum of **4** in  $\text{CD}_3\text{OD}$ .

Sample : 04. 2308-M-A4  
 (+) ESI-MS  
 Range : 150-260 m/z



#### Elemental Composition Report

##### Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

##### Monoisotopic Mass, Even Electron Ions

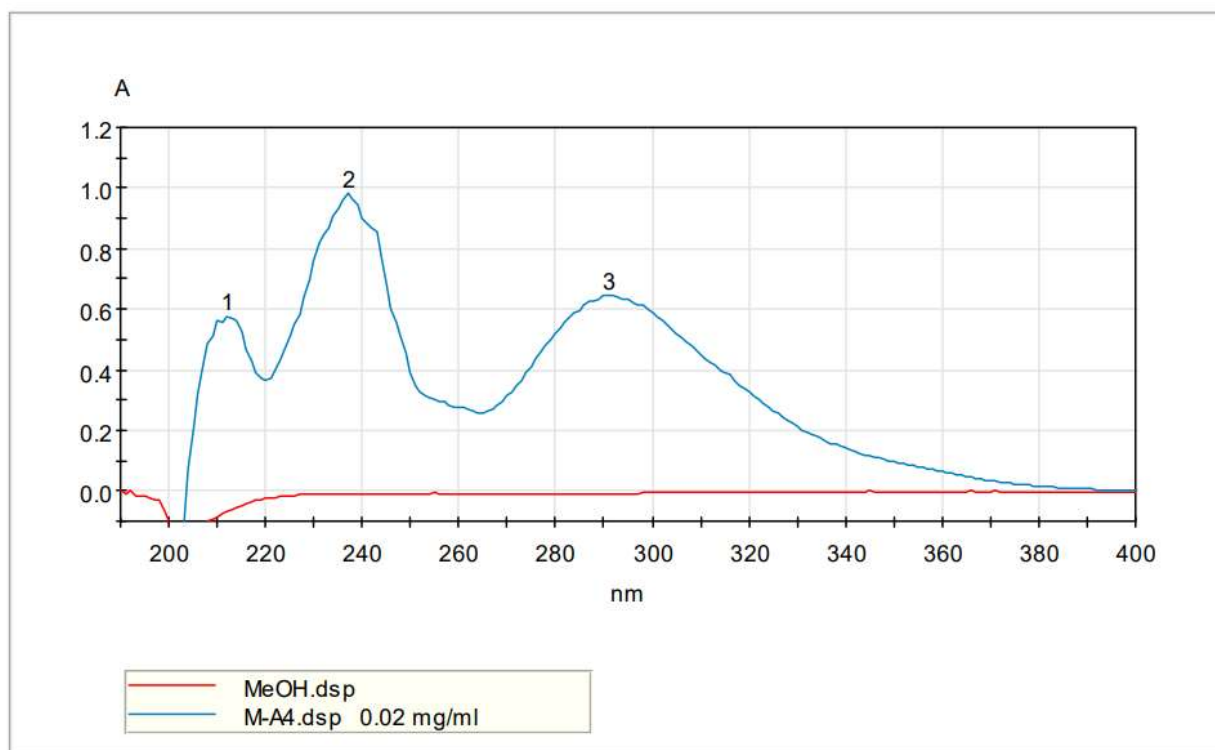
61 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-10 H: 0-300 N: 0-2 O: 0-5 Na: 0-1 Pt: 0-1

Minimum:					-1.5			
Maximum:			5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
203.0322	203.0320	0.2	1.0	5.5	652.1	n/a	n/a	C9 H8 O4 Na

Figure S28. HR-ESIMS spectrum of **4**.



M-A4.dsp      0.02 mg/ml

Maxima      Threshold: 0.1 A  
1 212 nm;      0.578 A      2 237 nm;      0.983 A      3 291 nm;      0.647 A

Figure S29. UV spectrum of 4.

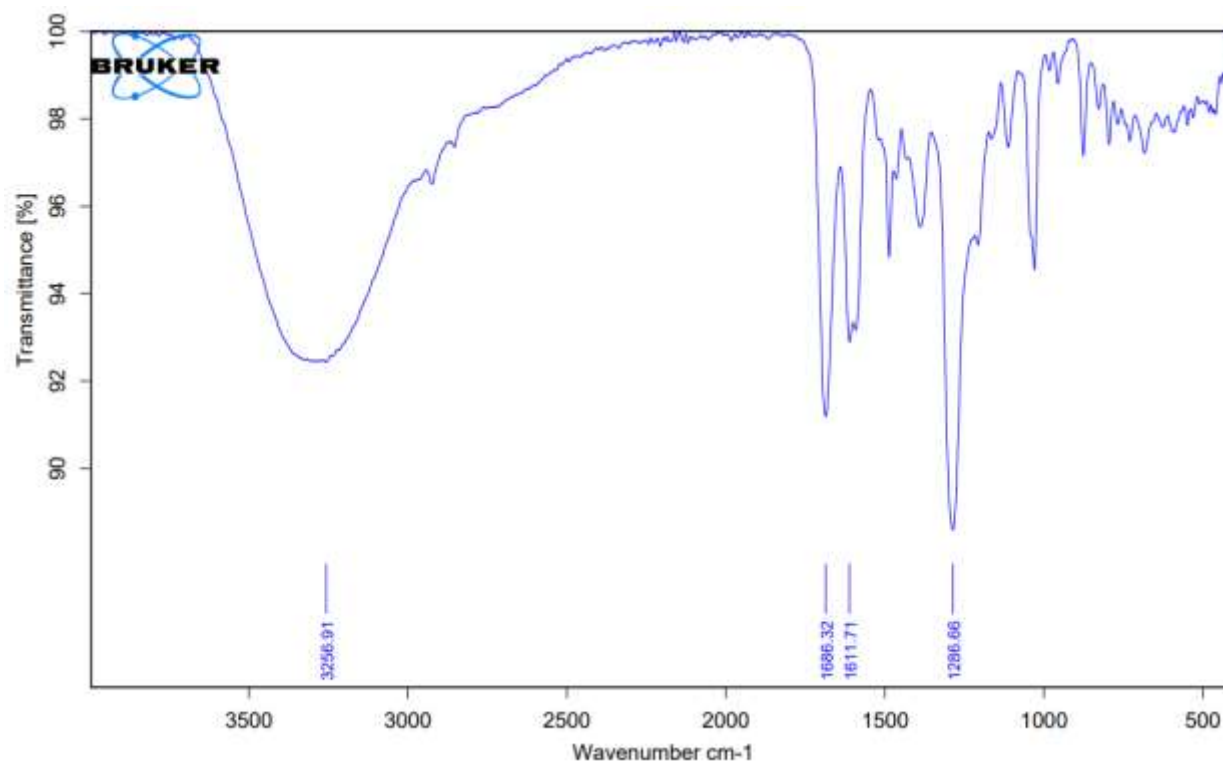


Figure S30. IR spectrum of **4**.



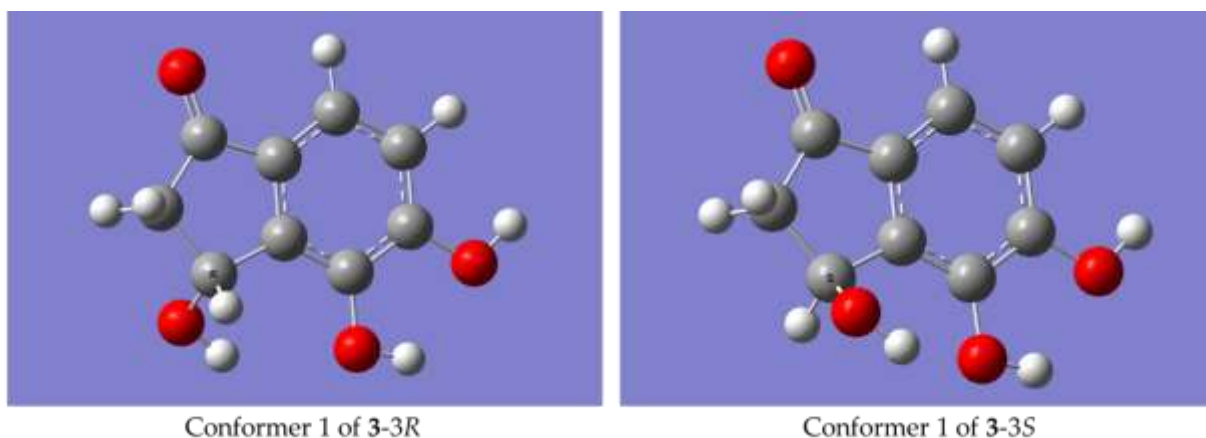


Figure S31. Initial geometry optimized conformers of **3**.

Table S1. Total Gibbs Free Energy and Boltzmann population of initial geometry optimized conformers of **3**.

Compound	Conformer	Total Gibbs Free Energy (KCAL/MOL)	Boltzmann population (%)
<b>3-3R</b>	1	86.85337	99.98721
<b>3-3S</b>	1	86.85337	99.98721

Table S2. The cartesian coordinates of conformers of **3**.

		Coordinates (Angstroms)					Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
Conformer 1 of <b>3-3R</b>	C	-0.13935	0.35933	-0.15283	Conformer 1 of <b>3-3S</b>	C	0.13934	0.35935	-0.15269
	C	1.22404	0.58074	-0.12869		C	-1.22404	0.58079	-0.12858
	C	2.07715	-0.51859	0.02033		C	-2.0772	-0.51851	0.02041
	C	1.56865	-1.81474	0.14007		C	-1.56873	-1.81469	0.14013
	C	0.19733	-2.03407	0.11963		C	-0.19741	-2.03405	0.11972
	C	-0.64369	-0.93326	-0.02294		C	0.64364	-0.93326	-0.02279
	H	2.2602	-2.64382	0.25386		H	-2.26034	-2.64373	0.25381
	H	-0.20618	-3.0356	0.21872		H	0.20607	-3.03559	0.21876
	C	-2.52303	0.59145	-0.11556		C	2.52305	0.59133	-0.11576
	C	-2.11533	-0.87483	-0.04662		C	2.11527	-0.8749	-0.04665
	O	-2.88715	-1.81987	-0.01033		O	2.88705	-1.81998	-0.01036
	O	1.70662	1.85003	-0.24188		O	-1.70654	1.8501	-0.2417
	O	3.40294	-0.2145	0.03601		O	-3.40294	-0.21443	0.0358
	H	2.6748	1.83643	-0.19793		H	-2.67475	1.83646	-0.19865
	H	3.95222	-1.0034	0.13717		H	-3.95227	-1.00332	0.1367
	H	-3.266	0.74618	-0.90068		H	3.26587	0.74596	-0.90105
	H	-2.98227	0.87118	0.83818		H	2.98247	0.87115	0.83786
	C	-1.23005	1.39211	-0.3165		C	1.23007	1.39208	-0.3165
	H	-1.18955	1.82497	-1.32352		H	1.18941	1.8249	-1.32354
	O	-1.15192	2.43797	0.64824		O	1.15219	2.43795	0.64822
	H	-0.30135	2.88635	0.5365		H	0.30157	2.88633	0.53672

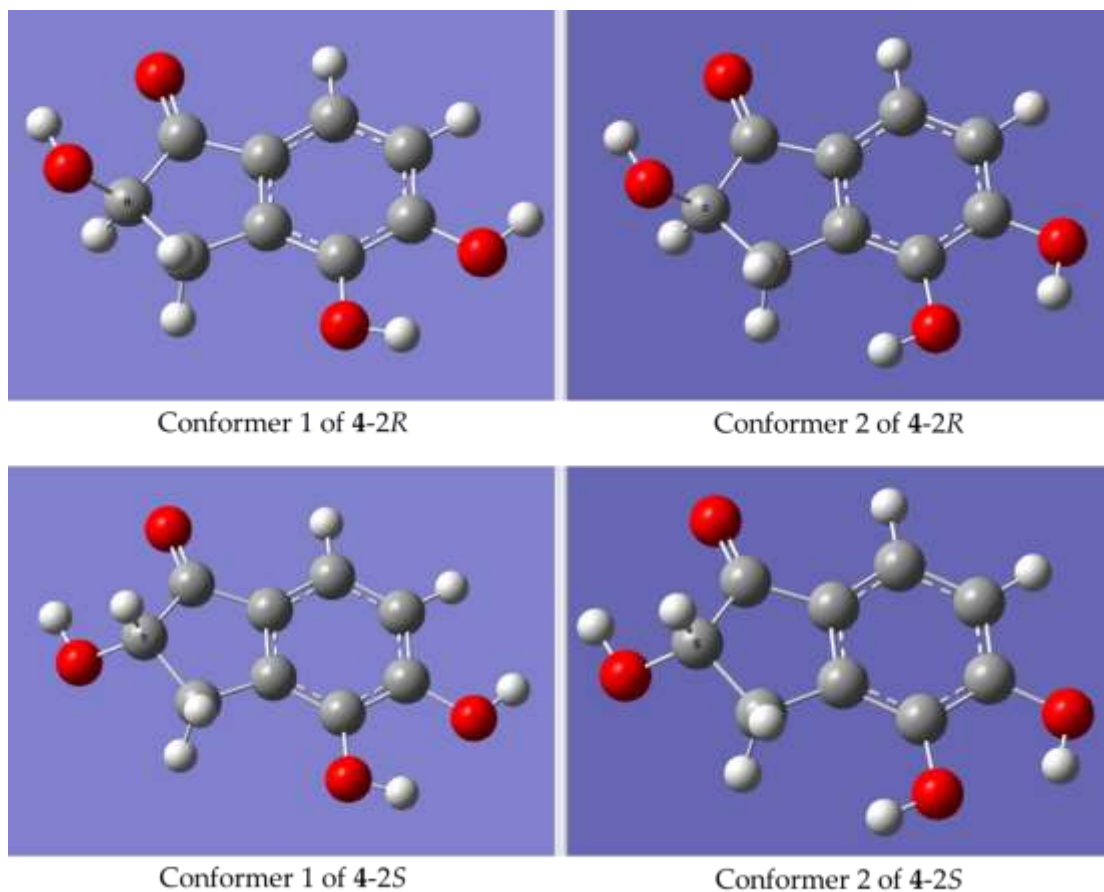


Figure S32. Initial geometry optimized conformers of **4**.

Table S3. Total Gibbs Free Energy and Boltzmann population of initial geometry optimized conformers of **4**.

Compound	Conformers	Total Gibbs Free Energy (KCAL/MOL)	Boltzmann population (%)
4-2R	1	119.3421	83.75961
	2	120.2777	16.14874
4-2S	1	119.3421	83.75961
	2	120.2777	16.14874

Table S4. The cartesian coordinates of conformers of 4.

		Coordinates (Angstroms)					Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
Conformer 1 of 4-2R	C	-0.06733	-0.51437	0.04284	Conformer 1 of 4-2S	C	0.06733	-0.51437	0.04284
	C	-1.42593	-0.76952	0.00497		C	1.42593	-0.76952	0.00497
	C	-2.3109	0.3163	-0.02761		C	2.3109	0.3163	-0.02761
	C	-1.85078	1.63557	-0.02646		C	1.85078	1.63557	-0.02646
	C	-0.48834	1.89374	0.00949		C	0.48834	1.89374	0.00949
	C	0.38668	0.81046	0.05192		C	-0.38668	0.81046	0.05192
	H	-2.57061	2.44789	-0.051		H	2.57061	2.44789	-0.051
	H	-0.11499	2.91178	0.0144		H	0.11499	2.91178	0.0144
	C	2.28939	-0.64388	0.37068		C	-2.28939	-0.64388	0.37068
	C	1.84886	0.7967	0.09485		C	-1.84886	0.7967	0.09485
	O	2.63487	1.71834	-0.0626		O	-2.63487	1.71834	-0.0626
	O	3.42835	-1.00697	-0.37827		O	1.88836	-2.04924	-0.01138
	H	4.05832	-0.27227	-0.32996		O	3.62656	-0.02718	-0.06452
	O	-1.88836	-2.04924	-0.01138		H	2.85715	-2.03781	-0.03804
	O	-3.62656	-0.02718	-0.06452		H	4.2009	0.74925	-0.10249
	H	-2.85715	-2.03781	-0.03804		O	-3.42835	-1.00697	-0.37827
	H	-4.2009	0.74925	-0.10249		H	-4.05832	-0.27227	-0.32996
	H	2.50444	-0.70149	1.44869		H	-2.50444	-0.70149	1.44869
	C	1.06673	-1.50829	0.04336		C	-1.06673	-1.50829	0.04336
	H	0.91312	-2.32073	0.75668		H	-1.19107	-1.95649	-0.94826
	H	1.19107	-1.95649	-0.94826		H	-0.91312	-2.32073	0.75668
Conformer 2 of 4-2R	C	-0.07855	-0.509	0.04886	Conformer 2 of 4-2S	C	0.07855	-0.509	0.04886
	C	-1.43978	-0.74557	0.0056		C	1.43978	-0.74557	0.0056
	C	-2.32037	0.34504	-0.02926		C	2.32037	0.34504	-0.02926
	C	-1.84608	1.65901	-0.02737		C	1.84608	1.65901	-0.02737
	C	-0.48249	1.90336	0.00939		C	0.48249	1.90336	0.00939
	C	0.38567	0.81404	0.05435		C	-0.38567	0.81404	0.05435
	H	-2.56723	2.46816	-0.05611		H	2.56723	2.46816	-0.05611
	H	-0.09809	2.9174	0.01233		H	0.09809	2.9174	0.01233
	C	2.28301	-0.64686	0.37229		C	-2.28301	-0.64686	0.37229
	C	1.84564	0.79422	0.09605		C	-1.84564	0.79422	0.09605
	O	2.63639	1.71192	-0.06279		O	-2.63639	1.71192	-0.06279
	O	3.41081	-1.01801	-0.38898		O	2.03823	-1.97503	-0.01278
	H	4.04289	-0.28422	-0.35405		O	3.65568	0.12767	-0.07231
	O	-2.03823	-1.97503	-0.01278		H	1.39376	-2.69297	-0.0547
	O	-3.65568	0.12767	-0.07231		H	3.82526	-0.82755	-0.08087
	H	-1.39376	-2.69297	-0.0547		O	-3.41081	-1.01801	-0.38898
	H	-3.82526	-0.82755	-0.08087		H	-4.04289	-0.28422	-0.35405
	H	2.50932	-0.70431	1.44763		H	-2.50932	-0.70431	1.44763
	C	1.0548	-1.50898	0.05723		C	-1.0548	-1.50898	0.05723
	H	0.91406	-2.31106	0.78661		H	-1.18072	-1.96935	-0.92875
	H	1.18072	-1.96935	-0.92875		H	-0.91406	-2.31106	0.78661