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Photochemical Transformations of Chalcone-Vitamin E Hybrids

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Supplementary Information

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

ISSN-e 2594-0317

Table of contents

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

ISSN-e 2594-0317

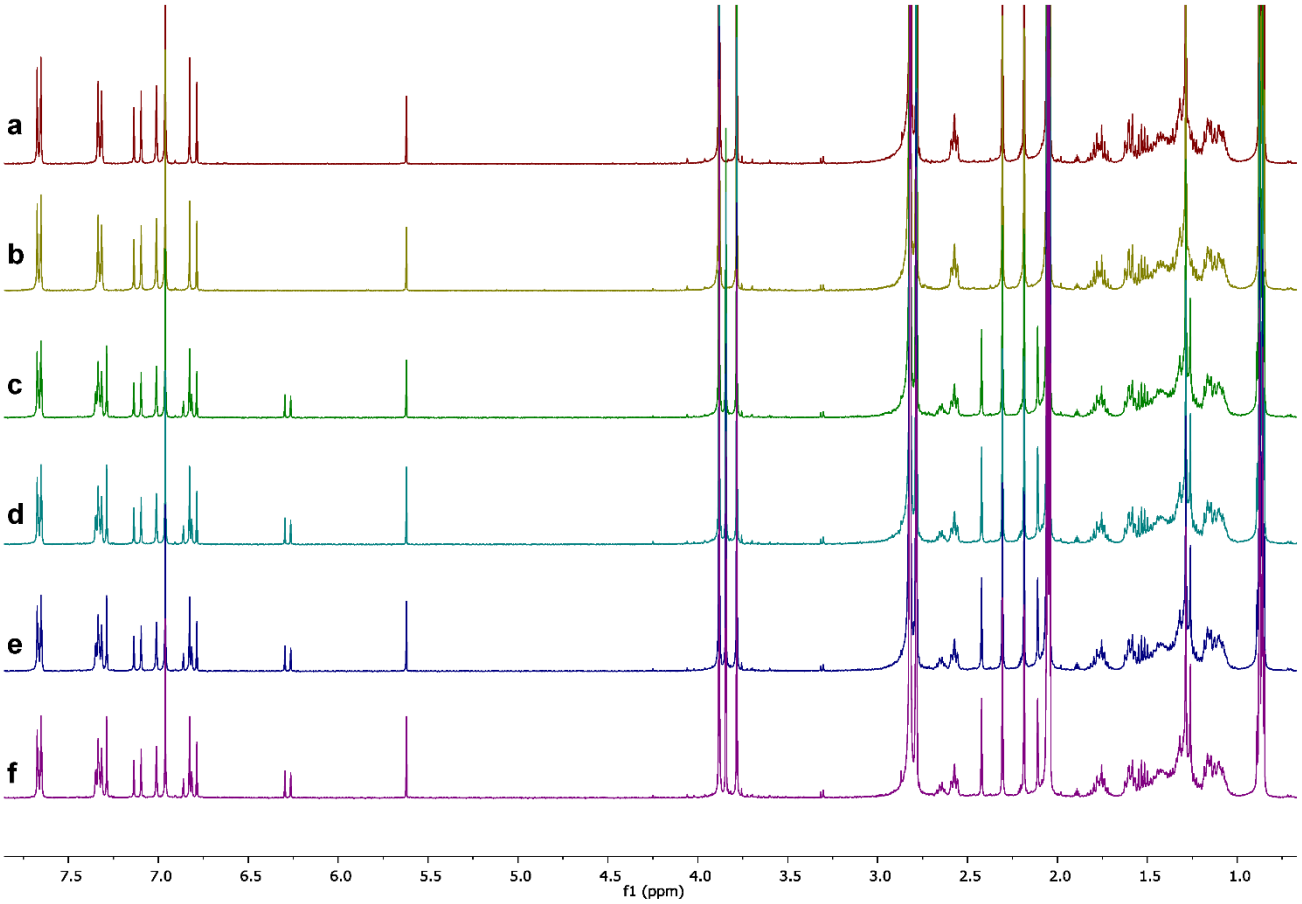

Fig. 1S. Stacked ^{1}H-NMR spectra (400 MHz, acetone-d6) from time-course study monitoring sunlight irradiation of 6'-*O*-tosyl-3,4,5-trimethoxy-*δ*-tocopherol-chalcone (**1**). **(a)** t=0 min, **(b)** t=60 min darkness, **(c)** t=5 min sunlight, **(d)** t=10 min sunlight, **(e)** t=15 min sunlight, **(f)** t=20 min sunlight.

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

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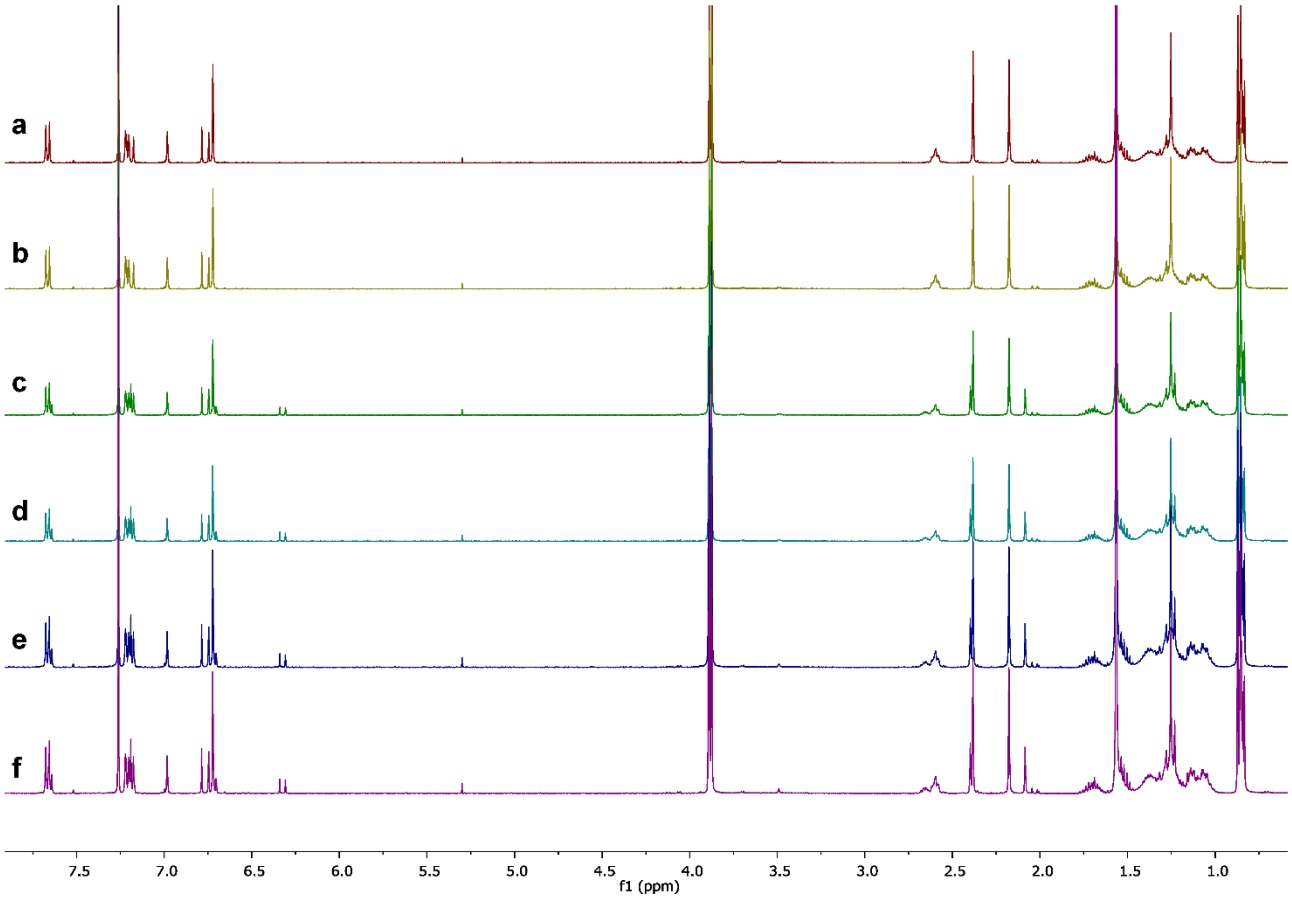

Fig. 2S. Stacked ^{1}H-NMR spectra (400 MHz, $CDCl_3$) from time-course study monitoring sunlight irradiation of 6'-*O*-tosyl-3,4,5-trimethoxy-*δ*-tocopherol-chalcone (**1**). **(a)** t=0 min, **(b)** t=60 min darkness, **(c)** t=5 min sunlight, **(d)** t=10 min sunlight, **(e)** t=15 min sunlight, **(f)** t=20 min sunlight.

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

ISSN-e 2594-0317

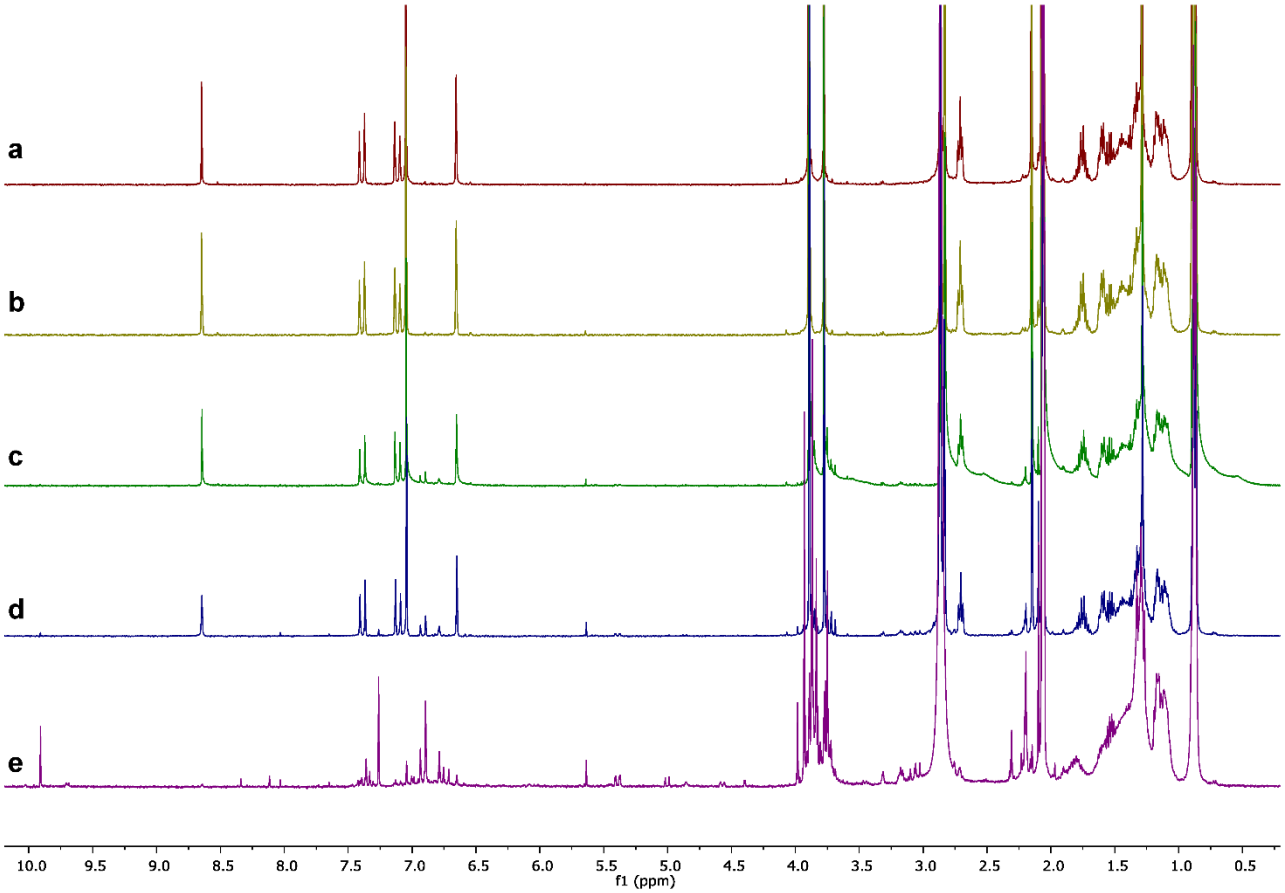

Fig. 3S. Stacked ^{1}H-NMR spectra (400 MHz, acetone-d6) from time-course study monitoring sunlight irradiation of 3,4,5-trimethoxy-*δ*-tocopherol-chalcone (**2**). **(a)** t=0 min, **(b)** t=60 min darkness, **(c)** t=5 min sunlight, **(d)** t=10 min sunlight, **(e)** t=60 min sunlight

J. Mex. Chem. Soc. **2022**, *66*(1)
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ISSN-e 2594-0317

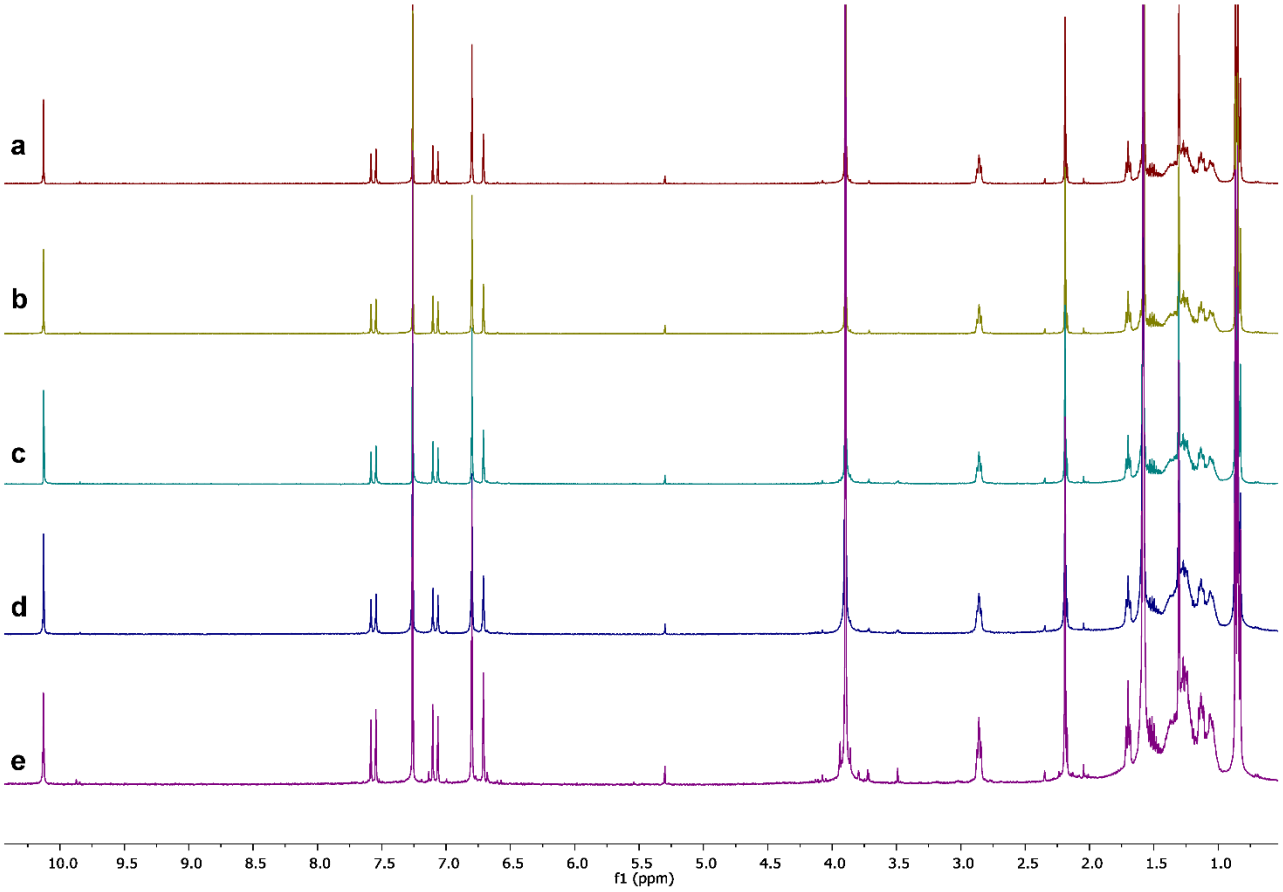

Fig. 4S. Stacked ^{1}H-NMR spectra (400 MHz, $CDCl_3$) from time-course study monitoring sunlight irradiation of 3,4,5-trimethoxy-*δ*-tocopherol-chalcone (**2**). **(a)** t=0 min, **(b)** t=60 min darkness, **(c)** t=5 min sunlight, **(d)** t=10 min sunlight, **(e)** t=60 min sunlight.

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

ISSN-e 2594-0317

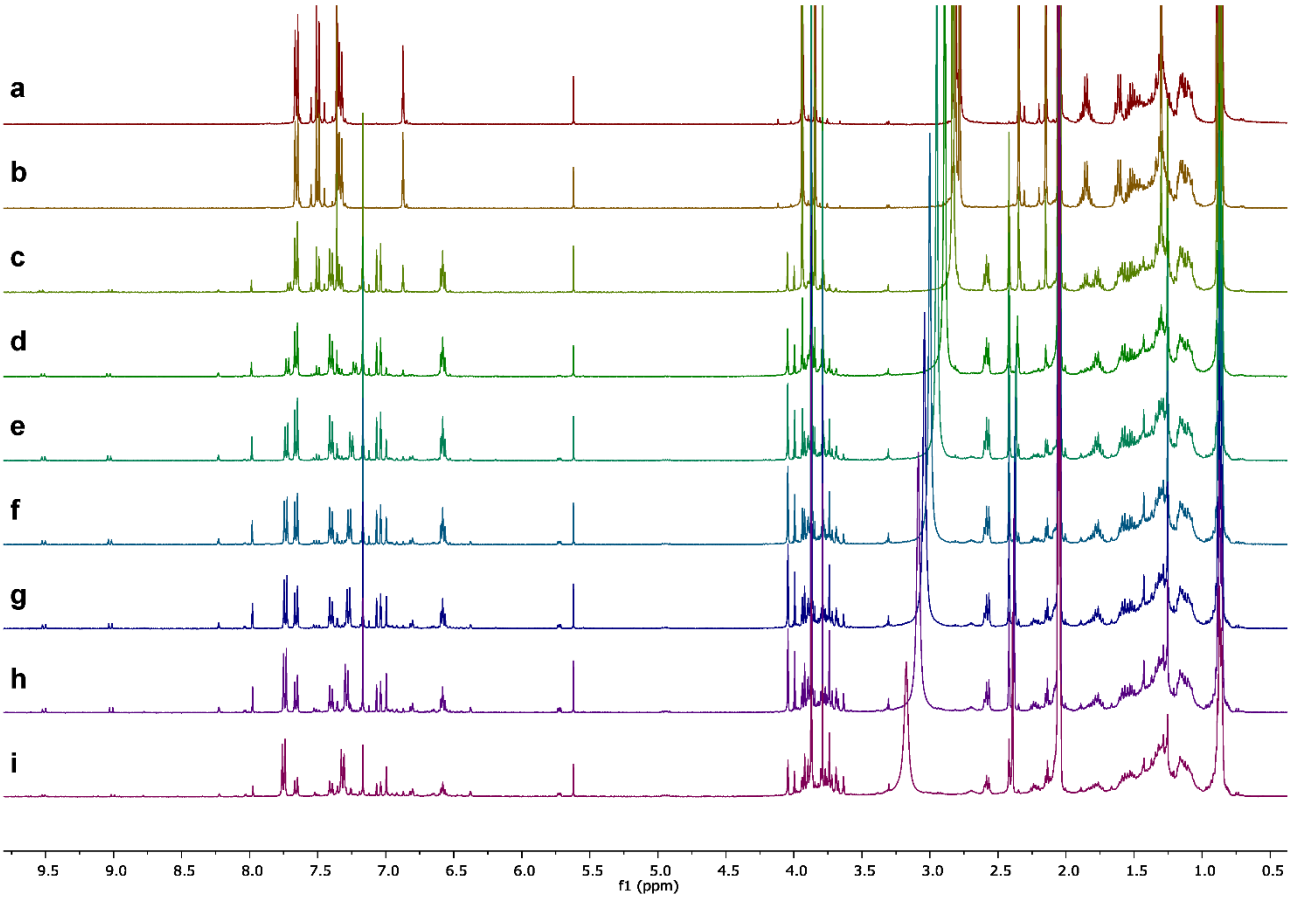

Fig. 5S. Stacked ^{1}H-NMR spectra (400 MHz, acetone-d6) from time-course study monitoring sunlight irradiation of 6'-*O*-tosyl-3,4,5-trimethoxy-*δ*-tocopherol-*retro*chalcone (**3**). **(a)** t=0 min, **(b)** t=60 min darkness, **(c)** t=5 min sunlight, **(d)** t=10 min sunlight, **(e)** t=15 min sunlight, **(f)** t=20 min sunlight, **(g)** t=25 min sunlight, **(h)** t=30 min sunlight, **(i)** t=60 min sunlight.

J. Mex. Chem. Soc. **2022**, *66*(1)
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ISSN-e 2594-0317

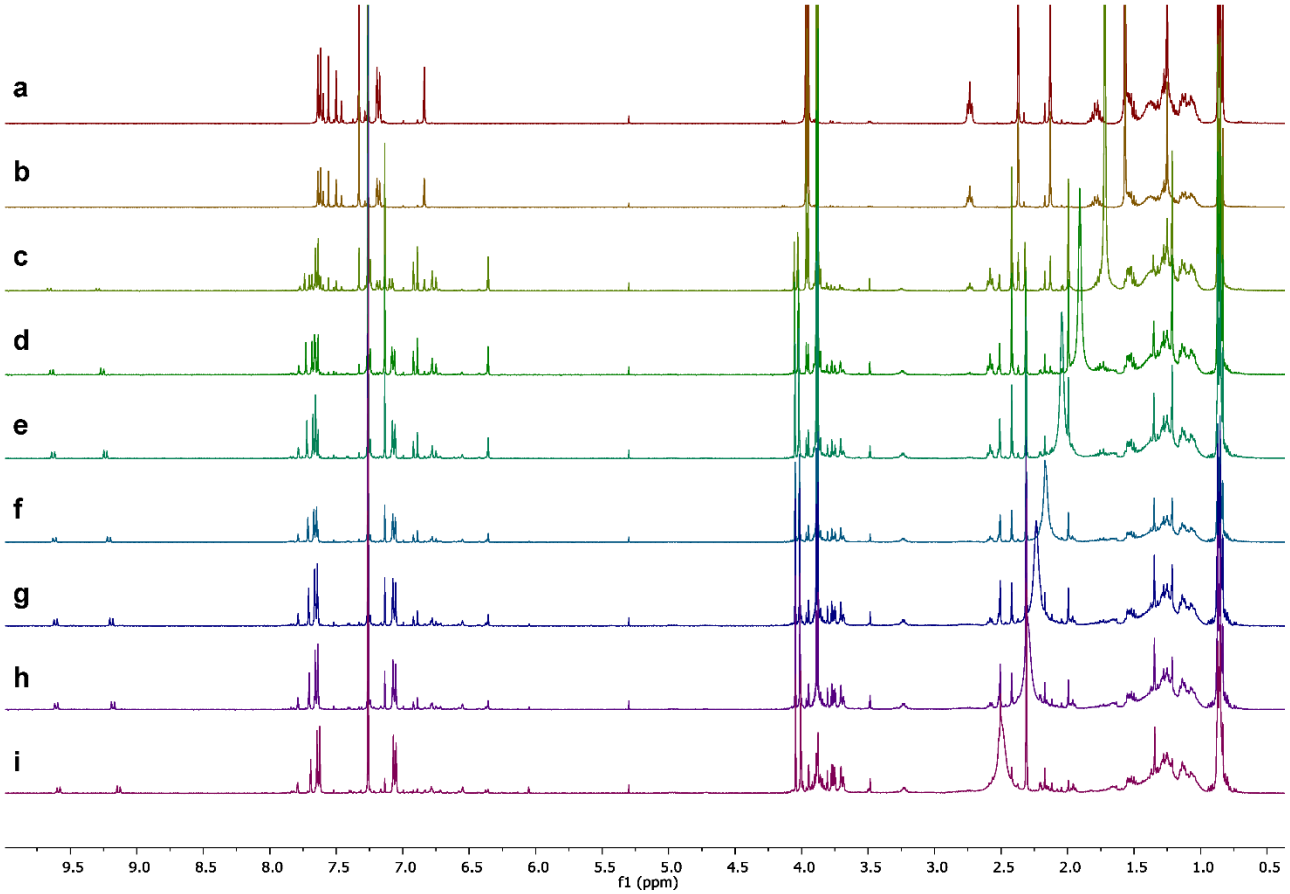

Fig. 6S. Stacked ^{1}H-NMR spectra (400 MHz, $CDCl_3$) from time-course study monitoring sunlight irradiation of 6'-*O*-tosyl-3,4,5-trimethoxy-*δ*-tocopherol-*retro*chalcone (**3**). **(a)** t=0 min, **(b)** t=60 min darkness, **(c)** t=5 min sunlight, **(d)** t=10 min sunlight, **(e)** t=15 min sunlight, **(f)** t=20 min sunlight, **(g)** t=25 min sunlight, **(h)** t=30 min sunlight, **(i)** t=60 min sunlight.

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

ISSN-e 2594-0317

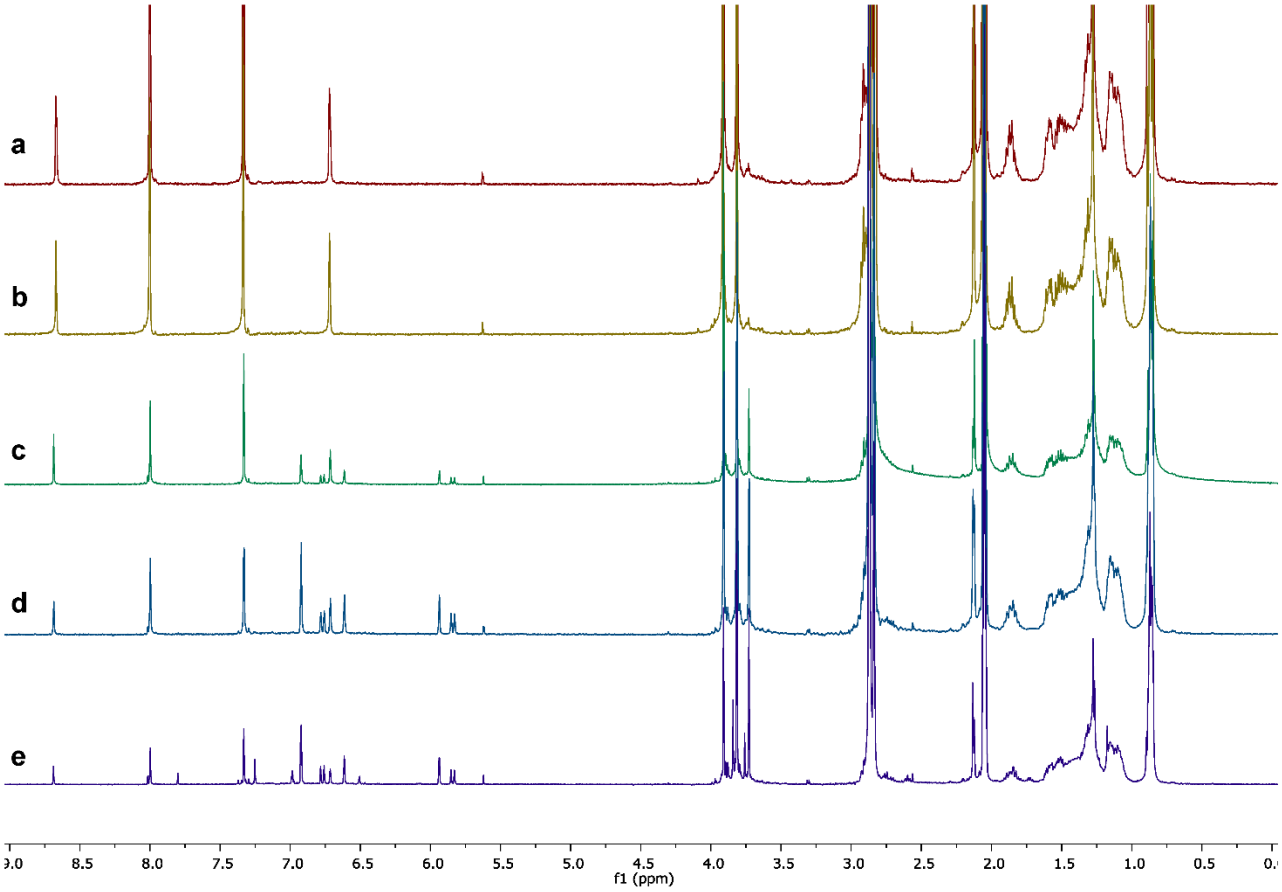

Fig. 7S. Stacked ^{1}H-NMR spectra (400 MHz, acetone-d6) from time-course study monitoring sunlight irradiation of 3,4,5-trimethoxy-*δ*-tocopherol-retrochalcone (**4**). **(a)** t=0 min, **(b)** t=60 min darkness, **(c)** t=5 min sunlight, **(d)** t=10 min sunlight, **(e)** t=15 min sunlight.

J. Mex. Chem. Soc. **2022**, *66*(1)
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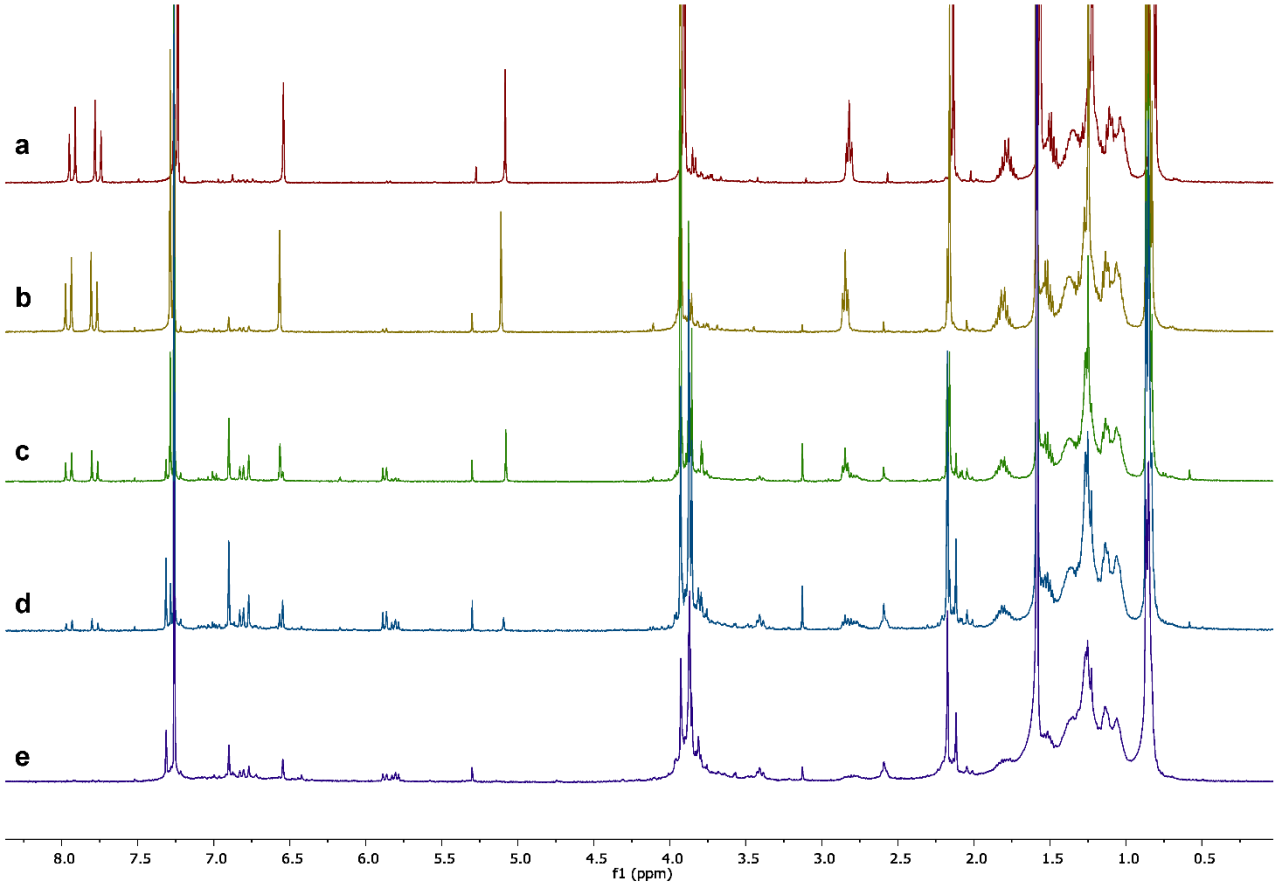


Fig. 8S. Stacked ^{1}H-NMR spectra (400 MHz, CDCl3) from time-course study monitoring sunlight irradiation of 3,4,5-trimethoxy-*δ*-tocopherol-retrochalcone (**4**). **(a)** t=0 min, **(b)** t=60 min darkness, **(c)** t=5 min sunlight, **(d)** t=10 min sunlight, **(e)** t=15 min sunlight.

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

ISSN-e 2594-0317

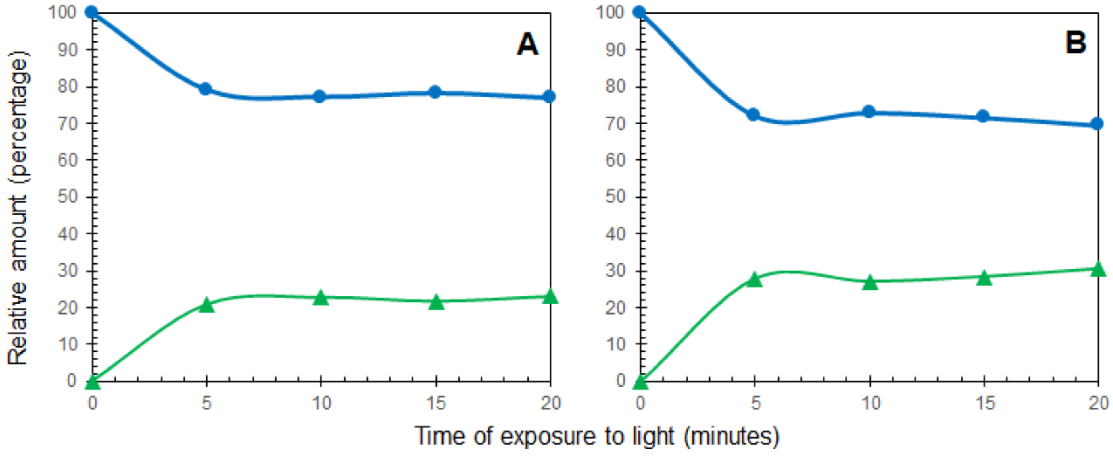
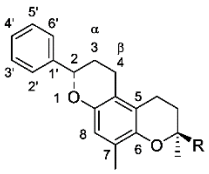


Fig. 9S. Photoisomerization process monitoring for *E*-chalcone **1**: **(A)** in deuterated chloroform, **(B)** in acetone-*d*6; *E*-chalcone ●, *Z*-chalcone **5** ▲).



	CDCl₃*			
Position	*E-retro*chalcone (**3**)	*Z-retro*chalcone (**7**)	3-deoxyanthocyanidin (**8**)	dimer
α (3)	7.48 d (15.9)	6.79 d (12.1)	9.66 d (9.2)	4.96**
β (**4**)	7.58 d (15.9)	6.90 d (12.1)	9.29 d (9.1)	4.71**
8	6.84 s	6.36 s	7.77 s	u
2' y 6'	7.33 s	7.14 s	7.74 s	u
MeO 3' y 5'	3.97 s	3.88 s	4.03 s	u
MeO 4'	3.95 s	3.89 s	4.06 s	u

	An-d₆*			
Position	*E-retro*chalcone (**3**)	*Z-retro*chalcone (**7**)	3-deoxyanthocyanidin (**8**)	dimer
α (3)	7.47 d (15.9)	6.58 d (12.1)	9.53 d (9.2)	4.94**
β (**4**)	7.53 d (16.0)	7.05 d (12.1)	9.02 d (9.1)	5.72**
8	6.87 s	6.58 s	8.23 s	u
2' y 6'	7.36 s	7.17 s	7.99 s	u
MeO 3' y 5'	3.94 s	3.87 s	4.05 s	u
MeO 4'	3.85 s	3.79 s	4.00 s	u

*Spectroscopic data collected at 5 min of exposure to light
**Protons characteristic of cyclobutane core
u - unassigned

Fig.10S. Characteristic 1H-NMR signals (chemical shifts in δ; coupling constants in Hz) of photoisomerization products **7** and **8**.

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

ISSN-e 2594-0317

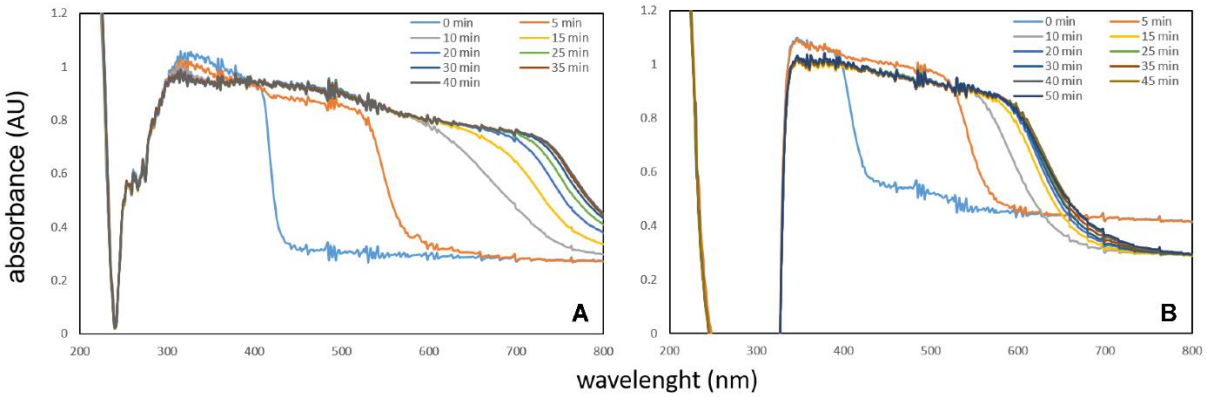


Fig. 11S. Stacked UV-vis spectra from time-course study monitoring sunlight irradiation of 6'-*O*-tosyl-3,4,5- trimethoxy-*δ*-tocopherol-retrochalcone (**3**). **(A)** In chloroform, **(B)** In acetone.

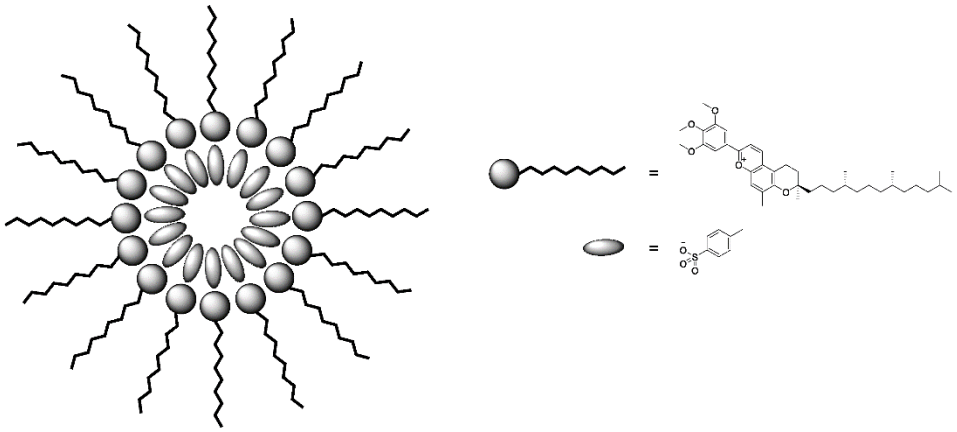


Fig. 12S. Schematic illustration for the distribution of 3-deoxyanthocyanidin (**8**) in reverse micelle-like aggregates, encapsulating moisture. The number of monomers shown in the aggregate are for visualization purposes only.

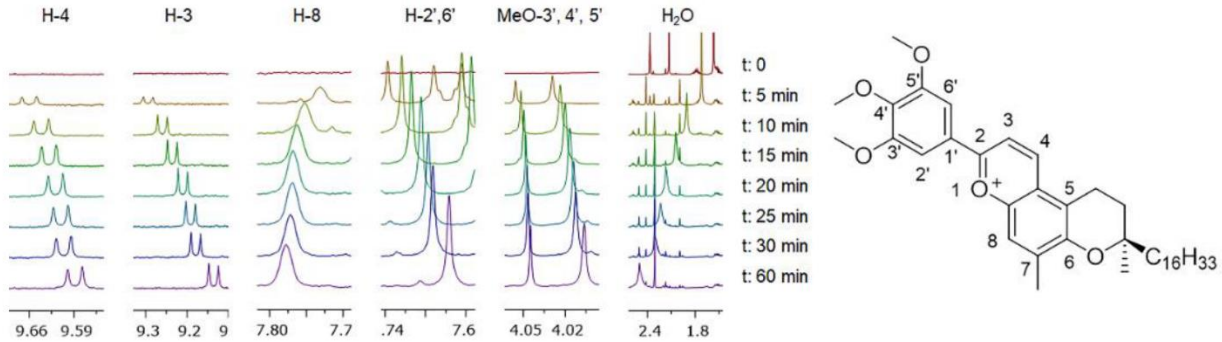


Fig. 13S. Stacked ^{1}H-NMR spectra (400 MHz, $CDCl_3$) showing changes in chemical shift values of key proton signals of 3-deoxyanthocyanidin **8** (evidence of aggregation process during time-course study).

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

ISSN-e 2594-0317

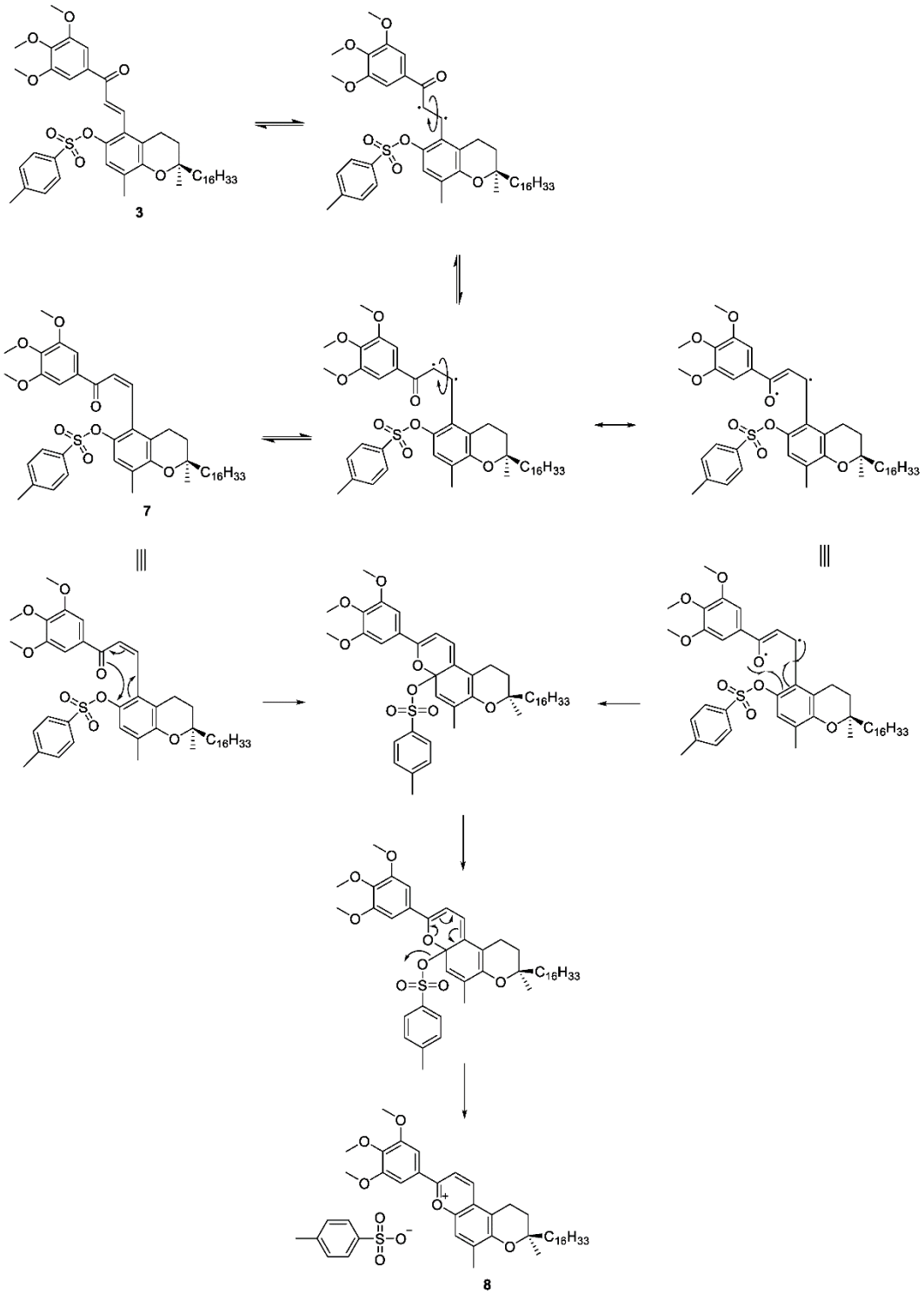


Fig. 14S. Proposed reaction pathways for the conversion of 6'-*O*-tosyl-3,4,5-trimethoxy-*δ*-tocopherol- retrochalcone (**3**) to 3-deoxyanthocyanidin (**8**).

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

ISSN-e 2594-0317

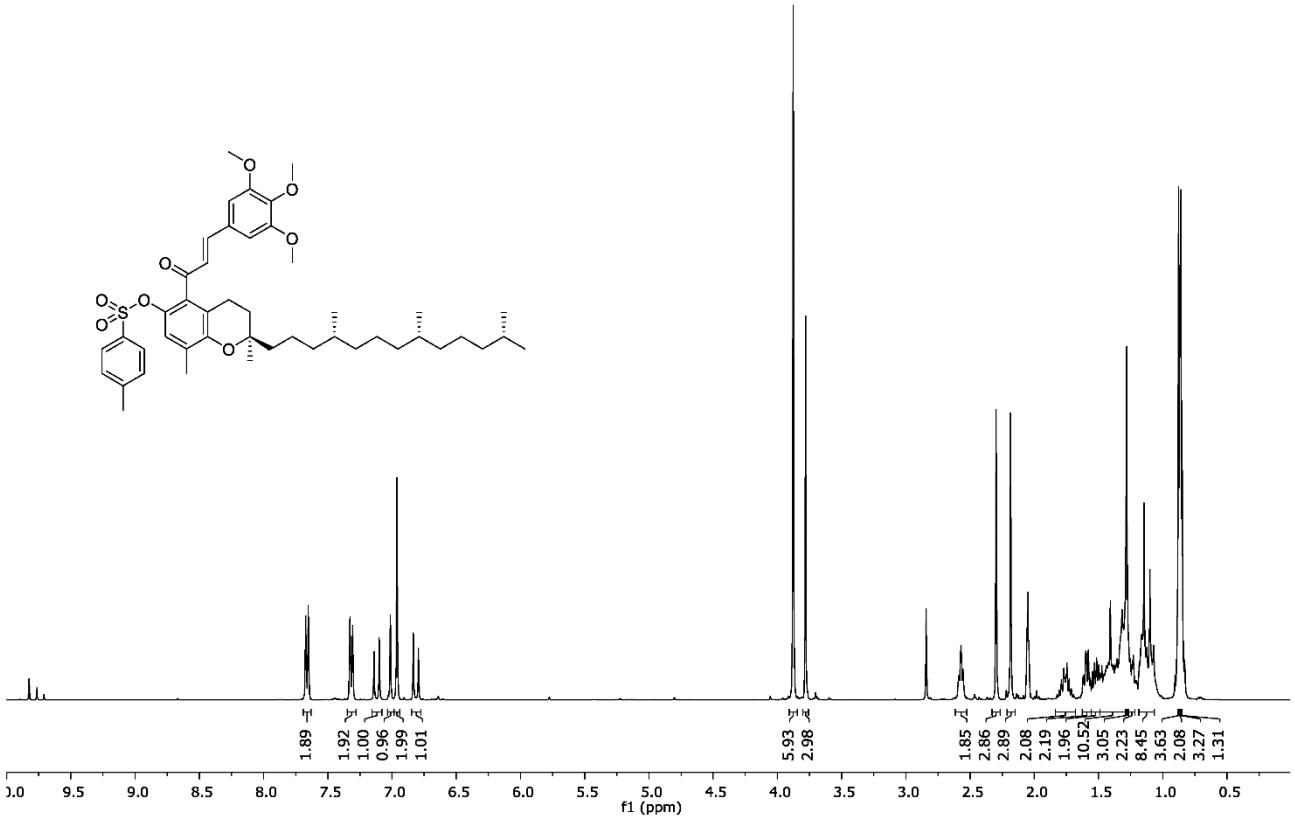


Fig. 15S. ^{1}H-NMR spectrum (400 MHz, acetone-d_6) of 6'-*O*-tosyl-3,4,5-trimethoxy-*δ*-tocopherol-chalcone (**1**).

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

ISSN-e 2594-0317

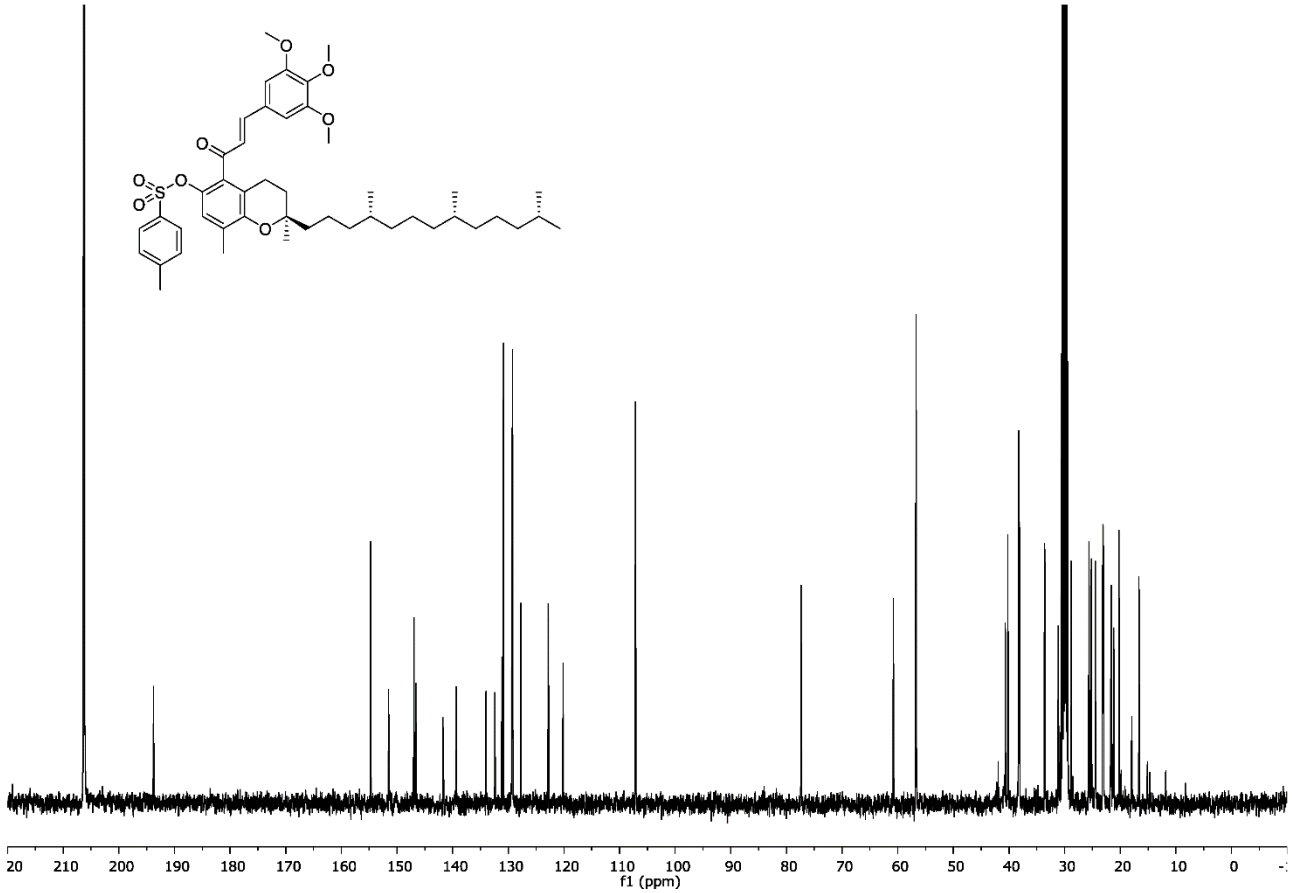


Fig. 16S. ^{13}C-NMR spectrum (100 MHz, acetone-d_6) of 6'-*O*-tosyl-3,4,5-trimethoxy-*δ*-tocopherol-chalcone (**1**).

J. Mex. Chem. Soc. **2022**, *66*(1)
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ISSN-e 2594-0317

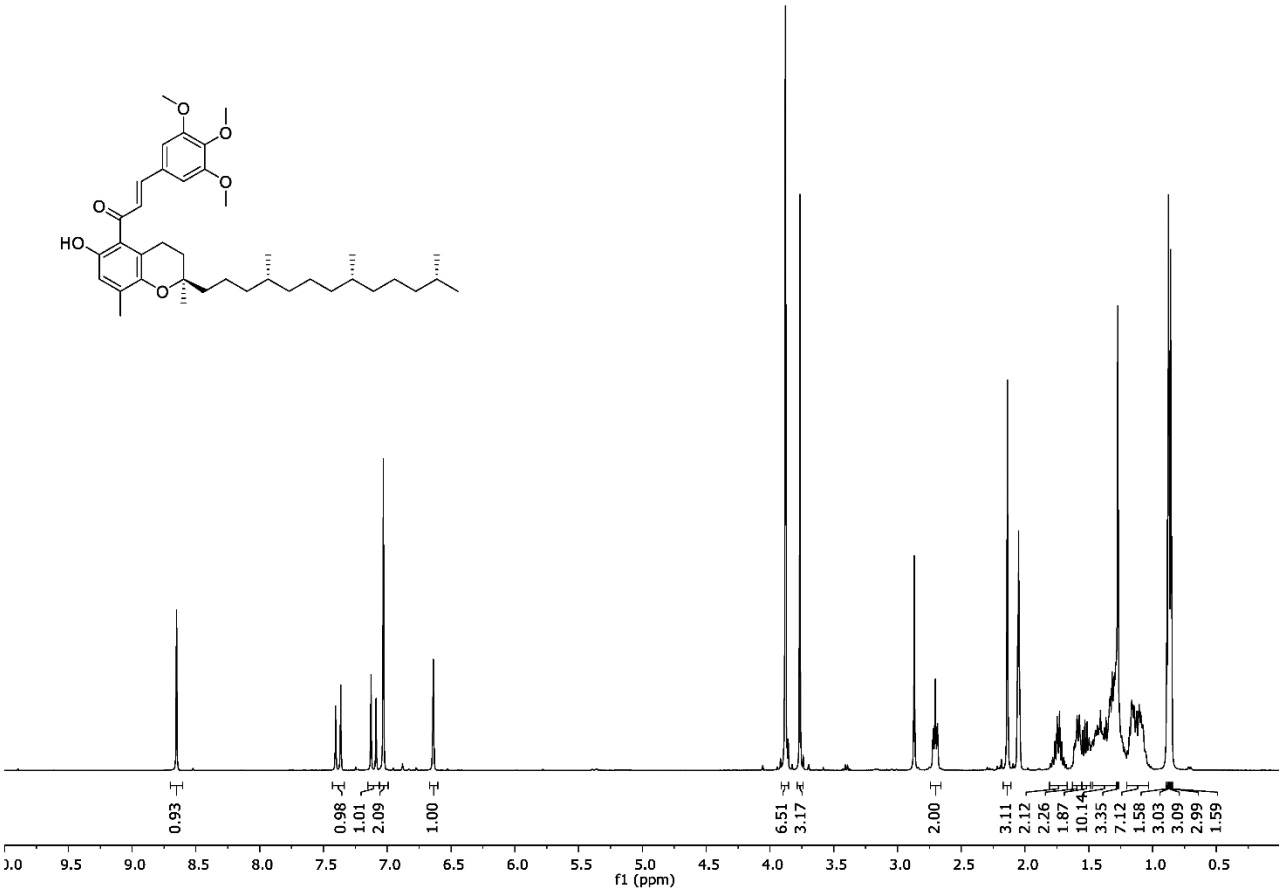

Fig. 17S. ^{1}H-NMR spectrum (400 MHz, acetone-d_6) of 3,4,5-trimethoxy-*δ*-tocopherol-chalcone (**2**).

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

ISSN-e 2594-0317

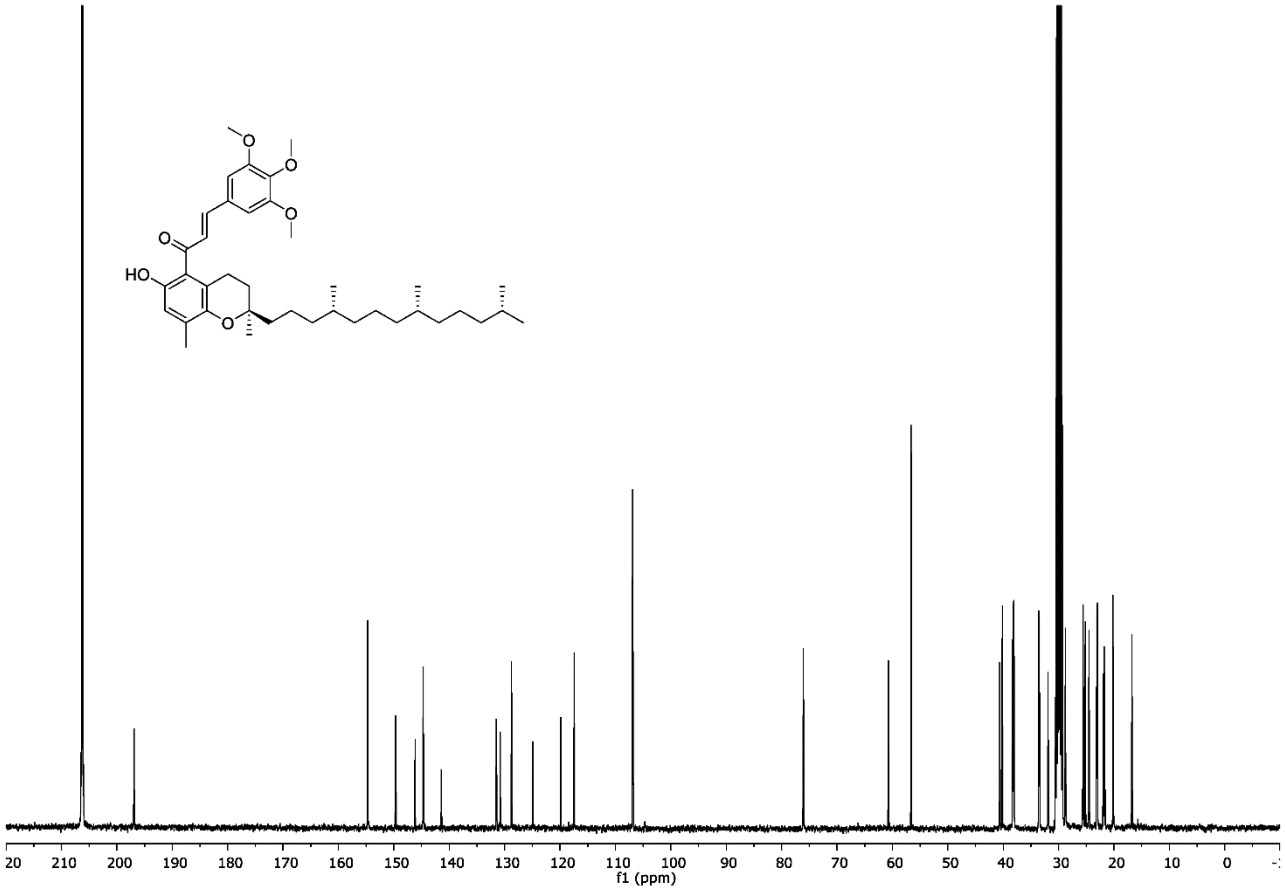

Fig. 18S. ^{13}C-NMR spectrum (100 MHz, acetone-d_6) of 3,4,5-trimethoxy-*δ*-tocopherol-chalcone (**2**).

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

ISSN-e 2594-0317

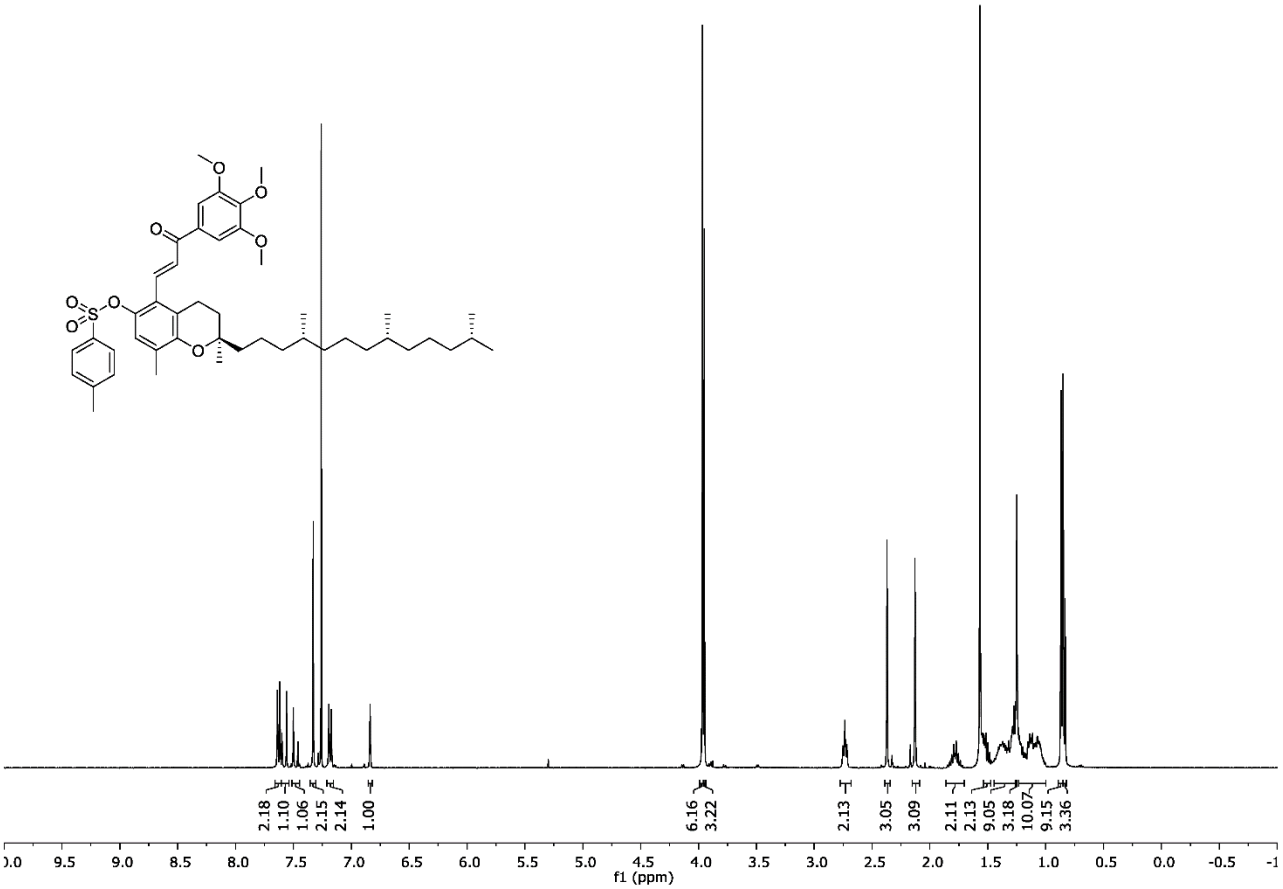

Fig. 19S. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of 6'-*O*-tosyl-3,4,5-trimethoxy-*δ*-tocopherol-retrochalcone (**3**).

J. Mex. Chem. Soc. **2022**, *66*(1)
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ISSN-e 2594-0317

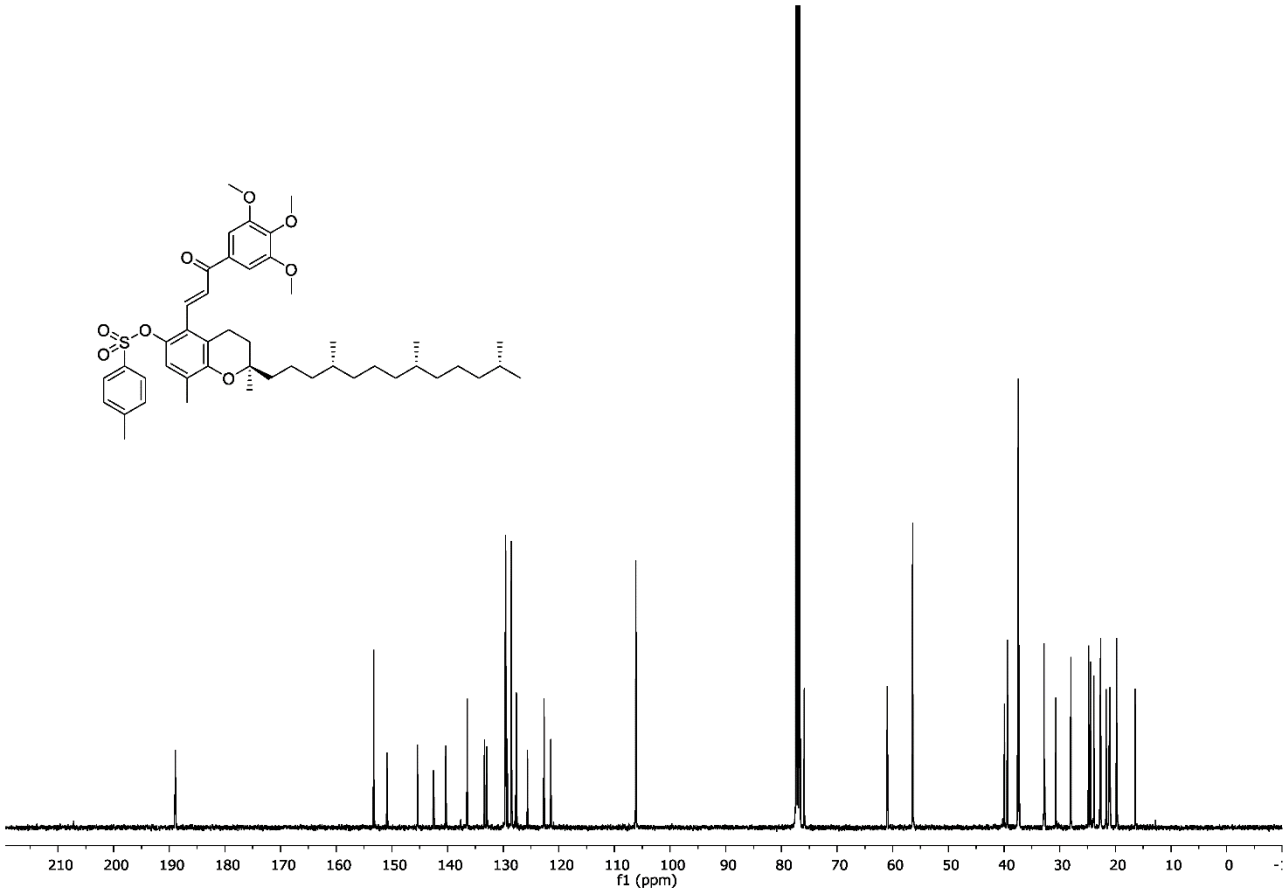

Fig. 20S. ^{13}C-NMR spectrum (100 MHz, $CDCl_3$) of 6'-*O*-tosyl-3,4,5-trimethoxy-*δ*-tocopherol-retrochalcone (**3**).

J. Mex. Chem. Soc. **2022**, *66*(1)
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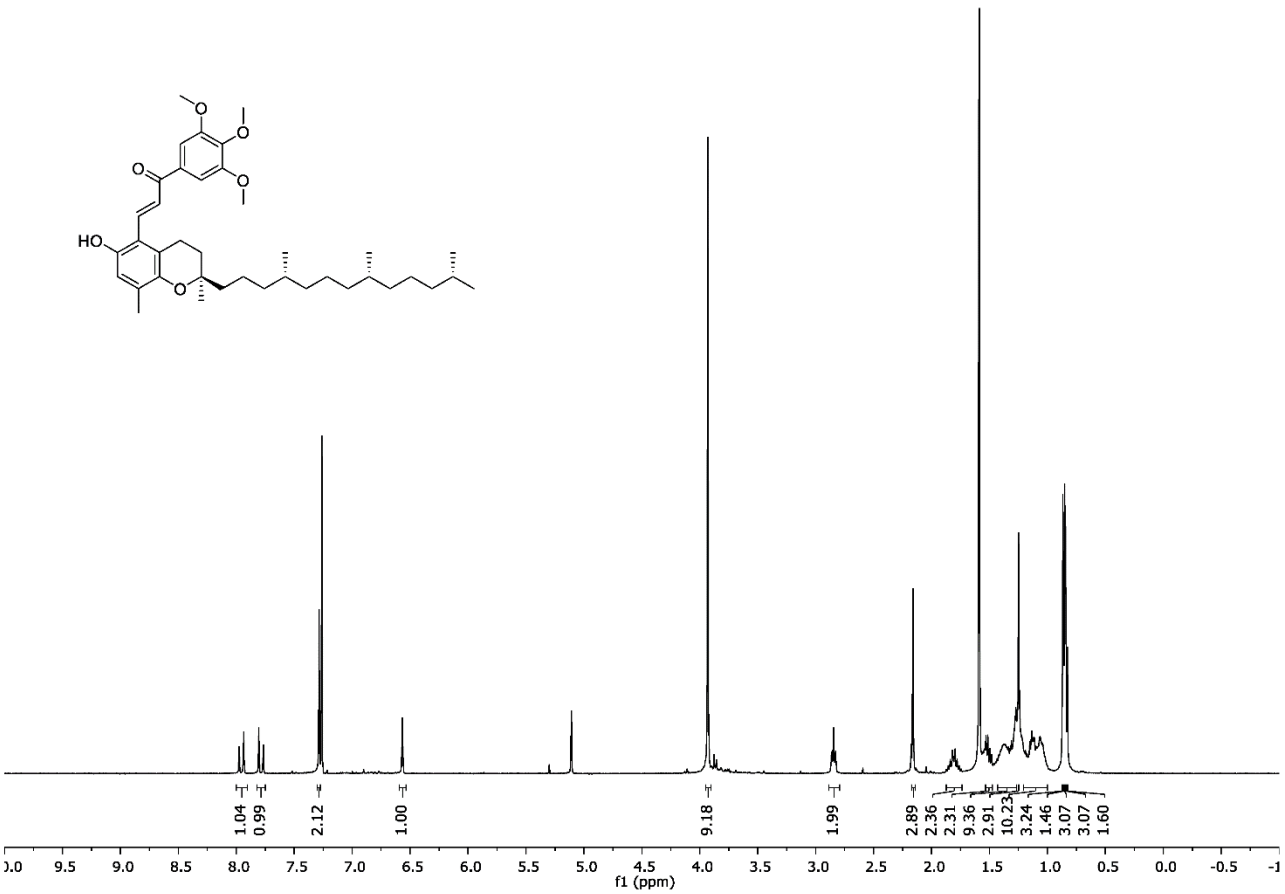

Fig. 21S. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of 3,4,5-trimethoxy-*δ*-tocopherol-retrochalcone (**4**).

J. Mex. Chem. Soc. **2022**, *66*(1)
Regular Issue

ISSN-e 2594-0317

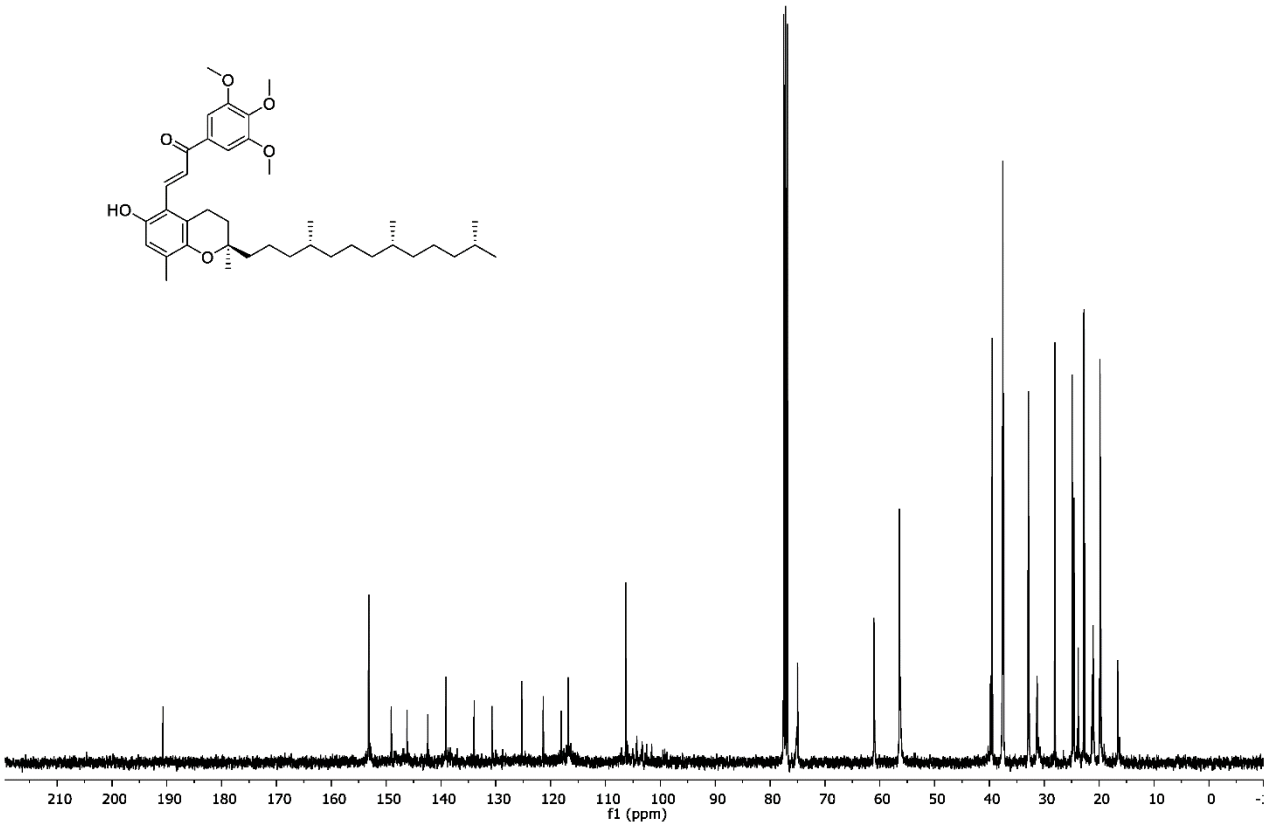

Fig. 22S. ^{13}C-NMR spectrum (100 MHz, $CDCl_3$) of 3,4,5-trimethoxy-*δ*-tocopherol-retrochalcone (**4**).