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Supplementary Information

Conformational Analysis of 2,2'-arylmethylene bis(3-hydroxy-5,5-dimethyl-2-cyclohexene-1-one) by NMR and Molecular Modeling

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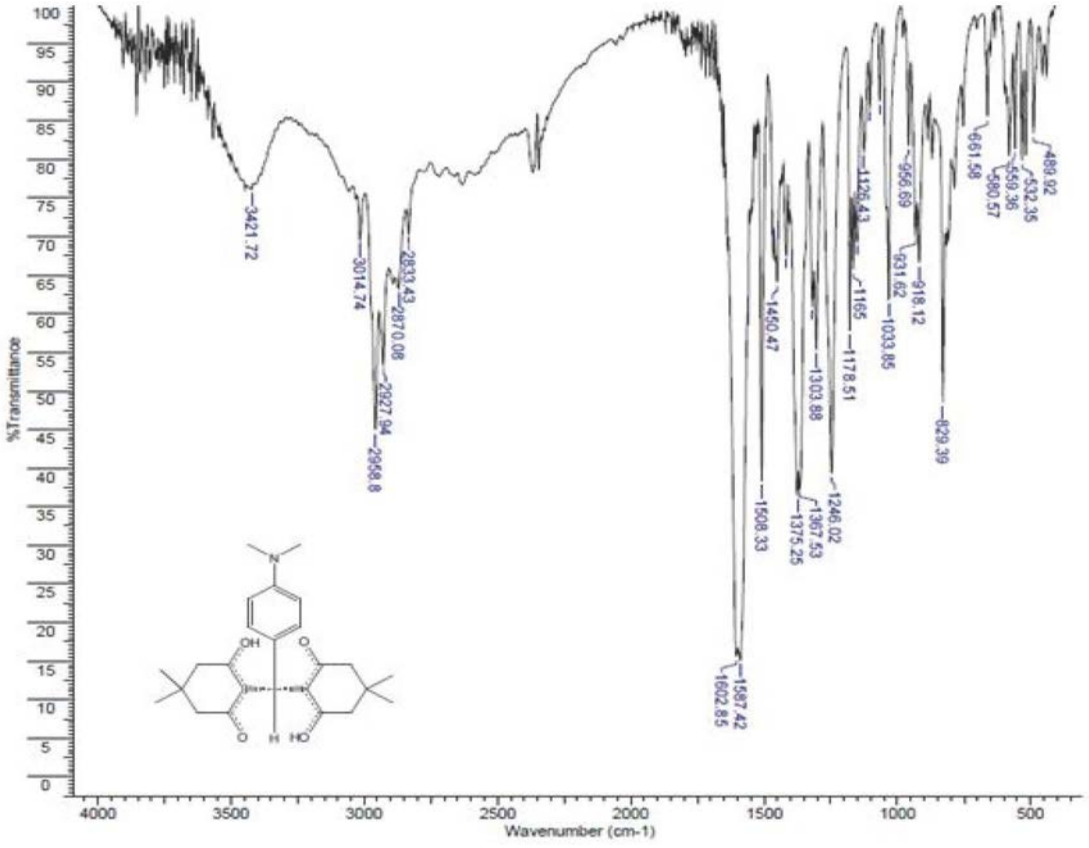

FigureS1. IR (KBr) of compound **3a.**

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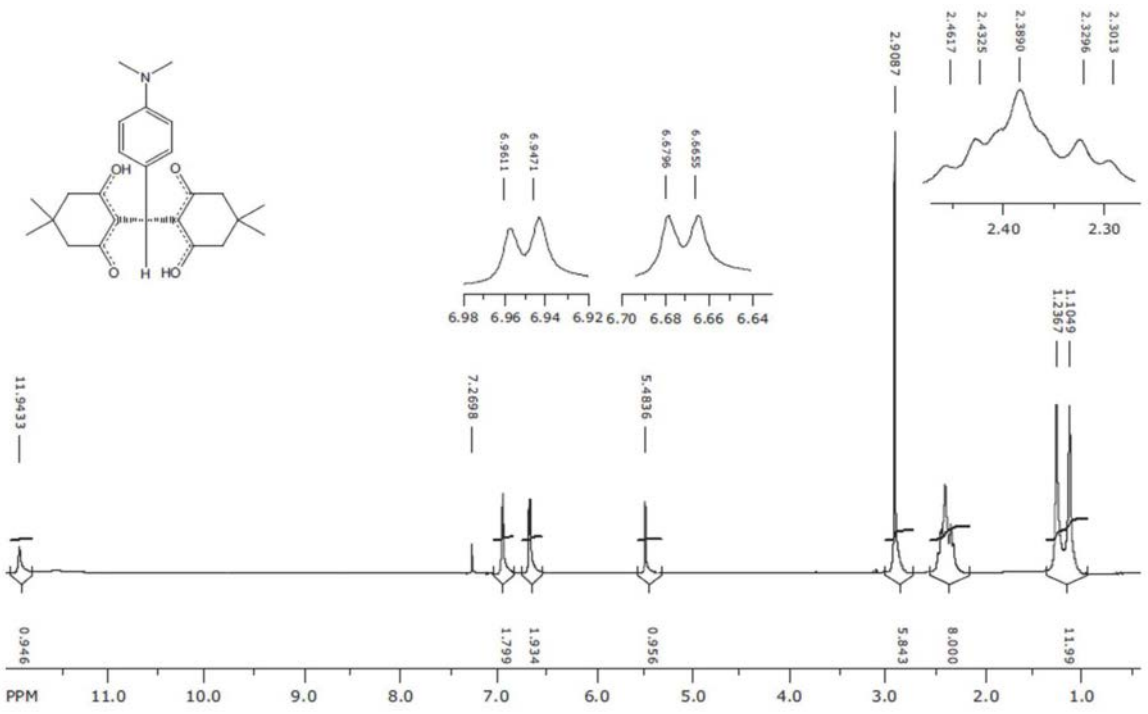

Figure S2. ^{1}H RMN spectrum ($CDCl_3$, 600 MHz) of compound **3a.**

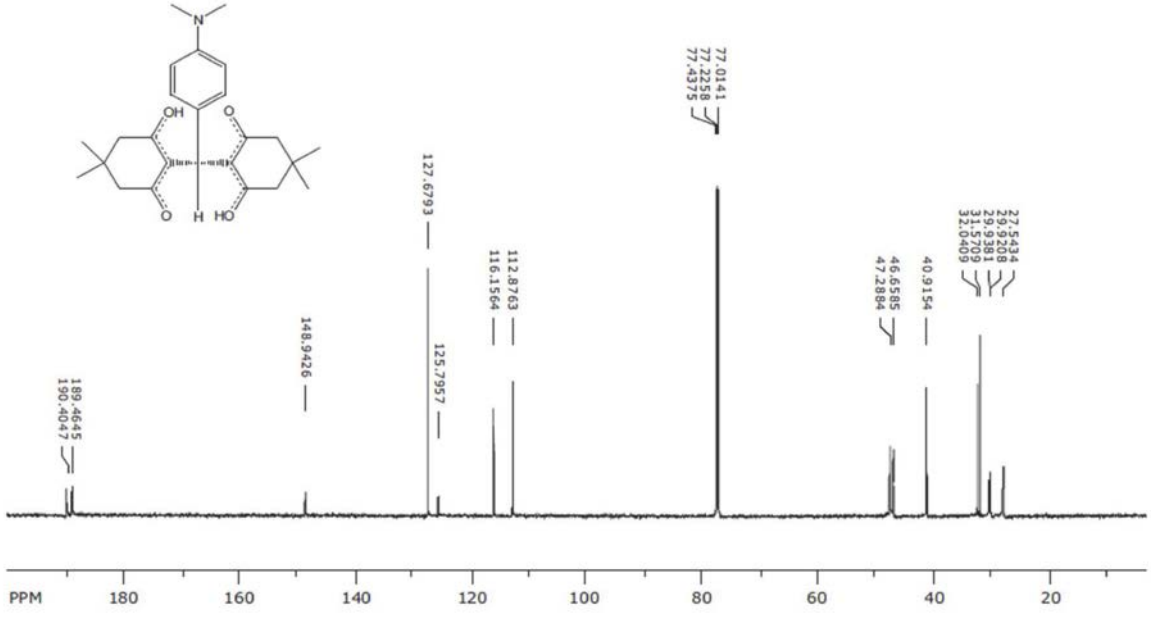

Figure S3. ^{13}C RMN spectrum ($CDCl_3$, 150 MHz) of compound **3a.**

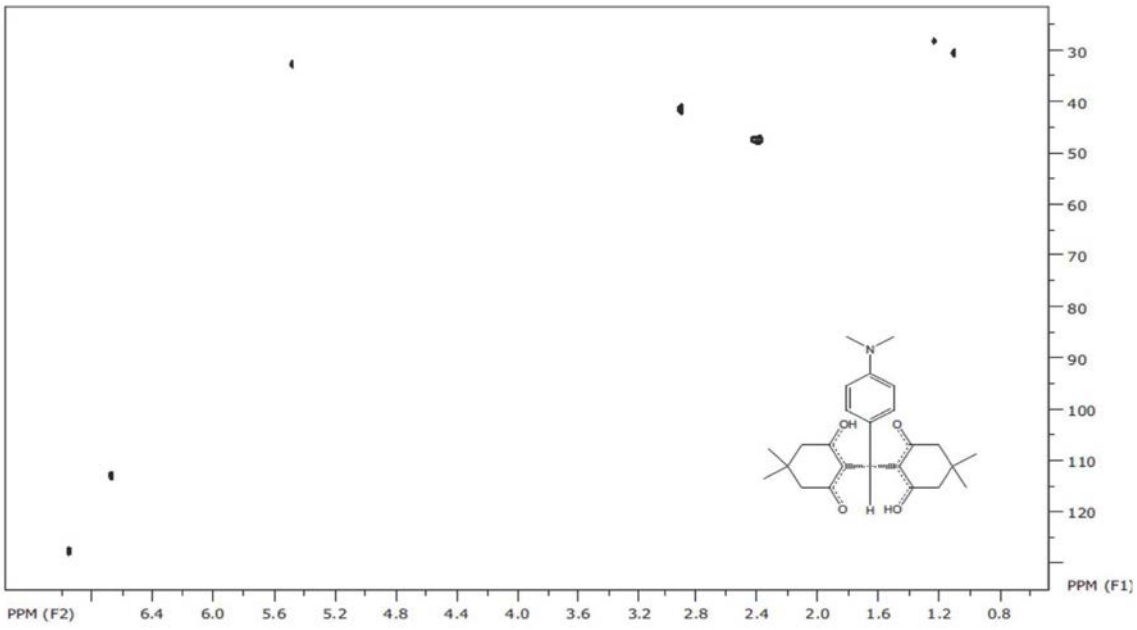

Figure S4. HSQC spectrum ($CDCl_3$, 600 MHz) of compound **3a.**

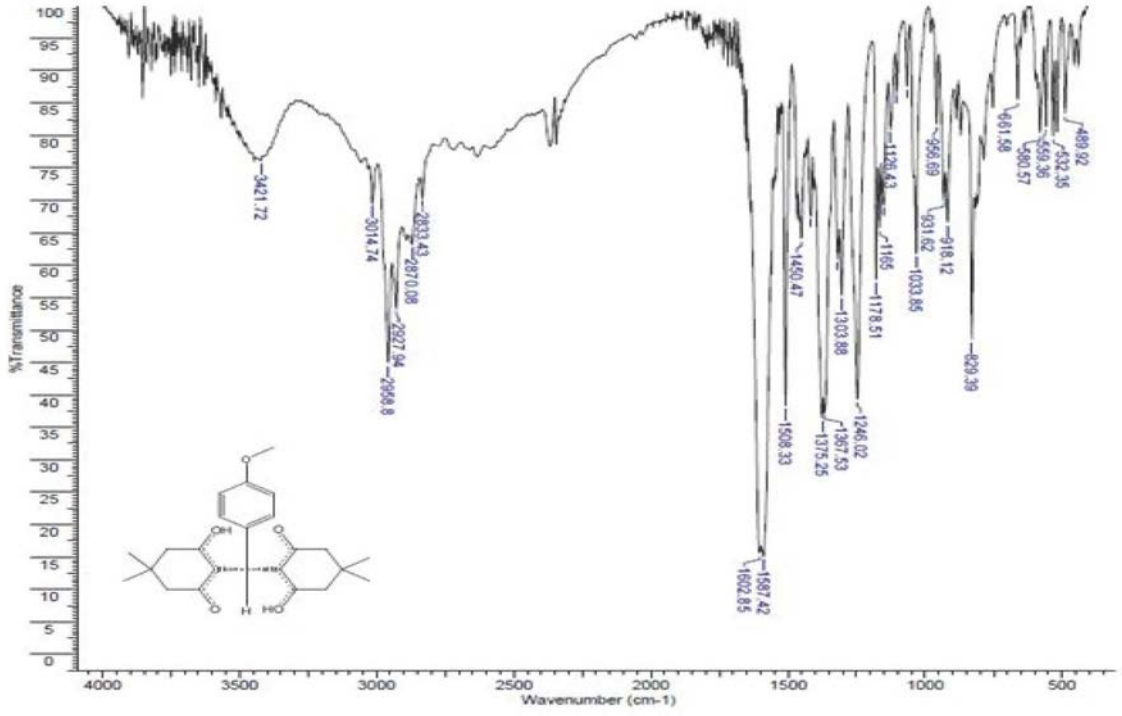

Figure S5. IR (KBr) of compound **3b.**

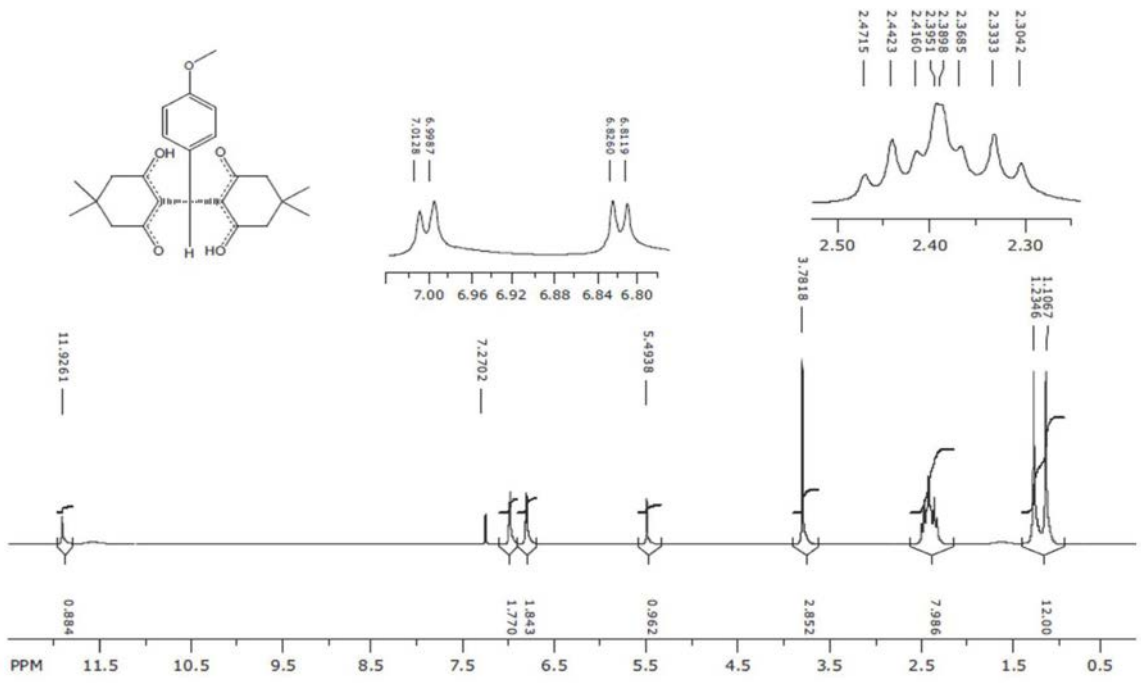

Figure S6. ^{1}H RMN spectrum ($CDCl_3$, 600 MHz) of compound **3b.**

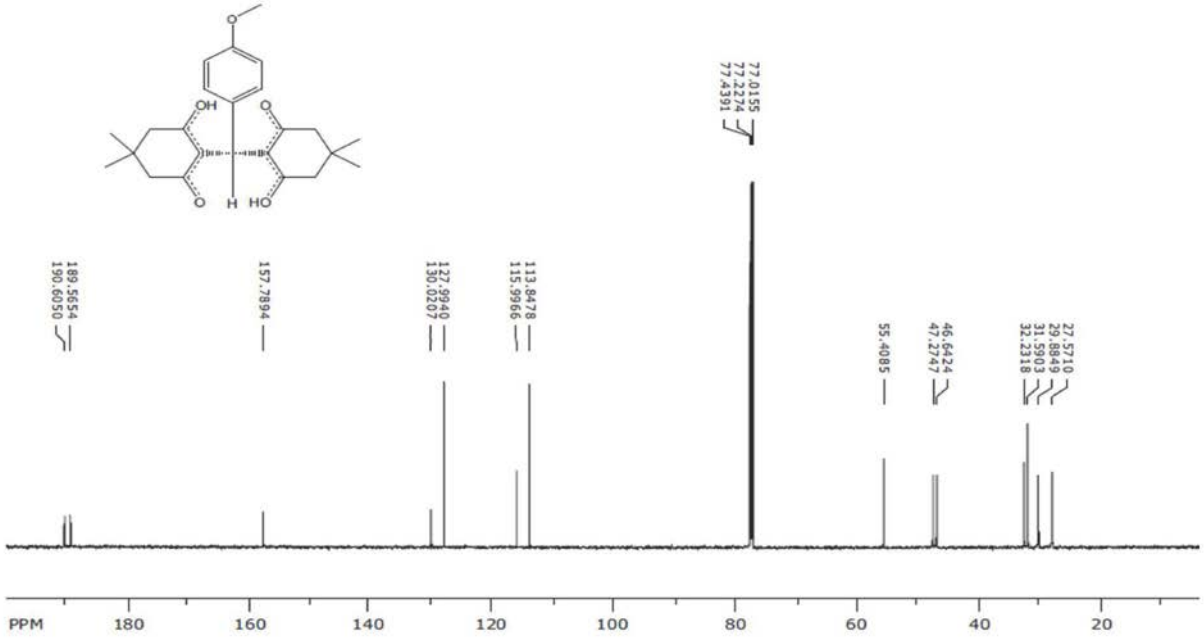

Figure S7. ^{13}C RMN spectrum ($CDCl_3$, 150 MHz) of compound **3b.**

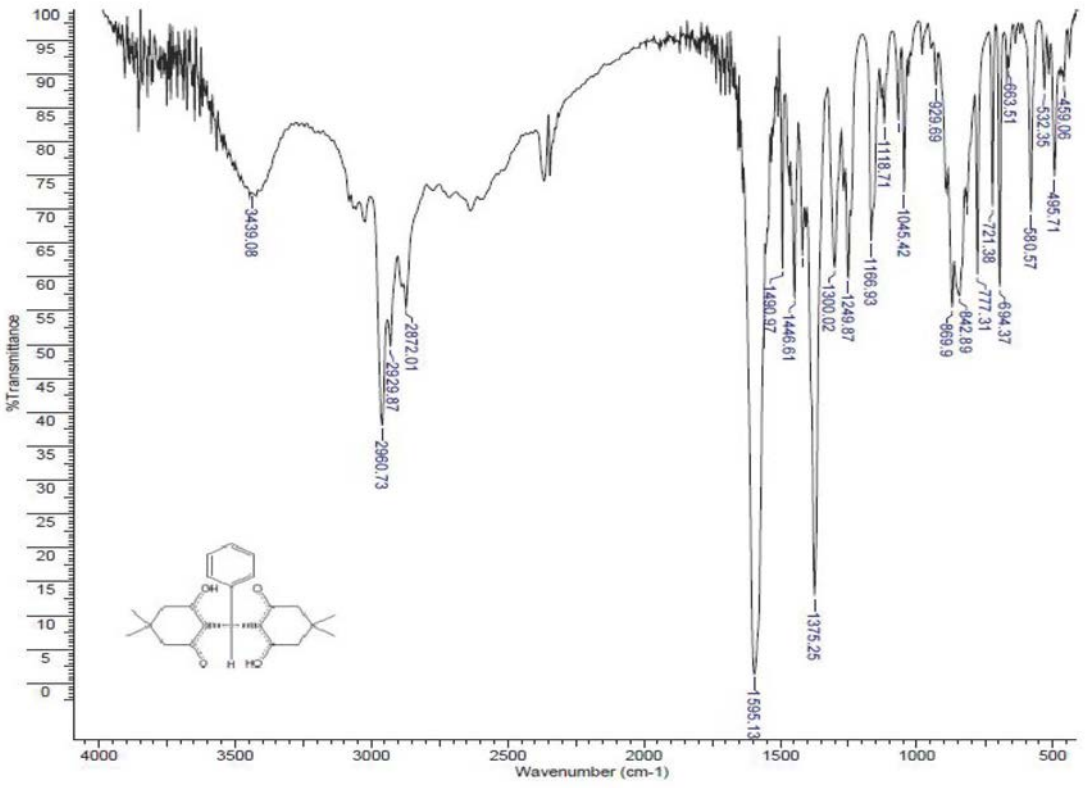

Figure S8. IR (KBr) of compound **3c.**

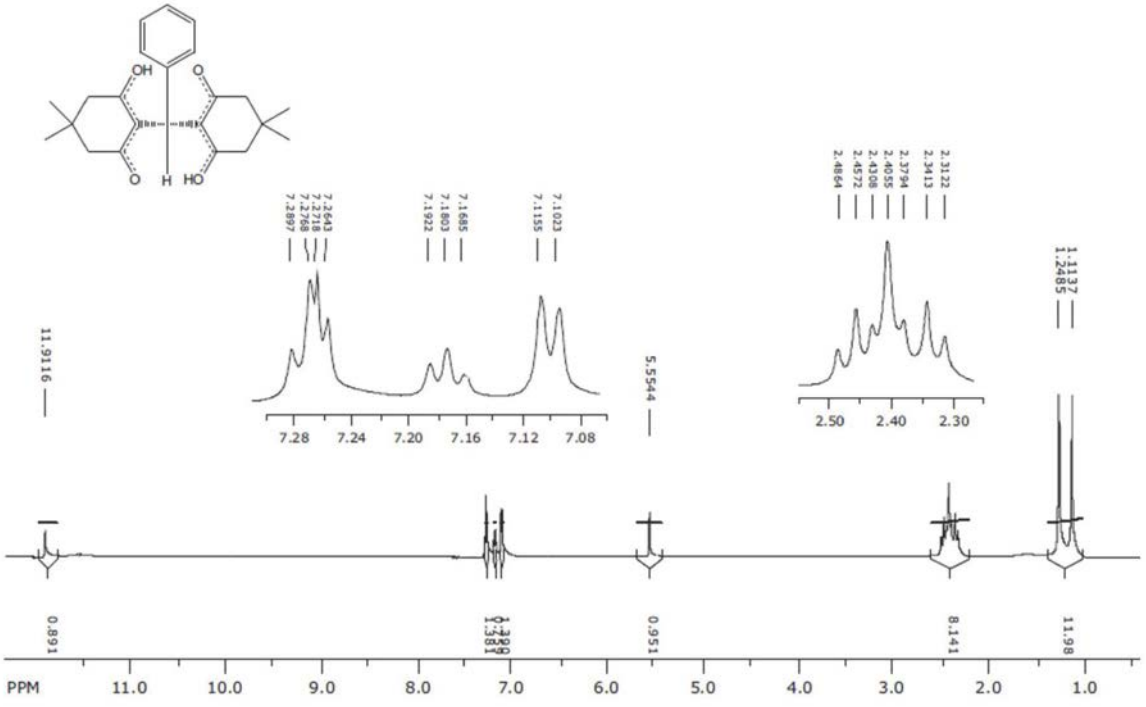

Figure S9. ^{1}H RMN spectrum ($CDCl_3$, 600 MHz) of compound **3c.**

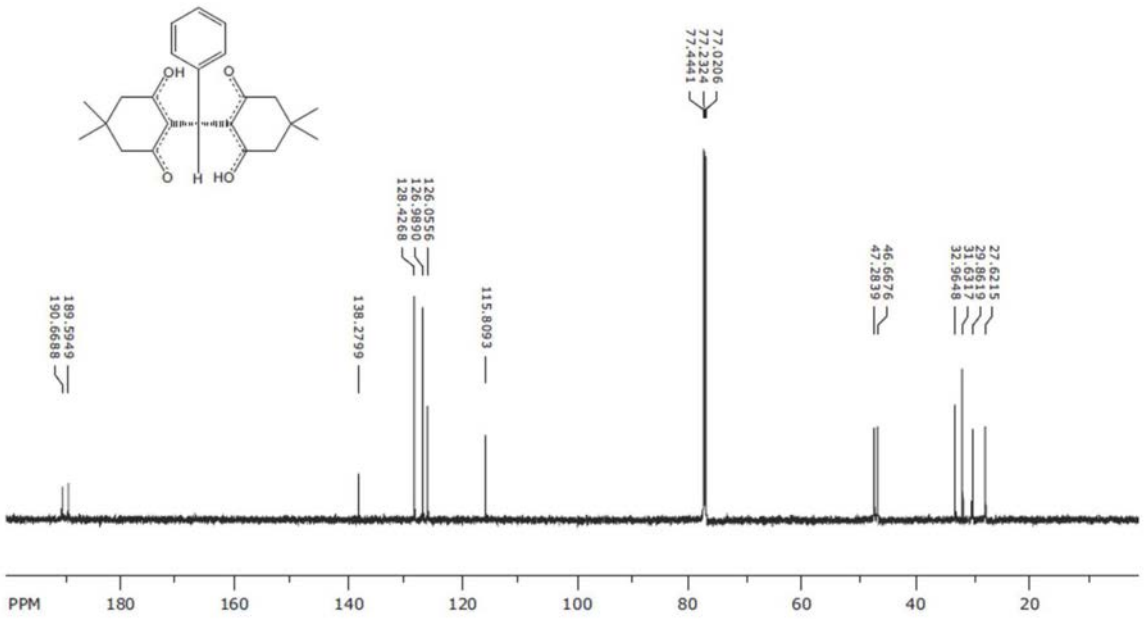

Figure S10. ^{13}C RMN spectrum ($CDCl_3$, 150 MHz) of compound **3c.**

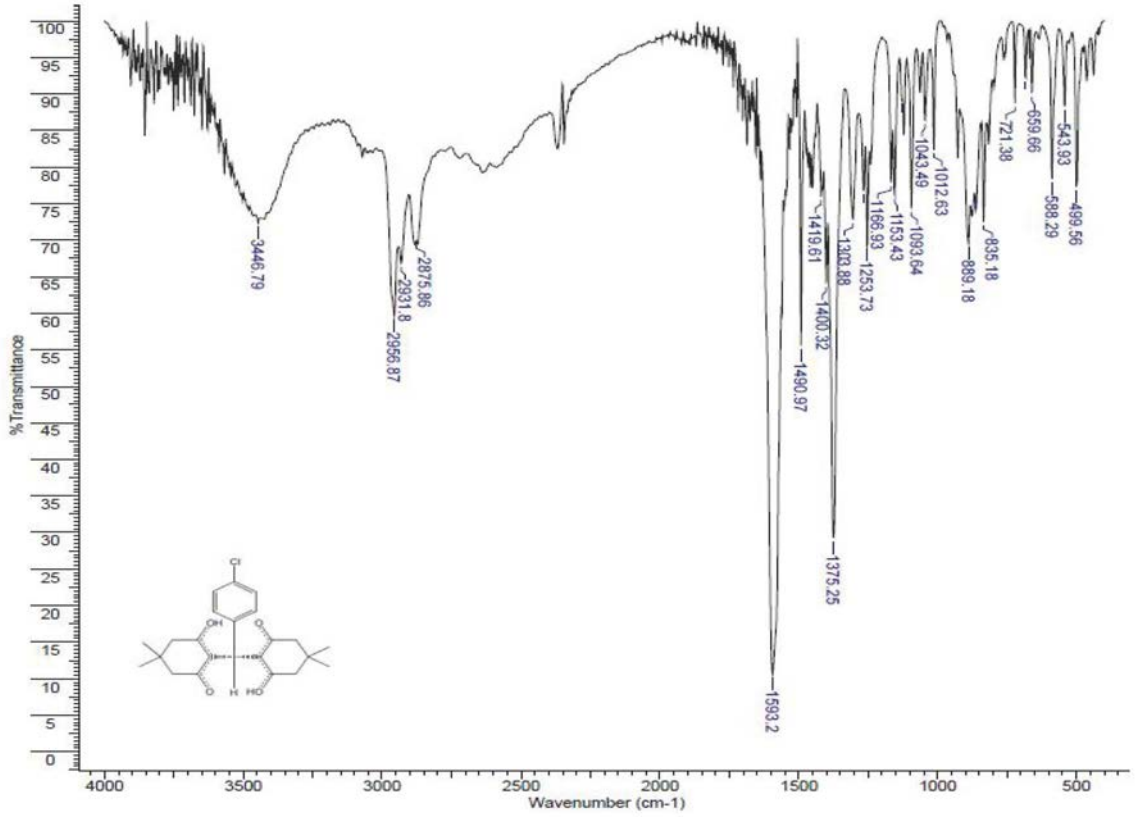

Figure S11. IR (KBr) of compound **3d.**

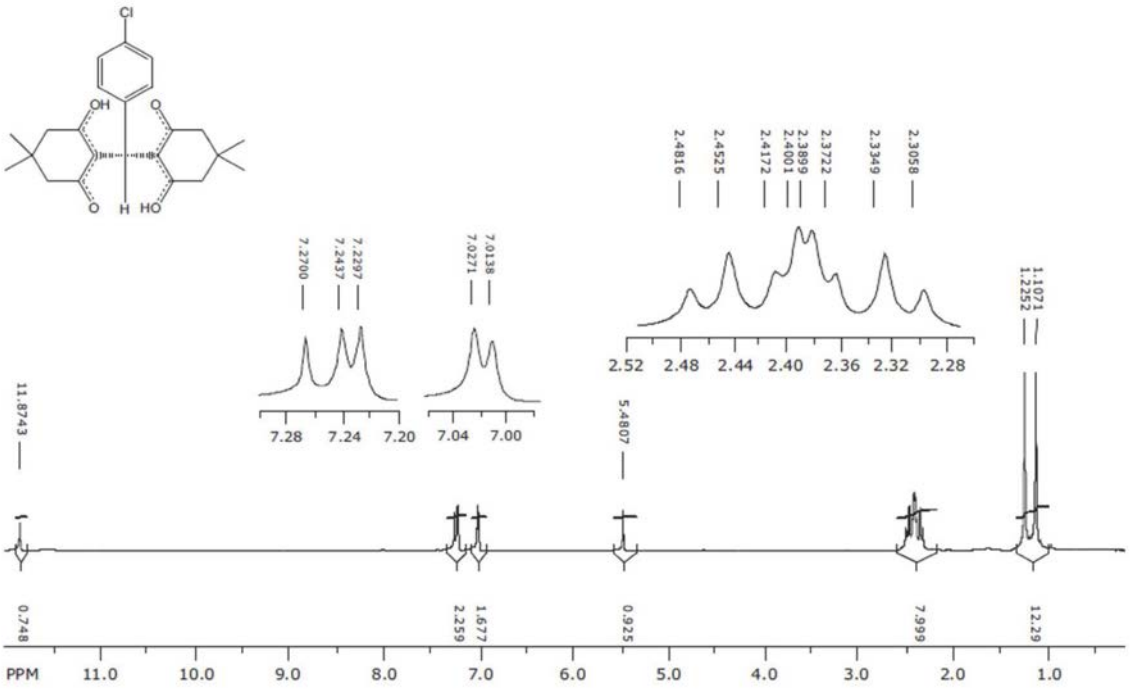

Figure S12. ^{1}H RMN spectrum ($CDCl_3$, 600 MHz) of compound **3d.**

Figure S13. ^{13}C RMN spectrum ($CDCl_3$, 150 MHz) of compound **3d.**

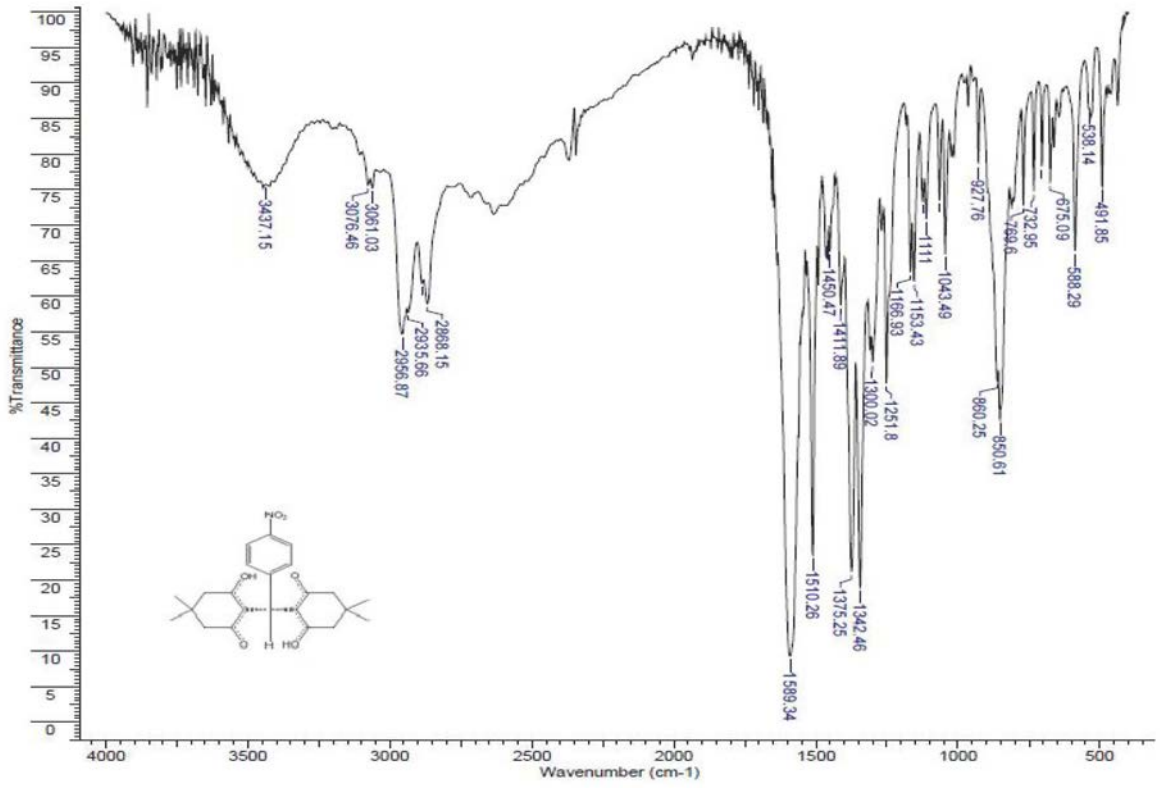

Figure S14. IR (KBr) of compound **3e.**

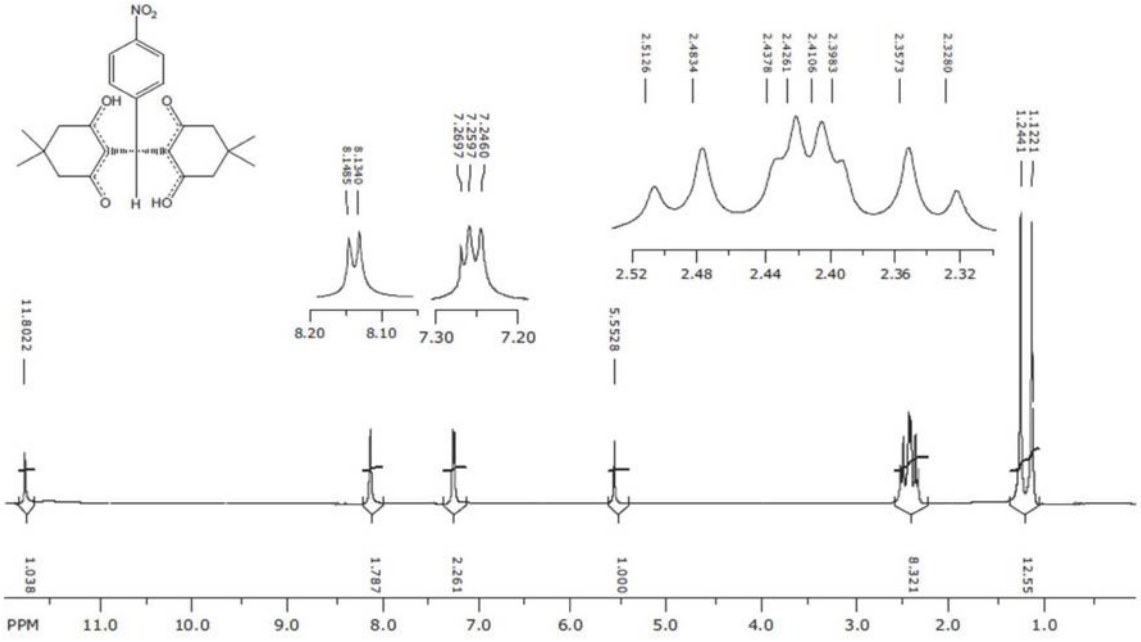

Figure S15. ^{1}H RMN spectrum ($CDCl_3$, 600 MHz) of compound **3e** at 20 °C.

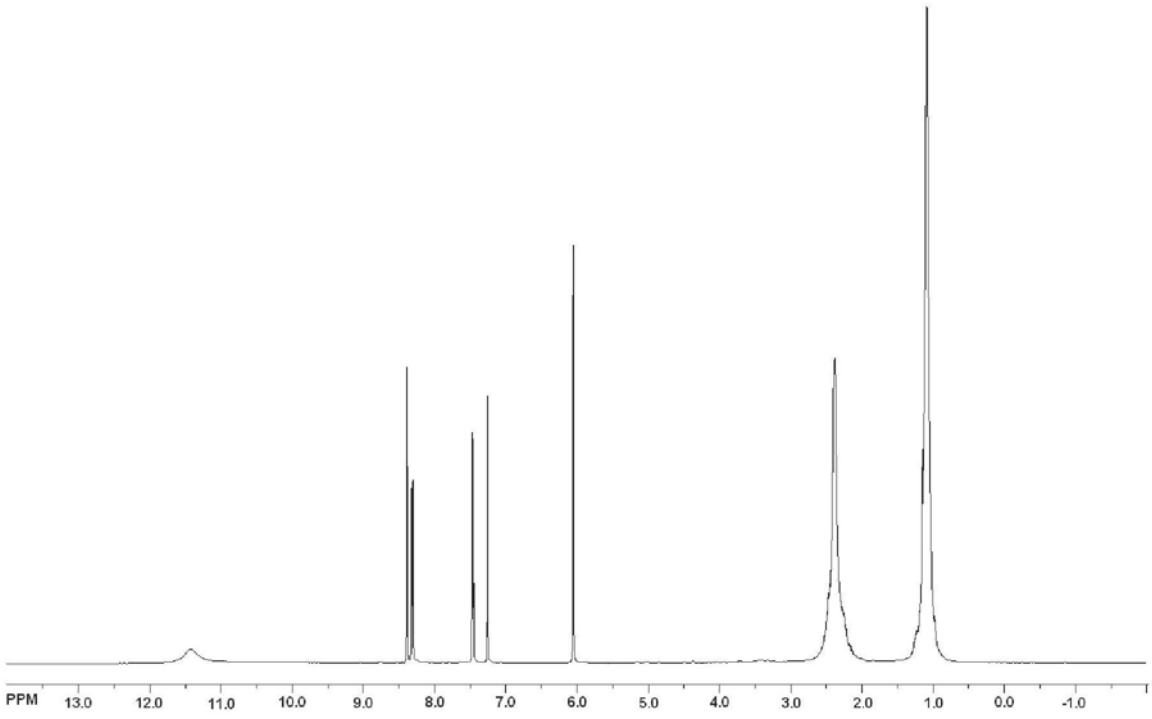

Figure S16. ^{1}H RMN spectrum ($CDCl_3$, 600 MHz) of compound **3e** at 50 °C.

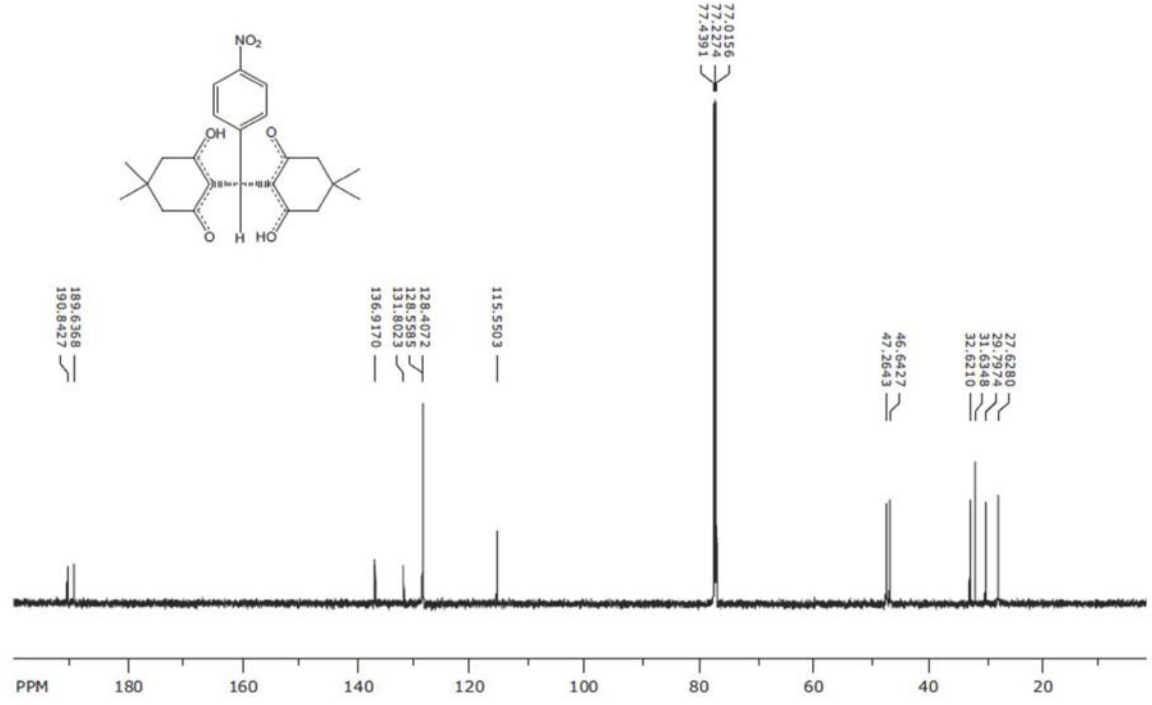

Figure S17. ^{13}C RMN spectrum ($CDCl_3$, 150 MHz) of compound **3e** at 20 °C.

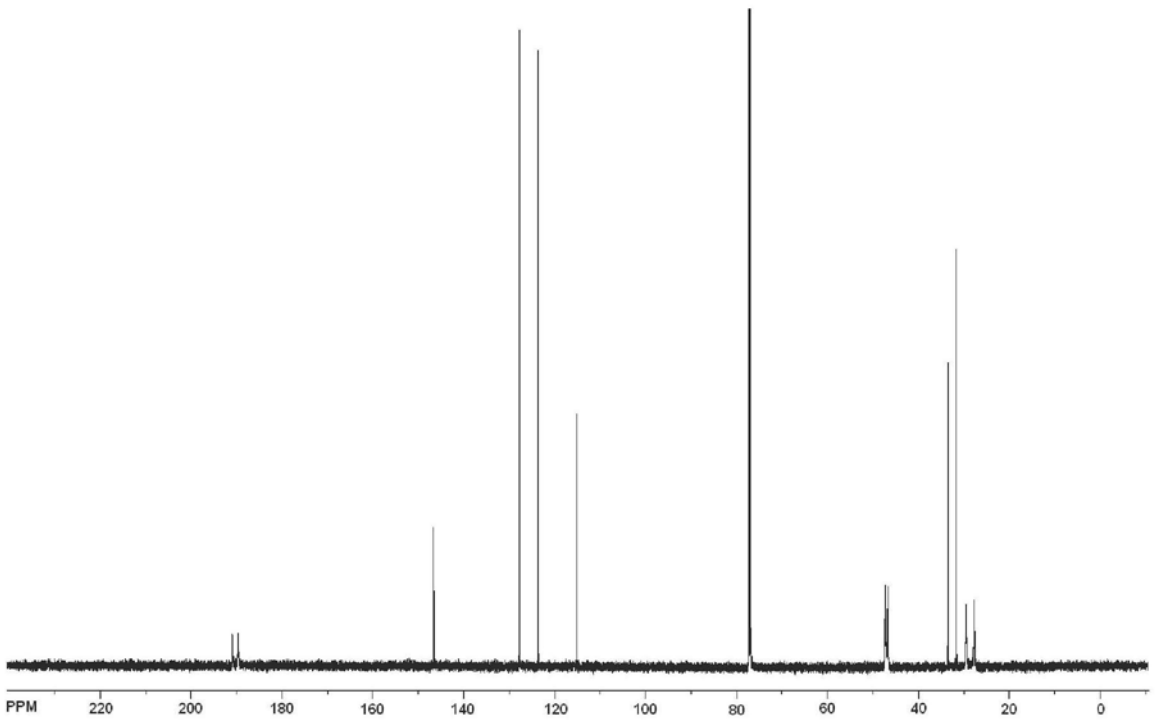

Figure S18. ^{13}C RMN spectrum ($CDCl_3$, 150 MHz) of compound **3e** at 50 °C.

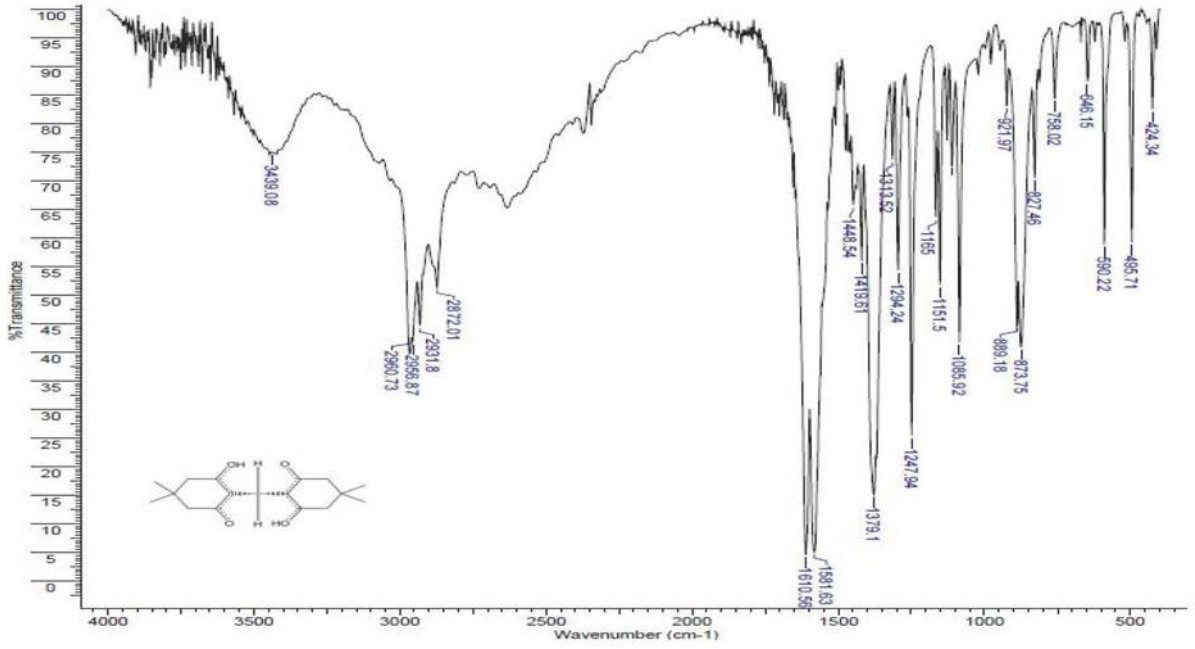

Figure S19. IR (KBr) of compound **3f.**

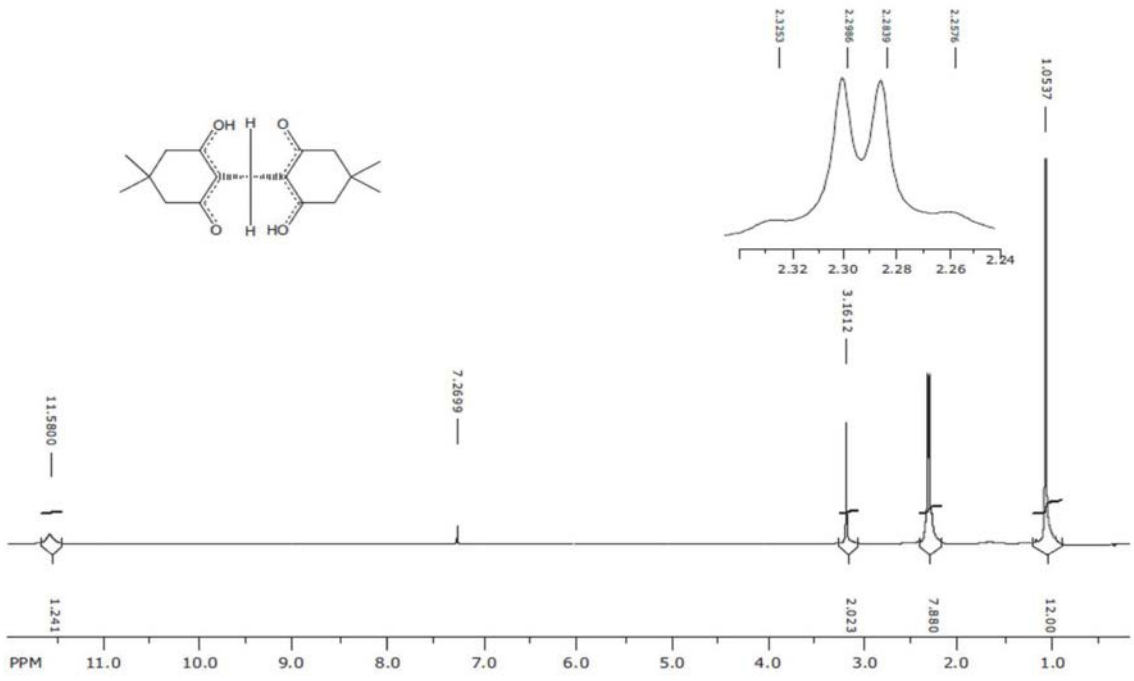

Figure S20. ^{1}H RMN spectrum ($CDCl_3$, 600 MHz) of compound **3f.**

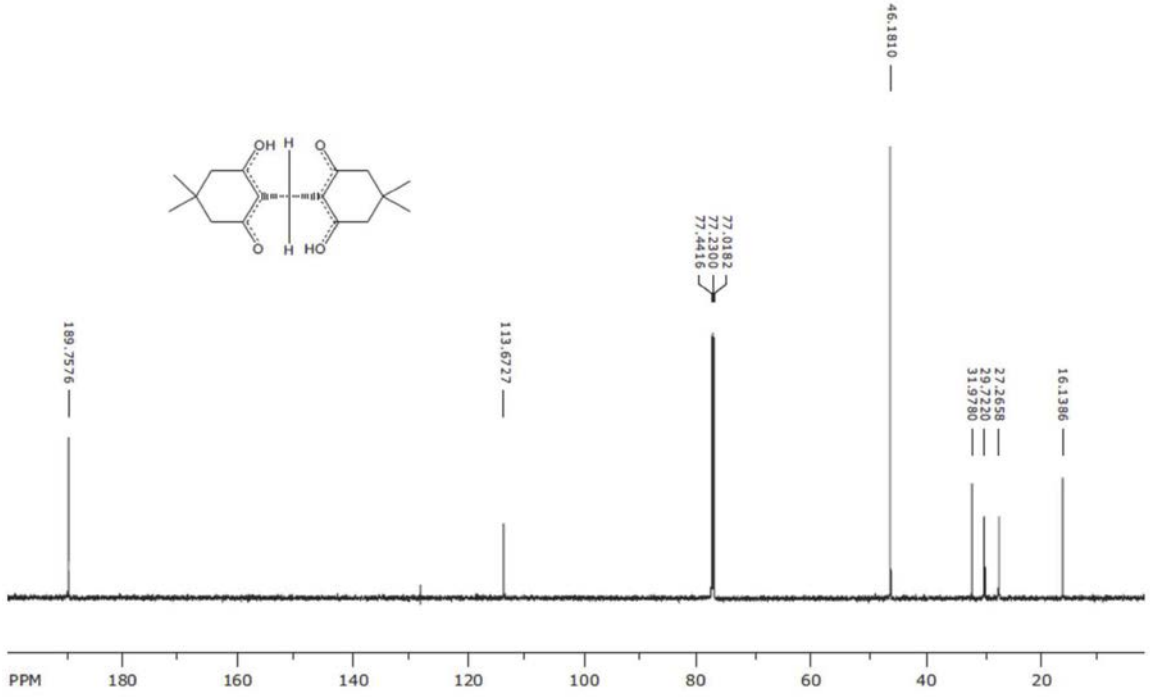

Figure S21. ^{13}C RMN spectrum ($CDCl_3$, 150 MHz) of compound **3f.**

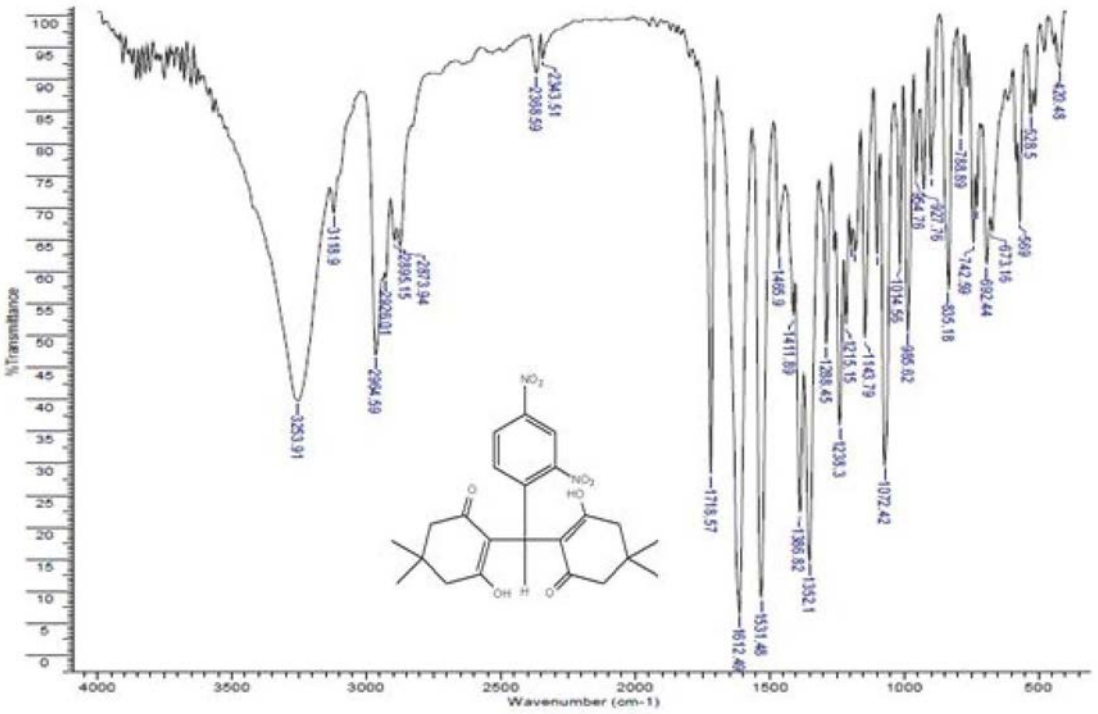

Figure S22. IR (KBr) of compound **3g.**

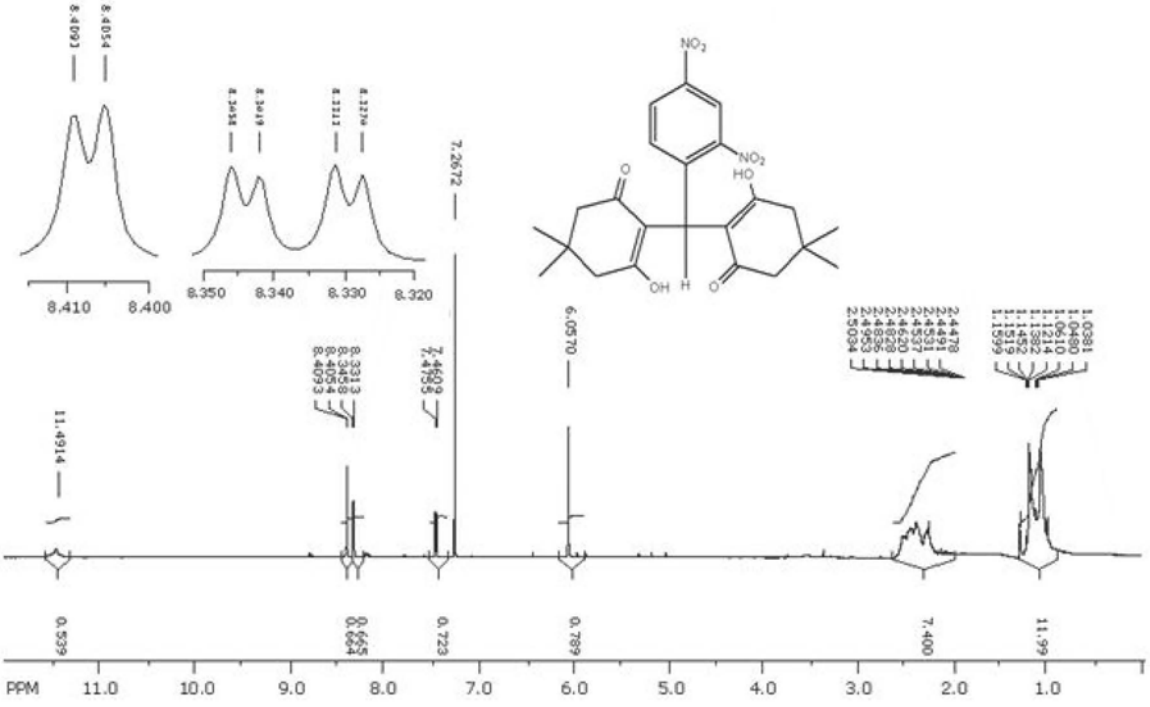

Figure S23. ^{1}H RMN spectrum ($CDCl_3$, 600 MHz) of compound **3g** at 20 °C.

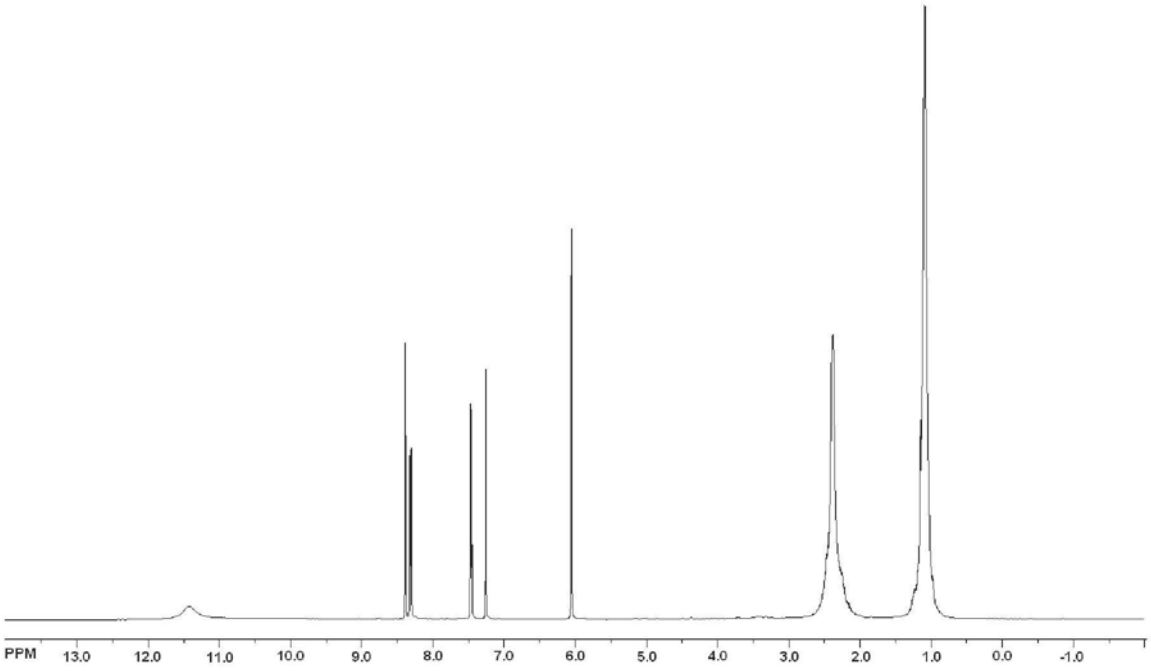

Figure S24. ^{1}H RMN spectrum ($CDCl_3$, 600 MHz) of compound **3g** at 50 °C.

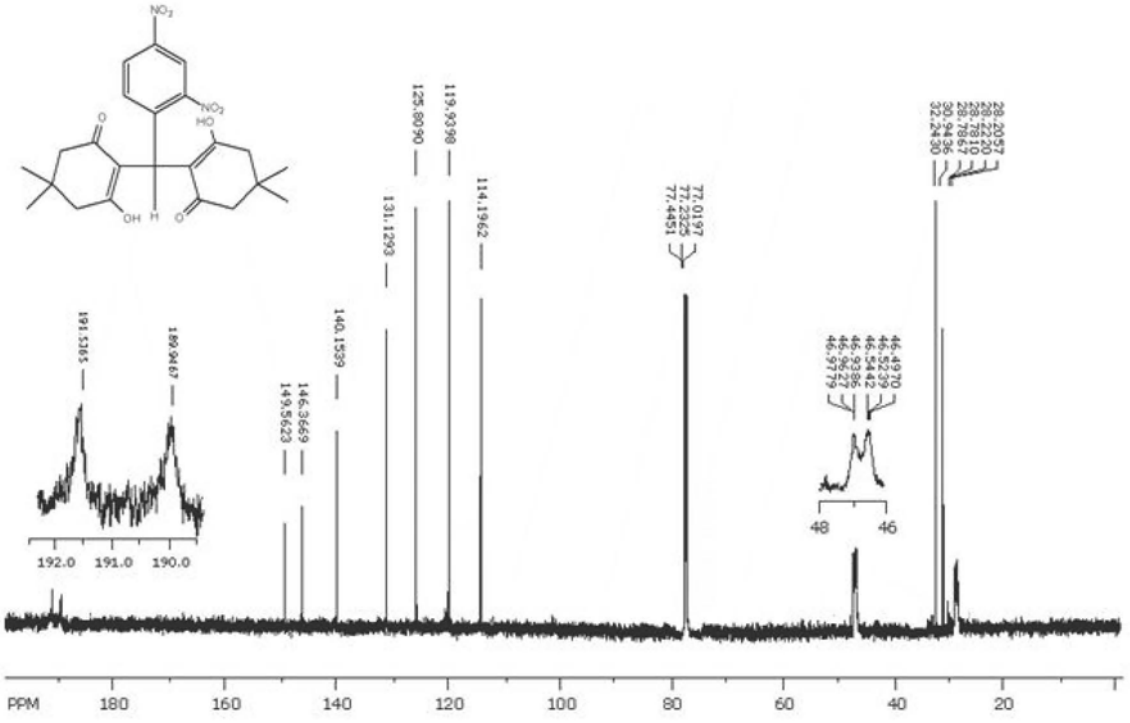

Figure S25. ^{13}C RMN spectrum ($CDCl_3$, 150 MHz) of compound **3g** at 20 °C.

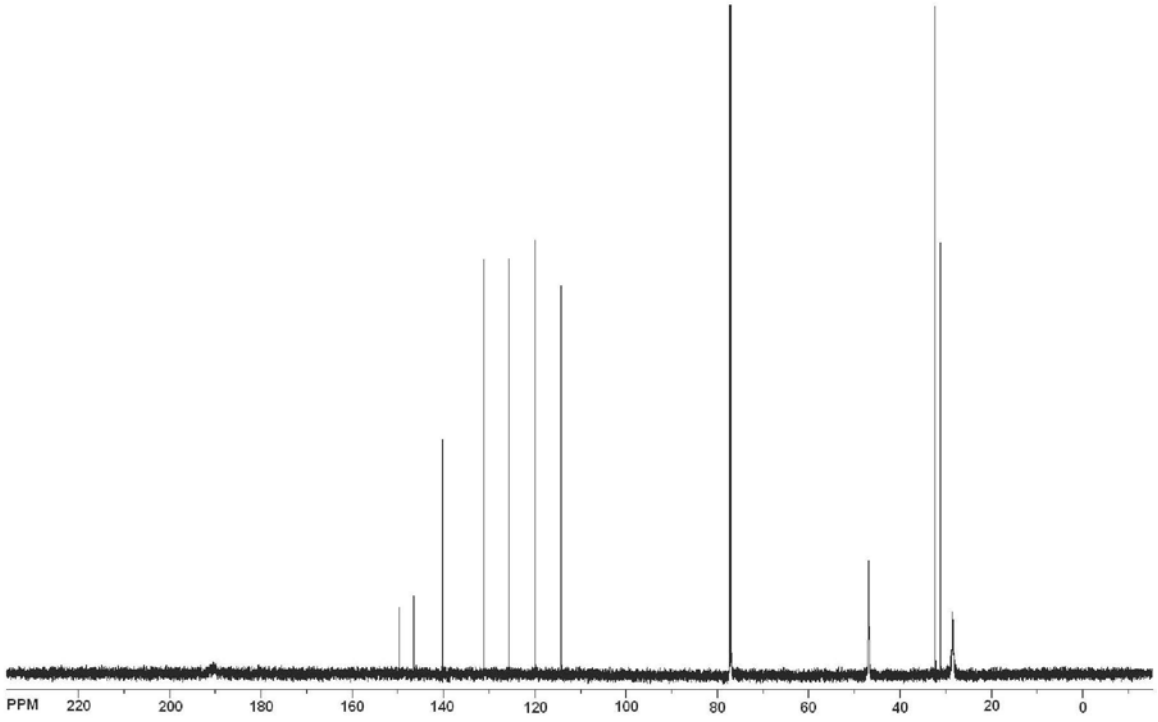

Figure S26. ^{13}C RMN spectrum ($CDCl_3$, 150 MHz) of compound **3g** at 50 °C.

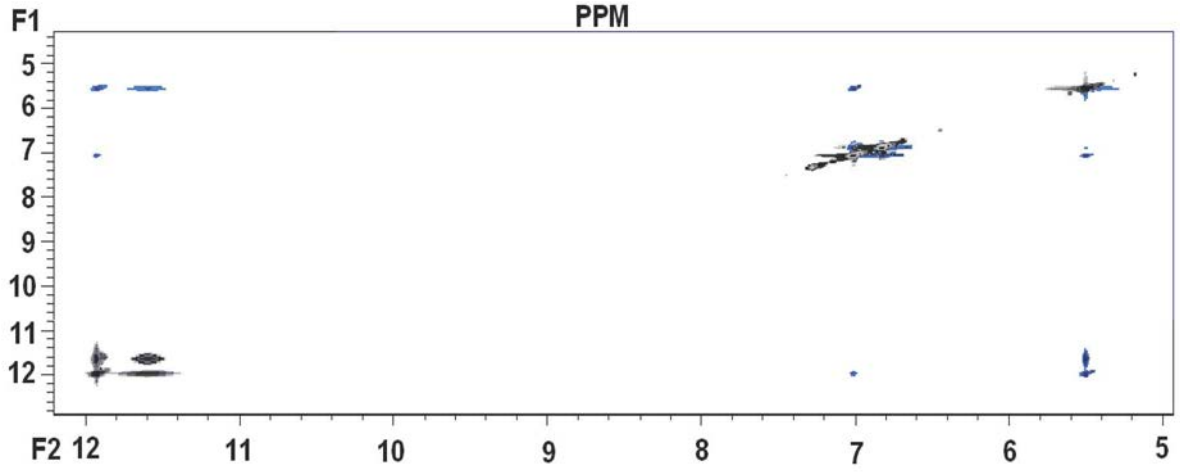

Figure S27. NOESY-2D spectrum ($CDCl_3$, 600 MHz) of compound **3b** showing the dipolar coupling interaction of the two intramolecular hydrogen bond signals (11.93 and 11.58 ppm) with H7 (5.48 ppm).

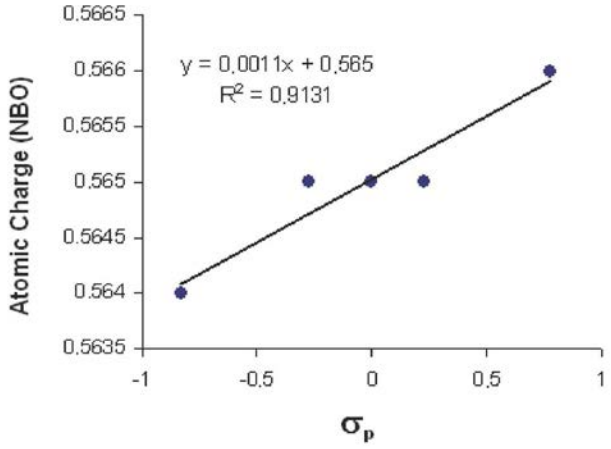

Figure S28. Graphic of correlation between the atomic charge (NBO) of C1 (**3a**-**e**) with the σ_p Hammett values of the R groups.

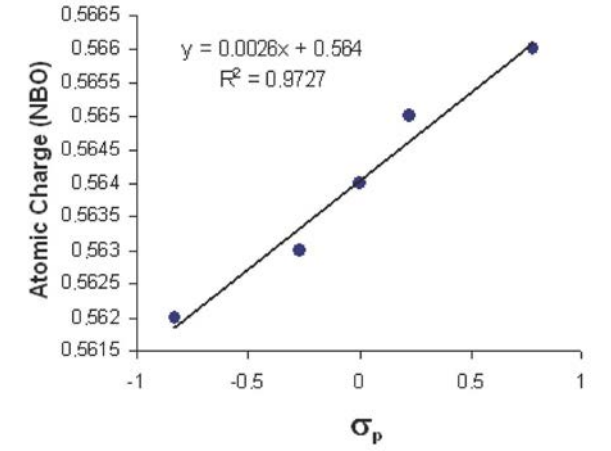

Figure S29. Graphic of correlation between the atomic charge (NBO) of C9 (**3a-e**) with the σ_p Hammett values of the R groups.

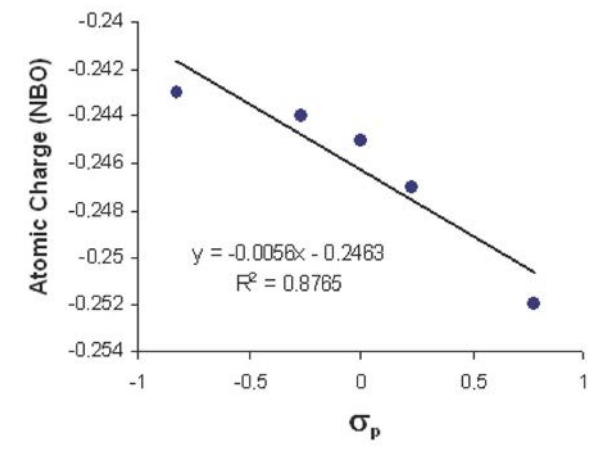

Figure S30. Graphic of correlation between the atomic charge (NBO) of C2 (**3a**-**e**) with the σ_p Hammett values of the R groups.

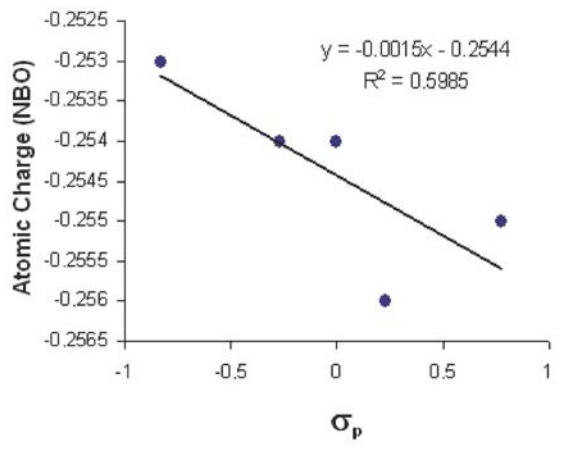

Figure S31. Graphic of correlation between the atomic charge (NBO) of C8 (**3a**-**e**) with the σ_p Hammett values of the R groups.

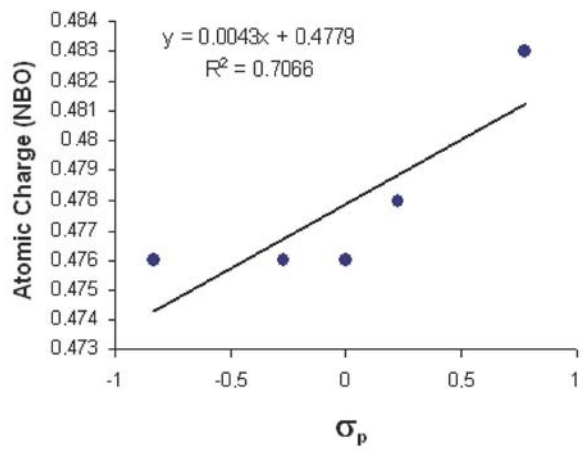

Figure S32. Graphic of correlation between the atomic charge (NBO) of C3 (**3a**-**e**) with the σ_p Hammett values of the R groups.

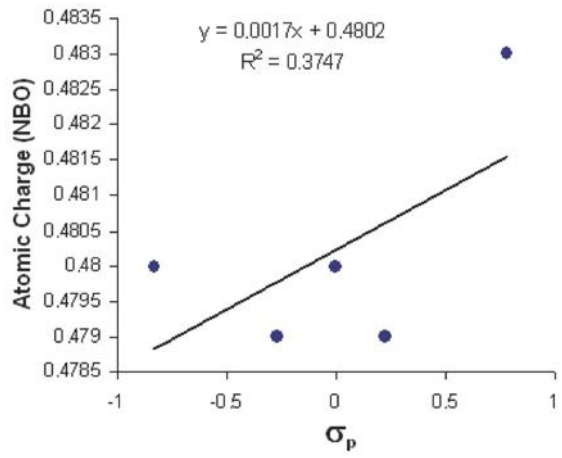

Figure S33. Graphic of correlation between the atomic charge (NBO) of C13 (**3a**-**e**) with the σ_p Hammett values of the R groups.

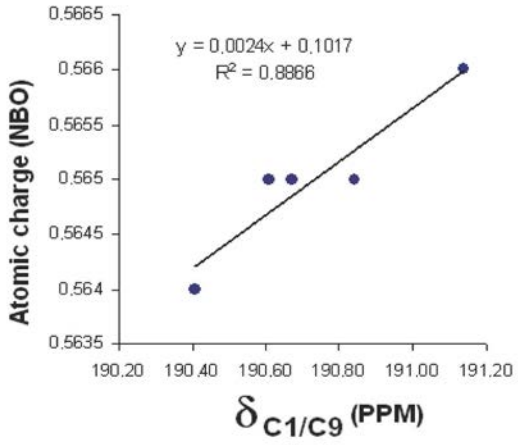

Figure S34. Graphic of correlation between the atomic charge (NBO) of C13 (**3a**-**e**) with the chemical shift $\delta_{C1/C9}$.

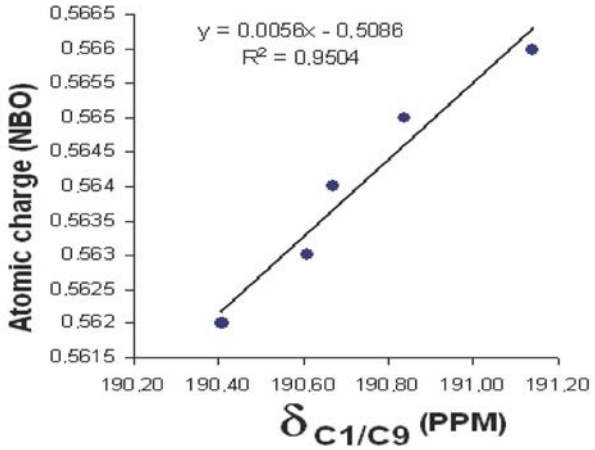

Figure S35. Graphic of correlation between the atomic charge (NBO) of C9 (**3a**-**e**) with the chemical shift $\delta_{C1/C9}$.

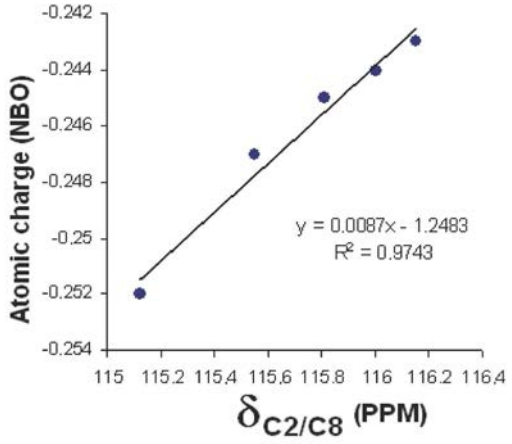

Figure S36. Graphic of correlation between the atomic charge (NBO) of C2 (**3a**-**e**) with the chemical shift δ_{C2}.

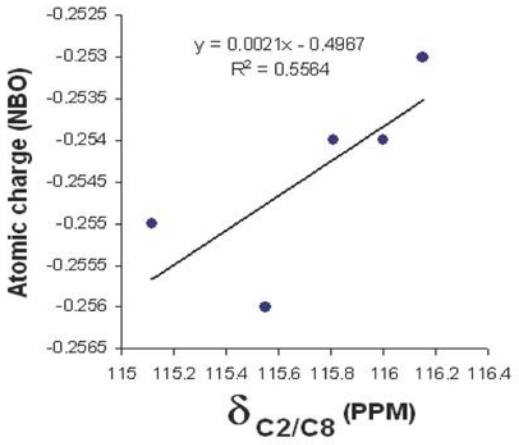

Figure S37. Graphic of correlation between the atomic charge (NBO) of C8 (**3a**-**e**) with the chemical shift δ_{C8}.

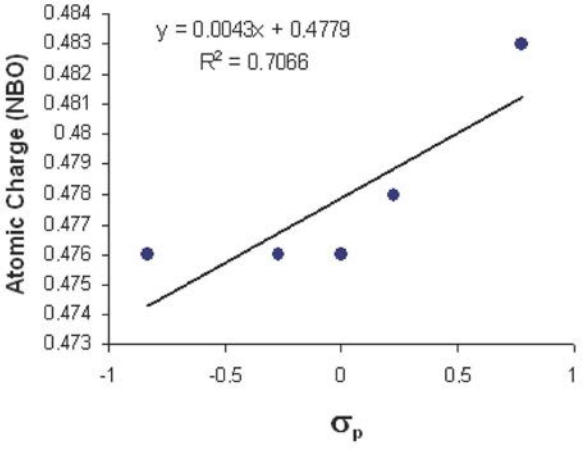

Figure S38. Graphic of correlation between the atomic charge (NBO) of C3 (**3a**-**e**) with the chemical shift $\delta_{C31/C13}$.

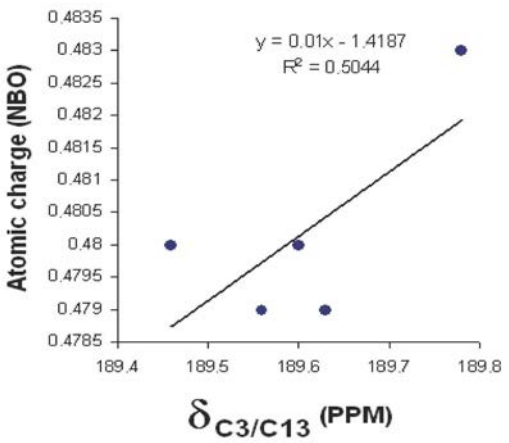

Figure S39. Graphic of correlation between the atomic charge (NBO) of C13 (**3a**-**e**) with the chemical shift $\delta_{C3/C13}$.

Table S1. ^{1}H NMR assignment ($CDCl_3$, 600 MHz) of compound **3a**

H	δ_H	Int.	Mult.	*J* / Hz	COSY	NOESY
OH	11.95	s	1H	–	–	5.48
OH	11.57*	bs	0.3H	–	–	–
H15/H-19	6.95	d	2H	8.4	6.97	6.67, 5.48, 1.24, 1.10
H16/H-18	6.67	d	2H	8.4	6.95	2.91
H7	5.48	s	1H	–	–	11.94, 6.95
R group	2.91	s	6H	–	–	6.67
H4a/H12a	2.45	d	2H	17.4	2.32	1.24, 1.10
H6a/H10a	2.40	d	2H	13.8	2.38	1.24, 1.10
H6b/H10b	2.38	d	2H	13.8	2.40	1.24, 1.10
H4b/H12b	2.32	d	2H	17.4	2.45	1.24, 1.10
H21/H23	1.24	s	6H	–	–	6.95, 2.45, 2.40, 2.38, 2.32
H20/H22	1.10	s	6H	–	–	6.95, 2.45, 2.40, 2.38, 2.32

Table S2. ^{13}C NMR assignment ($CDCl_3$, 150 MHz) of compound **3a**

C	δ_C	APT	HSQC	HMBC
C1/C9	190.41	C	–	2.45, 2.38
C3/C13	189.46	C	–	5.48, 2.40, 2.32
C17	148.95	C	–	**6.95**, 5.48, **2.91**
C15/C19	127.68	CH	6.95	**6.95**, **5.48**
C14	125.79	C	–	**6.67**, **5.48**
C2/C8	116.15	C	–	5.48
C-16/C18	112.88	CH	6.67	**6.67**. 5.48, 2.91
C6/C10	47.29	CH_2	2.40, 2.32	11.95, 2.45
C4/C12	46.66	CH_2	2.45, 2.38	2.40, **1.24**, 1.10
R group	40.91	CH_3	2.91	–
C7	32.04	CH	5.48	**6.95**
C5/C11	31.57	C	–	2.45, 2.40. 2.38, 2.32, 1.24, 1.10
C20/C22	29.91	CH_3	1.24	2.40, 2.38, 2.32, **1.24**
C21/C23	27.54	CH_3	1.10	2.45, 2.40, 2.39, 2.32, **1.10**

Table S3.^{1}H NMR assignment ($CDCl_3$, 600 MHz) of compound **3b**

H	δ_H	Int.	Mult	*J* / Hz	COSY	NOESY
OH	11.93	1H	s	–	–	7.01, 5.48 e 2.46
OH	11.58	0.6H	bs	–	–	7.01, 5.48 e 2.46
H15/H-19	7.01	2H	d	8.4	6.82	11.93, 6.82, 5.48, 2.40, **1.23** e **1.11**
H16/H-18	6.82	2H	d	8.4	7.01	**7.01**, **3.78**
H7	5.48	1H	s	–	–	**11.93**, **11.58**, **7.01**, 2.38, 1.23 e 1.11
R group	3.78	3H	s	–	–	6.82, 2.41
H4a/H12a	2.46	2H	d	18.0	2.32	7.01, **1.23**, **1.11**
H6a/H10a	2.40	2H	d	16.2	2.38	7.01, 5.48, 3.78, **1.23**, **1.11**
H6b/H10b	2.38	2H	d	16.2	2.40	7.01, **1.23**, **1.11**
H4b/H12b	2.32	2H	d	18.0	2.46	7.01, **1.23**, **1.11**
H21/H-23	1.23	6H	s	–	–	7.01, **2.41**, **1.11**
H20/H-22	1.11	6H	s	–	–	7.01, **2.41**, **1.23**

Table S4. ^{13}C NMR assignment ($CDCl_3$, 150 MHz) of compound **3b**

C	δ_C	APT	HSQC	HMBC
C1/C9	190.61	C	**–**	**5.48**, 2.46, 2.38
C3/C13	189.56	C	–	11.93, **5.48**, 2.40, 2.32
C17	157.79	C	**–**	**7.01**, 6.82
C14	130.02	C	–	**6.82**, **5.48**
C15/C19	127.99	CH	7.01	7.01, 5.48
C2/C8	116.00	C	–	11.93, **5.48**
C16/C-18	113.85	CH	6.82	6.82, 5.48
R group	54.41	CH_3	3.78	–
C6/C10	47.27	CH_2	2.40, 2.38	**11.93**, 2.46
C4/C12	46.69	CH_2	2.46, 2.32	2.40, 2.32, **1.23**, **1.11**
C7	32.23	CH	5.48	7.01
C5/C11	31.59	C	–	2.46, 2.40, 2.38, 2.32, **1.23**, **1,11**
C20/C22	29.88	CH_3	1.11	2.32, **1.23**
C21/C23	27.57	CH_3	1.23	2.46, 2.40, 2.38, 2.32, **1.11**

Table S5. ^{1}H NMR assignment ($CDCl_3$, 600 MHz) of compound **3c**

H	δ_H	Int.	m	*J* / Hz	COSY	NOESY
OH	11.91	1H	s	–	–	5.55
OH	11.57	0.3H	bs	–	–	5.55
H16/H-18	7.28	2H	t	7.8	7.18, 7.11	7.18, 7.11
H17	7.18	1H	t	7.2	7.28	7.28
H15/H-19	7.11	2H	d	8.4	7.28	7.28, 5.55, 1.25
H7	5.55	1H	s	–	–	11.91, 11.57, 7.11
H4a/H12a	2.49	2H	d	18.0	2.34	2.34, 2.402.38, 1.25, 1.11
H6a/H10a	2.40	2H	d	15.6	2.38	2.49, 2.38, 1.25, 1.11
H6b/H10b	2.38	2H	d	15.6	2.40	2.49, 2.34, 1.25, 1.11
H4b/H12b	2.34	2H	d	18.0	2.49	2.49, 2.38, 1.25, 1.11
H21/H23	1.25	6H	s	–	–	7.11, 2.49, 2.34, 2.28, 1.11
H20/H22	1.11	6H	s	–	–	2.49, 2.40, 2.34, 2.28, 1.25

Table S6. ^{13}C NMR assignment ($CDCl_3$, 150 MHz) of compound **3c**

C	δ_C	APT	HMBC	HMBC
C1/C9	190.67	C	–	**5.55**, 2.49, 2.38
C3/C13	189.60	C	–	11.91, **5.55**, 2.40, 2.34
C14	138.28	C	–	**7.28**, **5.55**
C16 /C18	128.42	CH	7.28	**7.28**, 5.55
C15 /C19	126.99	CH	7.11	7.28, **7.18**, **7.11**, **5.55**
C17	126.05	CH	7.18	**7.11**
C2/C8	115.81	C	–	**5.55**
C6/C10	47.28	CH_2	2.40, 2.38	11.91, 2.49, **1.25**, **1.11**
C4/C12	46.67	CH_2	2.49, 2.34	2.40, **1.25**, **1.11**
C7	32.96	CH	5.55	7.11
C5/C11	31.63	C	–	2.49, 2.38, 2.34, **1.25, 1.11**
C20/C22	29.86	CH_3	1.11	2.38, **1.25**
C21/C23	27.62	CH_3	1.25	**2.38**, 2.34, **1.11**

Table S7. ^{1}H NMR assignment ($CDCl_3$, 600 MHz) of compound **3d**

H	δ_H	Int.	Mult.	*J* / Hz	COSY	ROESY
OH	11.87	1H	s	–	–	5.48
OH	11.57	0.3H	bs	–	–	5.48
H16/H18	7.24	2H	d	8.4	7.02	7.02
H15/H19	7.02	2H	d	8.4	7.24	7.24, 5.48, 1.22
H7	5.48	1H	s	–	–	11.87, 11.57, 7.02
H4a/H12a	2.46	2H	d	17.4	2.32	2.41, 2.38, 2.32, 1.22, 1.11
H6a/H10a	2.41	2H	d	10.2	2.38	2.46, 2.38, 2.32, 1.22, 1.11
H6b/H10b	2.38	2H	d	10.2	2.41	2.46, 2.41. 2.32, 1.22, 1.11
H4b/H12b	2.32	2H	d	17.4	2.46	2.46, 2.41, 2.38, 1.22, 1.11
H21/H23	1.22	6H	s	–	–	7.02, 2.46, 2.41, 2.38, 2.32, 1.11
H20/H22	1.11	6H	s	–	–	2.46, 2.41, 2.38, 2.32, 1.22

Table S8. ^{13}C NMR assignment ($CDCl_3$, 150 MHz) of compound **3d**

C	δ_C	APT	HSQC	HMBC
C1/C9	190.84	C	–	5.48, **2.46**, **2.38**
C3/C13	189.63	C	–	11.87, 5.48, **2.41**, **2.32**
C14	136.91	C	**–**	**7.24**, **5.48**
C17	131.80	C	–	7.24, **7.02**, 5.48
C15/C19	128.56	CH	7.24	**7.24**
C16/C18	128.41	CH	7.02	**7.02**, **5.48**
C2/C8	115.55	C	–	11.87, **5.48**, **2.46**, 2.41, **2.38**, 2.32
C6/C10	47.25	CH_2	2.41, 2.32	**11.87**, **2.46**, 2.38, **1.22**, **1.11**
C4/C12	46.64	CH_2	2.48, 2.36	**2.41**, 2.32, **1.22**, **1.11**
C7	32.62	CH	5.48	**7.02**
C5/C11	31.63	C	**–**	**2.46**, **2.41**, **2.32**, **1.22**, **1.11**
C20/C22	29.80	CH_3	1.11	2.46, 2.41, **2.38**, **2.32**, **1.22**
C21/C23	27.63	CH_3	1.22	**2.46**, **2.41**, **2.38**, **2.32**, **1.11**

Table S9. ^{1}H NMR assignment ($CDCl_3$, 600 MHz) of compound **3e**

H	δ_H	Int.	Mult.	*J* / Hz	COSY	ROESY
OH	11.80	1H	s	–	–	–
OH	11.55	0.2H	bs	–	–	–
H16/H18	8.14	2H	d	8.4	7.25	7.25
H15/H19	7.25	2H	d	8.4	8.14	8.14, 5.55, 1.24
H7	5.55	1H	s	–	–	7.25
H4a/H12a	2.50	2H	d	17.4	2.41	1.24, 1.12
H6a/H10a	2.43	2H	d	16.2	2.34	**1.24, 1.12**
H6b/H10b	2.41	2H	d	17.4	2.50	**1.24, 1.12**
H4b/H12b	2.34	2H	d	16.2	2.43	1.24, 1.12
H21/H23	1.24	6H	s	–	–	7.25, 2.50, **2.43**, **2.41**, 2.34
H20/H22	1.12	6H	s	–	–	2.50, **2.43**, **2.41**, 2.34

Table S10. ^{13}C NMR assignment ($CDCl_3$, 150 MHz) of compound **3e**

C	δ_C	APT	HSQC	HMBC
C1/C9	191.14	C	–	**5.55**, **2.50**, **2.41**
C3/C13	189.78	C	–	11.80, **5.55**, **2.43**, **2.34**
C14	146.73	C	–	**8.14**, **5.55**
C17	146.34	C	–	**7.25**
C15/C19	127.85	CH	7.25	**7.25**, **5.55**
C16/C18	123.72	CH	8.14	8.14, **5.55**
C2/C8	115.12	C	–	11.80, **5.55**, **2.50**, **2.43**, **2.42**, **2.34**
C6/C10	47.20	CH_2	2.43. 2.34	11.80, 2.50, **1.24**, **1.12**
C4/C12	46.61	CH_2	2.50, 2.41	2.43, 2.41, 2.34, **1.24**, **1.12**
C7	33.47	CH	5.55	7.25
C5/C11	31.68	C	–	2.50, 2.43, 2.41, 2.34, **1.24**, **1.12**
C20/C22	29.50	CH_3	1.12	2.50, 2.43, **1.41**, **2.34**, **1.24**
C21/C23	27.68	CH_3	1.24	2.50, 2.43, 1.41, **2.34**, **1.12**

Table S11. ^{1}H NMR assignment ($CDCl_3$, 600 MHz) of compound **3f**

H	δ_H	Int.	Mult.	*J* / Hz
OH	11.58	2H	s	–
H7	3.16	2H	s	–
H4 e H12	2.30	4H	d	16.2
H6 e H10	2.28	4H	d	16.2
H20/H21 H22/H23	1.05	12H	s	–

Table S12: ^{13}C NMR assignment ($CDCl_3$, 150 MHz) of compound **3f**

C	δ_C	APT	HSQC	HMBC
C1/C3/C9/C13	189.76	C	–	**3.16**, **2.30**, **2.28**
C2/C8	113.67	C	–	**3.16**, 2.30, 2.28
C4/C6/C10/C12	46.18	CH_2	2.30, 2.28	**1.05**
C5/C11	31.98	C	–	2.30, 2.28, **1.05**
C20/C22	29.73	CH_2	1.05	2.30, 2.28, **1.05**
C21/C23	27.27	CH_2	1.05	2.30, 2.28, **1.05**
C7	16.14	CH_3	3.16	–

Table S13. ^{1}H NMR ($CDCl_3$, 600 MHz) and ^{13}C NMR spectra ($CDCl_3$, 150 MHz) of 2,2'-[(2,4-dinitrophenyl)methylene] bis(3-hydroxy-5,5-dimethylcyclohex-2-enone) (**3g**)

Atom	NMR spectra at 20 °C		NMR spectra at 50 °C	
	δ_H	δ_C	δ_H	δ_C
OH	11.49*	–	11.44*	–
1/9	–	191.54*	–	190.76
2/8	–	114.20	–	114.30
3/13	–	189.95*	–	190.76
4/12	2.20*	46.52	2.39*	46.88
5/11	–	32.24*	–	32.24
6/10	2.60*	46.96*	2.39*	46.88
7	6.06	30.94	6.07	31.06
14	–	140.15	–	140.22
15	–	149.56	–	149.74
16	8.40	119.94	8.40	119.91
17	–	146.37	–	146.55
18	8.34	125.81	8.32	125.73
19	7.46	131.13	7.48	131.17
20/22	1.20*	28.21*	1.10	28.49
21/23	0.80*	28.78*	1.10	28.49

*Broad signal

Table S14. ^{1}H NMR Chemical Assignment ($CDCl_3$, 600 MHz) of compounds **3a**-**g**

Hydrogen	**3a**	**3b**	**3c**	**3d**	**3e**	**3f**	**3g**
OH Side A	11.95	11.93	11.91	11.87	11.80	11.56	11.49*
OH Side B	11.57*	11.58*	11.57*	11.57*	11.55*	11.56	11.49*
R group	2.91	3.78	–	–	–	–	–
H15	6.95	7.01	7.11	7.02	7.25	–	
H16	6.67	6.82	7.28	7.24	8.14	–	8.40
H17	–	–	7.18	–		–	–
H18	6.67	6.82	7.28	7.24	8.14	–	8.34
H19	6.95	7.01	7.11	7.02	7.25	–	7.46
H20/H22	1.10	1.11	1.11	1.11	1.12	1.02	1.20*
H21/H23	1.24	1.23	1.25	1.22	1.24	1.04	0.80*
H6a/H10a	2.40	2.40	2.40	2.41	2.43	2.28	2.60*
H6b/H10b	2.38	2.38	2.38	2.38	2.41	2.26	2.60*
H4a/H12a	2.45	2.46	2.49	2.46	2.50	2.28	2.20*
H4b/H12b	2.32	2.32	2.34	2.32	2.34	2.26	2.20*
H7	5.48	5.48	5.55	5.48	5.55	3.14	6.06

*Broad signals

Table S15. ^{13}C NMR Chemical Shift Assignment ($CDCl_3$, 150 MHz) of compounds **3a**-**g**

Carbon	**3a**	**3b**	**3c**	**3d**	**3e**	**3f**	**3g**
R group	40.91	54.41	–	–	–	–	–
C14	125.79	130.02	138.28	136.91	146.73	–	140.15
C15	127.68	127.99	126.99	128.56	127.85	–	149.56
C16	112.88	113.85	128.42	128.41	123.72	–	119.94
C17	148.95	157.79	126.05	131.80	146.34	–	146.36
C18	112.88	113.85	128.42	128.41	123.72	–	125.81
C19	127.68	127.99	126.99	128.56	127.85	–	131.13
C20/C22	29.91	29.88	29.86	29.80	29.50	29.73	28.21*
C21/C23	27.54	27.57	27.62	27.63	27.68	27.27	28.78*
C3/C13	189.46	189.56	189.60	189.63	189.78	189.76	189.95*
C6/C10	47.29	47.27	47.28	47.25	47.20	46.18	46.96*
C5/C11	31.57	31.59	31.63	31.63	31.68	31.98	32.24*
C4/C12	46.66	46.69	46.67	46.64	46.61	46.18	46.52
C1/C9	190.41	190.61	190.67	190.84	191.14	189.76	191.54*
C2/C8	116.15	116.00	115.81	115.55	115.12	113.67	114.20
C7	32.04	32.23	32.96	32.62	33.47	16.14	30.94

*Broad signals

Table S16. Molecular modeling data (B3LYP/6-311+G(d,p)) of 2,2'-arylmethylene bis(3-hydroxy-5,5-dimethyl-2-cyclohexene-1-ones)

Angle	**3a**	**3b**	**3c**	**3d**	**3e**	**3f**	**3g**
C2C7C8	116.15	113.52	113.54	113.57	113.89	116.94	113.13
H7C7C14	103.01	102.72	102.38	102.47	101.91	–	102.58
H7C7C2	104.83	104.82	104.97	105.18	105.06	107.57	105.15
H7C7C8	103.41	103.32	103.38	103.25	103.36	109.06	103.73
C2C7C14	114.74	114.96	114.93	114.68	115.11	–	114.73
C8C7C14	115.27	115.43	115.54	115.64	115.31	–	115.60
C1C2C7	120.77	120.59	120.46	120.16	120.21	122.91	120.22
C7C8C13	125.29	125.53	125.58	125.61	125.48	117.75	126.56
C3C2C7	121.00	121.04	121.12	121.51	121.17	117.52	120.92
C7C8C9	116.15	115.99	115.90	115.79	115.84	122.82	114.96
C1C2C7C8	83.16	84.53	84.07	83.57	84.24	89.90	87.84
C2C7C8C13	84.17	82.23	82.71	83.32	82.57	88.86	73.66
C3C2C7C8	91.85	90.98	91.20	92.06	90.79	89.83	85.79
C2C7C8C9	94.22	94.85	94.39	94.00	94.45	90.56	99.66
C1C2C7C14	51.42	51.46	52.07	52.49	52.14	–	47.73
C13C8C7C14	52.18	53.55	53.15	52.30	53.71	–	61.50
C3C2C7H7	20.32	21.05	21.00	20.12	21.60	33.20	26.74
C9C8C7H7	18.81	18.09	18.77	19.34	18.95	31.71	13.72

Table S17. Natural atomic bound charges (Q_{NPA}) (B3LYP/6-311+G(d,p)) of the carbon atoms connecting the phenyl ring with the 1,3-dicarbonyl groups

	3a	**3b**	**3c**	**3d**	**3e**	**R^2 Q_{NPA} vs δ_C**	**R^2 Q_{NPA} vs σ_p**
C1	0.564	0.565	0.565	0.565	0.566	0.8860	0.9131
C2	–0.243	–0.244	–0.245	–0.247	–0.252	0.9743	0.8765
C3	0.476	0.476	0.476	0.478	0.483	0.6957	0.7066
C7	–0.267	–0.270	–0.274	–0.273	–0.279	0.9687	0.9435
C8	–0.253	–0.254	–0.254	–0.256	–0.255	0.5564	0.5985
C9	0.562	0.563	0.564	0.565	0.566	0.9504	0.9727
C13	0.480	0.479	0.480	0.479	0.483	0.3333	0.3747

Table S18. Calculated percentage of molecules (6-311+G(d,p)) for each conformation

Benzene Ring Rotation		Dimedone Rings Rotation		Side A OH---O oscillation		Side B OH---O oscillation	
Rel. E. (kJ/mol)	Molecules %	Rel. E. (kJ/mol)	Molecules %	Rel. E. (kJ/mol)	Molecules %	Rel. E. (kJ/mol)	Molecules %
16.23	2.0	55.80	0.9	2.04	8.8	3.91	4.7
12.50	2.6	19.74	2.6	0.89	13.8	1.81	9.2
6.53	5.0	0.79	42.3	0.04	15.0	0.49	12.3
1.92	16.9	0.00	50.7	0.01	18.0	0.03	16.7
0.00	32.5	96.73	0.5	0.40	17.8	0.00	18.4
1.40	23.2	94.94	0.5	1.47	12.2	0.42	18.2
3.93	8.3	95.56	0.5	2.94	6.1	1.67	8.0
7.06	4.6	93.55	0.5	4.90	3.7	3.07	6.0
10.53	3.1	78.52	0.6	7.06	2.5	4.74	3.9
15.72	2.1	65.32	0.8	9.40	1.9	6.70	2.7