## Supplementary Data for

# Synthesis, Characterization and Applications of (*E*)-3-((5-bromo-2-hydroxy-3-methoxycyclohexa-1,3-dienyl)methyleneamino)-6-(hydroxymethyl)-tetrahydro-2*H*-pyran-2,4,5-triol

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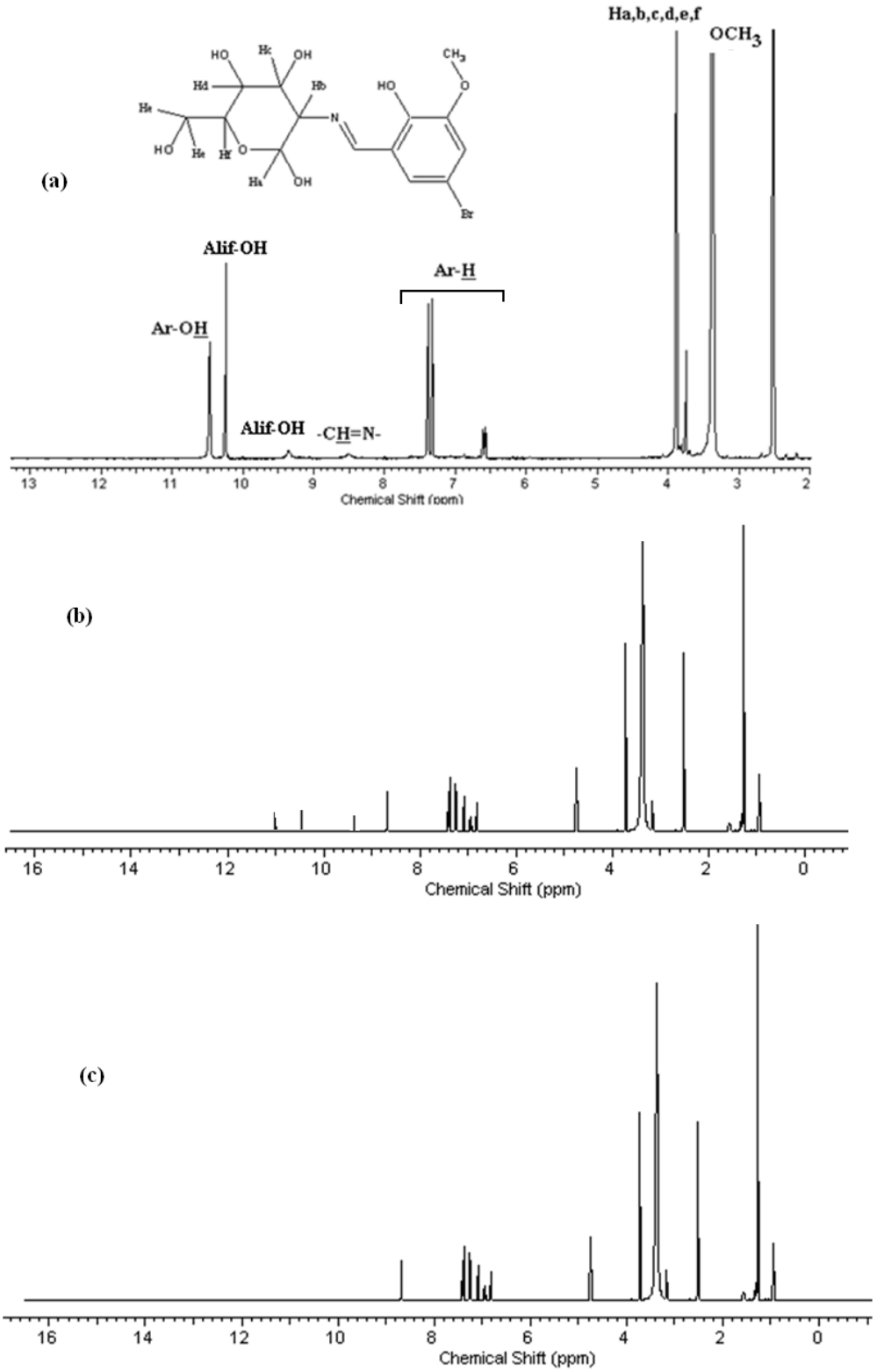


**Fig. S1** $^{1}$H-NMR Titration spectrum of the compound. **(a)** 0.0 eq $F^-$, **(b)** 0,5 eq $F^-$, **(c)** 3.0 eq $F^-$.

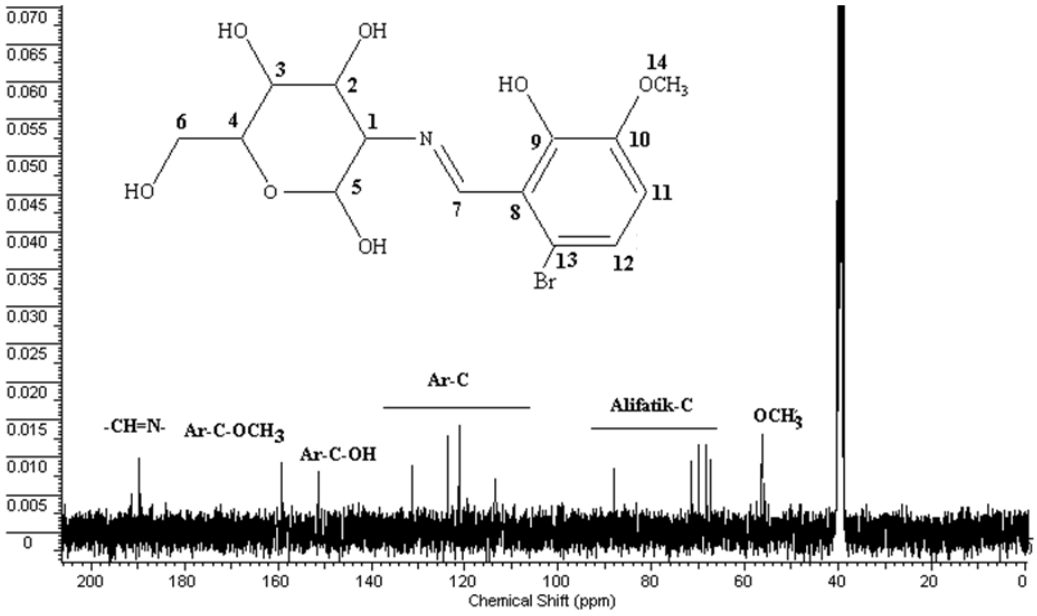


**Fig. S2** $^{13}$C- NMR spectrum of the compound.

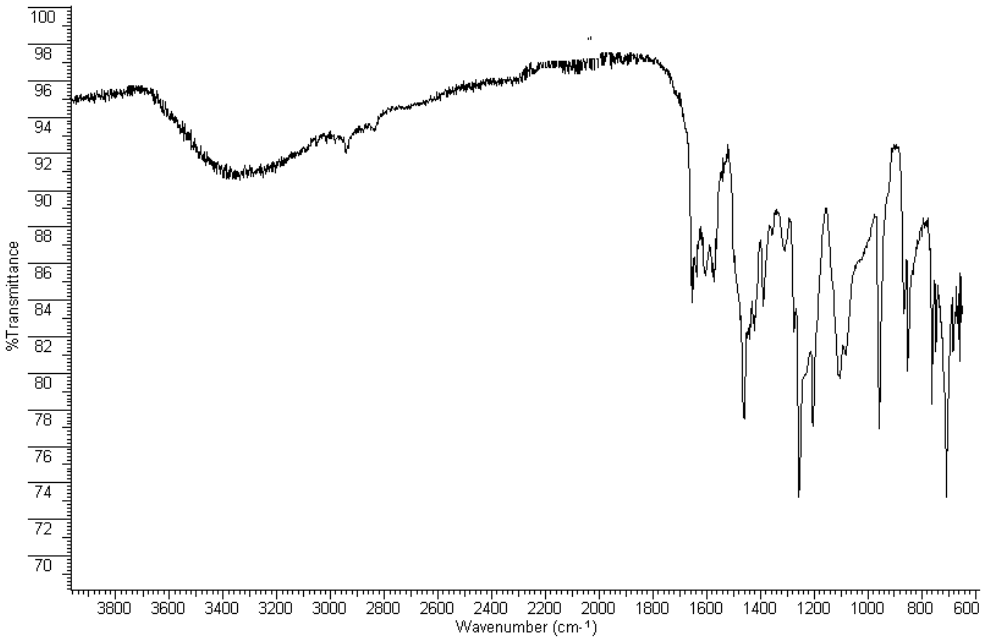


**Fig. S3** FT-IR spectrum of the title compound.

**Table S1** Comparison of the experimental and calculated vibrational frequencies ($cm^{-1}$).

| Vibrational assignments (PED %) | Exp. IR | Unscaled freq. | Scaled freq. | $I_{IR}$ |
|---|---|---|---|---|
| $\upsilon O_{30}H_{31}$ (100) | - | 3850.44 | 3088.72 | 55.112 |
| $\upsilon O_{30}H_{31}$ (89) | - | 3848.95 | 3687.29 | 48.768 |
| $\upsilon O_{30}H_{31}$ (99) | - | 3800.46 | 3640.84 | 60.302 |
| $\upsilon O_{30}H_{31}$ (100) | - | 3784.99 | 3626.02 | 67.800 |
| $\upsilon C_3H_8$ (98) | - | 3223.04 | 3087.67 | 2.387 |
| $\upsilon O_{11}H_{12}$ (12) + $\upsilon C_1H_7$ (86) | - | 3192.78 | 3058.68 | 71.129 |
| $\upsilon O_{11}H_{12}$ (87) | - | 3189.07 | 3055.13 | 550.857 |
| $\upsilon C_{14}H_{15}$ (100) | 2941 | 3064.26 | 2935.56 | 33.668 |
| υCH (97) | 2836 | 3000.97 | 2874.93 | 37.934 |
| υNC (69) | 1655 | 1683.80 | 1655.18 | 324.103 |
| βCCC(26)+ υCC (25)+ βHOC(18) | 1605 | 1651.27 | 1623.20 | 24.311 |
| υCC (42)+ βHCC(14) | 1573 | 1602.96 | 1575.71 | 52.262 |
| βHOC(18)+ βHCH(44)+ τHCOC(13) | - | 1505.46 | 1479.86 | 31.775 |
| υCC (13)+ βHOC(33)+ βHCH(22) | - | 1499.30 | 1473.81 | 73.021 |
| υCC (12)+ $\upsilon O_{11}C_5$(19)+ βHCH(23) | - | 1495.27 | 1469.86 | 169.440 |
| βHCH(75)+ τ HCOC(20) | 1460 | 1493.01 | 1467.63 | 18.957 |
| βHCC(15)+ βHCH(57) | - | 1474.75 | 1449.68 | 90.017 |
| βHOC(11)+ τ HCNC(18)+ τHCCC(10) | 1441 | 1460.03 | 1435.21 | 6.772 |
| τHCNC(14)+ τHCCC(10) | 1423 | 1455.61 | 1430.86 | 11.179 |
| βHCO(18)+ γCCCH(16) | 1391 | 1412.98 | 1388.96 | 13.567 |
| $\upsilon O_{11}C_5$ (42)+ βCCC(11) | 1259 | 1306.76 | 1284.55 | 140.904 |
| ρHCH(10)+ τHCOC(56) | - | 1206.98 | 1186.46 | 2.508 |
| ρHCN(25)+ τHCOC(74) | - | 1167.64 | 1147.79 | 0.749 |
| $\upsilon O_{30}C_{21}$ (16) | 1082 | 1111.18 | 1092.29 | 63.390 |
| $\upsilon O_{30}C_{21}$ (33) | - | 1083.06 | 1064.64 | 99.785 |
| $\upsilon O_{30}C_{21}$ (40) | - | 1077.14 | 1058.83 | 7.009 |
| υNC (33)+ $\upsilon O_{30}C_{21}$ (10) | - | 1065.85 | 1047.73 | 271.115 |
| $\upsilon O_{30}C_{21}$ (18)+ $\upsilon O_{36}C_{24}$ (40) | - | 1054.44 | 1036.52 | 89.557 |
| $\upsilon O_{30}C_{21}$ (20)+ $\upsilon O_{36}C_{24}$ (16) | 1023 | 1047.22 | 1029.42 | 62.326 |
| υCC (12)+ $\upsilon O_{30}C_{21}$ (10)+ $\upsilon O_{13}C_{14}$ (26) | 959 | 988.47 | 971.66 | 13.144 |
| υOC (12)+ βCCC(43) | 855 | 873.69 | 858.84 | 26.559 |
| υCC (18)+ υOC (16) | 764 | 783.37 | 770.05 | 29.615 |

Vibrational modes:υ, stretching; β, in-plane bending; δ, scissoring; γ, out of plane bending; τ, torsion; ρ, rocking. [a]Potential energy distribution (PED), less than 10% are not shown.

**Table S2** The calculated quantum molecular descriptors of the compound.

| **Parameter** | **B3LYP-6-311++G(d,p)** |
|---|---|
| $E_{HOMO}$(eV) | -6.03 |
| $E_{LUMO}$(eV) | -1.94 |
| $E_{HOMO}$–$E_{LUMO}$ | 4.09 |
| Ionization potential [$I$=–$E_{HOMO}$] (eV) | 6.03 |
| Electron affinity [$A$=–$E_{LUMO}$] (eV) | 1.94 |
| Chemical hardness [$\eta$=($I$–$A$)/2] (eV) | 2.04 |
| Electronegativity [$\mu$=–($I$+$A$)/2] (eV) | 3.99 |
| Softness [$\zeta$=1/2$\eta$] (eV) | 0.24 |
| Electrophilicity index [$\omega$=$\mu^2$/2$\eta$] (eV) | 3.88 |

**Table S3** The calculated results with second order perturbation theory of Fock matrix in NBO of the compound.

| ED(i)(e) | Donor (i) | ED(j)(e) | Acceptor (j) | E(2)[a] kcal/mol | E(j)-E(i)[b] a.u. | F(i,j)[c] a.u. |
|---|---|---|---|---|---|---|
| 1.75115 | π(C1-C2) | 0.36526 | π*(C3-C4) | 17.36 | 0.29 | 0.066 |
| 1.75115 | π(C1-C2) | 0.42805 | π*(C5-C6) | 14.53 | 0.29 | 0.061 |
| 1.96117 | σ(C1-C6) | 0.03421 | σ*(C2-Br18) | 5.93 | 0.78 | 0.061 |
| 1.97706 | σ(C1-H7) | 0.02577 | σ*(C2-C3) | 4.40 | 1.06 | 0.061 |
| 1.97014 | σ(C3-C4) | 0.02577 | σ*(C2-C3) | 4.13 | 1.26 | 0.064 |
| 1.97014 | σ(C3-C4) | 0.03421 | σ*(C2-Br18) | 4.79 | 0.81 | 0.056 |
| 1.70073 | π(C3-C4) | 0.37007 | π*(C1-C2) | 18.13 | 0.29 | 0.066 |
| 1.70073 | π(C3-C4) | 0.42805 | π*(C5-C6) | 17.94 | 0.29 | 0.067 |
| 1.97437 | σ(C3-H8) | 0.02335 | σ*(C1-C2) | 4.23 | 1.13 | 0.062 |
| 1.62387 | π(C5-C6) | 0.37007 | π*(C1-C2) | 21.98 | 0.28 | 0.070 |
| 1.62387 | π(C5-C6) | 0.36526 | π*(C3-C4) | 16.94 | 0.28 | 0.062 |
| 1.62387 | π(C5-C6) | 0.16023 | π*(C9-N10) | 20.05 | 0.27 | 0.069 |
| 1.97184 | σ(C6-C9) | 0.02248 | σ*(N10-C20) | 4.48 | 1.04 | 0.061 |
| 1.94658 | π(C9-N10) | 0.42805 | π*(C5-C6) | 6.54 | 0.36 | 0.048 |
| 1.98368 | σ(O11-H12) | 0.03449 | σ*(C4-C5) | 4.97 | 1.25 | 0.071 |
| 1.97809 | σ(C22-H29) | 0.03780 | σ*(C24-O36) | 4.27 | 0.80 | 0.052 |
| 1.97361 | σ(C23-H27) | 0.02267 | σ*(C21-O30) | 4.51 | 0.80 | 0.054 |
| 1.97961 | σ(C37-H38) | 0.03780 | σ*(C24-O36) | 5.27 | 0.79 | 0.058 |
| 1.99426 | σ(C37-O4) | 0.00462 | σ*(O40-H41) | 10.74 | 2.91 | 0.158 |
| 1.86700 | n(N10) | 0.03920 | σ*(C9-H19) | 11.01 | 0.76 | 0.084 |
| 1.86700 | n(N10) | 0.06477 | σ*(O11-H12) | 23.82 | 0.79 | 0.125 |
| 1.86700 | n(N10) | 0.02863 | σ*(C20-H25) | 5.65 | 0.77 | 0.060 |
| 1.97329 | n(O11) | 0.03169 | σ*(C5-C6) | 6.69 | 1.11 | 0.077 |
| 1.80757 | n(O11) | 0.42805 | π*(C5-C6) | 37.06 | 0.33 | 0.104 |
| 1.96068 | n(O13) | 0.02716 | σ*(C3-C4) | 6.89 | 1.10 | 0.078 |
| 1.83468 | n(O13) | 0.36526 | π*(C3-C4) | 30.98 | 0.33 | 0.096 |
| 1.83468 | n(O13) | 0.01863 | σ*(C14-H15) | 5.54 | 0.69 | 0.057 |
| 1.83468 | n(O13) | 0.01855 | σ*(C14-H17) | 5.50 | 0.69 | 0.057 |
| 1.97664 | n(Br18) | 0.02577 | σ*(C2-C3) | 3.25 | 0.83 | 0.046 |
| 1.94694 | n(Br18) | 0.37007 | π*(C1-C2) | 9.29 | 0.31 | 0.052 |
| 1.94990 | n(O30) | 0.04153 | σ*(C21-C23) | 5.45 | 0.67 | 0.054 |
| 1.94990 | n(O30) | 0.03343 | σ*(C21-H26) | 7.19 | 0.69 | 0.063 |
| 1.95907 | n(O32) | 0.04141 | σ*(C23-C24) | 7.36 | 0.69 | 0.064 |
| 1.93594 | n(O34) | 0.03896 | σ*(C22-H29) | 7.27 | 0.70 | 0.064 |
| 1.93594 | n(O34) | 0.05460 | σ*(C22-O36) | 8.57 | 0.62 | 0.065 |
| 1.90014 | n(O36) | 0.04581 | σ*(C20-C22) | 4.06 | 0.65 | 0.046 |
| 1.90014 | n(O36) | 0.05205 | σ*(C22-O34) | 13.58 | 0.60 | 0.081 |
| 1.90014 | n(O36) | 0.04141 | σ*(C23-C24) | 4.09 | 0.67 | 0.047 |
| 1.90014 | n(O36) | 0.03564 | σ*(C24-C37) | 6.73 | 0.68 | 0.061 |
| 1.96307 | n(O40) | 0.02492 | σ*(C37-H38) | 5.96 | 0.69 | 0.057 |
| 1.96307 | n(O40) | 0.02617 | σ*(C37-H39) | 6.12 | 0.72 | 0.060 |

ED is the electron density.
[a] E(2) is the energy of hyperconjugative interactions.
[b] Energy difference between donor (i) and acceptor (j) NBO.
[c] F(i,j) is the Fock matrix element between i and j NBO.

**Non-linear optical effects**

Non-linear optical materials continue to attract the attention of researchers due to their future potential applications in the optical technology and industrial applications. It is well known that the higher values of molecular polarizability and hyperpolarizability are important for more active NLO properties. To understand the NLO properties of the title compound, the linear polarizability ($\alpha$) and the first hyperpolarizability ($\beta$) were calculated at the B3LYP/6-311++G(d,p) level using Gaussian 09W program package. The polarizabilities and hyperpolarizability are reported in terms of atomic units (a.u.) and the calculated values have been converted by using 1 a.u$^3$ = (0.529)$^3$ Å$^3$ for α and 1 a.u = 8.641x10$^{-33}$ cm$^5$/esu for β.[30] The calculated polarizability ($\alpha$) and first hyperpolarizability ($\beta$) for the compound were found as 35.080 Å$^3$ and 4.920 x 10$^{-30}$ cm$^5$/esu, respectively (Table S4). Urea is one of the essential molecules used for determination of the NLO properties of molecular systems. Therefore, it is usually used as reference molecule in NLO studies. The calculated values of urea at the B3LYP/6-311++G(d,p) level were found as 4.90 Å$^3$ for $\alpha$ and 0.781x10$^{-30}$ cm$^5$/esu for $\beta$. The polarizability and first hyperpolarizability for title molecule is approximately 8.5 and 8-fold larger than those of urea, which implies that the compound is a good candidate material for NLO applications.

**Table S4** The electric dipole moment, polarizability and first order hyperpolarizability values of the compound.

| Parameters | Value (a.u.) | Parameters | Value (a.u.) |
|---|---|---|---|
| $\alpha_{xx}$ | 326.9116171 | $\beta_{xxx}$ | 38.7367578 |
| $\alpha_{xy}$ | -0.9075499 | $\beta_{xxy}$ | -143.5708925 |
| $\alpha_{xz}$ | 0.5716699 | $\beta_{xyy}$ | -65.0675367 |
| $\alpha_{yy}$ | 226.3044961 | $\beta_{yyy}$ | -377.2992885 |
| $\alpha_{yz}$ | -0.0598852 | $\beta_{xxz}$ | -36.6627469 |
| $\alpha_{zz}$ | 157.8739912 | $\beta_{yyz}$ | -15.3591404 |
| $\alpha_{total}$ | 711.0901044 | $\beta_{xzz}$ | 110.2477135 |
| $\Delta\alpha$ | 237.0300348 | $\beta_{yzz}$ | -32.0047425 |
| $\mu_x$ | -0.4707 | $\beta_{zzz}$ | -55.3257251 |
| $\mu_y$ | 1.8490 | $\beta_0$ | 569.417458 |
| $\mu_z$ | 0.0637 | | |
| $\mu_{total}$ | 1.9090 | | |

**Table S5** MIC (μg/mL) of the compound.

| **Microorganisms** | **Compound** | **Gentamicin** | **Ampicillin** | **Fluconasol** |
|---|---|---|---|---|
| ***S. aureus ATCC 25923*** | 128 | 1.25 | 0.50 | - |
| ***E. faecalis ATCC 29212*** | 32 | 20 | 8 | - |
| ***B. subtilis ATCC 6633*** | 64 | - | 2 | - |
| ***E. coli ATCC 25922*** | 256 | 2.50 | 4 | - |
| ***E. coli NRRL B-3704*** | 128 | 0.67 | 4 | - |
| ***P. aeruginosa ATCC 254992*** | - | - | 0.5 | - |
| ***P. vulgaris ATCC 13315*** | 128 | 2.50 | 8 | - |
| ***C. albicans ATCC 60193*** | 2 | - | - | 64 |
| ***C. tropicalis ATCC 13803*** | 64 | - | - | 128 |