

## Supporting information

### Design, Synthesis, and Evaluation of Benzofuran-based Chromenochalcones for Antihyperglycemic and Antidyslipidemic Activities

*Venkateswarlu Korthikunta<sup>a</sup>, Rohit Singh<sup>a,c,d</sup>, Rohit Srivastava<sup>b</sup>, Jyotsana Pandey<sup>b,c</sup>, Atul shrivastava<sup>b</sup>, Upma Chaturvedi<sup>b</sup>, Akansha Mishra<sup>b</sup>, Arvind K. Srivastava<sup>b</sup>, Akhilesh K. Tamrakar<sup>b,c</sup>, Narender Tadigoppula<sup>a,c\*</sup>*

<sup>a</sup>Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow (U.P.) - 226 031, India

<sup>b</sup>Division of Biochemistry, CSIR-Central Drug Research Institute, Lucknow (U.P.) - 226 031, India

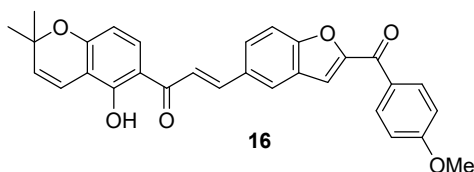
<sup>c</sup>Academy of Scientific and Innovative Research (AcSIR), Sector 19, Kamla Nehru Nagar Ghaziabad-201002, India

<sup>d</sup>Department of Pharmaceutical Chemistry, College of Pharmacy, JSS Academy of Technical Education, C-1/A, Sector-62, Noida, Uttar Pradesh-201309, India

\*Corresponding author Mailing address: Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow-226 031, U.P, India, Tel.: +91 522 2771940 (TN); fax: +91 522 2771941; E-mail addresses: [t\\_narendra@cdri.res.in](mailto:t_narendra@cdri.res.in), [tnarender@rediffmail.com](mailto:tnarender@rediffmail.com) (TN)

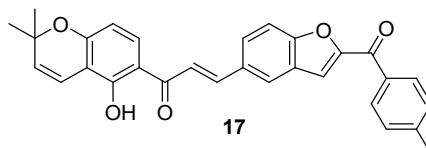
**Compounds characterization data**

**(E)-1-(5-hydroxy-2,2-dimethyl-2H-chromen-6-yl)-3-(2-(4-methoxybenzoyl) benzofuran-5-yl)prop-2-en-1-one (16).**



Yield 82%; MP: 180-182 °C; FT-IR (KBr,  $\text{cm}^{-1}$ ) 3395, 3023, 1641, 1367, 1217, 1114, 927, 763, 671;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 13.62 (s, 1H), 8.14 (d,  $J = 8.7\text{Hz}$ , 2H), 8.00 (d,  $J = 15.4\text{ Hz}$ , 1H), 7.99 (s, 1H), 7.82 (d,  $J = 8.6\text{ Hz}$ , 1H), 7.76 (d,  $J = 8.8\text{ Hz}$ , 1H), 7.68 (d,  $J = 8.6\text{Hz}$ , 1H), 7.60 (d,  $J = 15.4\text{ Hz}$ , 1H), 7.56 (s, 1H), 7.05 (d,  $J = 8.7\text{Hz}$ , 2H), 6.77 (d,  $J = 10.1\text{ Hz}$ , 1H), 6.42 (d,  $J = 8.8\text{Hz}$ , 1H), 5.62(d,  $J = 10.1\text{ Hz}$ , 1H), 3.95 (s, 3H), 1.49 (s, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 50 MHz)  $\delta$ : 191.66, 182.39, 163.82, 160.99, 159.95, 156.81, 153.76, 143.81, 132.03, 131.10, 130.66, 129.50, 128.16, 127.80, 124.07, 120.10, 115.82, 115.15, 113.94, 113.12, 109.43, 108.39, 77.91, 55.56, 28.39; HRESIMS:  $m/z$ calcd for  $[\text{M}+\text{H}]^+ \text{C}_{30}\text{H}_{25}\text{O}_6$  481.1646 found 481.1644.

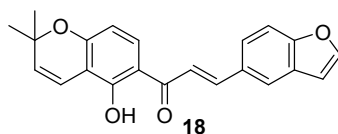
**(E)-1-(5-hydroxy-2,2-dimethyl-2H-chromen-6-yl)-3-(2-(4methylbenzoyl)benzofuran-5-yl)prop-2-en-1-one (17)**



Yield 90%; MP: 188-190°C; FT-IR (KBr,  $\text{cm}^{-1}$ ) : 3440, 1639, 1582, 1550, 1480, 1365, 1247, 1113, 1049, 977, 819, 770;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 13.66 (s, 1H), 8.02 (d,  $J = 15.4\text{Hz}$ , 1H), 8.02-7.89 (brd, 3H), 7.83 (d,  $J = 8.4\text{ Hz}$ , 1H), 7.75 (d,  $J = 8.4\text{ Hz}$ , 1H), 7.69 (d,  $J = 8.5\text{ Hz}$ , 1H), 7.66 (d,  $J = 15.4\text{Hz}$ , 1H), 7.56 (s, 1H), 7.37 (d,  $J = 15.4\text{Hz}$ , 2H), 6.78 (d,  $J = 10.1\text{Hz}$ , 1H),

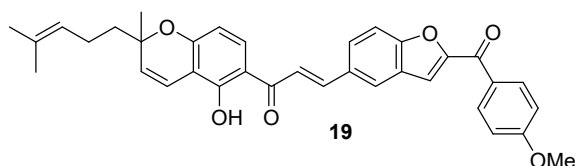
6.41 (d,  $J = 8.5\text{Hz}$ , 1H), 5.82 (d,  $J = 10.1\text{Hz}$ , 1H), 2.50 (s, 3H), 1.49 (s, 6H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.68, 183.69, 161.02, 159.98, 156.93, 153.52, 144.17, 143.78, 134.29, 131.19, 130.66, 129.69, 129.35, 128.19, 127.96, 127.77, 124.19, 120.20, 115.84, 115.69, 114.03, 113.21, 109.47, 108.41, 77.93, 28.40, 21.76. HRESIMS:  $m/z$ calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{30}\text{H}_{25}\text{O}_5$  465.1702 found 465.1697.

**(E)-3-(benzofuran-5-yl)-1-(5-hydroxy-2,2-dimethyl-2H-chromen-6-yl)prop-2-en-1-one (18).**



Yield 62%; MP: 116-118 °C; FT-IR (KBr,  $\text{cm}^{-1}$ ): 3446, 2926, 2807, 1633, 1470, 1360, 1109, 854, 773;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 13.77 (s, 1H), 8.01 (d,  $J = 15.4\text{Hz}$ , 1H), 7.89 (d,  $J = 1.1\text{ Hz}$ , 1H), 7.76 (d,  $J = 8.8\text{ Hz}$ , 1H), 7.68 (d,  $J = 7.1\text{ Hz}$ , 1H), 7.63 (s, 1H), 7.58 (d,  $J = 15.4\text{Hz}$ , 1H), 7.55 (d,  $J = 8.5\text{Hz}$ , 1H), 6.83 (d,  $J = 2.2\text{ Hz}$ , 1H), 6.78 (d,  $J = 10.1\text{Hz}$ , 1H), 6.42 (d,  $J = 8.8\text{ Hz}$ , 1H), 5.61 (d,  $J = 10.1\text{ Hz}$ , 1H), 1.49 (s, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 50 MHz)  $\delta$ : 191.95, 161.00, 159.82, 156.31, 146.18, 144.84, 130.68, 129.99, 128.13, 124.72, 122.32, 119.17, 115.94, 114.12, 112.06, 109.47, 108.31, 106.86, 77.85, 28.41; HRESIMS:  $m/z$ calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{22}\text{H}_{19}\text{O}_4$  347.1278 found 347.1284.

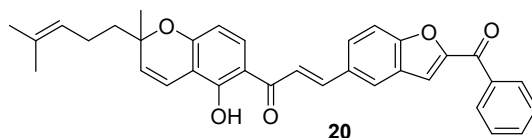
**(E)-1-(5-hydroxy-2-methyl-2-(4-methylpent-3-enyl)-2H-chromen-6-yl)-3-(2-(4-methoxybenzoyl)benzofuran-5-yl)prop-2-en-1-one (19)**



Yield 82%; MP: 130-132 °C; FT-IR (KBr,  $\text{cm}^{-1}$ ): 3456, 3067, 2922, 2854, 1635, 1579, 1480, 1362, 1110, 840, 764;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 13.65 (s, 1H), 8.14 (d,  $J = 9.0\text{Hz}$ , 2H), 8.01 (d,  $J = 15.4\text{ Hz}$ , 1H), 7.99 (s, 1H), 7.82 (dd,  $J = 8.7$  &  $1.3\text{ Hz}$ , 1H), 7.76 (d,  $J = 8.8\text{ Hz}$ , 1H), 7.68 (d,  $J = 8.7\text{Hz}$ , 1H), 7.60 (d,  $J = 15.4\text{ Hz}$ , 1H), 7.56 (s, 1H), 7.04 (d,  $J = 9.0\text{Hz}$ , 2H), 6.82 (d,  $J = 10.1\text{ Hz}$ , 1H), 6.42 (d,  $J = 8.8\text{Hz}$ , 1H), 5.56 (d,  $J = 10.1\text{ Hz}$ , 1H), 5.11 (t,  $J = 7.3\text{Hz}$ , 1H), 3.94

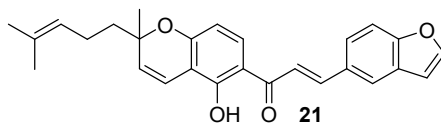
(s, 3H), 2.14 (m, 2H), 1.78 (m, 2H), 1.67 (s, 3H), 1.59 (s, 3H), 1.45 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 50 MHz)  $\delta$ : 191.78, 182.54, 164.05, 161.22, 160.59, 157.03, 153.98, 143.98, 132.27, 131.33, 130.98, 129.72, 128.07, 127.26, 124.33, 124.06, 120.29, 116.60, 115.42, 114.18, 113.32, 109.46, 108.47, 80.65, 55.80, 41.95, 27.43, 25.94, 22.93, 17.90; HRESIMS:  $m/z$ calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{35}\text{H}_{33}\text{O}_6$  549.2272 found 549.2271.

**(E)-3-(2-benzoylbenzofuran-5-yl)-1-(5-hydroxy-2-methyl-2-(4-methylpent-3-enyl)-2H-chromen-6-yl)prop-2-en-1-one (20)**



Yield 72%; MP: 141-143°C; FT-IR (KBr,  $\text{cm}^{-1}$ ): 3385, 3136, 2922, 1643, 1558, 1480, 1432, 1281, 1111, 798, 697;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 13.67 (s, 1H), 8.08 (d,  $J = 7.3$  Hz, 2H), 8.00 (s, 1H), 7.97 (d,  $J = 15.2$  Hz, 1H), 7.85 (d,  $J = 8.75$  Hz, 1H), 7.767-7.63 (m, 4H), 7.60 (d,  $J = 15.2$  Hz, 1H), 7.58 (m, 2H), 6.83 (d,  $J = 10.1$  Hz, 1H), 6.40 (d,  $J = 18.9$  Hz, 1H), 5.57 (d,  $J = 10.1$  Hz, 1H), 5.11 (t,  $J = 6.3$  Hz, 1H), 2.12 (m, 2H), 1.78 (m, 2H), 1.68 (s, 3H), 1.59 (s, 3H), 1.46 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 50 MHz)  $\delta$ : 191.58, 184.07, 160.99, 160.38, 156.99, 153.28, 143.63, 136.93, 133.16, 131.93, 131.28, 130.68, 129.48, 128.63, 128.09, 127.72, 127.04, 124.25, 123.77, 120.30, 116.33, 116.15, 113.92, 113.24, 109.23, 108.22, 80.44, 41.72, 27.21, 25.65, 22.67, 17.62; HRESIMS:  $m/z$ calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{34}\text{H}_{31}\text{O}_5$  519.2166 found 519.2173.

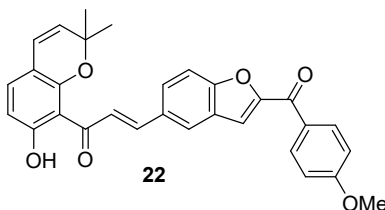
**(E)-3-(benzofuran-5-yl)-1-(5-hydroxy-2-methyl-2-(4-methylpent-3-enyl)-2H-chromen-6-yl)prop-2-en-1-one (21)**



Yield 63%; MP: 77-79 °C; FT-IR (KBr,  $\text{cm}^{-1}$ ): 3358, 2923, 1637, 1482, 1365, 1217, 1108, 767, 670;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 13.83 (s, 1H), 8.00 (d,  $J = 15.4$  Hz, 1H), 7.84 (s, 1H), 7.73 (d,  $J = 8.9$  Hz, 1H), 7.65 (d,  $J = 1.8$  Hz, 1H), 7.65 (d,  $J = 15.4$  Hz, 1H), 7.53 (m, 2H), 6.81 (d,  $J = 10.1$  Hz, 1H), 6.79 (s, 1H), 6.41 (d,  $J = 8.9$  Hz, 1H), 5.56 (d,  $J = 10.1$  Hz, 1H), 5.13 (t,  $J = 6.1$  Hz,

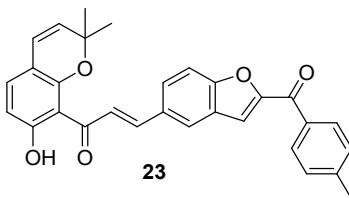
1H), 2.13 (m, 2H), 1.82 (m, 2H), 1.69 (s, 3H), 1.60 (s, 3H), 1.46 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ: 191.71, 160.99, 160.18, 156.26, 146.13, 144.75, 131.85, 130.71, 129.96, 128.18, 126.92, 124.70, 123.90, 122.30, 119.07, 116.48, 114.02, 112.00, 109.23, 108.10, 106.85, 80.32, 41.72, 27.17, 25.71, 22.73, 17.67; HRESIMS: *m/z*calcd for [M+H]<sup>+</sup> C<sub>27</sub>H<sub>27</sub>O<sub>4</sub> 415.1904 found 415.1910.

**(E)-1-(7-hydroxy-2,2-dimethyl-2H-chromen-8-yl)-3-(2-(4-methoxybenzoyl)benzofuran-5-yl)prop-2-en-1-one (22)**



Yield 92%; MP: 155-157 °C; FT-IR (KBr, cm<sup>-1</sup>): 3512, 2853, 1602, 1552, 1472, 1312, 1157, 767; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ: 13.11 (s, 1H), 8.14 (d, *J* = 8.1Hz, 2H), 8.09 (d, *J* = 15.2 Hz, 1H), 7.94 (s, 1H), 7.91 (d, *J* = 15.2 Hz, 1H), 7.79 (d, *J* = 8.6 Hz, 1H), 7.68 (d, *J* = 8.6Hz, 1H), 7.55 (s, 1H), 7.09 (d, *J* = 8.3Hz, 1H), 7.05 (d, *J* = 8.1 Hz, 2H), 6.52 (d, *J* = 8.3Hz, 1H), 6.29 (d, *J* = 9.9 Hz, 1H), 5.53 (d, *J* = 9.9 Hz, 1H), 3.93 (s, 3H), 1.58 (s, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 50 MHz) δ: 194.10, 182.40, 164.33, 163.79, 156.70, 154.74, 142.49, 133.60, 131.98, 131.65, 129.53, 127.79, 127.34, 126.30, 124.09, 122.30, 115.22, 113.94, 113.15, 111.70, 109.92, 78.25, 55.55, 28.33; HRESIMS: *m/z*calcd for [M+H]<sup>+</sup> C<sub>30</sub>H<sub>25</sub>O<sub>6</sub> 481.1646 found 481.1640.

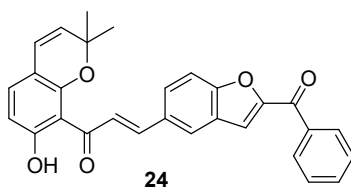
**(E)-1-(7-hydroxy-2,2-dimethyl-2H-chromen-8-yl)-3-(2-(4-methylbenzoyl)benzofuran-5-yl)prop-2-en-1-one (23)**



Yield 95%; MP: 168-170 °C; FT-IR (KBr, cm<sup>-1</sup>): 3455, 3021, 2927, 1640, 1601, 1475, 1362, 1215, 1113, 1021, 971, 892, 768, 671; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ: 13.08(s, 1H), 8.10 (d, *J* =

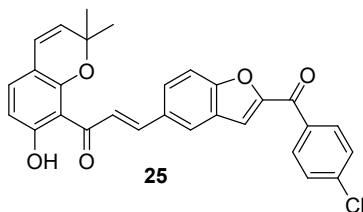
15.6Hz, 1H), 8.01 (d,  $J = 7.9$  Hz, 2H), 7.95 (s, 1H), 7.91 (d,  $J = 15.6$ Hz, 1H), 7.81 (d,  $J = 8.5$  Hz, 1H), 7.69 (d,  $J = 8.3$ Hz, 1H), 7.55 (s, 1H), 7.37(d,  $J = 7.9$  Hz, 2H), 7.10 (d,  $J = 8.3$  Hz, 1H), 6.25 (d,  $J = 8.3$ Hz, 1H), 6.30 (d,  $J = 9.9$  Hz, 1H), 5.54 (d,  $J = 9.9$  Hz, 1H), 2.49 (s, 3H), 1.58 (s, 6H); HRESIMS:  $m/z$ calcd for  $[M+H]^+$   $C_{30}H_{25}O_5$  465.1697 found 465.1697.

**(E)-3-(2-benzoylbenzofuran-5-yl)-1-(7-hydroxy-2,2-dimethyl-2H-chromen-8-yl)prop-2-en-1-one (24)**



Yield 82%; MP: 205-207 °C; FT-IR (KBr,  $cm^{-1}$ ): 3426, 3023, 1640, 1367, 1217, 1114, 927, 763, 670;  $^1H$  NMR ( $CDCl_3$ , 300 MHz)  $\delta$ : 13.10 (s, 1H), 8.11 (d,  $J = 15.4$ Hz, 1H), 8.07 (d,  $J = 8.7$  Hz, 2H), 7.95 (s, 1H), 7.91 (d,  $J = 15.4$ Hz, 1H), 7.82 (dd,  $J = 8.6$  & 1.4 Hz, 1H), 7.69 (m, 2H), 7.60-7.55 (m, 3H), 7.10 (d,  $J = 8.4$  Hz, 1H), 6.53 (d,  $J = 8.4$  Hz, 1H), 6.30 (d,  $J = 9.9$  Hz, 1H), 5.56 (d,  $J = 9.9$  Hz, 1H), 1.59 (s, 6H);  $^{13}C$  NMR ( $CDCl_3$ , 50 MHz)  $\delta$ : 194.16, 184.19, 164.32, 156.93, 154.77, 153.09, 142.41, 136.98, 133.65, 133.15, 131.82, 129.48, 128.64, 127.75, 127.67, 127.47, 126.32, 124.35, 118.12, 116.34, 113.30, 113.08, 111.72, 109.94, 78.30, 28.31; HRESIMS:  $m/z$ calcd for  $[M+H]^+$   $C_{29}H_{23}O_5$  451.1540 found 451.1549.

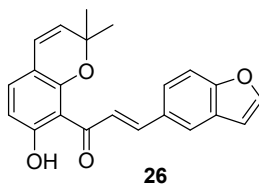
**(E)-3-(2-(4-chlorobenzoyl)benzofuran-5-yl)-1-(7-hydroxy-2,2-dimethyl-2H-chromen-8-yl)prop-2-en-1-one (25)**



Yield 85%; MP: 180-182 °C; FT-IR (KBr,  $cm^{-1}$ ): 3452, 2983, 2870, 1644, 1595, 1549, 1488, 1310, 1205, 1109, 814, 770, 628: 3395;  $^1H$  NMR ( $CDCl_3$ , 300 MHz)  $\delta$ : 13.08 (s, 1H), 8.11 (d,  $J = 15.6$  Hz, 1H), 8.05 (d,  $J = 8.7$  Hz, 2H), 7.96 (s, 1H), 7.92 (d,  $J = 15.6$ Hz, 1H), 7.83 (d,  $J = 8.8$

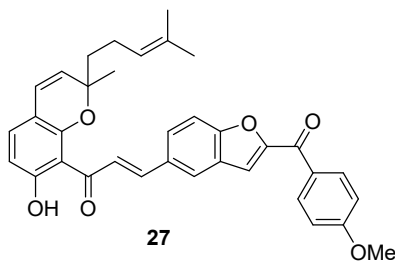
Hz, 1H), 7.70 (d,  $J = 8.8$  Hz, 1H), 7.59 (s, 1H), 7.56 (d,  $J = 8.7$  Hz, 2H), 7.11(d,  $J = 8.2$  Hz, 1H), 6.53 (d,  $J = 8.2$  Hz, 1H), 6.34 (d,  $J = 9.9$  Hz, 1H), 5.55 (d,  $J = 9.9$  Hz, 1H), 1.58 (s, 6H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$ : 194.14, 182.69, 164.34, 156.89, 154.77, 153.08, 142.23, 139.76, 135.15, 133.68, 131.97, 130.94, 129.02, 127.86, 127.66, 126.31, 124.24, 122.34, 116.20, 113.29, 113.08, 111.74, 109.98, 78.27, 28.36; HRESIMS:  $m/z$ calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{29}\text{H}_{22}\text{ClO}_5$  485.1150 found 485.1147.

**(E)-3-(benzofuran-5-yl)-1-(7-hydroxy-2,2-dimethyl-2H-chromen-8-yl)prop-2-en-1-one (26)**



Yield 60%; MP: 86-88 °C; FT-IR (KBr,  $\text{cm}^{-1}$ ) 3407, 3407, 109, 2937, 2848, 1635, 1478, 1360, 1116, 769, 643;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 13.20 (s, 1H), 8.09 (d,  $J = 15.5$  Hz, 1H), 7.94 (d,  $J = 15.5$  Hz, 2H), 7.85 (s, 1H), 7.68 (d,  $J = 2.1$  Hz, 1H), 7.63 (dd,  $J = 8.5$  & 1.4 Hz, 1H), 7.55 (d,  $J = 8.5$  Hz, 1H), 7.09 (d,  $J = 8.3$  Hz, 1H), 6.82 (d,  $J = 2.1$  Hz, 1H), 6.53 (d,  $J = 8.3$  Hz, 1H), 6.23 (d,  $J = 9.9$  Hz, 1H), 5.53 (d,  $J = 9.9$  Hz, 1H), 1.58 (s, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 50 MHz)  $\delta$ : 194.35, 164.37, 156.18, 154.79, 146.13, 143.65, 133.47, 130.55, 128.23, 126.49, 126.34, 124.23, 122.47, 122.37, 113.10, 112.13, 111.83, 109.93, 106.88, 78.21, 28.32; MS (ESI):  $m/z$  347 ( $\text{M} + \text{H}$ ) $^+$ .

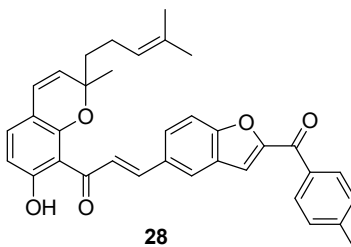
**(E)-1-(7-hydroxy-2-methyl-2-(4-methylpent-3-enyl)-2H-chromen-8-yl)-3-(2-(4-methoxybenzoyl)benzofuran-5-yl)prop-2-en-1-one (27)**



Yield 90%; MP: 152-154 °C; FT-IR (KBr,  $\text{cm}^{-1}$ ): 3440, 3065, 2854, 1635, 1580, 1480, 1349, 1110, 831, 753;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 13.12 (s, 1H), 8.13 (d,  $J = 8.9$ Hz, 2H), 8.07 (d,  $J$

= 15.6 Hz, 1H), 7.93 (s, 1H), 7.90 (d,  $J = 15.6$  Hz, 1H), 7.77 (dd,  $J = 8.6$  & 1.2 Hz, 1H), 7.58 (d,  $J = 8.6$  Hz, 1H), 7.53 (s, 1H), 7.07 (d,  $J = 8.3$  Hz, 1H), 7.04 (d,  $J = 8.9$  Hz, 2H), 6.50 (d,  $J = 8.4$  Hz, 1H), 6.32 (d,  $J = 9.9$  Hz, 1H), 5.48 (d,  $J = 9.9$  Hz, 1H), 5.10 (t,  $J = 5.5$  Hz, 1H), 3.93 (s, 3H), 2.16 (m, 2H), 1.86 (m, 2H), 1.63 (s, 3H), 1.52 (s, 3H), 1.48 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 50 MHz)  $\delta$ : 194.34, 182.70, 164.58, 164.05, 156.98, 155.32, 153.89, 142.76, 133.93, 132.51, 132.24, 131.87, 129.78, 128.04, 127.81, 127.65, 125.33, 124.32, 123.81, 123.15, 115.55, 114.20, 113.37, 113.09, 111.78, 109.94, 81.16, 55.83, 42.02, 27.30, 25.94, 23.32, 17.88; HRESIMS:  $m/z$  calcd for  $[\text{M}+\text{H}]^+ \text{C}_{35}\text{H}_{33}\text{O}_6$  549.2272 found 549.2272.

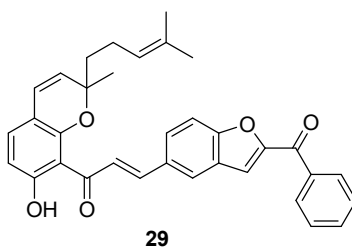
**(*E*)-1-(7-hydroxy-2-methyl-2-(4-methylpent-3-enyl)-2*H*-chromen-8-yl)-3-(2-(4-methylbenzoyl)benzofuran-5-yl)prop-2-en-1-one (28)**



Yield 92%; MP 107-109 °C; FT-IR (KBr,  $\text{cm}^{-1}$ ) 3440, 3019, 2922, 2854, 1640, 1604, 1560, 1470, 1313, 1120, 972, 765, 669;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 13.09 (s, 1H), 8.09 (d,  $J = 15.6$  Hz, 2H), 8.00 (d,  $J = 7.9$  Hz, 1H), 7.94 (s, 1H), 7.92 (d,  $J = 15.6$  Hz, 1H), 7.79 (dd,  $J = 8.5$  & 1.2 Hz, 1H), 7.67 (d,  $J = 8.5$  Hz, 1H), 7.54 (s, 1H), 7.37 (d,  $J = 7.9$  Hz, 2H), 7.09 (d,  $J = 8.2$  Hz, 1H), 6.51 (d,  $J = 8.2$  Hz, 1H), 6.34 (d,  $J = 9.9$  Hz, 1H), 5.49 (d,  $J = 9.9$  Hz, 1H), 5.10 (t,  $J = 6.3$  Hz, 1H), 2.49 (s, 3H), 2.19 (m, 2H), 1.86 (m, 2H), 1.60 (s, 3H), 1.53 (s, 3H), 1.49 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 50 MHz)  $\delta$ : 194.12, 183.77, 164.32, 156.83, 155.07, 153.38, 144.14, 142.43, 134.31, 133.67, 133.27, 131.69, 129.64, 129.34, 127.72, 127.49, 125.06, 124.15, 123.52, 122.90, 115.85, 113.19, 112.82, 111.53, 109.69, 80.90, 41.79, 27.07, 25.66, 23.06, 21.75, 17.61; HRESIMS:  $m/z$  calcd for  $[\text{M}+\text{H}]^+ \text{C}_{35}\text{H}_{33}\text{O}_5$  533.2323 found 533.2325.

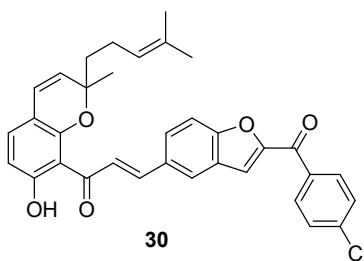


**(E)-3-(2-benzoylbenzofuran-5-yl)-1-(7-hydroxy-2-methyl-2-(4-methylpent-3-enyl)-2H-chromen-8-yl)prop-2-en-1-one (29)**



Yield 90%; MP: 130-132 °C; FT-IR (KBr,  $\text{cm}^{-1}$ ): 3485, 2926, 2854, 1641, 1602, 1549, 1473, 1296, 1112, 864, 765;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 13.10 (s, 1H), 8.10 (d,  $J = 14.6\text{Hz}$ , 1H), 8.07 (d,  $J = 8.8\text{ Hz}$ , 2H), 7.93 (s, 1H), 7.89 (d,  $J = 14.6\text{ Hz}$ , 1H), 7.80 (dd,  $J = 8.6$  & 1.2 Hz, 1H), 7.68 (d,  $J = 8.6\text{Hz}$ , 1H), 7.67 (s, 1H), 7.61-7.50 (m, 3H), 7.02 (d,  $J = 8.2\text{Hz}$ , 1H), 6.51 (d,  $J = 8.2\text{ Hz}$ , 1H), 6.32 (d,  $J = 9.9\text{ Hz}$ , 1H), 5.48 (d,  $J = 9.9\text{ Hz}$ , 1H), 5.10 (t,  $J = 6.1\text{ Hz}$ , 1H), 2.18 (m, 2H), 1.18 (m, 2H), 1.62 (s, 3H), 1.52 (s, 3H), 1.48 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 50 MHz)  $\delta$ : 194.07, 184.10, 164.34, 156.91, 155.07, 153.17, 142.37, 136.97, 133.70, 133.16, 132.27, 131.77, 129.45, 128.66, 127.90, 127.75, 127.54, 125.07, 124.22, 123.55, 122.91, 116.33, 113.22, 112.83, 111.54, 109.71, 80.91, 41.79, 27.06, 25.67, 23.08, 17.63; HRESIMS:  $m/z$  calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{34}\text{H}_{31}\text{O}_5$  519.2166 found 519.2168.

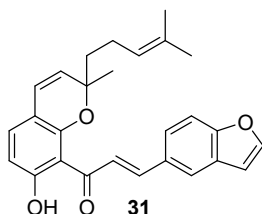
**(E)-3-(2-(4-chlorobenzoyl)benzofuran-5-yl)-1-(7-hydroxy-2-methyl-2-(4-methylpent-3-enyl)-2H-chromen-8-yl)prop-2-en-1-one (30)**



Yield 92%; Semi solid; FT-IR (Neat,  $\text{cm}^{-1}$ ): 3394, 3020, 1641, 1550, 1470, 1216, 763, 670;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 13.08(s, 1H), 8.06 (d,  $J = 15.6\text{Hz}$ , 1H), 8.04(d,  $J = 8.5\text{ Hz}$ , 2H), 7.93 (s, 1H), 7.88 (d,  $J = 15.6\text{ Hz}$ , 1H), 7.78 (d,  $J = 8.6\text{ Hz}$ , 1H), 7.65 (d,  $J = 8.7\text{Hz}$ , 1H), 7.55 (s, 1H), 7.53 (d,  $J = 8.5\text{ Hz}$ , 2H), 7.06 (d,  $J = 8.2\text{Hz}$ , 1H), 6.49 (d,  $J = 8.2\text{ Hz}$ , 1H), 6.32 (d,  $J = 9.9\text{ Hz}$ ,

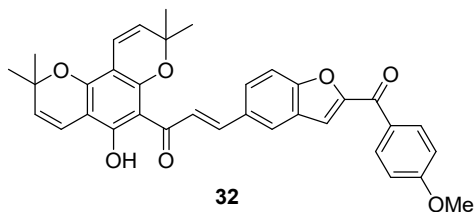
1H), 5.47 (d,  $J = 9.9$  Hz, 1H), 5.10 (t,  $J = 6.5$  Hz, 1H), 2.18 (m, 2H), 1.83 (m, 2H), 1.62 (s, 3H), 1.52 (s, 3H), 1.48 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 50 MHz)  $\delta$ : 194.02, 182.55, 164.34, 156.85, 155.04, 153.04, 142.22, 139.69, 135.11, 133.69, 132.23, 131.88, 130.91, 128.98, 128.01, 127.63, 125.03, 124.16, 123.55, 122.90, 116.19, 113.17, 112.81, 111.50, 109.7, 80.90, 41.77, 27.04, 25.65, 23.05, 17.60; MS (ESI):  $m/z$  553 ( $\text{M} + \text{H}$ ) $^+$ .

**(*E*)-3-(benzofuran-5-yl)-1-(7-hydroxy-2-methyl-2-(4-methylpent-3-enyl)-2*H*-chromen-8-yl)prop-2-en-1-one (31)**



Yield 72%; Semi solid; FT-IR (Neat,  $\text{cm}^{-1}$ ): 3453, 3019, 2964, 1723, 1633, 1601, 1555, 1472, 1364, 1216, 1027, 979, 859, 762, 668;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 13.19 (s, 1H), 8.08 (d,  $J = 15.6$  Hz, 1H), 7.95 (s, 1H), 7.85 (s, 1H), 7.68 (d,  $J = 2.1$  Hz, 1H), 7.61 (dd,  $J = 8.8$  & 1.4 Hz, 1H), 7.53 (d,  $J = 8.8$  Hz, 1H), 7.08 (d,  $J = 8.5$  Hz, 1H), 6.81 (d,  $J = 2.1$  Hz, 1H), 6.51 (d,  $J = 8.5$  Hz, 1H), 6.33 (d,  $J = 9.9$  Hz, 1H), 5.49 (d,  $J = 9.9$  Hz, 1H), 5.11 (t,  $J = 5.5$  Hz, 1H), 2.20 (m, 2H), 1.84 (m, 2H), 1.65 (s, 3H), 1.53 (s, 3H), 1.49 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 50 MHz)  $\delta$ : 194.33, 164.39, 156.20, 155.10, 146.11, 143.65, 133.50, 132.21, 130.53, 128.22, 126.59, 125.08, 124.48, 123.64, 122.96, 122.32, 112.84, 112.05, 111.65, 109.69, 106.86, 80.86, 41.80, 27.05, 25.68, 23.09, 17.61; HRESIMS:  $m/z$  calcd for  $[\text{M} + \text{H}]^+$   $\text{C}_{27}\text{H}_{27}\text{O}_4$  415.1904 found 415.1900.

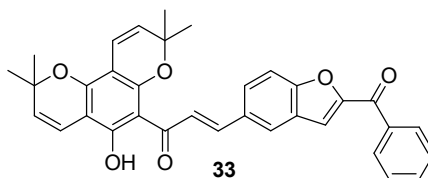
**C-2' and C-4'-hydroxyls engaged benzofuran-based chromenochalcones (32).**



Yield 95%; MP: 185-187  $^{\circ}\text{C}$ ; FT-IR (KBr,  $\text{cm}^{-1}$ ): 3438, 3019, 1638, 1547, 1510, 1463, 1421, 1360, 1262, 1174, 1031, 971, 771, 669;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 14.37 (s, 1H), 8.15 (brs ,

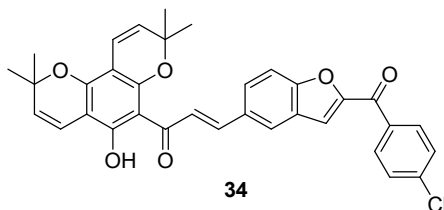
3H), 7.93 (s, 1H), 7.89 (d,  $J = 15.6$  Hz, 1H), 7.79 (d,  $J = 8.1$  Hz, 1H), 7.68 (d,  $J = 8.1$ Hz, 1H), 7.56 (s, 1H), 7.07 (d,  $J = 8.7$  Hz, 2H), 6.72 (d,  $J = 9.9$ Hz, 1H), 6.64 (d,  $J = 10.1$  Hz, 1H), 5.51(d,  $J = 9.9$  Hz, 2H), 3.94 (s, 3H), 1.59 (s, 6H), 1.48 (s, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$ : 192.63, 182.48, 163.79, 161.48, 156.60, 156.18, 155.38, 153.63, 141.67, 131.99, 129.60, 127.77, 127.46, 127.33, 125.43, 124.75, 123.85, 116.63, 116.21, 115.30, 113.94, 113.09, 105.94, 102.65, 102.57, 78.36, 78.32, 55.56, 28.43, 28.16; MS (ESI):  $m/z$  563 ( $\text{M} + \text{H}$ ) $^+$ .

**C-2' and C-4'-hydroxyls engaged benzofuran based chromenochalcone (33)**



Yield 90%; MP: 163-165 °C; FT-IR (KBr,  $\text{cm}^{-1}$ ): 3440, 3065, 2854, 1635, 1580, 1480, 1349, 1110, 831, 753;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 14.37 (s, 1H), 8.15 (d,  $J = 15.5$ Hz, 1H), 8.06 (d,  $J = 7.1$  Hz, 2H), 7.93 (s, 1H), 7.89 (d,  $J = 15.5$  Hz, 1H), 7.81 (d,  $J = 8.6$ Hz, 1H), 7.69 (d,  $J = 8.6$  Hz, 1H), 7.66 (s, 1H), 7.58 (m, 3H), 6.71(d,  $J = 10.1$ Hz, 1H), 6.64 (d,  $J = 9.9$  Hz, 1H), 5.51 (d,  $J = 9.9$  Hz, 1H), 5.50 (d,  $J = 10.1$  Hz, 1H), 1.59 (s, 6H), 1.48 (s, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$ : 192.62, 184.17, 161.46, 156.78, 156.18, 155.40, 153.10, 141.55, 137.00, 133.12, 132.09, 129.45, 128.64, 127.62, 125.46, 124.75, 124.07, 116.63, 116.38, 116.19, 113.22, 105.93, 102.58, 78.33, 28.42, 28.16; MS (ESI):  $m/z$  533 ( $\text{M} + \text{H}$ ) $^+$ .

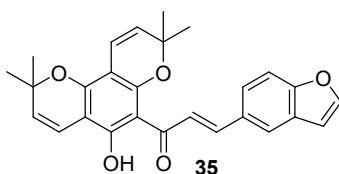
**C-2' and C-4'-hydroxyls engaged benzofuran based chromenochalcone (34).**



Yield 92%; MP: 114-116 °C; FT-IR (KBr,  $\text{cm}^{-1}$ ) 3459, 2798, 1642, 1581, 1420, 1292, 1133, 972, 867, 767;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 14.33 (s, 1H), 8.14 (d,  $J = 15.4$  Hz, 1H), 8.05 (d,  $J = 8.6$  Hz, 2H), 7.93 (s, 1H), 7.86 (d,  $J = 15.4$  Hz, 1H), 7.80 (d,  $J = 8.5$  Hz, 1H), 7.69 (d,  $J = 8.5$ Hz,

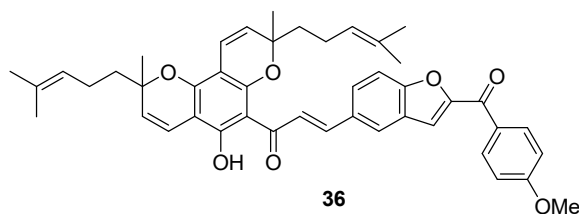
1H), 7.56 (m, 3H), 6.70 (d,  $J = 10.1$  Hz, 1H), 6.41 (d,  $J = 9.9$ Hz, 1H), 5.50 (brd,  $J = 9.9$  Hz, 2H), 1.58 (s, 6H), 1.48 (s, 6H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$ : 192.62, 182.72, 161.48, 156.78, 156.18, 155.44, 153.01, 141.39, 139.72, 135.19, 132.26, 130.94, 129.01, 127.82, 127.74, 127.62, 125.48, 124.74, 124.00, 116.66, 116.27, 116.20, 113.21, 105.95, 102.67, 102.58, 78.40, 78.33, 28.44, 28.18; HRESIMS:  $m/z$ calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{34}\text{H}_{28}\text{ClO}_6$  567.1569 found 567.1566.

### C-2' and C-4'-hydroxyls engaged benzofuran based chromenochalcone (35)



Yield 62%; MP: 124-126 °C; FT-IR (KBr,  $\text{cm}^{-1}$ ) 3465, 2965, 1636, 1589, 1461, 1422, 1257, 1133, 867, 764;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 14.46(s, 1H), 8.13 (d,  $J = 15.6$  Hz, 1H), 7.91(d,  $J = 15.6$  Hz, 1H), 7.83(s, 1H), 7.67 (d,  $J = 1.9$  Hz, 1H), 7.62 (d,  $J = 8.6$  Hz, 1H), 7.52 (d,  $J = 8.6$ Hz, 1H), 6.83 (d,  $J = 1.9$  Hz, 1H), 6.71 (d,  $J = 10.1$ Hz, 1H), 6.65 (d,  $J = 9.9$ Hz, 1H), 5.50 (d,  $J = 9.9$  Hz, 2H), 1.59 (s, 6H), 1.48 (s, 6H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$ : 192.90, 192.62, 161.50, 156.77, 156.19, 156.01, 155.44, 155.22, 153.01, 146.00, 142.74, 141.39, 139.72, 135.19, 132.26, 130.94, 130.82, 129.01, 128.14, 127.82, 127.74, 127.62, 126.56, 125.48, 125.38, 124.74, 124.11, 123.99, 122.20, 116.66, 116.29, 116.20, 113.21, 112.02, 106.85, 105.98, 102.67, 102.58, 102.54, 78.40, 78.33, 78.29, 78.24, 28.42, 28.18, 28.12. HRESIMS:  $m/z$ calcd for  $[\text{M}+\text{H}]^+$   $\text{C}_{27}\text{H}_{25}\text{O}_5$  429.1697 found 429.1696

### C-2' and C-4'-hydroxyls engaged benzofuran based chromenochalcone (36)

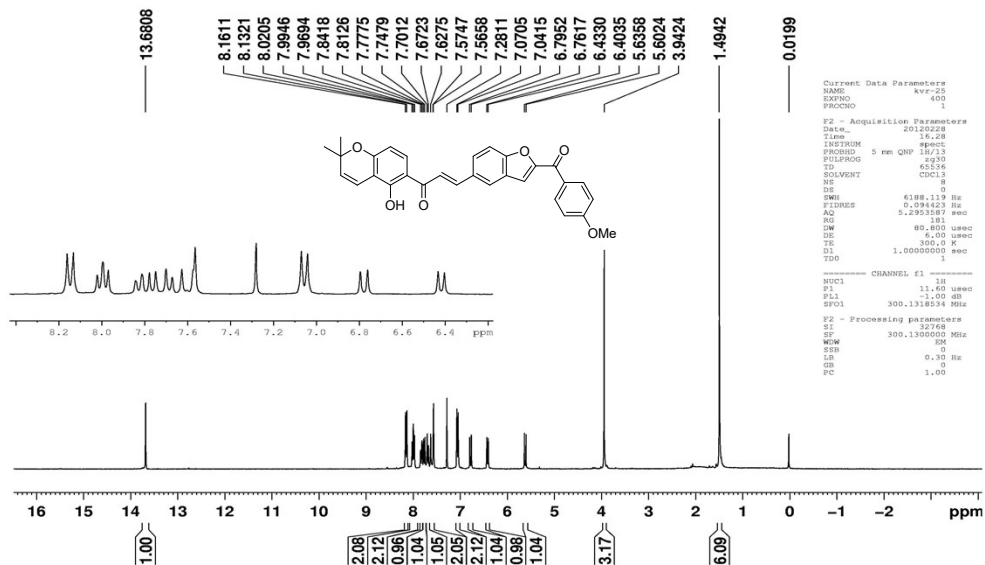


Yield 80%; MP: 160-162 °C; FT-IR (KBr,  $\text{cm}^{-1}$ ): 3503, 3026, 2961, 1636, 1549, 1450, 1217, 766, 670;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 14.39 (s, 1H), 8.14 (d,  $J = 8.9$ Hz, 2H), 8.12 (d,  $J = 15.6$

Hz, 1H), 7.93 (s, 1H), 7.88 (d,  $J = 15.6$  Hz, 1H), 7.77 (d,  $J = 8.6$  Hz, 1H), 7.65 (d,  $J = 8.6$  Hz, 1H), 7.54 (s, 1H), 7.06 (d,  $J = 8.9$  Hz, 2H), 6.75 (d,  $J = 9.8$  Hz, 1H), 6.68 (d,  $J = 10.1$  Hz, 1H), 5.49 (d,  $J = 9.8$  Hz, 1H), 5.48 (d,  $J = 10.1$  Hz, 1H), 5.12 (t,  $J = 6.3$  Hz, 2H), 3.94 (s, 3H), 2.14 (m, 4H), 1.76 (m, 4H), 1.68 (s, 3H), 1.64 (s, 3H), 1.60 (s, 3H), 1.52 (s, 3H), 1.49 (s, 3H), 1.45 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$ : 192.82, 182.76, 164.06, 161.72, 156.89, 156.76, 155.89, 153.88, 141.91, 132.48, 132.26, 132.10, 129.86, 128.04, 127.83, 124.55, 124.16, 124.04, 123.89, 123.75, 117.39, 116.95, 115.61, 114.21, 113.31, 105.97, 102.58, 102.34, 102.29, 81.24, 81.05, 55.83, 41.90, 27.33, 27.27, 25.95, 23.35, 22.91, 17.90, MS (ESI):  $m/z$  699 ( $\text{M} + \text{H}$ ) $^+$ .

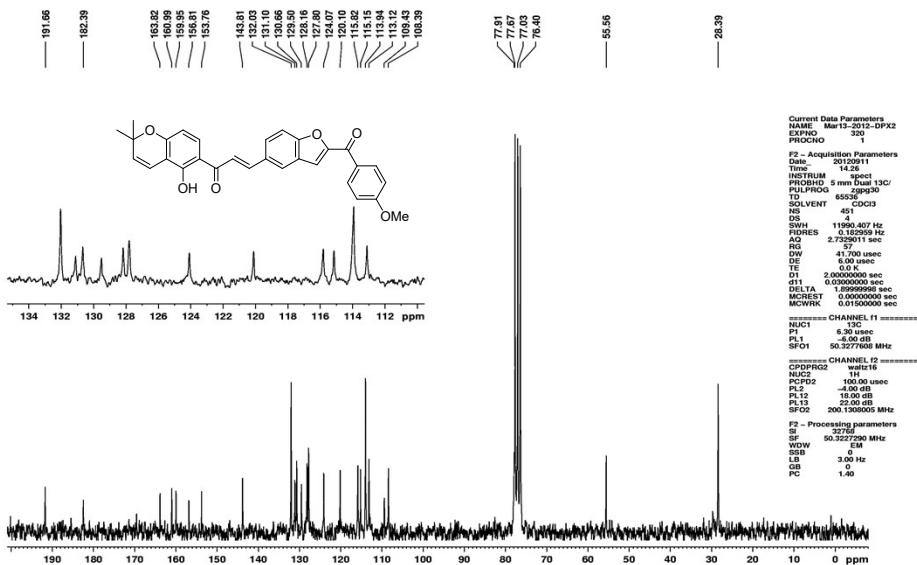
# NMR and HRMS spectra of the synthesized compounds

KVR-204/12

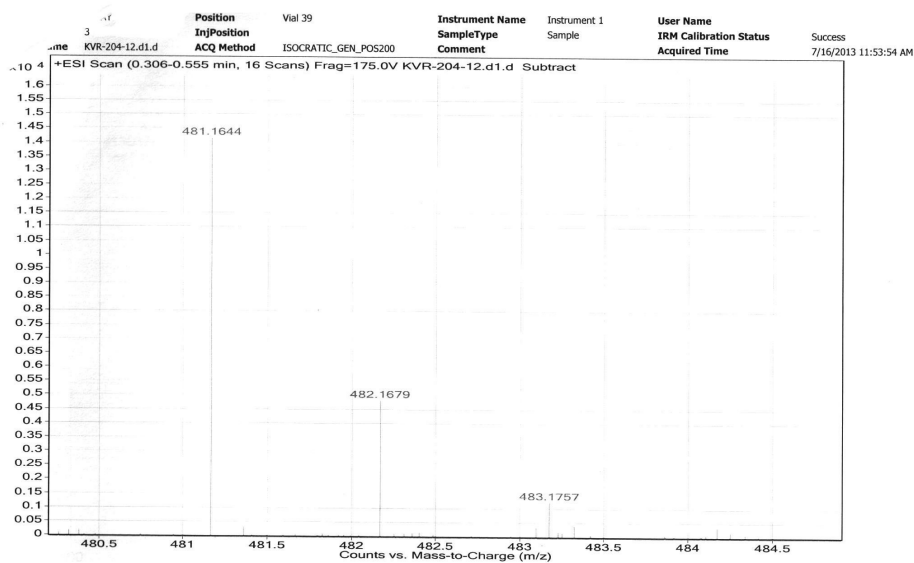


<sup>1</sup>H-NMR spectrum of **16** (300 MHz, CDCl<sub>3</sub>)

KVR-204/12

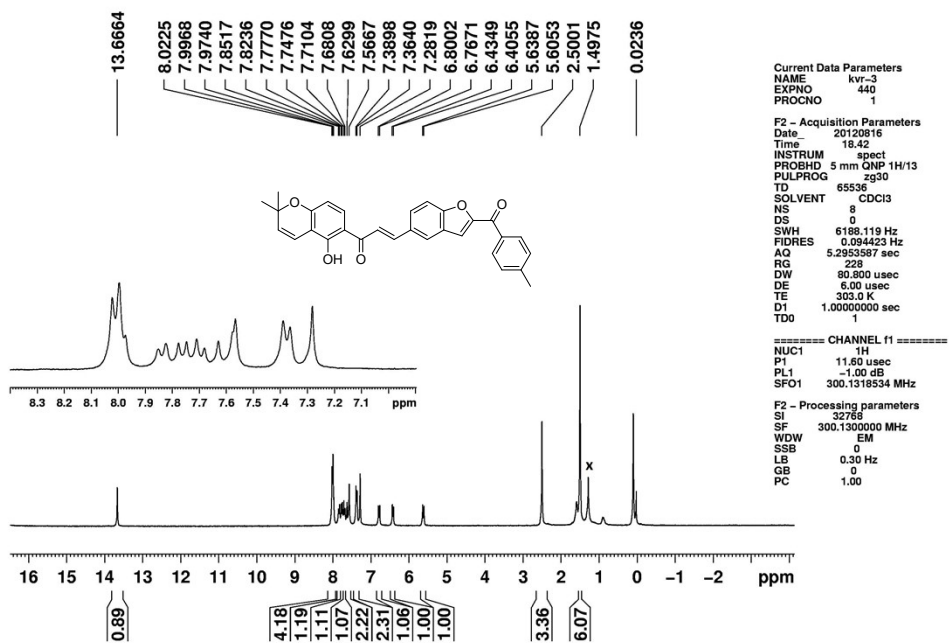


<sup>13</sup>C-NMR spectrum of **16** (50 MHz, CDCl<sub>3</sub>)

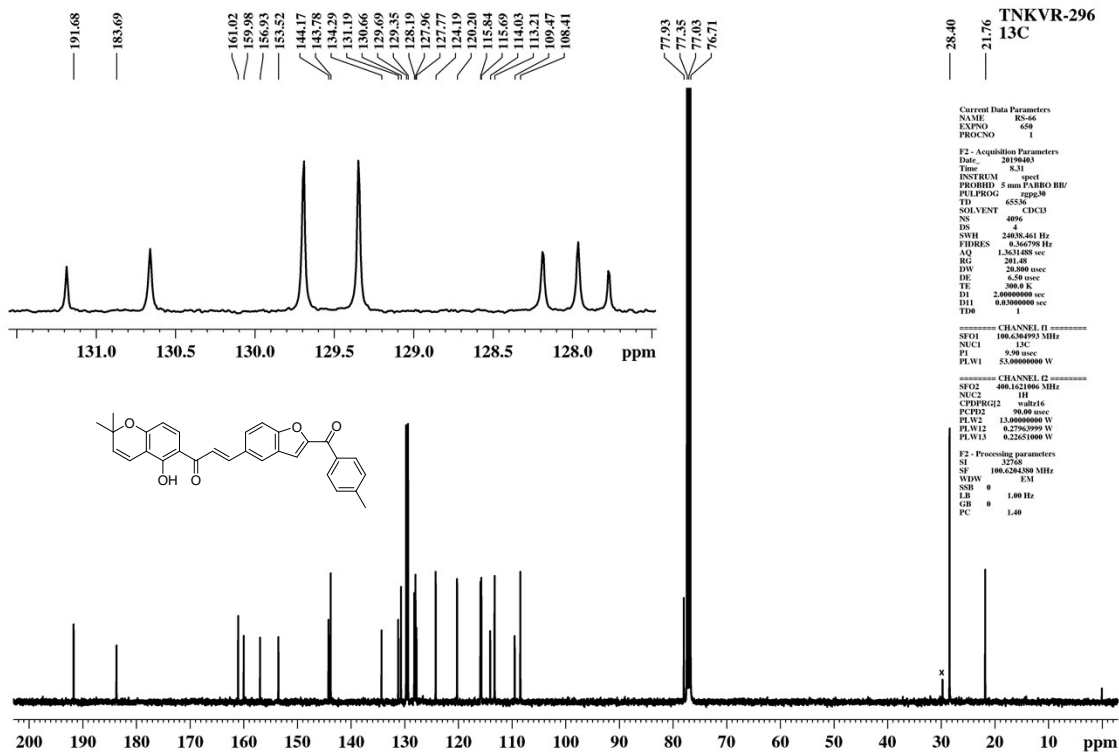


### HRMS Spectrum of compound 16

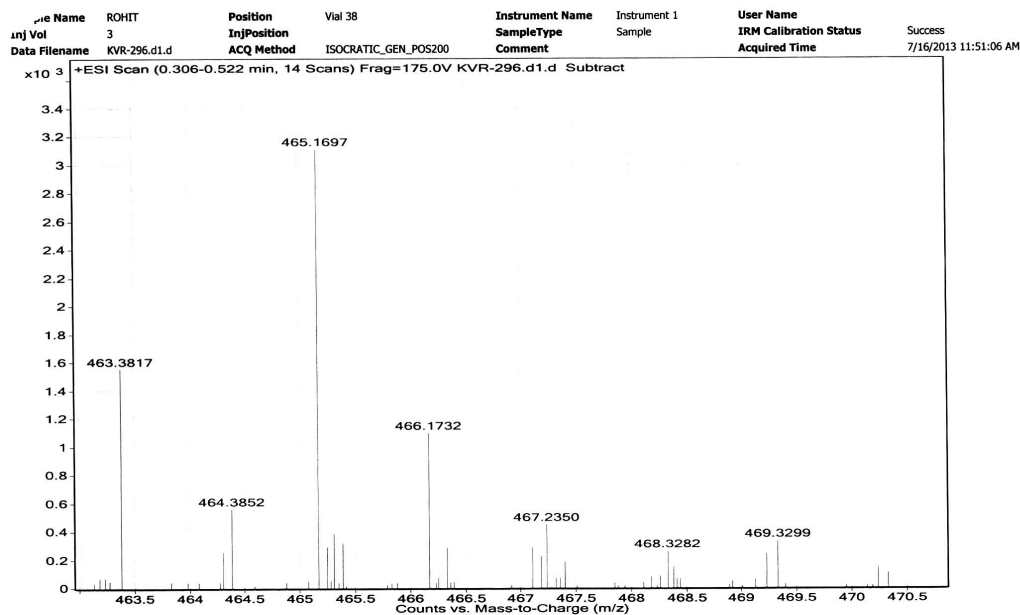
KVR-296



<sup>1</sup>H-NMR spectrum of 17 (300 MHz, CDCl<sub>3</sub>); X = Wax impurity



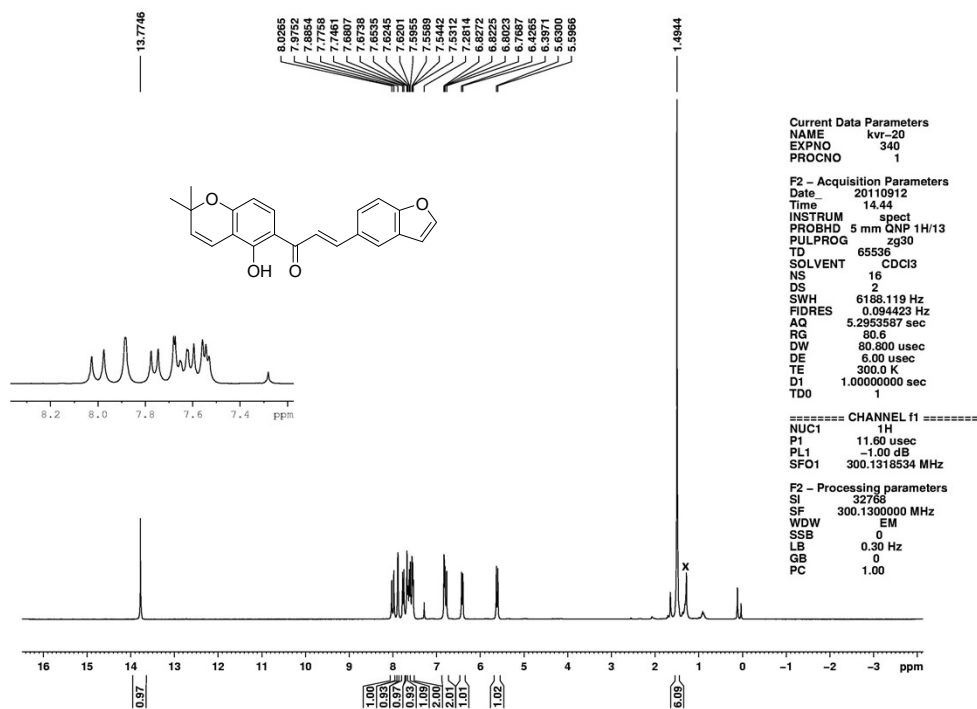
<sup>13</sup>C-NMR spectrum of **17** (75 MHz, CDCl<sub>3</sub>); X = Wax impurity



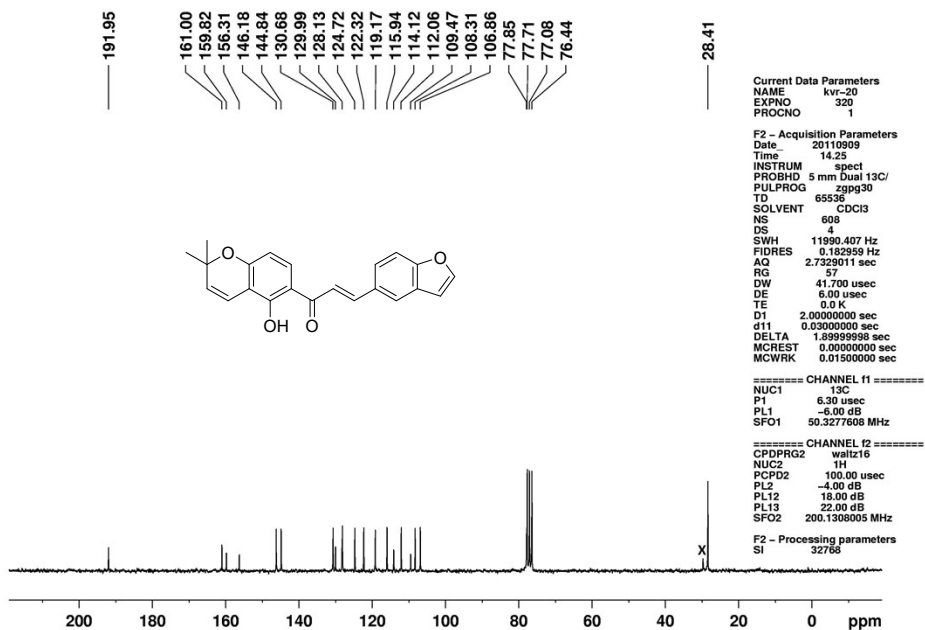
HRMS Spectrum of compound **17**



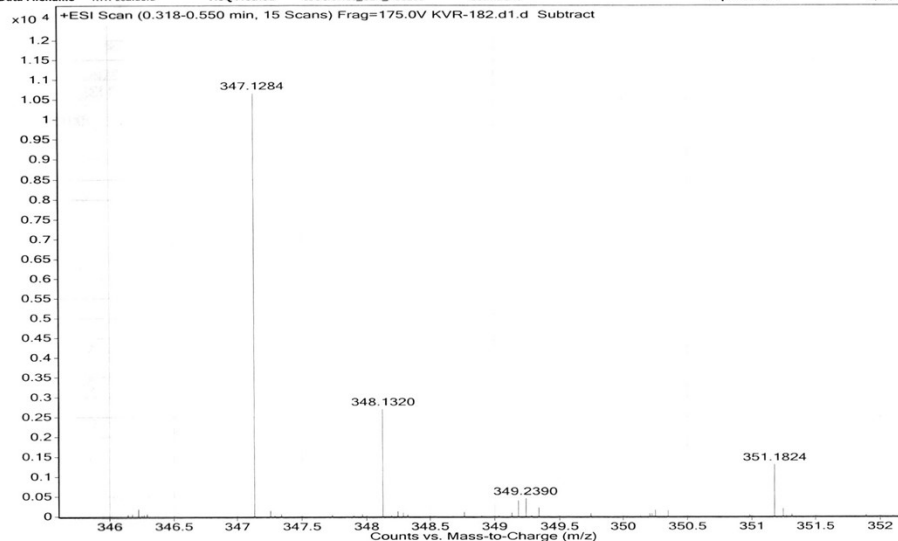
KVR-204

<sup>1</sup>H-NMR spectrum of **18** (300 MHz, CDCl<sub>3</sub>); X = Wax impurity

KVR-182

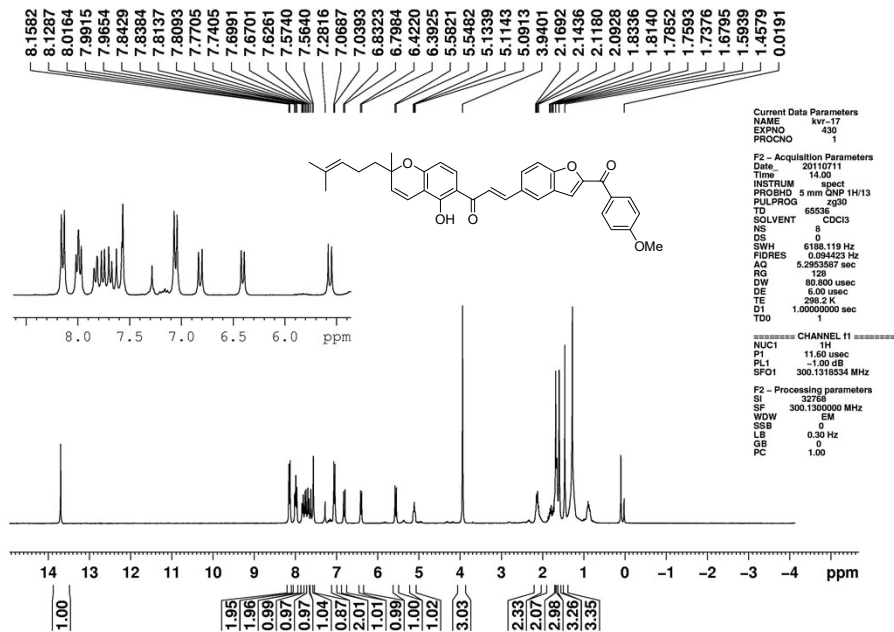
<sup>13</sup>C-NMR spectrum of **18** (50 MHz, CDCl<sub>3</sub>); X = Wax impurity

Sample Name SANDEEP Position Vial 47 Instrument Name Instrument 1 User Name  
 Inj Vol 3 InjPosition Sample IRM Calibration Status Success  
 Data Filename KVR-182.d1.d ACQ Method ISOCRATIC\_GEN\_POS200 Comment Acquired Time 7/16/2013 12:33:32 PM

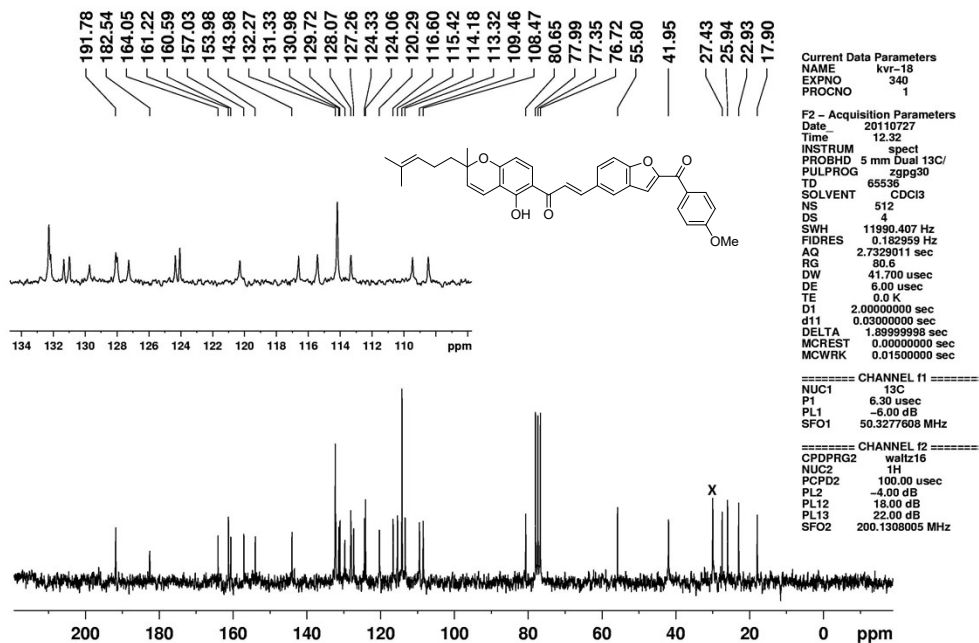


HRMS Spectrum of compound 18

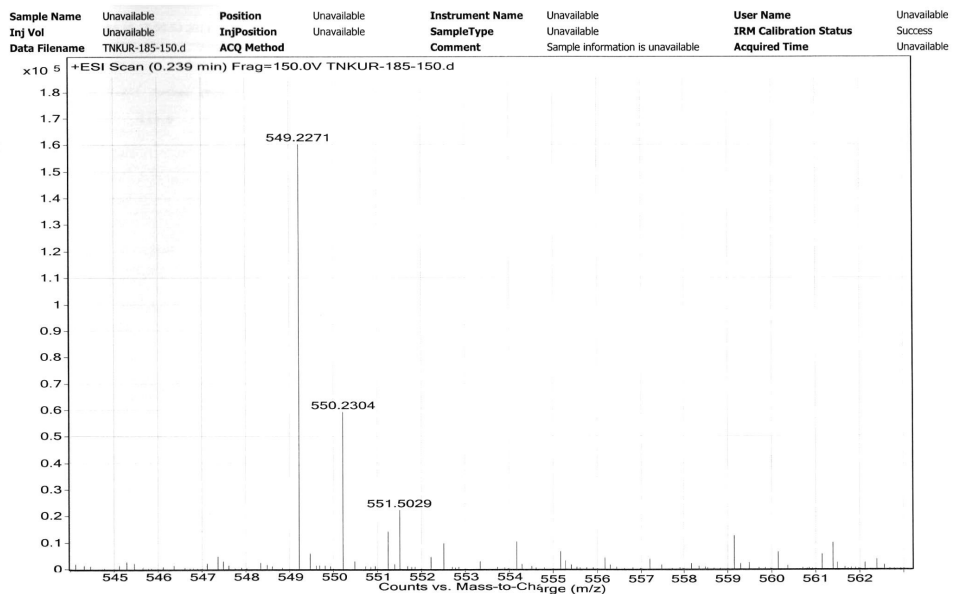
KVR-185



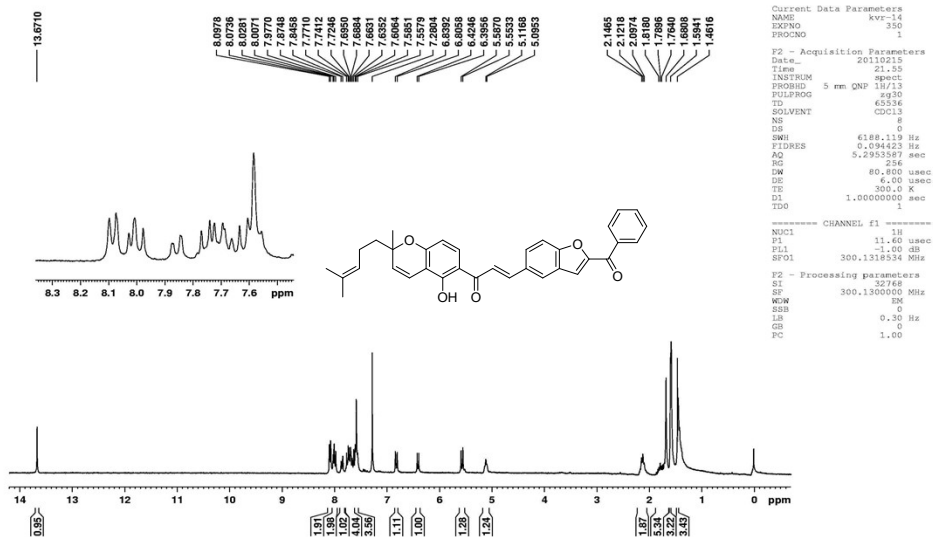
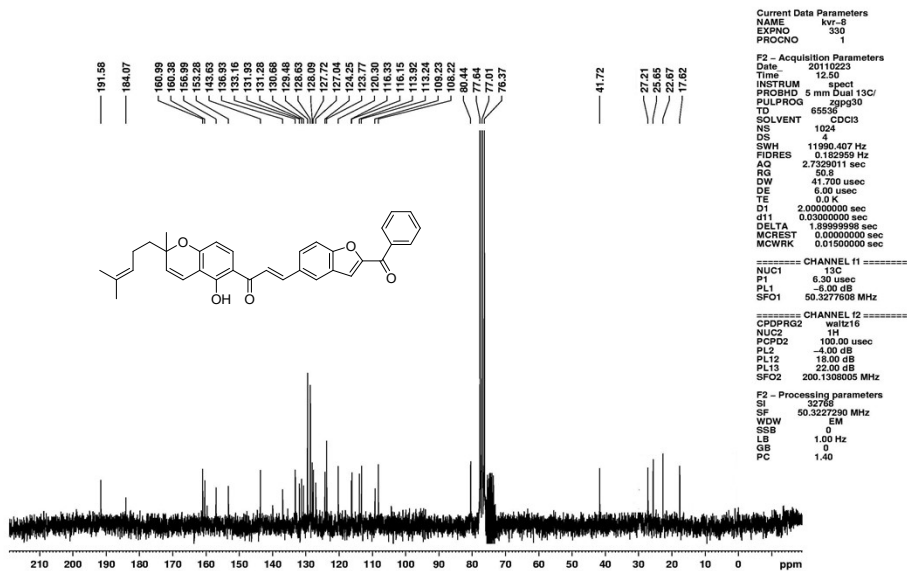
<sup>1</sup>H-NMR spectrum of 19 (300 MHz, CDCl<sub>3</sub>)

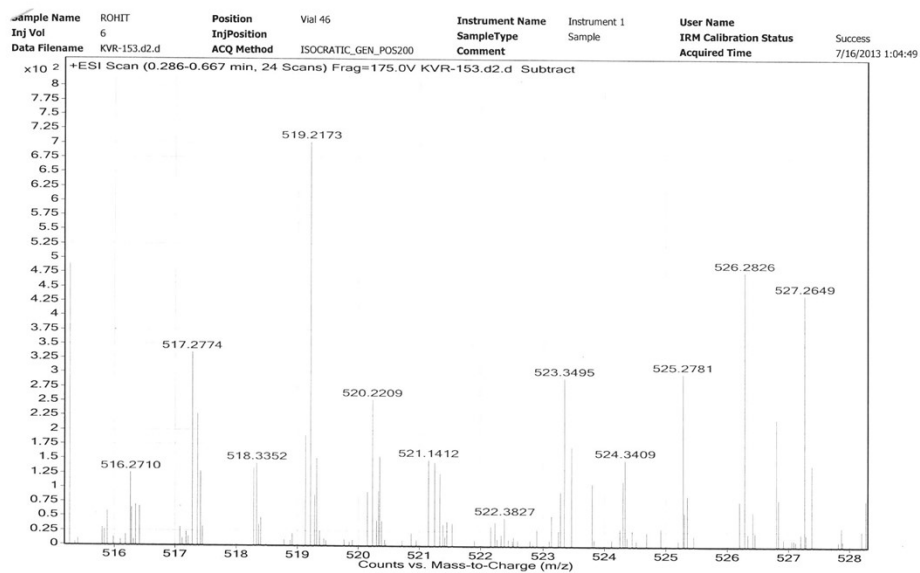


<sup>13</sup>C-NMR spectrum of **19** (50 MHz, CDCl<sub>3</sub>); X = Wax impurity



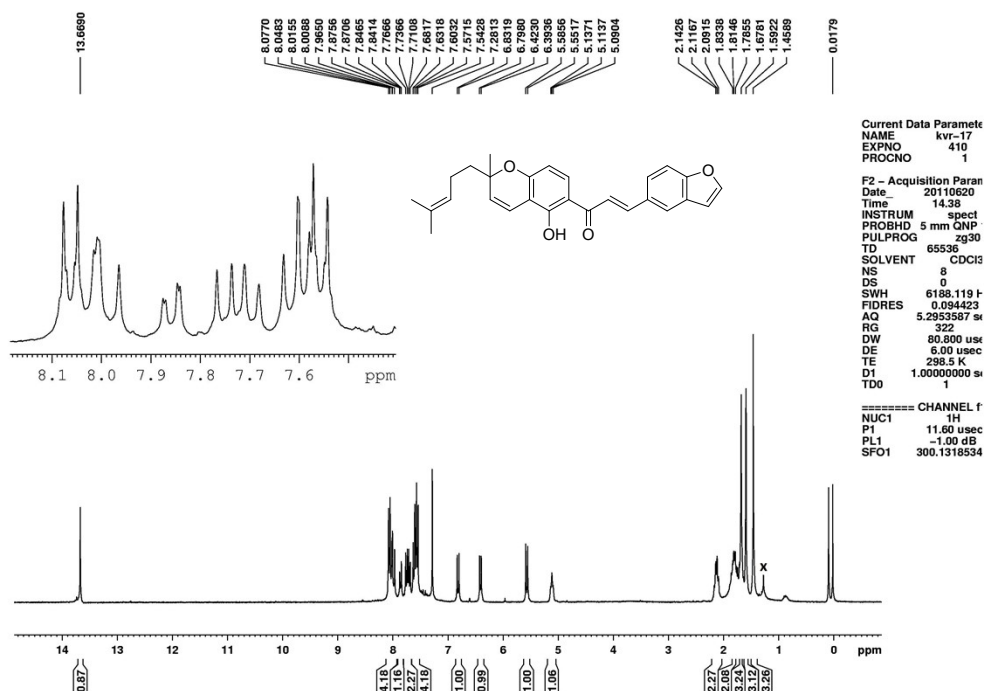
HRMS Spectrum of compound **19**

 $^1\text{H-NMR}$  spectrum of **20** (300 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C-NMR}$  spectrum of **20** (50 MHz,  $\text{CDCl}_3$ )



HRMS Spectrum of compound 20

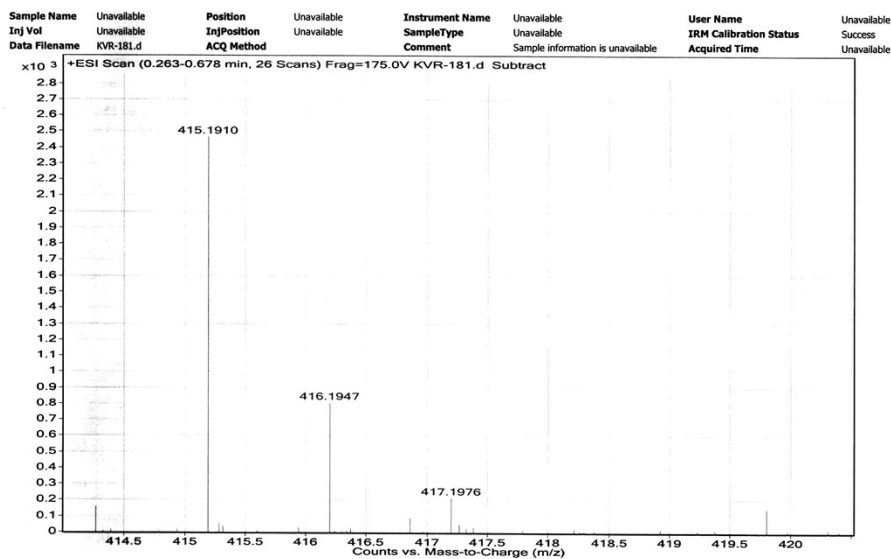
KVR-181



<sup>1</sup>H-NMR spectrum of 21 (300 MHz, CDCl<sub>3</sub>); X = Wax impurity

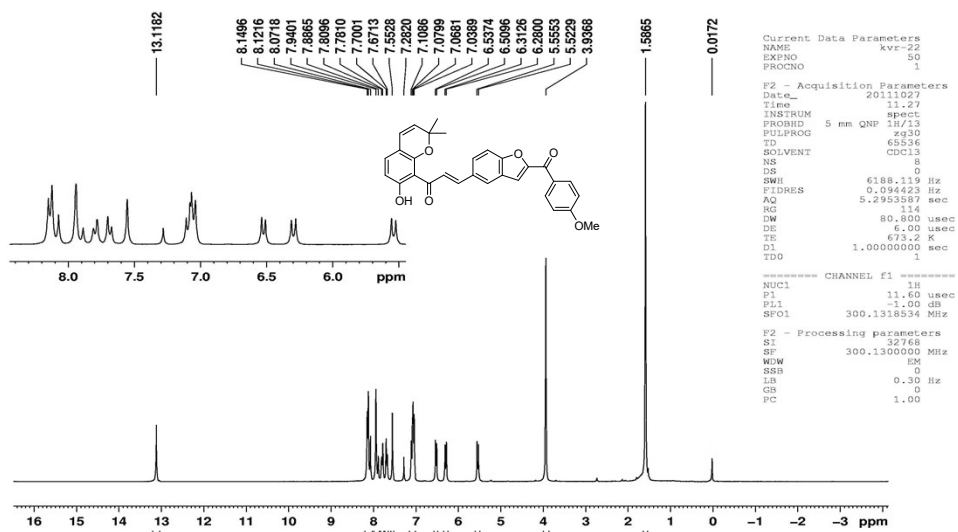


$^{13}\text{C}$ -NMR spectrum of **21** (50 MHz,  $\text{CDCl}_3$ ); X = Wax impurity

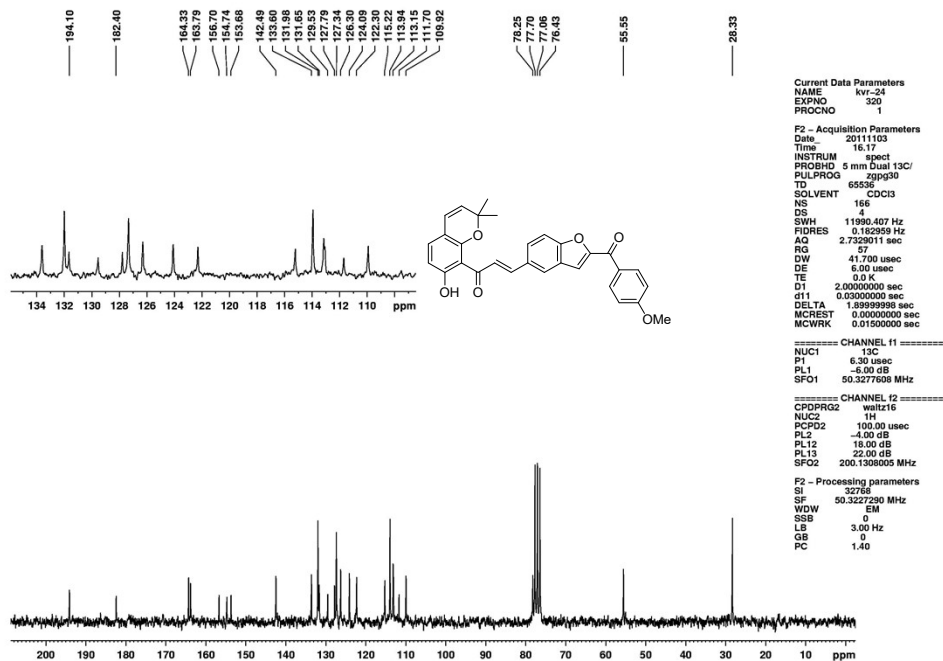


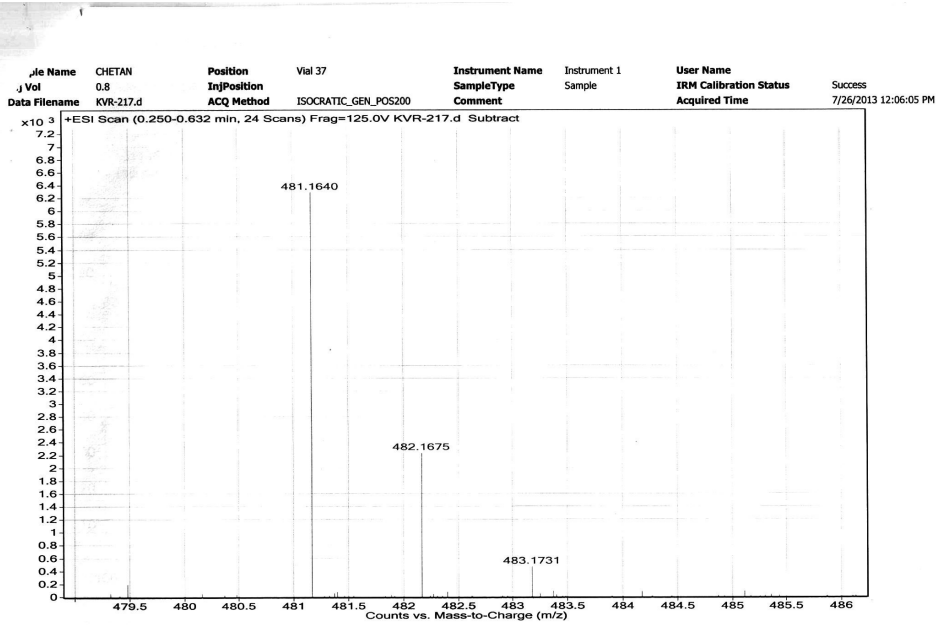
HRMS Spectrum of compound **21**

KVR-217

<sup>1</sup>H-NMR spectrum of **22** (300 MHz, CDCl<sub>3</sub>)

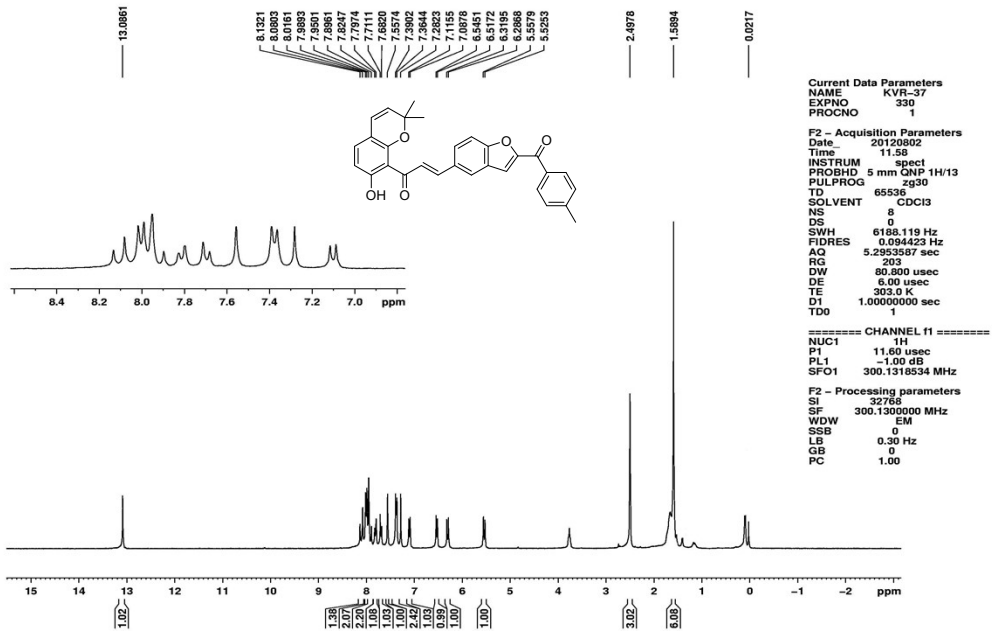
KVR-217

<sup>13</sup>C-NMR spectrum of **22** (50 MHz, CDCl<sub>3</sub>)



HRMS Spectrum of compound 22

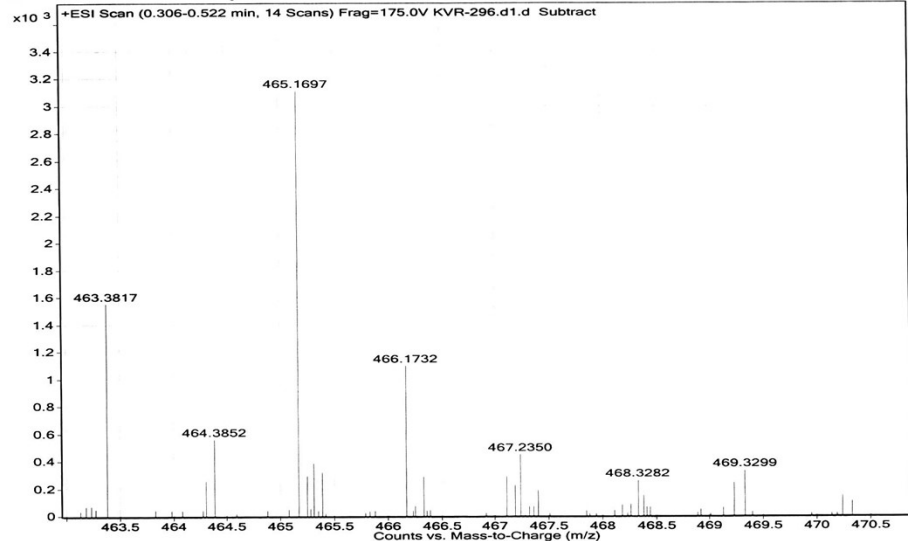
KVR 293



<sup>1</sup>H-NMR spectrum of 23 (300 MHz, CDCl<sub>3</sub>)

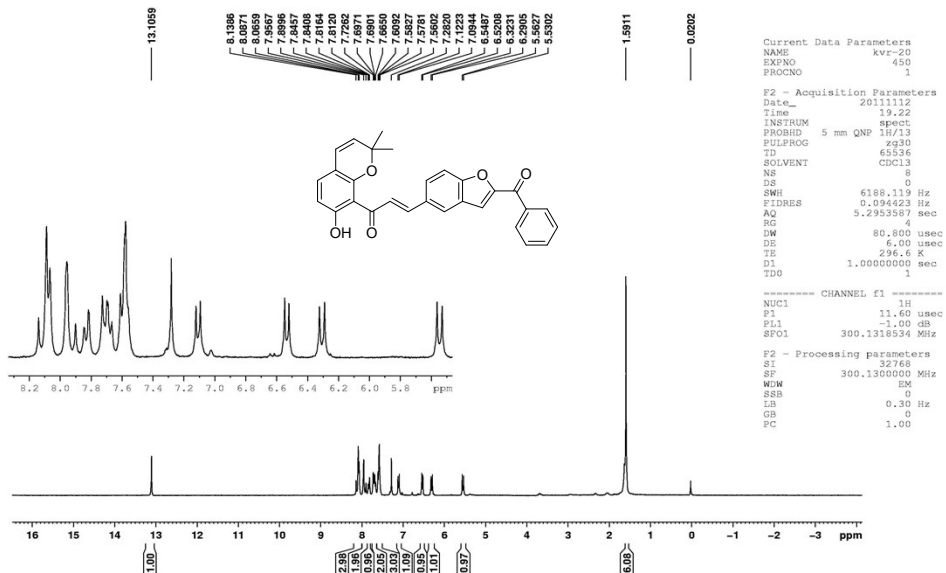


Sample Name	ROHIT	Position	Vial 38	Instrument Name	Instrument 1	User Name	Success
Inj Vol	3	InjPosition		SampleType	Sample	IRM Calibration Status	7/16/2013 11:51:06 AM
Data Filename	KVR-296.d1.d	ACQ Method	ISOCRATIC_GEN_POS200	Comment		Acquired Time	



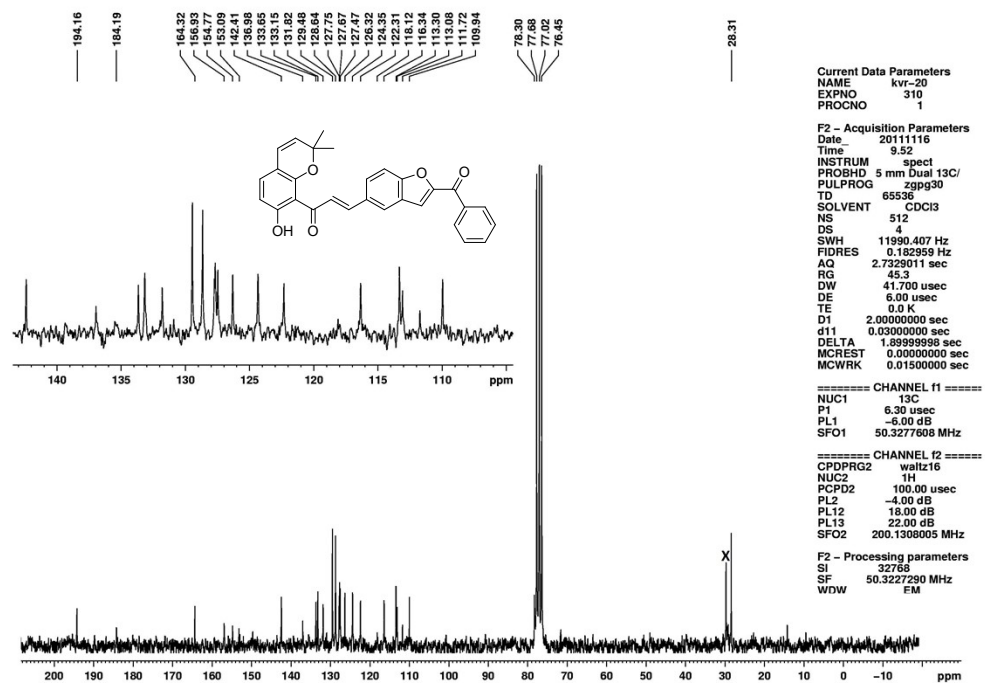
HRMS Spectrum of compound **23**

KVR-208A

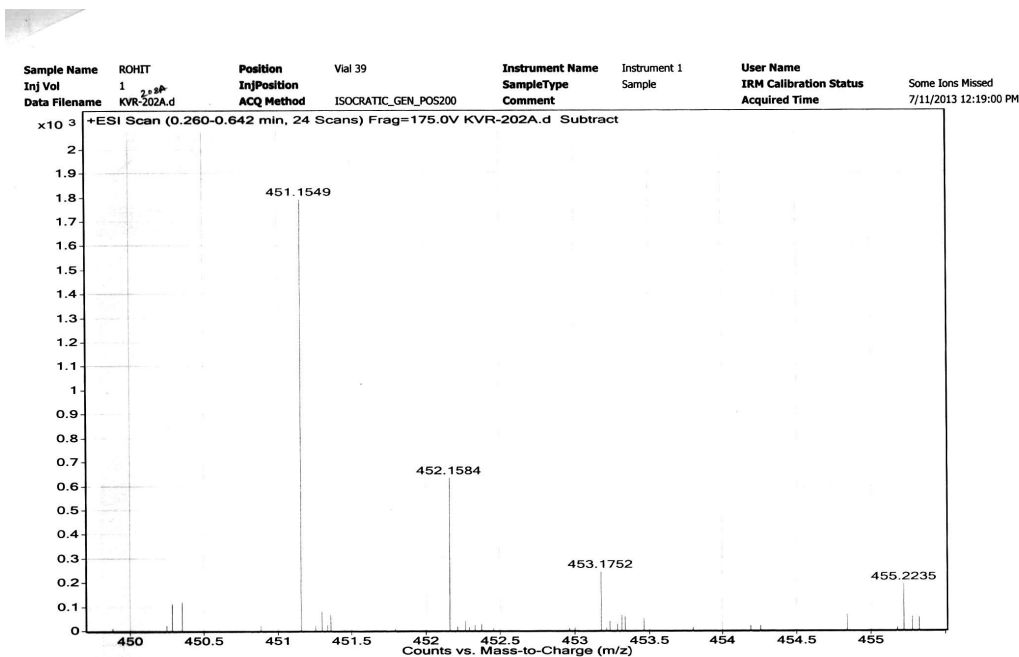


$^1\text{H-NMR}$  spectrum of **24** (300 MHz,  $\text{CDCl}_3$ )

KVR-208A

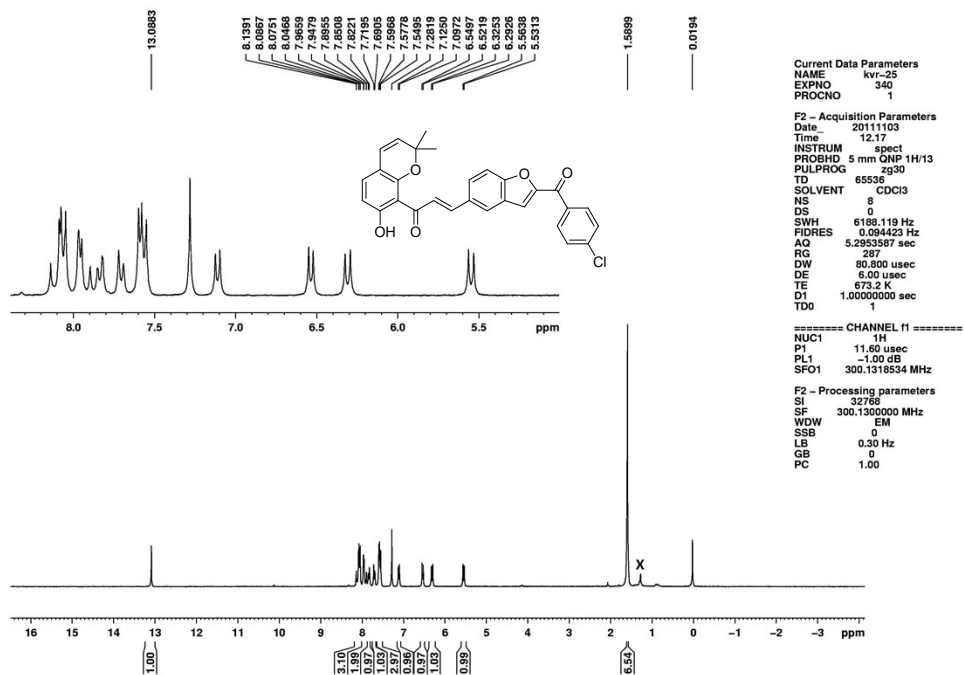


$^{13}\text{C}$ -NMR spectrum of **24** (50 MHz,  $\text{CDCl}_3$ ); X = Wax impurity

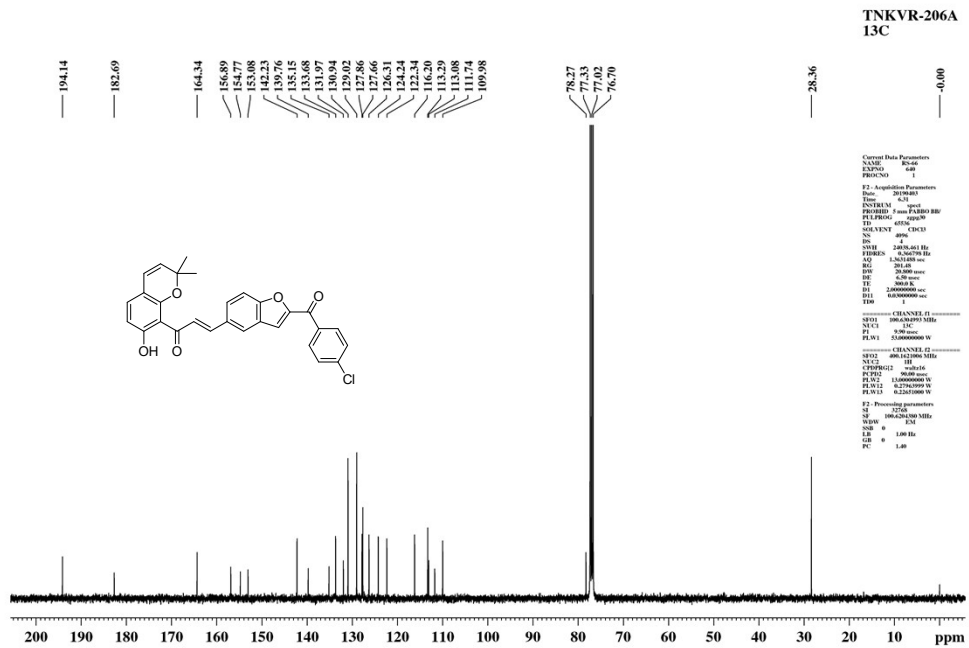


HRMS Spectrum of compound **24**

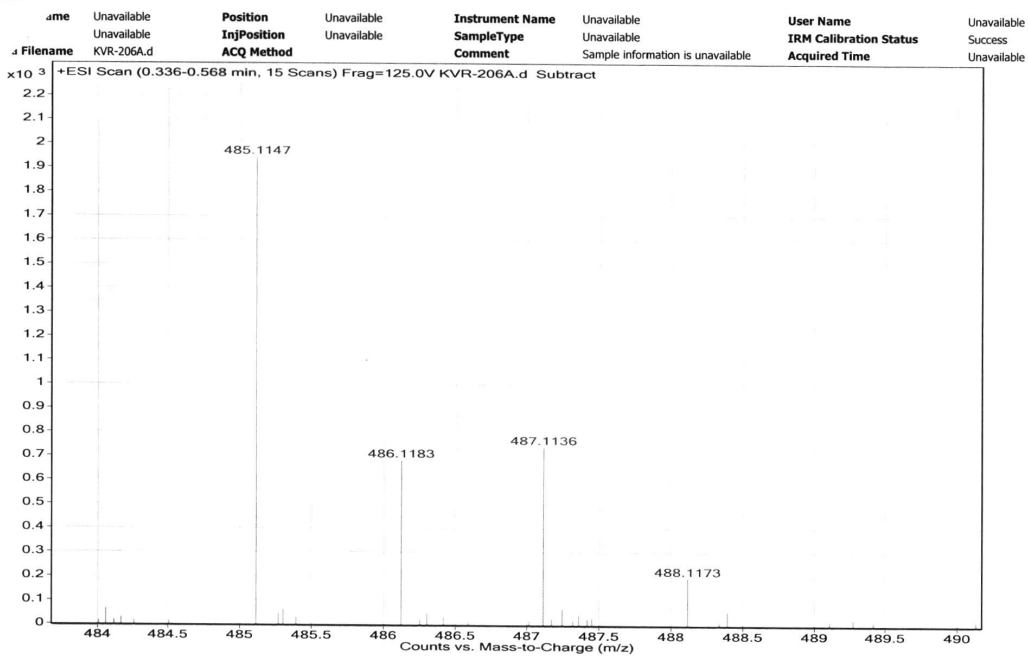
KVR-206A



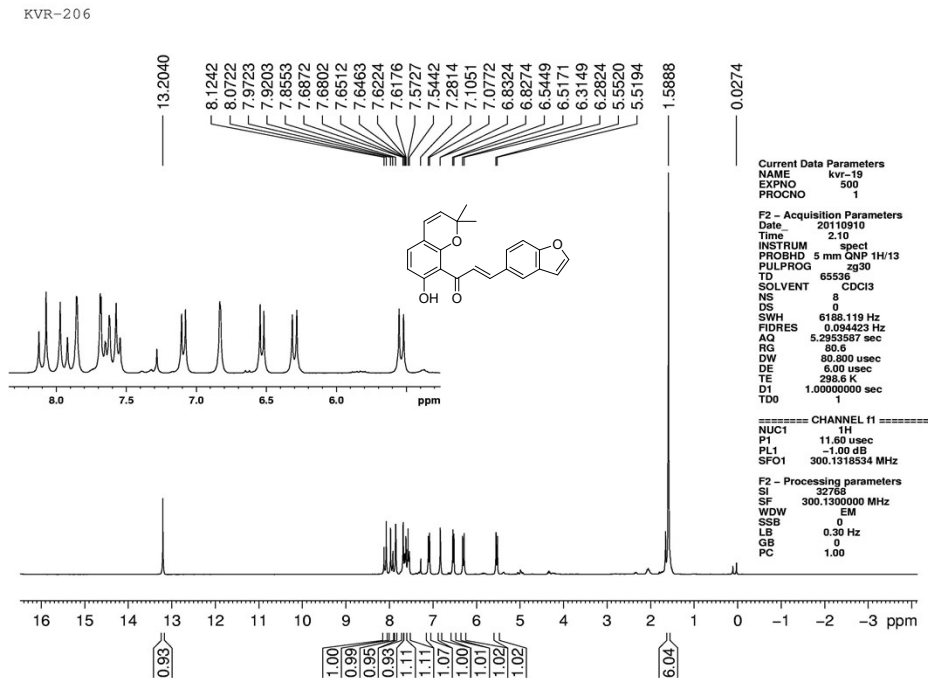
$^1\text{H-NMR}$  spectrum of **25** (300 MHz,  $\text{CDCl}_3$ ); X = Wax impurity



$^{13}\text{C-NMR}$  spectrum of **25** (100 MHz,  $\text{CDCl}_3$ )

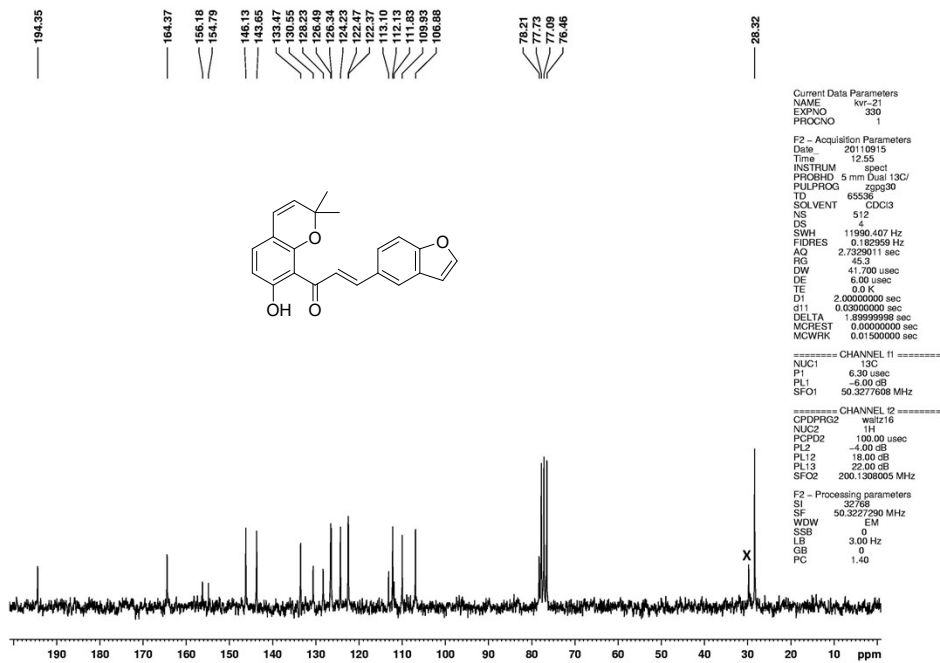


HRMS Spectrum of compound 25



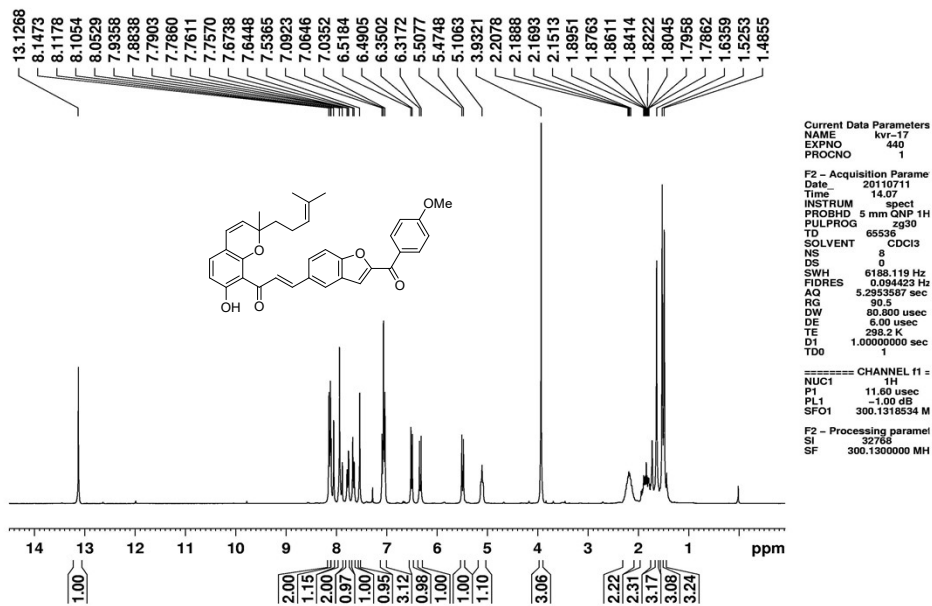
<sup>1</sup>H-NMR spectrum of 26 (300 MHz, CDCl<sub>3</sub>)

KVR-206



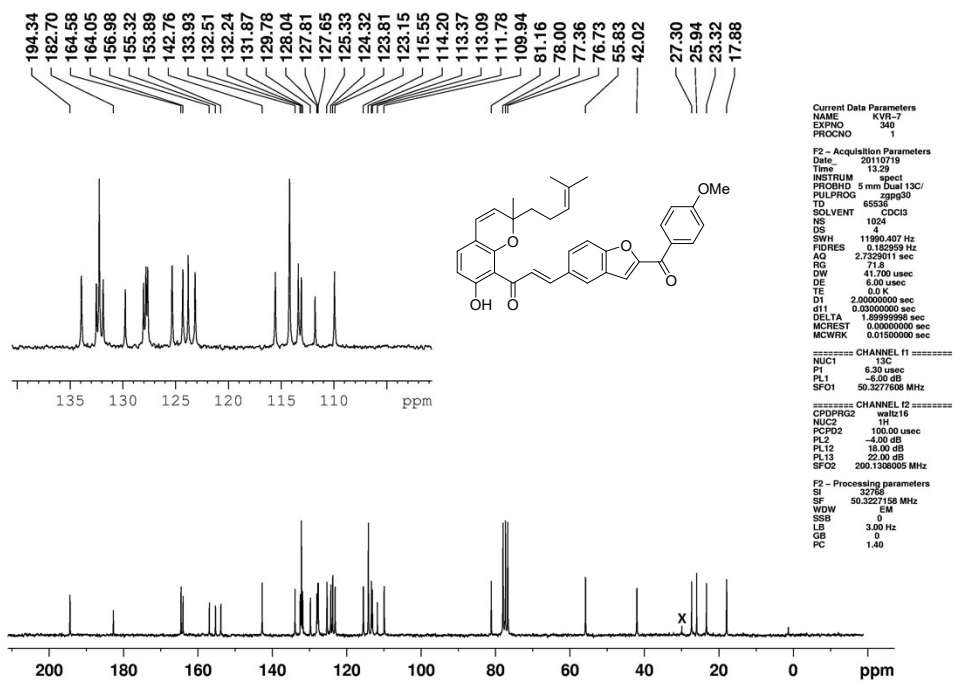
<sup>13</sup>C-NMR spectrum of **26** (50 MHz, CDCl<sub>3</sub>); X = Wax impurity

KVR-186

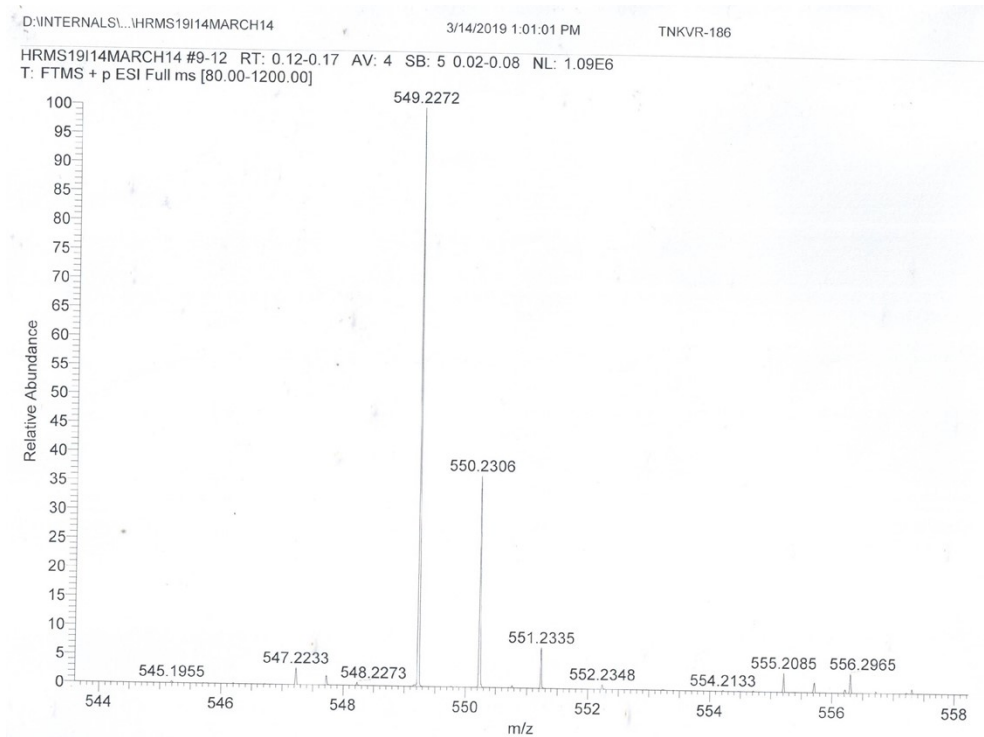


<sup>1</sup>H-NMR spectrum of **27** (300 MHz, CDCl<sub>3</sub>)  
 S-29

KVR-186

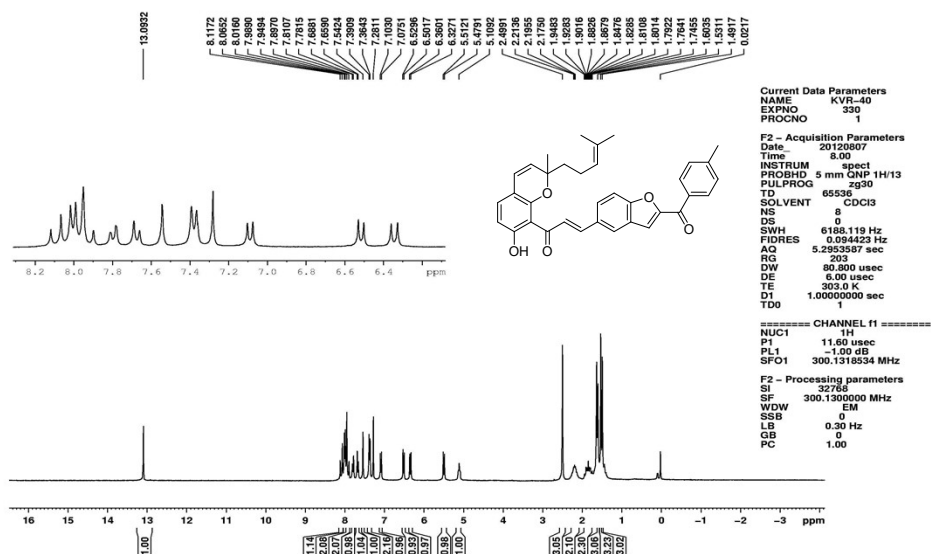


<sup>13</sup>C-NMR spectrum of **27** (50 MHz, CDCl<sub>3</sub>); X = Wax impurity



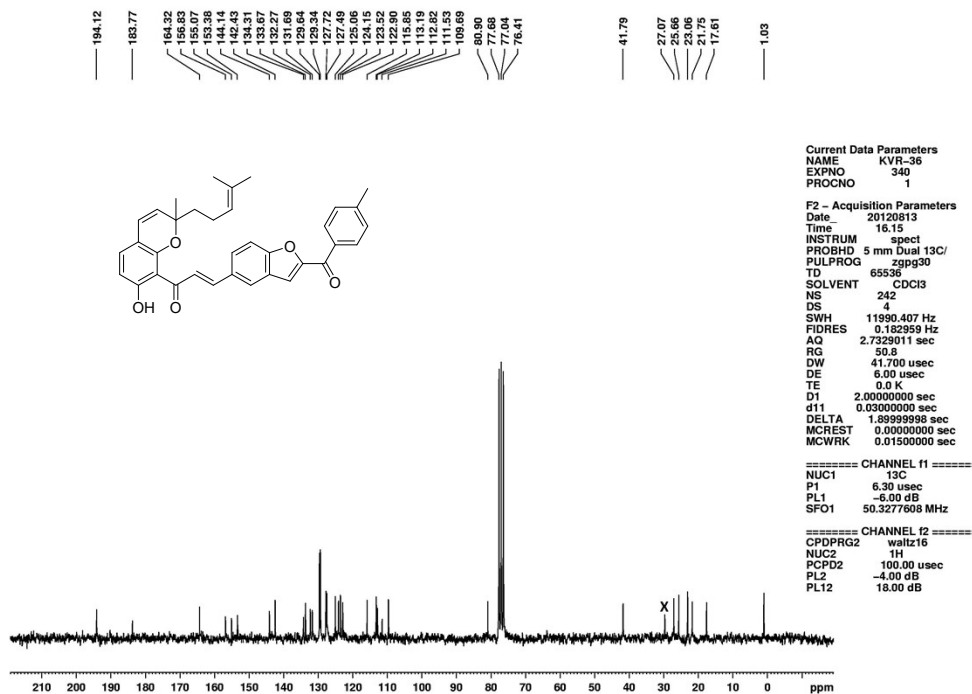
HRMS Spectrum of compound **27**

KVR-294



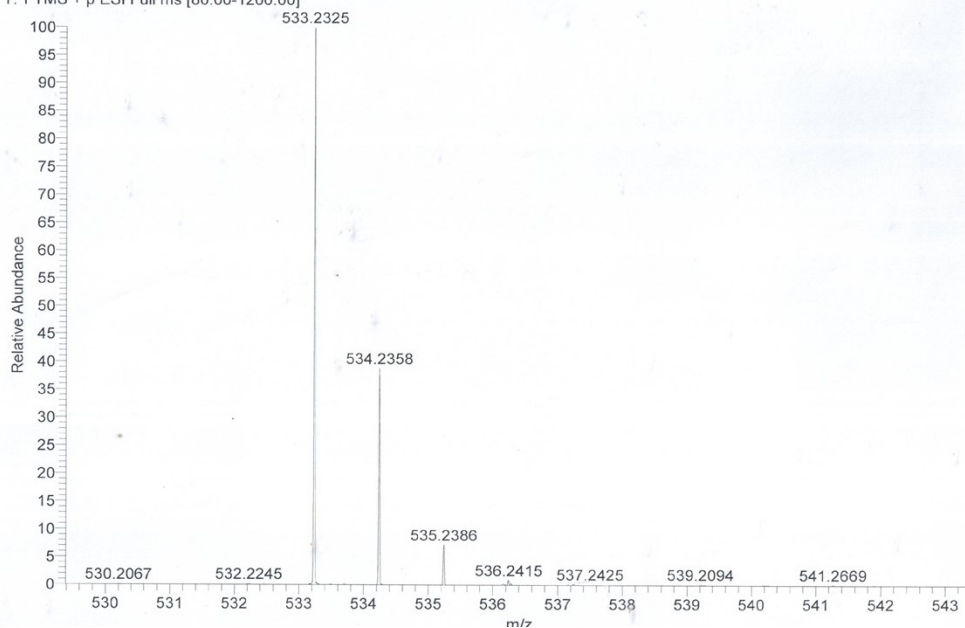
<sup>1</sup>H-NMR spectrum of **28** (300 MHz, CDCl<sub>3</sub>)

KVR-294



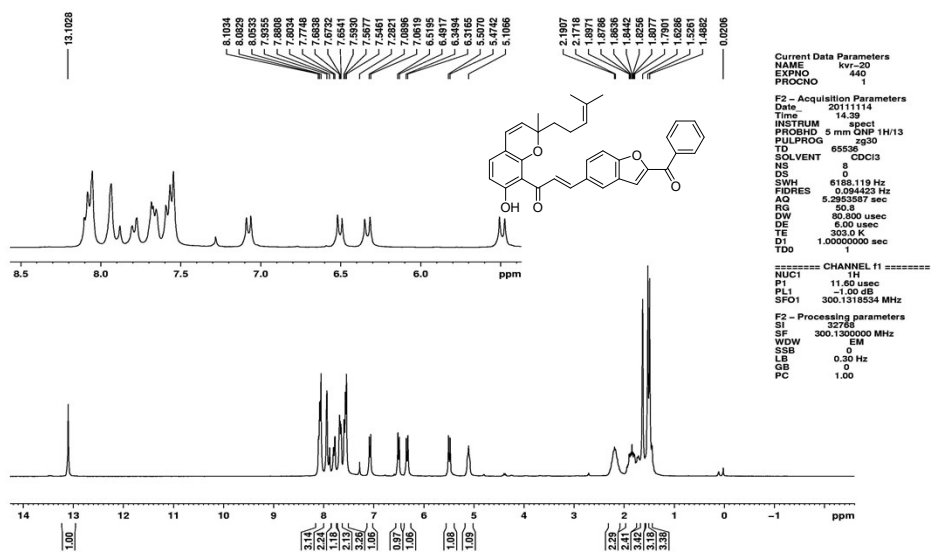
<sup>13</sup>C-NMR spectrum of **28** (50 MHz, CDCl<sub>3</sub>); X = Wax impurity

HRMS19114MARCH16 #10 RT: 0.14 AV: 1 SB: 5 0.02-0.08 NL: 2.51E6  
T: FTMS + p ESI Full ms [80.00-1200.00]



HRMS Spectrum of compound 28

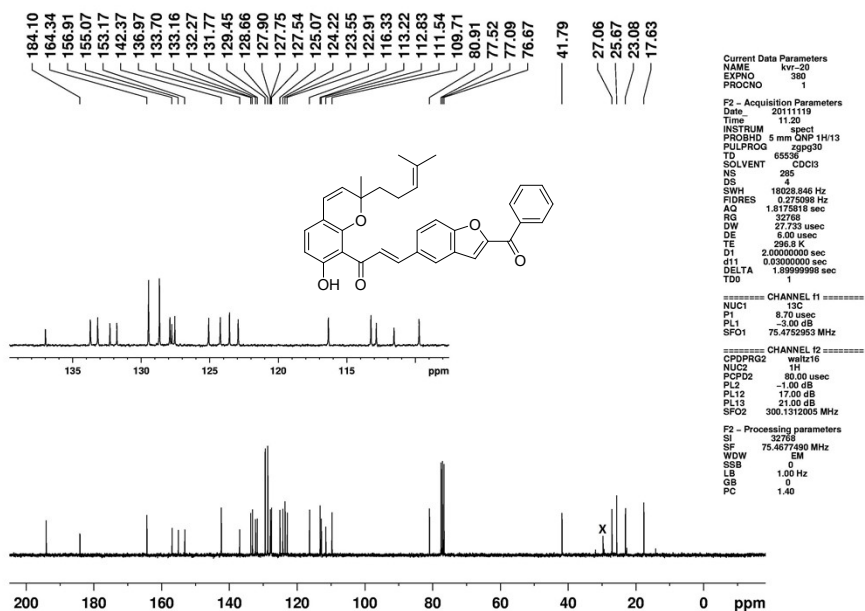
KVR-209A



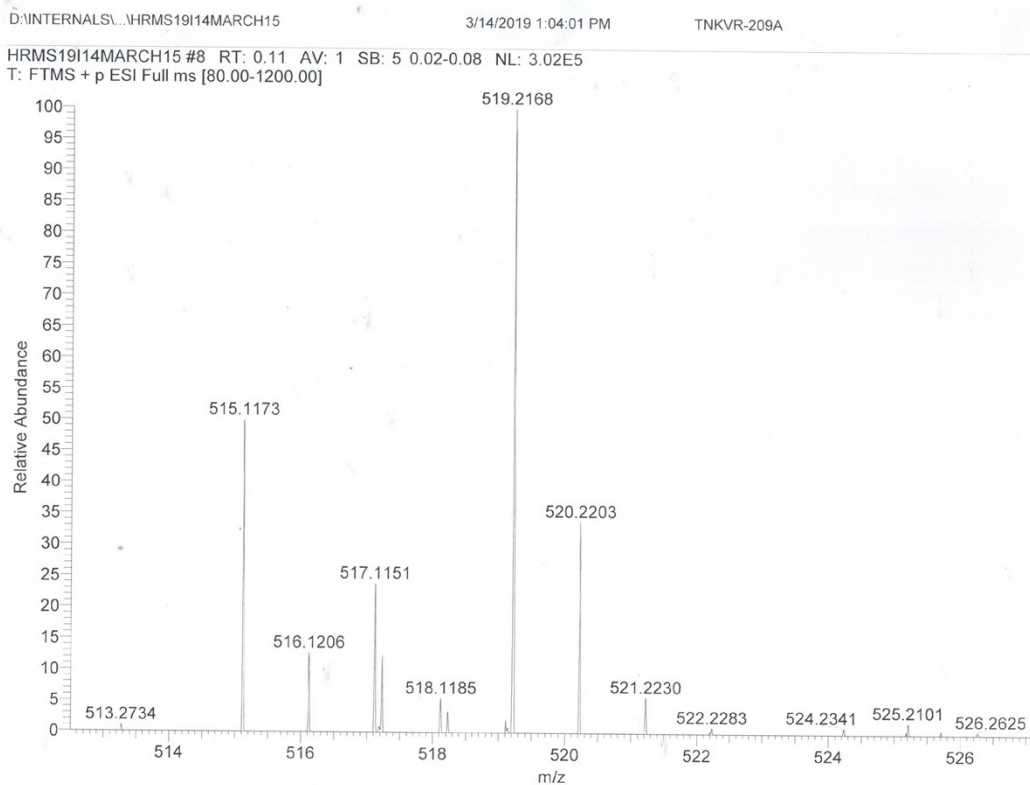
<sup>1</sup>H-NMR spectrum of 29 (300 MHz, CDCl<sub>3</sub>)



KVR-209A

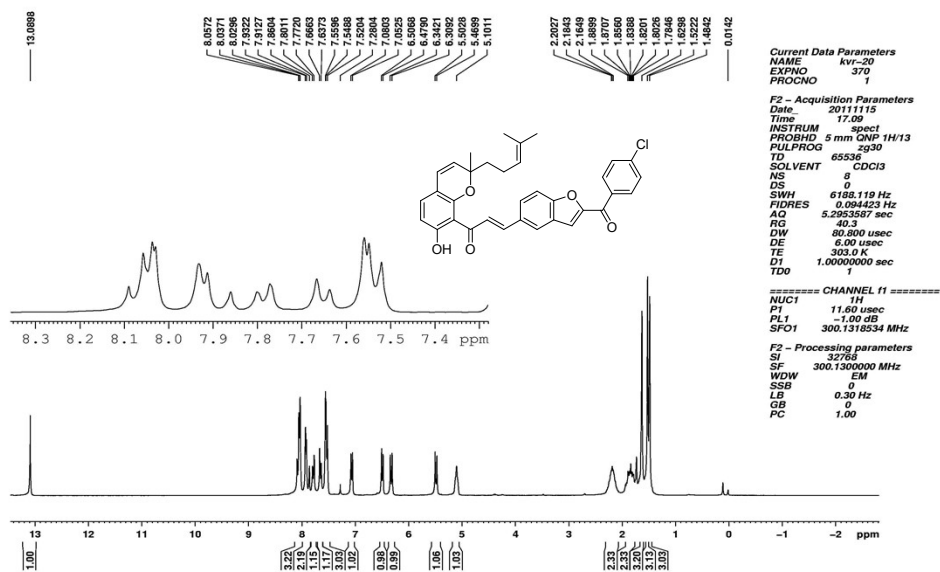


$^{13}\text{C}$ -NMR spectrum of **29** (50 MHz,  $\text{CDCl}_3$ ); X = Wax impurity



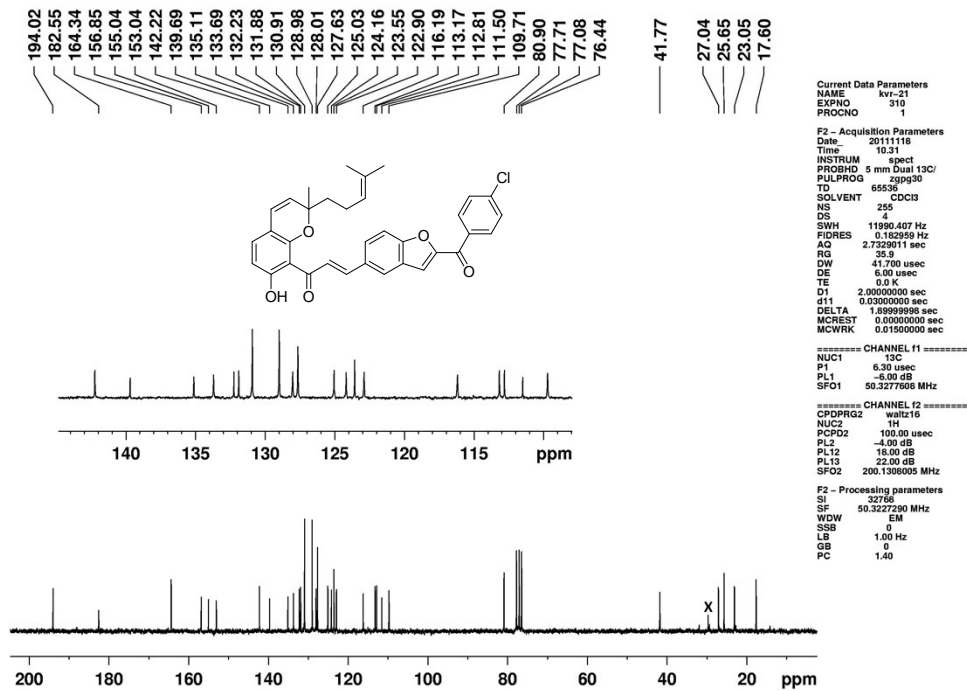
HRMS Spectrum of compound **29**

KVR-202



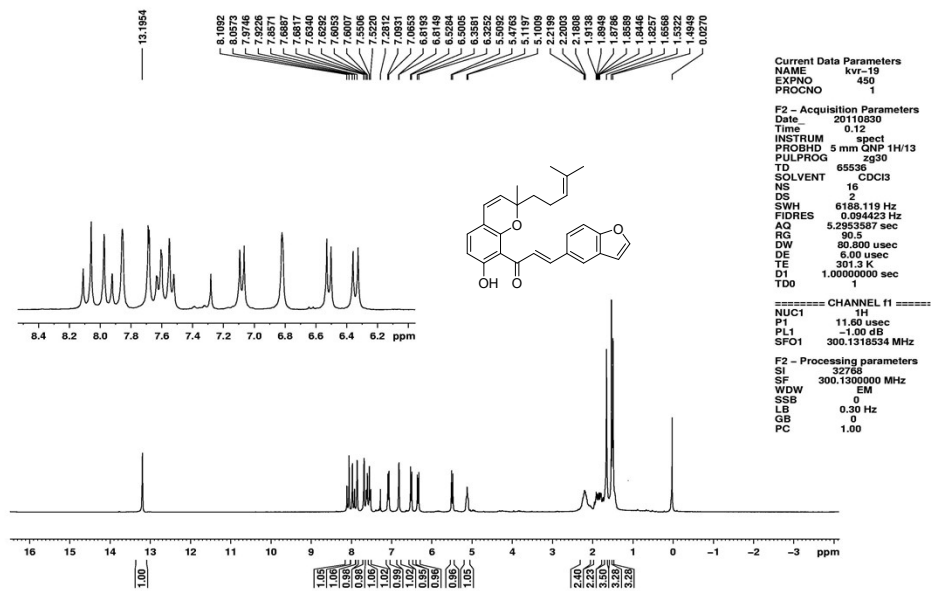
<sup>1</sup>H-NMR spectrum of **30** (300 MHz, CDCl<sub>3</sub>)

KVR-202



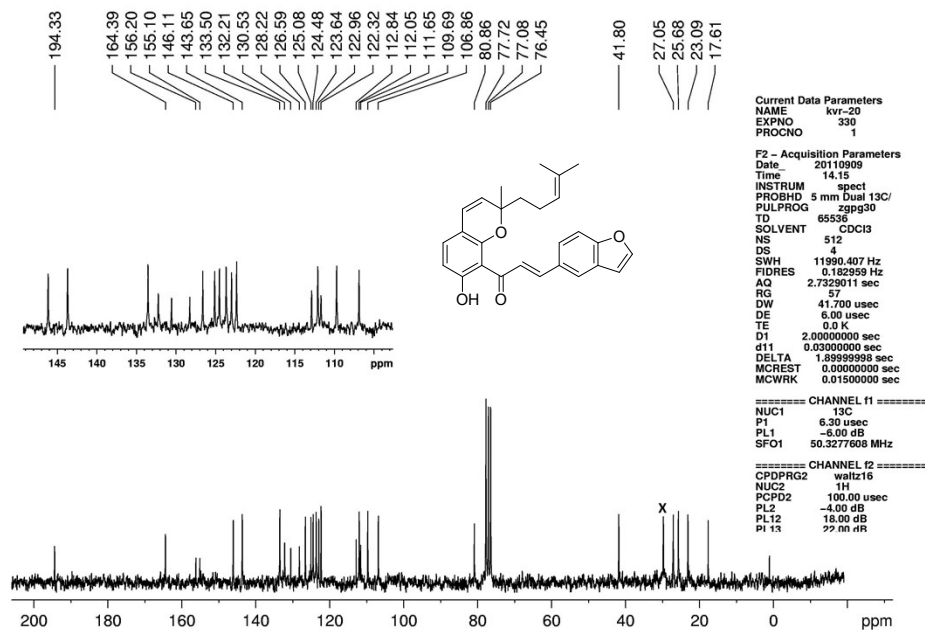
<sup>13</sup>C-NMR spectrum of **30** (50 MHz, CDCl<sub>3</sub>); X = Wax impurity

KVR-202A

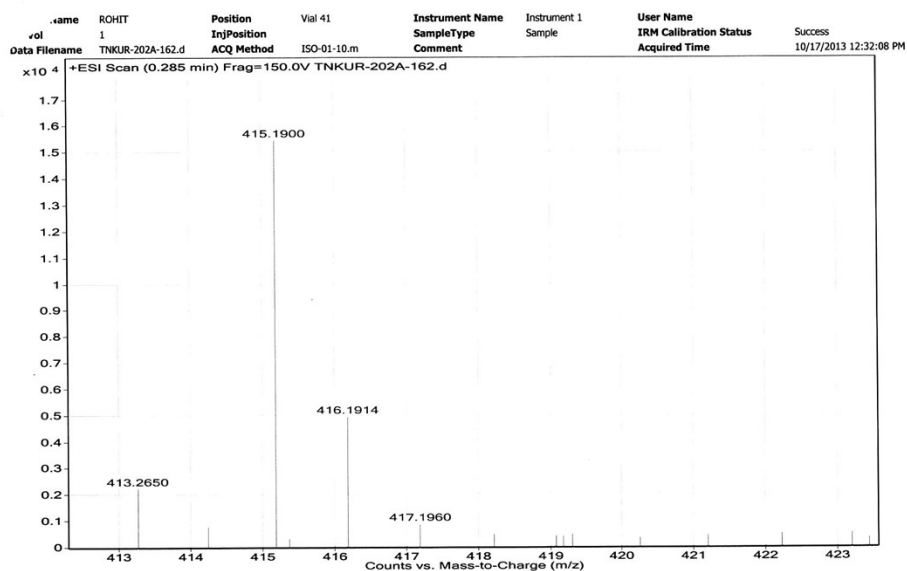


<sup>1</sup>H-NMR spectrum of **31** (300 MHz, CDCl<sub>3</sub>)

KVR-202A

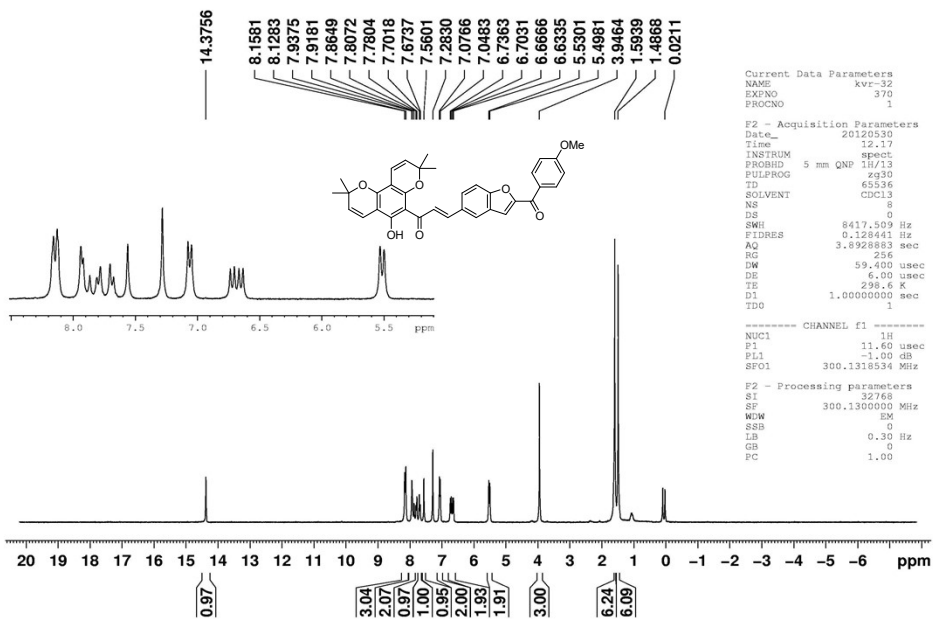


<sup>13</sup>C-NMR spectrum of **31** (50 MHz, CDCl<sub>3</sub>); X = Wax impurity



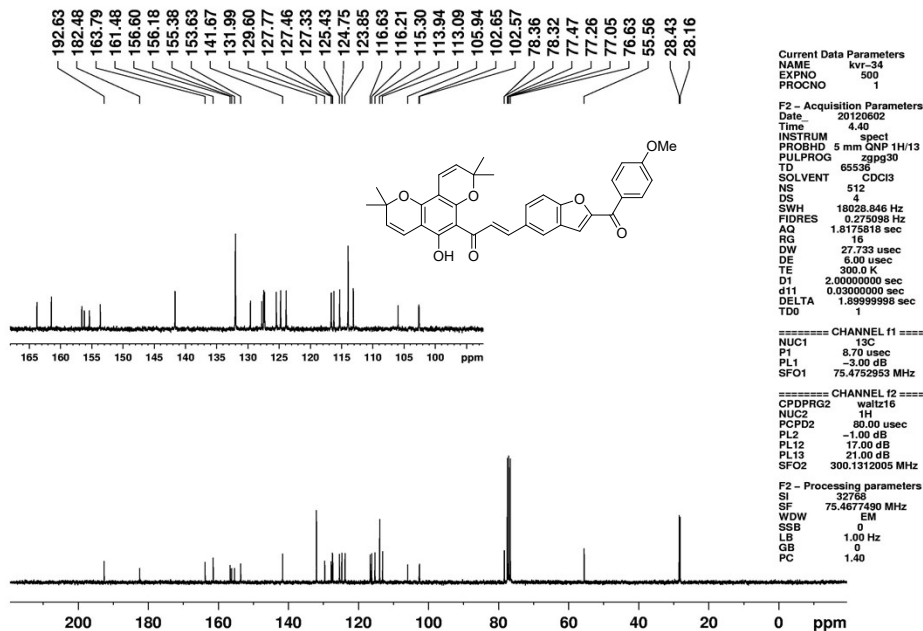
HRMS Spectrum of compound 31

KVR-270



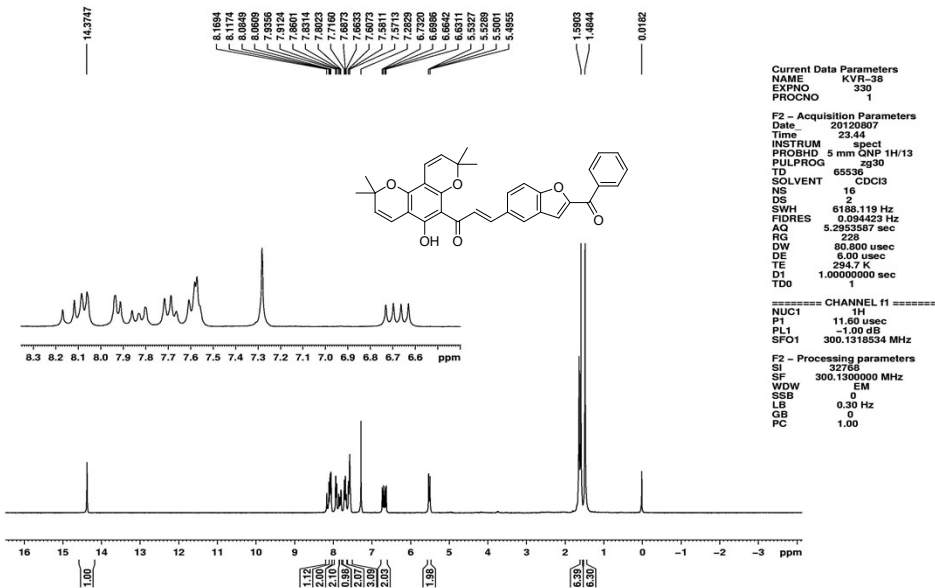
<sup>1</sup>H-NMR spectrum of 32 (300 MHz, CDCl<sub>3</sub>)

KVR-270



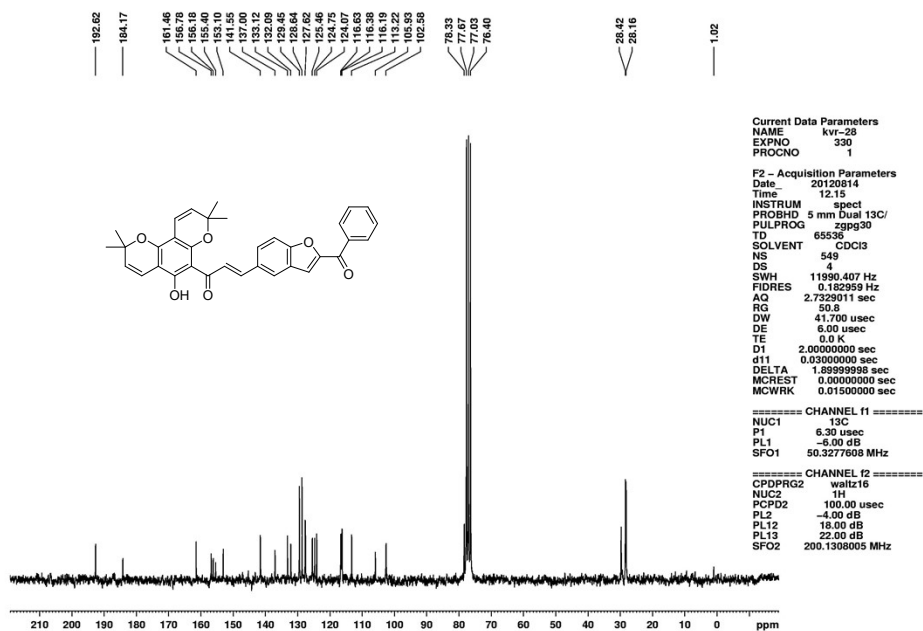
<sup>13</sup>C-NMR spectrum of **32** (50 MHz, CDCl<sub>3</sub>)

KVR-272



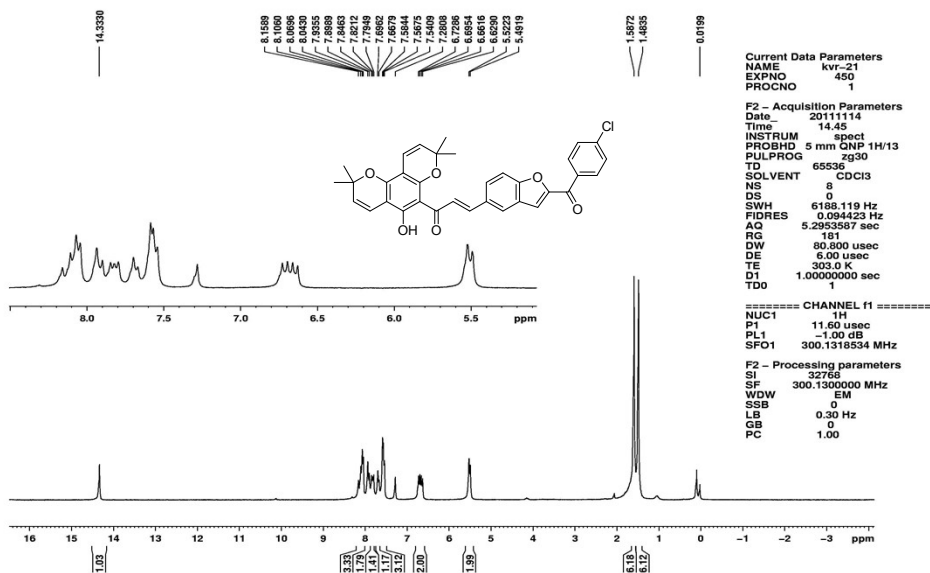
<sup>1</sup>H-NMR spectrum of **33** (300 MHz, CDCl<sub>3</sub>)

KVR-272

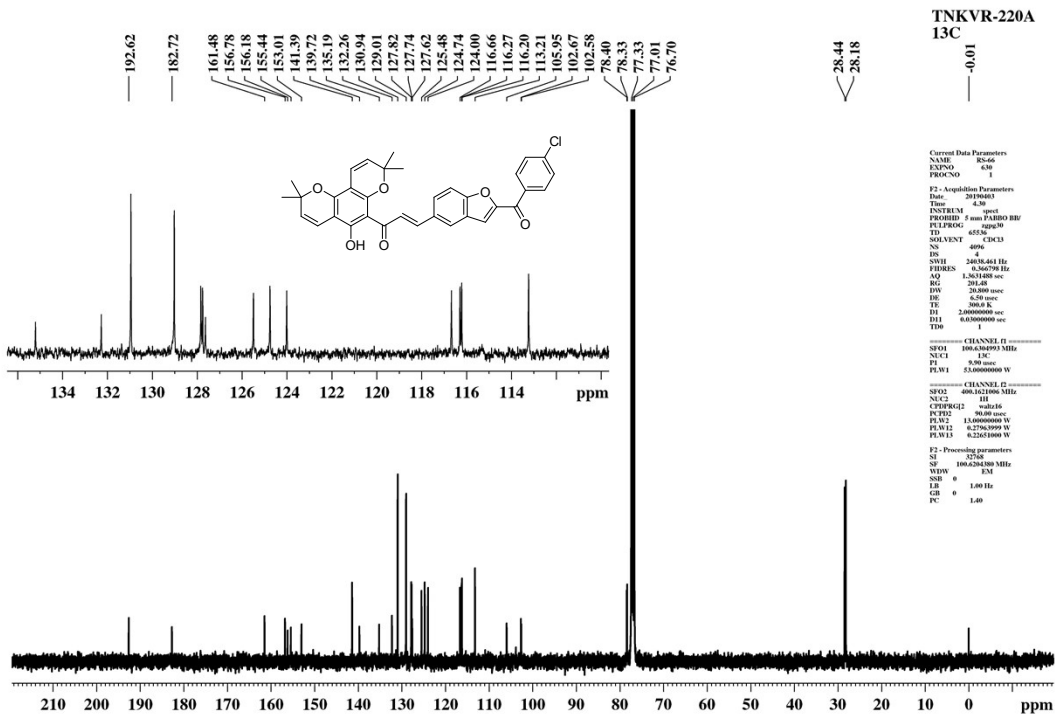


<sup>13</sup>C-NMR spectrum of **33** (50 MHz, CDCl<sub>3</sub>)

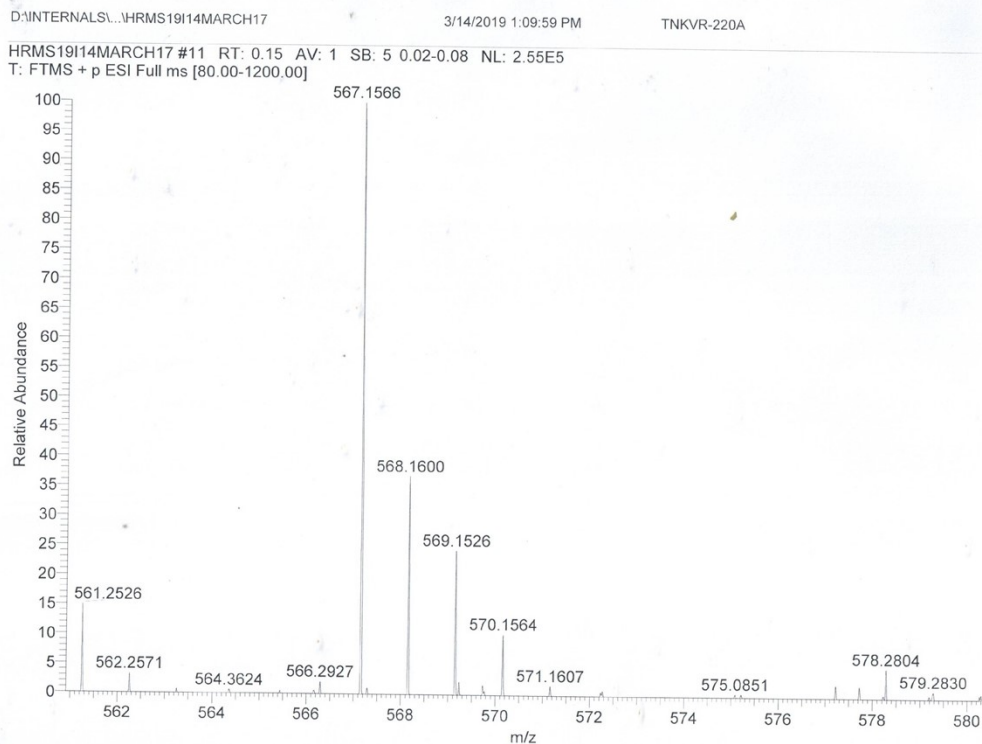
KVR-220A



<sup>1</sup>H-NMR spectrum of **34** (300 MHz, CDCl<sub>3</sub>)

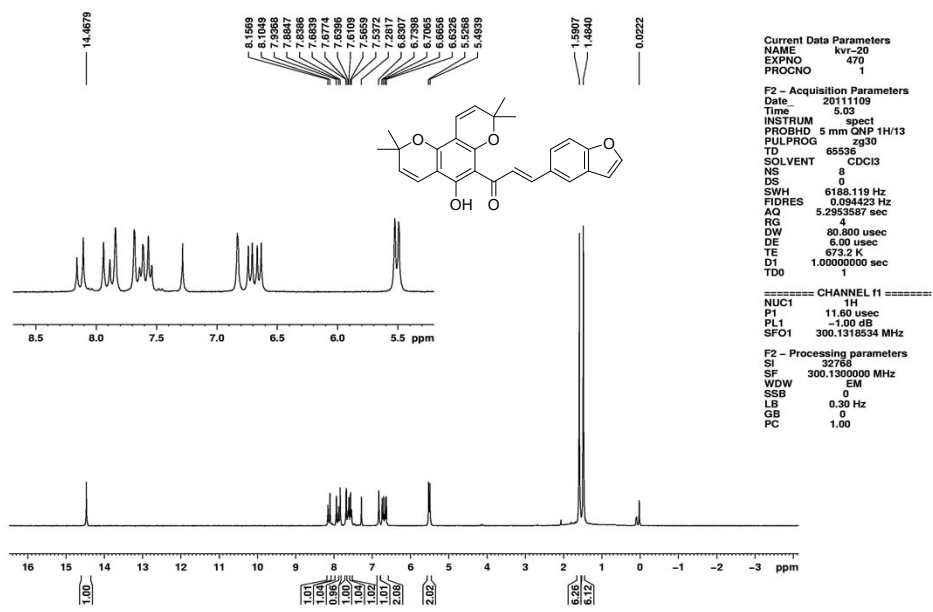


<sup>13</sup>C-NMR spectrum of **34** (100 MHz, CDCl<sub>3</sub>)

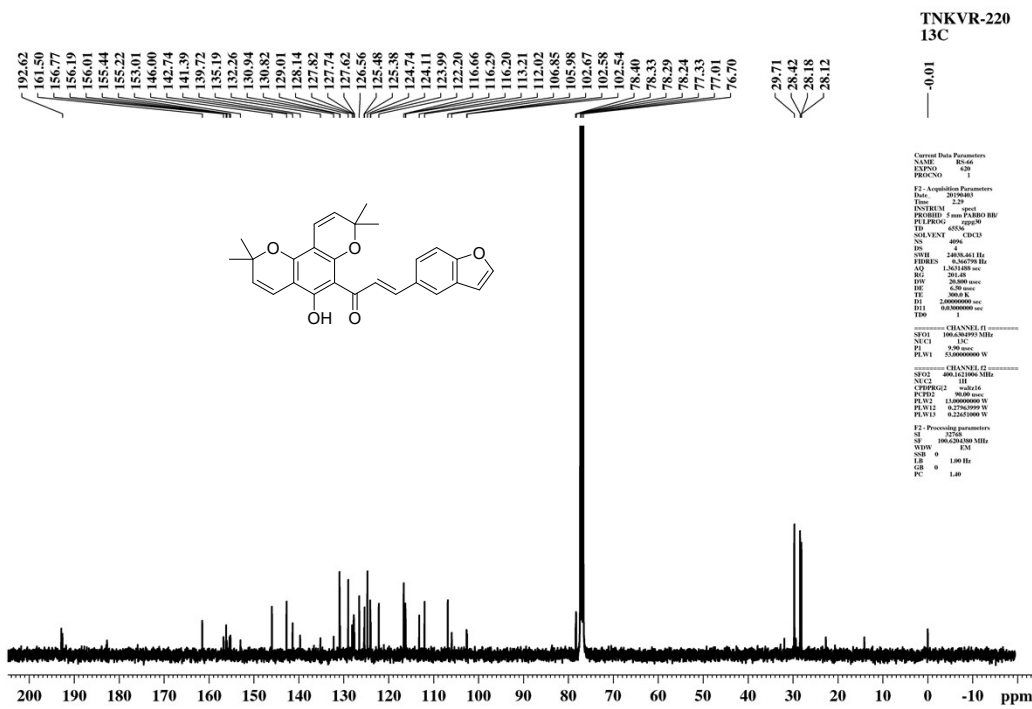


HRMS Spectrum of compound **34**

KVR-220



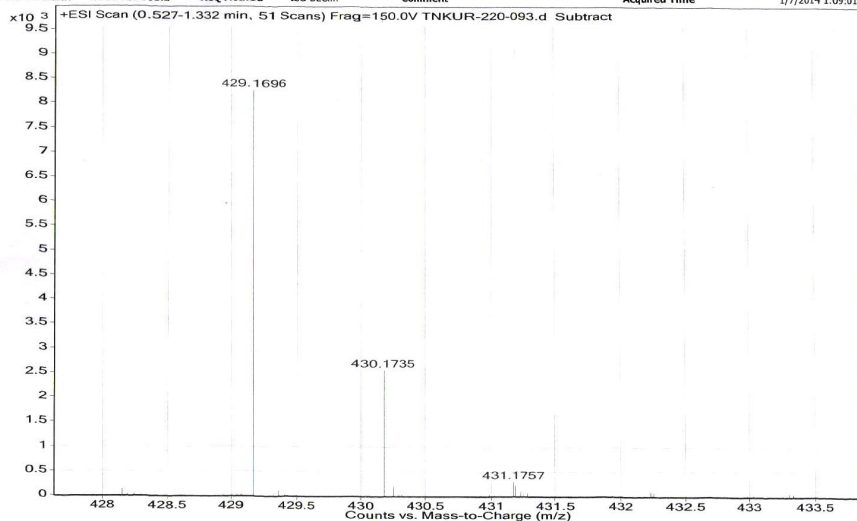
<sup>1</sup>H-NMR spectrum of **35** (300 MHz, CDCl<sub>3</sub>)



<sup>13</sup>C-NMR spectrum of **35** (100 MHz, CDCl<sub>3</sub>)

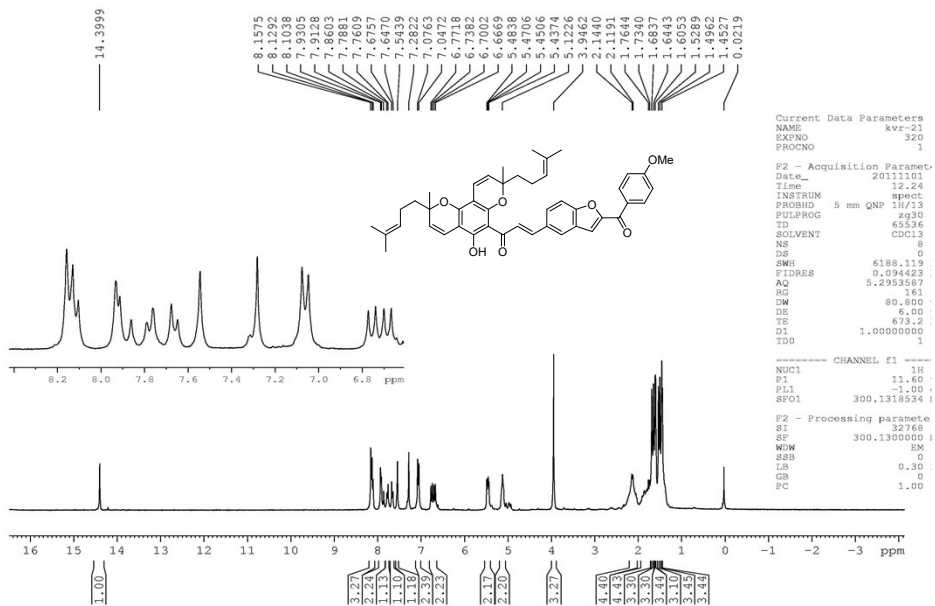


Sample Name	Dr.T. NARENDER	Position	Vial 22	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	TNKUR-220-093.d	ACQ Method	ISO-DEC.m	Comment		Acquired Time	1/7/2014 1:09:01 PM



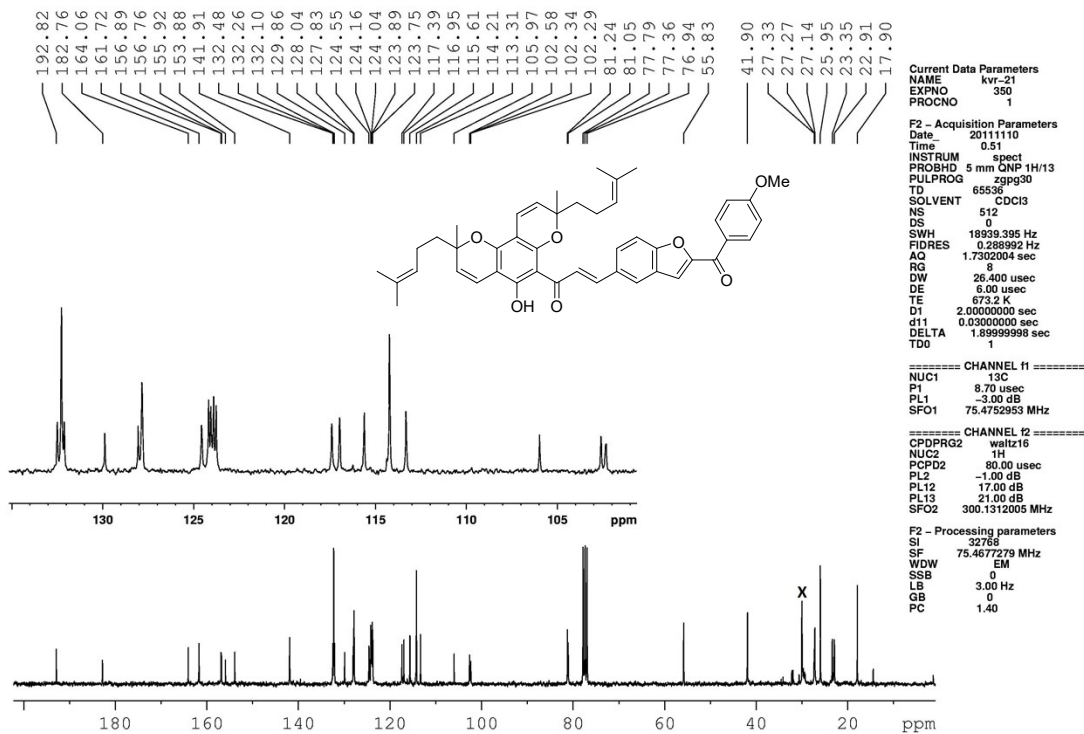
### HRMS Spectrum of compound 35

KVR-218



### <sup>1</sup>H-NMR spectrum of 36 (300 MHz, CDCl<sub>3</sub>)

KVR-218



<sup>13</sup>C-NMR spectrum of **36** (75 MHz, CDCl<sub>3</sub>); X = Wax impurity