Electronic Supplementary Material (ESI) for RSC Advances.

Ionic liquid [Dabco-H][AcO] as a highly efficient and recyclable catalyst for the synthesis of various bisenol derivatives *via* domino Knoevenagel–Michael reaction in aqueous media

Supporting Information

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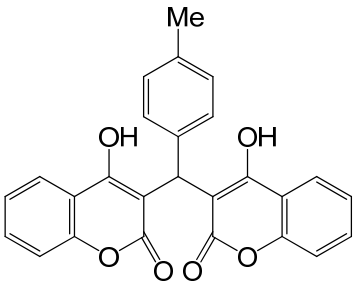
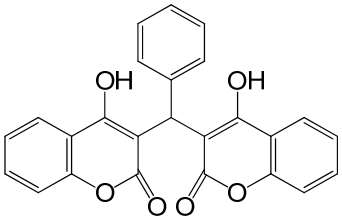
1.0 Data of compounds



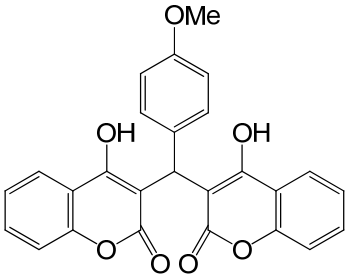
3,3'-(p-tolylmethylene)bis(4-hydroxy-2H-chromen-2-one) (3a)[1]

White solid, mp 265-267 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 2.29 (s, 3H, CH_3), 6.41 (s, 1H, CH), 7.10 (s, 4H, ArH), 7.39 (t, 2H, *J* = 7.6 Hz, ArH), 7.44 (d, 2H, *J* = 8.4 Hz, ArH), 7.66 (t, 2H, *J* = 8.0 Hz, ArH), 7.98 (d, 2H, *J* = 8.0 Hz, ArH), 12.19 (brs, 2H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 20.55, 35.60, 104.47, 116.13, 117.39, 123.87, 124.02, 126.67, 128.83, 132.19, 134.75, 136.01, 152.14, 164.60, 164.98.



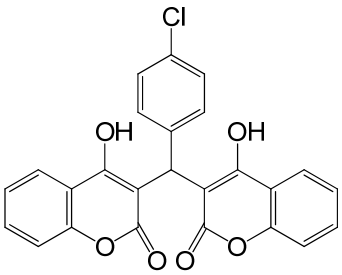
3,3'-(phenylmethylene)bis(4-hydroxy-2H-chromen-2-one) (3b)[1]

White solid, mp 232-234 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 6.61 (s, 1H, CH), 7.34-7.38 (m, 3H, ArH), 7.42-7.44 (m, 2H, ArH), 7.54 (t, 2H, *J* = 7.6 Hz, ArH), 7.59 (d, 2H, *J* = 8.0 Hz, ArH), 7.80 (t, 2H, *J* = 7.2 Hz, ArH), 8.13 (d, 2H, *J* = 7.6 Hz, ArH), 12.53 (brs, 2H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 36.08, 104.44, 116.23, 117.60, 124.02, 124.10, 125.91, 126.87, 128.32, 132.29, 139.45, 152.30, 164.92, 165.09.



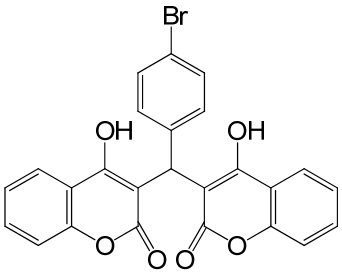
3,3'-((4-methoxyphenyl)methylene)bis(4-hydroxy-2H-chromen-2-one) (3c)[1]

White solid, mp 225-226 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 3.89 (s, 3H, CH_3), 6.52 (s, 1H, CH), 7.01 (d, 2H, *J* = 8.8 Hz, ArH), 7.27 (d, 2H, *J* = 8.4 Hz, ArH), 7.53 (t, 2H, *J* = 7.2 Hz, ArH), 7.58 (d, 2H, *J* = 8.0 Hz, ArH), 7.80 (t, 2H, *J* = 8.0 Hz, ArH), 8.12 (d, 2H, *J* = 7.6 Hz, ArH), 12.62 (brs, 2H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 35.36, 55.10, 104.70, 113.73, 116.22, 117.53, 123.97, 124.11, 127.95, 130.90, 132.27, 152.25, 157.60, 164.67, 165.05.



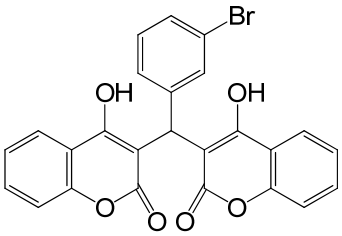
3,3'-((4-chlorophenyl)methylene)bis(4-hydroxy-2H-chromen-2-one) (3d)[1]

White solid, mp 242-245 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 6.35 (s, 1H, CH), 7.16 (d, 2H, *J* = 8.4 Hz, ArH), 7.32-7.44 (m, 6H, ArH), 7.61 (t, 2H, *J* = 7.6 Hz, ArH), 7.94 (d, 2H, *J* = 7.6 Hz, ArH), 13.01 (brs, 2H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 35.77, 103.95, 116.05, 117.76, 118.69, 123.86, 123.94, 129.19 130.92, 132.08, 139.54, 152. 24, 164.75, 165.23.



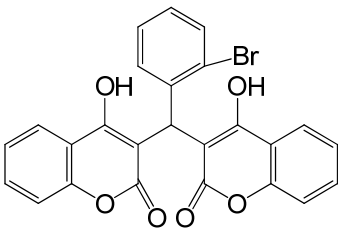
3,3'-((4-bromophenyl)methylene)bis(4-hydroxy-2H-chromen-2-one) (3e)[1]

White solid, mp 248-250 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 6.53 (s, 1H, CH), 7.34 (d, 2H, *J* = 8.0 Hz, ArH), 7.50-7.62 (m, 6H, ArH), 7.79 (t, 2H, *J* = 7.2 Hz, ArH), 8.12 (d, 2H, *J* = 8.0 Hz, ArH), 13.18 (brs, 2H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 35.90, 104.10, 116.18, 117.83, 118.83, 124.00, 124.06, 129.31, 131.05, 132.21, 139.60, 152.36, 164.88, 165.29.



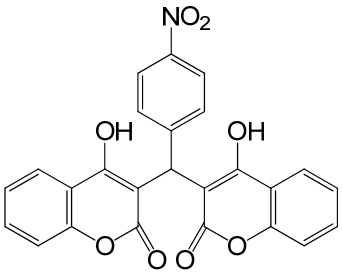
3,3'-((3-bromophenyl)methylene)bis(4-hydroxy-2H-chromen-2-one) (3f) [1]

White solid, mp 210-217 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 6.39 (s, 1H, CH), 7.22-7.26 (m, 2H, ArH), 7.35-7.41 (m, 6H, ArH), 7.63 (t, 2H, *J* = 7.6 Hz, ArH), 7.95 (d, 2H, *J* = 7.6 Hz, ArH), 12.75 (brs, 2H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 35.97, 103.64, 115.95, 117.99, 121.56, 123.69, 123.93, 126.03, 128.49, 129.31, 130.18, 131.90, 143.49, 152.25, 164.57, 165.57.



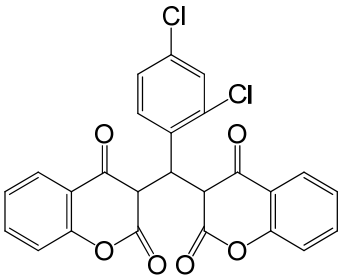
3,3'-((2-bromophenyl)methylene)bis(4-hydroxy-2H-chromen-2-one) (3g)[2]

White solid, mp 202-208 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 6.10 (s, 1H, CH), 7.13 (t, 1H, *J* = 7.6 Hz, ArH), 7.26-7.38 (m, 6H, ArH), 7.52 (d, 1H, *J* = 7.6 Hz, ArH), 7.59 (t, 2H, *J* = 7.6 Hz, ArH), 7.93 (d, 2H, *J* = 7.6 Hz, ArH), 11.96 (brs, 2H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 38.67, 104.33, 115.98, 117.57, 123.50, 123.60, 126.96, 127.84, 130.27, 131,69, 132.66, 140.40, 152.16, 163.33, 164.19.



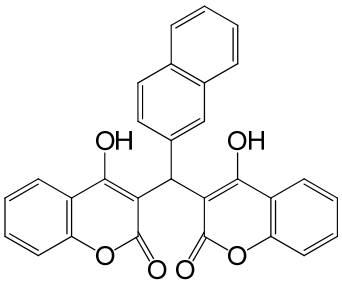
3,3'-((4-nitrophenyl)methylene)bis(4-hydroxy-2H-chromen-2-one) (3h) [1]

Yellow solid, mp 238-240 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 6.45 (s, 1H, CH), 7.32-7.44 (m, 4H, ArH), 7.47 (d, 2H, *J* = 8.4 Hz, ArH), 7.62 (d, 2H, *J* = 8.0 Hz, ArH), 7.93 (d, 2H, *J* = 8.0 Hz, ArH), 8.13 (d, 2H, *J* = 8.8 Hz, ArH), 11.51 (brs, 2H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 36.84, 103.51, 116.06, 118.53, 123.37, 123.72, 124.18, 128.23, 131.98, 145.70, 150.09, 152.53, 164.58, 166.38.



3,3'-((2,4-dichlorophenyl)methylene)bis(chroman-2,4-dione) (3i) [3]

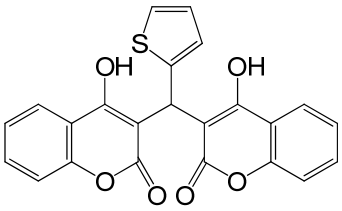
White solid, mp 169-170 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 6.33 (s, 3H, CH), 7.48 (m, 5H, ArH), 7.60 (m, 2H, ArH), 7.74 (t, 2H, *J* = 8.4 Hz, ArH), 8.07 (d, 2H, *J* = 7.6 Hz, ArH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 36.15, 43.08, 103.26, 115.91, 118.89, 123.47, 124.04, 126.48, 128.77, 130.99, 131.53, 131.75, 133.70, 139.21, 152.47, 163.70, 166.34.



3,3'-(naphthalen-2-ylmethylene)bis(4-hydroxy-2H-chromen-2-one) (3j)[4]

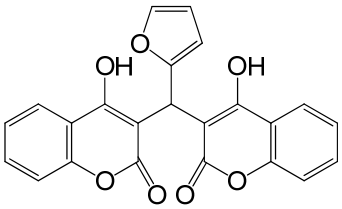
Yellow solid, mp 275-278 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 6.53 (s, 1H, CH), 7.35 (t, 3H, *J* = 8.0 Hz, ArH), 7.41-7.44 (m, 4H, ArH), 7.61-7.67 (m, 3H, ArH), 7.77-7.86 (m, 3H, ArH), 7.94 (d,

2H, *J* = 7.2 Hz, ArH), 9.07 (brs, 2H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 36.38, 104.12, 115.98, 118.04, 123.72, 123.93, 124.38, 125.16, 125.76, 126.08, 127.19, 127.52, 127.56, 131.56, 131.88, 133.04, 137.85, 152.28, 164.78, 165.48.



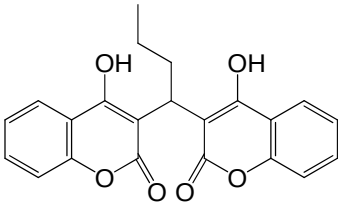
3,3'-(thiophen-2-ylmethylene)bis(4-hydroxy-2H-chromen-2-one) (3k)[5]

Yellow solid, mp 212-214 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 6.71 (s, 1H, CH), 6.90 (s, 1H, ArH), 7.03 (d, 1H, *J* = 3.2 Hz, ArH), 7.41-7.53 (m, 5H, ArH), 7.74 (t, 2H, *J* = 7.6 Hz, ArH), 8.10 (d, 2H, *J* = 7.6 Hz, ArH), 13.44 (brs, 2H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 32.86, 104.55, 116.163, 117.95, 123.88, 124.00, 124.20, 126.68, 132.29, 145.23, 152.34, 164.62, 165.63.



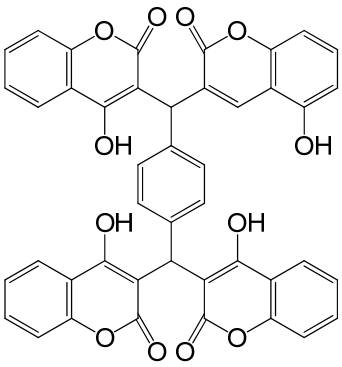
3,3'-(furan-2-ylmethylene)bis(4-hydroxy-2H-chromen-2-one) (3l)[1]

Grey solid, mp 200-202 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 6.15 (s, 1H, CH), 6.36-7.40 (m, 2H, ArH), 7.36-7.43 (m, 4H, ArH), 7.54 (s, 1H, ArH), 7.65 (t, 2H, *J* = 8.4 Hz, ArH), 7.99 (d, 2H, *J* = 6.8 Hz, ArH), 12.97 (brs, 2H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 31.98, 103.19, 106.60, 110.74, 116.51, 118.03, 124.36, 132.61, 142.03, 152.60, 153.19, 164.81, 165.54.



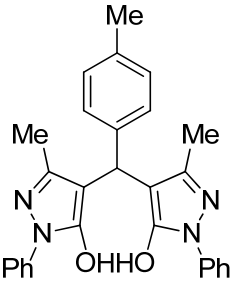
3,3'-(butane-1,1-diyl)bis(4-hydroxy-2H-chromen-2-one) (3m)[1]

White solid, mp 116-118 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 0.90 (t, 3H, CH_3), 1.25-1.31 (m, 2H, CH_2), 2.13 (q, 2H, *J* = 7.2 Hz, CH_2), 4,96 (d, 1H, *J* = 8.0 Hz, CH), 7.38-7.41 (m, 4H, ArH), 7.63 (t, 2H, *J* = 7.2 Hz, ArH), 7.99 (d, 2H, *J* = 7.2 Hz, ArH), 11,97 (brs, 2H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 14.36, 21.42, 31.89, 31.96, 105.93, 116.47, 117.65, 124.06, 124.45, 132.43, 152.30, 164.29, 165.46.



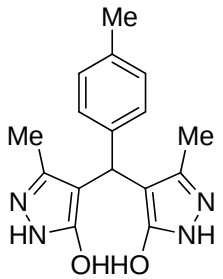
3,3'-((4-((4-hydroxy-2-oxo-2H-chromen-3-yl)(5-hydroxy-2-oxo-2H-chromen-3-yl)methyl)phenyl)methylene)bis(4-hydroxy-2H-chromen-2-one) (3n)[6]

White solid, mp 298-300 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 6.34 (s, 2H, CH), 7.05 (s, 4H, ArH), 7.31-7.38 (m, 8H, ArH), 7.58-7.62 (m, 4H, ArH), 7.90-7.92 (m, 4H, ArH), 10.90 (brs, 2H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 35.60, 104.14, 115.91, 117.78, 123.73, 123.87, 126.52, 131.87, 136.88, 152.13, 164.80, 165.04.



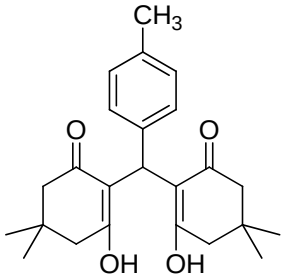
4,4'-(p-tolylmethylene)bis(3-methyl-1-phenyl-1H-pyrazol-5-ol) (4)[7]

White solid, mp 165-167 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 2.43 (s, 3H, CH_3), 2.51 (s, 6H, CH_3), 5.11 (s, 1H, CH), 7.27 (d, 2H, *J* = 6.8 Hz, ArH), 7.34 (d, 2H, *J* = 6.8 Hz, ArH), 7.43 (d, 2H, *J* = 6.4 Hz, ArH), 7.63 (t, 4H, *J* = 6.8 Hz, ArH), 7.91 (d, 4H, *J* = 7.6 Hz, ArH), 12,58 (brs, 1H, OH), 14.16 (brs, 1H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 11.80, 20.68, 32.92, 120.64, 125.67, 127.24, 128.84, 129.06, 134.96, 137.55, 139.32, 146.37.



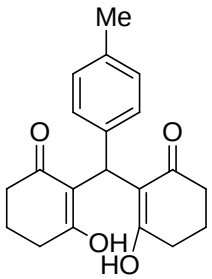
4,4'-(p-tolylmethylene)bis(3-methyl-1H-pyrazol-5-ol) (5)[8]

White solid, mp 213-215 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 2.06 (s, 6H, CH_3), 2.22 (s, 3H, CH_3), 4.76 (s, 1H, CH), 7.00 (s, 4H, ArH), 11.34 (brs, 4H, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 10.35, 20.50, 32.28, 44.18, 55.99, 104.33, 127.32, 128.24, 134.14, 140.22.



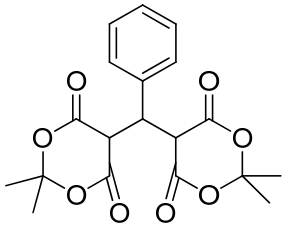
2,2'-(4-methylphenylmethylene)bis(3-hydroxy-5,5-dimethyl-2-cyclohexene-1-one) (6)[7]

white solid，mp 138-140 °C. ^{1}H NMR (400MHz, $CDCl_3$): δ = 1.09 (s, 6H, CH_3), 1.22 (s, 6H, CH_3), 2.29 (s, 3H, CH_3), 2.32-2.47 (m, 8H, CH_2), 5.50 (s, 1H, CHPh), 6.97 (d, 2H, *J* = 7.6 Hz, ArH), 7.07 (d, 2H, *J* = 8.0 Hz, ArH), 11.91 (s, 2H, OH). ^{13}C NMR (100MHz, $CDCl_3$): δ = 20.92, 27.40, 29.69, 31.43, 32.42, 46.45, 47.07, 115.73, 126.68, 128.97, 134.93, 135.26, 189.39, 190.43.



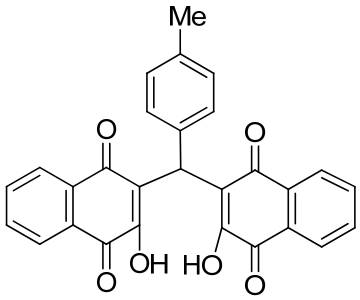
2,2'-(p-tolylmethylene)bis(3-hydroxycyclohex-2-enone) (7)[9]

white solid，mp 191-192 °C. ^{1}H NMR (400MHz, $CDCl_3$): δ = 2.00-2.03 (m, 4H, CH_2), 2.29 (s, 3H, CH_3), 2.33-2.48 (m, 4H, CH_2), 2.54-2.64 (m, 4H, CH_2), 5.42 (s, 1H, CH), 6.98 (d, 2H, *J* = 7.6 Hz, ArH), 7.06 (d, 2H, *J* = 8.0 Hz, ArH), 11.97 (brs, OH), 12.37 (s, OH); ^{13}C NMR (100MHz, $CDCl_3$): δ = 20.13, 21.11, 27.17, 31.24, 33.03, 37.00, 117.02, 126.38, 128.86, 135.27, 141.53, 163.84, 192.09, 196.66.



5,5'-(phenylmethylene)bis(2,2-dimethyl-1,3-dioxane-4,6-dione) (8)[10]

White solid, mp 134-136 °C. ^{1}H NMR (400MHz, $CDCl_3$): δ = 1.71 (s, 6H, CH_3), 1.77 (s, 6H, CH_3), 4.03 (s, 2H, OH), 7.51 (t, 2H, *J* = 8.0 Hz, ArH), 7.59 (t, 1H, *J* = 7.2 Hz, ArH), 8.01 (d, 2H, *J* = 7.2 Hz, ArH), 8.37 (s, 1H, CH); ^{13}C NMR (100MHz, $CDCl_3$): δ = 26.91, 27.00, 30.66, 36.56, 104.60, 105.72, 115.67, 128.44, 132.80, 133.01, 156.54, 164.07.



3,3'-(p-tolylmethylene)bis(2-hydroxynaphthalene-1,4-dione) (9)[11]

Orange solid, mp 165-167 °C; ^{1}H NMR (400MHz, DMSO-d_6): δ = 2.24 (s, 3H, CH_3), 6.11 (s, 1H), 7.00 (d, 2H, *J* = 7.6 Hz, ArH), 7.11 (d, 2H, *J* = 8.0 Hz, ArH), 7.75 (t, 2H, *J* = 7.2 Hz, ArH), 7.80 (t, 2H, *J* = 7.2 Hz, ArH), 7.94 (d, 2H, *J* = 7.6 Hz, ArH), 7.97 (d, 2H, *J* = 7.6 Hz, ArH), 10.89 (brs, OH); ^{13}C NMR (100MHz, DMSO-d_6): δ = 21.07, 36.95, 123.65, 125.94, 126.44, 128.31, 128.74, 130.50, 132.86, 133.32, 134.60, 134.95, 138.33, 158.18, 182.16, 183.85.

2.0 References

1 B. Karmakar, A. Nayak and J. Banerji, *Tetrahedron Lett.*, 2012, **53**, 4343-4346.

2 K. M. Khan, S. Iqbal, M. A. Lodhi, G. M. Maharvi, Z. Ullah, M. I. Choudhary, A. Rahmana and S. Perveen, *Bioorg. Med. Chem.*, 2004, **12**, 1963–1968.

3 P. Singh, P. Kumar, A. Katyal, R. Kalra, S. K. Dass, S. Prakash and R. Chandra, *Catal. Lett.*, 2010, **134**, 303-308.

4 K. A. Nolan, J. R. Doncaster, M. S. Dunstan, K. A. Scott, A. D. Frenkel, D. Siegel, D. Ross, J. Barnes, C. Levy, D. Leys, R. C. Whitehead, I. J. Stratford and R. A. Bryce, *J. Med. Chem.*, 2009, **52**, 7142-7156.

5 K. P. Boroujeni, P. Ghasemi and Z. Rafienia, *Monatsh Chem.*, 2014, **145**, 1023-1026.

6 A. R. Karimi, Z. Eftekhari, M. Karimi and Z. Dalirnasab, *Synthesis*, 2014, **46**, 3180-3184.

7 M. Kour and S. Paul, *New J. Chem.*, 2015, **39**, 6338-6350.

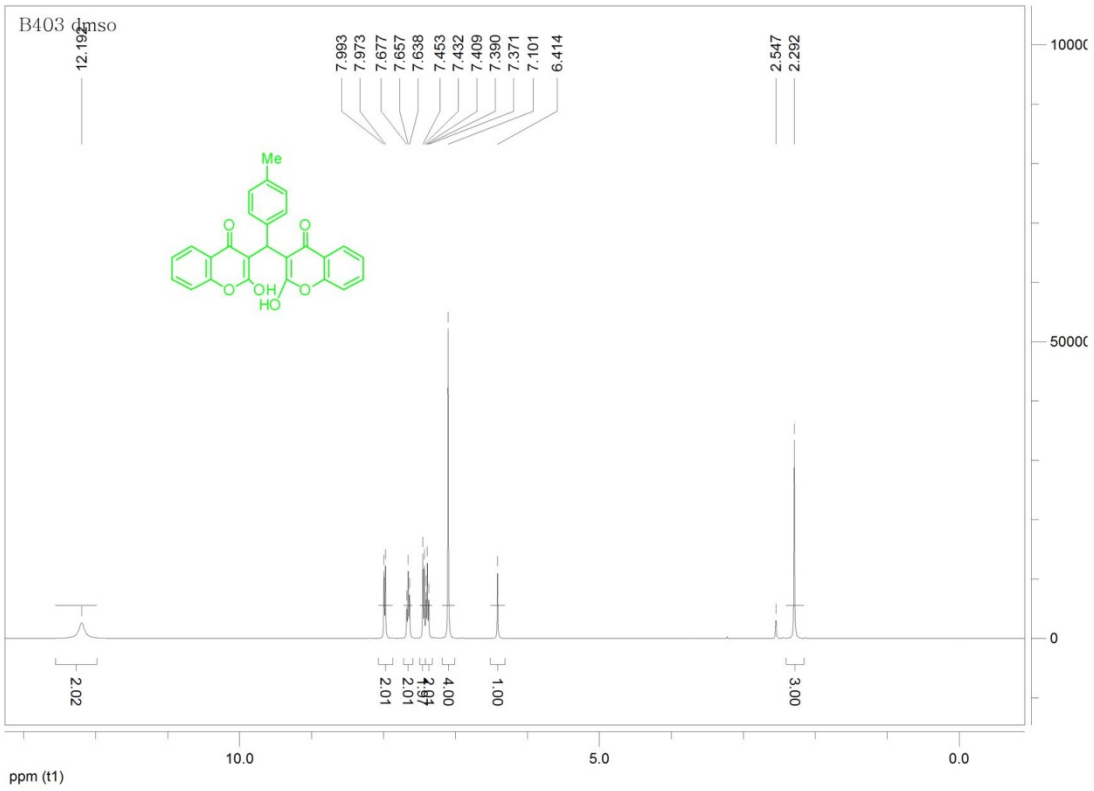
8 M. Zarghani and B. Akhlaghinia, *RSC Adv.*, 2015, **5**, 87769-87780.

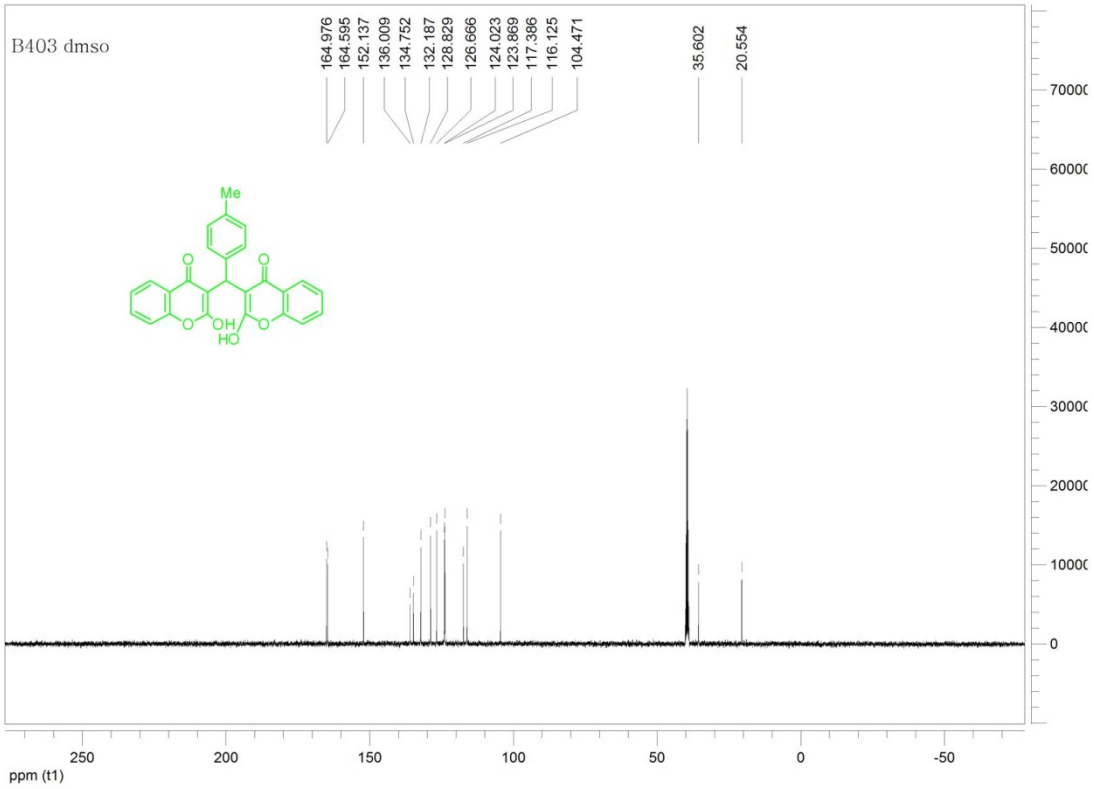
9 K M. Khan, G. M. Maharvi, M. T. H. Khan, A. J. Shaikh, S. Perveen, S. Begum and M. I. Choudhary, *Bioorg. Med. Chem.*, 2006, **14**, 344-351.

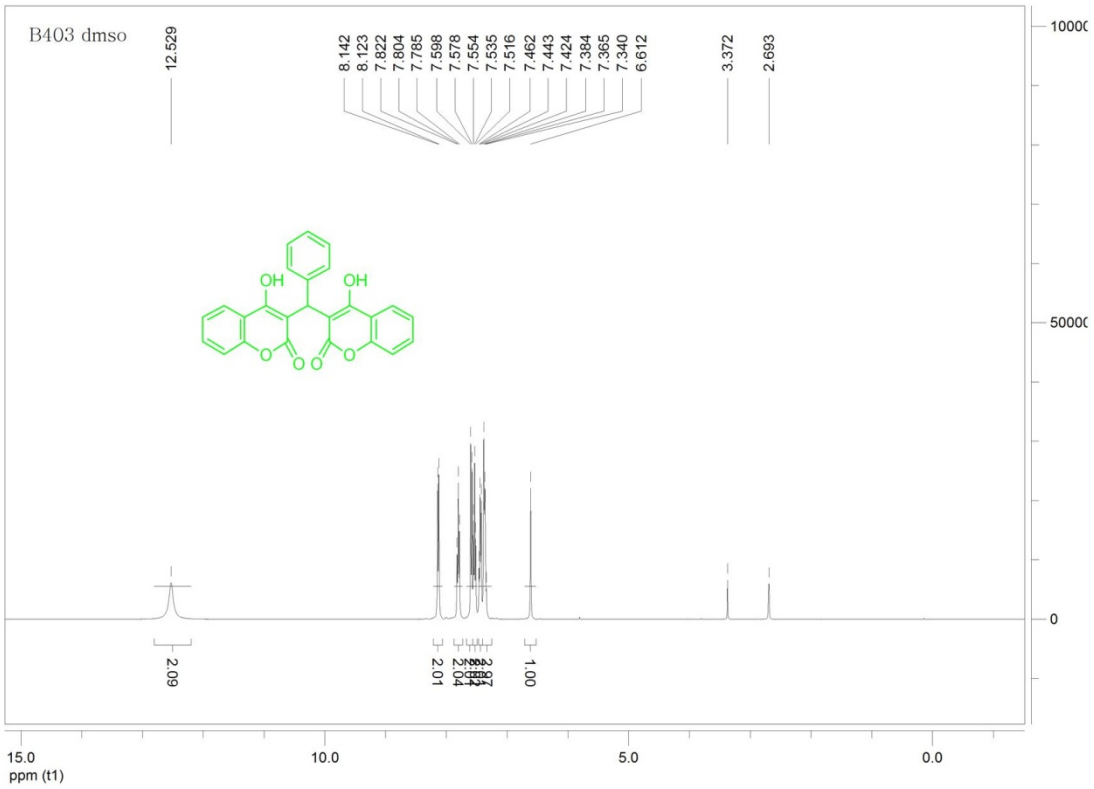
10 W.-J. Le, H.-F. Lu, J.-T. Zhou, H.-L. Cheng and Y.-H. Gao, *Tetrahedron Lett.*, 2013, **54**, 5370-5373.

11 H. Wang, Z. Wang, C. Wang, F. Yang, H. Zhang, H. Yue and L. Wang, *RSC Adv.*, 2014, **4**, 35686-35689.

3.0 NMR spectra of compounds



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6.612
3.372
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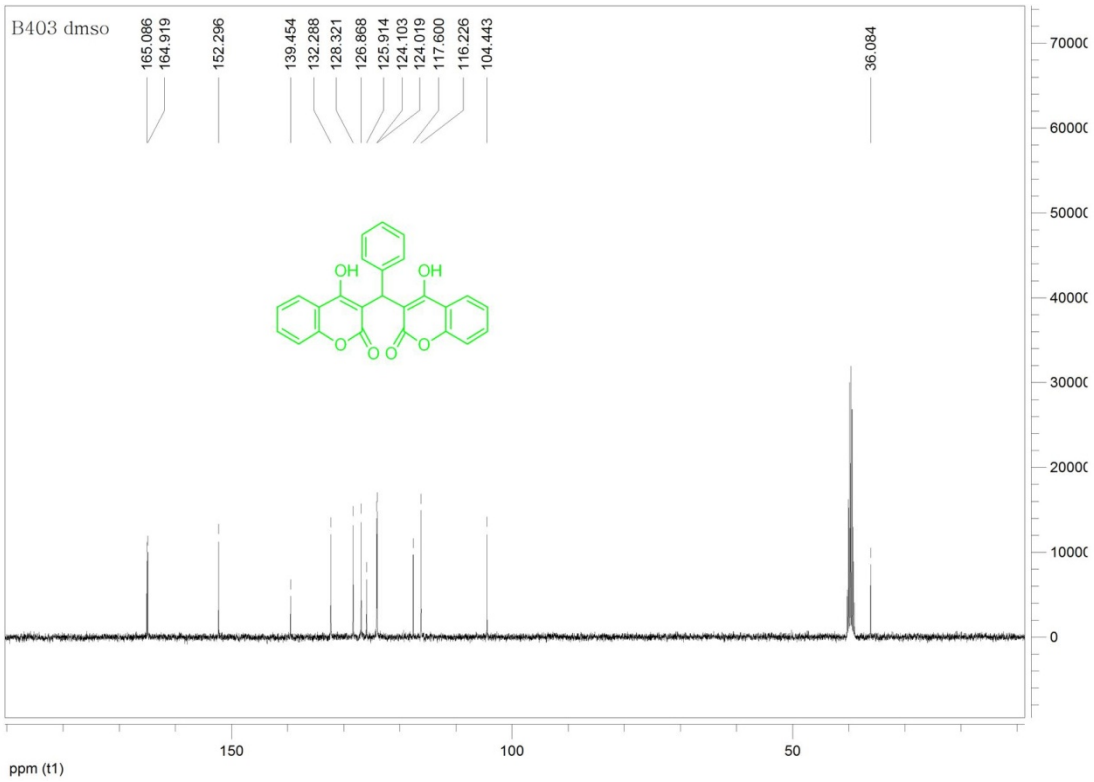
0.0
ppm (t1)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126.868
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36.084
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O
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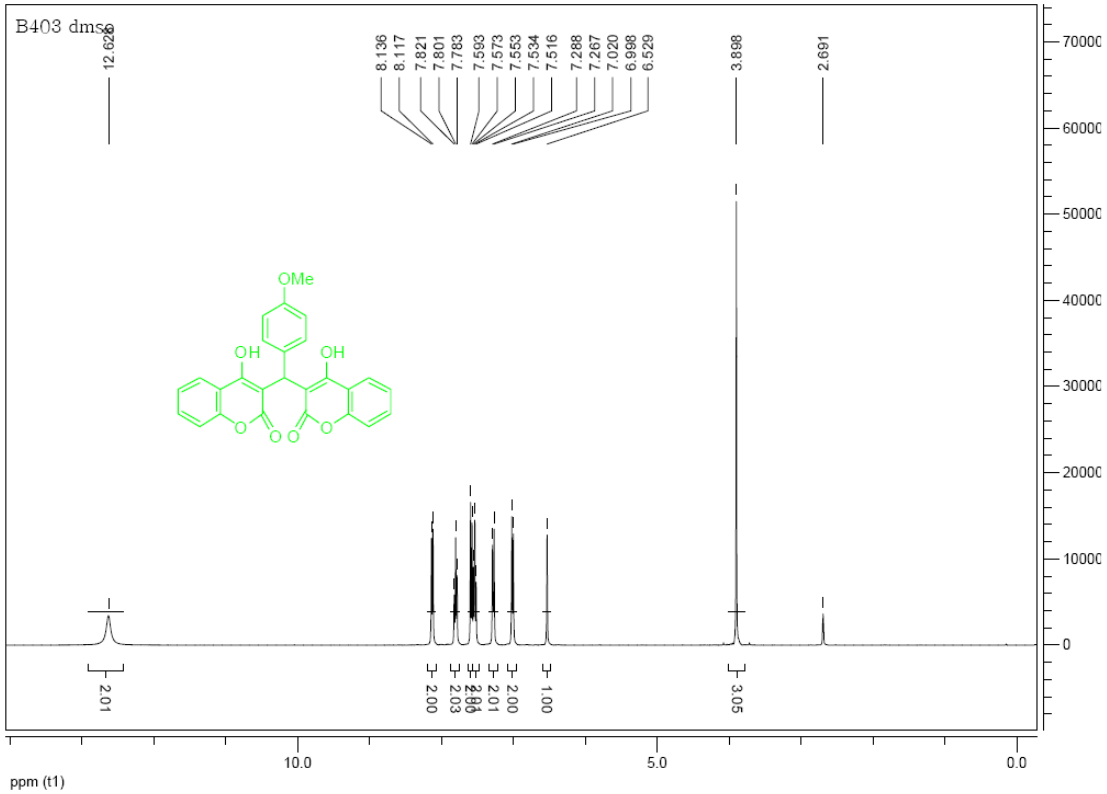
50
ppm (t1)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6.529
3.898
2.691
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O
O
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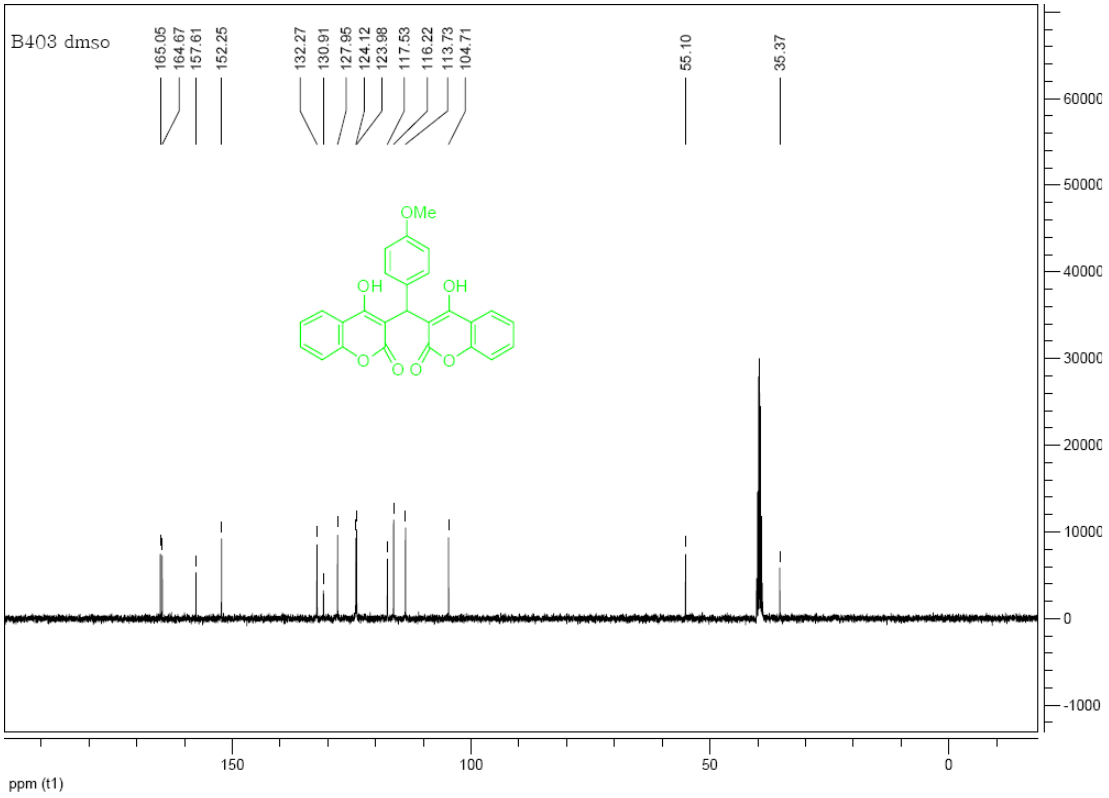
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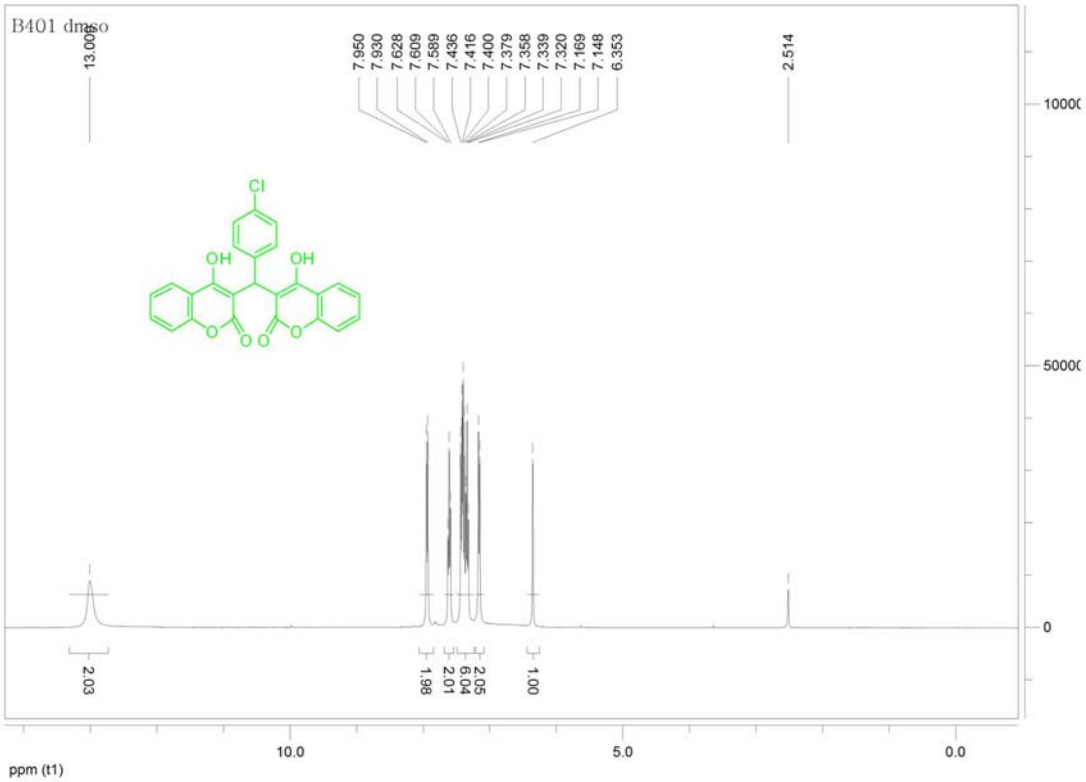
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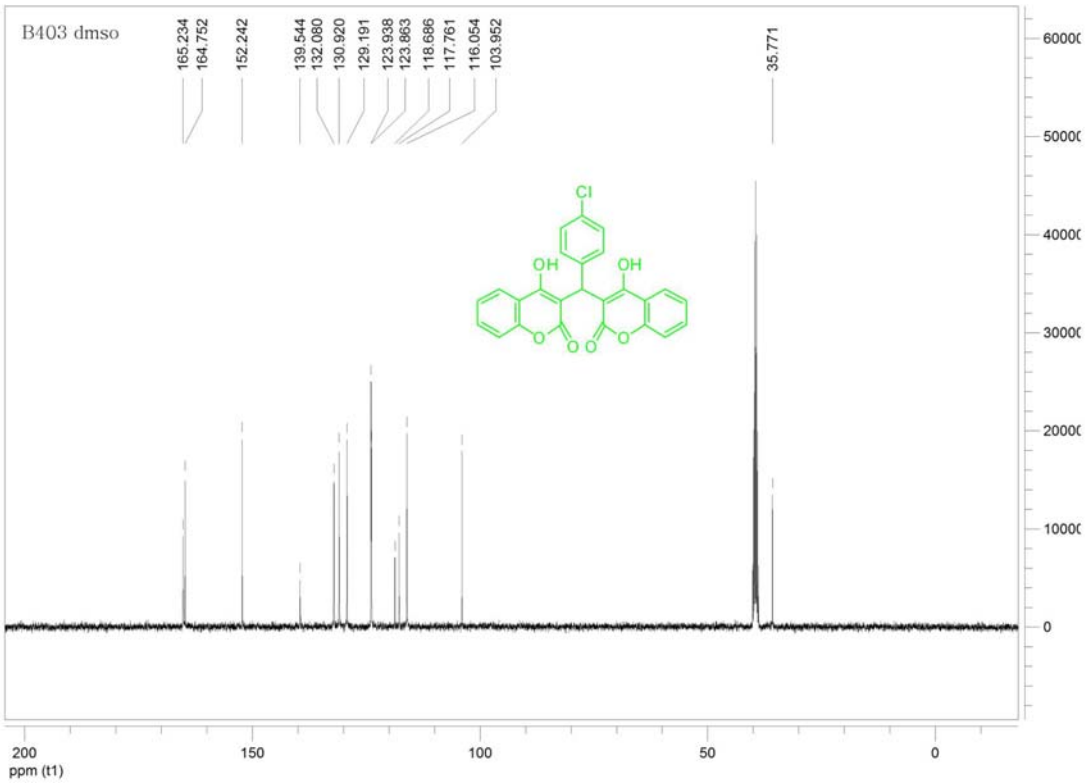
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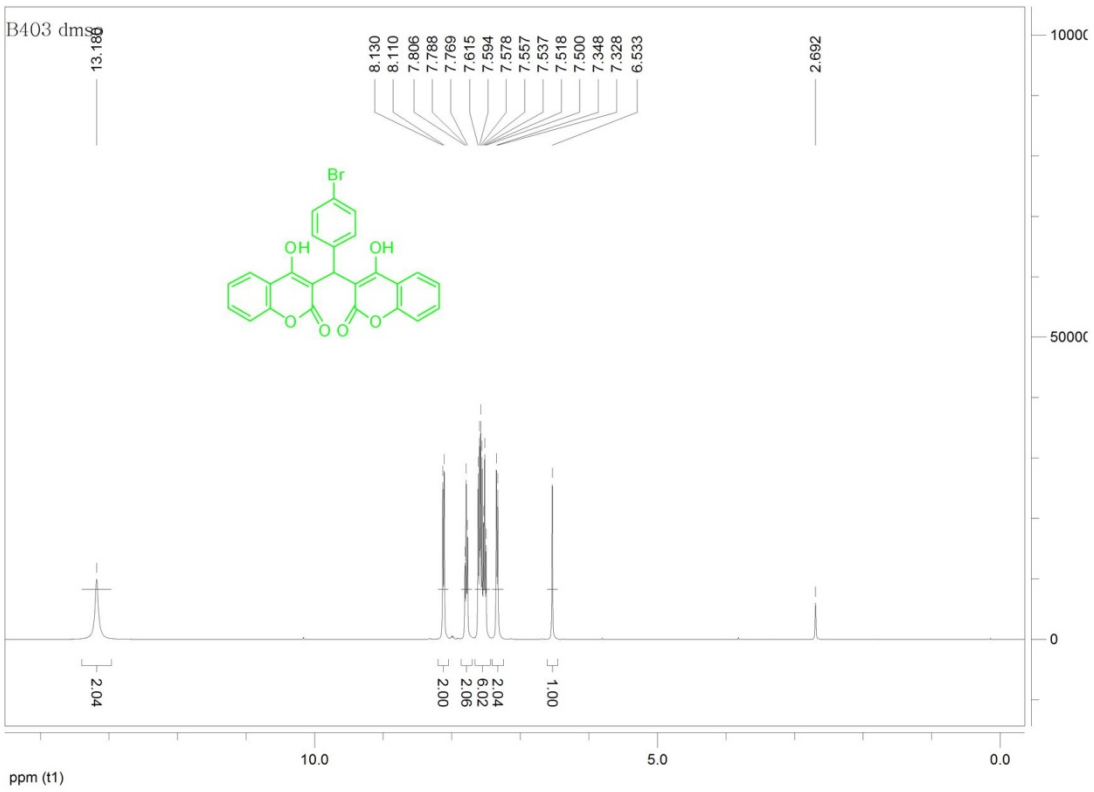
ppm (t1)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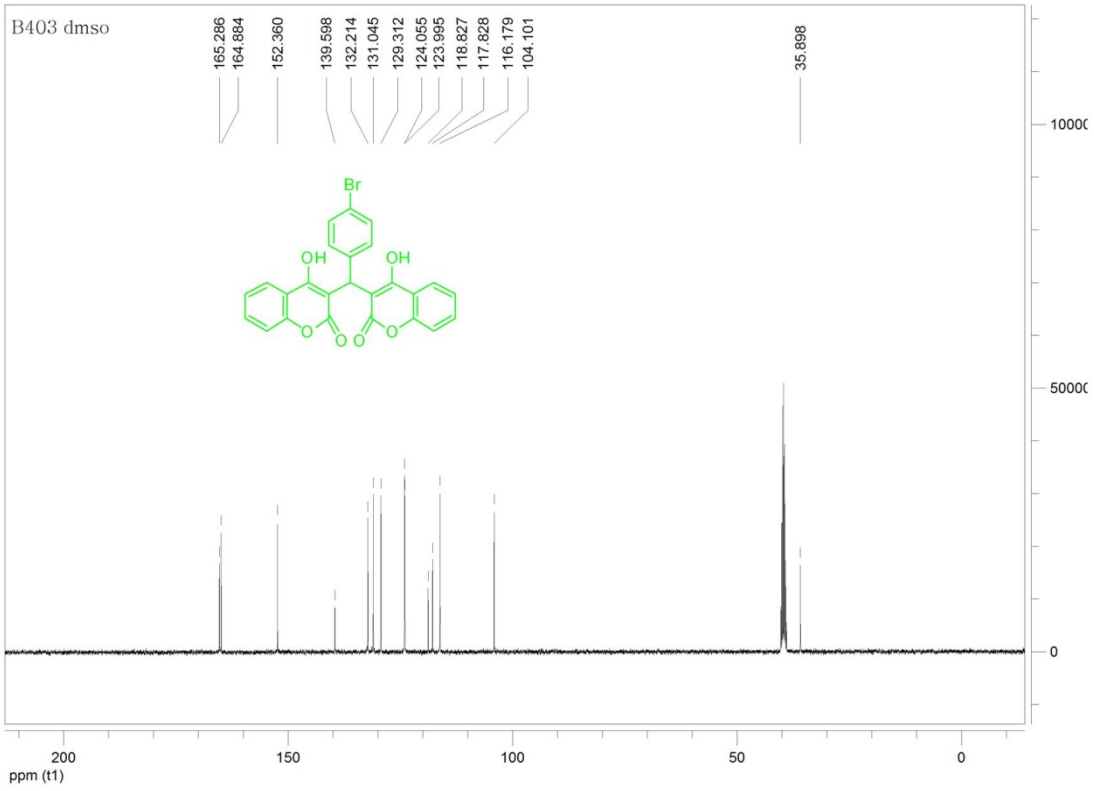
ppm (t1)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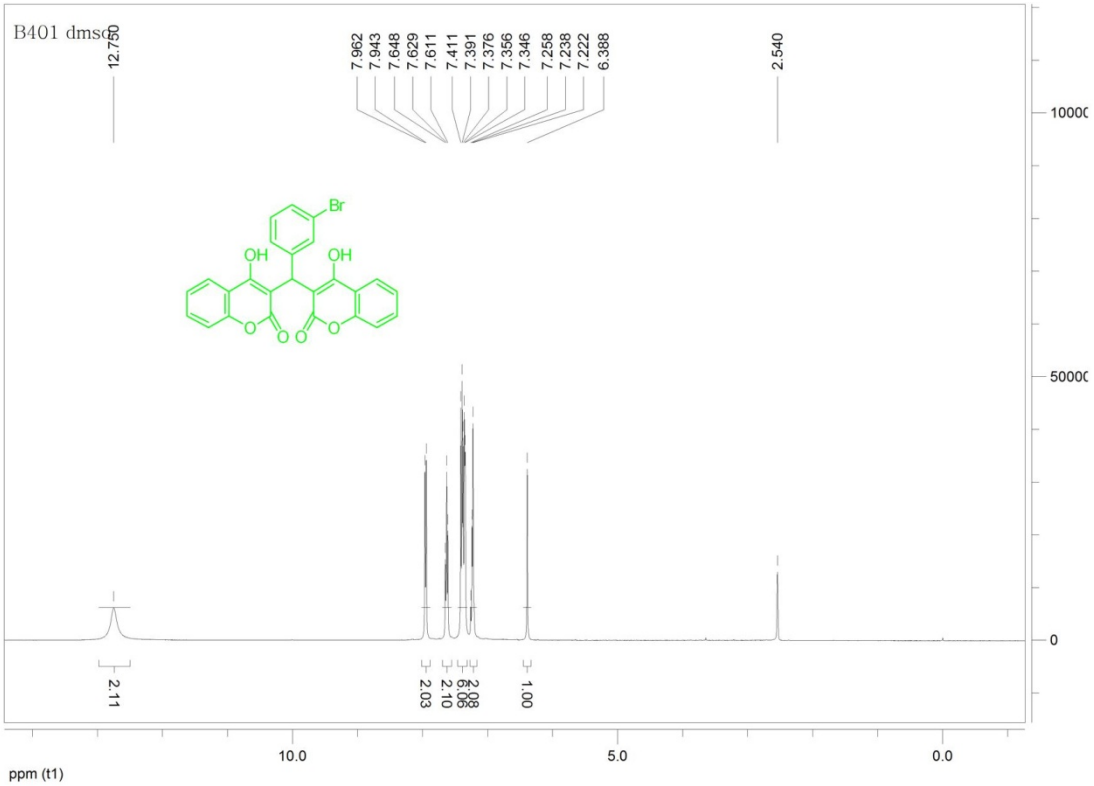
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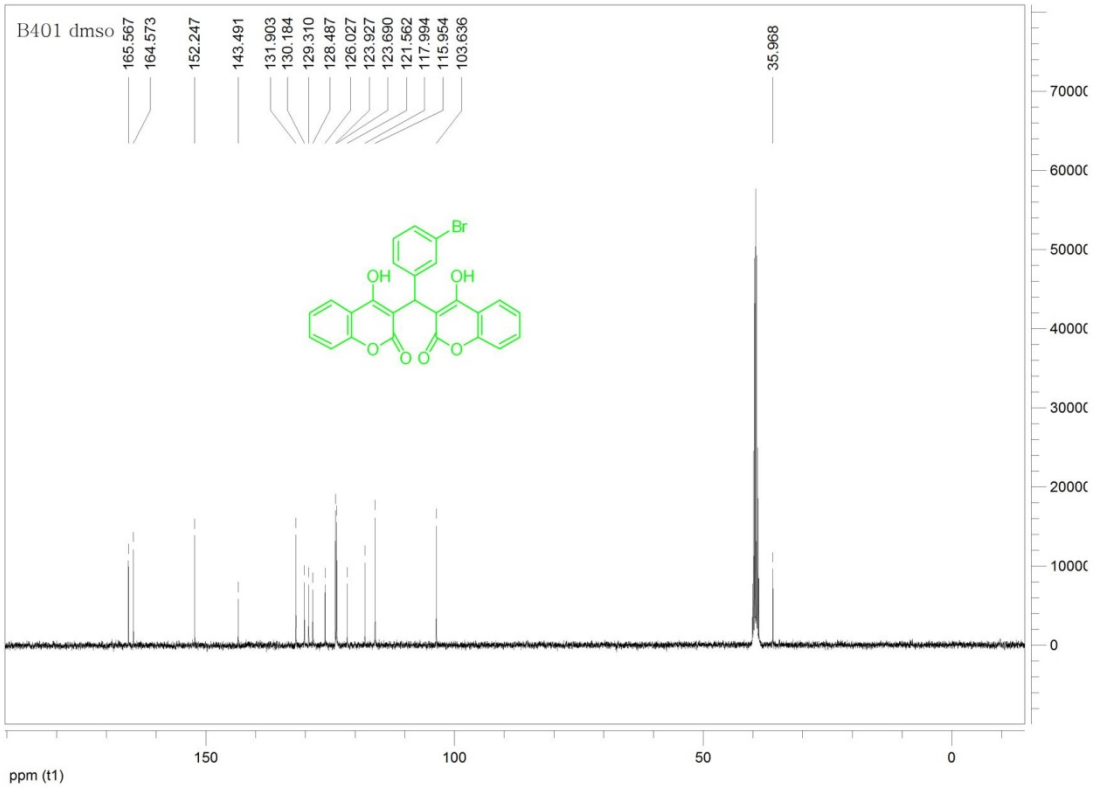
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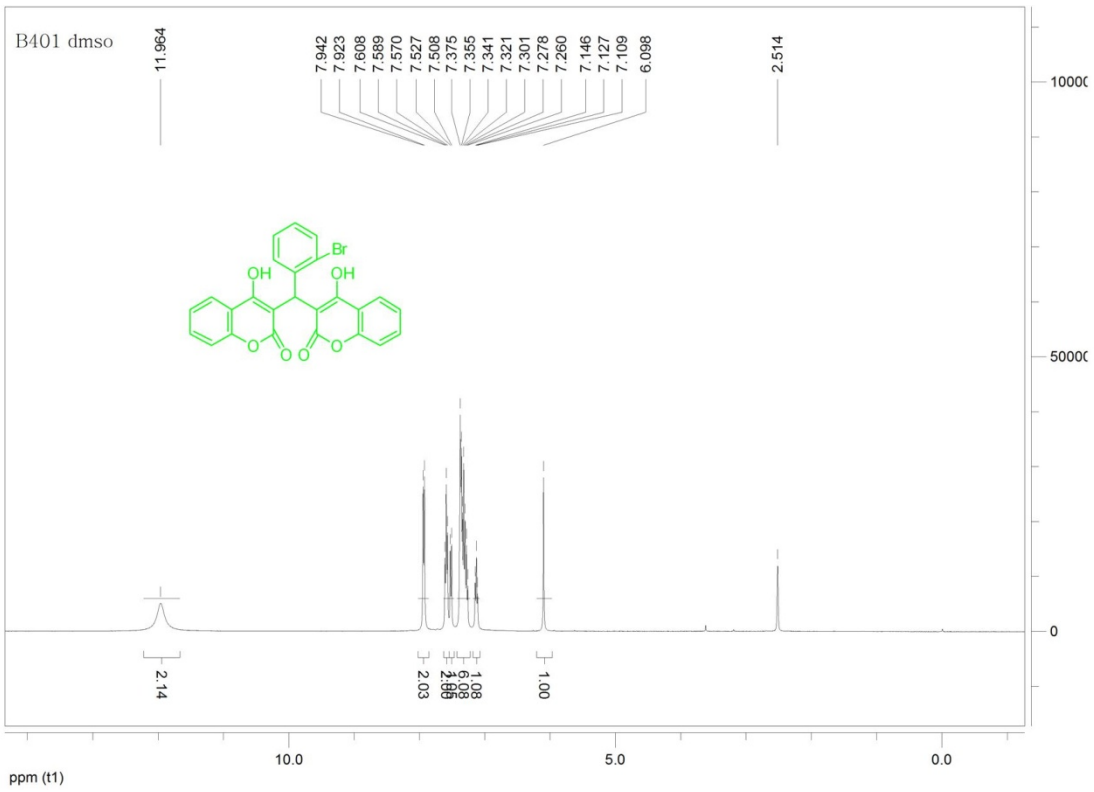
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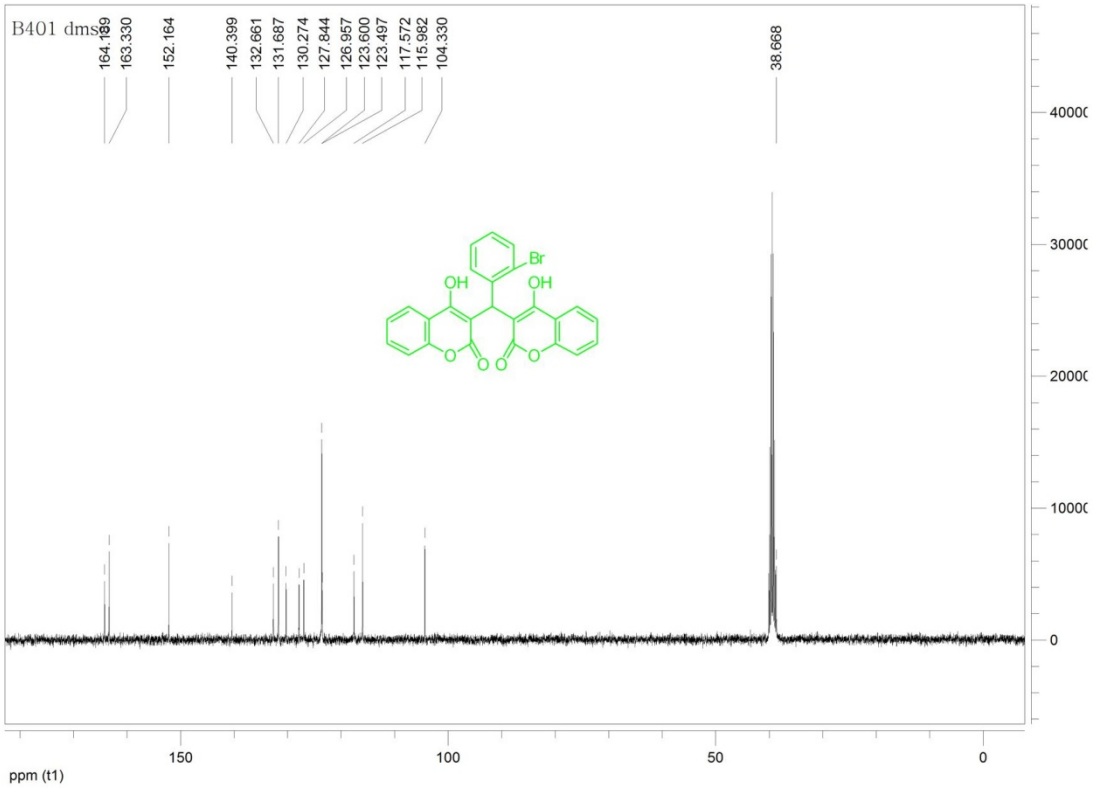
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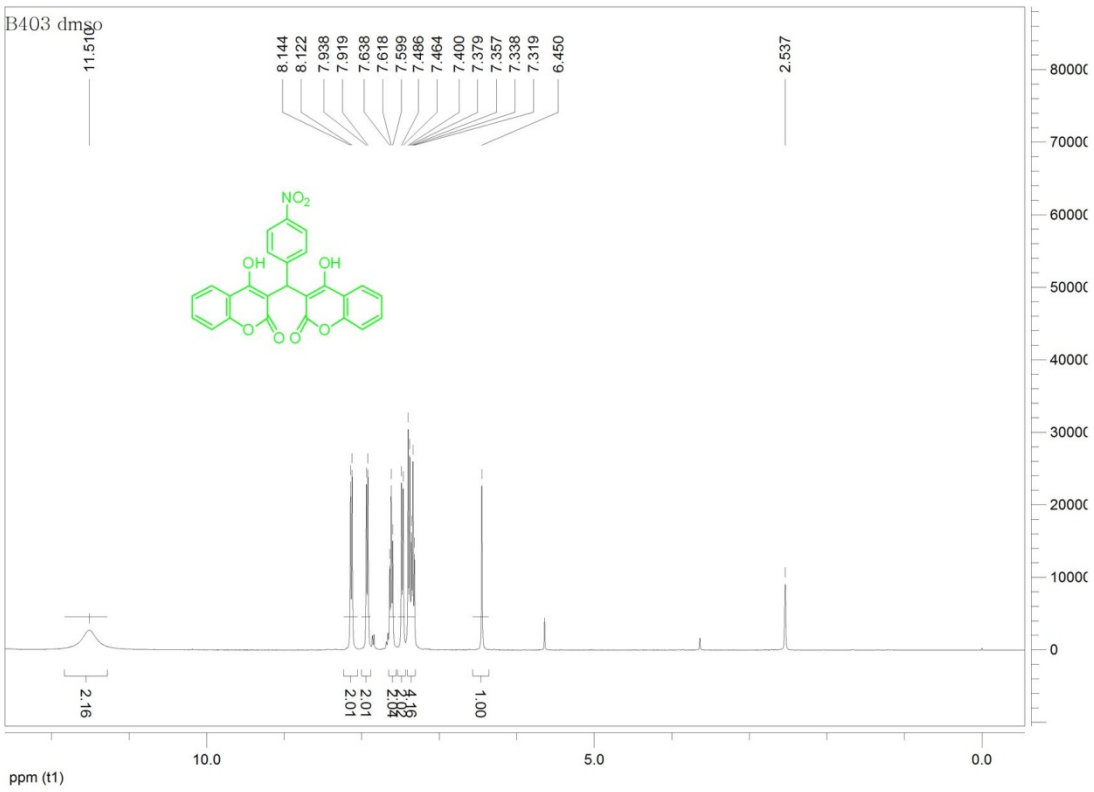
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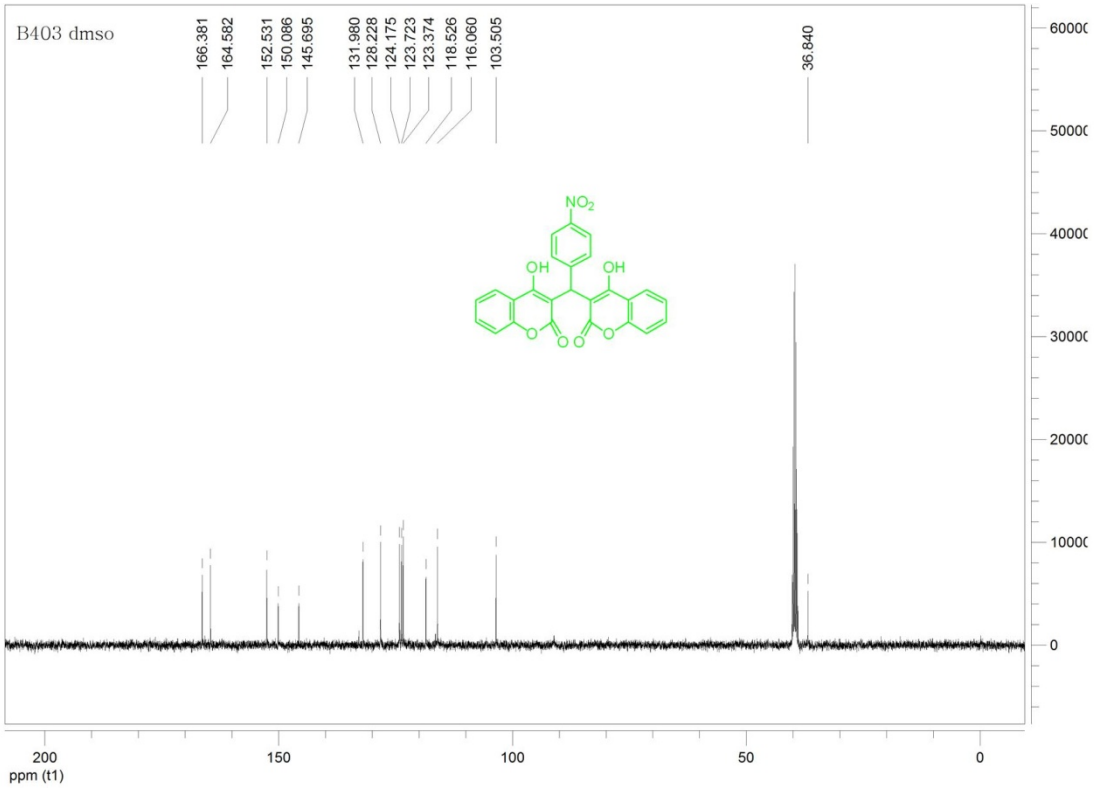
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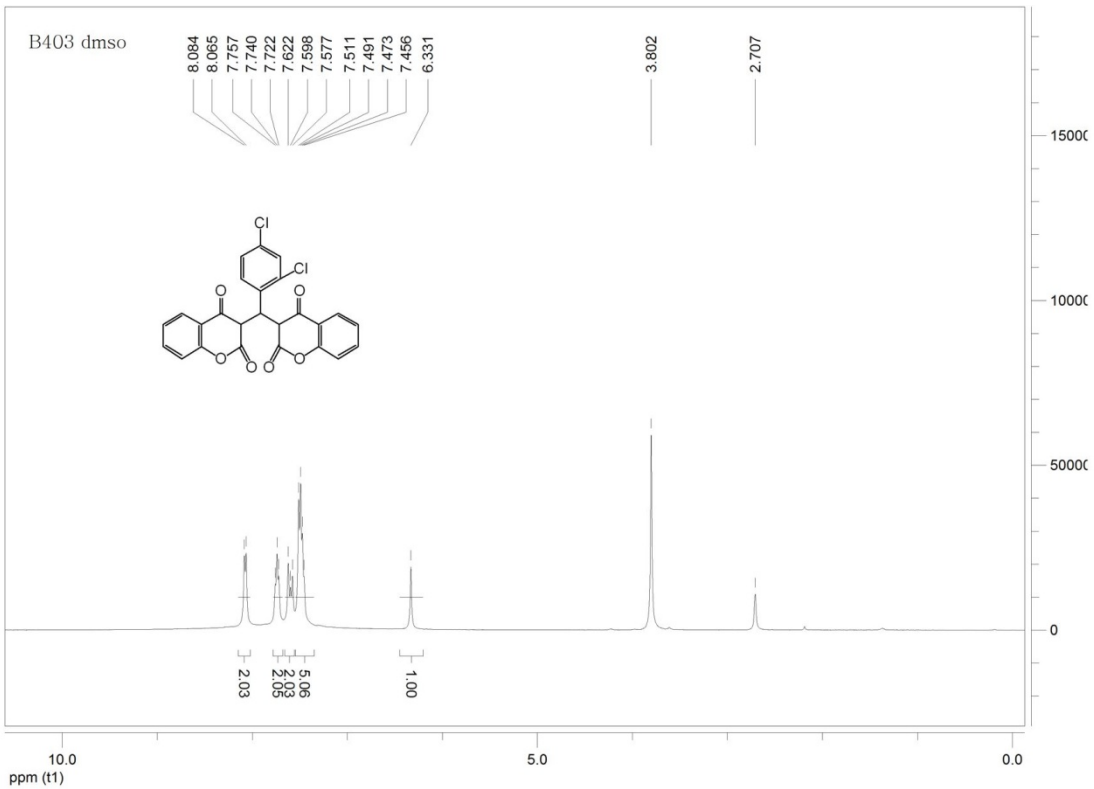
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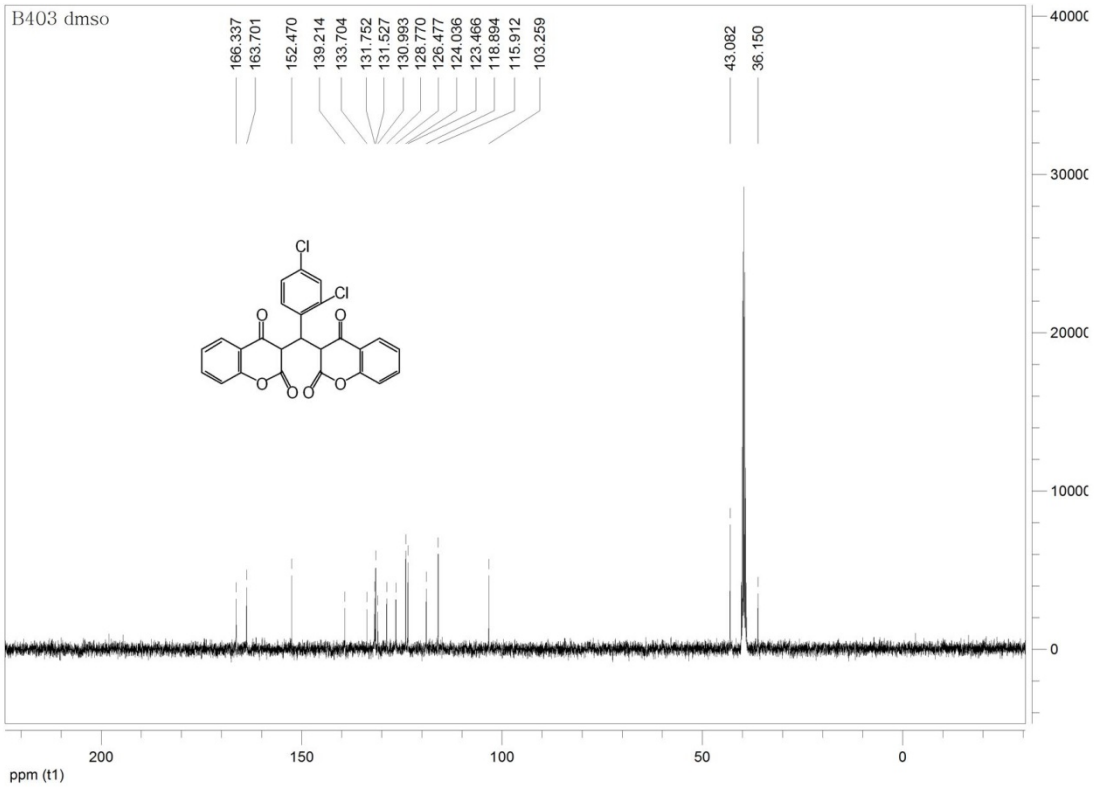
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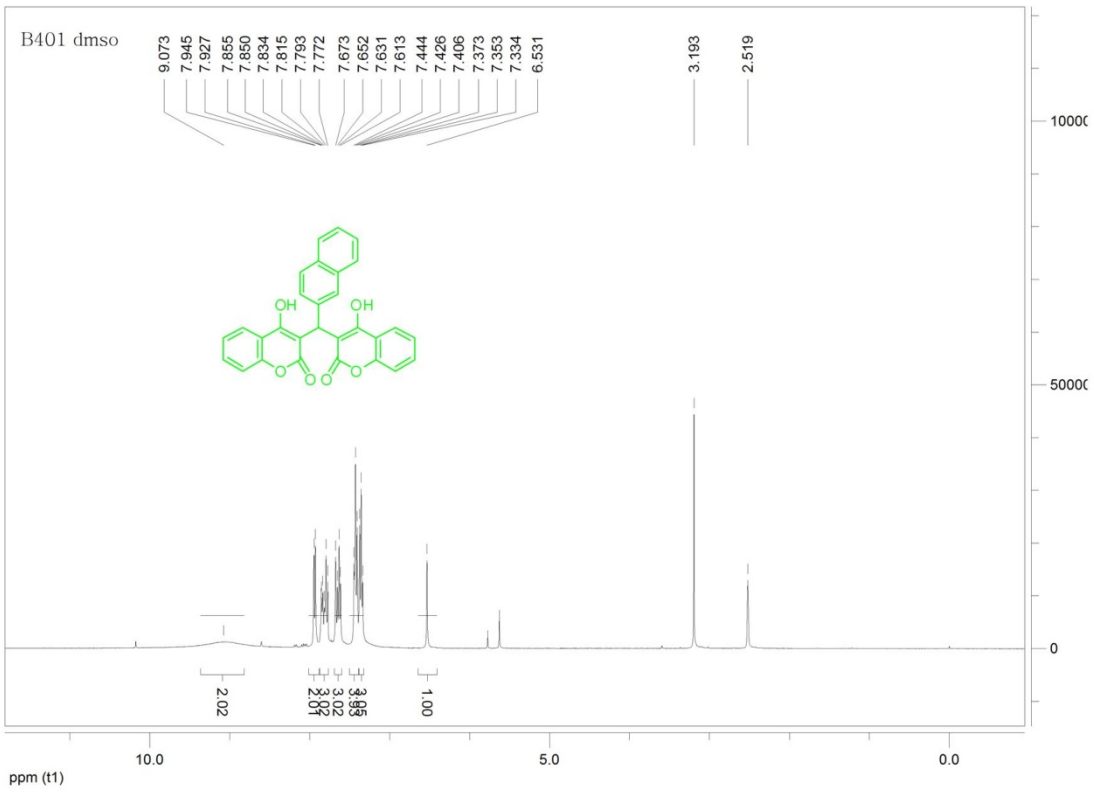
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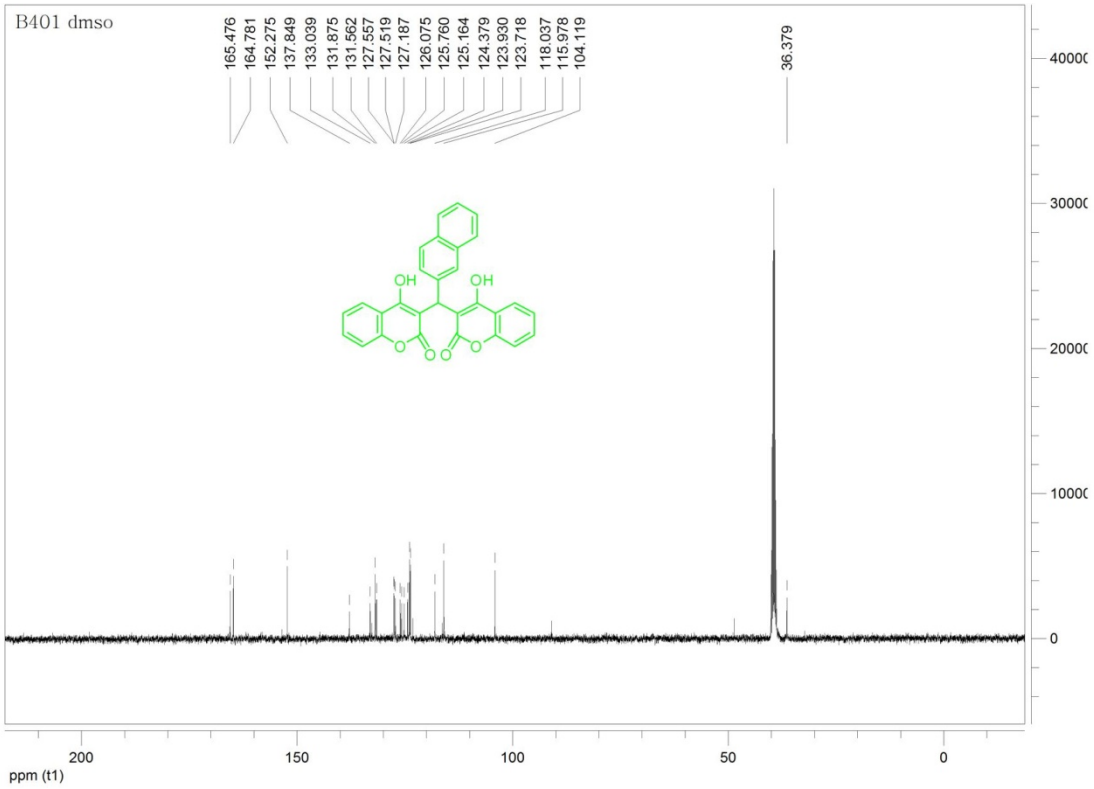
ppm (t1)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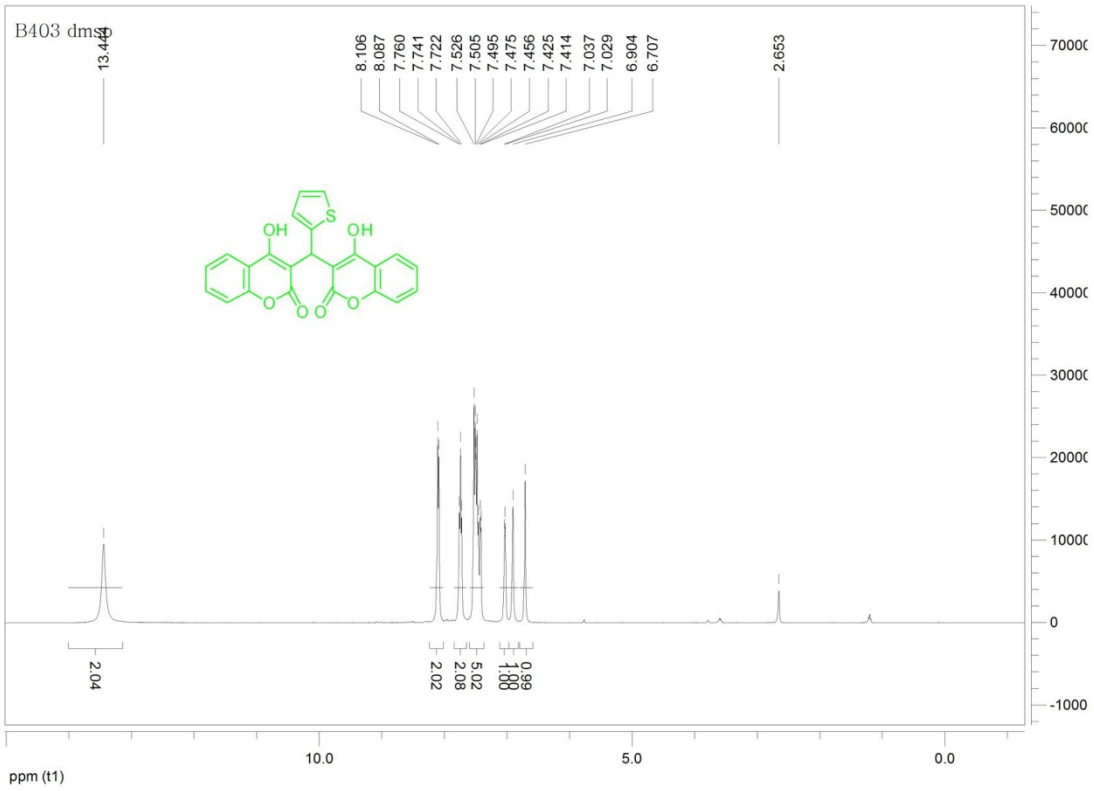
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7.029
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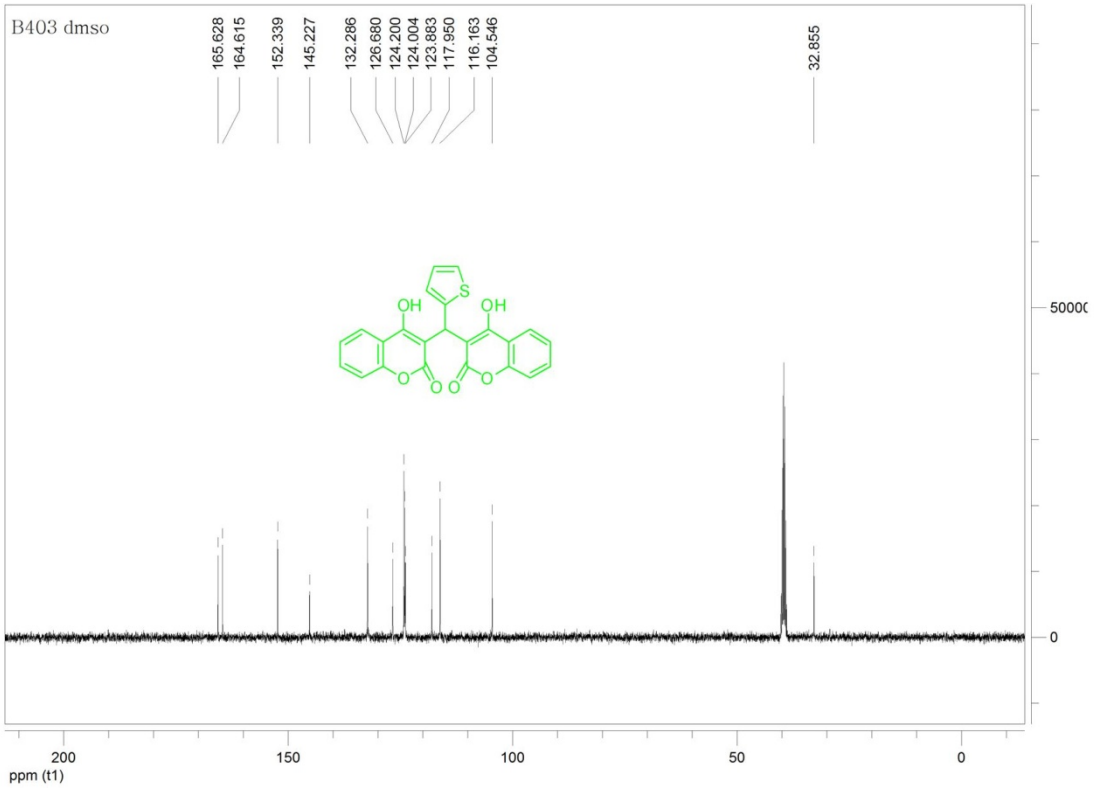
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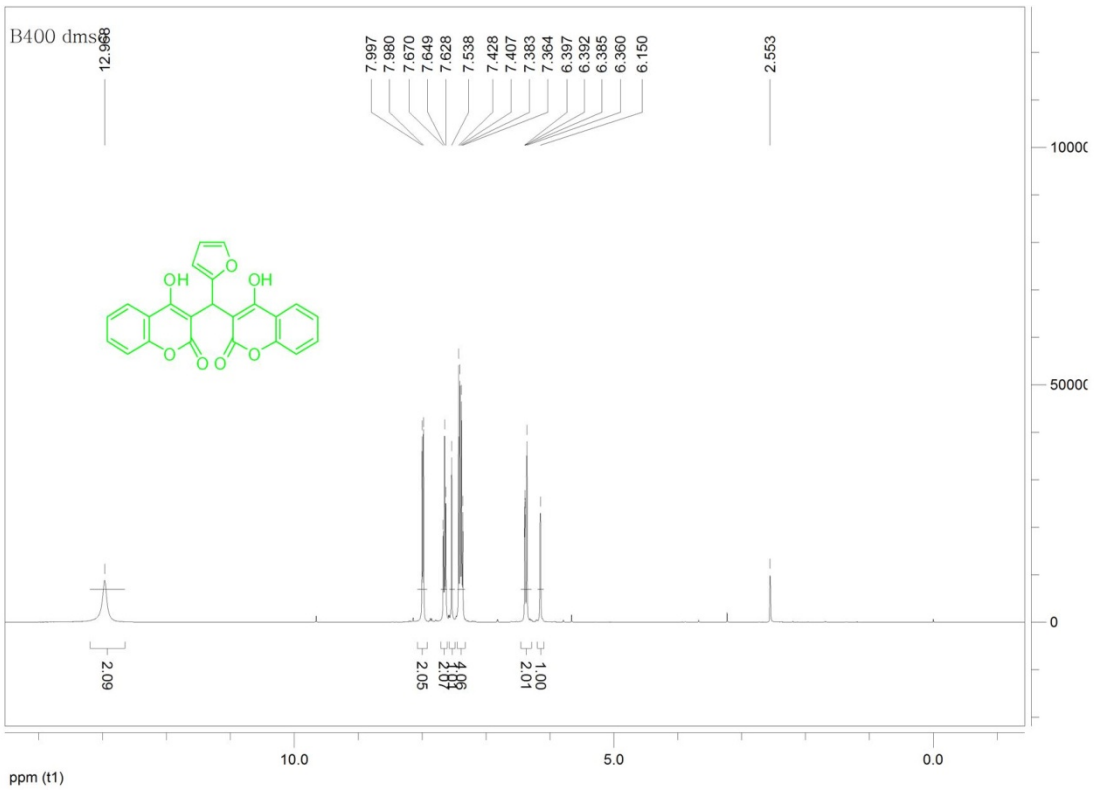
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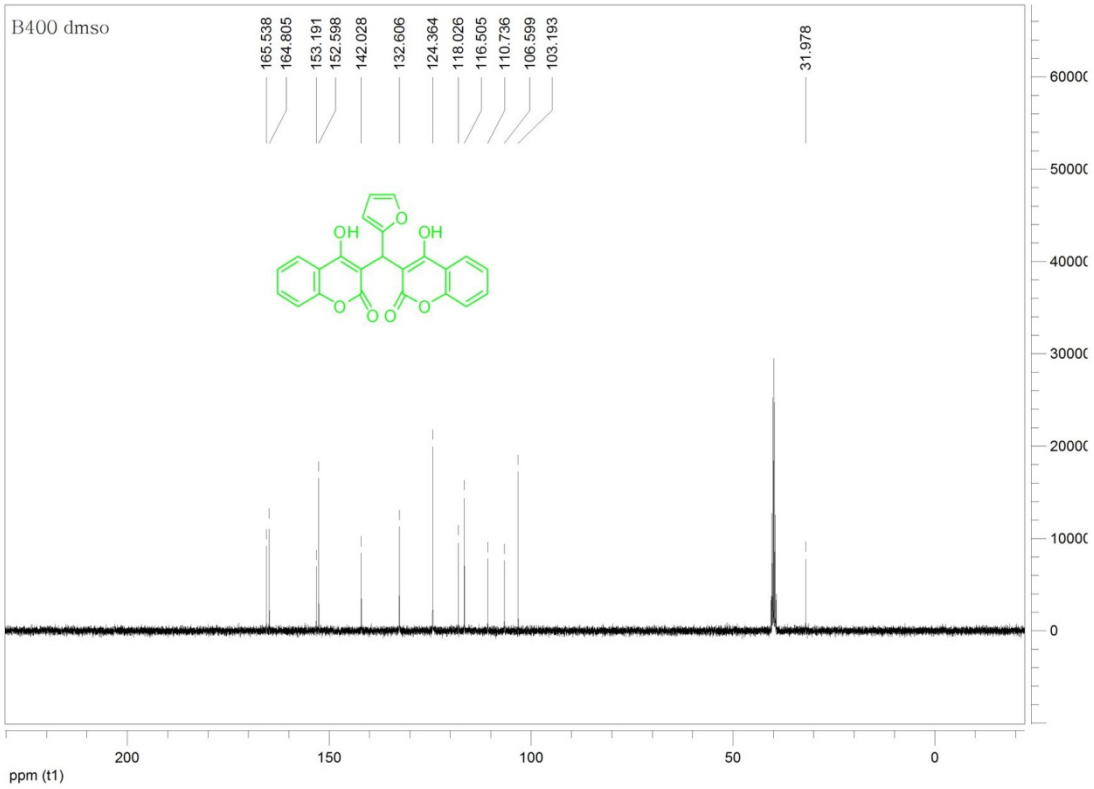
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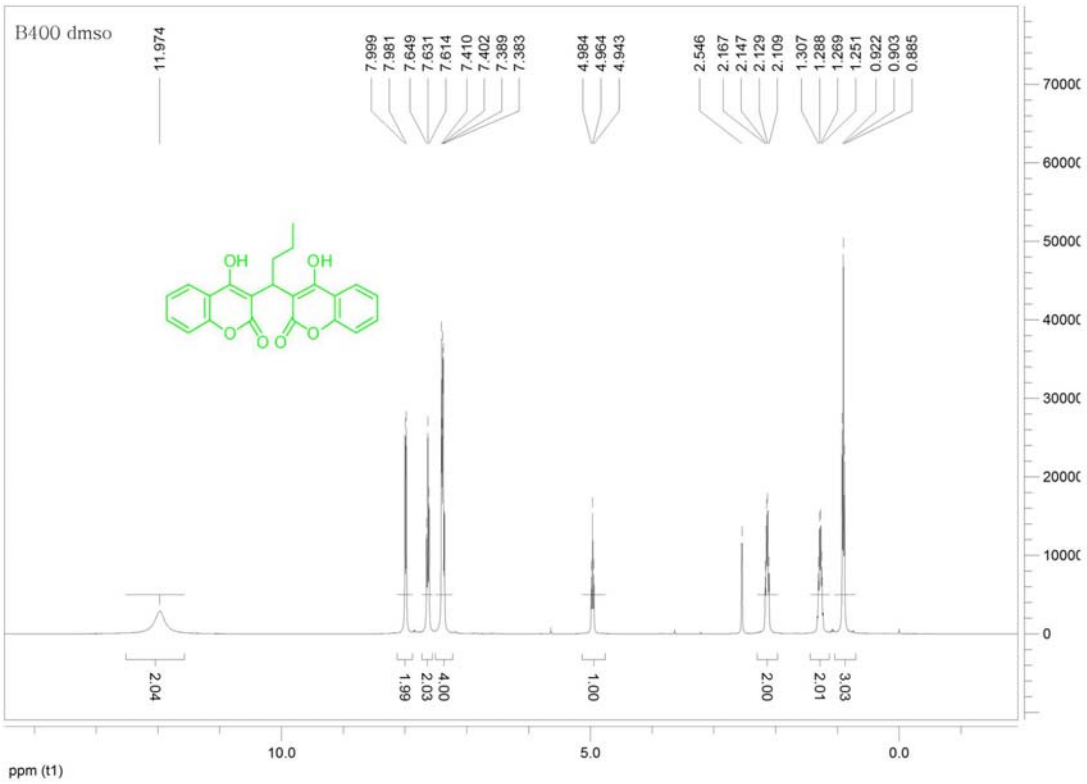
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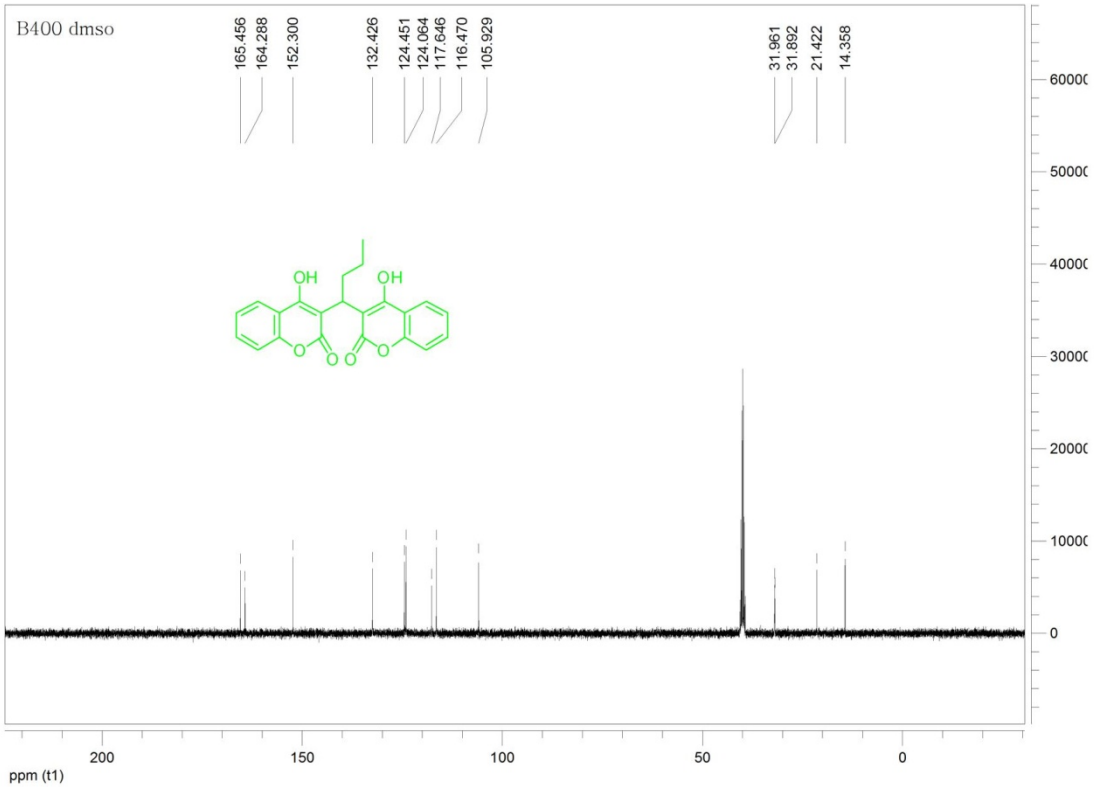
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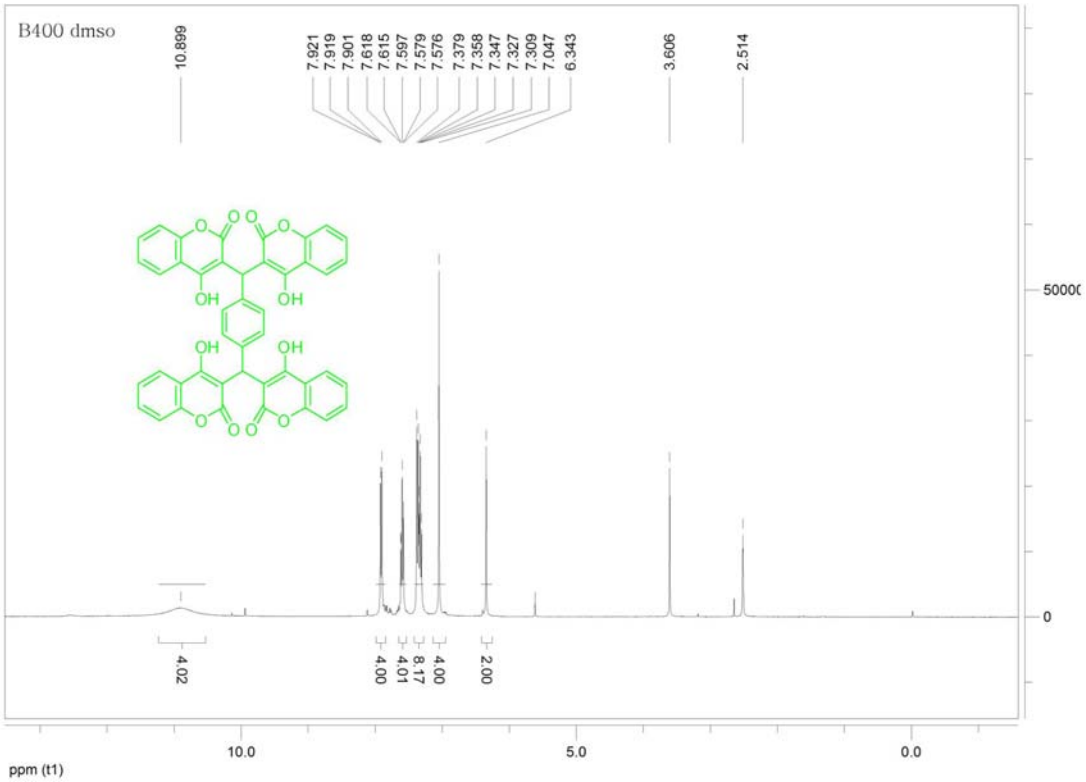
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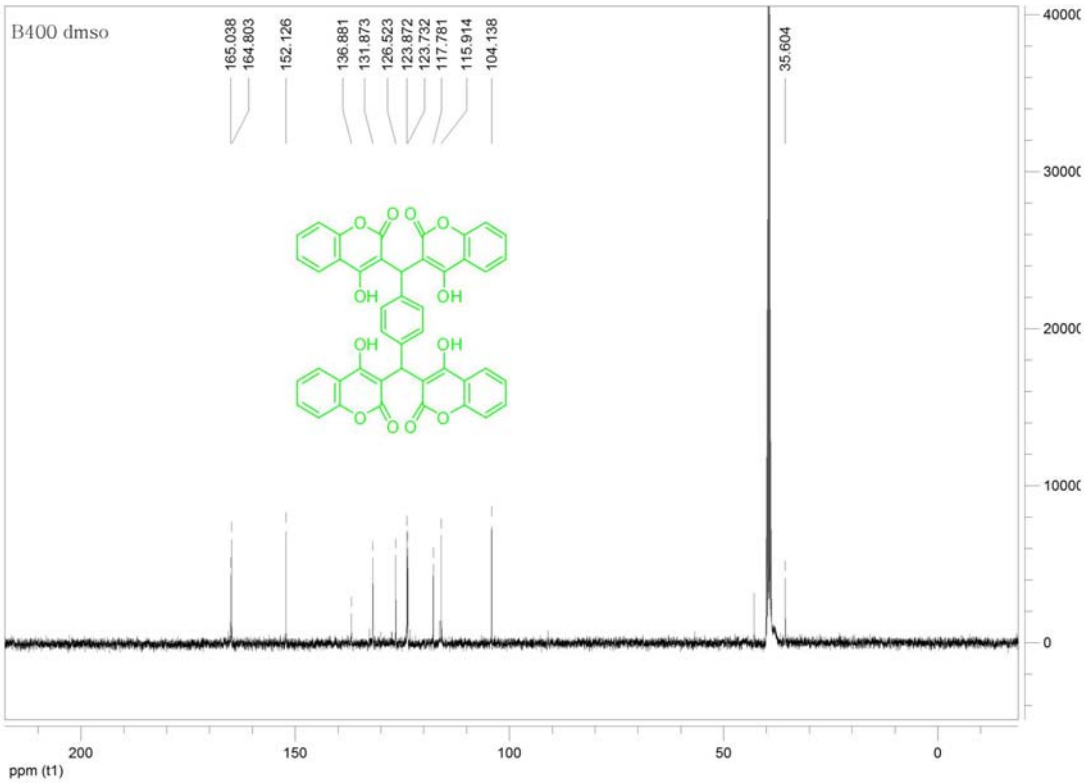
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150
100
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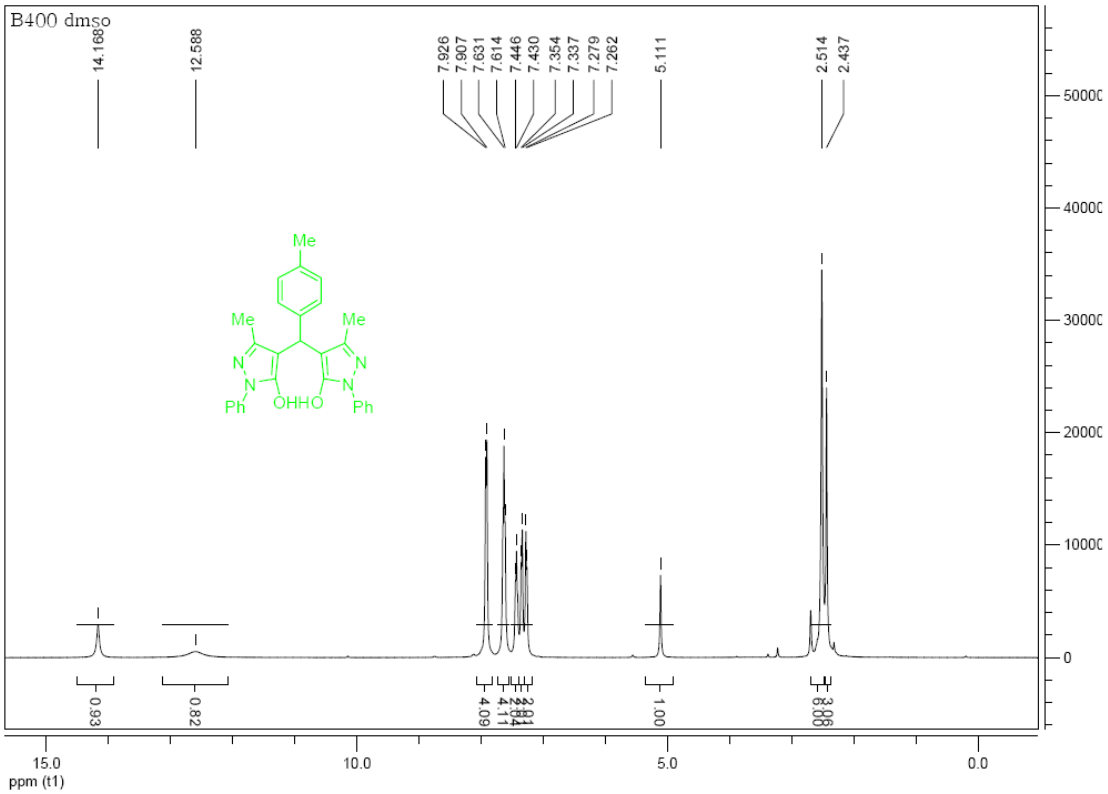
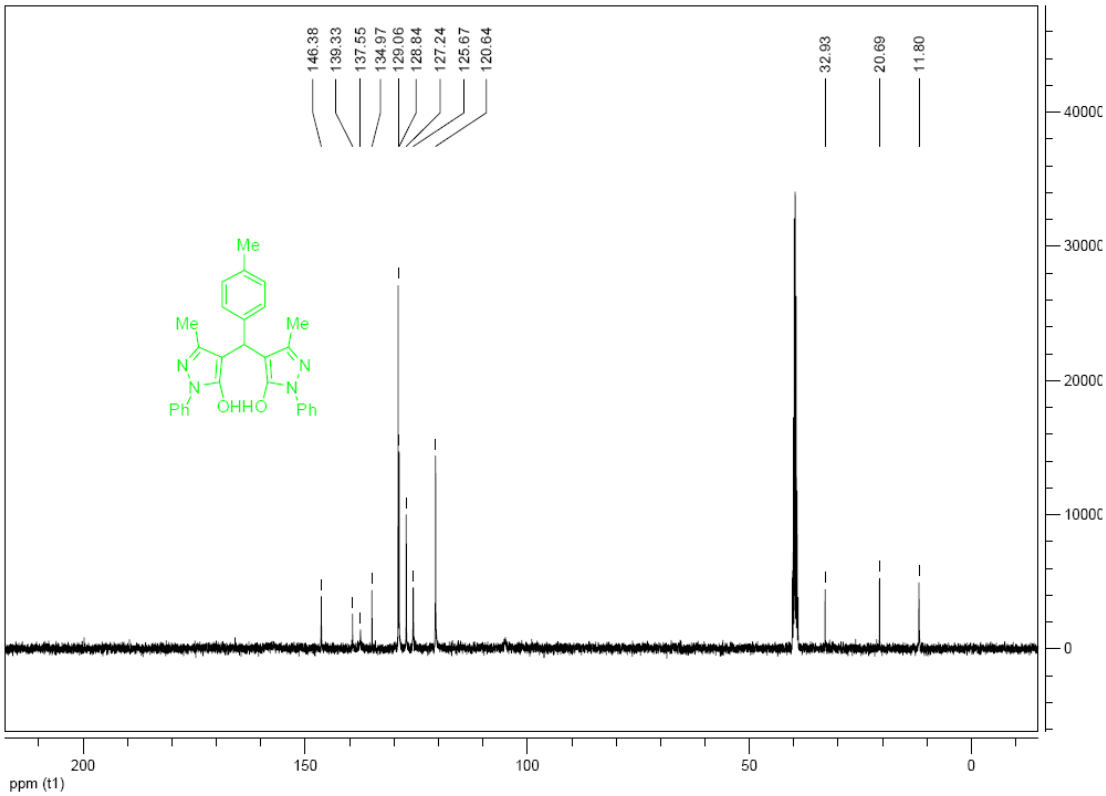
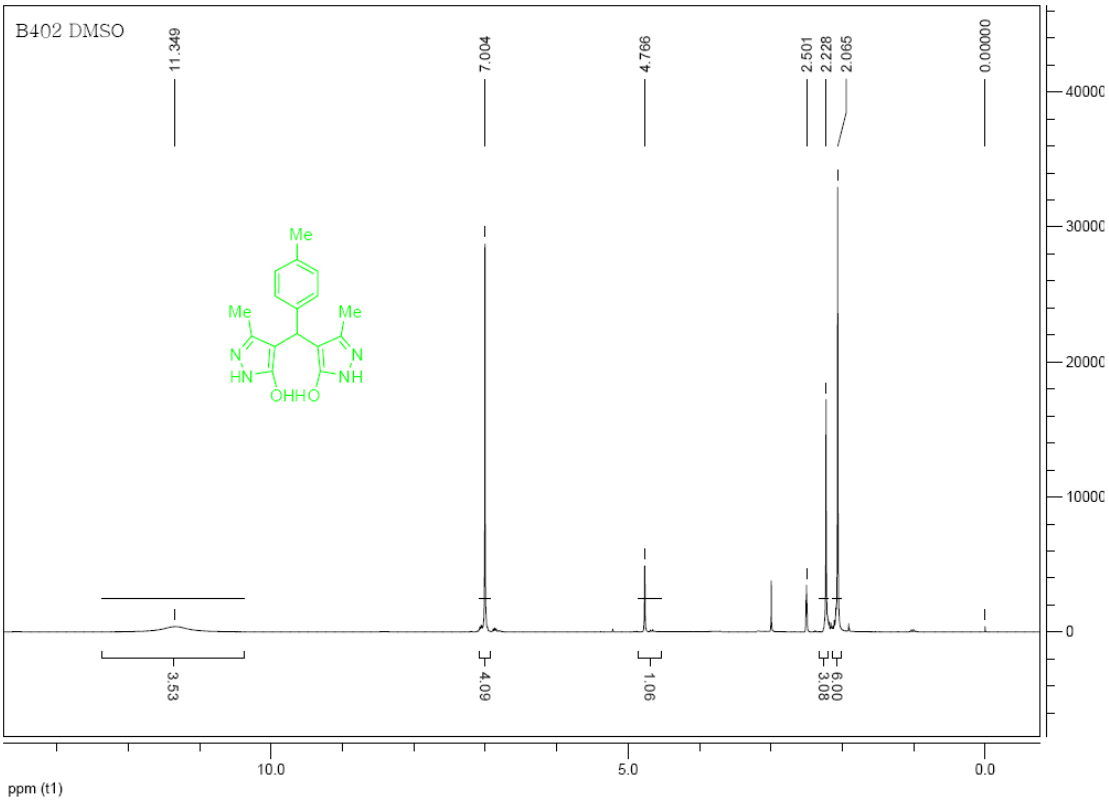
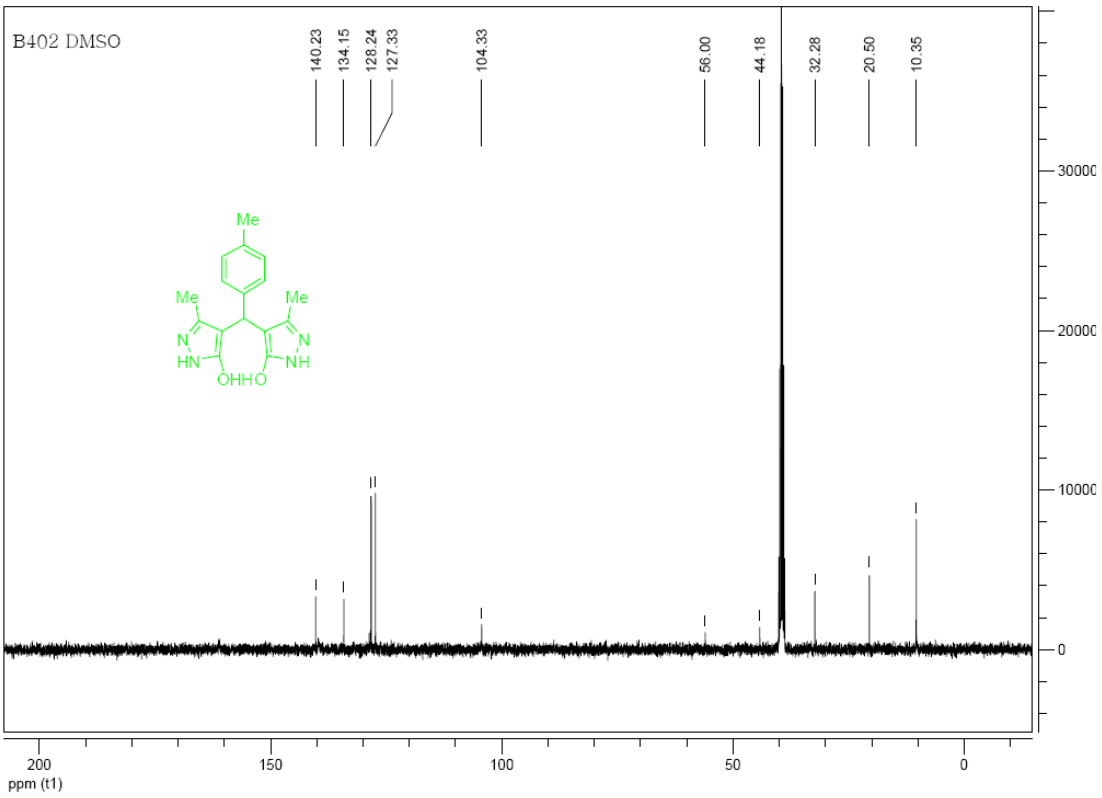
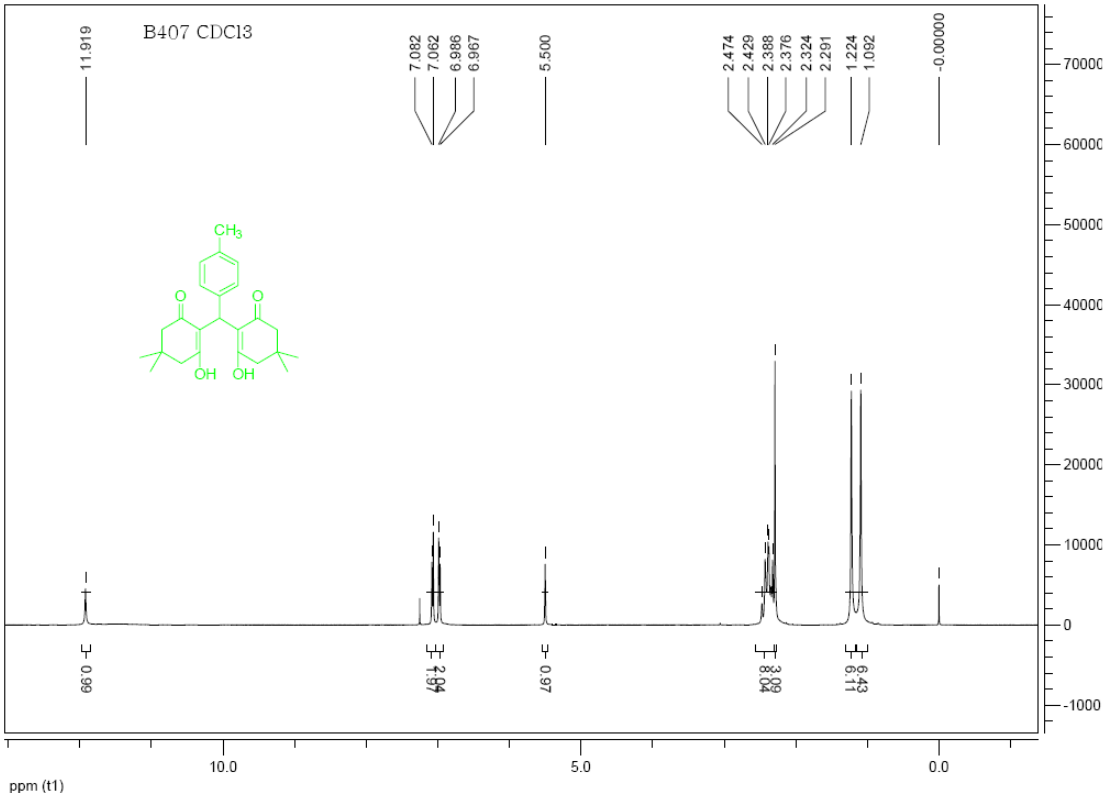
0
ppm (t1)

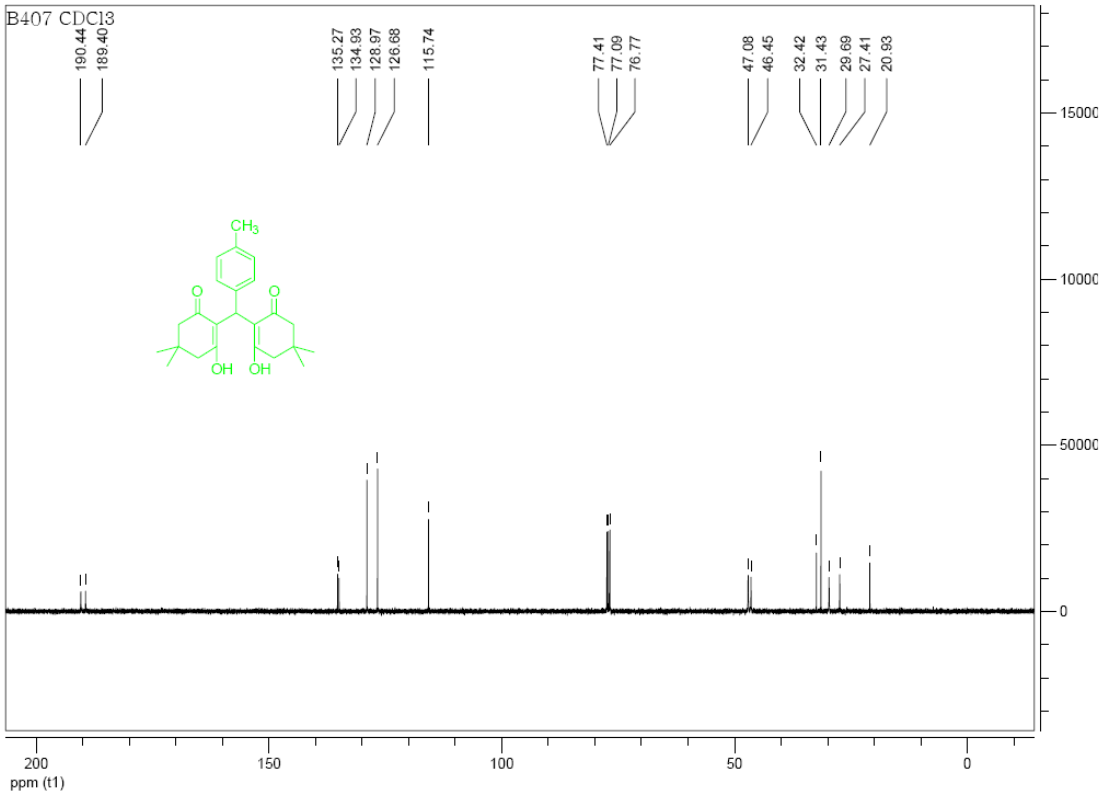

B400 dmso
14.168
12.588
7.926
7.907
7.631
7.614
7.446
7.430
7.354
7.337
7.279
7.262
5.111
2.514
2.437
Me
Me
Me
N
N
Ph
OHHO
Ph
0.93
0.82
4.09
1.00
6.06
15.0
10.0
5.0
0.0
ppm (t1)

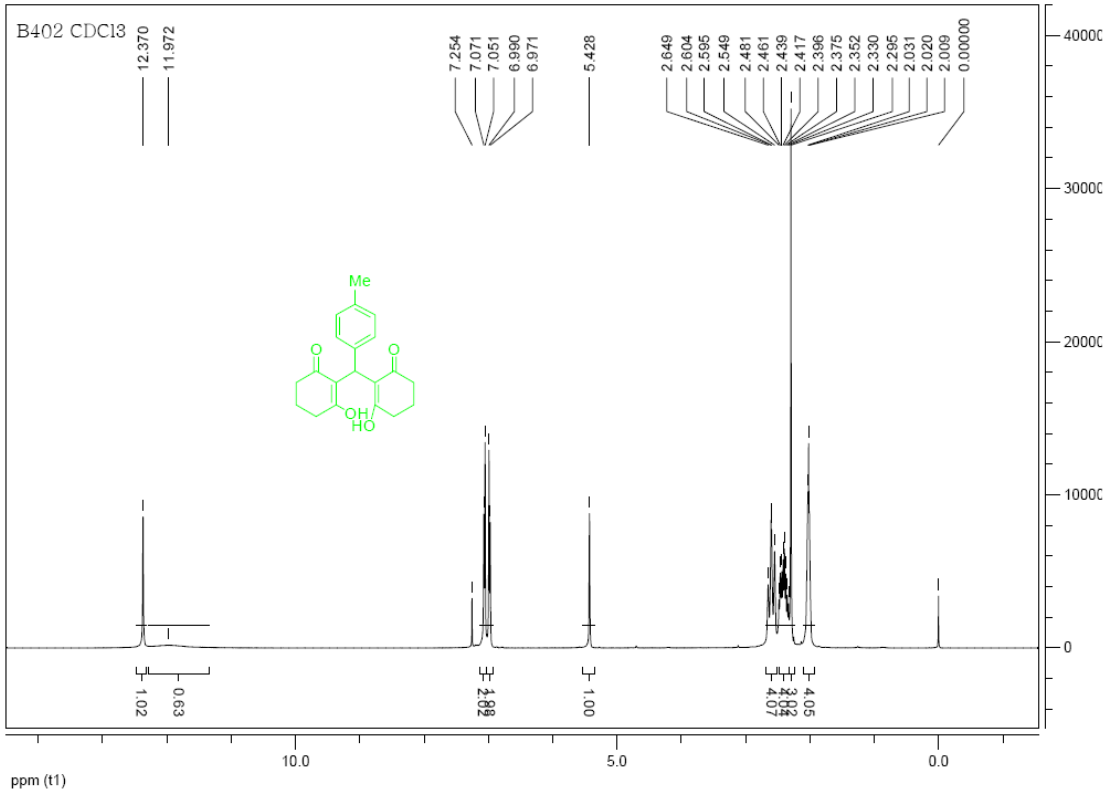

146.38
139.33
137.55
134.97
129.06
128.84
127.24
125.67
120.64
32.93
20.69
11.80
Me
Me
Me
N
N
Ph
OHHO
Ph
200
150
100
50
0
ppm (t1)

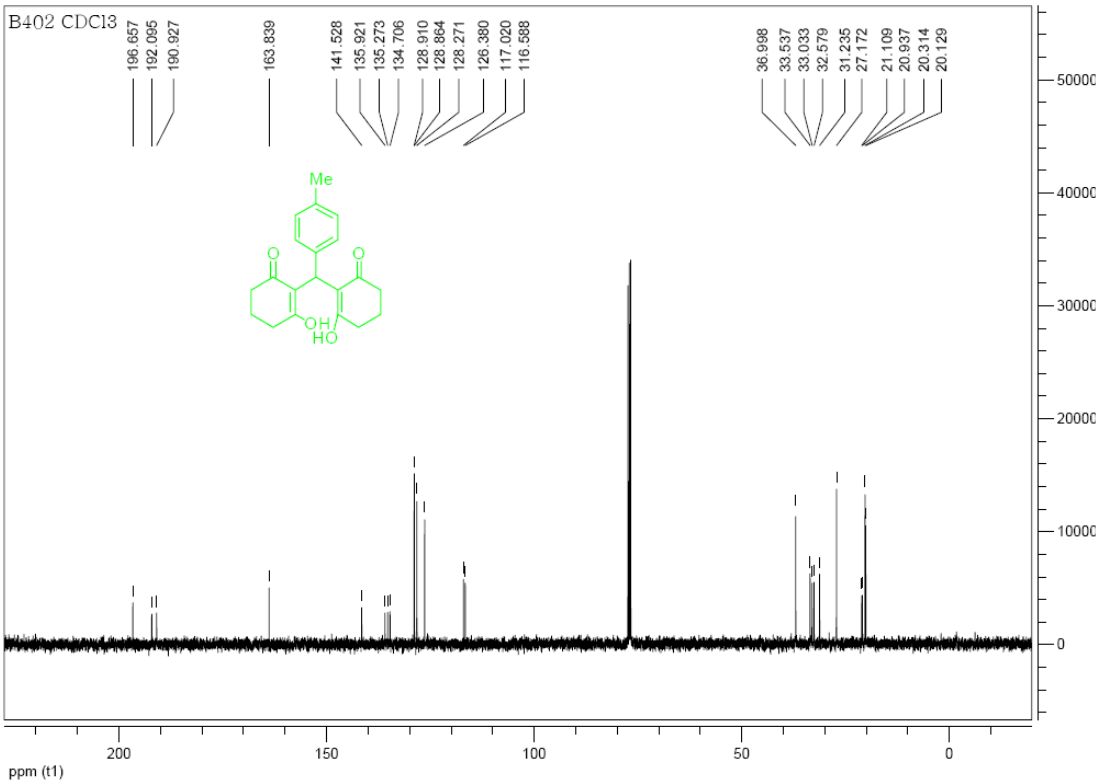

B402 DMSO
11.349
7.004
4.766
2.501
2.228
2.065
0.00000
Me
Me
Me
N
HN
NH
N
OHHO
3.53
4.09
1.06
3.08
6.00
40000
30000
20000
10000
0
10.0
5.0
0.0
ppm (t1)

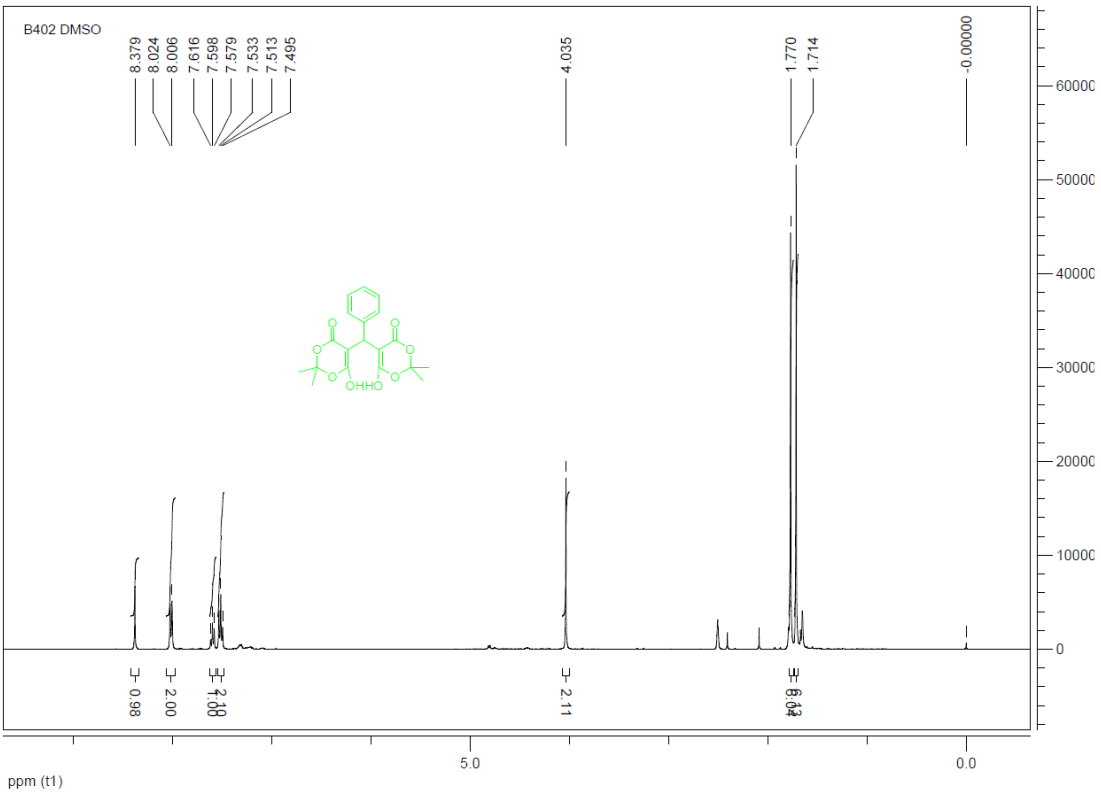

B402 DMSO
140.23
134.15
128.24
127.33
104.33
56.00
44.18
32.28
20.50
10.35
Me
Me
Me
N
HN
NH
N
OHHO
30000
20000
10000
0
200
150
100
50
0
ppm (t1)

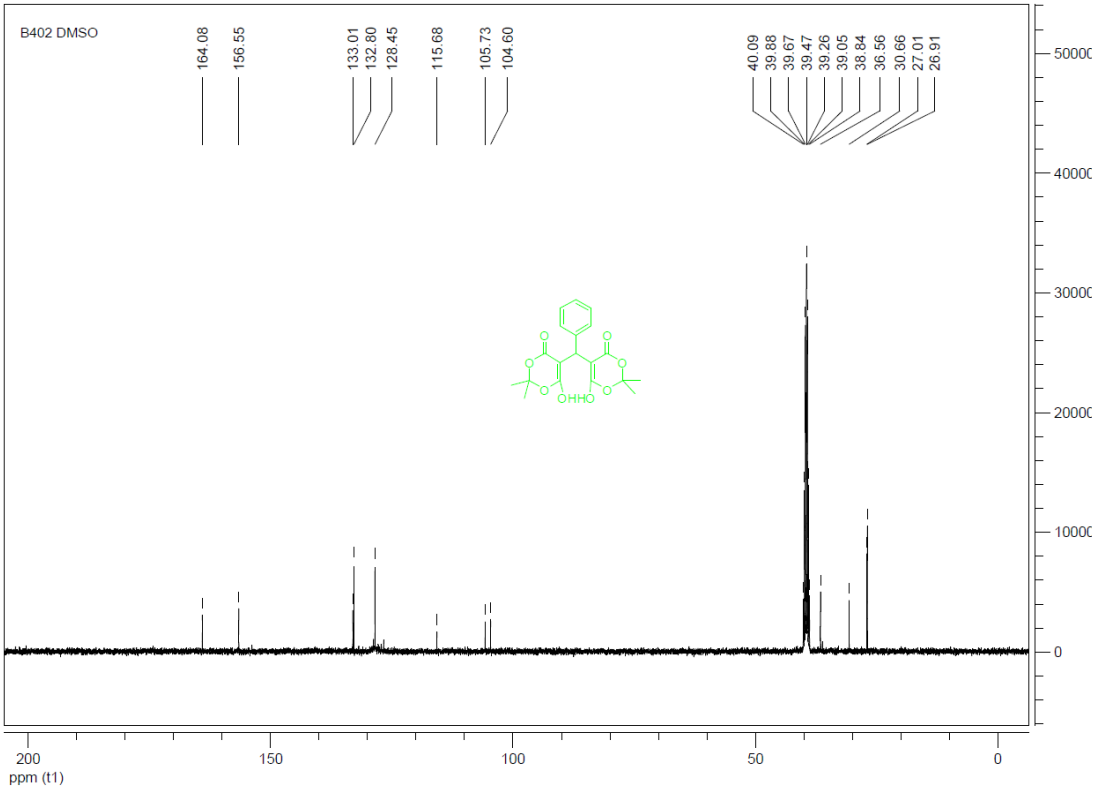

B407 CDCl3
11.919
7.082
7.062
6.986
6.967
5.500
2.474
2.429
2.388
2.376
2.324
2.291
1.224
1.092
-0.00000
CH3
O
O
OH
OH
0.99
2.97
0.97
8.04
6.11
ppm (t1)

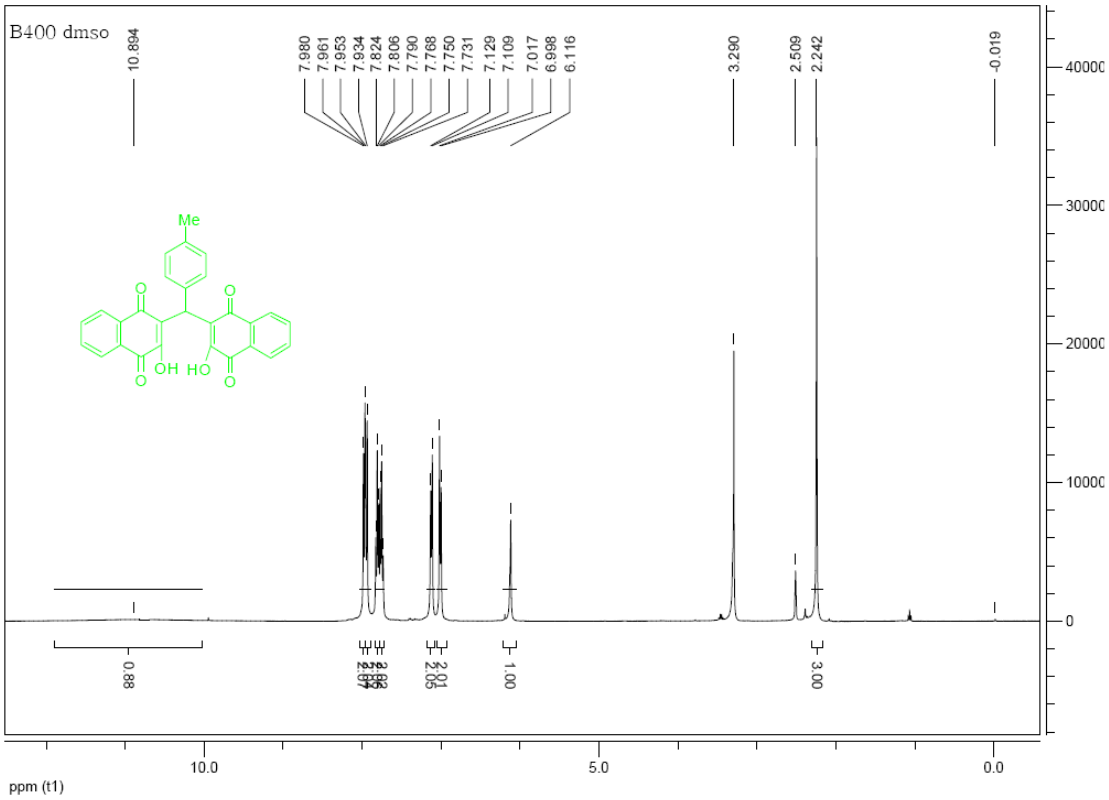

B407 CDCl3
190.44
189.40
135.27
134.93
128.97
126.68
115.74
77.41
77.09
76.77
47.08
46.45
32.42
31.43
29.69
27.41
20.93
CH3
O
O
OH
OH
ppm (t1)

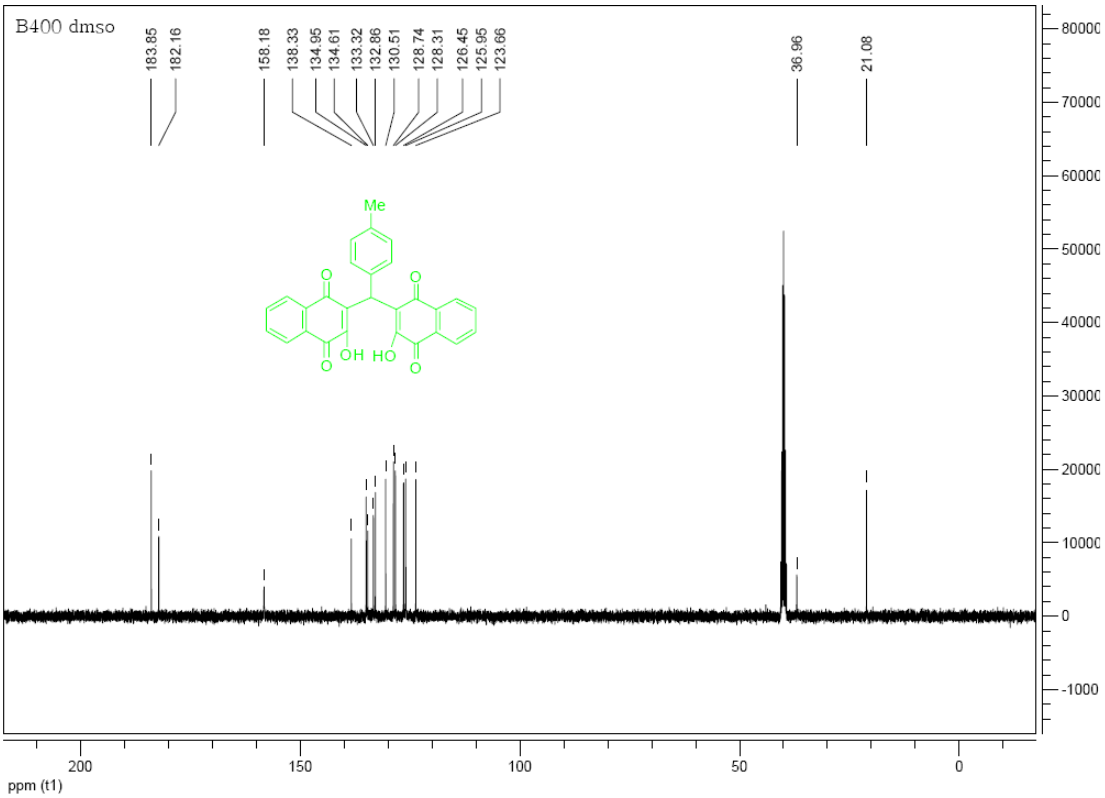

B402 CDCl3
12.370
11.972
7.254
7.071
7.051
6.990
6.971
5.428
2.649
2.604
2.595
2.549
2.481
2.461
2.439
2.417
2.396
2.375
2.352
2.330
2.295
2.031
2.020
2.009
0.00000
Me
O
O
OH
HO
1.02
0.63
2.82
1.00
4.07
4.05
10.0
5.0
0.0
ppm (t1)


B402 CDCl3
196.657
192.095
190.927
163.839
141.528
135.921
135.273
134.706
128.910
128.864
128.271
126.380
117.020
116.588
36.998
33.537
33.033
32.579
31.235
27.172
21.109
20.937
20.314
20.129
Me
O
O
OH
HO
200
150
100
50
0
ppm (t1)


B402 DMSO
8.379
8.024
8.006
7.616
7.598
7.579
7.533
7.513
7.495
4.035
1.770
1.714
-0.00000
OHHO
0.98
2.00
7.08
2.11
6.04
3.13
5.0
0.0
ppm (t1)


B402 DMSO
164.08
156.55
133.01
132.80
128.45
115.68
105.73
104.60
40.09
39.88
39.67
39.47
39.26
39.05
38.84
36.56
30.66
27.01
26.91
OHHO
200
150
100
50
0
ppm (t1)


B400 dmso
10.894
7.980
7.961
7.953
7.934
7.824
7.806
7.790
7.768
7.750
7.731
7.129
7.109
7.017
6.998
6.116
3.290
2.509
2.242
-0.019
Me
OH
HO
0.88
2.01
1.00
3.00
ppm (t1)


B400 dmso
183.85
182.16
158.18
138.33
134.95
134.61
133.32
132.86
130.51
128.74
128.31
126.45
125.95
123.66
36.96
21.08
Me
OH
HO
ppm (t1)