Electronic Supplementary Information for

Enantio- and diastereoselective asymmetric allylic alkylation catalyzed by planar-chiral cyclopentadienyl ruthenium complex

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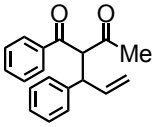
General Information: All reactions were carried out under Ar atmosphere using Schlenk technique, whereas the work up was performed in air. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on Varian Mercury 300, JEOL ECS400 and ECA500 spectrometers. Enantiomeric excess was determined by HPLC analysis using Shimadzu LC-10 and SPD-10AV equipped with DAICEL Chiralcel OJ-H, OD-H, OB-H and Chiralpak AD-H, AS-H columns. Optical rotation was measured on JASCO DIP-1000. HRMS measurements were carried out Thermo Fisher Schientific LTQ-Orbitrap XL.

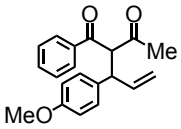
Materials: All solvents used for reactions were passed through purification columns just before use. Planar-chiral Cp'Ru complexes **1** were prepared as reported previously.[1] Cinnamyl chloride **2a** was purchased from TCI. Allylic chlorides were prepared by Corey-Kim chlorination of the corresponding allylic alcohols.[2] All allylic chlorides were purified by distillation using glass tube oven. 1,3-Diketone (**3e**,[3] **3f**,[4] **3g**,[5] **3h**,[6] **3i**,[7] **3j**,[8] **3k**,[9] **3l**[7] and **3m**[10] were synthesized according to the literature procedure.

Standard method of the catalytic reaction. To a solution of cinnamyl chloride (**2a**: 152.6 mg, 1.0 mmol), (*S*)-**1a** (10.0μmol, 2 mol%), $NaHCO_3$ (100.8 mg, 1.20 mmol), and MS 3A (50 mg) in THF (2.0 mL) was added 1-phenylbutene-1,3-dione (**3a**: 81 mg, 0.50 mmol). The mixture was stirred for 24 h at 25 ºC. After dilution with ether, the insoluble parts were filtered off. The solvent was evaporated under reduced pressure and the residue oil was placed on a column of silica gel to give allylic compound **4a**.



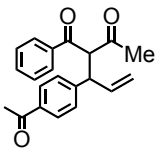
1-phenyl-2-(1-phenylallyl)butane-1,3-dione (4a)

Flash chromatography over silica gel using hexane: ether (20:1) successively to give white solid (99% yield). After recrystallization of the product with hexane, the single diastereomer of **4a** was obtained in 60% yield. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.07 (d, 2H, *J* = 8.4 Hz, Ar), 7.64-7.47 (m, 3H, Ar), 7.36-7.18 (m, 5H, Ar), 5.83 (ddd, 1H, *J* = 17.2, 10.1, 7.0 Hz, -C*H*=CH_2), 5.12 (d, 2H, *J* = 11.3 Hz, PhCHC*H*-), 4.96 (dt, 2H, *J* = 17.2, 1.2 Hz, -CH=CH_2), 4.93 (dt, 1H, *J* = 10.1, 1.2 Hz, =CH_2), 4.49 (dd, 1H, *J* = 11.3, 7.0 Hz, PhC*H*-), 1.94 (s, 3H, -CH_3). ^{13}C NMR ($CDCl_3$, 101 MHz): δ 202.5, 194.3, 139.7, 138.4, 137.1, 133.8, 128.9, 128.6, 128.3, 127.3, 116.3, 68.2, 50.0, 28.0. One carbon peak was missing due to overlapping. HPLC analysis: Chiralcel OJ-H column, 100/4 (v/v), 0.75 mL/min, 254 nm; major enantiomer *t* = 28.0 min, minor enantiomer *t* = 35.2 min. 97% ee (*S*, *S*). $[\alpha]_D^{27}$ = –8.5 (*c* 0.11, $CHCl_3$). Calcd for $C_{19}H_{18}O_2Na$ [M+Na$^+$]: 301.1205, found: *m/z* = 301.1205.



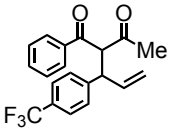
1-phenyl- 2-(1-(4-methoxyphenyl)allyl)butane-1,3-dione (4b)

White solid (99%). ^{1}H NMR ($CDCl_3$, 300 MHz): major diastereomer: δ 8.07 (d, 2H, *J* = 7.2 Hz, Ar), 7.61-7.37 (m, 6H, Ar), 7.21 (d, 2H, *J* = 8.7 Hz, Ar), 6.87 (d, 2H, *J* = 8.7 Hz, Ar), 5.81 (ddd, 1H, *J* = 17.0, 10.3, 7.0 Hz, -C*H*=CH_2), 5.21-4.90 (m, 6H, COC*H*-, -CH=CH_2), 4.44 (dd, 1H, *J* =11.4, 7.0 Hz, ArC*H*-), 3.78 (s, 3H, O -*CH_3*), 1.95 (s, 3H, -*CH_3*). minor diastereomer: δ 7.84 (d, 2H, *J* =7.3 Hz, Ar), 7.61-7.37 (m, 6H, Ar), 7.11 (d, 2H, *J* = 8.7 Hz, Ar), 6.72 (d, 2H, *J* = 8.7 Hz, Ar), 5.98 (ddd, 1H, *J* = 17.0, 10.3, 7.0 Hz, -C*H*=CH_2), 5.21-4.90 (m, 6H, COC*H*-, -CH=CH_2), 4.38 (dd, 1H, *J* = 11.4, 7.0 Hz, ArC*H*-), 3.70 (s, 3H, O -*CH_3*), 2.22 (s, 3H, -*CH_3*). ^{13}C NMR ($CDCl_3$, 101 MHz): δ 202.6, 194.3, 158.6, 138.7, 137.1, 133.7, 131.5, 129.3, 128.8, 128.6, 1 15.8, 114.3, 68.4, 55.2, 49.1, 27.9. $[\alpha]_D^{26}$ = –6.3 (*c* 0.19, $CHCl_3$). Calcd for $C_{20}H_{20}O_3Na$ [M+Na$^+$]: 331.1310, found: *m/z* = 331.1306.



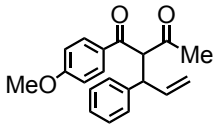
1-phenyl-2-(1-(4-acetylphenyl)allyl)butane-1,3-dione (4c)

White solid (99%). ^{1}H NMR ($CDCl_3$, 300 MHz): major diastereomer: δ 8.08 (d, 2H, *J* = 8.3 Hz, Ar), 7.94 (d, 2H, *J* = 8.3 Hz, Ar), 7.63 (t, 1H, *J* = 7.5 Hz, Ar), 7.52 (t, 2H, *J* = 7.5 Hz, Ar), 7.40 (d, 2H, *J* = 7.5 Hz, Ar), 5.81 (ddd, 1H, *J* = 17.2, 10.0, 7.2 Hz, -C*H*=CH_2), 5.15 (d, 1H, *J* = 11.3 Hz, COC*H*-), 4.98 (d, 1H, *J* = 17.2 Hz, CH=CH_2), 4.98 (d, 1H, *J* = 10.8 Hz, CH=CH_2), 4.56 (dd, 1H, *J* = 11.3, 7.2 Hz, ArC*H*-), 2.59 (s, 3H, CH_3CO-), 1.95 (s, 3H, CH_3). minor diastereomer: δ 7.86 (d, 2H, *J* = 8.5 Hz, Ar), 7.79 (d, 2H, *J* = 8.5 Hz, Ar), 7.52 (t, 1H, *J* = 8.3 Hz, Ar), 7.40 (t, 2H, *J* = 8.3 Hz, Ar), 7.31 (d, 2H, *J* = 8.3 Hz, Ar), 5.98 (ddd, 1H, *J* = 17.0, 10.2, 8.5 Hz, -C*H*=CH_2), 5.22 (d, 1H, *J* = 17.0 Hz, CH=CH_2), 5.16 (d, 1H, *J* = 10.2 Hz, CH=CH_2), 5.09 (d, 1H, *J* = 11.2 Hz, COC*H*-), 4.50 (dd, 1H, *J* = 11.2, 8.5 Hz, ArC*H*-), 2.50 (s, 3H, CH_3CO-), 2.23 (s, 3H, CH_3). ^{13}C NMR ($CDCl_3$, 126 MHz): δ 202.7, 194.3, 158.6, 138.7, 137.1, 133.7, 131.5, 129.3, 128.8, 128.6, 128.5, 115.8, 114.3, 68.4, 55.2, 49.1, 27.9. HPLC analysis: Chiralcel OD-H column, 100/1 (v/v), 1.0 mL/min, 254 nm; major enantiomer *t* = 59.4 min, minor enantiomer *t* = 48.9 min. 93% ee. $[\alpha]_D^{28}$= -16.0 (c 0.20, $CHCl_3$). HRMS (ESI): Calcd for $C_{21}H_{20}O_3Na$ [M+Na$^+$]: 343.1310, found: *m/z* = 343.1309.



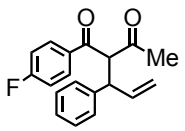
1-phenyl-2-(1-(4-(trifluoromethyl)phenyl)allyl)butane-1,3-dione (4d)

White solid (99%). ^{1}H NMR ($CDCl_3$, 300 MHz): major diastereomer:δ 8.08-8.05 (m, 2H, Ar), 7.65-7.31 (m, 7H, Ar), 5.80 (ddd, 1H, *J* = 17.6, 9.7, 7.0 Hz, -C*H*=CH_2), 5.13 (d, 1H, *J* = 11.4 Hz, COC*H*-), 4.98 (d, 1H, *J* = 9.7 Hz, -CH=CH_2), 4.97 (d, 1H, *J* = 17.6 Hz, -CH=CH_2), 4.56 (dd, 1H, *J* = 11.4, 7.0 Hz, ArC*H*-), 1.98 (s, 3H, -CH_3). minor diastereomer: δ 7.86-7.83 (m, 2H, Ar), 7.65-7.31 (m, 7H, Ar), 5.97 (ddd, 1H, *J* = 17.9, 9.7, 7.0 Hz, -C*H*=CH_2), 5.21 (d, 1H, *J* = 17.9 Hz, -CH=CH_2), 5.06 (d, 1H, *J* = 11.1 Hz, COC*H*-), 4.49 (dd, 1H, *J* = 11.1, 7.0 Hz, ArC*H*-), 2.22 (s, 3H, -CH_3). One proton peak of minor diastereomer was missing due to overlapping with major diastereomer. ^{13}C NMR ($CDCl_3$, 101 MHz):δ 201.7, 193.8, 144.0, 137.4, 136.8, 133.9, 129.4 (q, *J* = 30.8 Hz), 128.9, 128.8, 128.6, 125.7, 123.94 (q, *J* = 273.3 Hz) 117.1, 67.7, 49.5, 28.2. HPLC analysis: Chiralpak AD-H column, 100/4 (v/v), 0.75 mL/min, 254 nm; major enantiomer *t* = 12.8 min, minor enantiomer *t* = 13.6 min. 92% ee. $[\alpha]_D^{26}$ = –49.8 (*c* 0.18, $CHCl_3$). HRMS (ESI): Calcd for $C_{20}H_{17}F_3O_2Na$ [M+Na$^+$]: 369.1078, found: *m/z* = 369.1079.



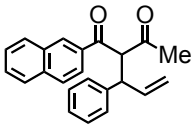
1-(4-methoxyphenyl)-2-(1-phenylallyl)butane-1,3-dione (4e)

White solid (99%). ^{1}H NMR ($CDCl_3$, 300 MHz): major diastereomer: δ 8.07 (d, 2H, *J* = 9.1 Hz, Ar), 7.38-7.18 (m, 5H, Ar), 6.96 (d, 2H, *J* = 9.1 Hz, Ar), 5.82 (ddd, 1H, *J* = 17.1, 10.1, 7.0 Hz, -C*H*=CH_2), 5.06 (d, 1H, *J* = 11.3 Hz, COC*H*-), 4.94 (dt, 1H, *J* = 17.1, 1.4 Hz, -CH=CH_2), 4.93 (dt, 1H, *J* = 10.1, 1.4 Hz, -CH=CH_2), 4.48 (dd, 1H, *J* = 11.3, 7.0 Hz, ArC*H*-), 3.88 (s, 3H, OCH_3), 2.20 (s, 3H, -CH_3). minor diastereomer: δ 7.85 (d, 2H, *J* = 9.1 Hz, Ar), 7.38-7.18 (m, 5H, Ar), 6.84 (d, 2H, *J* = 9.1 Hz, Ar), 6.06 (ddd, 1H, *J* = 17.1, 10.1, 7.0 Hz, -C*H*=CH_2), 5.35 (dt, 1H, *J* = 17.1, 1.4 Hz, -CH=CH_2), 5.20 (dt, 1H, *J* = 10.1, 1.4 Hz, -CH=CH_2), 5.00 (d, 1H, *J* = 11.7 Hz, COC*H*-), 4.42 (dd, 1H, *J* = 11.7, 7.0 Hz, ArC*H*-), 3.82 (s, 3H, OCH_3), 1.94 (s, 3H, CH_3). ^{13}C NMR ($CDCl_3$, 101 MHz): δ 202.9, 192.4, 164.1, 139.7, 138.5, 131.3, 130.0, 128.8, 128.2, 127.1, 116.1, 114.0, 67.8, 55.5, 49.7, 27.7. HPLC analysis: Chiralpak AD-H column, 100/4 (v/v), 0.75 mL/min, 254 nm; major enantiomer *t* = 18.5 min, minor enantiomer *t* = 21.6 min. 92% ee. $[\alpha]_D^{27}$ = –45.0 (*c* 0.27, $CHCl_3$). Calcd for $C_{20}H_{20}O_3Na$ [M+Na$^+$]: 331.1310, found: *m/z* = 331.1310.



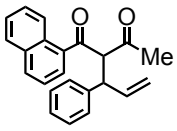
1-(4-fluorophenyl)-2-(1-phenylallyl)butane-1,3-dione (4f)

Yellow solid (88%).^{1}H NMR ($CDCl_3$, 300 MHz): major diastereomer: δ 8.12 (d, 2H, *J* = 8.8 Hz, Ar), 8.11 (d, 2H, *J* = 8.8 Hz, Ar), 7.36-7.01 (m, 5H, Ar), 5.81 (ddd, 1H, *J* = 17.3, 10.0, 7.3 Hz, -C*H*=CH_2), 5.06 (d, 1H, *J* = 11.1 Hz, COC*H*-), 4.95 (d, 1H, *J* = 17.3 Hz, -CH=CH_2), 4.94 (d, 1H, *J* = 10.0 Hz, -CH=CH_2), 4.47 (dd, 1H, *J* = 11.1, 7.3 Hz, ArC*H*-), 1.94 (s, 3H, CH_3). minor diastereomer: δ 7.87 (d, 2H, *J* = 8.8 Hz, Ar), 7.86 (d, 2H, *J* = 8.8 Hz, Ar), 7.36-7.01 (m, 5H, Ar), 5.99 (ddd, 17.3, 10.0, 7.3 Hz, -C*H*=CH_2), 5.20 (d, 1H, *J* = 17.3 Hz, -CH=CH_2), 5.13 (d, 1H, *J* = 10.0 Hz, -CH=CH_2), 5.00 (d, 1H, *J* = 10.9 Hz, COC*H*-), 4.40 (dd, 1H, *J* = 10.9, 7.3 Hz, ArC*H*-), 2.23 (s, 3H, CH_3). ^{13}C NMR ($CDCl_3$, 101 MHz): δ 202.5, 192.7, 167.2, 164.7, 133.5, 131.7, 131.2, 128.9,128.2, 127.4 (d, *J* = 30.8 Hz), 116.3, 116.1, 68.1, 49.9, 27.7. HPLC analysis: Chiralcel OJ-H column, 100/1 (v/v), 0.75 mL/min, 254 nm; major enantiomer *t* = 44.0 min, minor enantiomer *t* = 83.4 min. 86% ee. $[\alpha]_D^{27}$ = 5.2 (*c* 0.14, $CHCl_3$). Calcd for $C_{19}H_{17}O_2FNa$ [M+Na$^+$]: 319.1110, found: *m/z* = 319.1109.



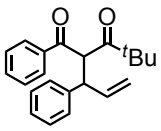
1-(naphthalen-2-yl)-2-(1-phenylallyl)butane-1,3-dione (4g)

White solid (91%).^{1}H NMR ($CDCl_3$, 300 MHz): major diastereomer: δ 8.63 (s, 1H, Ar), 8.09 (d, 1H, *J* = 8.5 Hz, Ar), 8.03 (d, 1H, *J* = 8.5 Hz, Ar), 7.92 (d, 1H, *J* = 8.5 Hz, Ar), 7.88 (d, 1H, *J* = 8.5 Hz, Ar), 7.66-7.51 (m, 2H, Ar), 7.38-7.03 (m, 5H, Ar), 5.86 (ddd, *J* = 17.1, 10.1, 7.0 Hz, -C*H*=CH_2), 5.28 (d, *J* = 11.4 Hz, COC*H*-), 4.99 (d, 1H, *J* = 17.1 Hz, -CH=CH_2), 4.94 (d, 1H, *J* = 10.1 Hz, -CH=CH_2), 4.55 (dd, 1H, *J* = 11.4, 7.0 Hz, ArC*H*-), 1.99 (s, 3H, CH_3). minor diastereomer: δ 8.42 (s, 1H, Ar), 7.66-7.51 (m, 2H, Ar), 7.38-7.03 (m, 2H, Ar), 6.12-5.98 (m, 1H, -C*H*=CH_2), 5.36 (d, 1H, *J* = 17.3 Hz, -C*H*=CH_2), 5.22 (d, 1H, *J* = 11.4 Hz, COC*H*-), 5.15 (d, 1H, *J* = 10.3 Hz, -CH=CH_2), 4.48 (dd, 1H, *J* = 11.4, 7.0 Hz, ArC*H*-), 2.26 (s, 3H, CH_3). Four proton peaks of minor diastereomer were missing due to overlapping with major diastereomer. ^{13}C NMR ($CDCl_3$, 126 MHz): δ 202.6, 194.1, 139.6, 138.4, 135.7, 134.4, 132.4, 131.0, 129.8, 129.0. 128.9, 128.8, 128.3, 127.7, 127.2, 126.9, 124.0, 116.3, 68.2, 50.0, 27.9. HPLC analysis: Chiralcel OD-H column, 100/2 (v/v), 0.75 mL/min, 254 nm; major enantiomer *t* = 19.5 min, minor enantiomer *t* = 17.6 min. 84% ee. $[\alpha]_D^{27}$ = –97.4 (*c* 0.14, $CHCl_3$). Calcd for $C_{23}H_{20}O_2Na$ [M+Na^+]: 351.1361, found: *m/z* = 351.1361.



1-(naphthalen-1-yl)-2-(1-phenylallyl)butane-1,3-dione (4h)

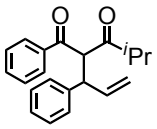
Colorless oil (92%).^{1}H NMR ($CDCl_3$, 300 MHz): δ major diastereomer: δ 8.59 (d, 1H, Ar), 8.13 (d, 1H, *J* = 7.3 Hz, Ar), 8.04 (d, 1H, *J* = 7.3 Hz, Ar), 7.90 (d, 1H, *J* = 7.3 Hz, Ar), 7.66-7.05 (m, 7H, Ar), 5.90 (ddd, *J* = 17.2, 10.0, 7.6 Hz, -C*H*=CH_2), 5.17 (d, *J* = 11.4 Hz, COC*H*-), 5.10 (d, 1H, *J* = 17.2 Hz, -CH=CH_2), 4.97 (d, 1H, *J* = 10.0 Hz, -CH=CH_2), 4.56 (dd, 1H, *J* = 11.4, 7.6 Hz, ArC*H*-), 2.04 (s, 3H, CH_3). minor diastereomer: δ 7.99 (d, 1H, *J* = 7.3 Hz, Ar), 7.79 (d, 1H, *J* = 7.3 Hz, Ar), 7.66-7.05 (m, 7H, Ar), 6.10-5.96 (m, 1H, -C*H*=CH_2), 5.15 (d, 1H, *J* = 10.0 Hz, -CH=CH_2), 5.08 (d, 1H, *J* = 11.1 Hz, COC*H*-), 4.49 (dd, 1H, *J* = 11.1, 7.6 Hz, ArC*H*-), 2.34 (s, 3H, CH_3). Three proton peaks of minor diastereomer were missing due to overlapping with major diastereomer. ^{13}C NMR ($CDCl_3$, 126 MHz): δ 202.9, 197.2, 139.7, 138.3, 133.9, 133.7, 133.2, 130.1, 129.8, 128.9, 128.4, 127.2, 126.7, 125.6, 124.3, 116.6, 71.5, 51.1, 28.4. Two carbon peaks were missing due to overlapping. HPLC analysis: Chiralcel OJ-H column, 200/1 (v/v), 1.0 mL/min, 254 nm; major enantiomer *t* = 106.8 min, minor enantiomer *t* = 90.2 min. 90% ee. $[\alpha]_D^{27}$ = 15.7 (*c* 0.12, $CHCl_3$). Calcd for $C_{23}H_{20}O_2Na$ [M+Na^+]: 351.1361, found: *m/z* = 351.1360.



4,4-dimethyl-1-phenyl-2-(1-phenylallyl)pentane-1,3-dione (4i)

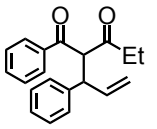
White solid (79%).^{1}H NMR ($CDCl_3$, 300 MHz): major diastereomer: δ 8.07 (d, 2H, *J* = 7.3 Hz, Ar), 7.61 (t, 1H, *J* = 7.3 Hz, Ar), 7.53 (t, 1H, *J* = 7.3 Hz, Ar), 7.33-7.26 (m, 4H, Ar), 5.90 (ddd, 1H, *J* = 16.8, 10.0, 8.9 Hz, -C*H*=CH_2), 5.51 (d, 1H, *J* = 11.0 Hz, COC*H*-), 4.98 (d, 1H, *J* = 16.8 Hz, -CH=CH_2), 4.84 (d, 1H, *J* = 10.0 Hz, -CH=CH_2), 4.43 (dd, 1H, *J* = 11.0, 8.9 Hz, ArC*H*-), 1.06 (s, 9H, ^{t}Bu). minor diastereomer: δ 7.69 (d, 2H, *J* = 7.3 Hz, Ar), 7.42 (t, 1H, *J* = 7.3 Hz, Ar), 7.33-7.26 (m, 3H, Ar), 7.20 (t, 1H, *J* = 7.3 Hz, Ar), 7.10 (t, 2H, *J* = 7.3 Hz, Ar), 6.99 (t, 1H, *J* = 7.3 Hz, Ar), 6.12 (ddd, 1H, *J* = 16.8, 10.5, 8.5 Hz, -C*H*=CH_2), 5.47 (d, 1H, *J* = 10.3 Hz, COC*H*-), 5.09 (d, 1H, *J* = 10.5 Hz, -CH=CH_2), 5.08 (d, 1H, *J* = 16.9 Hz, -CH=CH_2), 4.40 (dd, 1H, *J* = 10.3, 8.5 Hz, ArC*H*-), 0.77 (s, 9H, ^{t}Bu). ^{13}C NMR

($CDCl_3$, 101 MHz): δ 206.4, 194.0, 141.3, 137.5, 137.2, 133.3, 128.8, 128.7, 128.4, 128.2, 126.8, 117.3, 60.5, 52.4, 44.8, 25.8. HPLC analysis: Chiralcel OJ-H column, 100/1 (v/v), 0.75 mL/min, 254 nm; major enantiomer t = 14.6 min, minor enantiomer t = 13.9 min. 70% ee. $[\alpha]_D^{27}$ = –161.9 (c 0.15, $CHCl_3$). Calcd for $C_{22}H_{24}O_2Na$ [M+Na^+]: 343.1674, found: m/z = 343.1673.



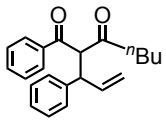
4-methyl-1-phenyl-2-(1-phenylallyl)pentane-1,3-dione (4j)

White solid (93%).^{1}H NMR ($CDCl_3$, 300 MHz): major diastereomer: δ 8.08 (d, 2H, J = 7.1 Hz, Ar), 7.60 (t, 1H, J = 7.1 Hz, Ar), 7.50 (t, 2H, J = 7.1 Hz, Ar), 7.38-7.13 (m, 5H, Ar), 5.86 (ddd, 1H, J = 17.1, 10.1, 7.6 Hz, -C*H*=CH_2), 5.27 (d, 1H, J = 11.0 Hz, COC*H*-), 4.97 (dt, 1H, J = 17.1, 1.1 Hz, -CH=CH_2), 4.92 (dt, 1H, J = 10.0, 1.1 Hz, -CH=CH_2), 4.52 (dd, 1H, J = 11.0, 7.6 Hz, ArC*H*-), 2.57 (hept, 1H, J = 6.9 Hz, C*H*), 0.66 (d, 3H, J = 6.9 Hz, CH_3), 0.64 (d, 3H, J = 6.9 Hz, CH_3). minor diastereomer: δ 7.80 (d, 2H, J = 7.1 Hz, Ar), 7.49 (t, 1H, J = 7.1 Hz, Ar), 7.38-7.03 (m, 7H, Ar), 6.01 (ddd, 1H, J = 17.1, 10.1, 8.2 Hz, -C*H*=CH_2), 5.22 (d, 1H, J = 11.0 Hz, COC*H*-), 5.11 (dt, 1H, J = 17.1, 1.1 Hz, -CH=CH_2), 5.09 (d, 1H, J = 10.1, 1.1 Hz, -CH=CH_2), 4.47 (dd, 1H, J = 11.0, 8.2 Hz, ArC*H*-), 2.87 (hept, 1H, J = 6.9 Hz, C*H*), 1.00 (d, 3H, J = 6.9 Hz, CH_3), 0.99 (d, 3H, J = 6.9 Hz, CH_3). ^{13}C NMR ($CDCl_3$, 101 MHz): δ 207.3, 194.0, 140.4, 138.1, 137.3, 133.5, 128.8, 128.6, 128.4, 126.9, 116.4, 66.2, 50.3, 40.4, 18.5, 17.7. HPLC analysis: Chiralpak AD-H column, 100/1 (v/v), 0.75 mL/min, 254 nm; major enantiomer t = 17.4 min, minor enantiomer t = 18.9 min. 94% ee. $[\alpha]_D^{26}$ = –63.3 (c 0.11, $CHCl_3$). Calcd for $C_{21}H_{22}O_2Na$ [M+Na^+]: 329.1518, found: m/z = 329.1518.



1-phenyl-2-(1-phenylallyl)pentane-1,3-dione (4k)

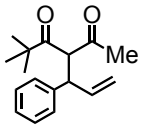
Colorless oil (84%).^{1}H NMR ($CDCl_3$, 300 MHz): major diastereomer: δ 8.07 (d, 2H, J = 7.3 Hz, Ar), 7.60 (t, 1H, J = 7.3 Hz, Ar), 7.50 (t, 2H, J = 7.3 Hz, Ar), 7.39-7.17 (m, 5H, Ar), 5.85 (ddd, 1H, J = 17.2, 10.1, 7.2 Hz, -C*H*=CH_2), 5.14 (d, 1H, J = 11.4 Hz, COC*H*-), 4.96 (dt, 1H, J = 17.2, 1.1 Hz, -CH=CH_2), 4.94 (dt, 1H, J = 10.1, 1.1 Hz, -CH=CH_2), 4.50 (dd, 1H, J = 11.4, 7.2 Hz, ArC*H*-), 2.29 (t, 1H, J = 7.3 Hz, CH_2), 2.26 (t, 1H, J = 7.3 Hz, CH_2), 0.68 (t, 3H, J = 7.3 Hz, CH_3). minor diastereomer: δ 7.83 (d, 2H, J = 7.3 Hz, Ar), 7.39-7.10 (m, 7H, Ar), 5.99 (ddd, 1H, J = 17.2, 10.1, 7.2 Hz, -C*H*=CH_2), 5.10 (d, 1H, J = 11.4 Hz, COC*H*-), 4.45 (dd, 1H, J = 11.4, 7.2 Hz, ArC*H*-), 0.97 (t, 1H, J = 7.3 Hz, CH_2). Five proton peaks of minor diastereomer were missing due to overlapping with major diastereomer. ^{13}C NMR ($CDCl_3$, 101 MHz): δ 204.8, 194.3, 139.9, 138.4, 137.1, 133.7, 128.9, 128.6, 128.5, 128.3, 127.2, 116.3, 67.5, 50.0, 34.6, 7.3. HPLC analysis: Chiralcel OJ-H column, 200/1 (v/v), 0.5 mL/min, 254 nm; major enantiomer t = 61.1 min, minor enantiomer t = 44.5 min. 92% ee. $[\alpha]_D^{27}$ = –7.6 (c 0.18, $CHCl_3$). Calcd for $C_{20}H_{20}O_2Na$ [M+Na^+]: 315.1361, found: m/z = 315.1361.



1-phenyl-2-(1-phenylallyl)heptane-1,3-dione (4l)

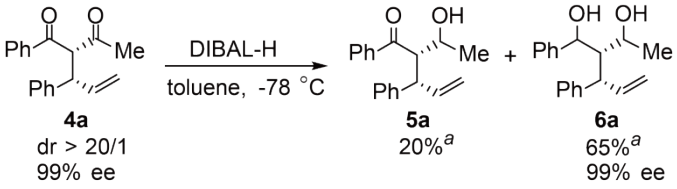
Colorless oil (127 mg, 79%). ^{1}H NMR ($CDCl_3$, 500 MHz): major diastereomer: δ 8.07 (d, 2H, J = 7.5 Hz, Ar), 7.60 (t, 1H, J = 7.5 Hz, Ar), 7.50 (t, 2H, J = 7.5 Hz, Ar), 7.34-7.16 (m, 5H, Ar), 5.84 (ddd, 1H, J = 17.0, 10.1, 7.2 Hz, -C*H*=CH_2), 5.15 (d, 1H, J = 11.0 Hz, COC*H*-), 4.96 (dt, 1H, J = 17.0 Hz, -CH=CH_2), 4.93 (dt, 1H, J = 10.1 Hz, -CH=CH_2), 4.50 (dd, 1H, J = 11.0, 7.2 Hz,

ArC*H*-), 2.25 (t, 1H, *J* = 7.3 Hz, CH_2), 1.23-1.08 (m, 2H, CH_2), 0.95 (hex, 2H, *J* = 7.3 Hz, CH_2), 0.67 (t, 3H, *J* = 7.3 Hz, CH_3). minor diastereomer: δ 7.83 (d, 2H, *J* = 7.5 Hz, Ar), 7.37 (t, 2H, *J* = 7.5 Hz, Ar), 7.34-7.07 (m, 6H, Ar), 5.99 (ddd, 1H, *J* = 17.2, 10.1, 7.2 Hz, -C*H*=CH_2), 5.09 (d, 1H, *J* = 11.1 Hz, COC*H*-), 4.54 (dd, 1H, *J* = 11.0, 7.2 Hz, ArC*H*-), 2.56 (t, 2H, *J* = 7.3 Hz, CH_2), 1.46 (pent, 2H, *J* = 7.3 Hz, CH_2), 1.23-1.08 (m, 2H, CH_2), 0.83 (t, 1H, *J* = 7.3 Hz, CH_2). ^{13}C NMR ($CDCl_3$, 126 MHz): δ 204.3, 194.3, 139.9, 138.5, 137.2, 133.7, 128.8, 128.8, 128.4, 127.1, 116.2, 67.7, 50.0, 40.9, 25.0, 21.7, 13.6. HPLC analysis: Chiralpak AD-H column, 100/1 (v/v), 1.0 mL/min, 254 nm; major enantiomer *t* = 13.6 min, minor enantiomer *t* = 19.2 min. 90% ee. $[\alpha]_D^{32}$= -81.6 (c 0.055, $CHCl_3$). HRMS (ESI): Calcd for $C_{22}H_{24}O_2Na$ [M+Na^+]: 343.1674, found: *m/z* = 343.1673.



5,5-dimethyl-3-(1-phenylallyl)hexane-2,4-dione (4m)

Colorless oil (81%).^{1}H NMR ($CDCl_3$, 300 MHz): major diastereomer: δ 7.39-7.14 (m, 5H, Ar), 5.78 (ddd, 1H, *J* = 17.1, 10.0, 8.0 Hz, -C*H*=CH_2), 5.00 (d, 1H, *J* = 17.1 Hz, -CH=CH_2), 4.98 (d, 1H, *J* = 10.1 Hz, -CH=CH_2), 4.45 (d, 1H, *J* = 11.5 Hz, COC*H*-), 4.22 (dd, 1H, *J* = 11.5, 8.0 Hz, ArC*H*-), 1.88 (s, 3H, CH_3), 1.14 (s, 9H, ^{t}Bu). minor diastereomer: δ 7.39-7.14 (m, 5H, Ar), 6.01 (ddd, 1H, *J* = 17.2, 10.2, 9.0 Hz, -C*H*=CH_2), 5.20 (d, 1H, *J* = 17.2 Hz, -CH=CH_2), 5.12 (d, 1H, *J* = 10.2 Hz, -CH=CH_2), 4.61 (d, 1H, *J* = 11.3 Hz, COC*H*-), 4.18 (dd, 1H, *J* = 11.3, 9.0 Hz, ArC*H*-), 2.19 (s, 3H, CH_3), 0.75 (s, 9H, ^{t}Bu). ^{13}C NMR ($CDCl_3$, 101 MHz): δ 208.7, 203.5, 140.6, 138.6, 128.9, 128.1, 127.2, 116.8, 70.2, 51.8, 45.8, 27.4, 26.0. HPLC analysis: Chiralcel OJ-H column, 100/1 (v/v), 0.75 mL/min, 254 nm; major enantiomer *t* = 11.5 min, minor enantiomer *t* = 15.2 min. 92% ee. $[\alpha]_D^{26}$ = –15.4 (*c* 0.12, $CHCl_3$). Calcd for $C_{17}H_{22}O_2Na$ [M+Na^+]: 281.1518, found: *m/z* = 281.1513.



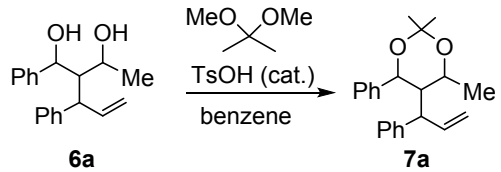
The diastereoselective reduction of 4a: To a toluene solution (0.25 mL) of **4a** (30 mg, 0.11 mmol) was

added dropwise a 1.0 M toluene solution of diisobutylaluminium hydride (0.5 mL, 0.5 mmol) at –78 ºC, and the mixture was stirred for 1 h. The reaction was warmed to room temperature, and stirred for 12 h. The mixture was cooled to -78 ºC and, quenched by the addition of a saturated potassium sodium tartrate solution (5.0 mL) and the mixture was allowed to warm to room temperature and stirred for 1 h. The reaction mixture was extracted with ethyl acetate. Combined organic layer was washed with brine and dried over Na_2SO_4. The solvent was removed by evaporation to give yellow oil. The oil was purified by silica gel column chromatography (eluent: dichloromethane/ethyl acetate = 8/2) to give colorless oil of **5a** (4 mg, 26%) and **6a** (20 mg, 65%).

2-(1-hydroxyethyl)-1,3-diphenylpent-4-en-1-one (5a): White solid (26%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.96 (dd, 2H, *J* = 7.3, 1.3 Hz, Ar), 7.61 (dt, 1H, *J* = 7.3, 1.3 Hz, Ar), 7.51 (t, 2H, *J* = 7.3 Hz, Ar), 7.38-7.35 (m, 4H, Ar), 7.20-7.23 (m, 1H, Ar), 5.89 (ddd, 1H, *J* = 16.9, 10.1, 8.9 Hz, -C*H*=CH_2), 4.97 (dt, 1H, *J* = 16.9, 1.3 Hz, -CH=CH_2), 4.83 (ddd, 1H, *J* = 10.1, 1.3, 0.7 Hz, -CH=CH_2), 4.07 (t, 1H, *J* = 11.0 Hz, -C*H*Ph), 3.89 (dd, 1H, *J* = 11.0, 2.8 Hz, C*H*), 3.63 (m, 1H, -(OH)C*H*CH_3), 3.21 (d, 1H, *J* = 10.7 Hz, -(O*H*)$CHCH_3$), 1.05 (d, 3H, *J* = 6.6 Hz, -(OH)CHCH_3). ^{13}C NMR ($CDCl_3$, 101 MHz): δ 206.4, 141.4, 139.1, 138.5, 133.6, 128.8, 128.4, 128.2, 126.9, 116.7, 77.2, 670 54.5, 51.0, 22.9.

1-phenyl-2-(1-phenylallyl)butane-1,3-diol (6a): Colorless oil (65%).^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.40-7.18 (m, 10H, Ar), 5.58 (ddd, 1H, *J* = 17.0, 10.1, 8.7 Hz, -C*H*=CH_2), 5.35 (br, 1H, -(OH)C*H*Ph), 4.82 (ddd, 1H, *J* = 17.0, 1.6, 1.1. Hz, -CH=CH_2), 4.69(ddd, 1H, *J* =10.1, 1.6, 0.7 Hz, -CH=CH_2), 3.98 (qd, 1H, *J* = 6.5, 2.3 Hz, -(OH)C*H*CH_3), 3.91 (t, 1H, *J* = 8.5 Hz, -C*H*Ph), 3.46 (br, 1H, -(O*H*)CHPh), 2.26 (dt, 1H, *J* = 8.5, 2.3 Hz, C*H*), 1.94 (br, 1H, -(O*H*)$CHCH_3$), 1.27 (d, 3H, *J* = 6.5 Hz, CH_3), ^{13}C NMR ($CDCl_3$, 101 MHz): δ 143.7, 143.6, 140.9, 128.7, 128.3, 128.0, 126.6, 126.4, 126.2, 114.8, 71.6, 68.6, 53.9, 48.0, 22.2. HPLC analysis: Chiralcel OJ-H column, 90/10 (v/v), 0.5 mL/min, 230 nm; major enantiomer *t* = 17.2 min, minor enantiomer *t* = 21.9 min. 99% ee. $[\alpha]_D^{21}$ = –13.5 (*c* 0.16, $CHCl_3$). Calcd for $C_{19}H_{22}O_2Na$ [M+Na^+]: 305.1518, found: *m/z* = 281.1515.

<u>Determination of the relative configuration of 6a by Rychnovsky's method.</u>

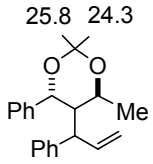


6a **7a**

Synthesis of 7: A solution of **6a** (46 mg, 0.16 mmol), 2,2-dimethoxypropane (1.0 mL) and a catalytic amount of *p*-toluenesulfonic acid in benzene (1.0 mL) was stirred for 4 h at room temperature. To the solution was added sodium hydrogen carbonate aqueous solution, and the mixture was diluted with ethyl acetate, and the organic layer was washed with water and dried with Na_2SO_4. After removal of the solvents, the residue was purified by silica gel column chromatography (*n*-hexane/diethyl ether = 50/1) to give

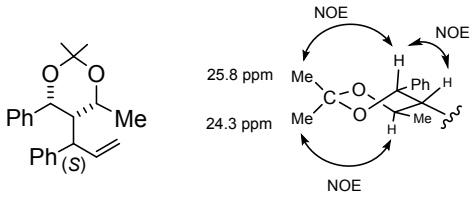
colorless oil (50 mg, 98%). ^{1}H NMR ($CDCl_3$, 400 MHz): 7.22-7.05 (m, 8H, Ar), 6.90 (d, 2H, *J* = 6.9 Hz, Ar), 5.77 (ddd, 1H, *J* = 16.9, 10.2, 8.9 Hz, -C*H*=CH_2), 5.26 (d, 1H, *J* = 4.4 Hz, -CHC*H*(-O)Ph), 4.61 (dd, 1H, *J* = 10.2, 1.4 Hz, -CH=CH_2), 4.56 (dd, 1H, *J* = 16.9, 1.4 Hz, -CH=CH_2), 3.73 (quin, 1H, *J* = 6.4 Hz, -C*H*C(-O)CH_3), 3.45 (dd, 1H, *J* = 8.9, 6.4 Hz, PhC*H*-), 2.38 (td, 1H, *J* = 6.4, 4.4 Hz, -CH(-C*H*)CH-), 1.40 (s, 3H, CH_3), 1.34 (s, 3H, CH_3), 1.16 (d, 3H, *J* = 6.4 Hz, -CHC(-O)CH_3), ^{13}C NMR ($CDCl_3$, 101 MHz): 145.5, 140.0, 139.8, 128.2, 128.0, 127.6, 126.4, 125.7, 114.4, 100.9, 69.9, 67.7, 53.5, 48.9, 25.8, 24.3, 21.8. Two carbon peaks were missing due to overlapping. $[\alpha]_D^{25}$ = +10.5 (*c* 0.29, $CHCl_3$). Calcd for $C_{22}H_{26}O_2Na$ [M+Na^+]: 345.1830, found: *m/z* = 345.1829.

^{13}C chemical shifts of methyl groups in 1,3-diol acetonides.



<u>Determination of the absolute configuration of 7 by NOE analysis.</u>

2,2,4-trimethyl-6-phenyl-5-((*S*)-1-phenylallyl)-1,3-dioxane (7)



NOESY Spectrum of 7

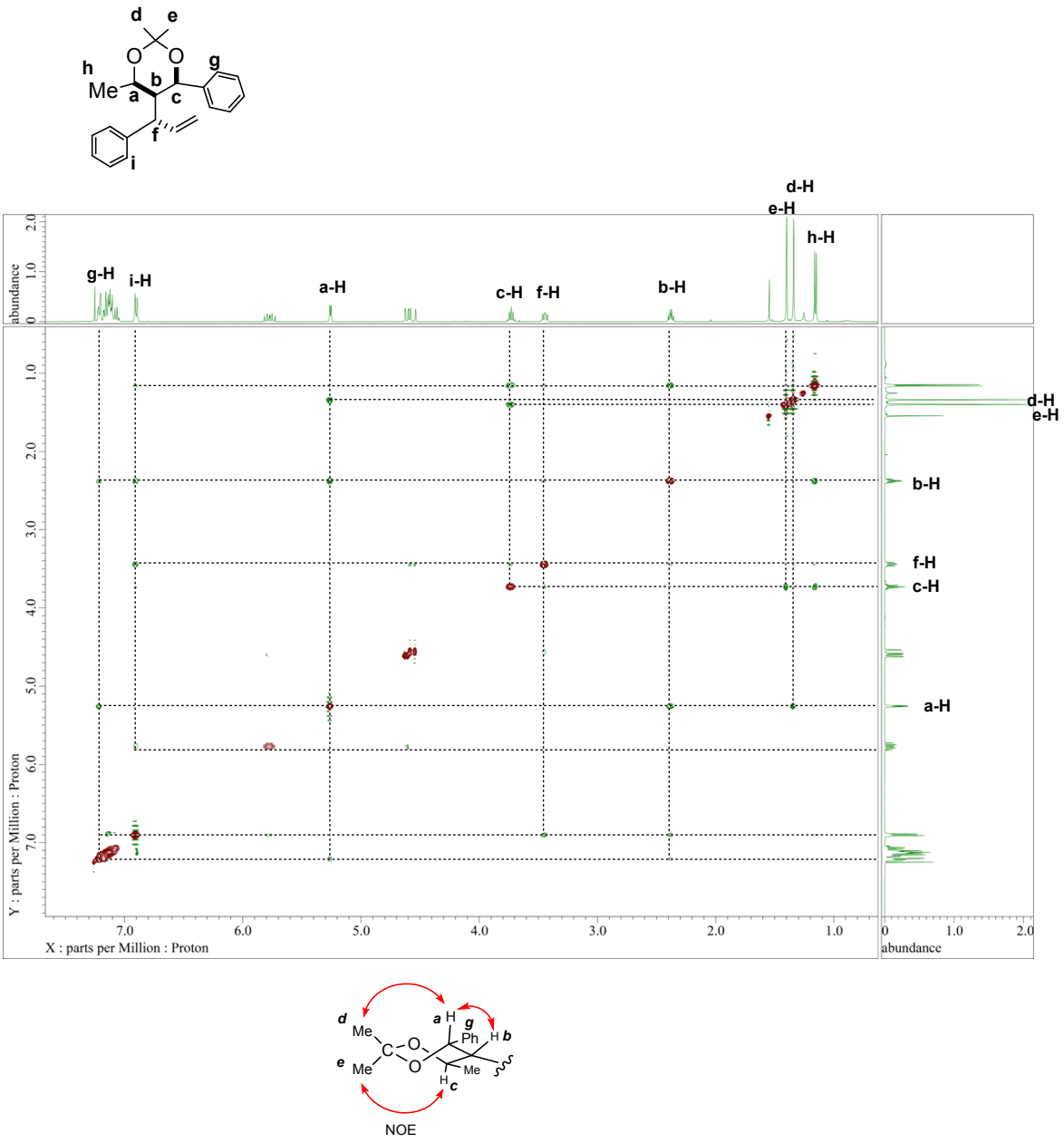


Figure S1. NOESY (400 MHz, in $CDCl_3$ at 303 K) spectrum of **7**.

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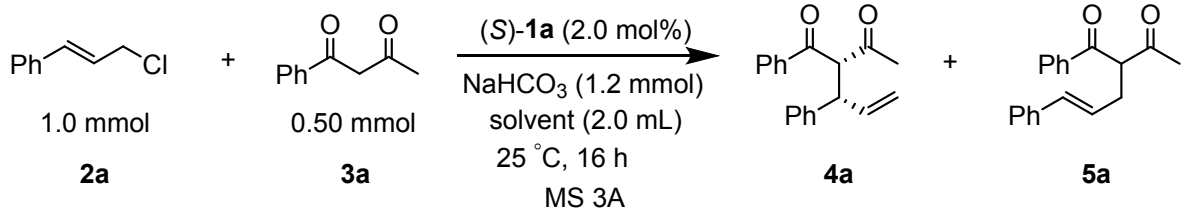
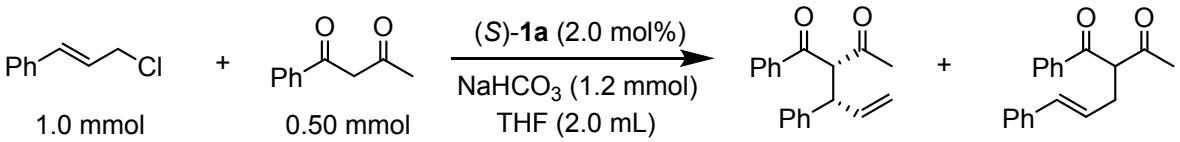
Table S1. Screening of Solvent[a].



entry	solvent	yield[b]	**4a**/**5a**[b]	dr of **4a**[b]	ee of **4a**[c]
1	THF	99	>20/1	5/1	97
2	Dioxane	99	>20/1	3/1	91
3	DME	99	>20/1	6/1	89
4	Acetone	92	>20/1	6/1	84
5	DMF	99	>20/1	1/1	94
6	CH_2Cl_2	99	>20/1	3/1	79
7	Toluene	trace	–	–	–

[a]cat/$NaHCO_3$/**2a**/**3a** = 0.0072/1.2/0.50/1.0 mmol in solvent (2.0 mL) at 25 °C. [b]Determined by ^1H NMR spectroscopic analysis of crude reaction mixtures. [c]Determined by HPLC analysis on a chiral stationary phase.

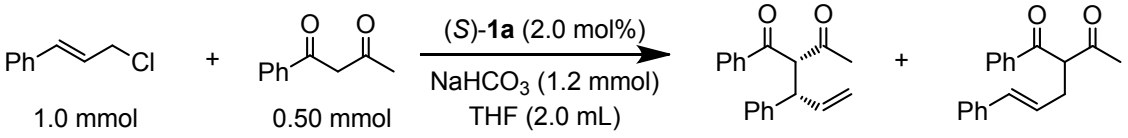
Table S2. Effect of Temperature[a].



entry	temperature (°C)	yield[b]	**4a**/**5a**[b]	dr of **4a**[b]	ee of **4a**[c]
1	30	99	>20/1	5/1	93
2	25	99	>20/1	5/1	97
3	20	99	>20/1	5/1	93
4	15	99	>20/1	6/1	95
5[d]	10	99	>20/1	6/1	91
6[d]	5	99	>20/1	6/1	92
7[e]	0	99	>20/1	7/1	92

[a]cat/$NaHCO_3$/**2a**/**3a** = 0.0072/1.2/0.50/1.0 mmol in THF (2.0 mL). [b]Determined by ^1H NMR spectroscopic analysis of crude reaction mixtures. [c]Determined by HPLC analysis on a chiral stationary phase.[d]Reaction time for 2 days. [e]Reaction time for 3 days.

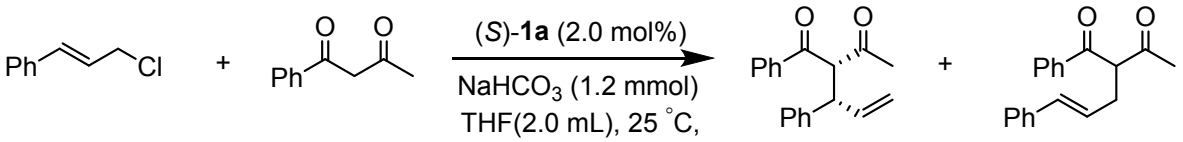
Table S3. Screening of Reaction Time[a].



entry	Reaction time (h)	yield(%)[b]	**4a**/**5a**[b]	dr of **4a**[b]	ee of **4a**[c]
1	4	42	>20/1	5/1	–
2	8	94	>20/1	5/1	90
3	12	99	>20/1	5/1	95
4	24	99	>20/1	5/1	97

[a]cat/$NaHCO_3$/**2a**/**3a** = 0.0072/1.2/0.50/1.0 mmol in THF (2.0 mL) at 25 °C. [b]Determined by ^1H NMR spectroscopic analysis of crude reaction mixtures. [c]Determined by HPLC analysis on a chiral stationary phase.

Table S4. Stoichiometry of Substarates[a].

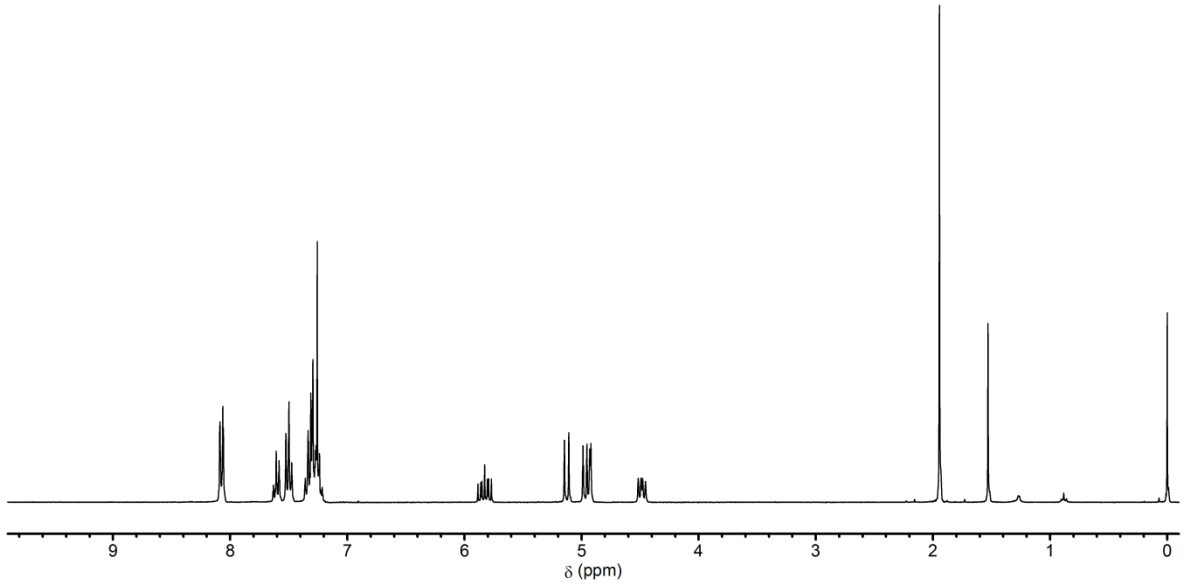


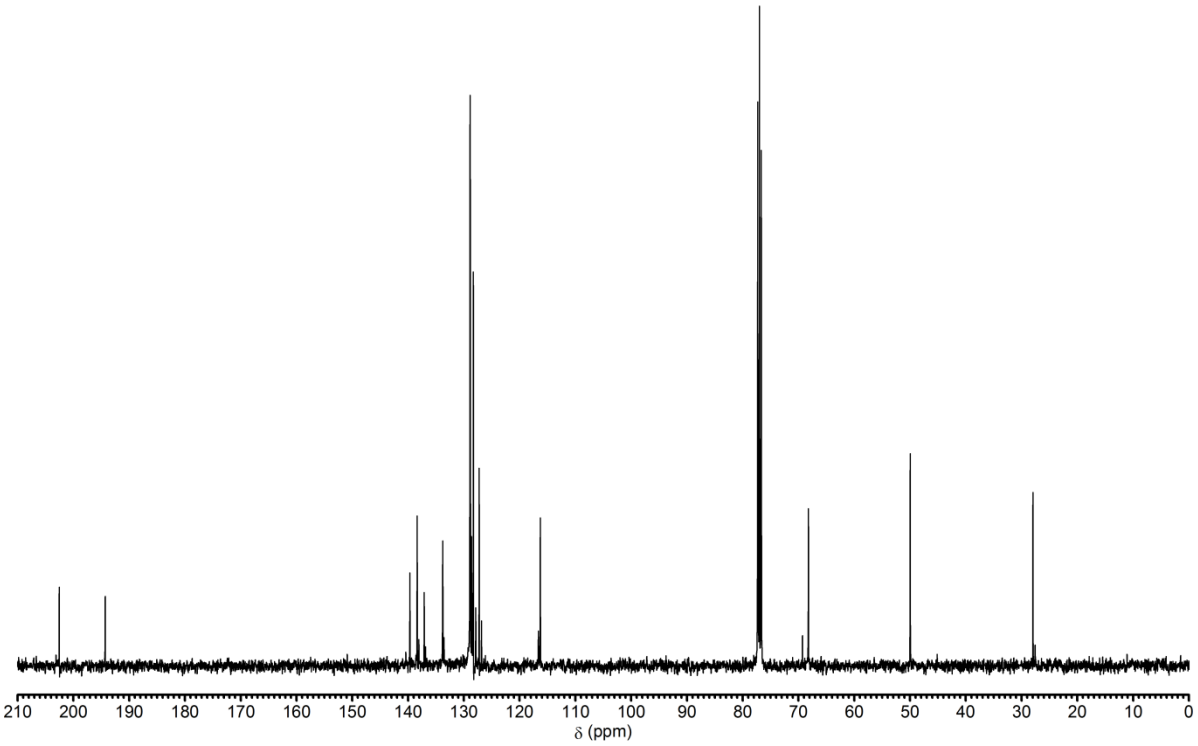
2a **3a** **4a** **5a**

entry	**2a** : **3a** (mmol)	yield(%)[b]	**4a**/**5a**[b]	dr of **4a**[b]	ee of **4a**[c]
1	1.0 : 0.50	99	>20/1	5/1	97
2	0.60 : 0.50	90	>20/1	5/1	91
3	0.50 : 1.0	90	>20/1	5/1	96

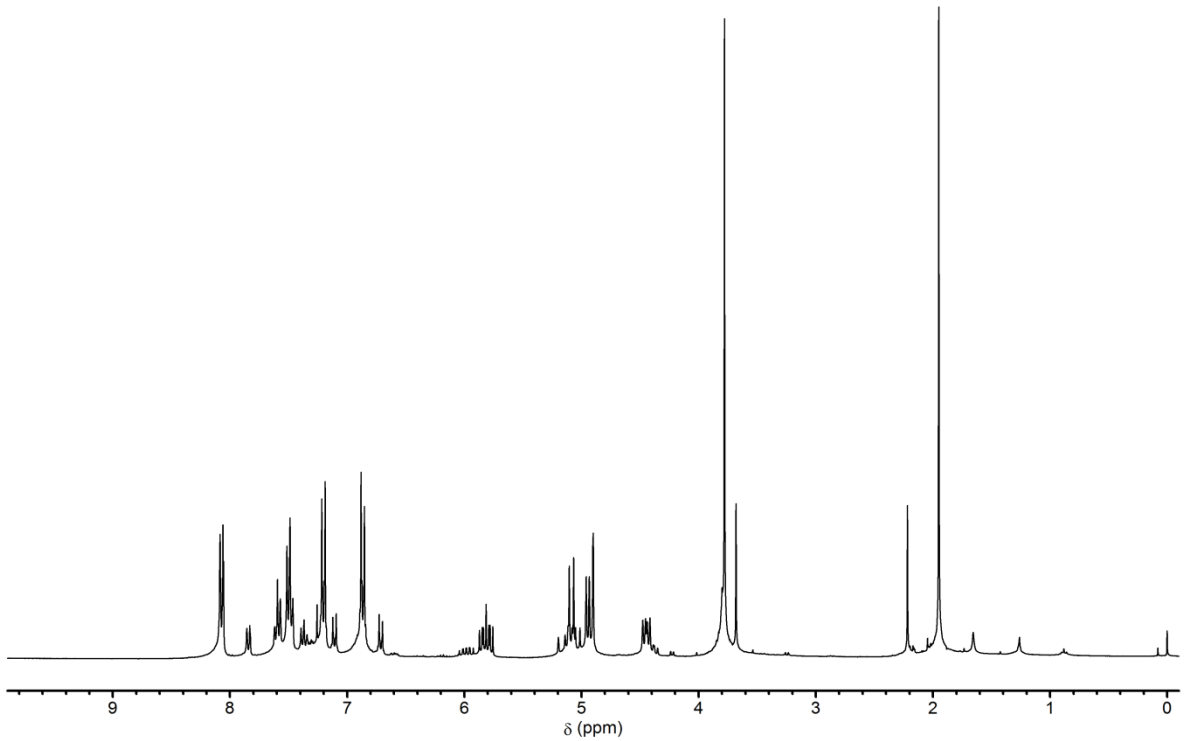
[a]cat/$NaHCO_3$ = 0.0072/1.2 mmol in THF (2.0 mL) at 25 °C. [b]Determined by ^1H NMR spectroscopic analysis of crude reaction mixtures. [c]Determined by HPLC analysis on a chiral stationary phase.

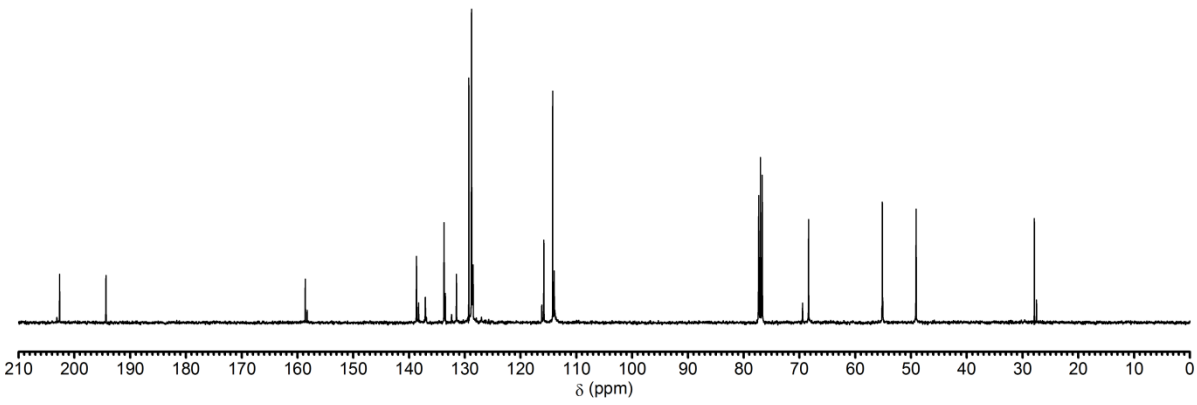
1-phenyl-2-(1-phenylallyl)butane-1,3-dione (4a)



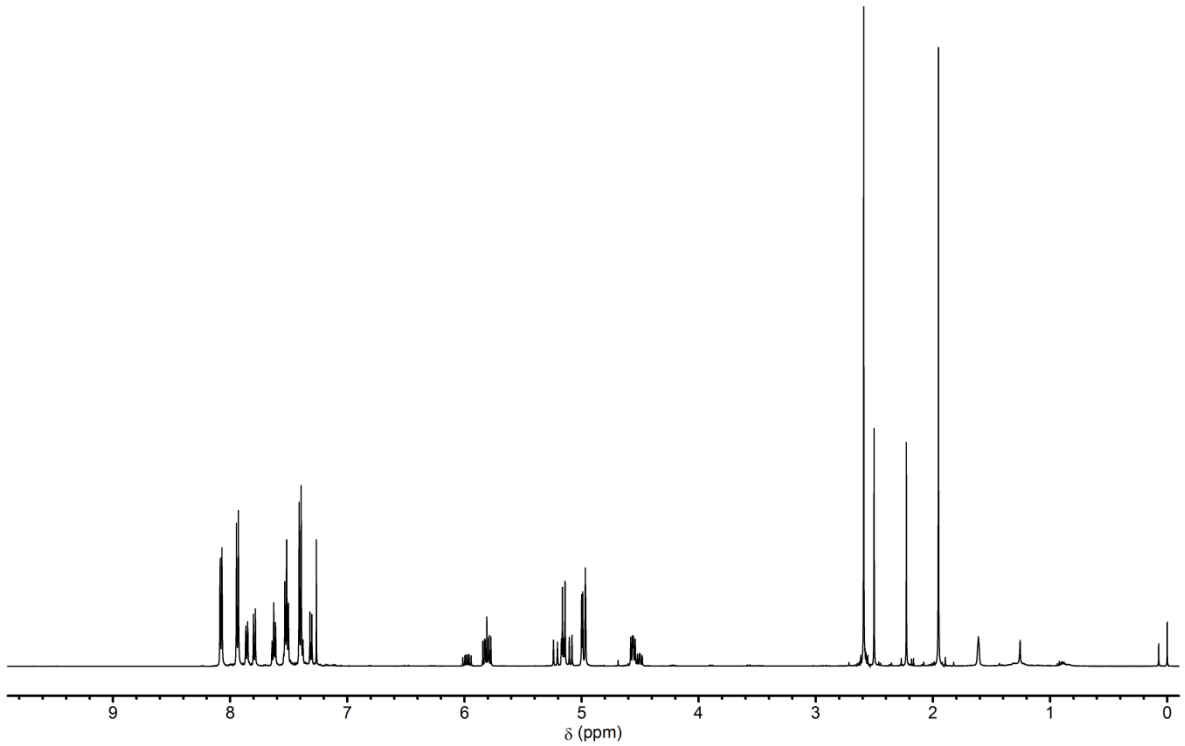


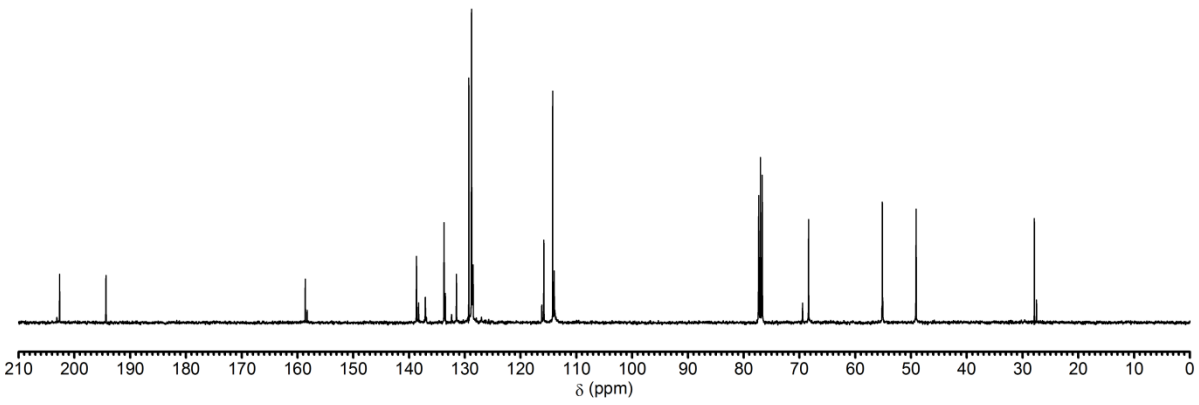
1-phenyl- 2-(1-(4-methoxyphenyl)allyl)butane-1,3-dione (4b)



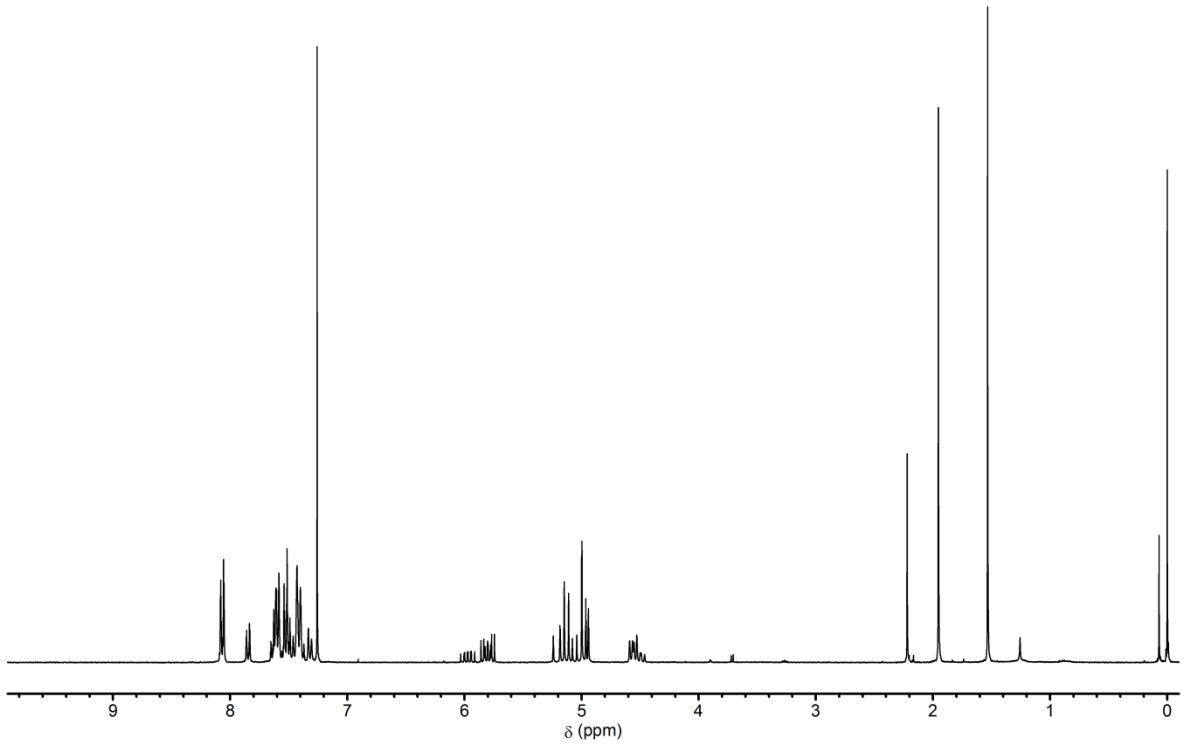


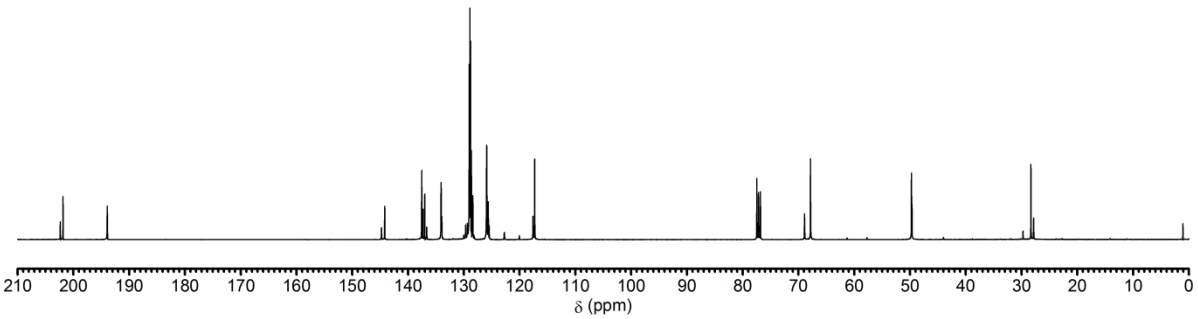
1-phenyl-2-(1-(4-acetylphenyl)allyl)butane-1,3-dione (4c)



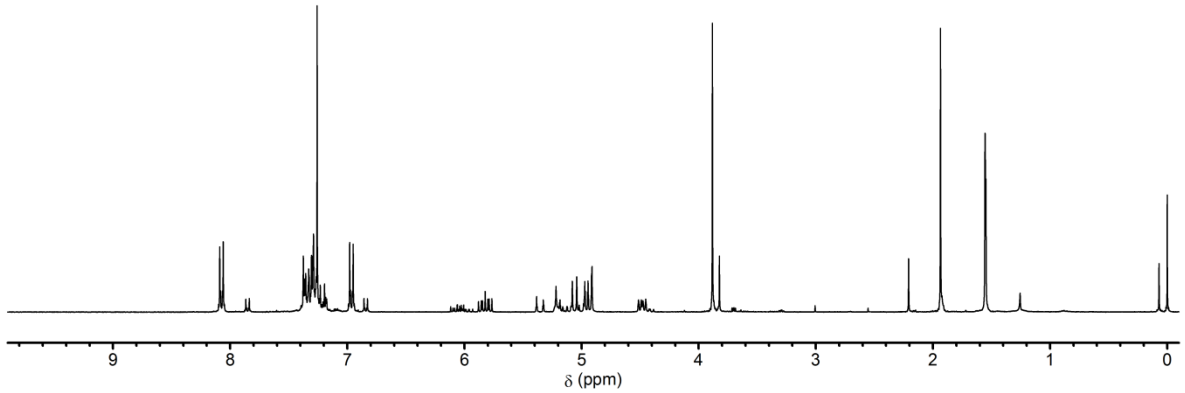


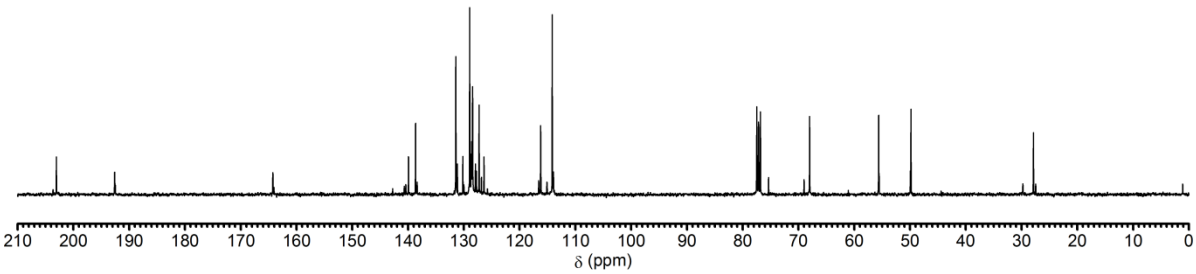
1-phenyl-2-(1-(4-(trifluoromethyl)phenyl)allyl)butane-1,3-dione (4d)



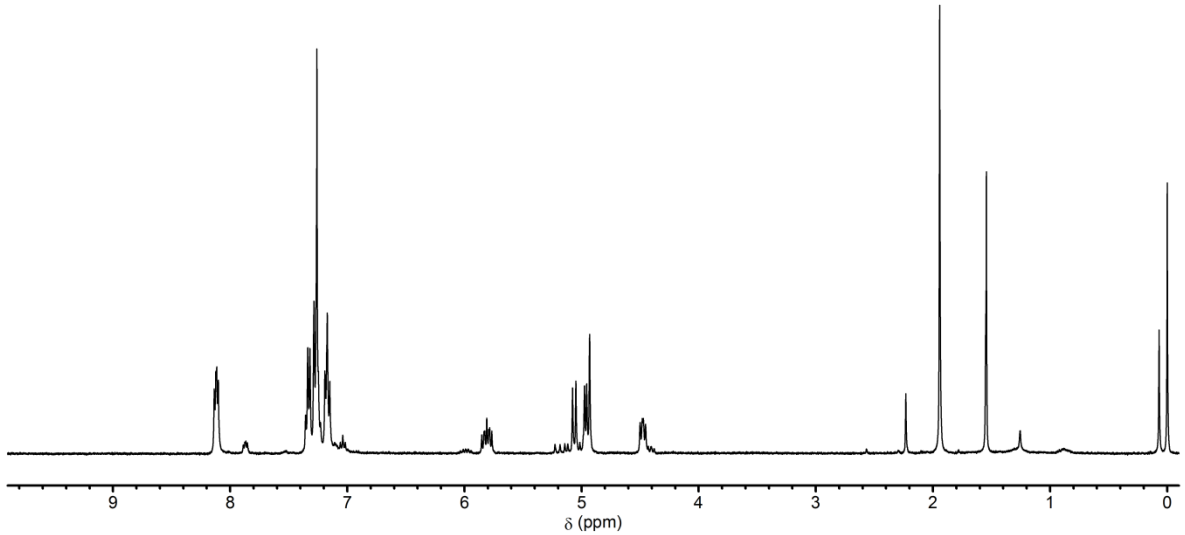


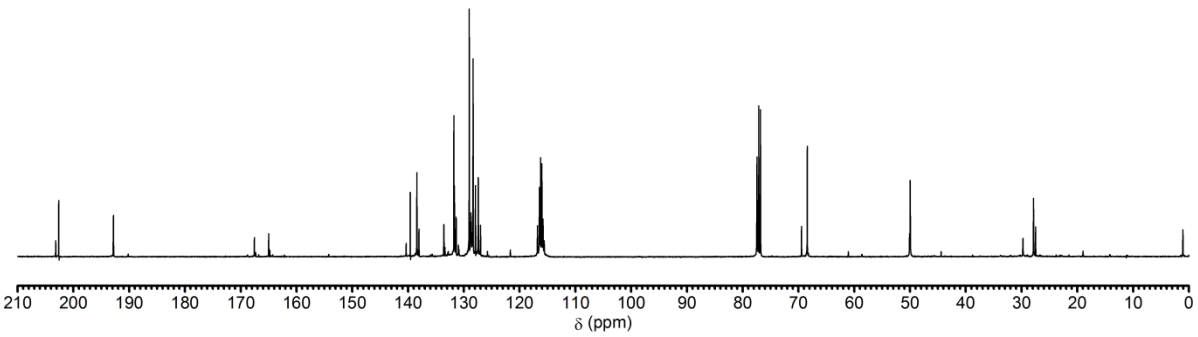
1-(4-methoxyphenyl)-2-(1-phenylallyl)butane-1,3-dione (4e)



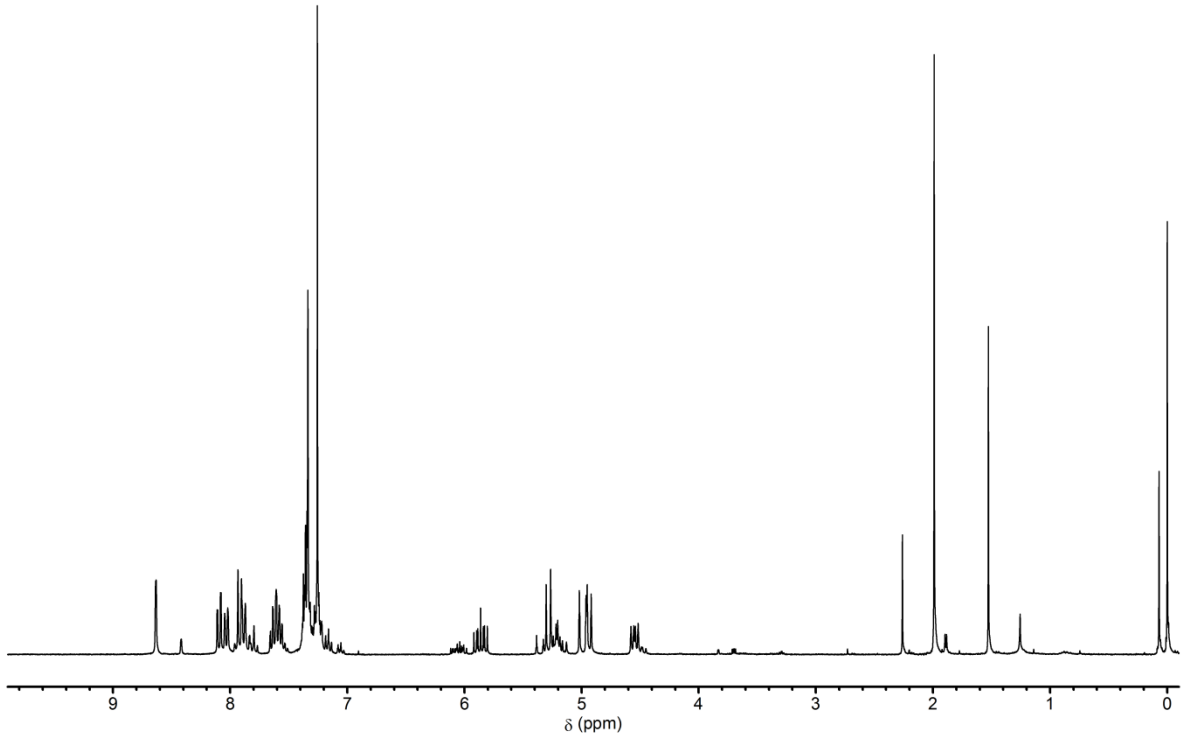


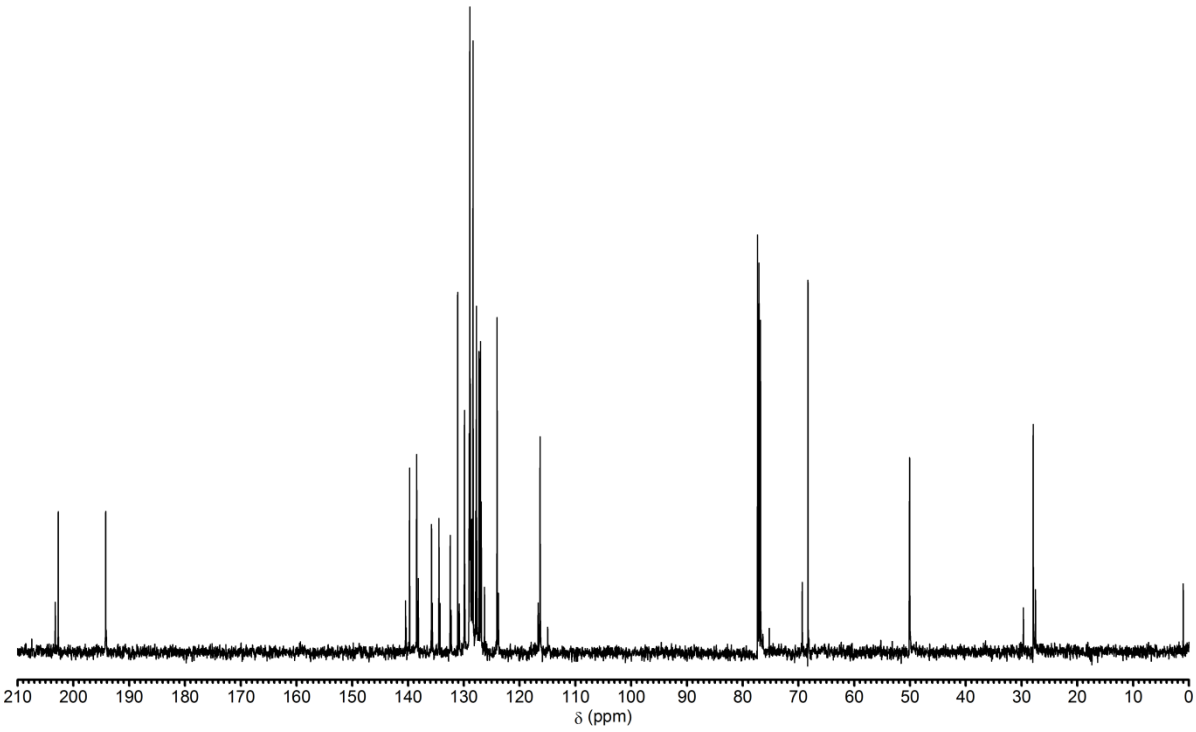
1-(4-fluorophenyl)-2-(1-phenylallyl)butane-1,3-dione (4f)



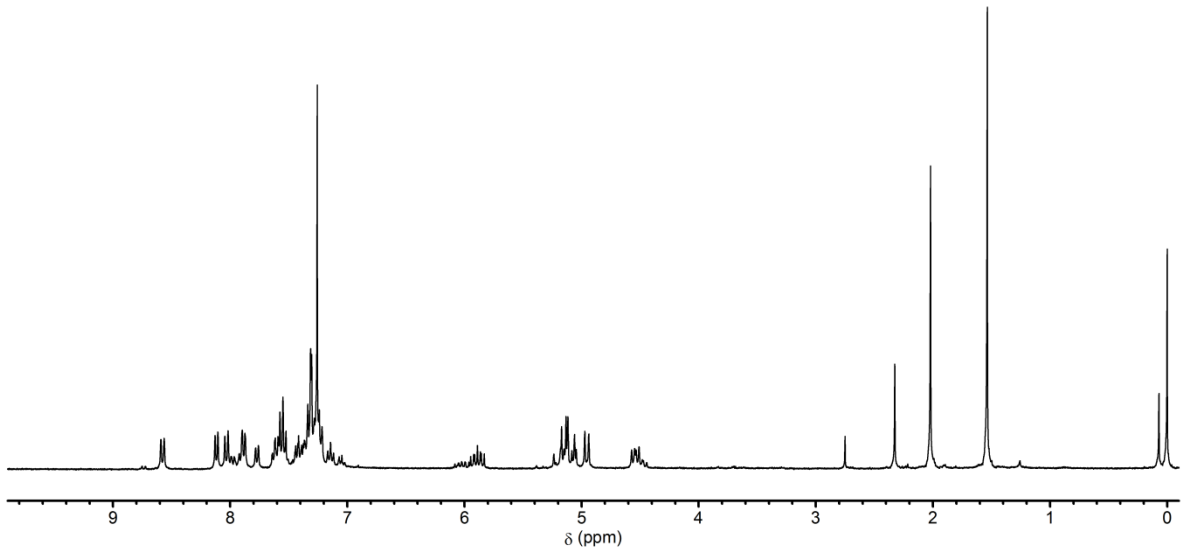


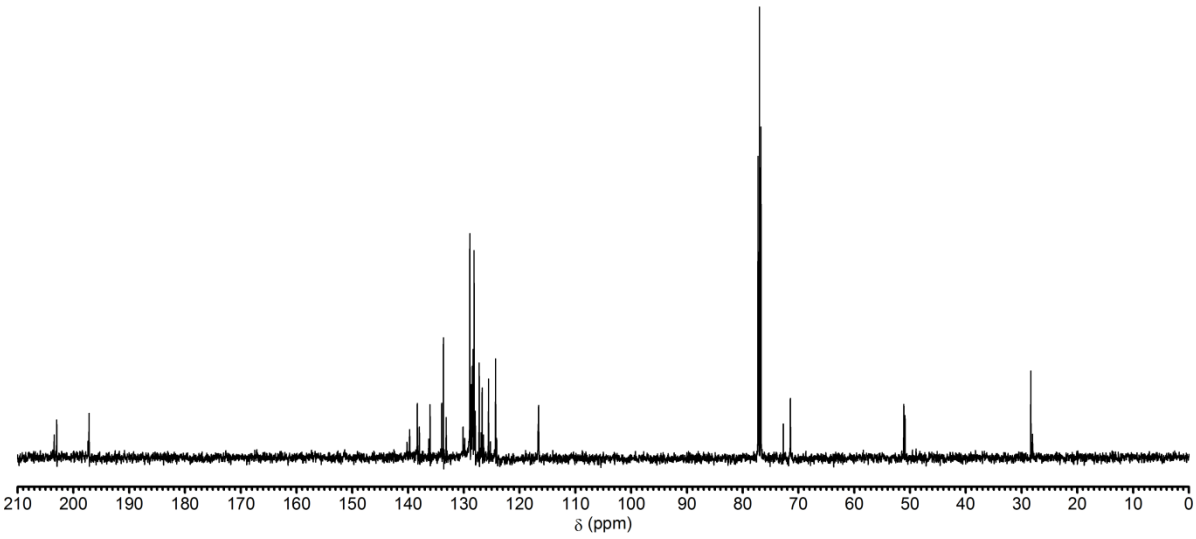
1-(naphthalen-2-yl)-2-(1-phenylallyl)butane-1,3-dione (4g)



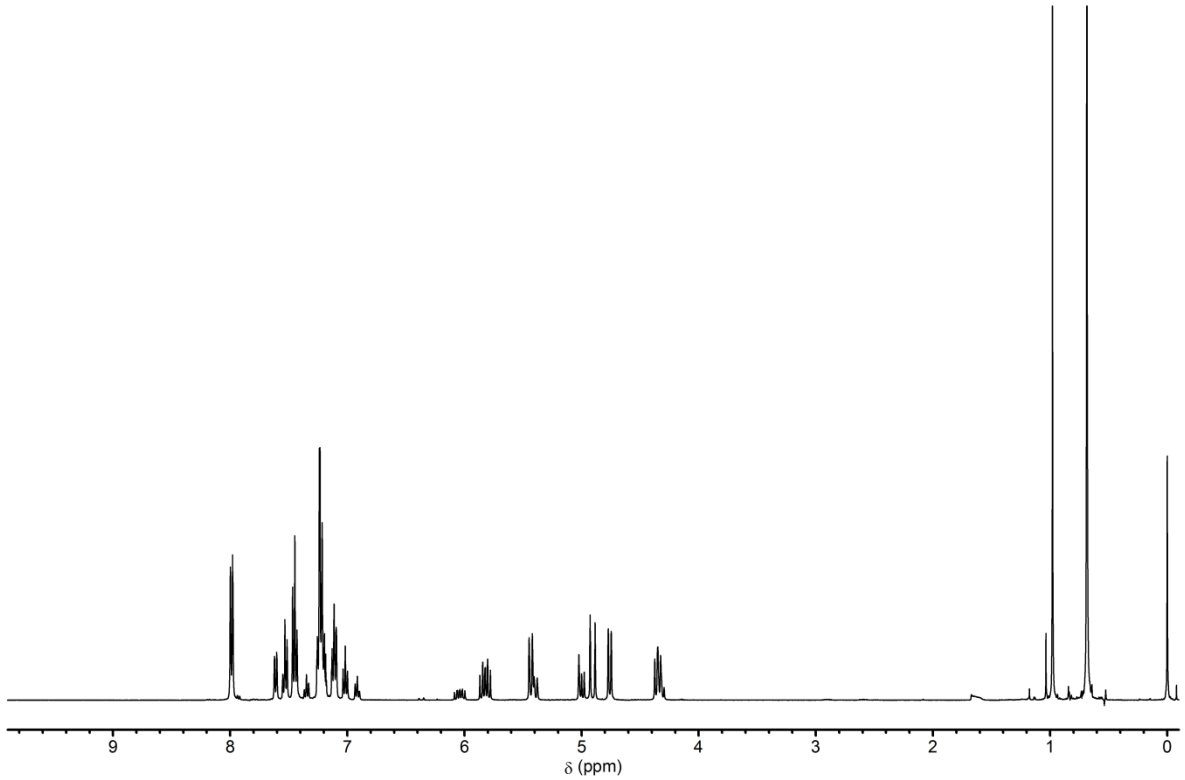


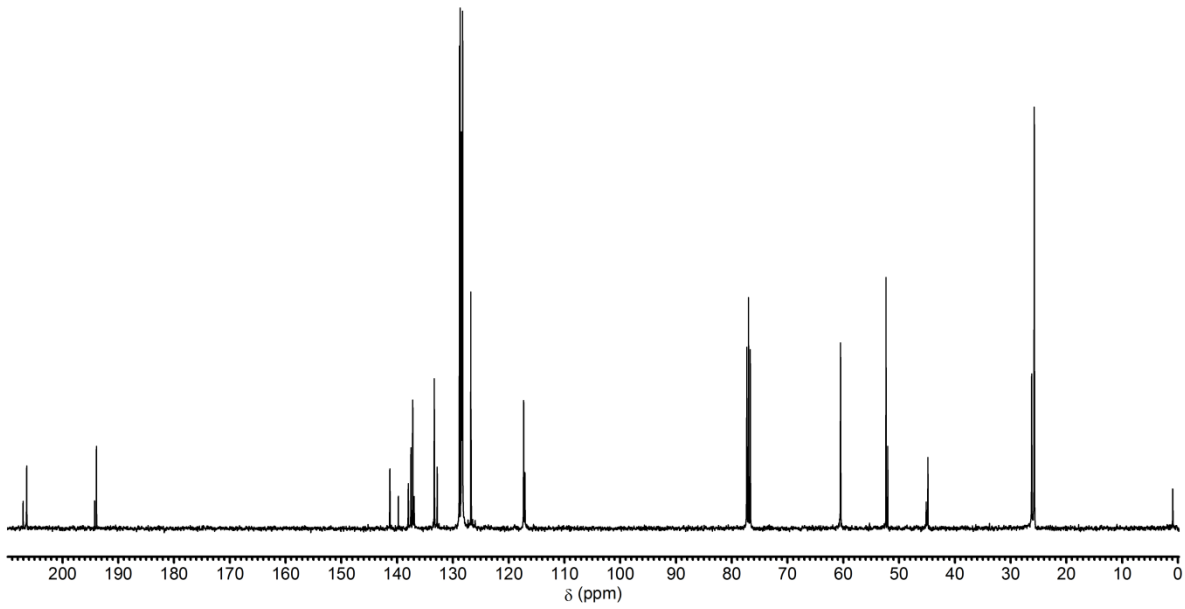
1-(naphthalen-1-yl)-2-(1-phenylallyl)butane-1,3-dione (4h)



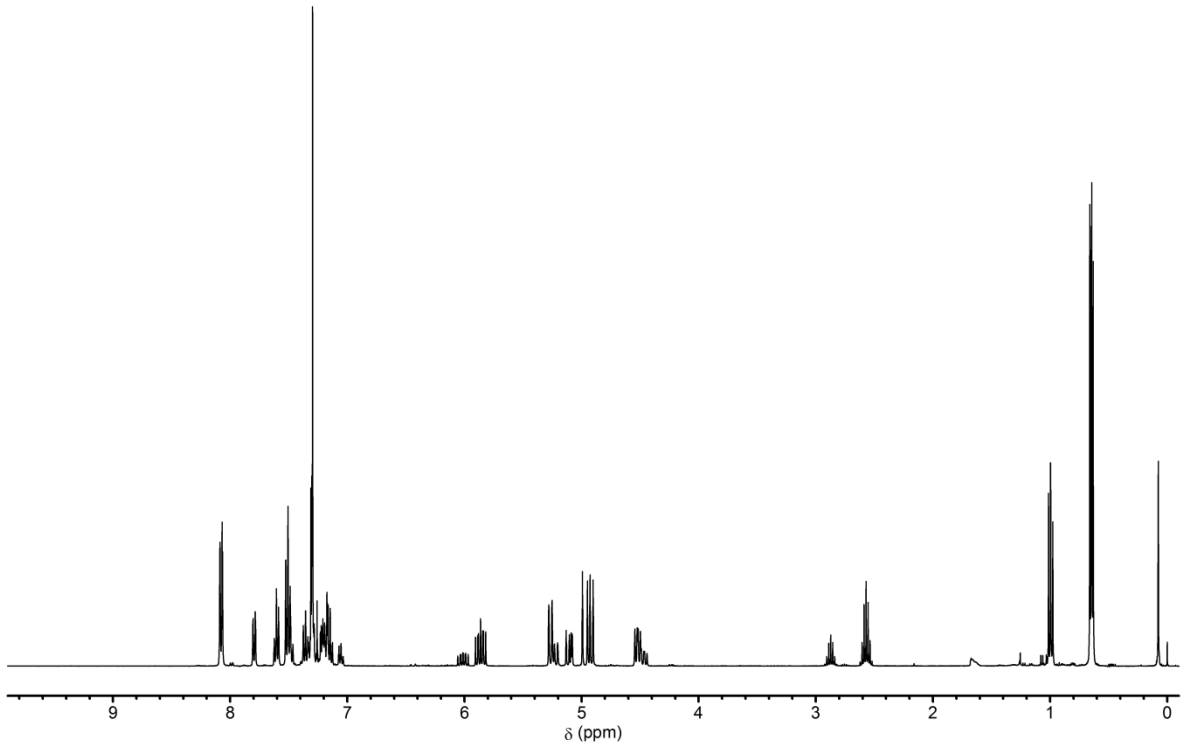


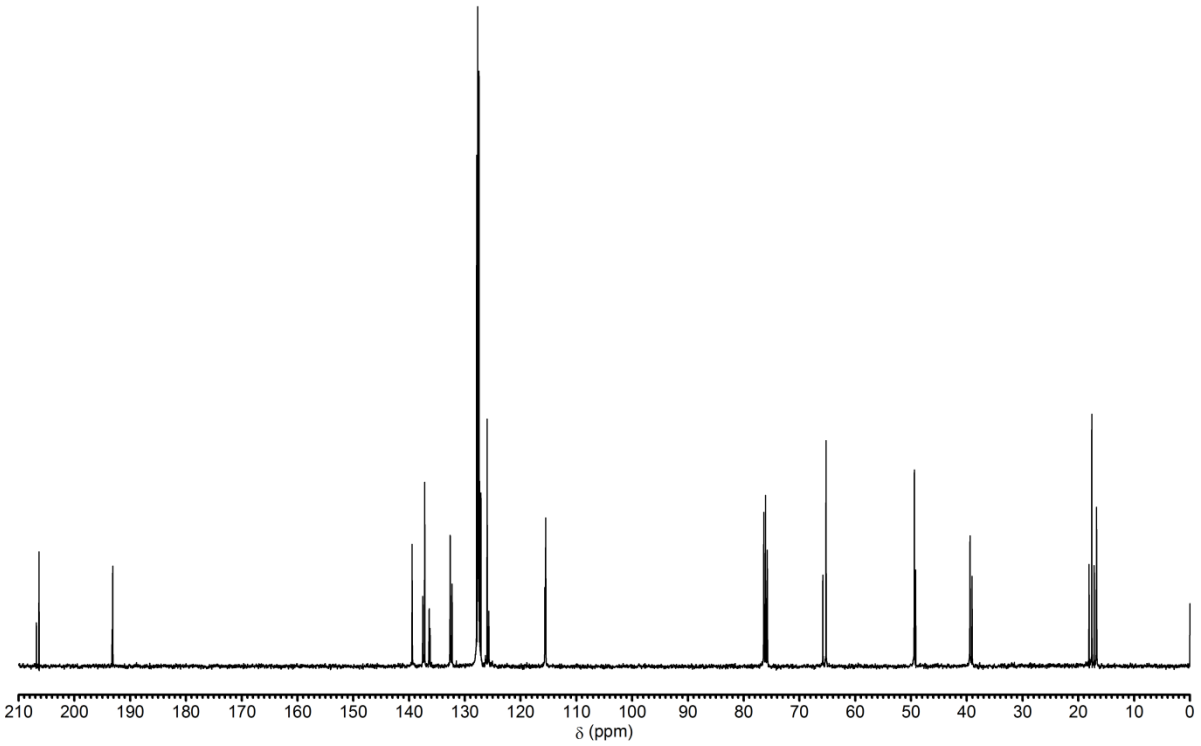
4,4-dimethyl-1-phenyl-2-(1-phenylallyl)pentane-1,3-dione (4i)



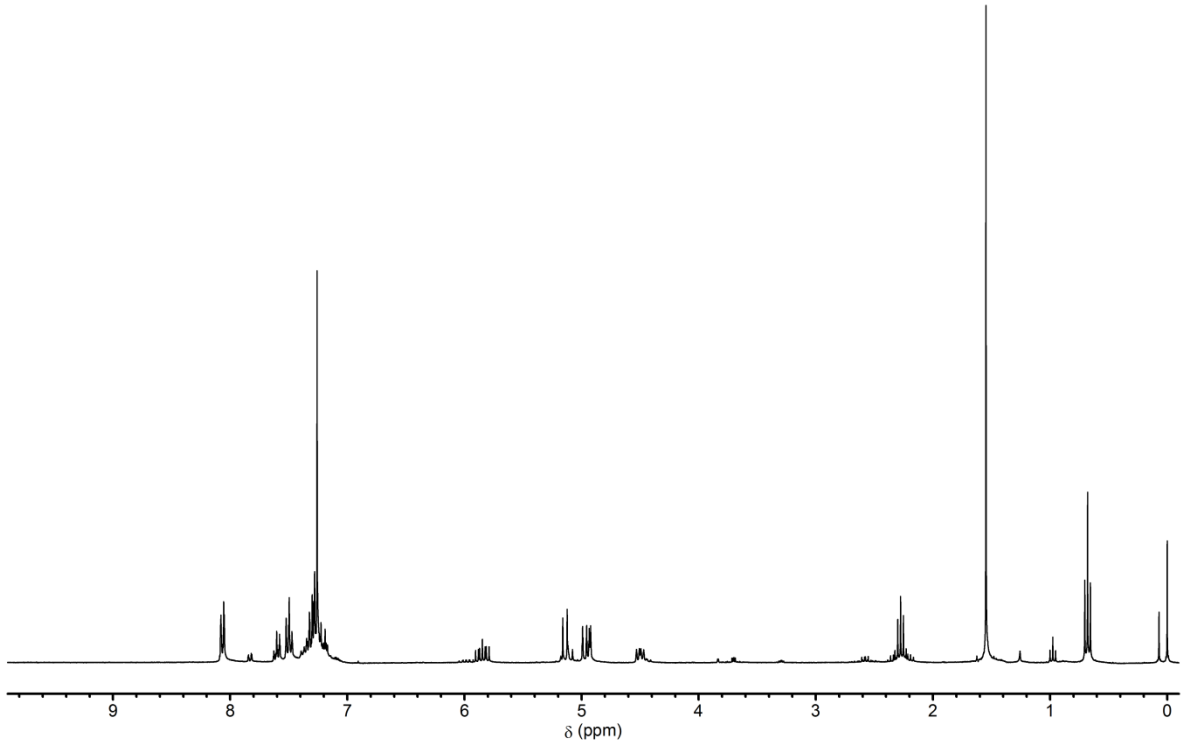


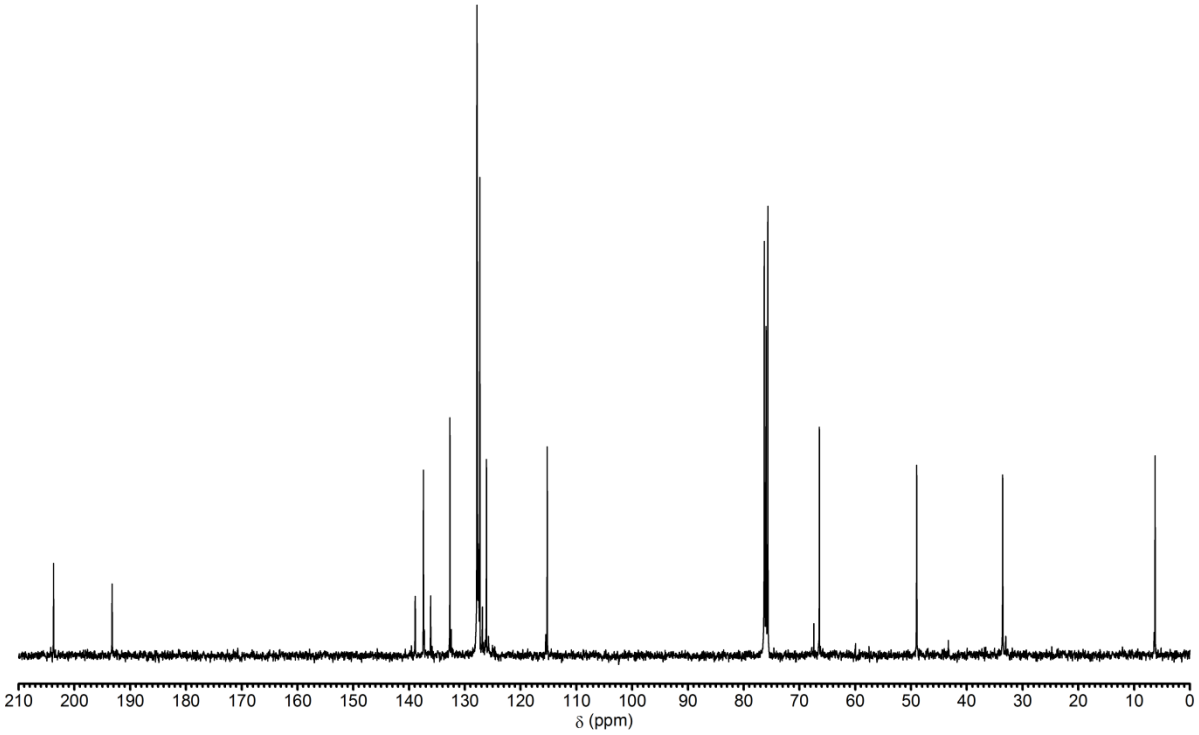
4-methyl-1-phenyl-2-(1-phenylallyl)pentane-1,3-dione (4j)



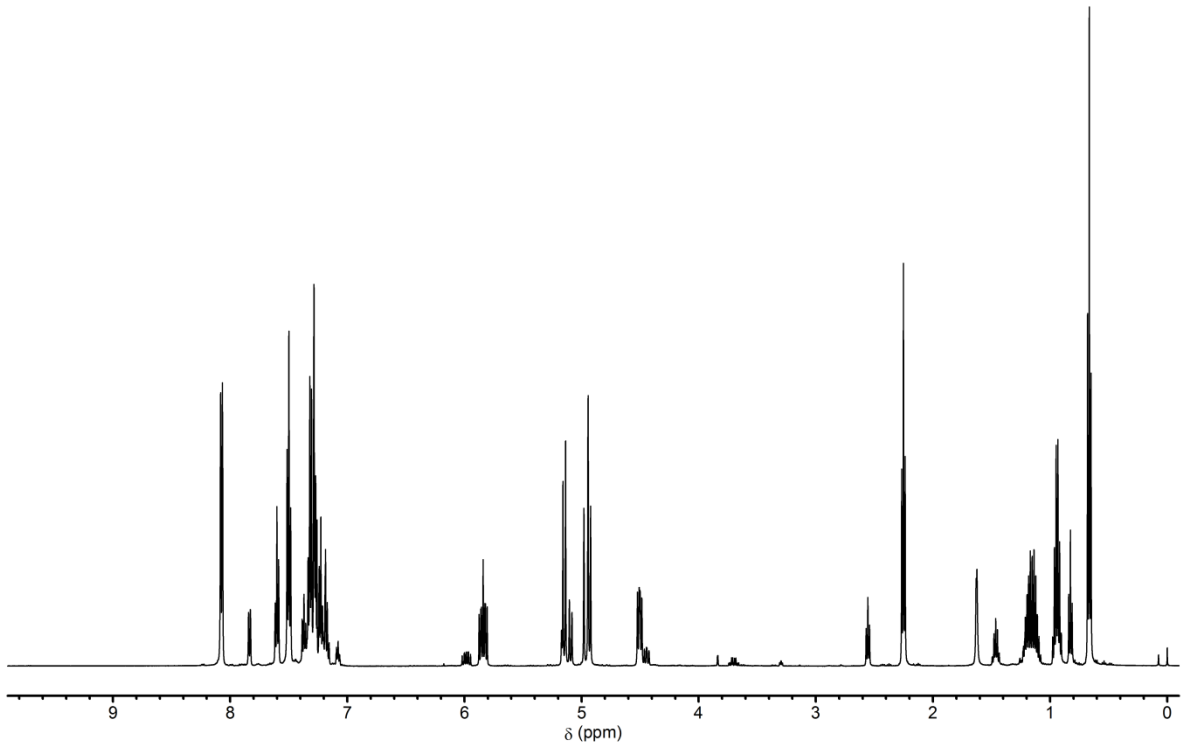


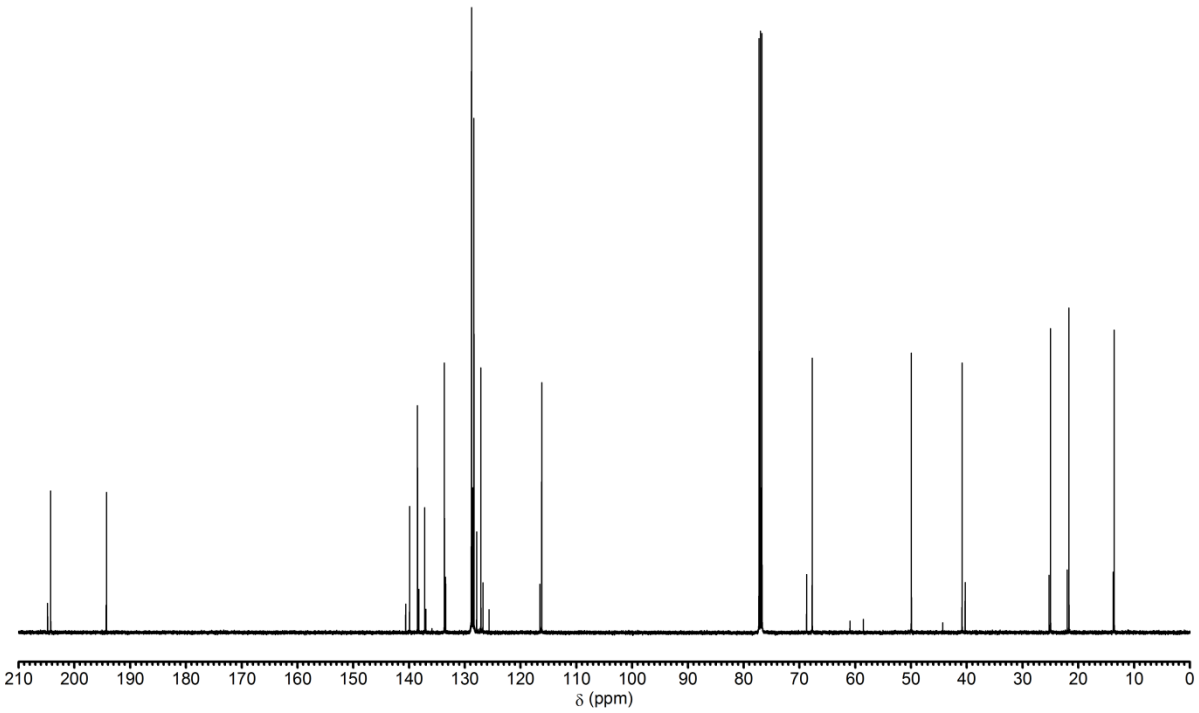
1-phenyl-2-(1-phenylallyl)pentane-1,3-dione (4k)



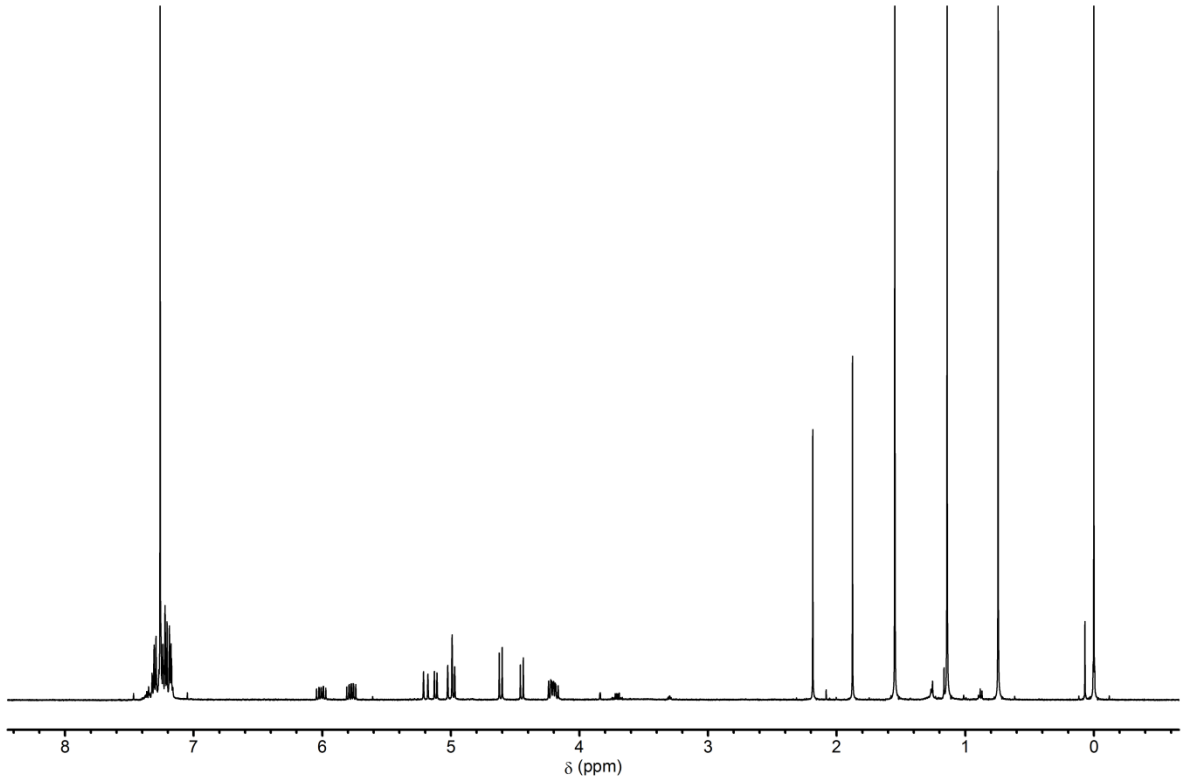


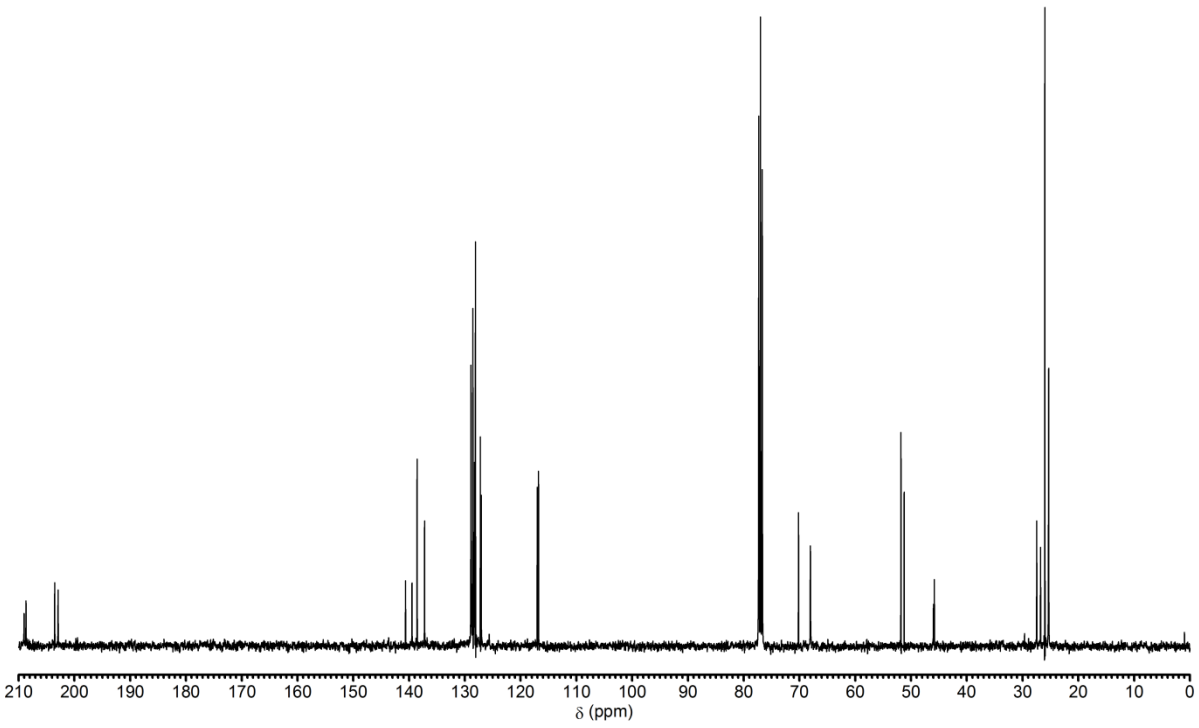
1-phenyl-2-(1-phenylallyl)heptane-1,3-dione (4l)



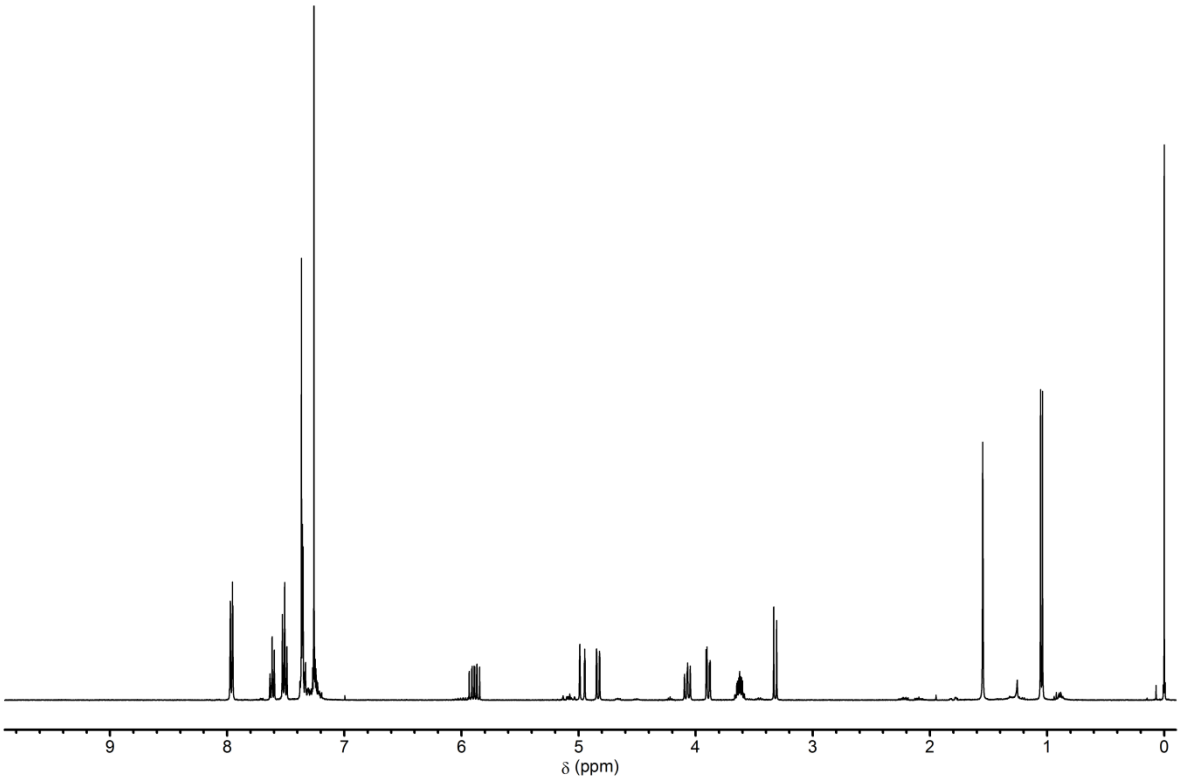


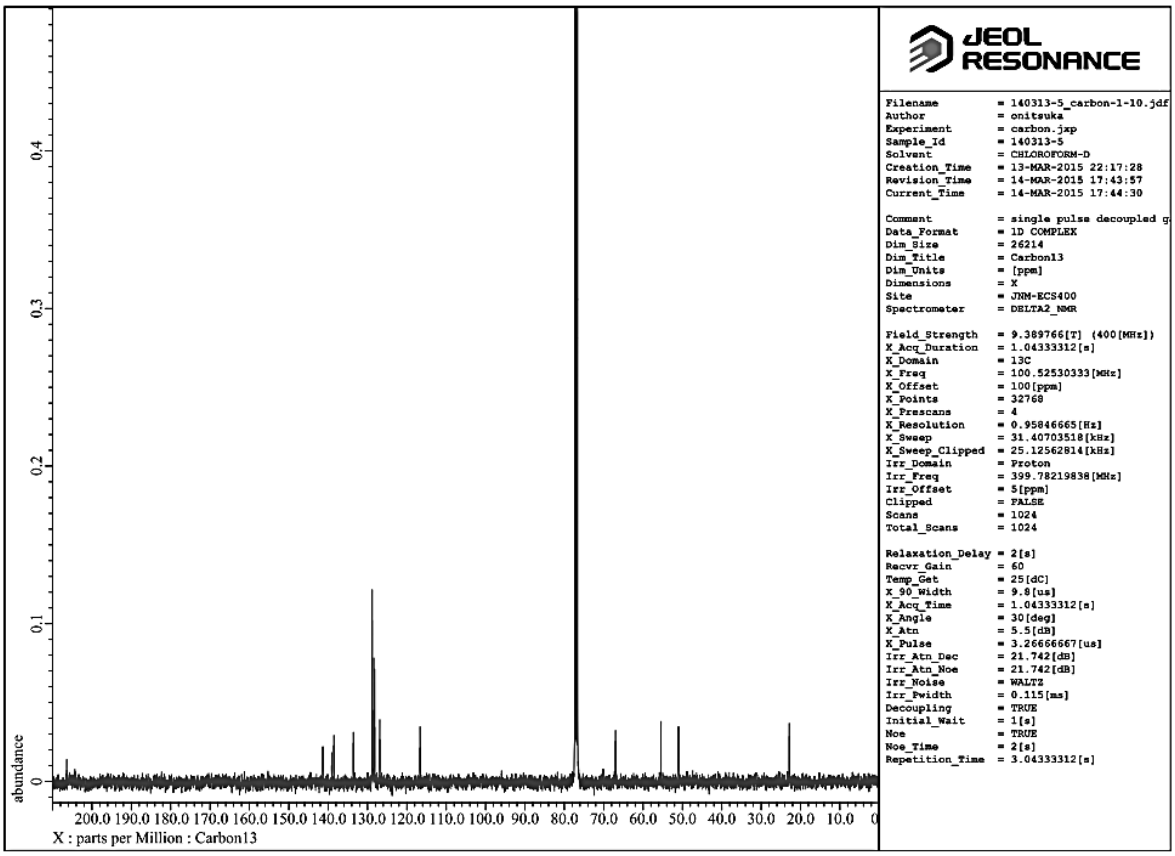
5,5-dimethyl-3-(1-phenylallyl)hexane-2,4-dione (4m)



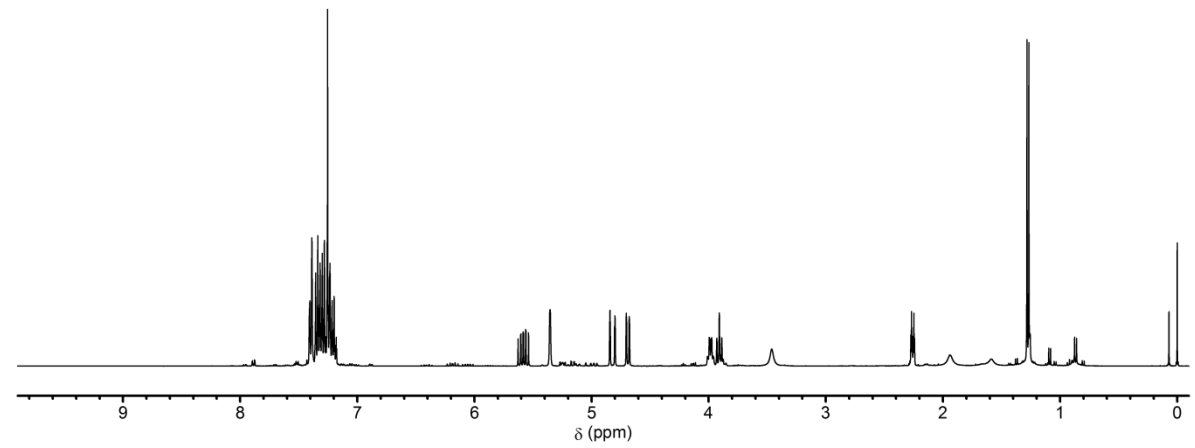


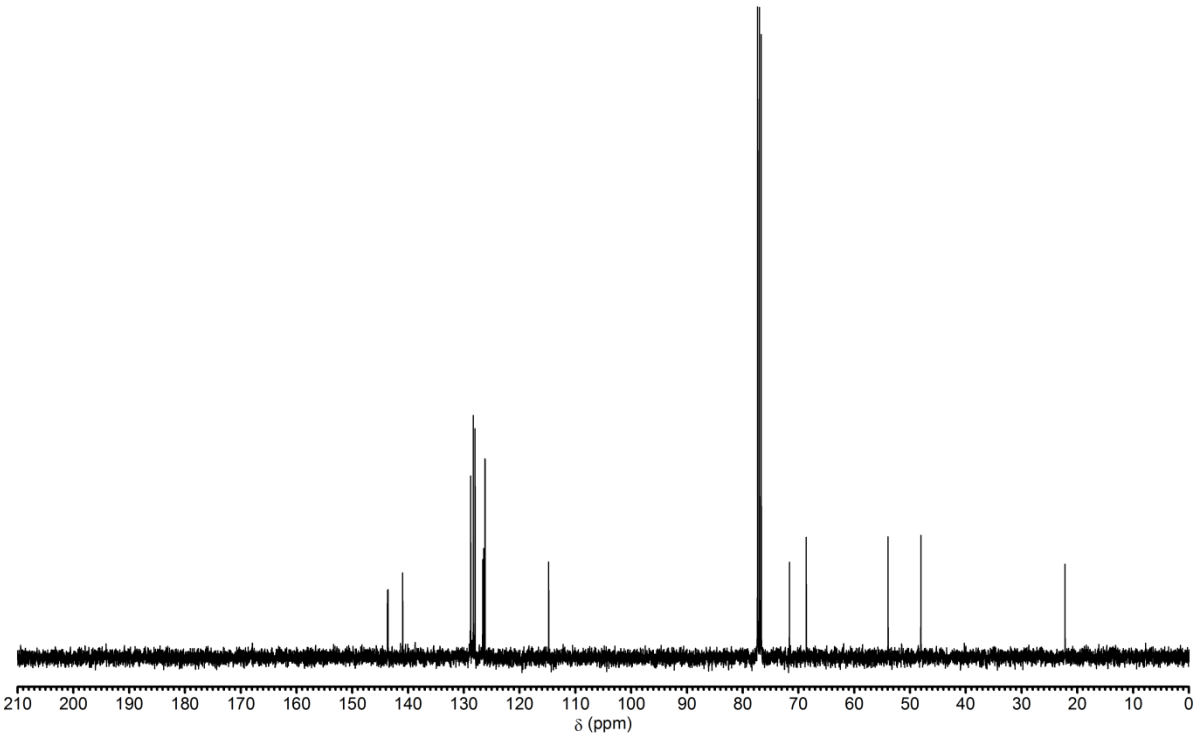
(1-hydroxyethyl)-1,3-diphenylpent-4-en-1-one (5a)


9
8
7
6
5
4
3
2
1
0
δ (ppm)

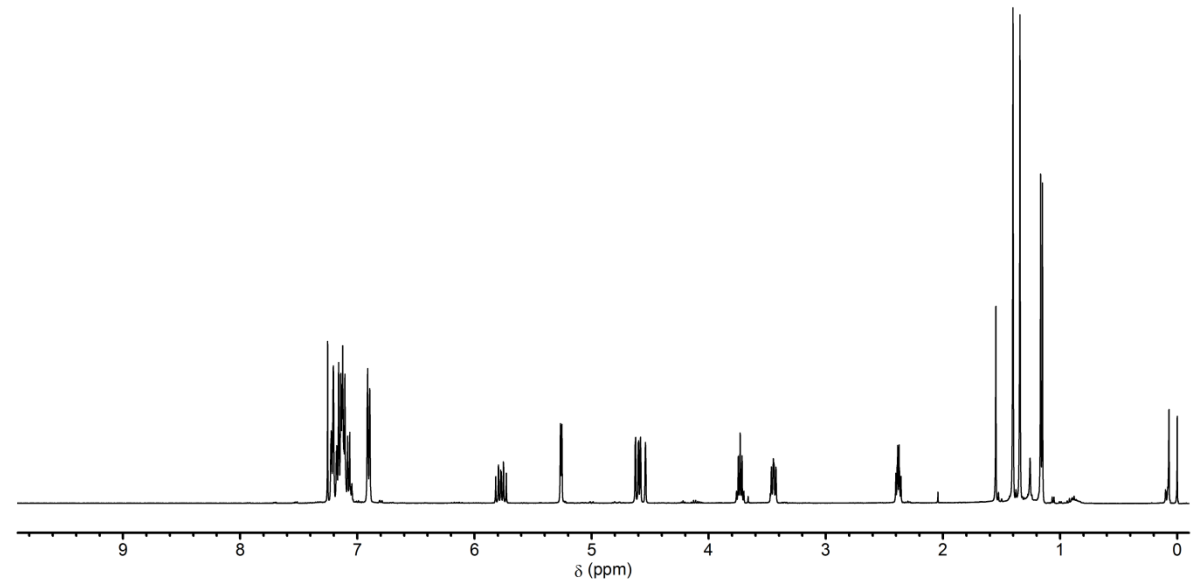

abundance
0
0.1
0.2
0.3
0.4
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = 140313-5_carbon-1-10.jdf
Author = onitsuka
Experiment = carbon.jxp
Sample_Id = 140313-5
Solvent = CHLOROFORM-D
Creation_Time = 13-MAR-2015 22:17:28
Revision_Time = 14-MAR-2015 17:43:57
Current_Time = 14-MAR-2015 17:44:30
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 25[dC]
X_90_Width = 9.8[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 5.5[dB]
X_Pulse = 3.26666667[us]
Irr_Atn_Dec = 21.742[dB]
Irr_Atn_Noe = 21.742[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

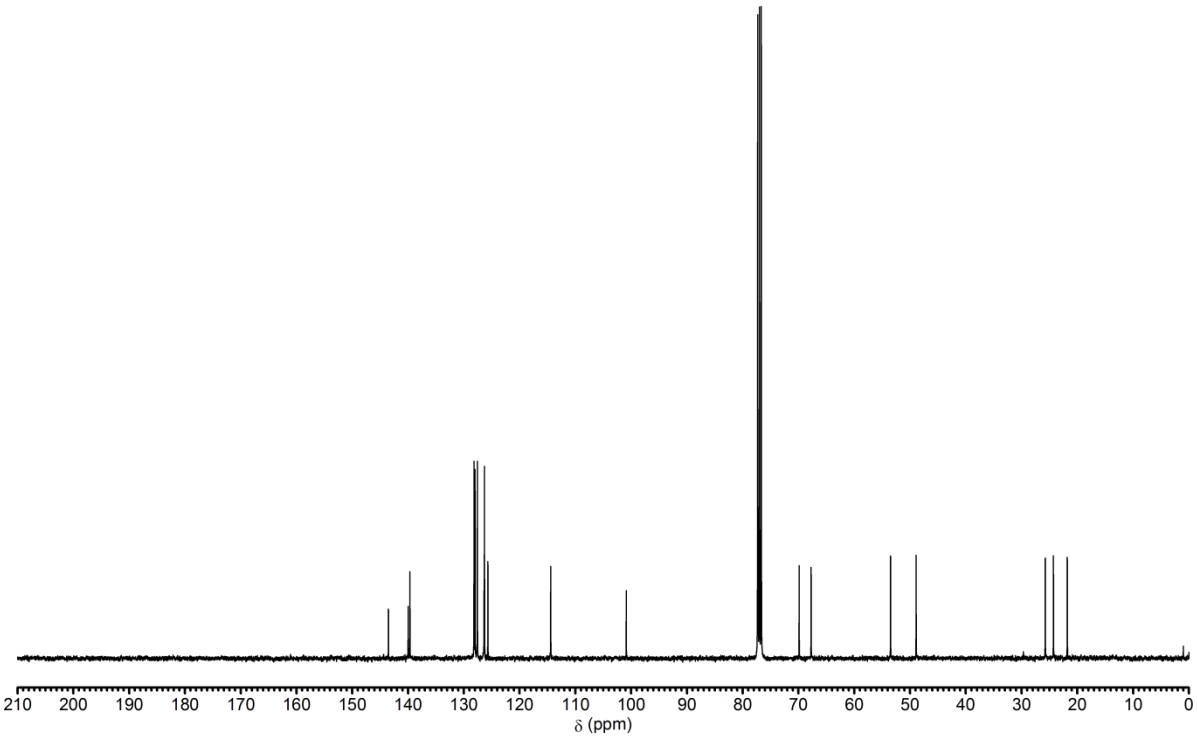
1-phenyl-2-(1-phenylallyl)butane-1,3-diol (6a)



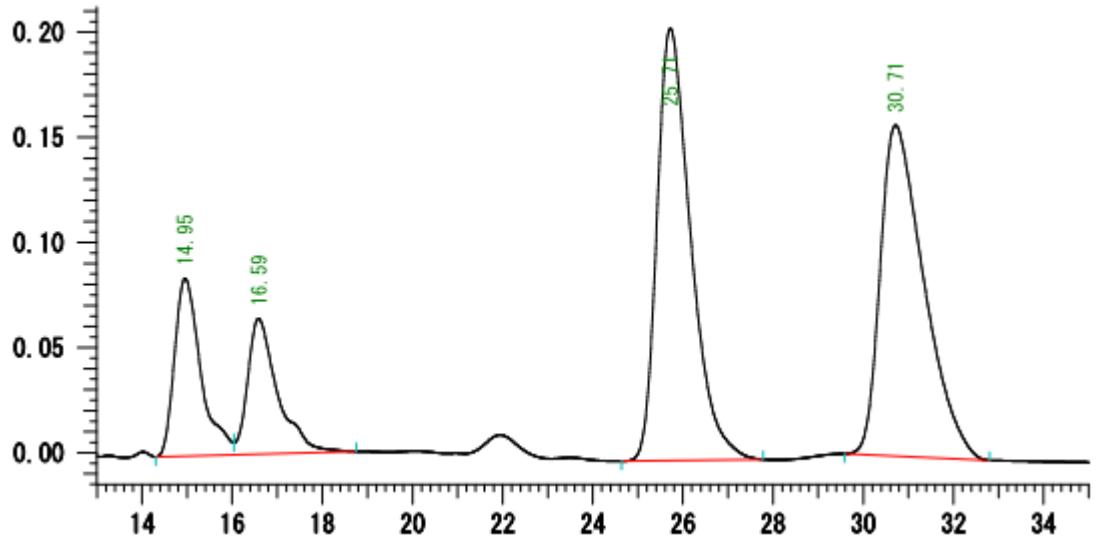


(4*S*,5*S*,6*R*)-2,2,4-trimethyl-6-phenyl-5-((*S*)-1-phenylallyl)-1,3-dioxane (7a)

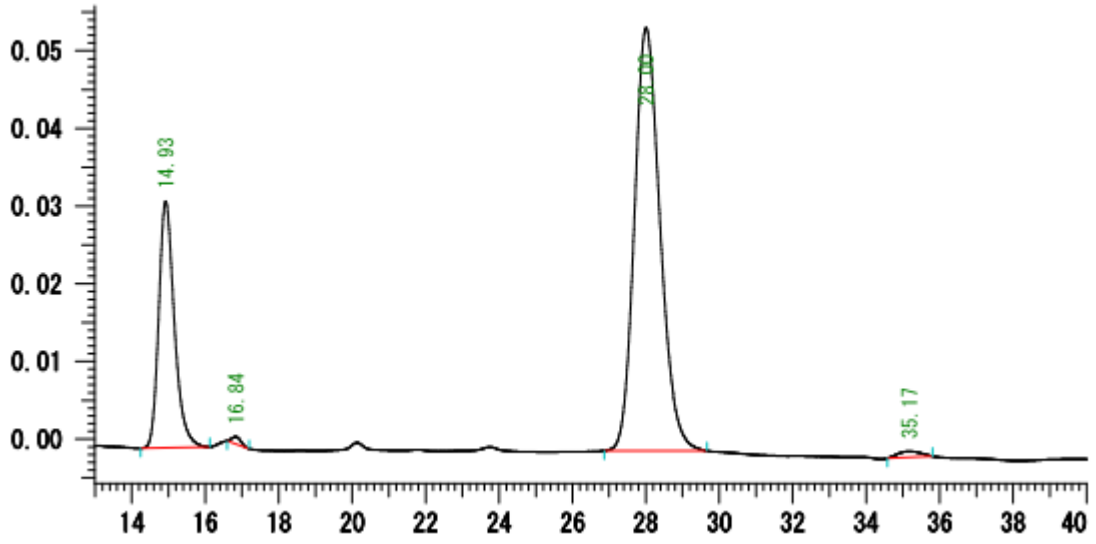




1-phenyl-2-(1-phenylallyl)butane-1,3-dione (4a)

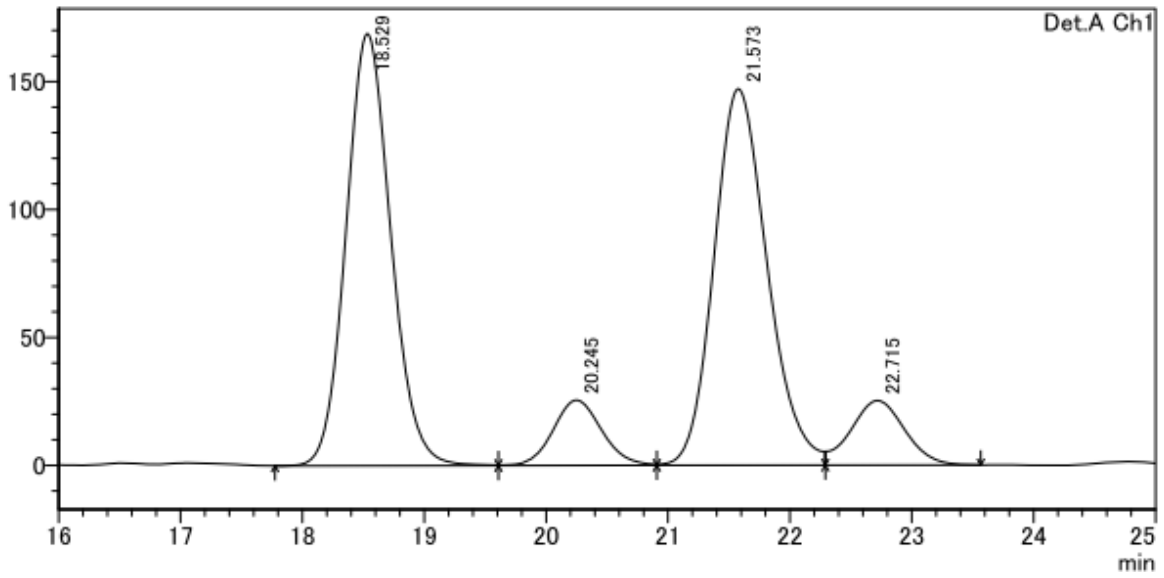


NO	RT	面積	濃度1	BC
1	14.95	1710744	12.340	BV
2	16.59	1479855	10.675	VB
3	25.71	5368841	38.727	BB
4	30.71	5303731	38.258	BB
		13863171	100.000	



NO	RT	面積	濃度1	BC
1	14.93	464083	25.674	BB
2	16.84	7688	0.425	BB
3	28.00	1319037	72.972	BB
4	35.17	16794	0.929	BB
		1807602	100.000	

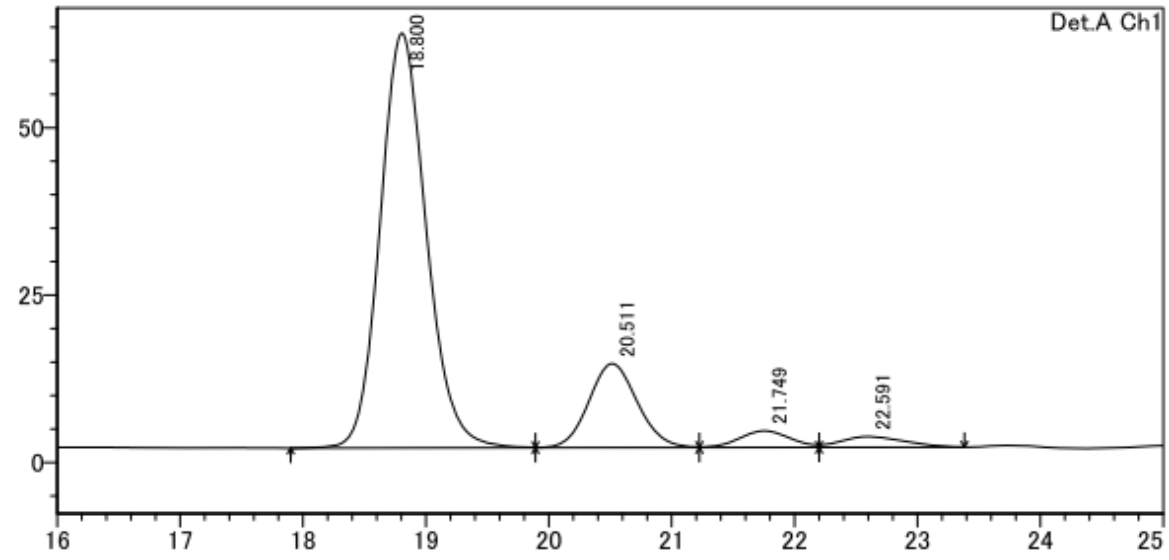
1-phenyl-2-(1-(4-acetylphenyl)allyl)butane-1,3-dione (4c)



Peak Table

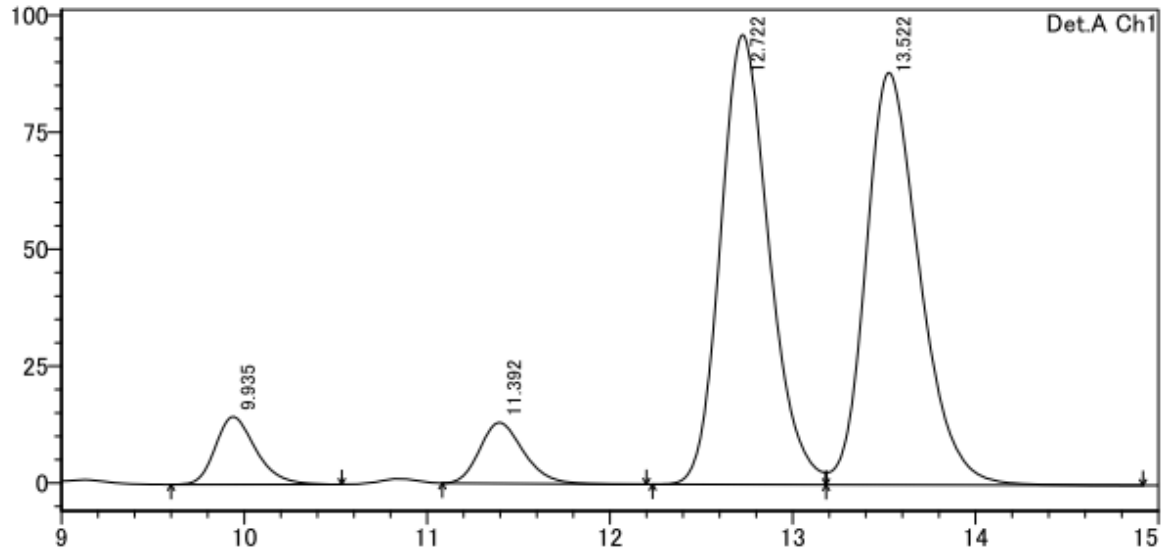
UV-Vis Ch1 254nm

Peak	Retention Time	Area	High	Area Percent
1	18.529	4310296	168793	42.074
2	20.245	704183	25507	6.874
3	21.573	4462192	147072	43.556
4	22.715	767975	25193	7.496
合計		10244647	366564	100.000

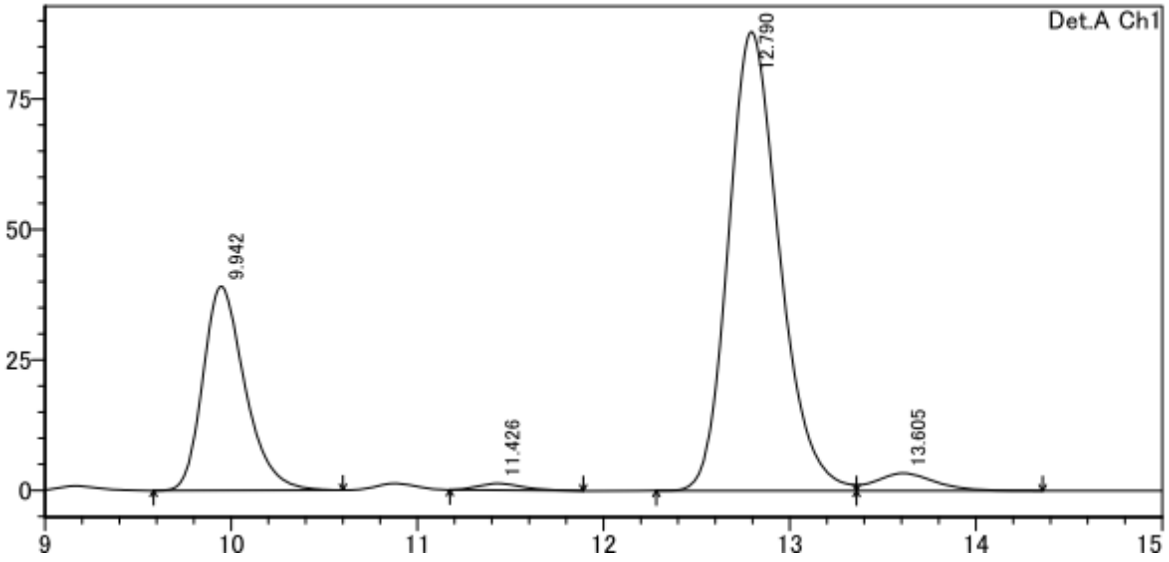


Peak	Retention Time	Area	High	Area Percent
1	18.800	1615766	61932	77.462
2	20.511	343559	12545	16.471
3	21.749	70188	2478	3.365
4	22.591	56360	1593	2.702
合計		2085873	78548	100.000

1-phenyl-2-(1-(4-(trifluoromethyl)phenyl)allyl)butane-1,3-dione (4d)

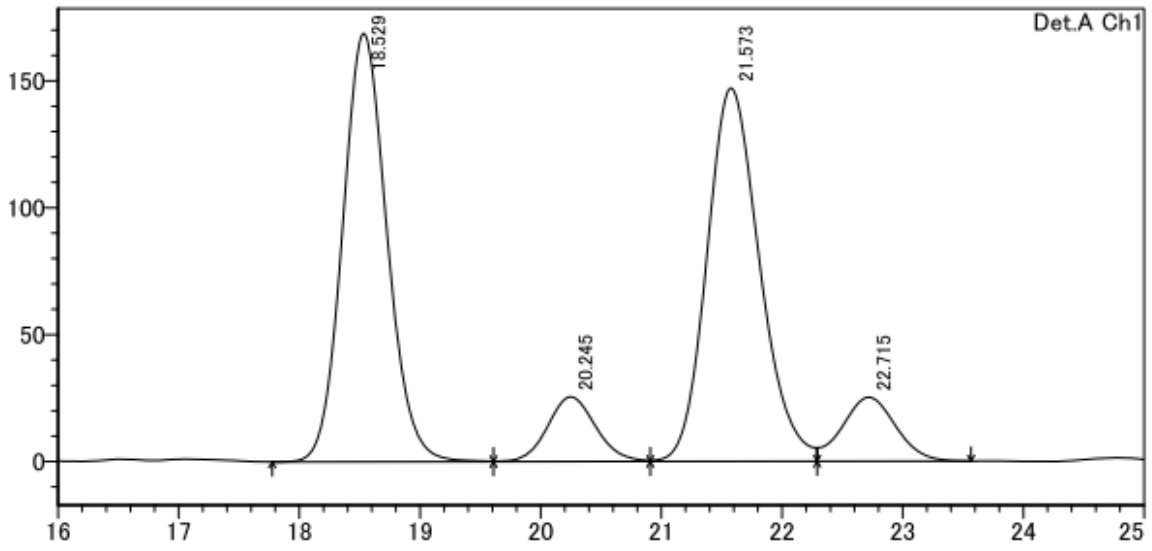


Peak	Retention Time	Area	High	Area Percent
1	9.935	222907	14466	5.557
2	11.392	216807	12999	5.405
3	12.722	1775144	96151	44.256
4	13.522	1796266	88136	44.782
合計		4011124	211752	100.000

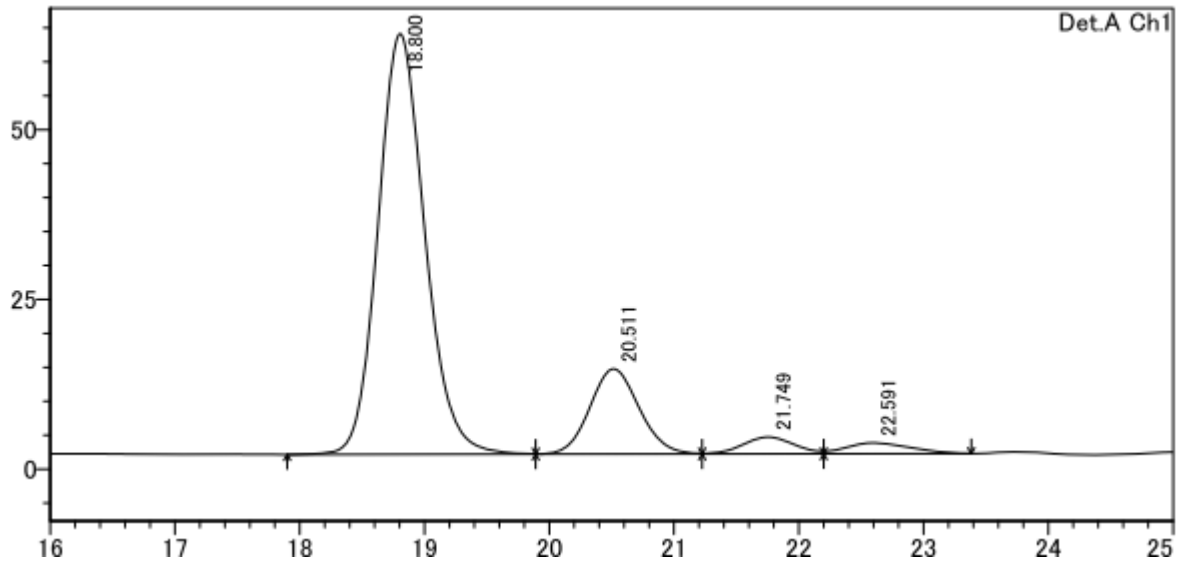


Peak	Retention Time	Area	High	Area Percent
1	9.942	613860	39103	25.799
2	11.426	20374	1270	0.856
3	12.790	1672628	87936	70.296
4	13.605	72556	3355	3.049
合計		2379418	131665	100.000

1-(4-methoxyphenyl)-2-(1-phenylallyl)butane-1,3-dione (4e)

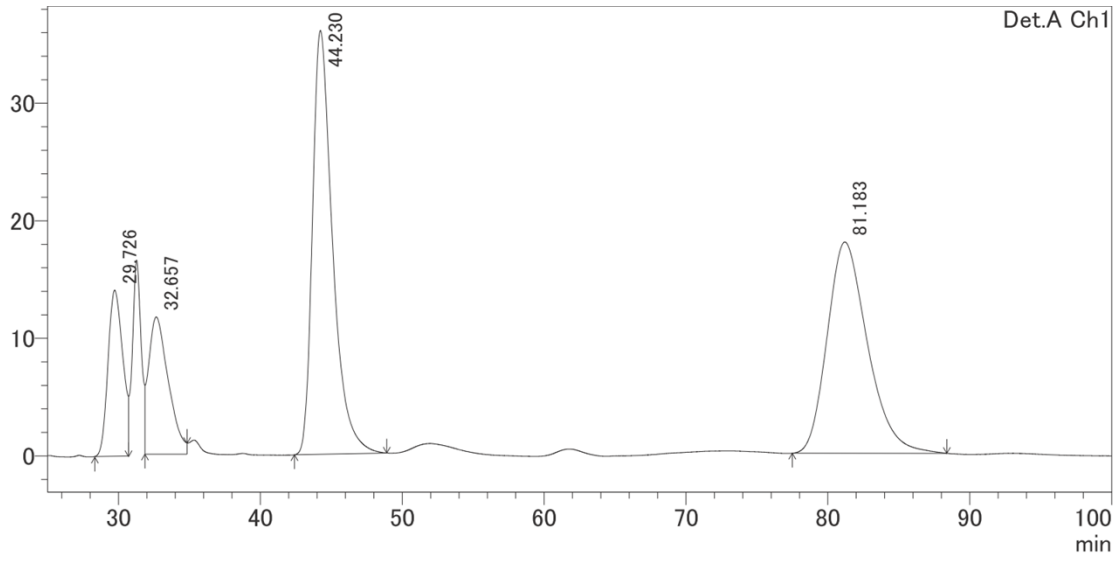


Peak	Retention Time	Area	High	Area Percent
1	18.529	4310296	168793	42.074
2	20.245	704183	25507	6.874
3	21.573	4462192	147072	43.556
4	22.715	767975	25193	7.496
合計		10244647	366564	100.000



Peak	Retention Time	Area	High	Area Percent
1	18.800	1615766	61932	77.462
2	20.511	343559	12545	16.471
3	21.749	70188	2478	3.365
4	22.591	56360	1593	2.702
合計		2085873	78548	100.000

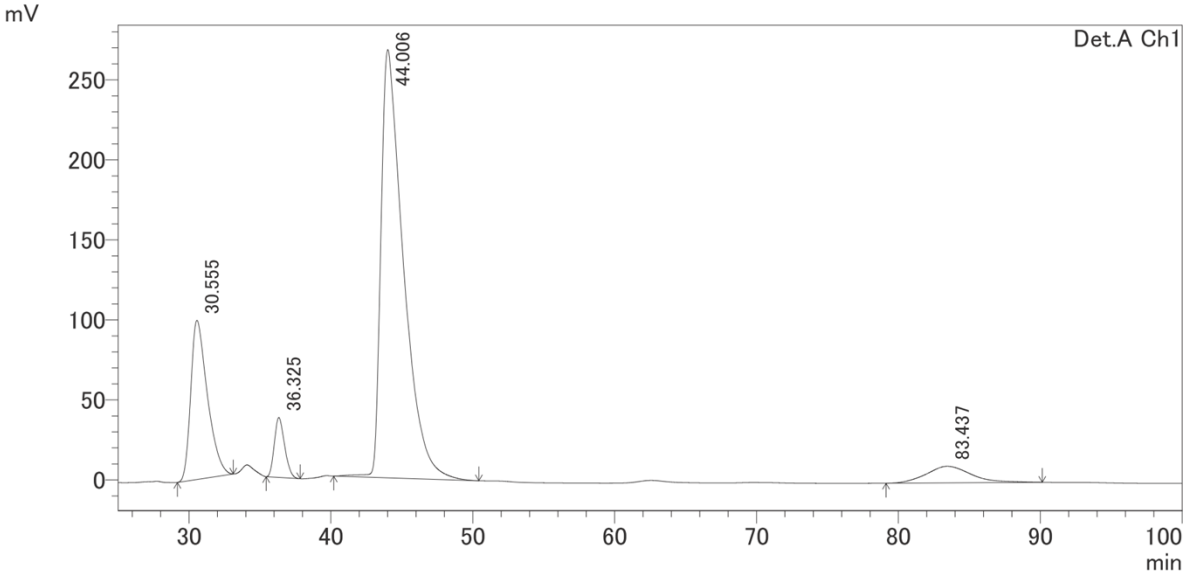
1-(4-fluorophenyl)-2-(1-phenylallyl)butane-1,3-dione (4f)



Peak Table

UV-Vis Ch1 254nm

Peak	Retention Time	Area	High	Area Percent
1	29.726	993501	13907	10.958
2	32.657	976991	11009	10.776
3	44.230	3546201	36052	39.114
4	81.183	3549673	17969	39.152
合計		9066366	78937	100.000

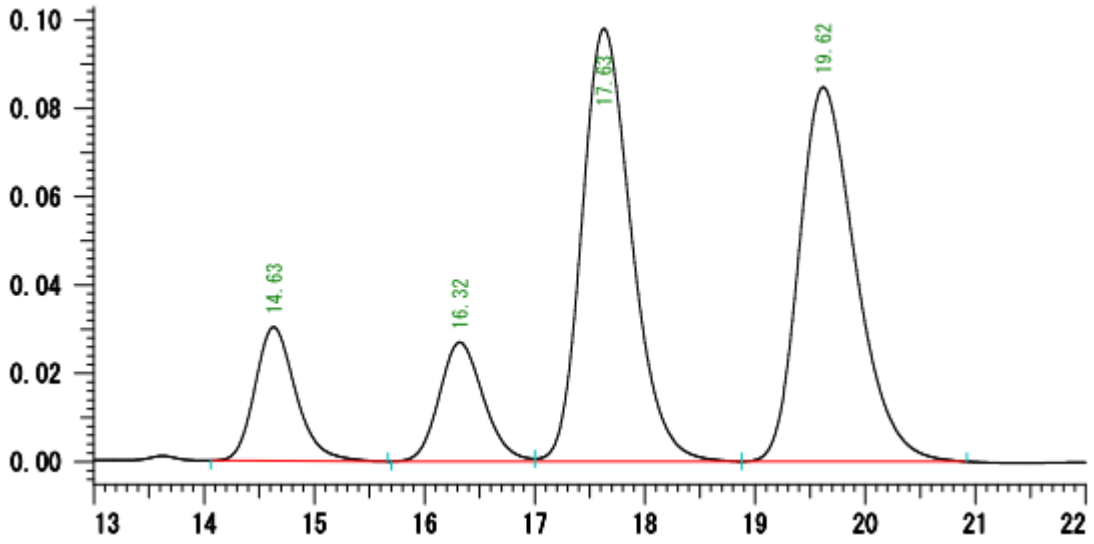


Peak Table

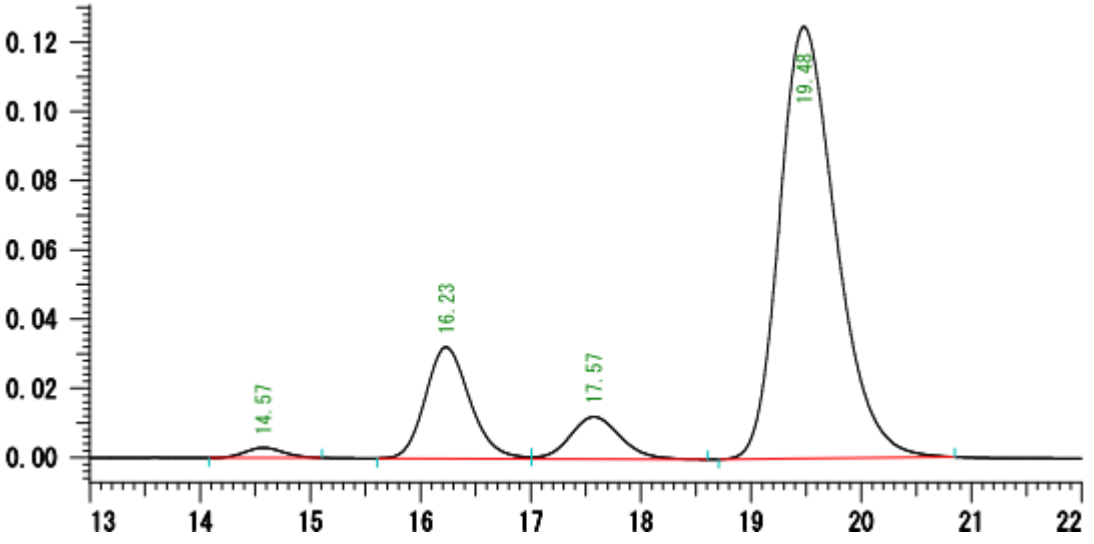
UV-Vis Ch1 254nm

Peak	Retention Time	Area	High	Area Percent
1	30.555	8126337	99485	19.464
2	36.325	1885612	37504	4.516
3	44.006	29455604	267633	70.550
4	83.437	2283763	10376	5.470
合計		41751317	414999	100.000

1-(naphthalen-2-yl)-2-(1-phenylallyl)butane-1,3-dione (4g)

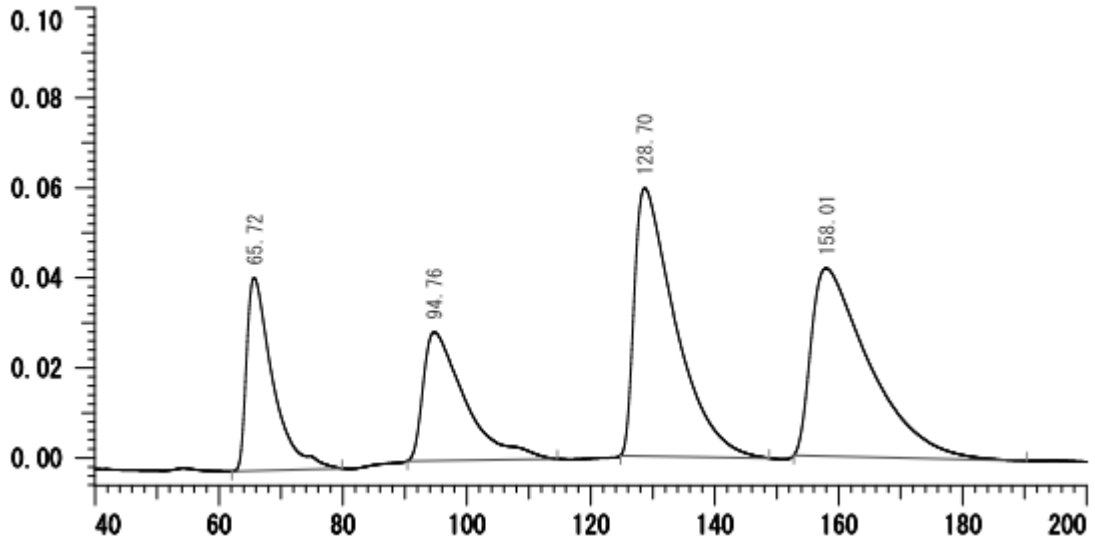


NO	RT	面積	濃度1	BC
1	14.63	387326	10.201	BB
2	16.32	374820	9.871	BV
3	17.63	1525036	40.164	VB
4	19.62	1509885	39.764	BB
		3797067	100.000	

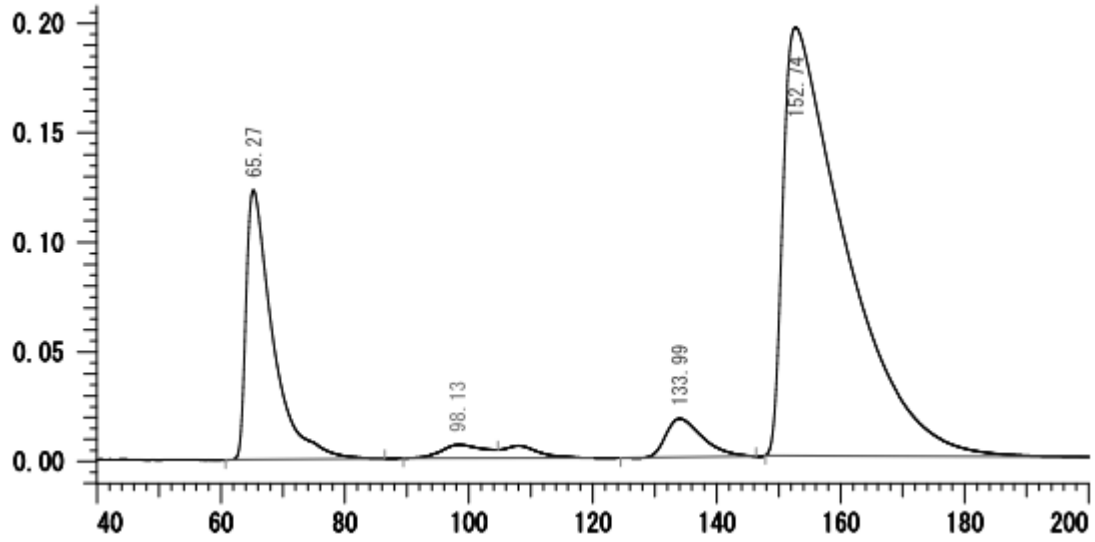


NO	RT	面積	濃度1	BC
1	14.57	35923	1.238	BB
2	16.23	451832	15.575	BV
3	17.57	192332	6.630	VB
4	19.48	2220927	76.557	BB
		2901014	100.000	

1-(naphthalen-1-yl)-2-(1-phenylallyl)butane-1,3-dione (4h)

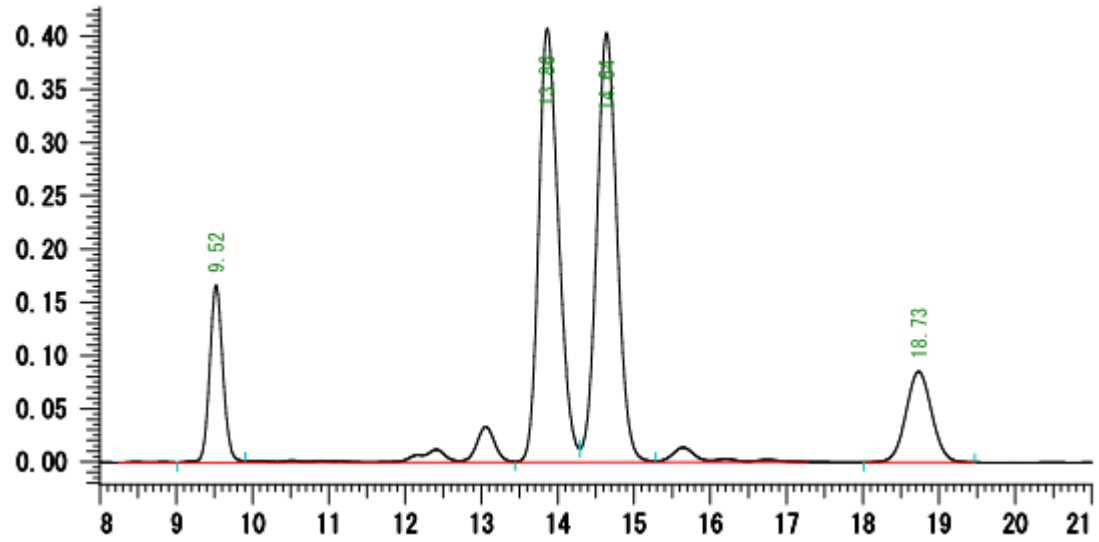


NO	RT	面積	濃度1	BC
1	65.72	6222124	15.555	MC
2	94.76	6648510	16.621	MC
3	128.70	13618554	34.046	MC
4	158.01	13511486	33.778	MC
		40000674	100.000	

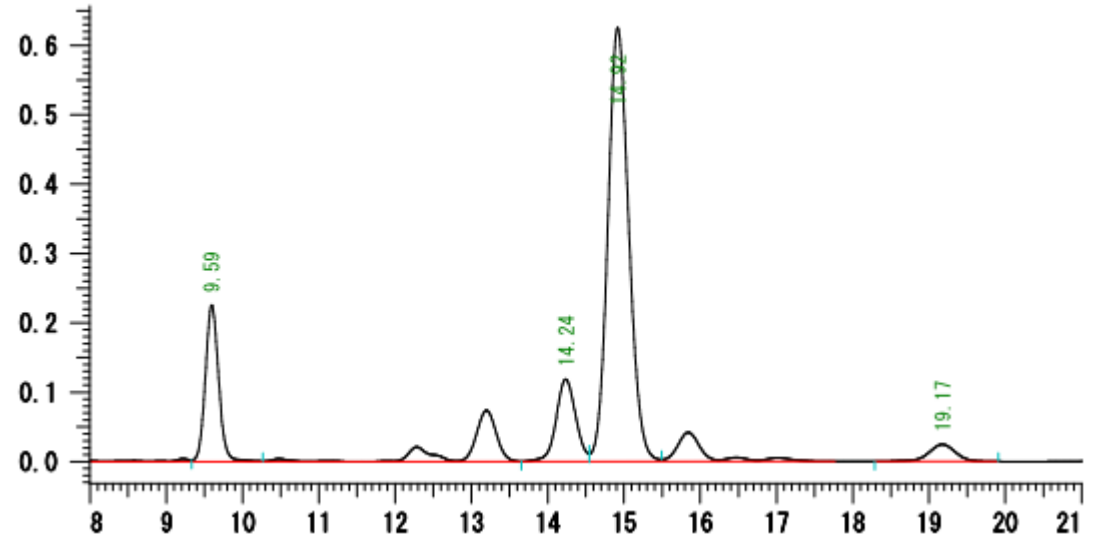


NO	RT	面積	濃度1	BC
1	65.27	18116972	19.766	MC
2	98.13	1510369	1.648	MC
3	133.99	3586357	3.913	MC
4	152.74	68444175	74.674	MC
		91657873	100.000	

4,4-dimethyl-1-phenyl-2-(1-phenylallyl)pentane-1,3-dione (4i)

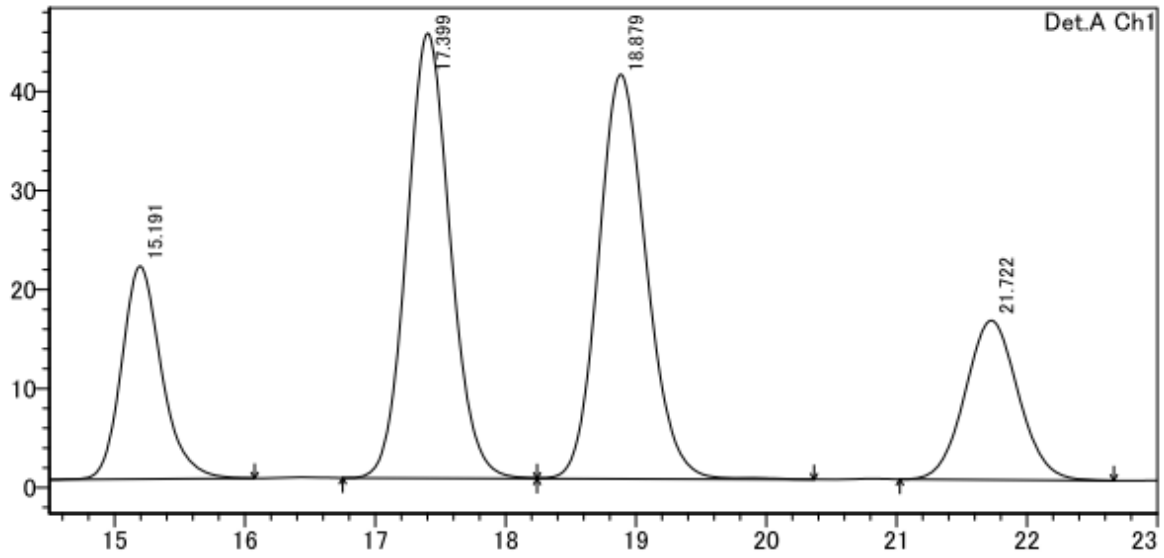


NO	RT	面積	濃度1	BC
1	9.52	1001642	10.632	BV
2	13.86	3690076	39.170	VV
3	14.64	3726234	39.554	VV
4	18.73	1002751	10.644	BB
		9420703	100.000	

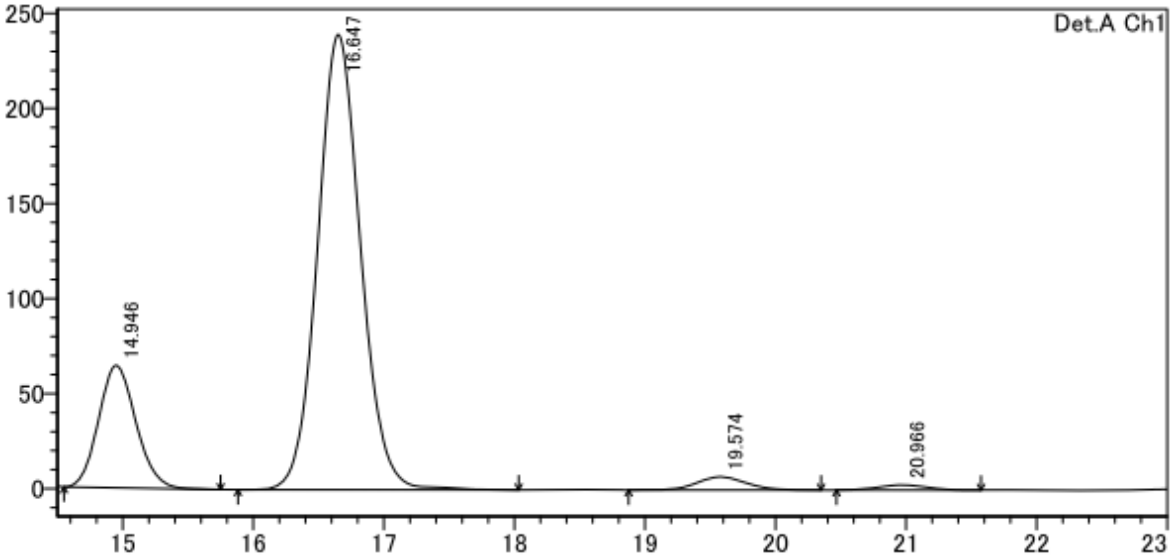


NO	RT	面積	濃度1	BC
1	9.59	1387654	15.906	VV
2	14.24	1068516	12.248	VV
3	14.92	5960807	68.326	VV
4	19.17	307059	3.520	BB
		8724036	100.000	

4-methyl-1-phenyl-2-(1-phenylallyl)pentane-1,3-dione (4j)

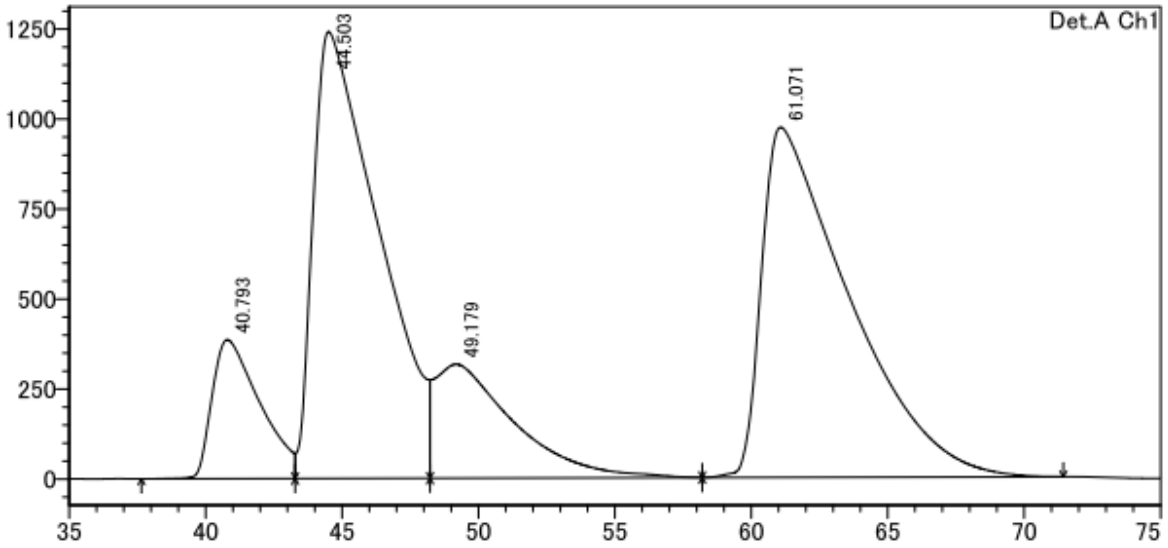


Peak	Retention Time	Area	High	Area Percent
1	15.191	458349	21498	15.271
2	17.399	1043075	44924	34.753
3	18.879	1044223	40843	34.791
4	21.722	455773	16088	15.185
合計		3001419	123353	100.000

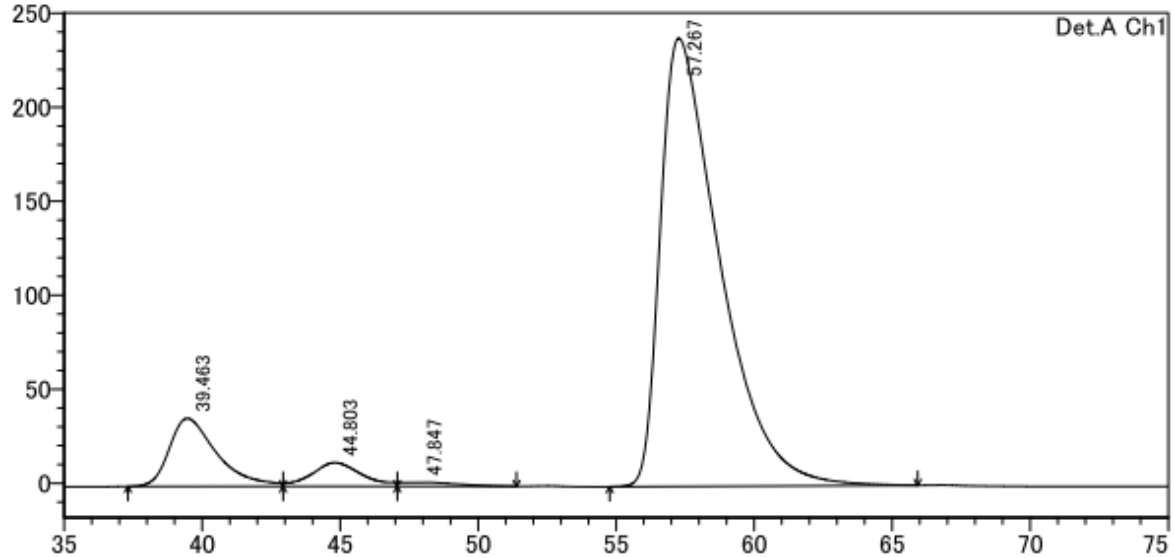


Peak	Retention Time	Area	High	Area Percent
1	14.946	1280568	64378	18.268
2	16.647	5477475	239488	78.139
3	19.574	182166	6948	2.599
4	20.966	69735	2687	0.995
合計		7009944	313500	100.000

1-phenyl-2-(1-phenylallyl)pentane-1,3-dione (4k)

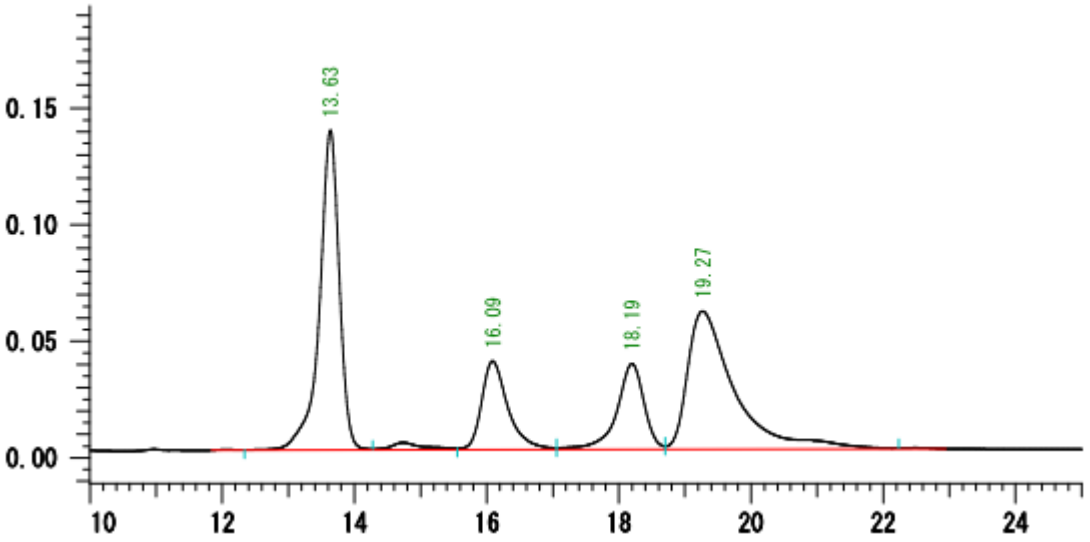


Peak	Retention Time	Area	High	Area Percent
1	40.793	46919211	385782	8.765
2	44.503	207242047	1240786	38.714
3	49.179	63862212	316390	11.930
4	61.071	217289790	972556	40.591
合計		535313260	2915514	100.000

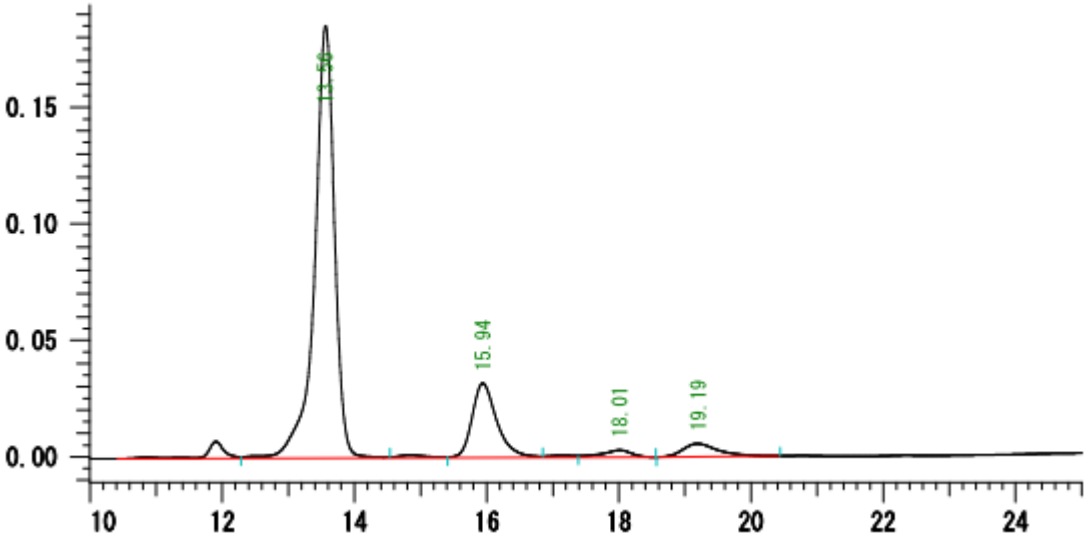


Peak	Retention Time	Area	High	Area Percent
1	39.463	4308659	36168	10.315
2	44.803	1563219	12593	3.742
3	47.847	298351	2152	0.714
4	57.267	35599716	238361	85.228
合計		41769946	289275	100.000

1-phenyl-2-(1-phenylallyl)heptane-1,3-dione (4l)

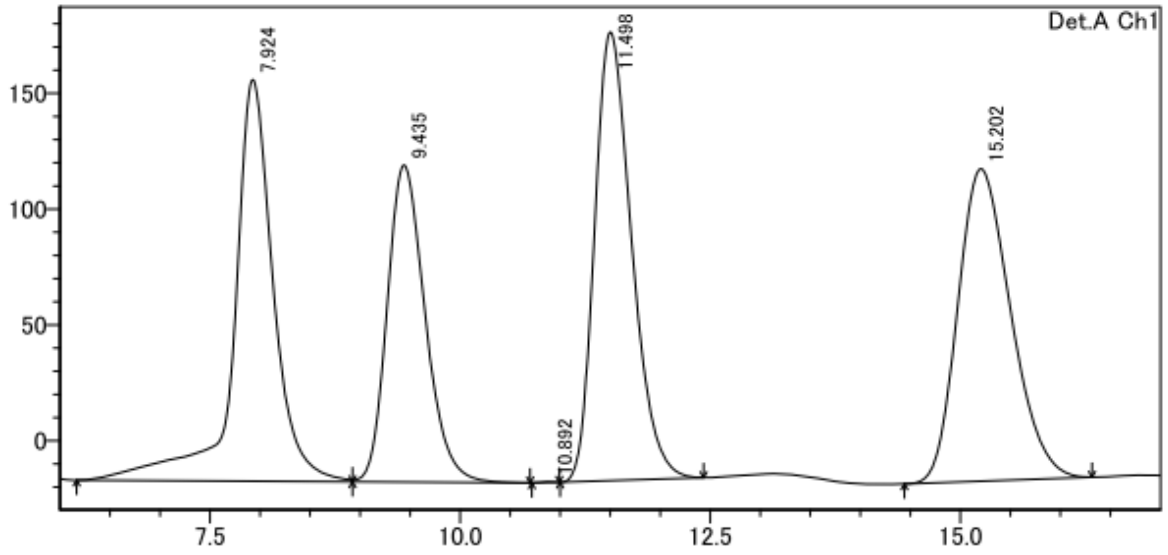


NO	RT	面積	濃度1	BC
1	13.63	1445303	36.631	BV
2	16.09	523356	13.264	VV
3	18.19	523444	13.267	VV
4	19.27	1453503	36.839	VV
		3945606	100.000	

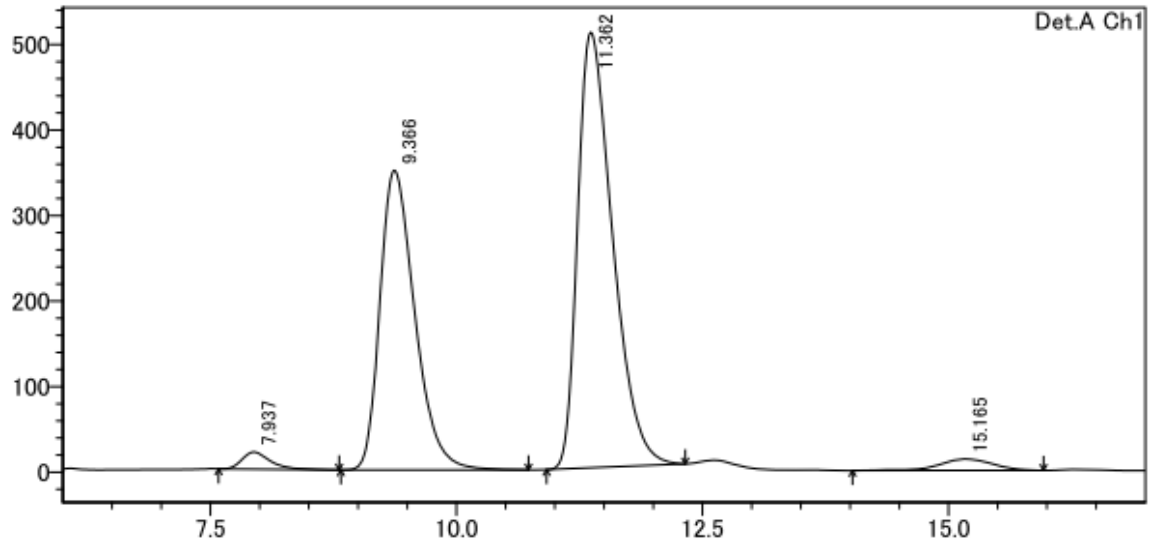


NO	RT	面積	濃度1	BC
1	13.56	1958772	77.645	VV
2	15.94	413146	16.377	VV
3	18.01	46663	1.850	VB
4	19.19	104135	4.128	BB
		2522716	100.000	

5,5-dimethyl-3-(1-phenylallyl)hexane-2,4-dione (4m)

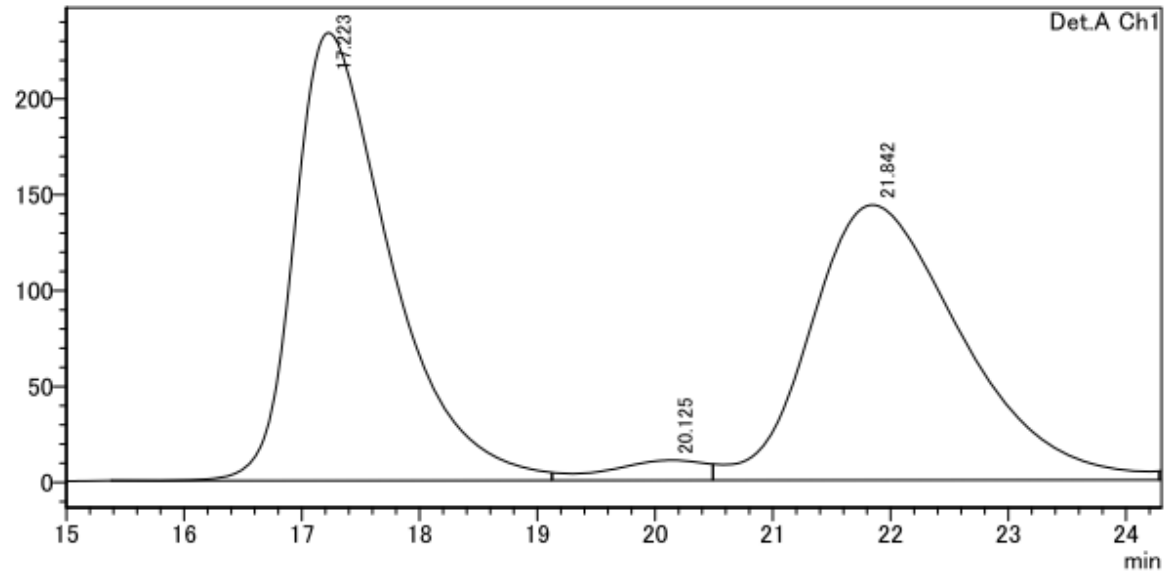


Peak	Retention Time	Area	High	Area Percent
1	7.924	4779124	173343	26.086
2	9.435	3606999	136822	19.688
3	10.892	2359	269	0.013
4	11.498	4988885	193622	27.231
5	15.202	4943359	134847	26.982
合計		18320727	638902	100.000

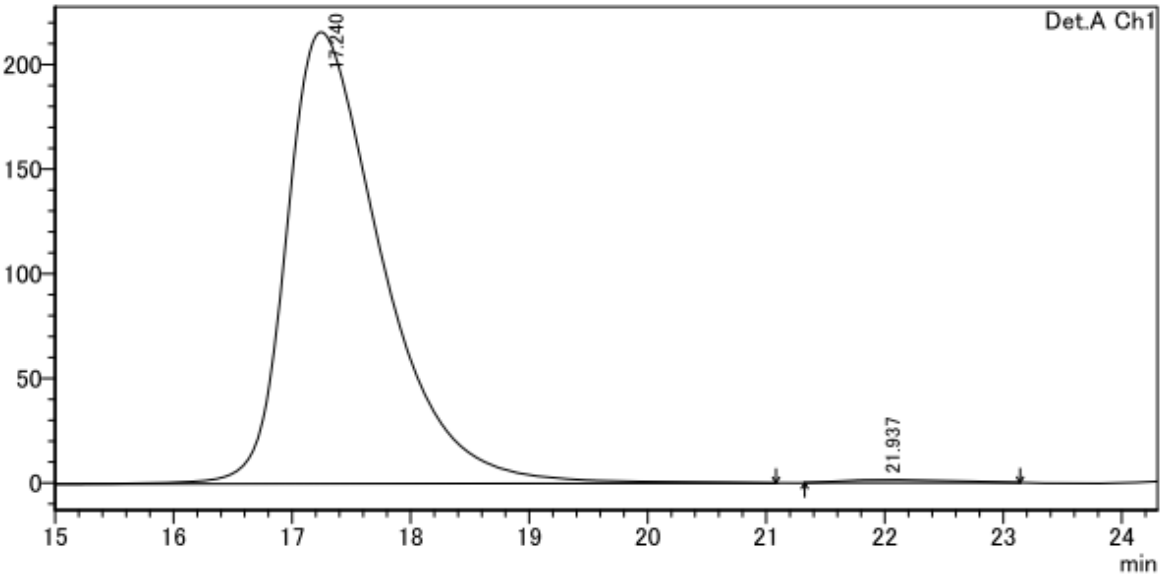


Peak	Retention Time	Area	High	Area Percent
1	7.937	400597	20046	1.813
2	9.366	8620138	350151	39.010
3	11.362	12575151	509185	56.908
4	15.165	501256	13196	2.268
合計		22097142	892578	100.000

1-phenyl-2-(1-phenylallyl)butane-1,3-diol (6a)



Peak	Retention Time	Area	High	Area Percent
1	17.223	13197490	233377	48.787
2	20.125	586623	10379	2.169
3	21.842	12780845	143414	47.247
4	24.740	486435	11035	1.798
合計		27051392	398206	100.000



Peak	Retention Time	Area	High	Area Percent
1	17.240	12091384	215877	99.272
2	21.937	88614	1315	0.728
合計		12179998	217192	100.000

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