Supporting Information

Catalytic Asymmetric Michael Addition with Curcumin Derivative

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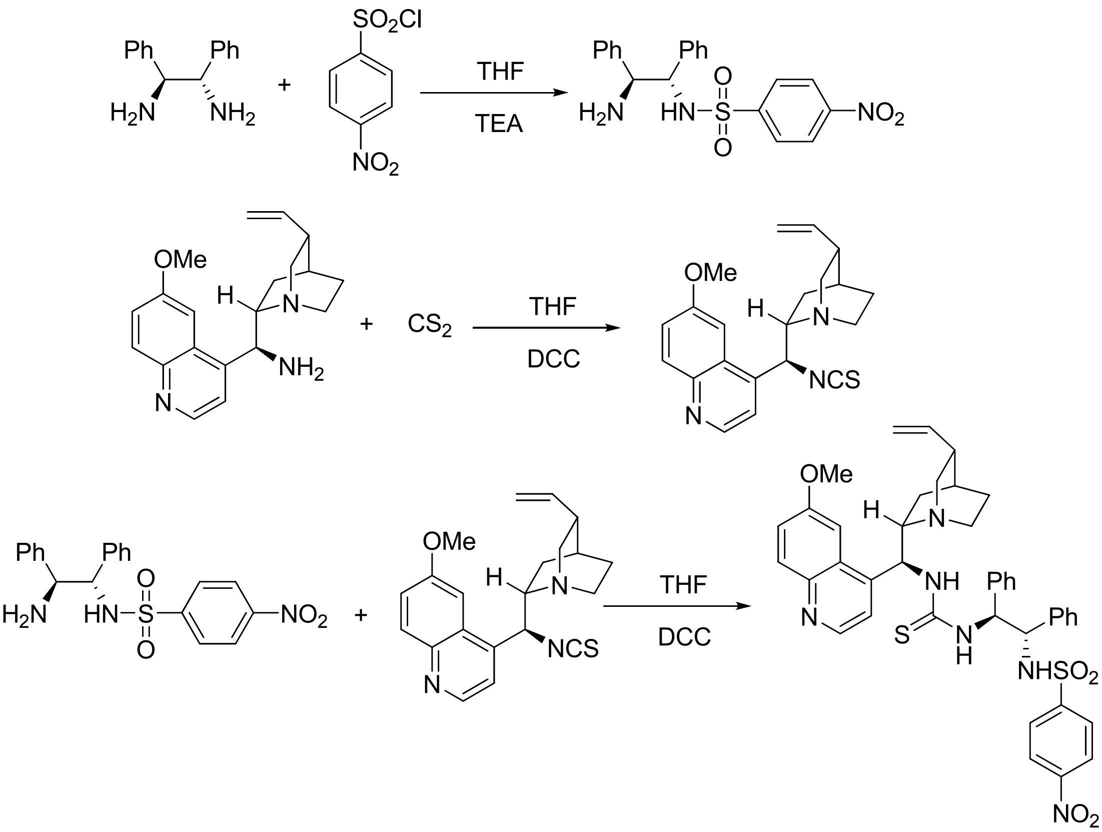
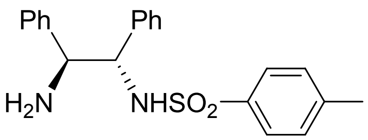
Contents

A: Procedure and Characterization for the Synthesis of Organocatalysts

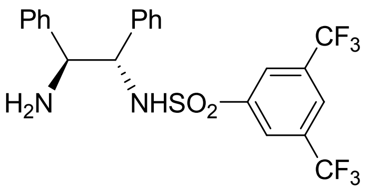
Organocatalysts **1a-1d** were prepared following the literature procedures [1-4].
The synthesis of tertiary amine-thiourea organocatalysts (**1e-1n**) were depicted in the following.



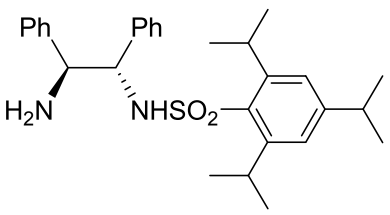
The characterization data of sulfonamides were depicted in the following.



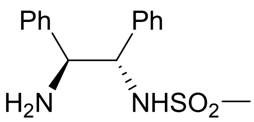
The product was obtained in 95% yield, yellow solid. Mp = 142-143 °C; $[\alpha]_D^{22}$ = 30.0 (*c* = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.33 (d, *J* = 8.0 Hz, 2H), 7.17-7.12 (m, 10H), 6.98 (d, *J* = 8.0 Hz, 2H), 4.39 (d, *J* = 5.2 Hz, 1H), 4.14 (d, *J* = 5.2 Hz, 1H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 142.5, 141.5, 139.3, 137.2, 129.1, 128.3, 128.2, 127.4, 127.3, 127.0, 126.8, 126.6, 63.5, 60.6, 21.4. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{21}H_{23}N_2O_2S$) requires m/z 367.1480, found m/z 367.1476.



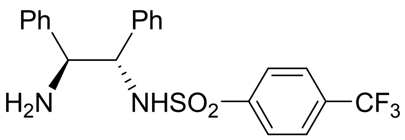
The product was obtained in 94% yield, yellow solid. Mp = 158-159 °C; $[\alpha]_D^{22}$ = 38.3 (*c* = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.87 (s, 2H), 7.80 (s, 1H), 7.17-7.09 (m, 10H), 4.53 (d, *J* = 4.8 Hz, 1H), 4.18 (d, *J* = 4.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): d (ppm) 143.2, 140.9, 138.1, 132.3, 131.9, 128.7, 128.5, 127.9, 127.8, 127.1, 126.9, 126.2, 125.5, 125.4, 123.7, 121.0, 63.4, 60.1. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{22}H_{19}F_6N_2O_2S$) requires m/z 489.1071, found m/z 489.1065.



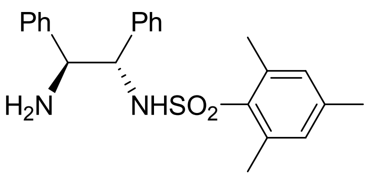
The product was obtained in 93% yield, yellow solid. Mp = 166-167 °C; $[\alpha]_D^{22}$ = 25.2 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.31-7.29 (m, 2H), 7.10-7.09 (m, 3H), 6.88-6.78 (m, 7H), 5.03 (d, J = 10.8 Hz, 1H), 4.90 (d, J = 10.8 Hz, 1H), 4.13-4.07 (m, 2H), 2.78-2.72 (m, 1H), 1.16-1.12 (m, 12H), 1.06 (d, J = 6.4 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 152.2, 149.8, 136.2, 134.2, 133.7, 128.6, 128.5, 127.8, 127.3, 123.1, 61.7, 59.2, 34.0, 29.6, 25.1, 24.8, 23.6. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{29}H_{39}N_2O_2S$) requires m/z 479.2732, found m/z 479.2732.



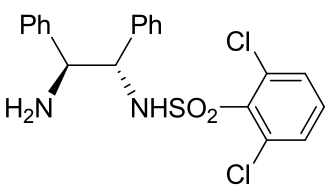
The product was obtained in 96% yield, yellow solid. Mp = 124-125 °C; $[\alpha]_D^{22}$ = 18.7 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.35-7.27 (m, 10H), 4.57 (d, J = 5.2 Hz, 1H), 4.30 (d, J = 5.2 Hz, 1H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 141.8, 139.7, 128.7, 128.6, 127.8, 127.0, 126.9, 63.7, 60.3, 40.8. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{15}H_{19}N_2O_2S$) requires m/z 291.1167, found m/z 291.1167.



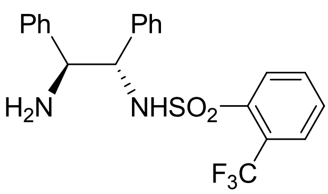
The product was obtained in 91% yield, yellow solid. Mp = 155-156 °C; $[\alpha]_D^{22}$ = 32.3 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.50 (d, J = 8.0 Hz, 2H), 7.41 (d, J = 8.0 Hz, 2H), 7.21-7.16 (m, 10H), 4.57 (d, J = 4.4 Hz, 1H), 4.21 (d, J = 4.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 143.6, 141.1, 139.0, 128.5, 128.4, 127.8, 127.7, 127.1, 126.8, 126.2, 125.6, 125.5, 63.2, 60.1. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{21}H_{20}F_3N_2O_2S$) requires m/z 421.1198, found m/z 421.1190.



The product was obtained in 92% yield, yellow solid. Mp = 158-159 °C; $[\alpha]_D^{22}$ = 14.5 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.15-7.14 (m, 3H), 7.06-7.00 (m, 5H), 6.94-6.92 (m, 2H), 6.70 (s, 2H), 4.33 (d, J = 6.8 Hz, 1H), 4.00 (d, J = 6.8 Hz, 1H), 2.41 (s, 6H), 2.21 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 141.7, 141.6, 138.7, 134.1, 131.6, 128.3, 127.8, 127.3, 127.2, 127.2, 126.6, 63.9, 60.8, 22.9, 20.8. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{23}H_{27}N_2O_2S$) requires m/z 395.1793, found m/z 395.1784.

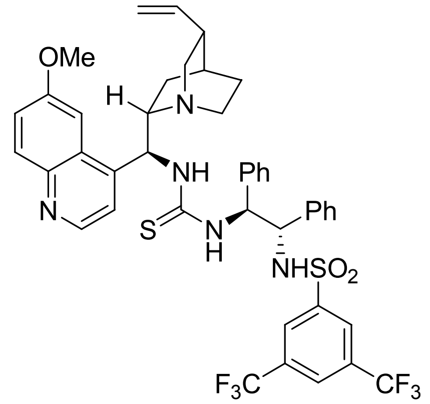


The product was obtained in 95% yield, yellow solid. Mp = 138-139 °C; $[\alpha]_D^{22}$ = 28.8 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.27-7.23 (m, 2H), 7.18-7.06 (m, 11H), 4.70 (d, J = 4.8 Hz, 1H), 4.27 (d, J = 4.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 141.1, 138.7, 136.0, 134.4, 131.7, 131.0, 128.3, 128.2, 127.6, 126.6, 126.4, 64.2, 59.9. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{20}H_{19}Cl_2N_2O_2S$) requires m/z 421.0544, found m/z 421.0547.

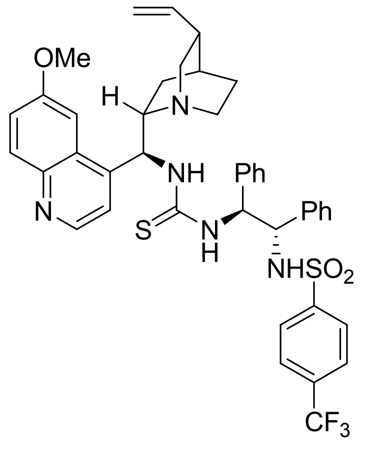


The product was obtained in 94% yield, yellow solid. Mp = 133-135 °C; $[\alpha]_D^{22}$ = 29.1 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.64 (t, J = 8.0 Hz, 2H), 7.46 (t, J = 8.0 Hz, 2H), 7.31 (t, J = 8.0 Hz, 2H), 7.21-7.06 (m, 10H), 4.54 (d, J = 4.4 Hz, 1H), 4.22 (d, J = 4.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 141.0, 139.3, 138.8, 131.9, 131.8, 130.8, 128.4, 128.3, 128.1, 128.0, 127.9, 127.5, 127.0, 126.7, 126.3, 124.3, 121.6, 63.9, 60.0. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{21}H_{20}F_3N_2O_2S$) requires m/z 421.1198, found m/z 421.1192.

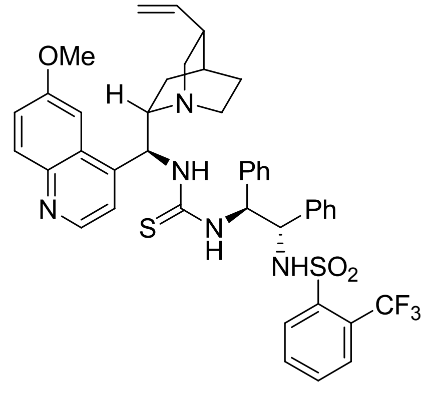
The characterization data of organocatalysts were depicted in the following.



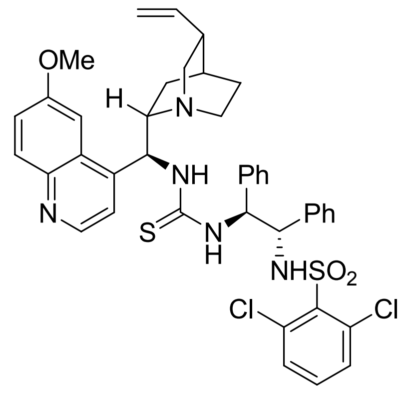
Catalyst **1e**: The product was obtained in 84% yield, yellow solid. Mp = 143-144 °C; $[\alpha]_D^{22}$ = - 1.6 (c = 1.0, $CHCl_3$); ^{1}H-NMR (400 MHz, $(CD_3)_2CO$): δ (ppm) 8.66 (d, J = 4.4 Hz, 1H), 8.03-7.93 (m, 5H), 7.48 (d, J = 4.4 Hz, 1H), 7.39-7.36 (m, 1H), 7.10-7.02 (m, 5H), 6.94-6.90 (m, 5H), 5.86-5.77 (m, 3H), 5.01-4.89 (m, 3H), 3.97 (s, 3H), 3.29-3.23 (m, 3H), 2.77-2.70 (m, 2H), 2.34 (br, 1H), 1.76-1.65 (m, 3H), 1.41-1.35 (m, 1H), 1.08-1.03 (m, 1H). ^{13}C-NMR (100 MHz, $(CD_3)_2CO$): δ (ppm) 205.4, 183.5, 170.1, 157.6, 147.5, 144.8, 144.5, 141.8, 138.1, 136.8, 131.7, 131.5, 131.3, 128.3, 128.0, 127.8, 127.5, 127.2, 125.4, 124.0, 121.4, 113.7, 102.8, 63.1, 62.2, 62.1, 60.5, 59.7, 55.5, 55.3, 40.9, 39.7, 27.7, 27.6, 25.7, 19.9, 13.6. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{43}H_{42}N_5O_3F_6S_2$) requires m/z 854.2633, found m/z 854.2632.



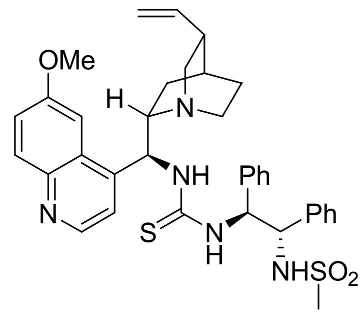
Catalyst **1f**: The product was obtained in 82% yield, yellow solid. Mp = 154-155 °C; $[\alpha]_D^{22}$ = 9.8 (c = 1.0, $CHCl_3$); ^{1}H-NMR (400 MHz, $(CD_3)_2CO$): δ (ppm) 8.75-8.74 (m, 1H), 8.03-8.00 (m, 2H), 7.65-7.63 (m, 2H), 7.51-7.43 (m, 4H), 7.09-6.89 (m, 10H), 5.84-5.70 (m, 3H), 4.99-4.88 (m, 2H), 4.74-4.71 (m, 1H), 4.05 (s, 3H), 3.26-3.18 (m, 3H), 2.68 (br, 2H), 2.30 (br, 1H), 1.69-1.57 (m, 3H), 1.40-1.34 (m, 1H), 1.05-1.00 (m, 1H). ^{13}C-NMR (100 MHz, $(CD_3)_2CO$): δ (ppm) 205.5, 183.2, 170.1, 157.8, 147.7, 145.2, 144.8, 141.8, 138.5, 137.9, 132.6, 132.3, 131.6, 128.1, 127.8, 127.7, 127.4, 127.2, 125.6, 124.9, 122.3, 121.6, 113.7, 102.7, 63.3, 62.5, 59.7, 55.4, 40.9, 39.6, 27.6, 25.7, 20.0, 13.7. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{42}H_{43}N_5O_3S_2F_3$) requires m/z 786.2759, found m/z 786.2753.



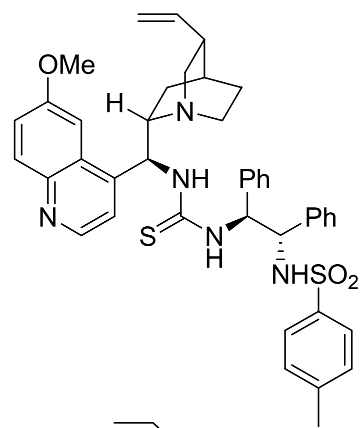
Catalyst **1g:** The product was obtained in 85% yield, yellow solid. Mp = 151-152 °C; $[\alpha]_D^{22}$ = - 8.7 (c = 1.0, $CHCl_3$); ^{1}H-NMR (400 MHz, $(CD_3)_2CO$): δ (ppm) 8.70-8.69 (m, 1H), 7.99-7.93 (m, 2H), 7.76-7.69 (m, 3H), 7.59-7.55 (m, 1H), 7.50-7.40 (m, 3H), 7.08 (br, 3H), 6.95-6.90 (m, 6H), 5.84-5.75 (m, 3H), 5.00-4.88 (m, 2H), 4.77-4.75 (m, 1H), 4.03 (s, 3H), 3.23 (br, 3H), 2.71 (br, 2H), 2.31 (br, 1H), 1.73-1.59 (m, 3H), 1.37-1.30 (m, 1H), 1.09-1.04 (m, 1H). ^{13}C-NMR (100 MHz, $(CD_3)_2CO$): δ (ppm) 205.5, 157.8, 147.7, 144.8, 141.8, 139.8, 137.8, 132.2, 131.0, 128.1, 127.8, 127.7, 127.4, 127.2, 124.5, 121.8, 121.5, 113.7, 102.6, 63.7, 62.5, 59.7, 55.4, 40.8, 39.6, 27.6, 25.6, 20.0, 13.7. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{42}H_{43}N_5O_3S_2F_3$) requires m/z 786.2759, found m/z 786.2760.



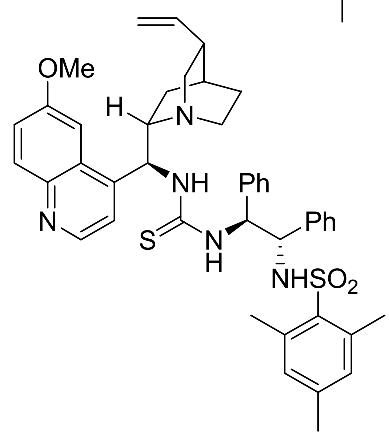
Catalyst **1h:** The product was obtained in 84% yield, yellow solid. Mp = 157-158 °C; $[\alpha]_D^{22}$ = 7.6 (c = 1.0, $CHCl_3$); ^{1}H-NMR (400 MHz, $(CD_3)_2CO$): δ (ppm) 8.72-8.71 (m, 1H), 7.99-7.93 (m, 3H), 7.53 (br, 1H), 7.43-7.40 (m, 1H), 7.20-6.96 (m, 9H), 6.88-6.86 (m, 3H), 5.85-5.75 (m, 3H), 5.00-4.74 (m, 3H), 4.04 (s, 3H), 3.23 (br, 3H), 2.93-2.71 (m, 3H), 2.30 (br, 1H), 1.71-1.59 (m, 3H), 1.36-1.30 (m, 1H), 1.10-1.05 (m, 1H). ^{13}C-NMR (100 MHz, $(CD_3)_2CO$): δ (ppm) 205.4, 170.1, 157.7, 147.7, 144.8, 141.8, 137.2, 136.2, 133.9, 132.2, 131.6, 131.0, 128.2, 128.1, 127.7, 127.4, 127.3, 121.3, 113.7, 64.1, 59.6, 55.3, 40.8, 39.6, 27.6, 27.5, 25.5, 19.9, 13.6. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{41}H_{42}N_5O_3S_2Cl_2$) requires m/z 786.2106, found m/z 786.2090.



Catalyst **1j**: The product was obtained in 84% yield, yellow solid. Mp = 138-139 °C; $[\alpha]_D^{22}$ = 4.5 (c = 1.0, $CHCl_3$); ^{1}H-NMR (400 MHz, $(CD_3)_2CO$): δ (ppm) 8.70-8.68 (m, 1H), 8.00-7.95 (m, 2H), 7.50-7.27 (m, 5H), 7.24-7.13 (m, 7H), 5.84-5.75 (m, 2H), 4.99-4.73 (m, 3H), 4.02 (s, 3H), 3.26-3.20 (m, 3H), 2.89 (s, 3H), 2.50 (br, 2H), 2.39 (s, 1H), 2.30 (br, 1H), 1.77-1.49 (m, 3H), 1.37-1.30 (m, 1H), 1.08-1.03 (m, 1H). ^{13}C-NMR (100 MHz, $(CD_3)_2CO$): δ (ppm) 205.5, 170.1, 157.7, 147.6, 144.8, 141.8, 139.7, 138.7, 131.6, 128.2, 127.9, 127.8, 127.5, 127.0, 121.5, 113.7, 102.7, 68.5, 64.4, 63.3, 62.5, 59.7, 55.4, 40.8, 40.6, 40.4, 39.6, 27.6, 25.6, 20.0, 13.7. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{36}H_{42}N_5O_3S_2$) requires m/z 656.2729, found m/z 656.2733.

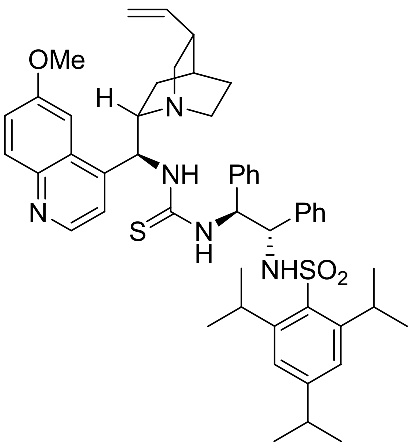


Catalyst **1k**: The product was obtained in 84% yield, yellow solid. Mp = 145-146 °C; $[\alpha]_D^{22}$ = -12.2 (c = 1.0, $CHCl_3$); ^{1}H-NMR (400 MHz, $(CD_3)_2CO$): δ (ppm) 8.73-8.74 (m, 1H), 8.00-8.03 (m, 2H), 7.51-7.39 (m, 5H), 7.13-6.90 (m, 11H), 5.85-5.76 (m, 1H), 5.69-5.63 (m, 1H), 5.00-4.88 (m, 2H), 4.62-4.60 (m, 1H), 4.06 (s, 3H), 3.29-3.18 (m, 3H), 2.93 (br, 2H), 2.69 (br, 2H), 2.28 (s, 3H), 1.69-1.58 (m, 3H), 1.40-1.35 (m, 1H), 1.03-1.02 (m, 1H).^{13}C-NMR (100 MHz, $(CD_3)_2CO$): δ (ppm) 205.5, 157.9, 147.7, 144.8, 142.4, 141.8, 138.5, 131.6, 129.0, 128.0, 127.8, 127.7, 127.4, 127.0, 126.7, 121.6, 113.7, 63.2, 62.7, 59.7, 55.5, 40.9, 39.6, 27.7, 25.7, 20.5, 20.0, 13.6. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{42}H_{46}N_5O_3S_2$) requires m/z 732.3042, found m/z 732.3055.

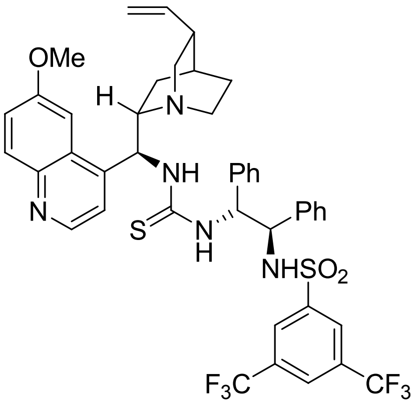


Catalyst **1l**: The product was obtained in 84% yield, yellow solid. Mp = 148-149 °C; $[\alpha]_D^{22}$ = 1.7 (c = 1.0, $CHCl_3$); ^{1}H-NMR (400

MHz, $(CD_3)_2CO$): δ (ppm) 8.71 (br, 1H), 8.00-7.93 (m, 3H), 7.54-7.41 (m, 2H), 7.06-6.82 (m, 9H), 6.71 (s, 2H), 5.84-5.68 (m, 3H), 5.01-4.89 (m, 2H), 4.54-4.52 (m, 1H), 4.03 (s, 3H), 3.28-3.25 (m, 3H), 2.35 (s, 6H), 2.17 (s, 3H), 1.73-1.61 (m, 3H), 1.35-1.30 (m, 3H), 1.10-1.07 (m, 1H), 0.89-0.87 (m, 1H). ^{13}C-NMR (100 MHz, $(CD_3)_2CO$): δ (ppm) 205.6, 170.1, 157.8, 147.8, 144.8, 141.6, 141.5, 138.7, 138.4, 135.2, 131.6, 131.4, 128.1, 127.9, 127.6, 127.4, 127.0, 121.5, 113.9, 102.8, 63.1, 62.7, 59.7, 55.4, 55.3, 40.9, 39.5, 27.6, 25.6, 22.3, 20.0, 13.8. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{44}H_{50}N_5O_3S_2$) requires m/z 760.3355, found m/z 760.3365.

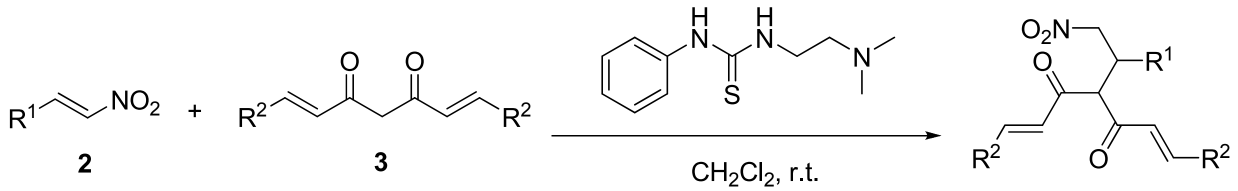


Catalyst **1m**: The product was obtained in 84% yield, yellow solid. Mp = 185-186 °C; $[\alpha]_D^{22}$ = 5.3 (*c* = 1.0, $CHCl_3$); ^{1}H-NMR (400 MHz, $(CD_3)_2CO$): δ (ppm) 8.72 (s, 1H), 8.02-7.86 (m, 4H), 7.43 (br, 1H), 7.06-6.92 (m, 9H), 6.79-6.76 (m, 2H), 5.83-5.75 (m, 3H), 5.01-4.88 (m, 2H), 4.65 (br, 1H), 4.03 (s, 3H), 3.24 (br, 3H), 2.93-2.73 (m, 5H), 2.32 (br, 1H), 1.73-1.61 (m, 3H), 1.34-1.30 (m, 2H), 1.18 (d, J = 6.8 Hz, 6H), 1.08-1.00 (m, 12H). ^{13}C-NMR (100 MHz, $(CD_3)_2CO$): δ (ppm) 205.4, 157.7, 152.3, 149.5, 147.8, 144.8, 141.7, 138.7, 138.5, 134.5, 131.7, 128.0, 127.7, 127.4, 127.3, 126.3, 123.3, 121.5, 121.4, 113.8, 102.6, 62.9, 59.7, 55.3, 40.7, 39.6, 27.7, 25.5, 24.4, 24.2, 23.1, 20.1, 13.7. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{50}H_{62}N_5O_3S_2$) requires m/z 844.4294, found m/z 844.4295.



Catalyst **1n**: The product was obtained in 84% yield, yellow solid. Mp = 152-153 °C; $[\alpha]_D^{22}$ = 2.5 (*c* = 1.0, $CHCl_3$); ^{1}H-NMR (400 MHz, $(CD_3)_2CO$): δ (ppm) 8.66 (d, J = 4.4 Hz, 1H), 8.03-7.93 (m, 5H), 7.48 (d, J = 4.4 Hz, 1H), 7.39-7.36 (m, 1H), 7.10-7.02 (m, 5H), 6.94-6.90 (m, 5H), 5.86-5.77 (m, 3H), 5.01-4.89 (m, 3H), 3.97 (s, 3H), 3.29-3.23 (m, 3H), 2.77-2.70 (m, 2H), 2.34 (br, 1H), 1.76-1.65 (m, 3H), 1.41-1.35 (m, 1H), 1.08-1.03 (m, 1H). ^{13}C-NMR (100 MHz, $(CD_3)_2CO$): δ (ppm) 205.4, 183.5, 170.1, 157.6, 147.5, 144.8, 144.5, 141.8, 138.1, 136.8, 131.7, 131.5, 131.3, 128.3, 128.0, 127.8, 127.5, 127.2, 125.4, 124.0, 121.4, 113.7, 102.8, 63.1, 62.2, 62.1, 60.5, 59.7, 55.5, 55.3, 40.9, 39.7, 27.7, 27.6, 25.7, 19.9, 13.6. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{43}H_{42}N_5O_3F_6S_2$) requires m/z 854.2633, found m/z 854.2638.

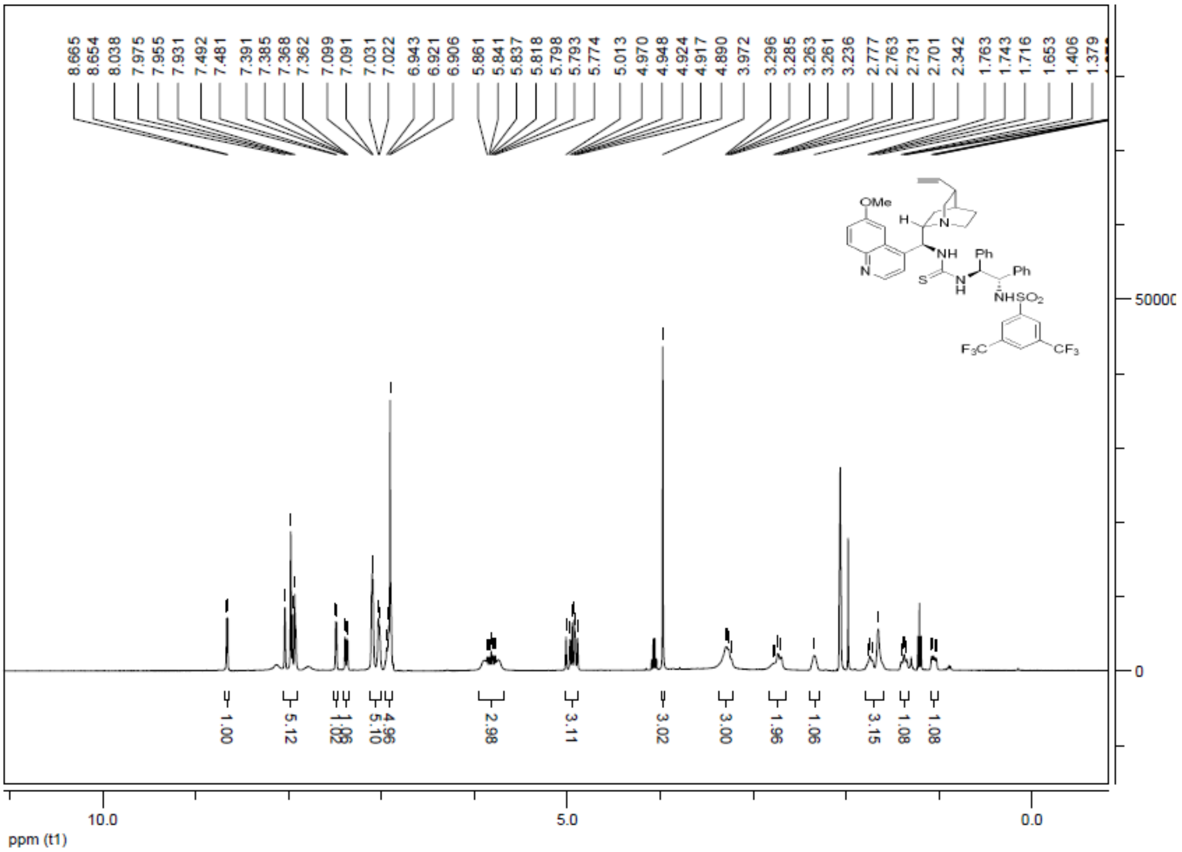
B: Procedure for the Synthesis of Racemic Products

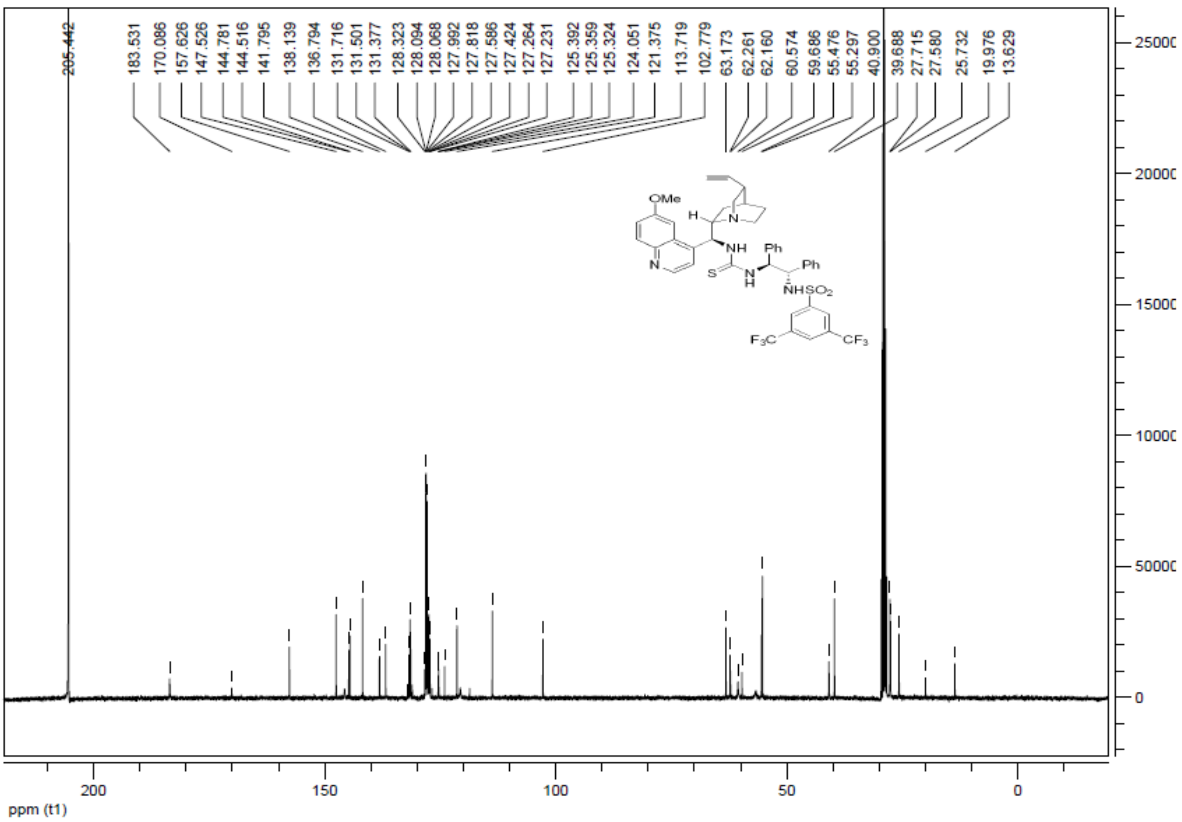


To a solution of trans-β-substituted nitroolefins **2** (0.10 mmol) in dichloromethane (0.2 mL) were added curcumin derivates **3** (0.10 mmol) and catalyst (0.01 mmol). The reaction mixture was stirred at room temperature for 72h and then the solvent was removed under vacuum. The residues were purified by silica gel chromatography to yield the desired addition products.

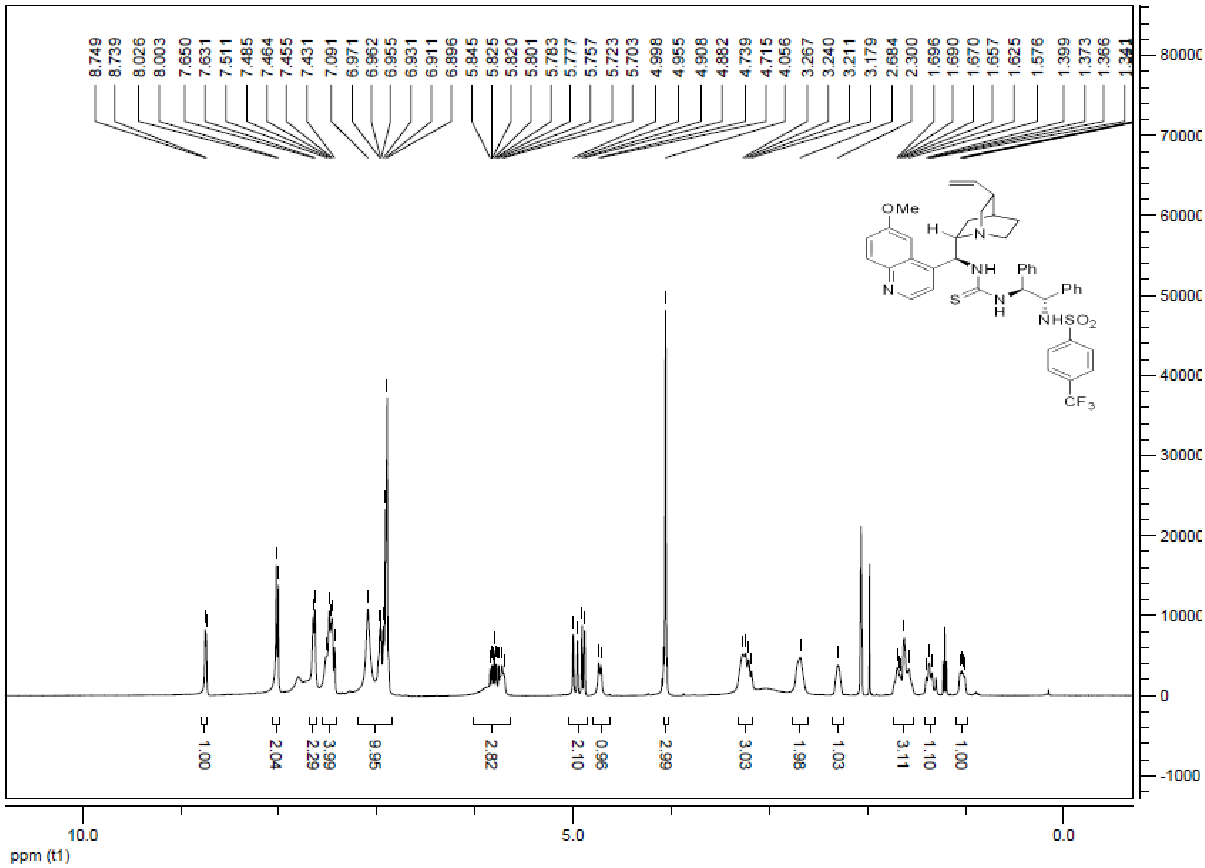
C: NMR Spectra of Organocatalysts

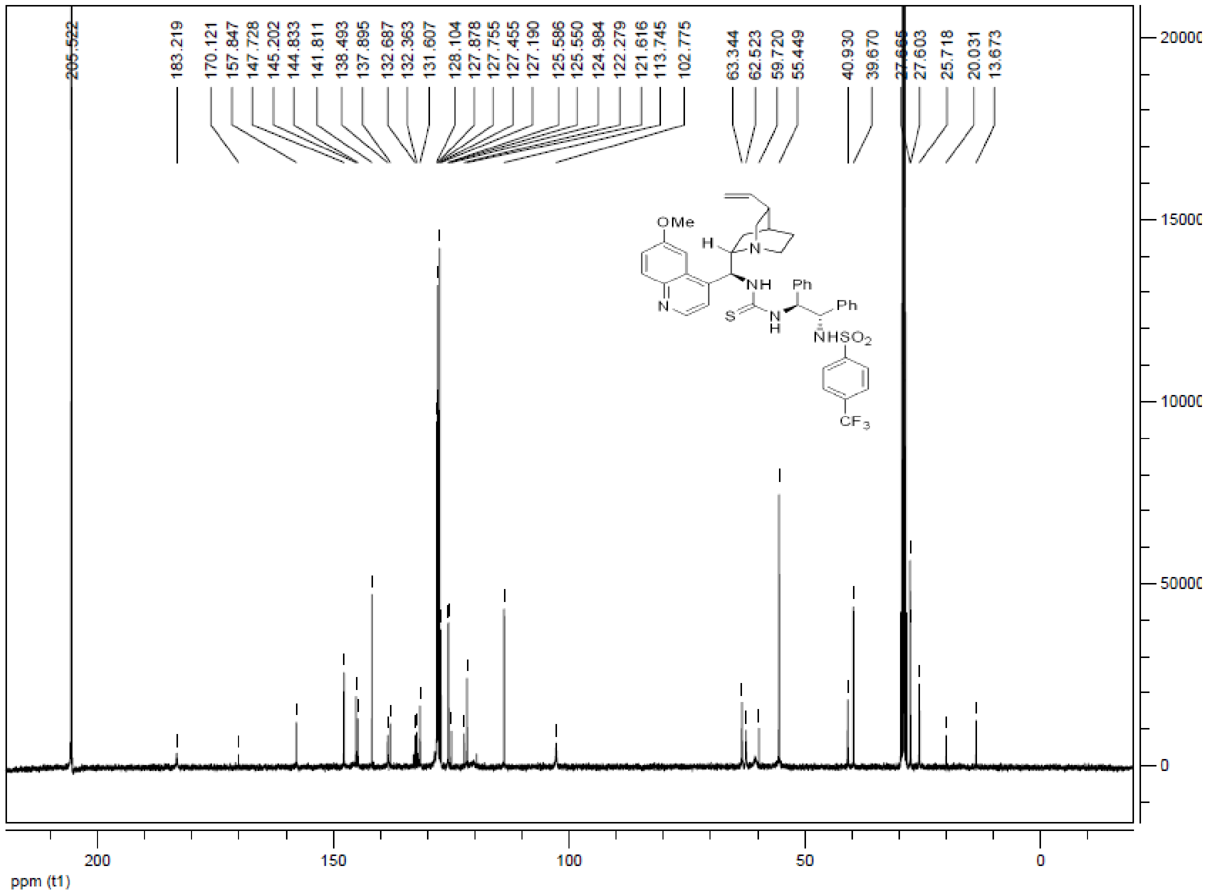
Catalyst 1e



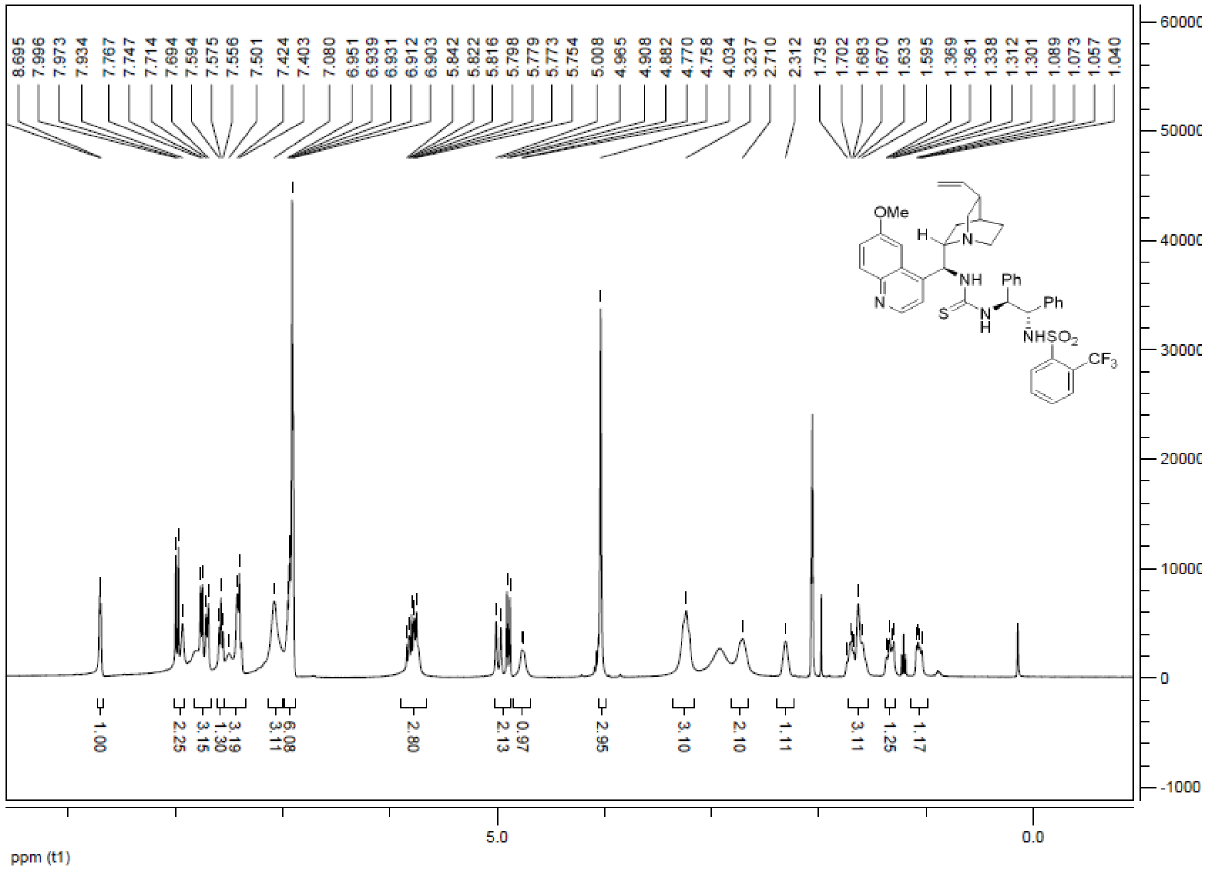


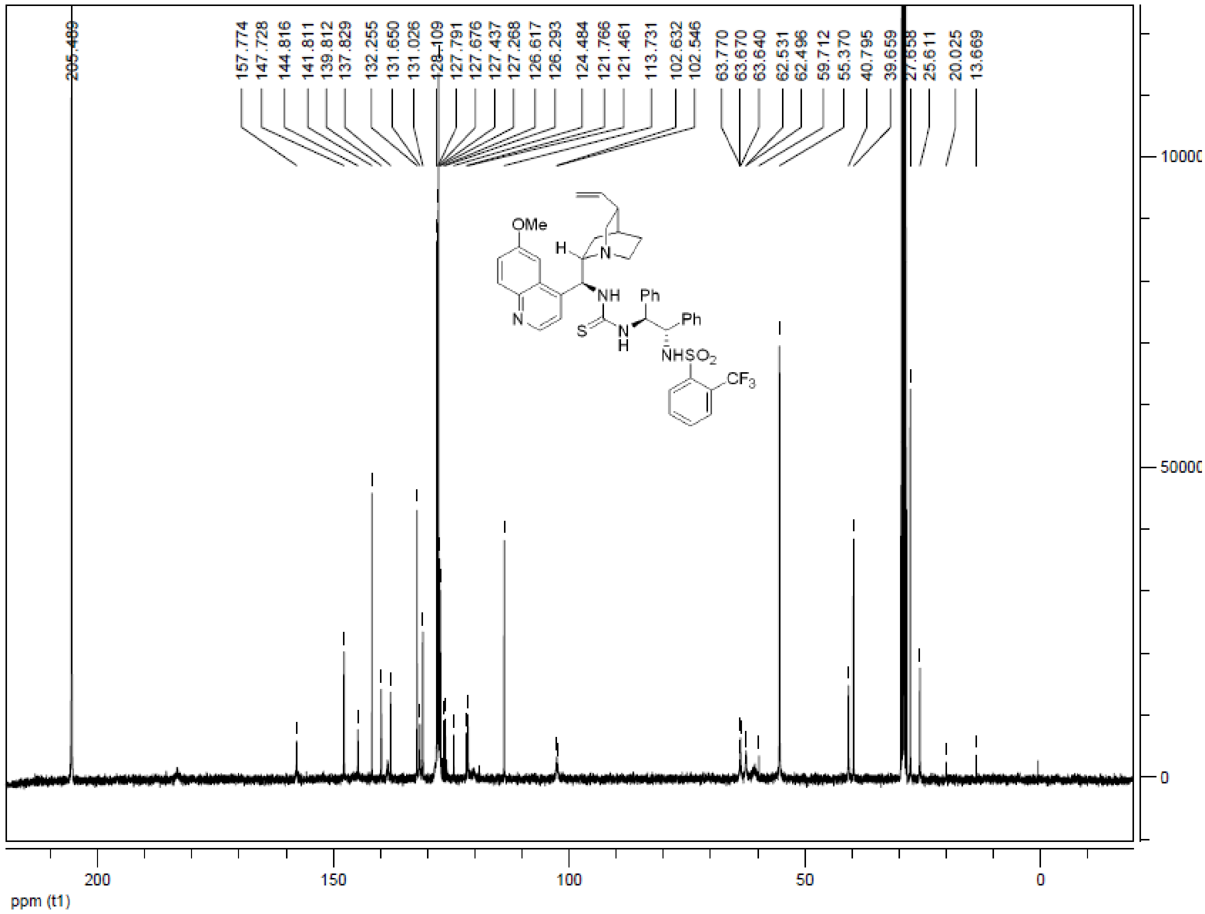
Catalyst 1f



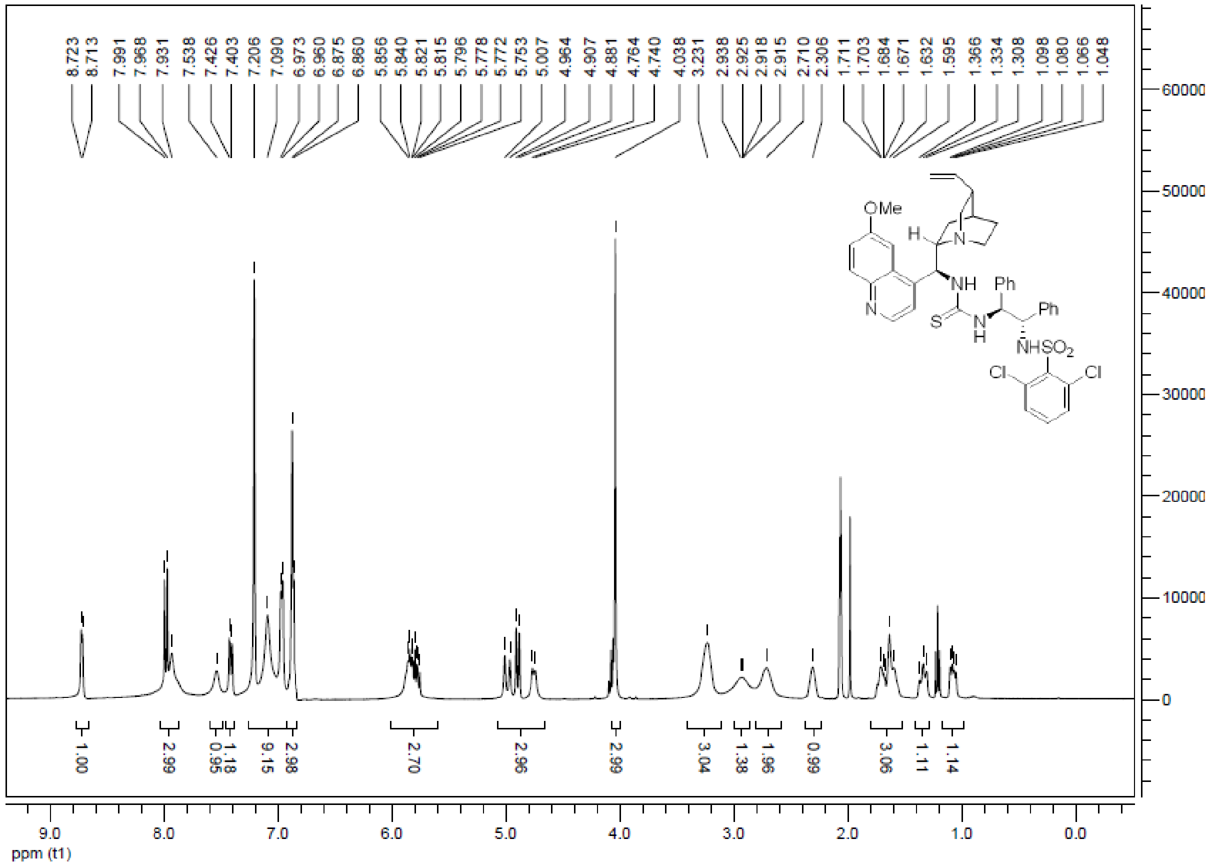


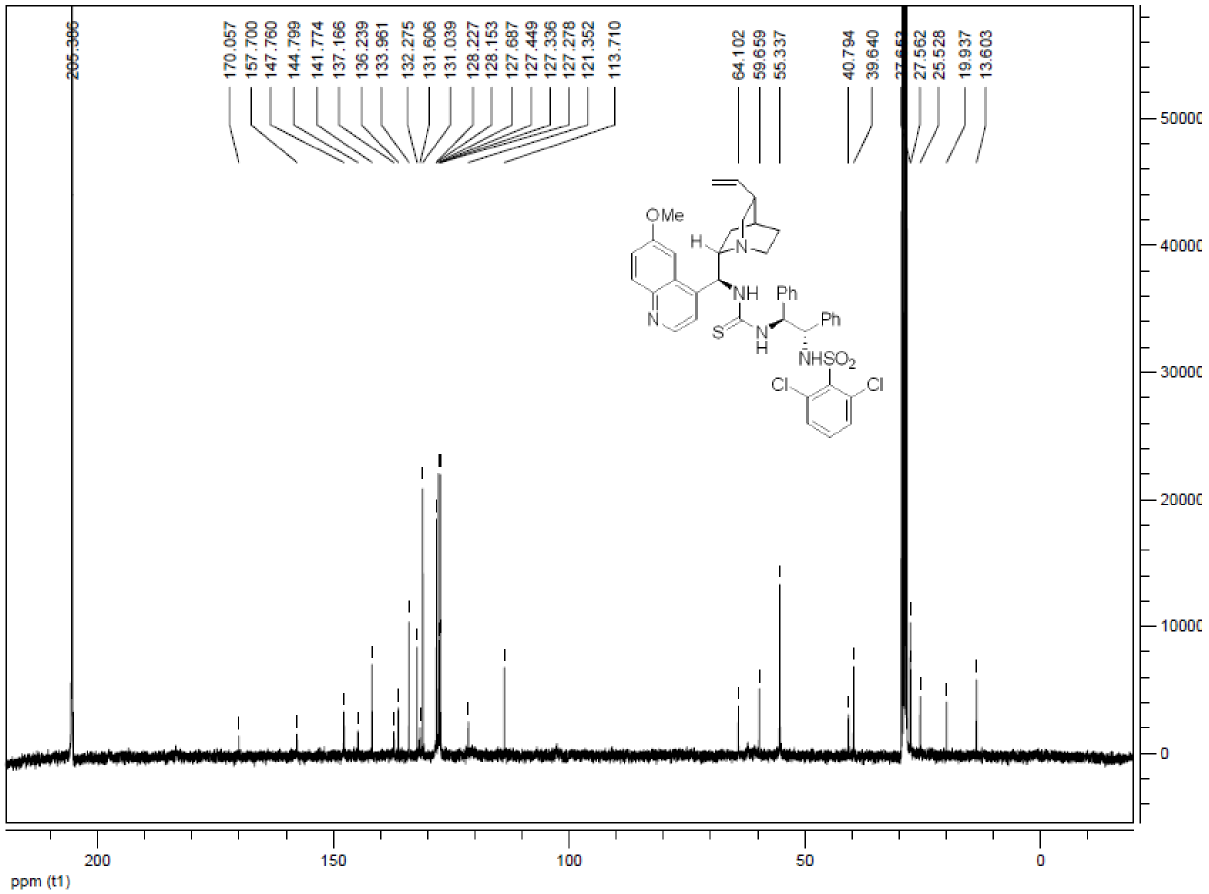
Catalyst 1g



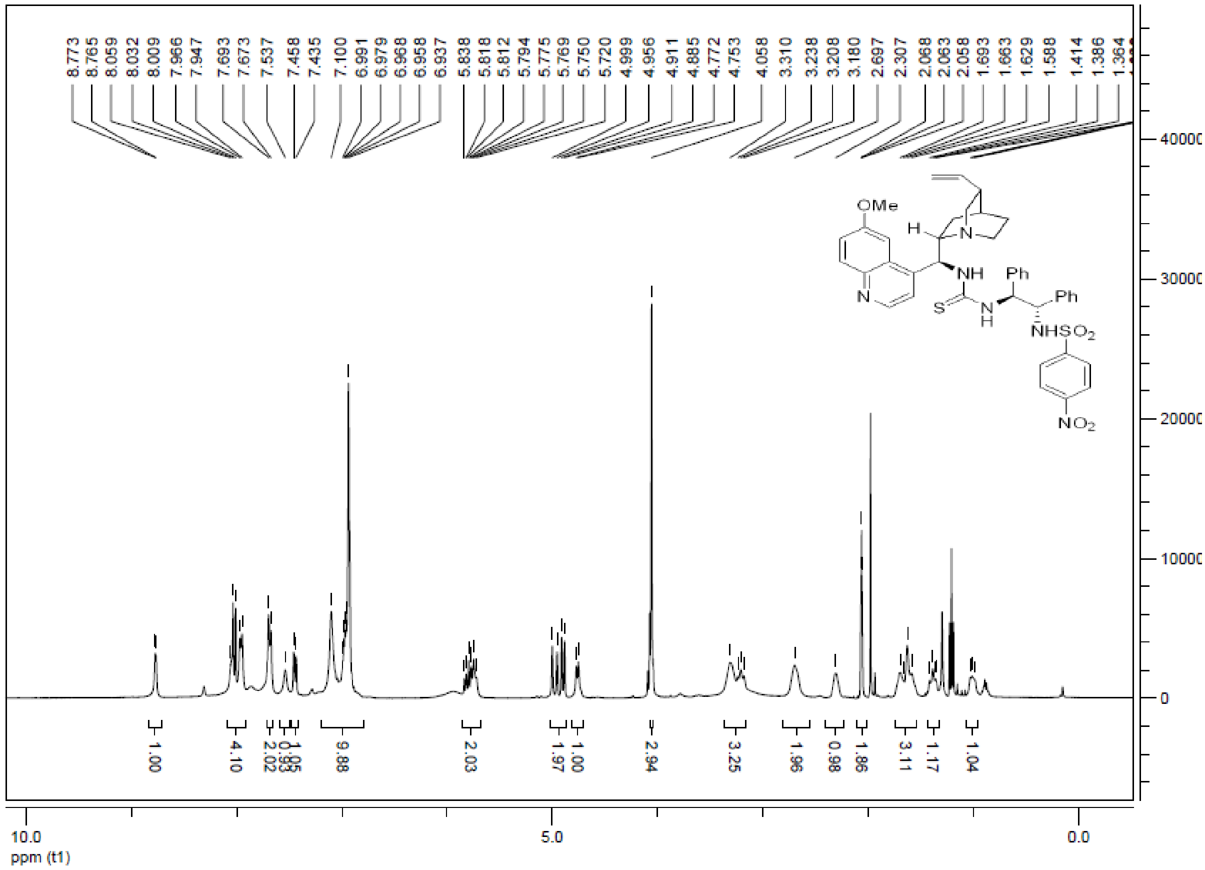


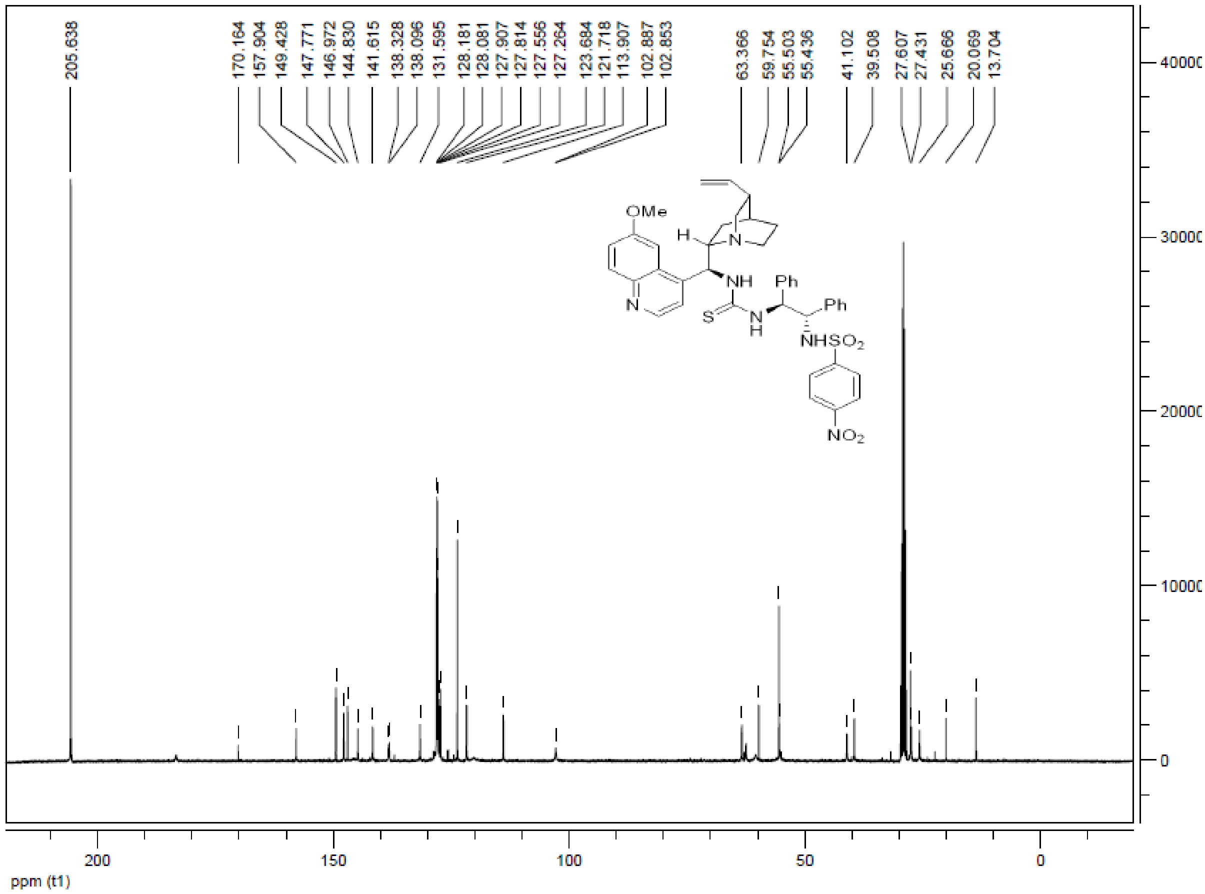
Catalyst 1h



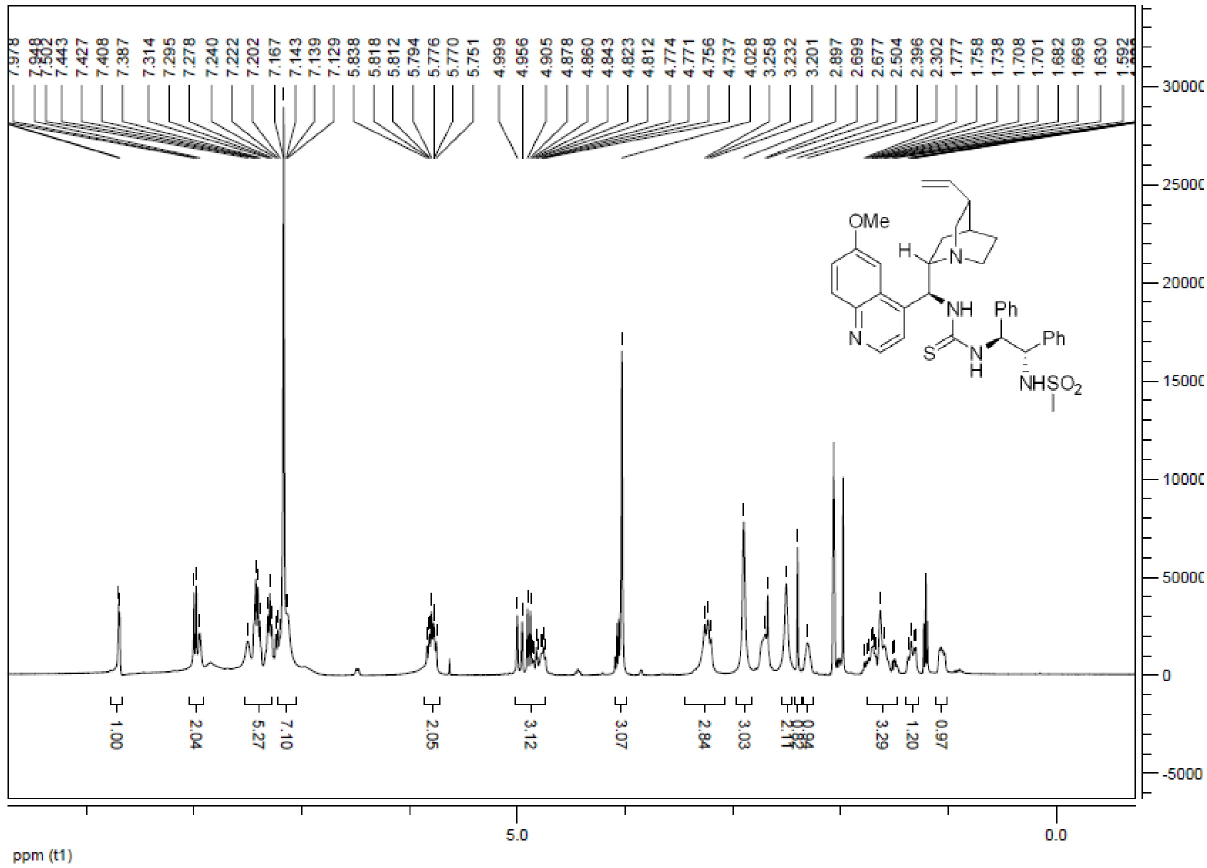


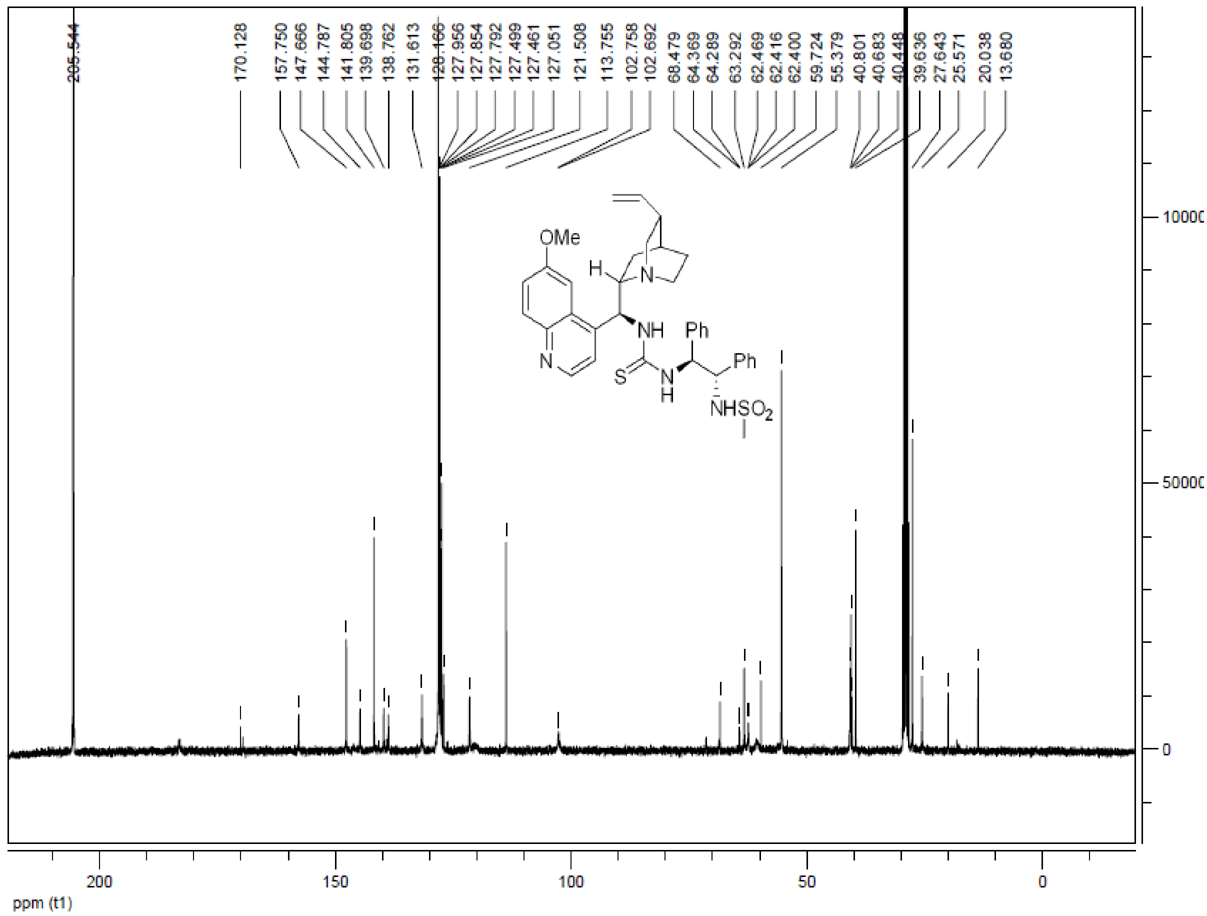
Catalyst 1i



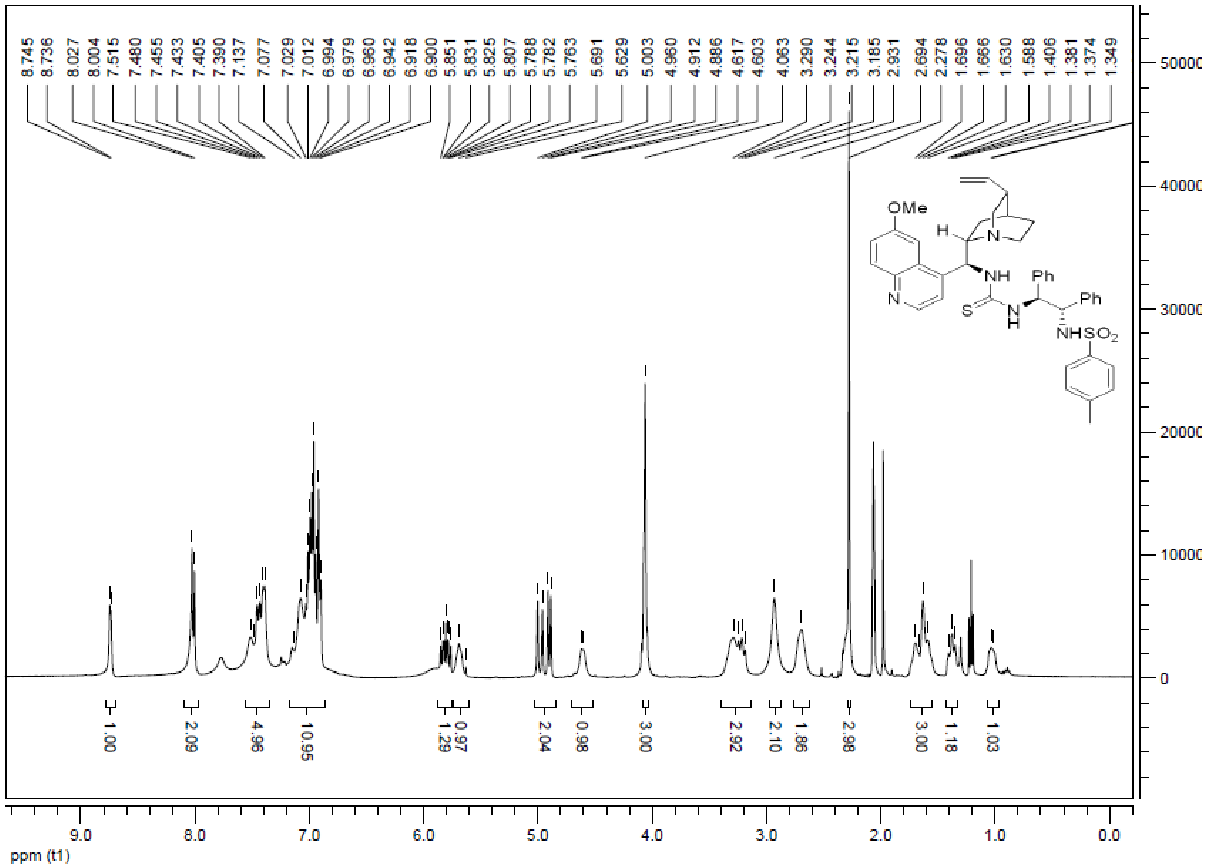


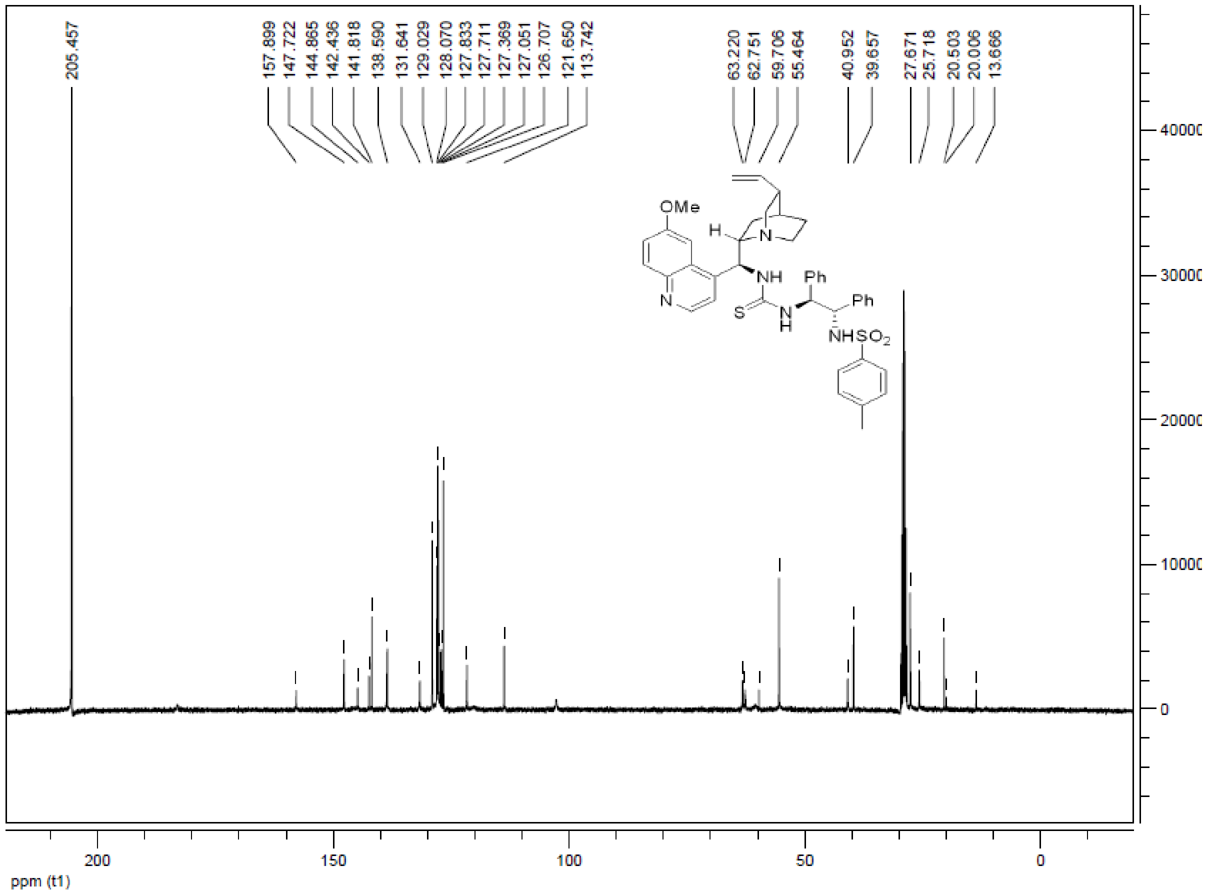
Catalyst 1j



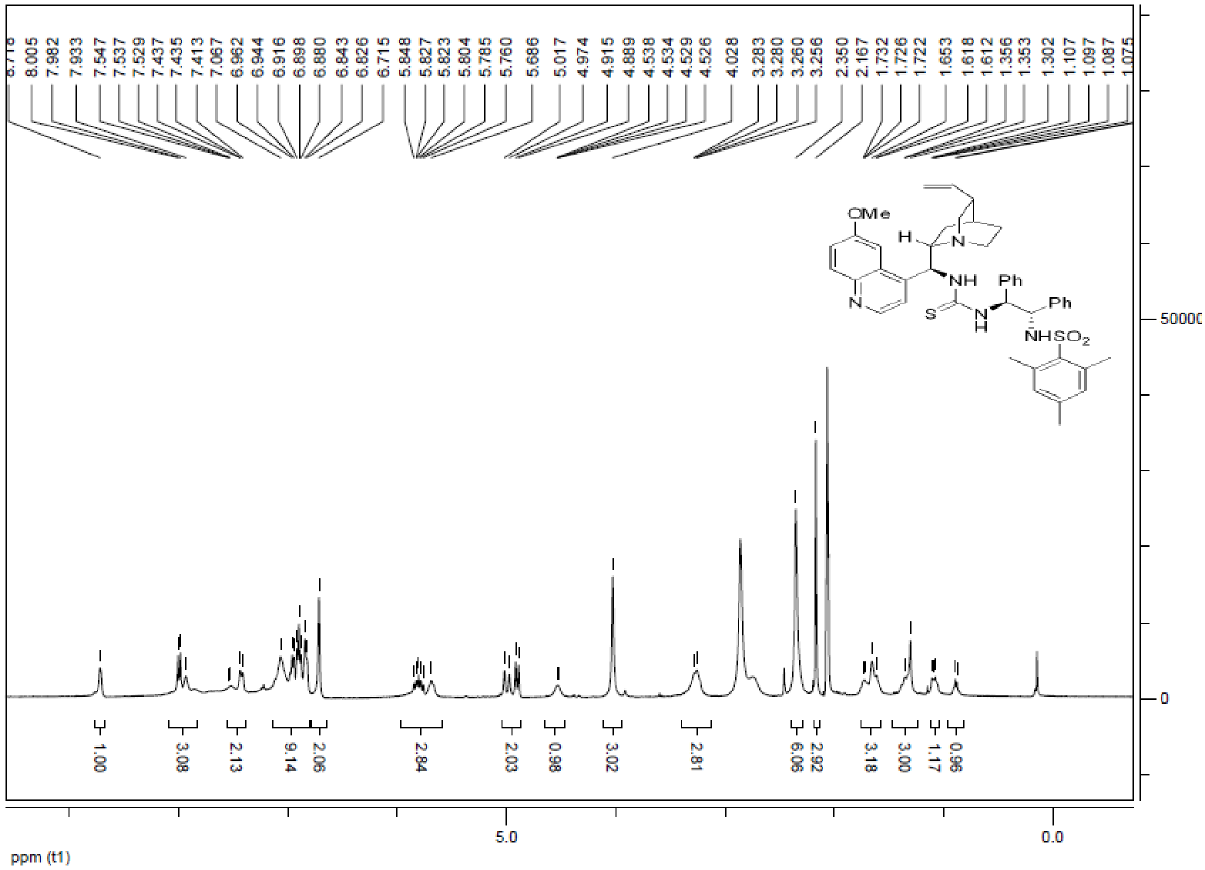


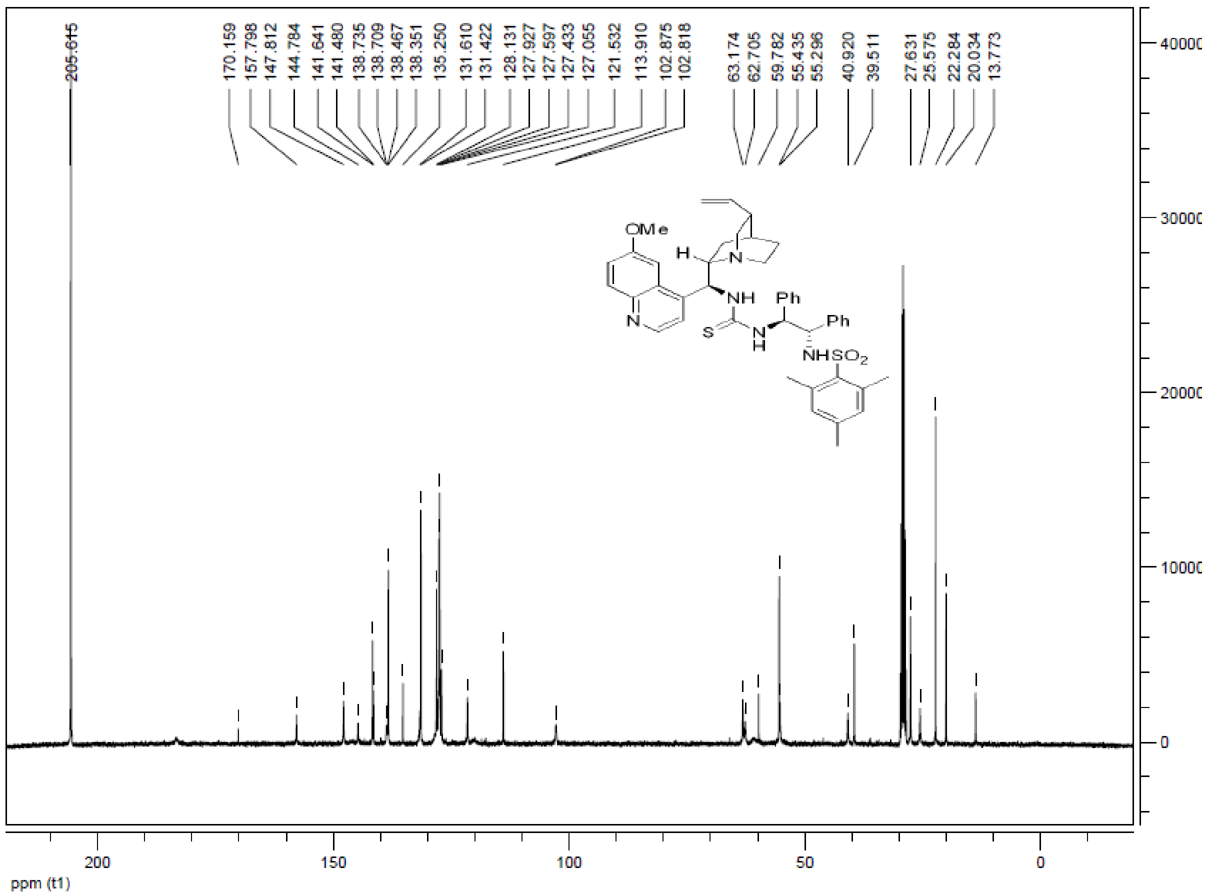
Catalyst 1k


8.745 8.736 8.027 8.004 7.515 7.480 7.455 7.433 7.405 7.390 7.137 7.077 7.029 7.012 6.994 6.979 6.960 6.942 6.918 6.900 5.851 5.831 5.825 5.807 5.788 5.782 5.763 5.691 5.629 5.003 4.960 4.912 4.886 4.617 4.603 4.063 3.290 3.244 3.215 3.185 2.931 2.694 2.278 1.696 1.666 1.630 1.588 1.406 1.381 1.374 1.349
OMe
H
N
NH
Ph
N
S
N
H
Ph
NHSO2
1.00 2.09 4.96 10.95 1.29 0.97 2.04 0.98 3.00 2.92 2.10 1.86 2.98 3.00 1.18 1.03
ppm (t1)

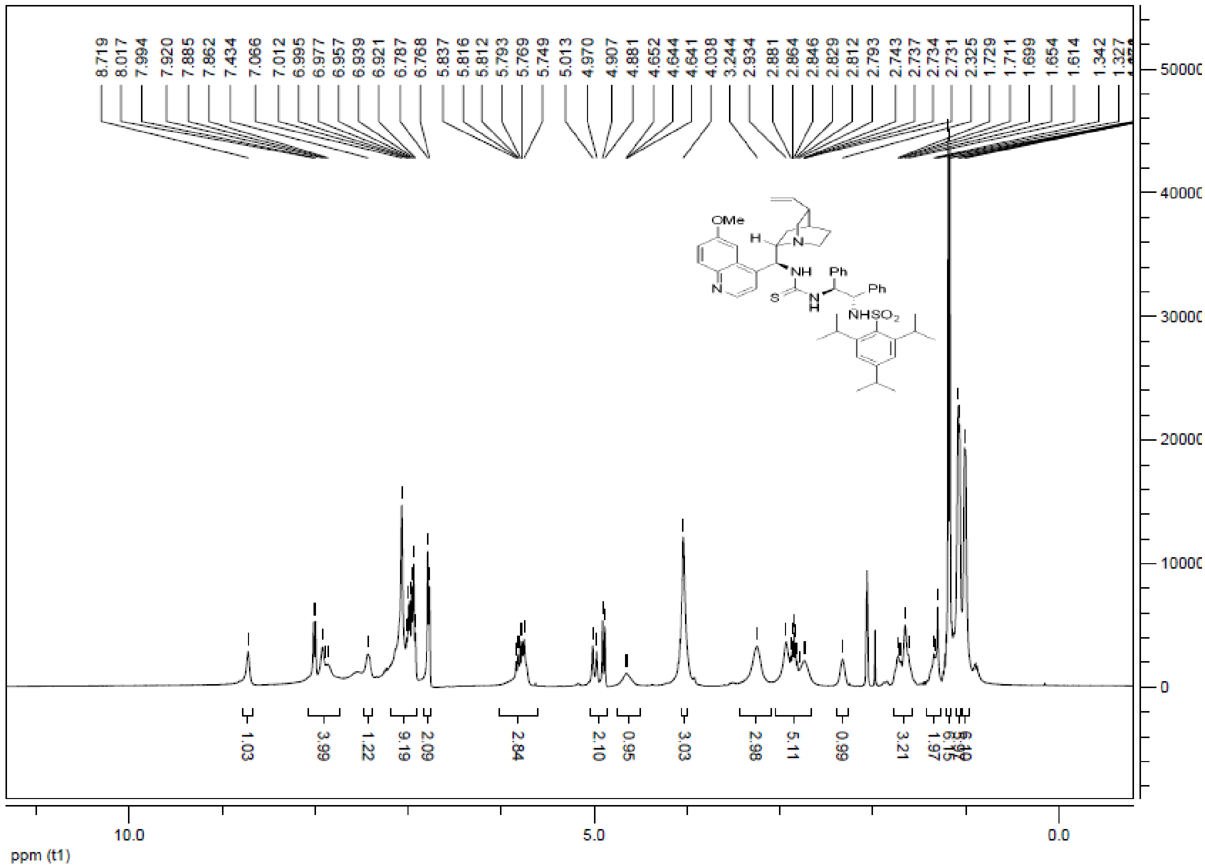

205.457
157.899 147.722 144.865 142.436 141.818 138.590 131.641 129.029 128.070 127.833 127.711 127.369 127.051 126.707 121.650 113.742
63.220 62.751 59.706 55.464 40.952 39.657 27.671 25.718 20.503 20.006 13.666
OMe
H
N
NH
Ph
N
S
N
H
Ph
NHSO2
ppm (t1)

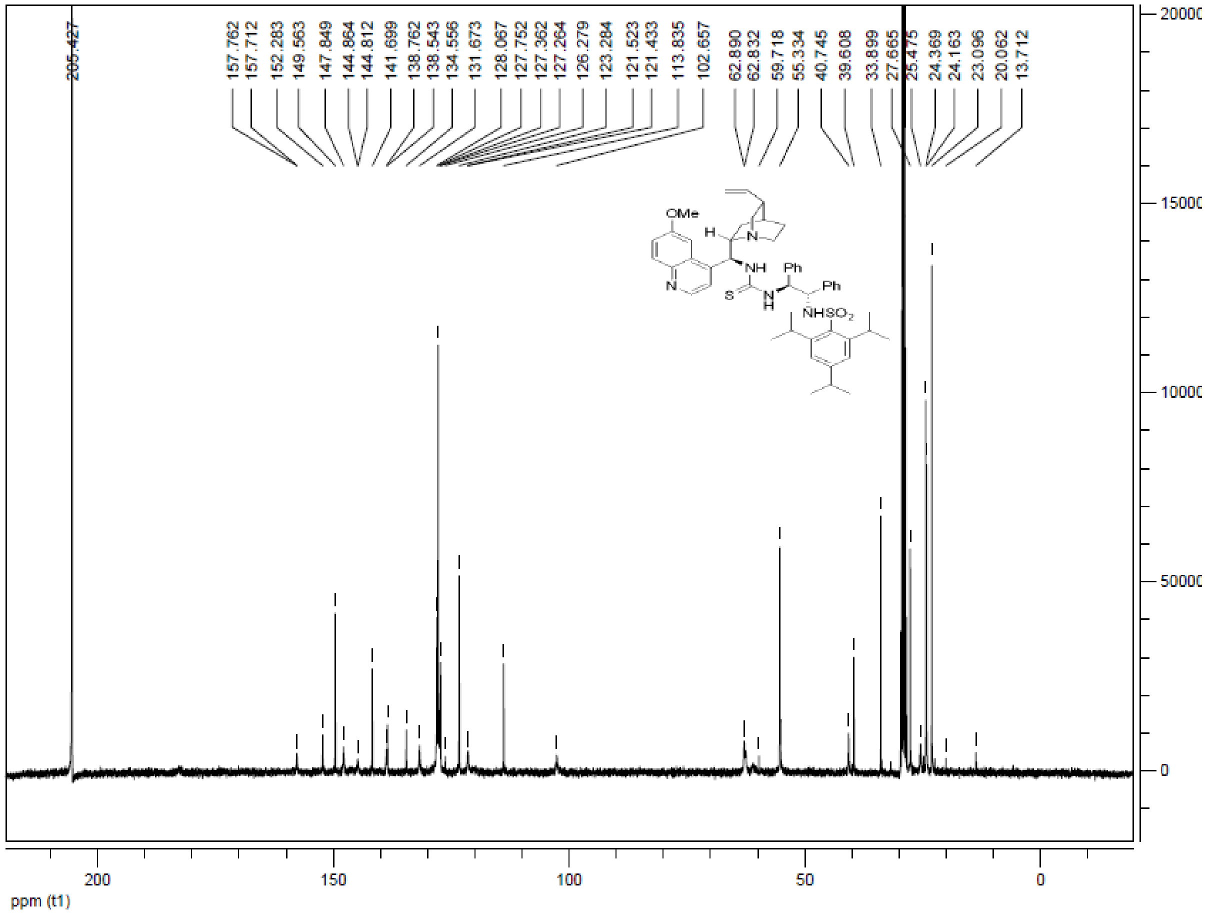
Catalyst 1l



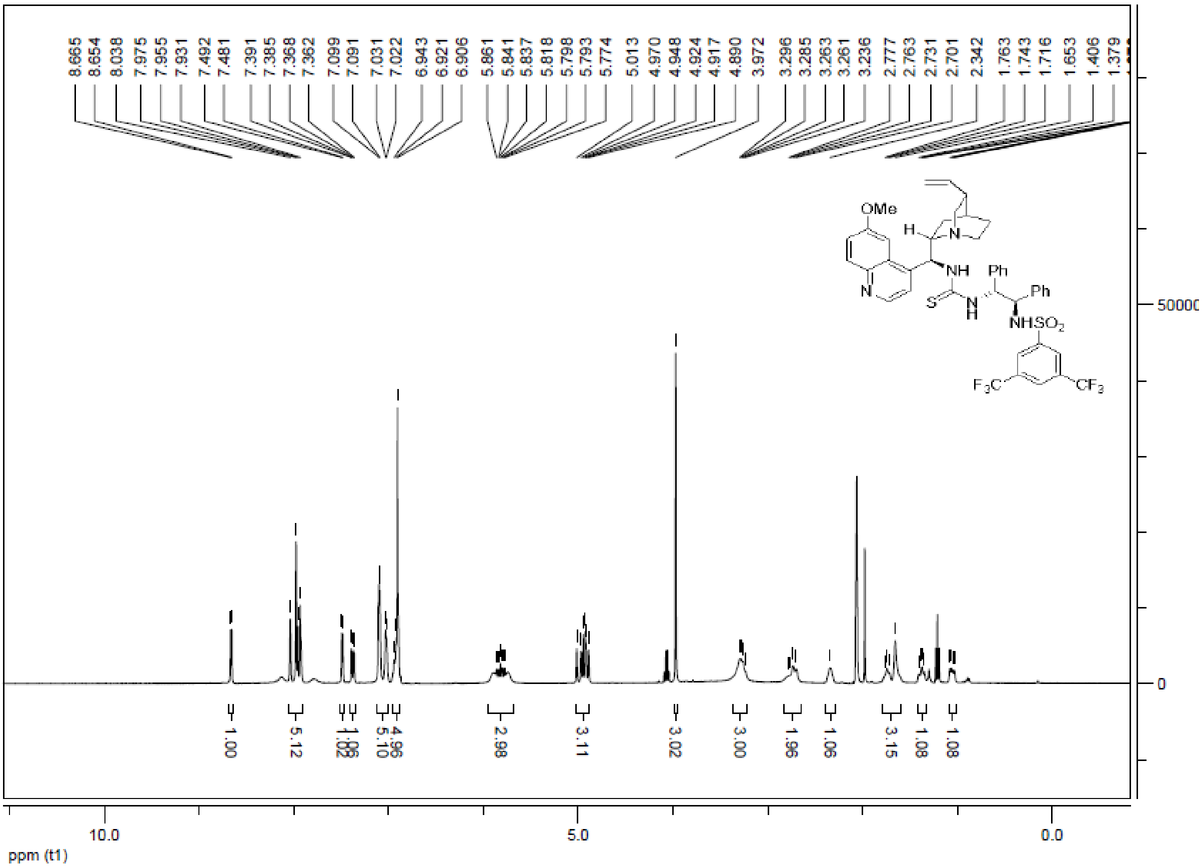


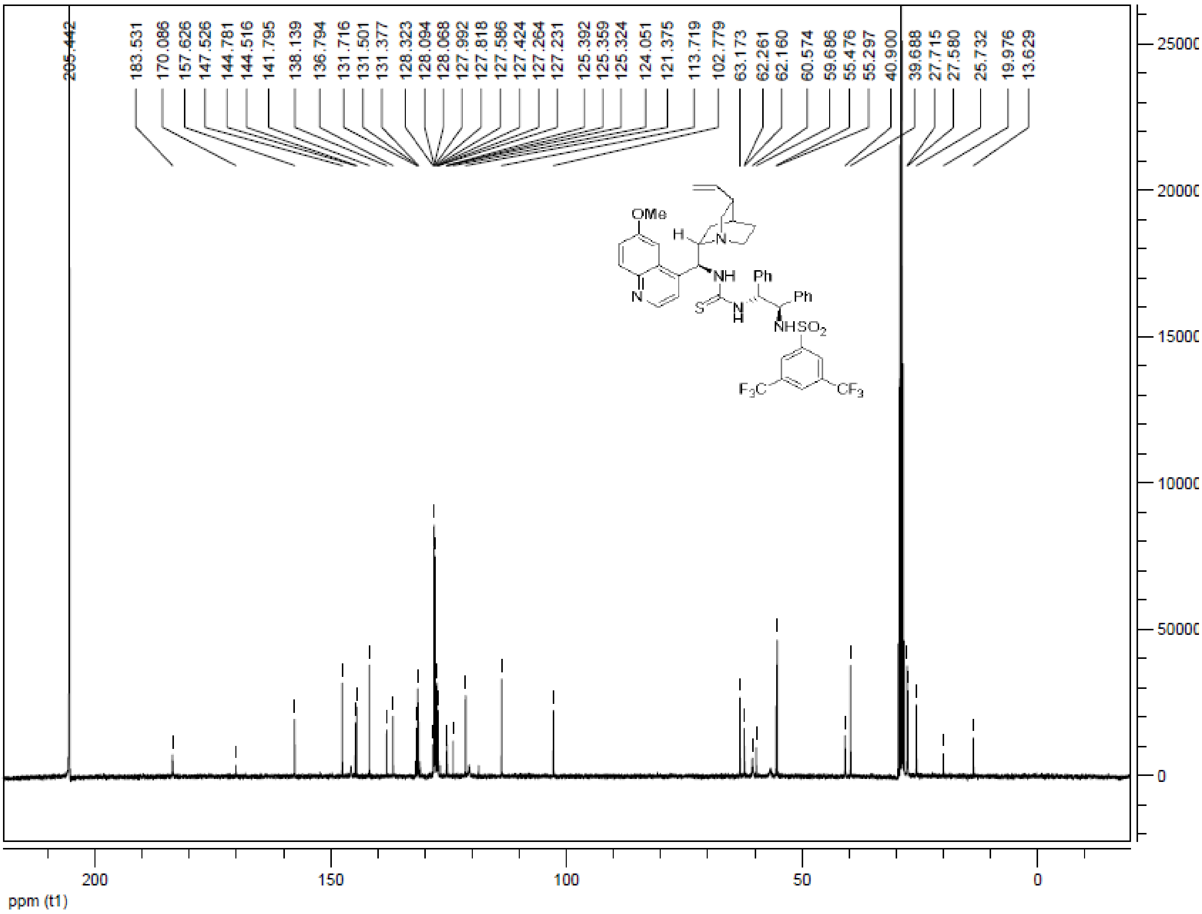
Catalyst 1m





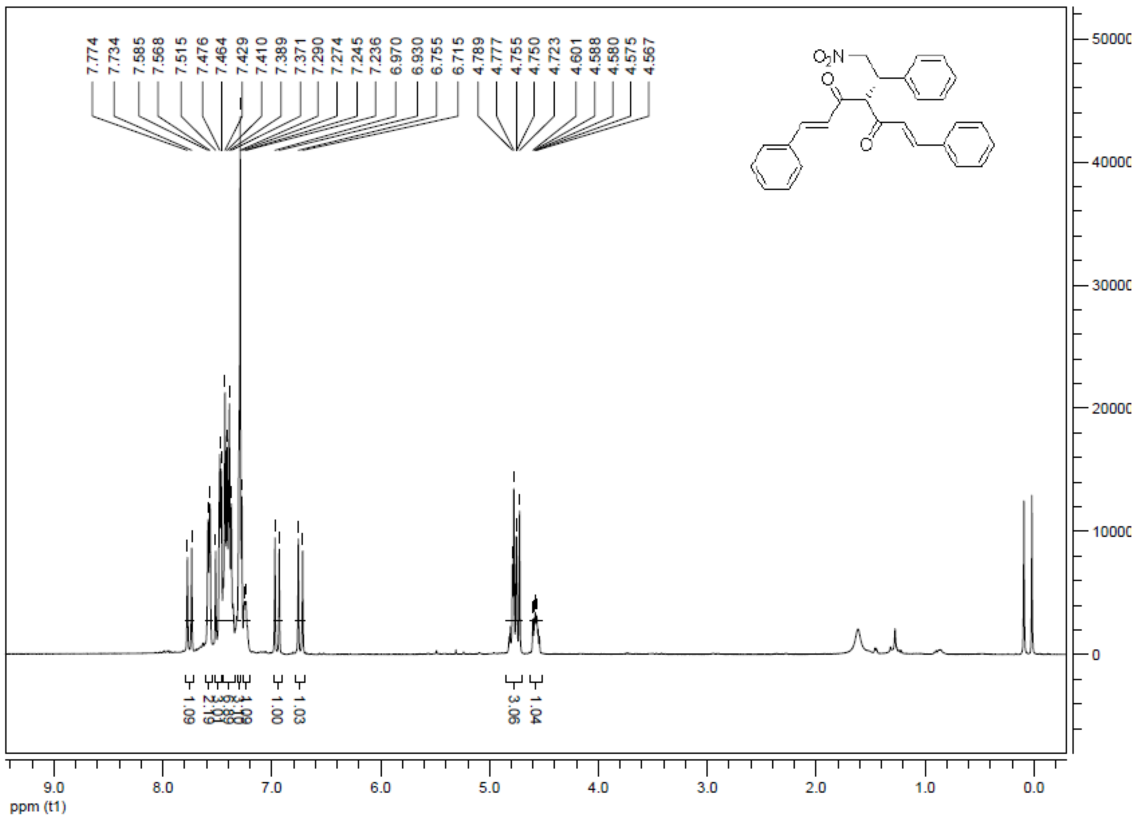
Catalyst 1n

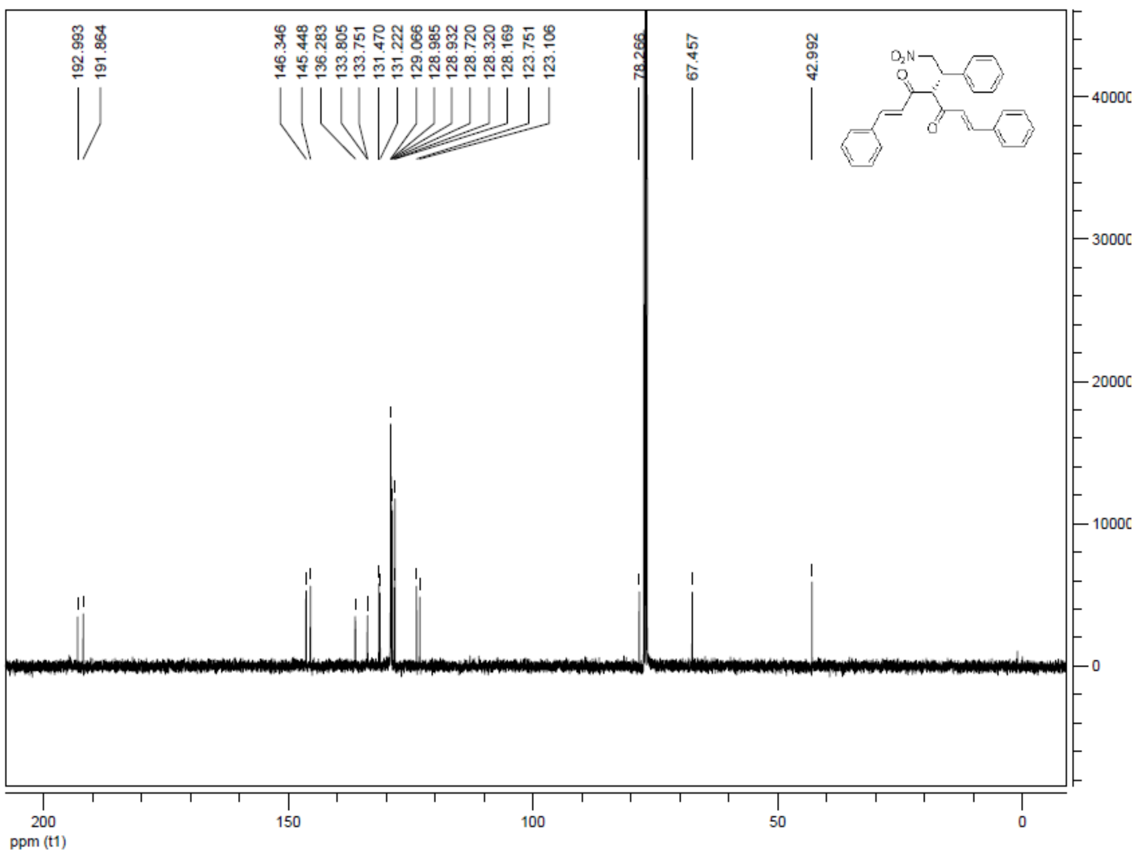




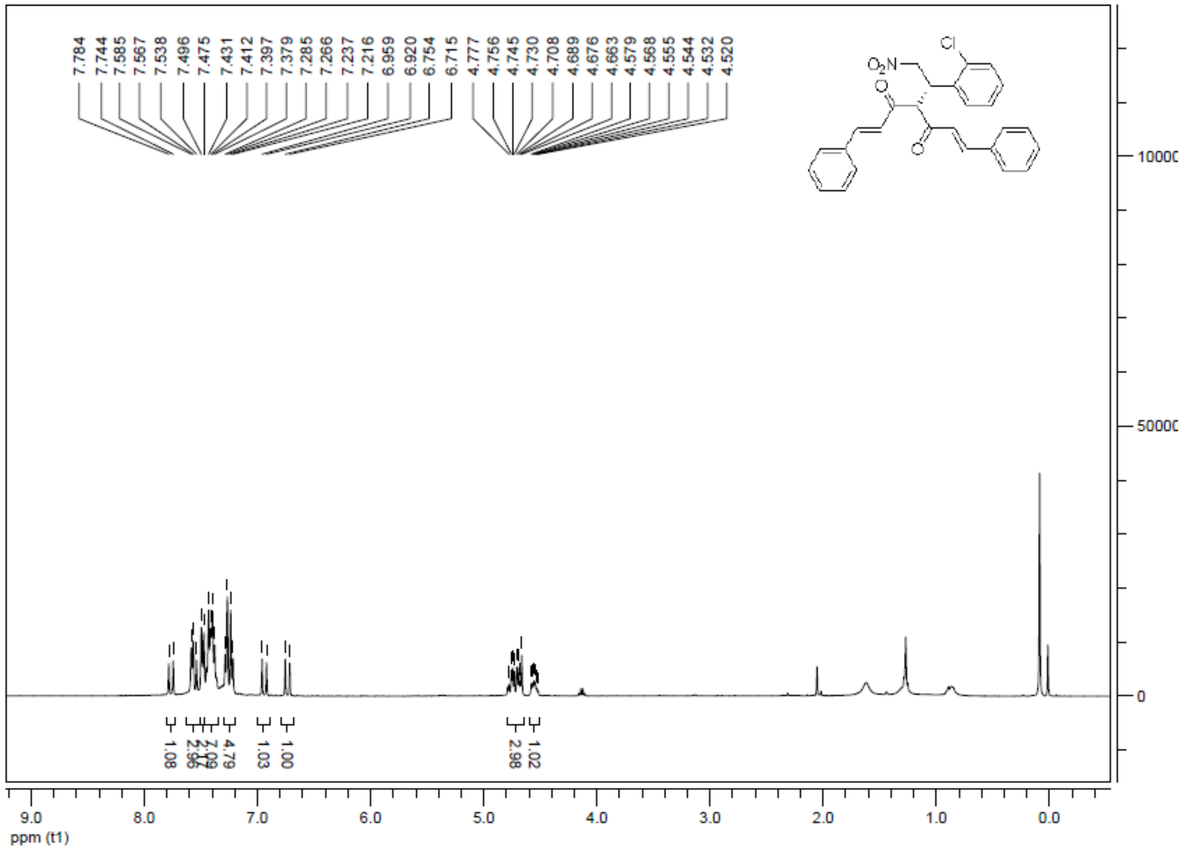
D: NMR Spectra of Michael Addition Products

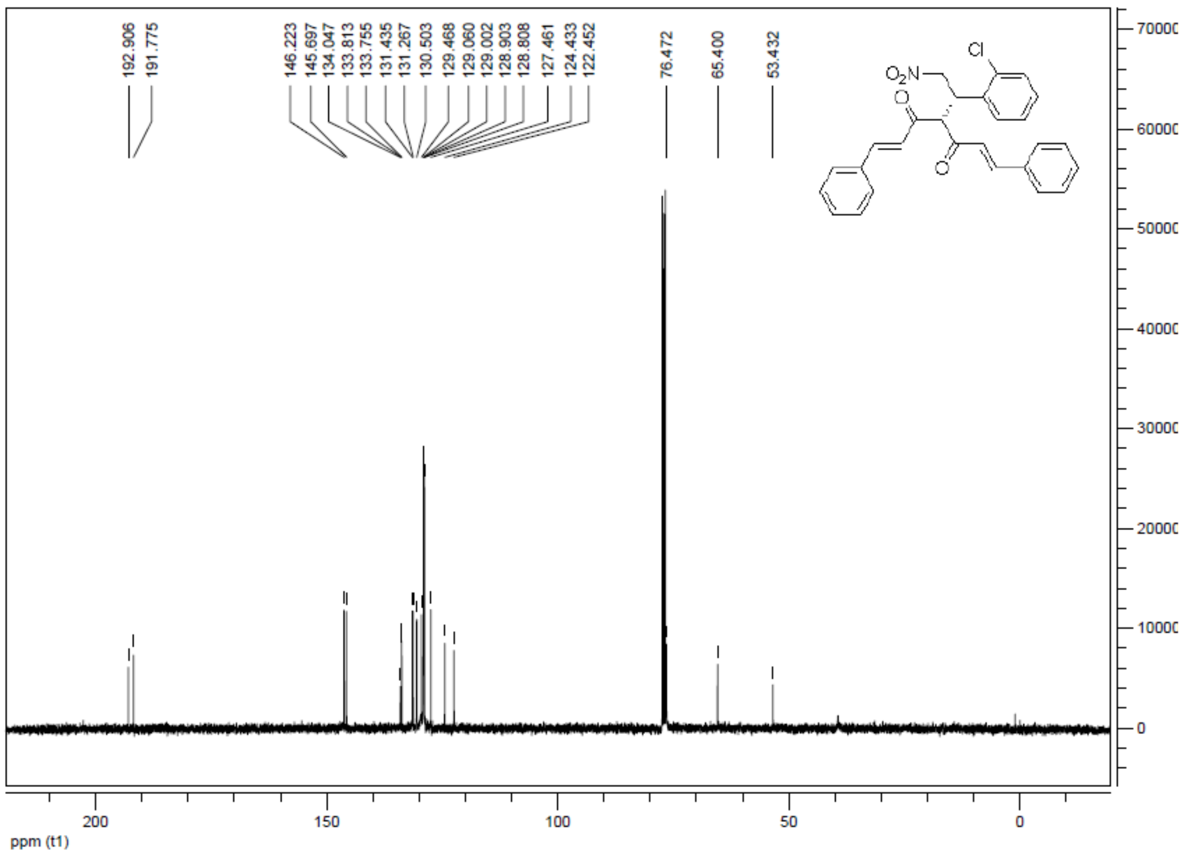
4-(2-nitro-1-phenylethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione(4aa)



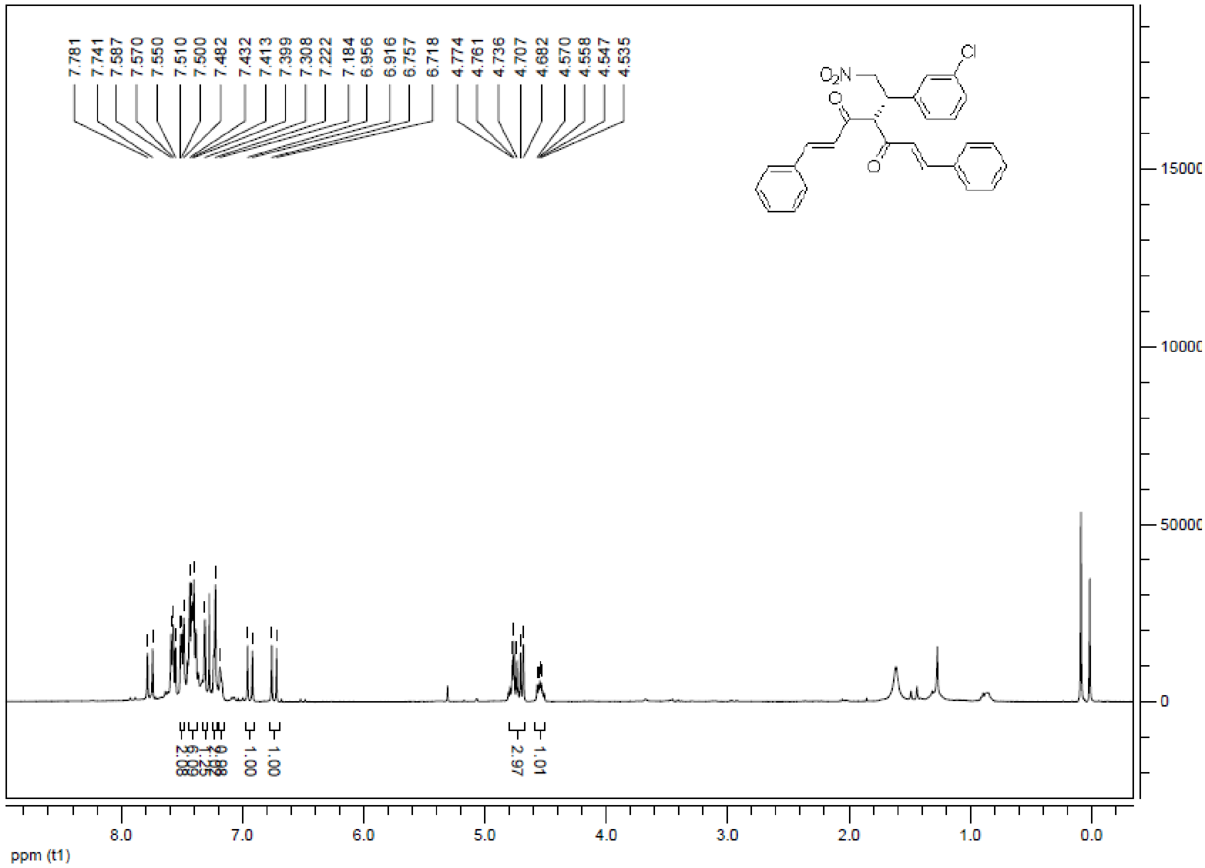


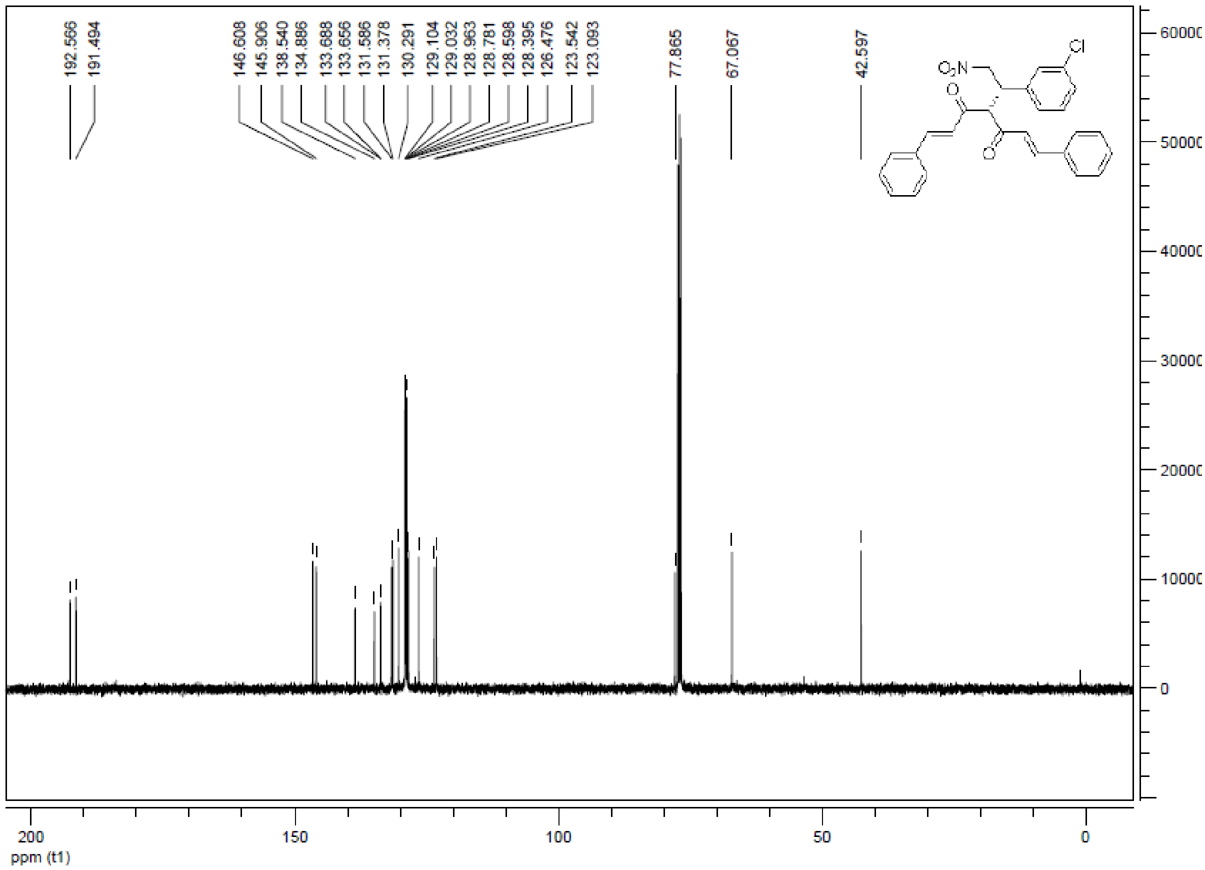
4-(1-(2-chlorophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ba)



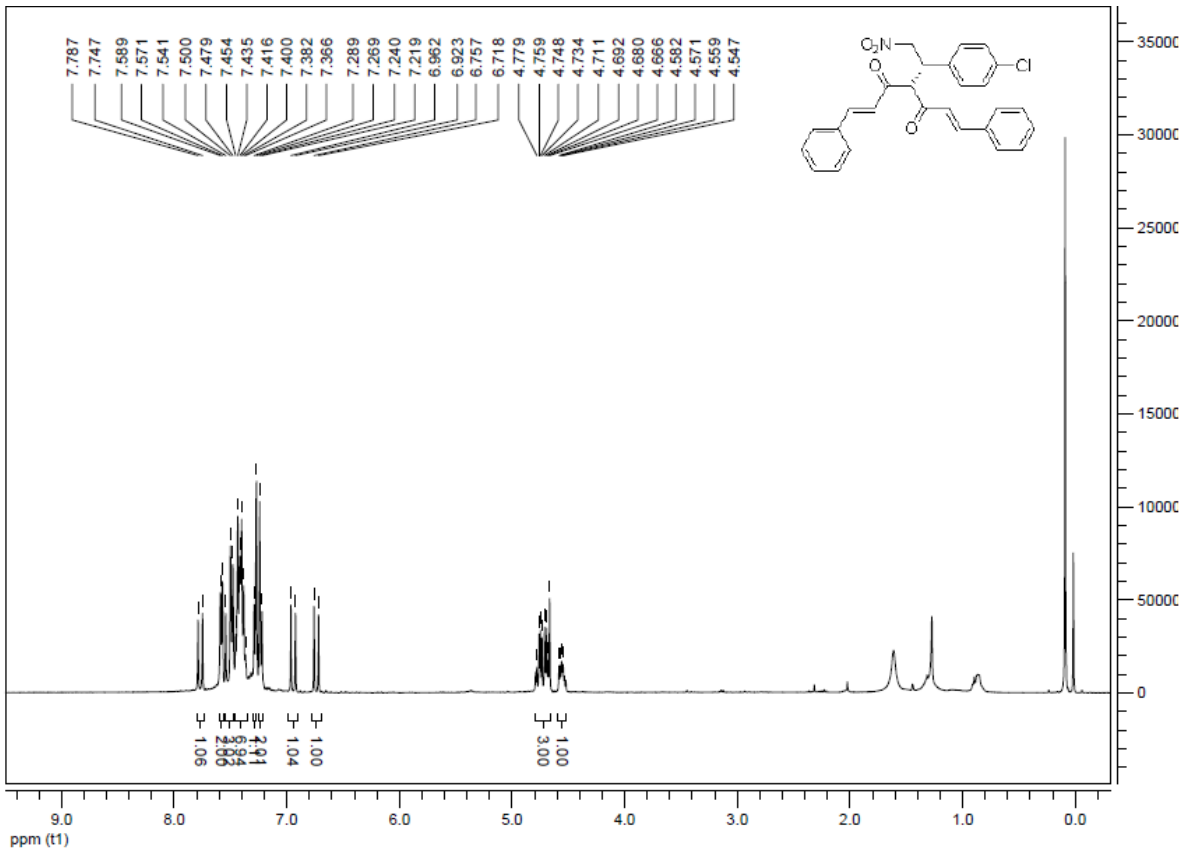


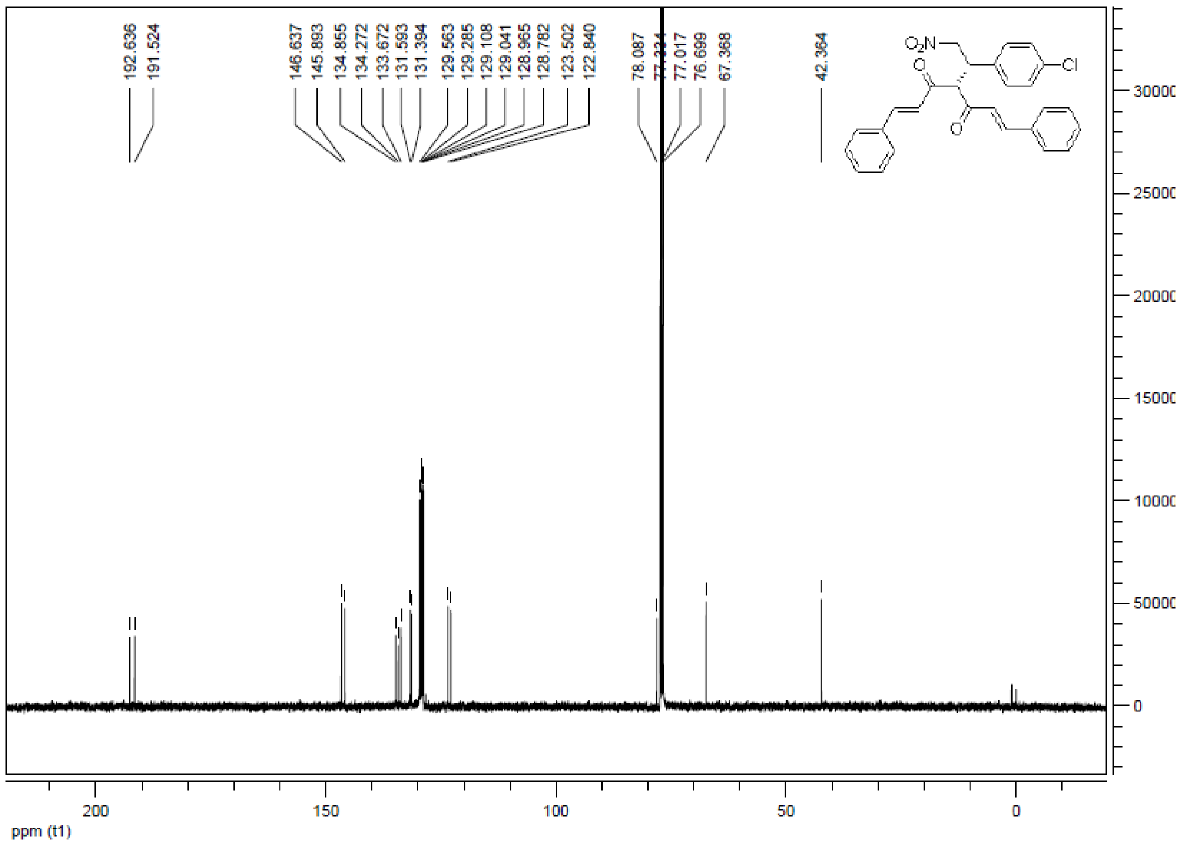
4-(1-(3-chlorophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ca)



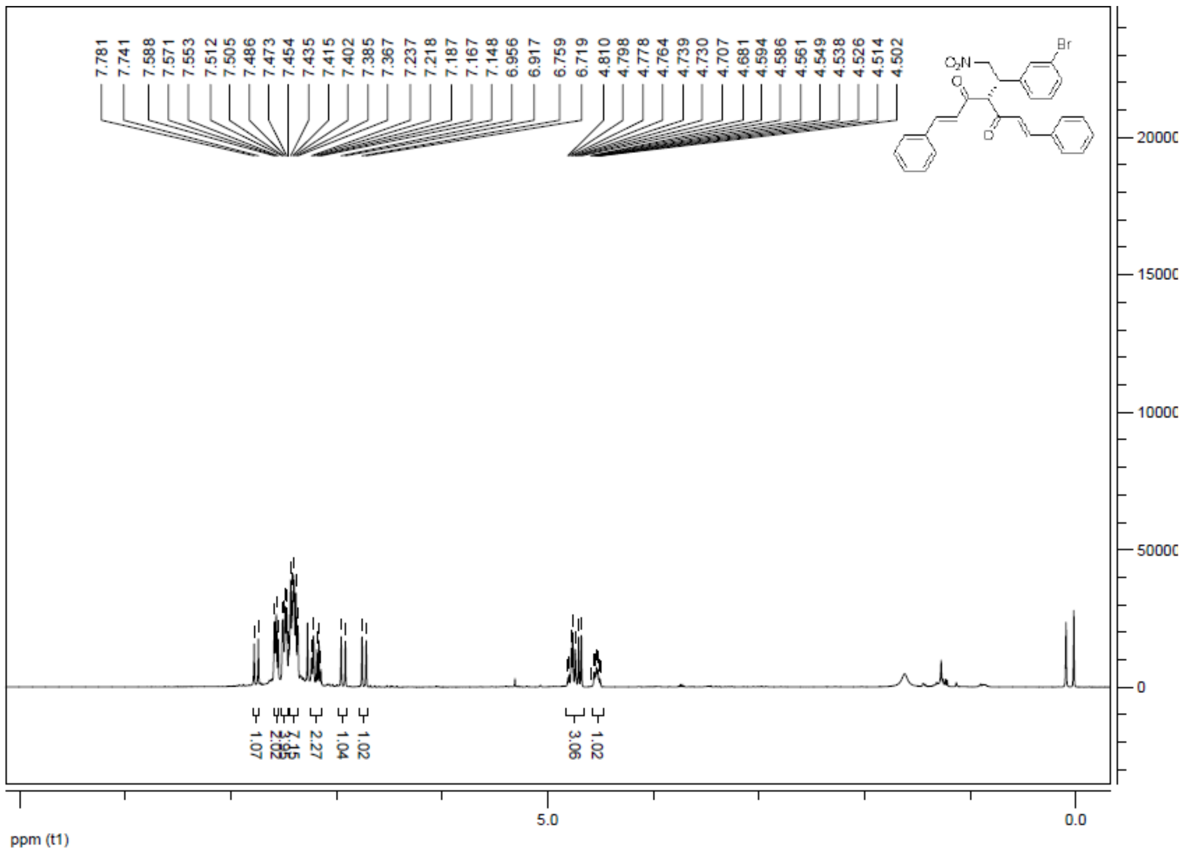


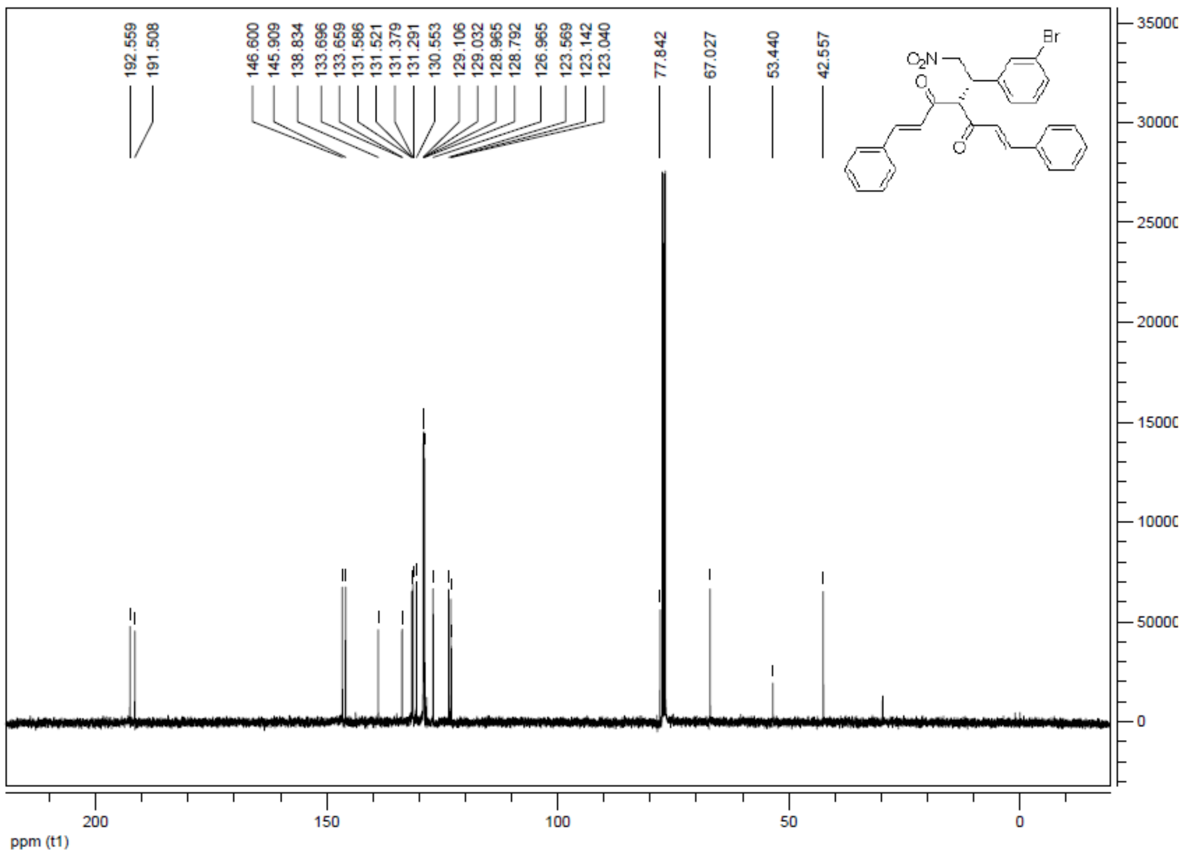
4-(1-(4-chlorophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4da)



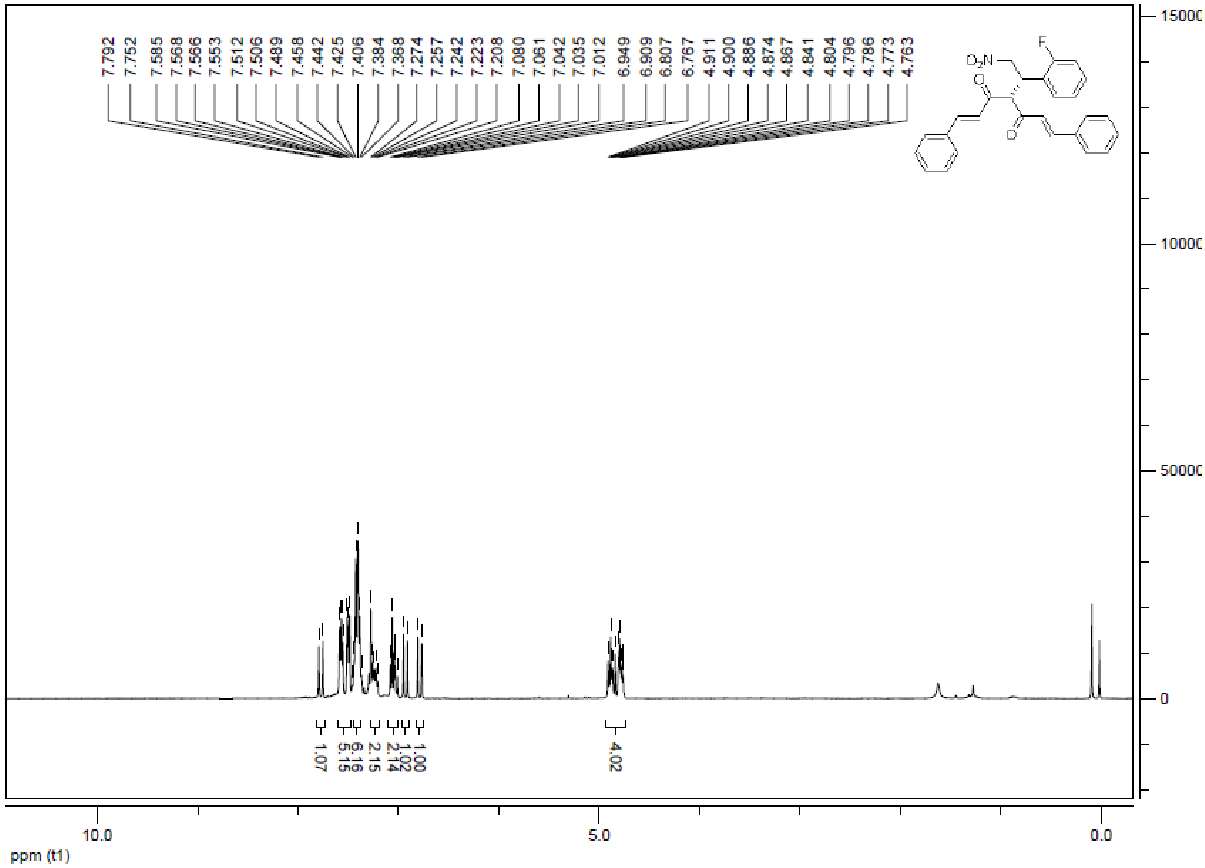


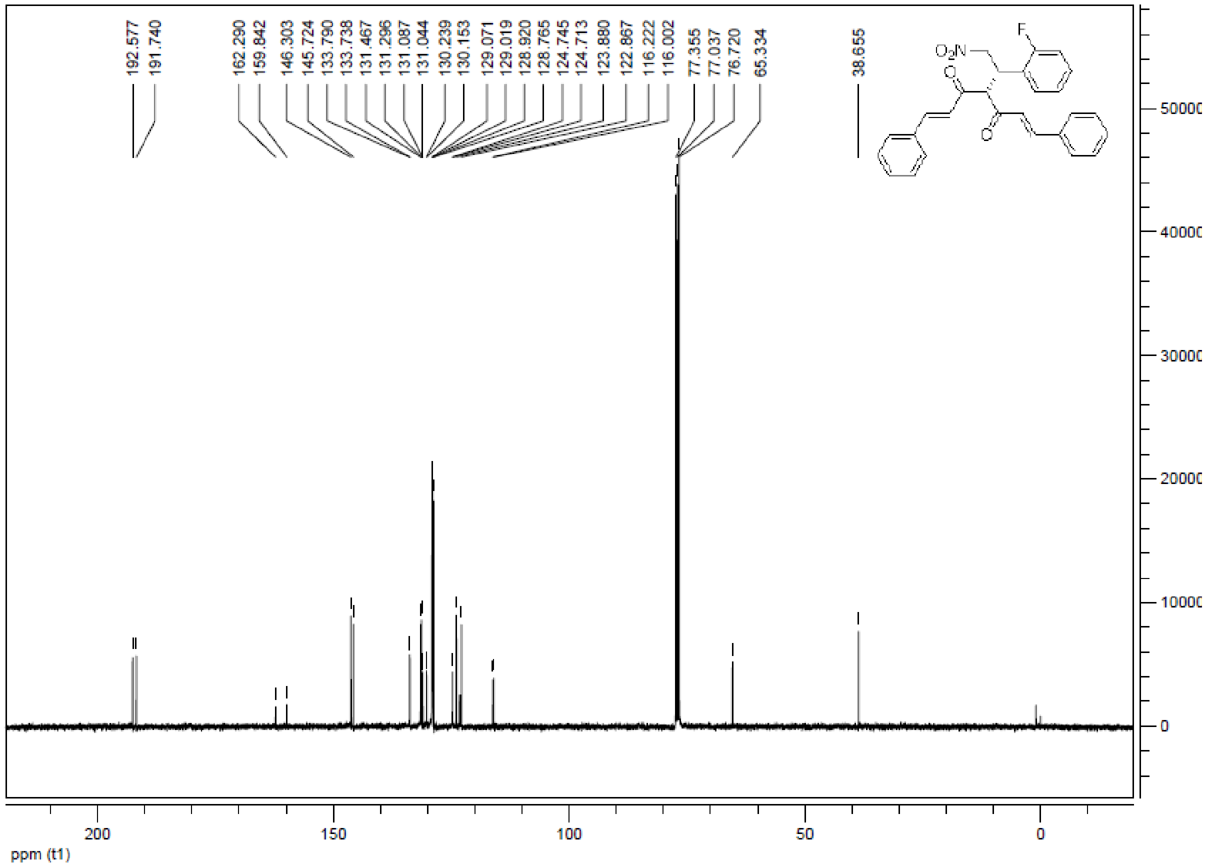
4-(1-(3-bromophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ea)



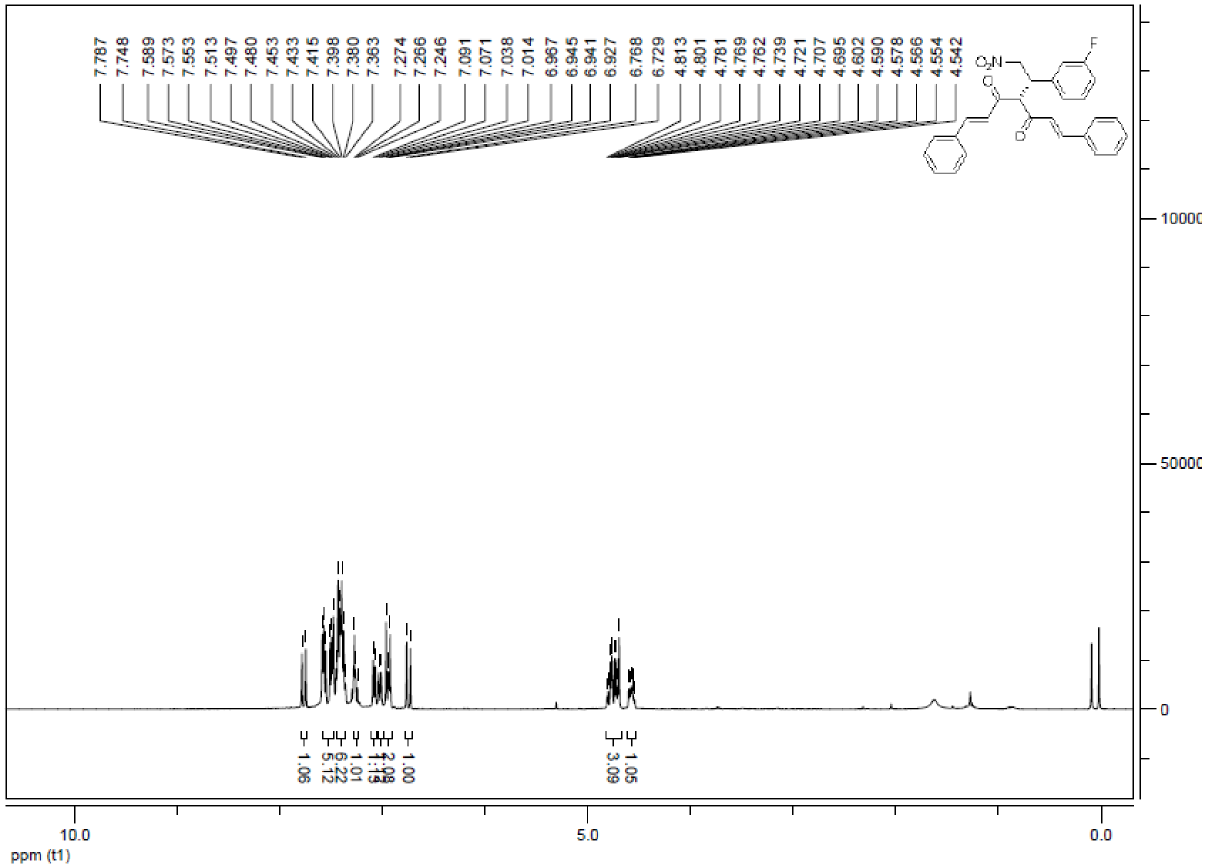


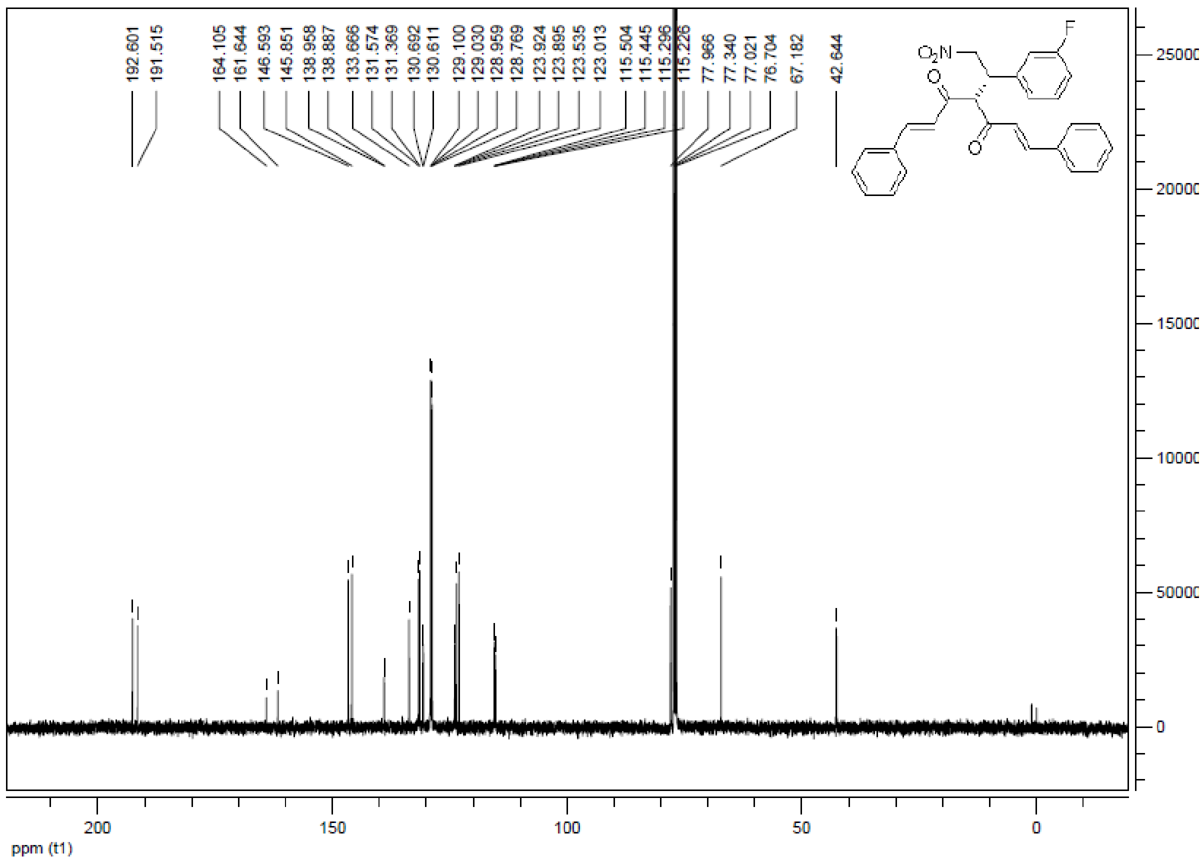
4-(1-(2-fluorophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4fa)



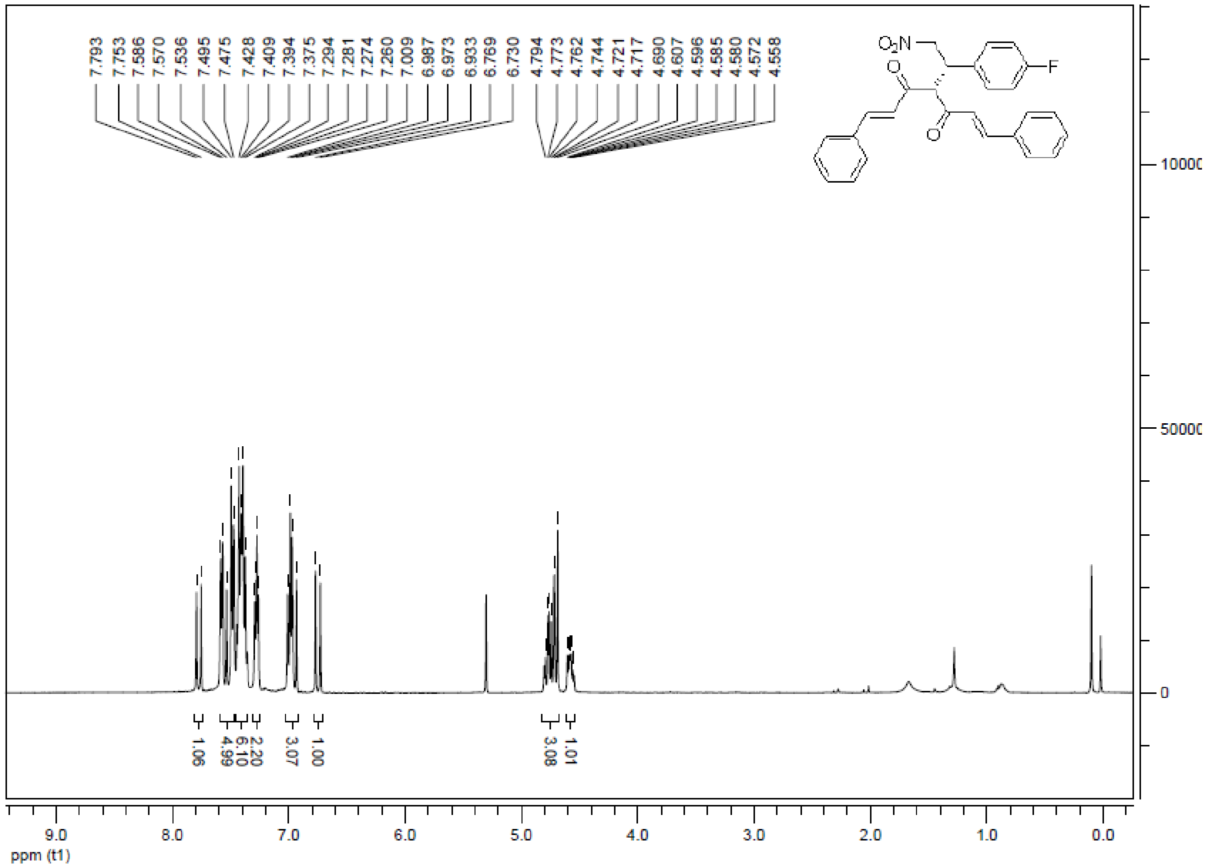


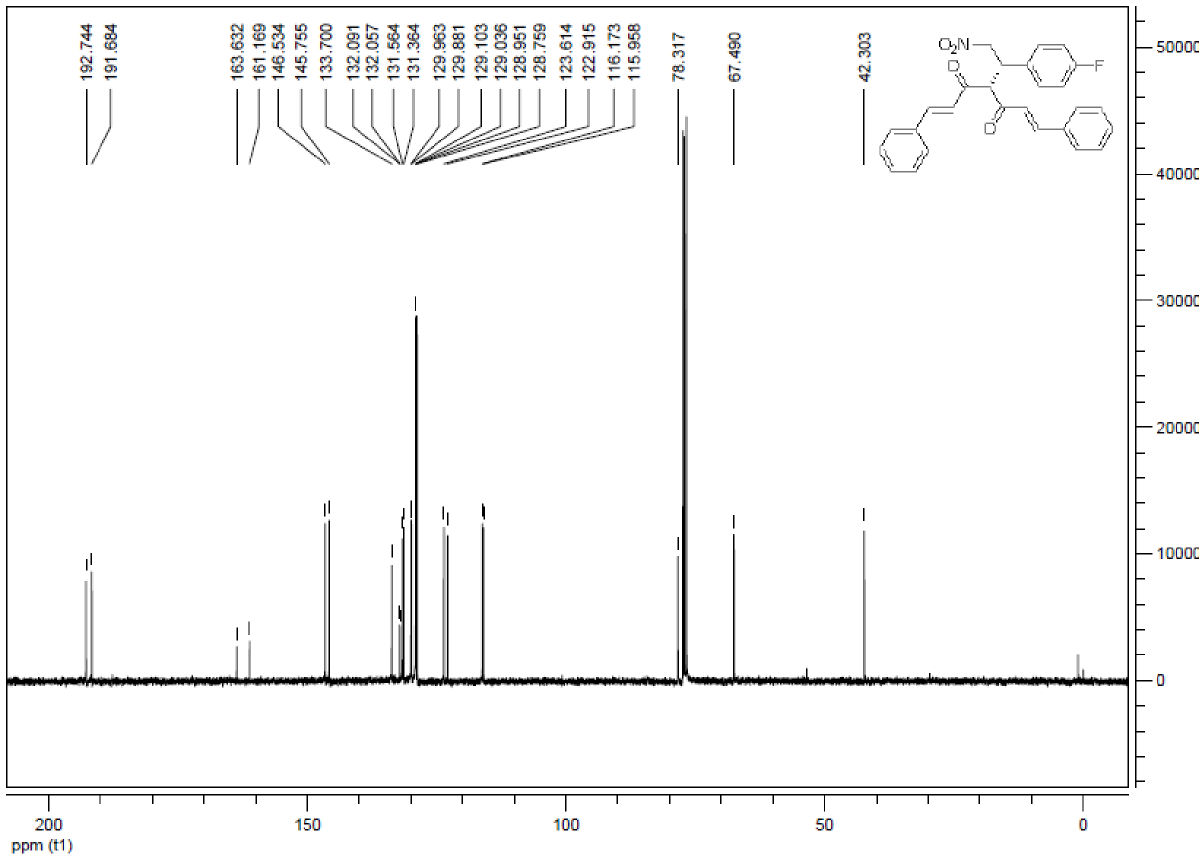
4-(1-(3-fluorophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ga)



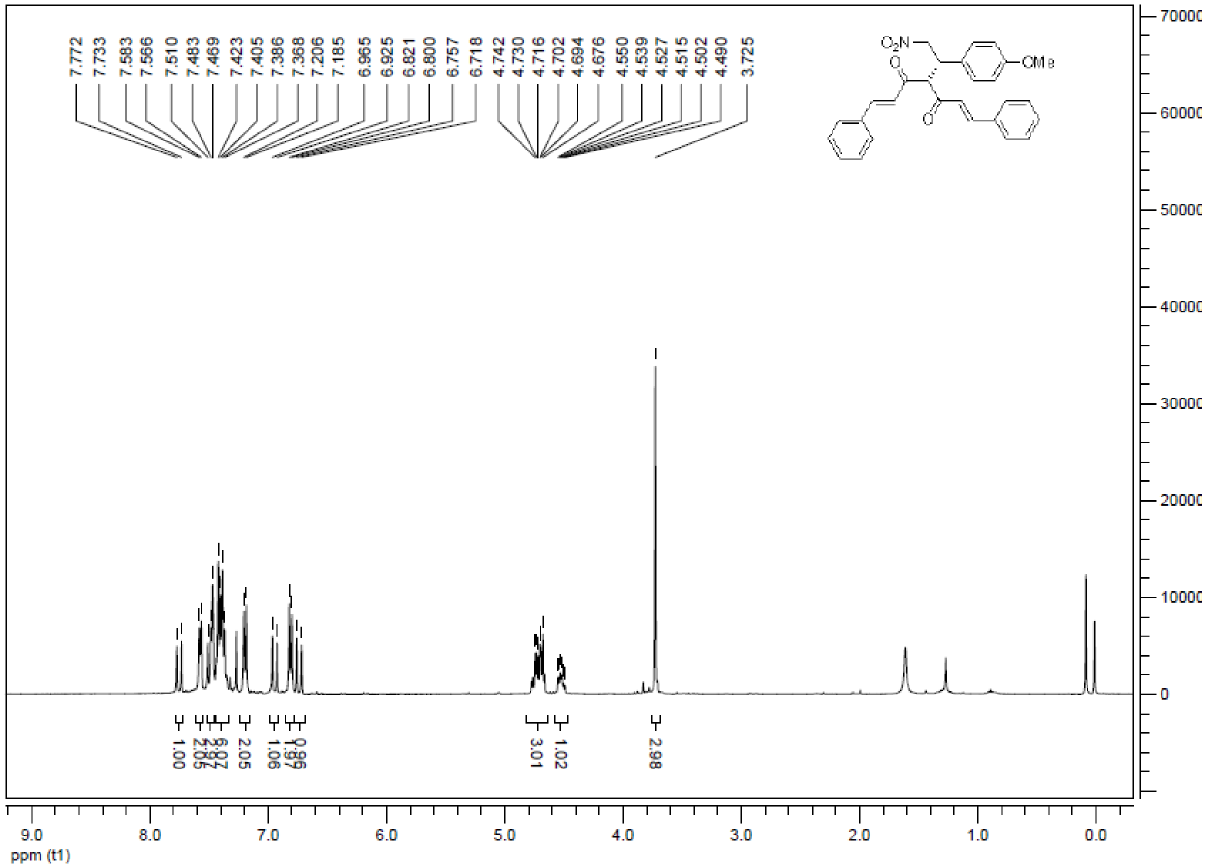


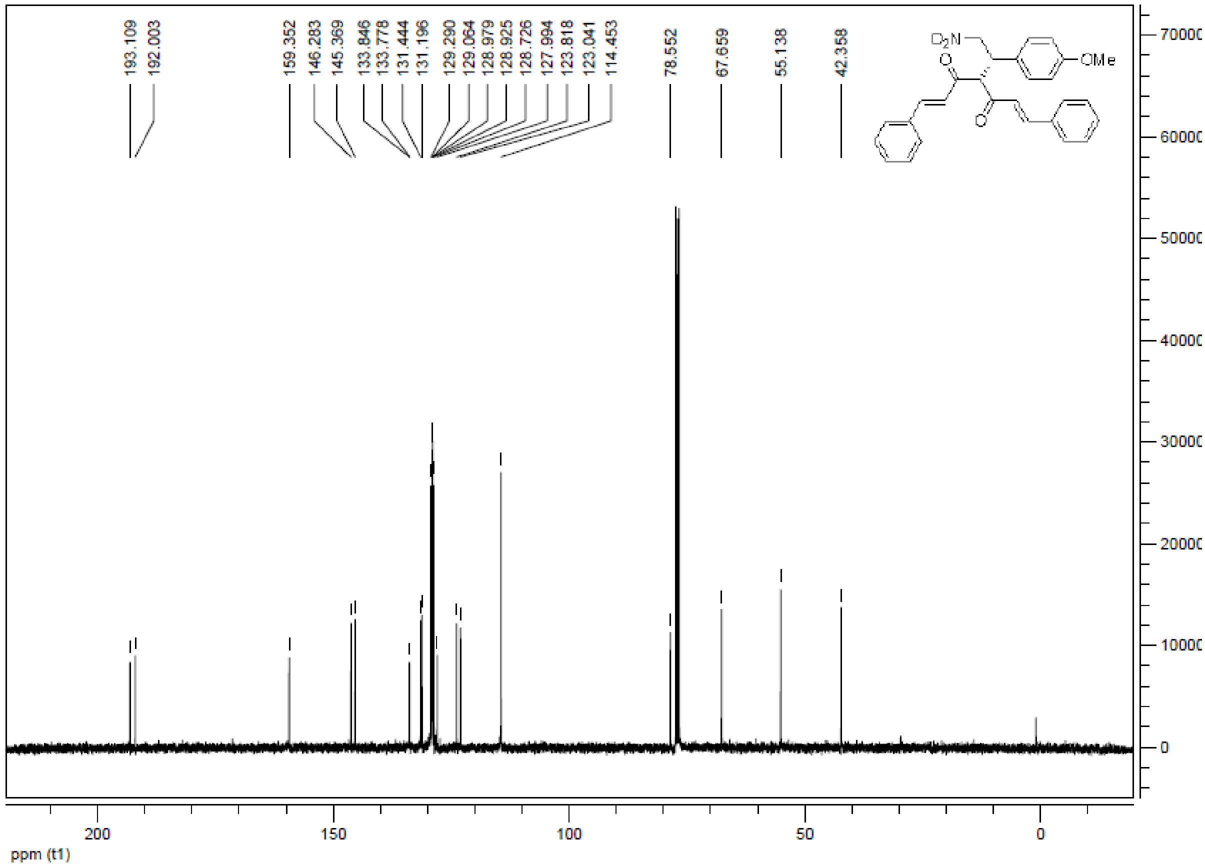
4-(1-(4-fluorophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ha)



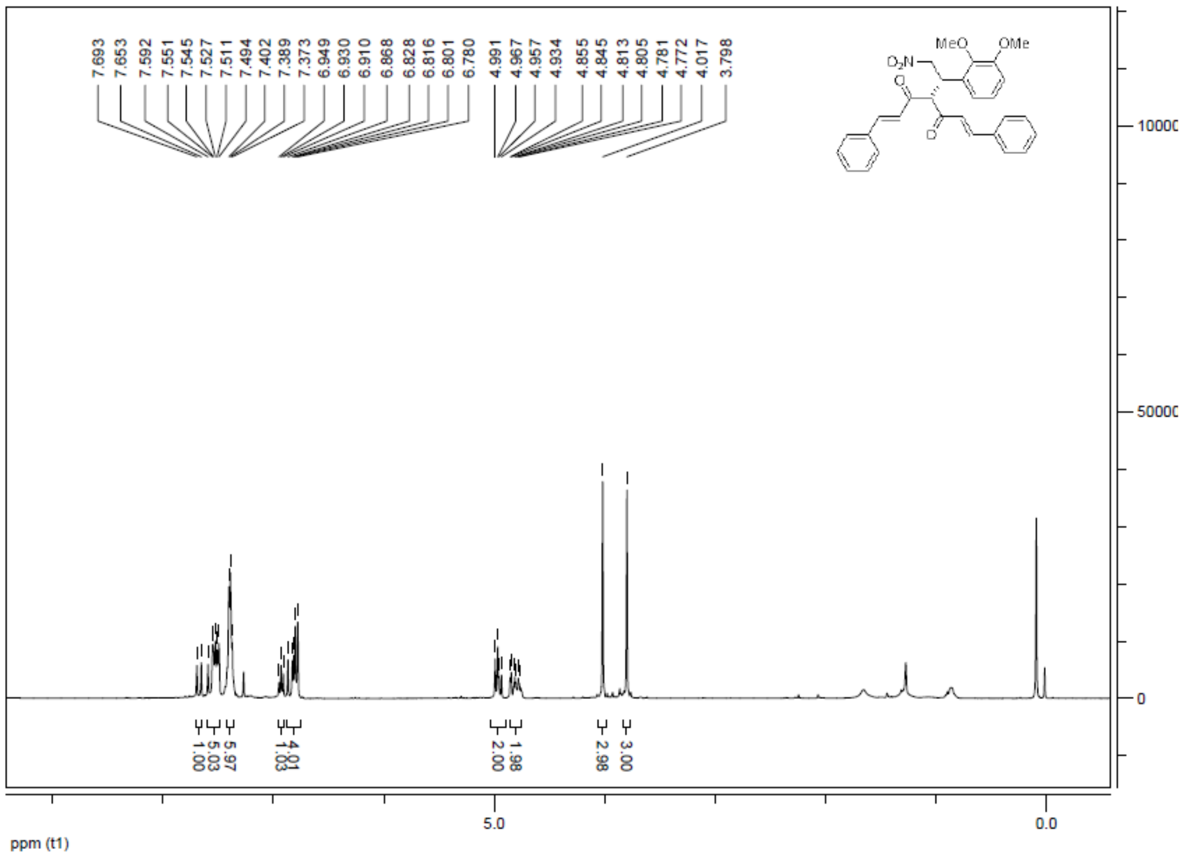


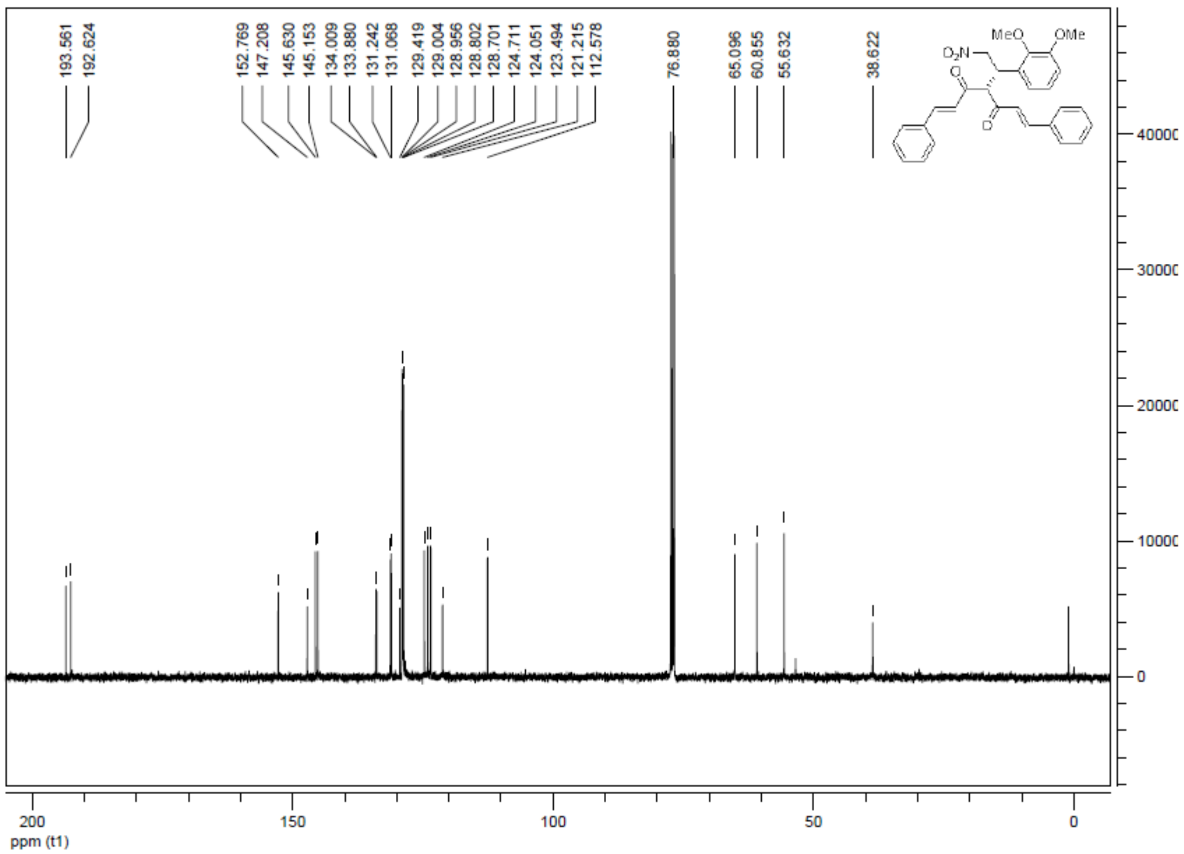
4-(1-(4-methoxyphenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ia)



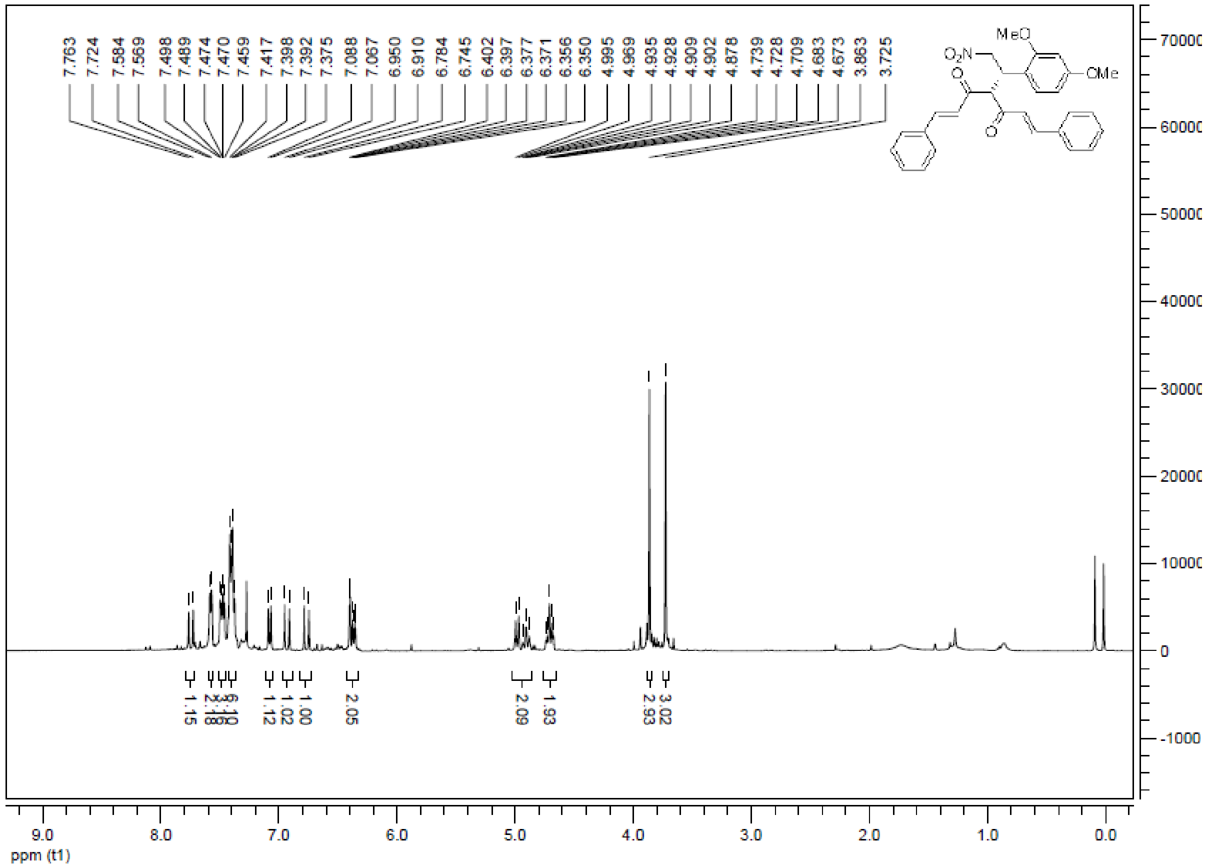


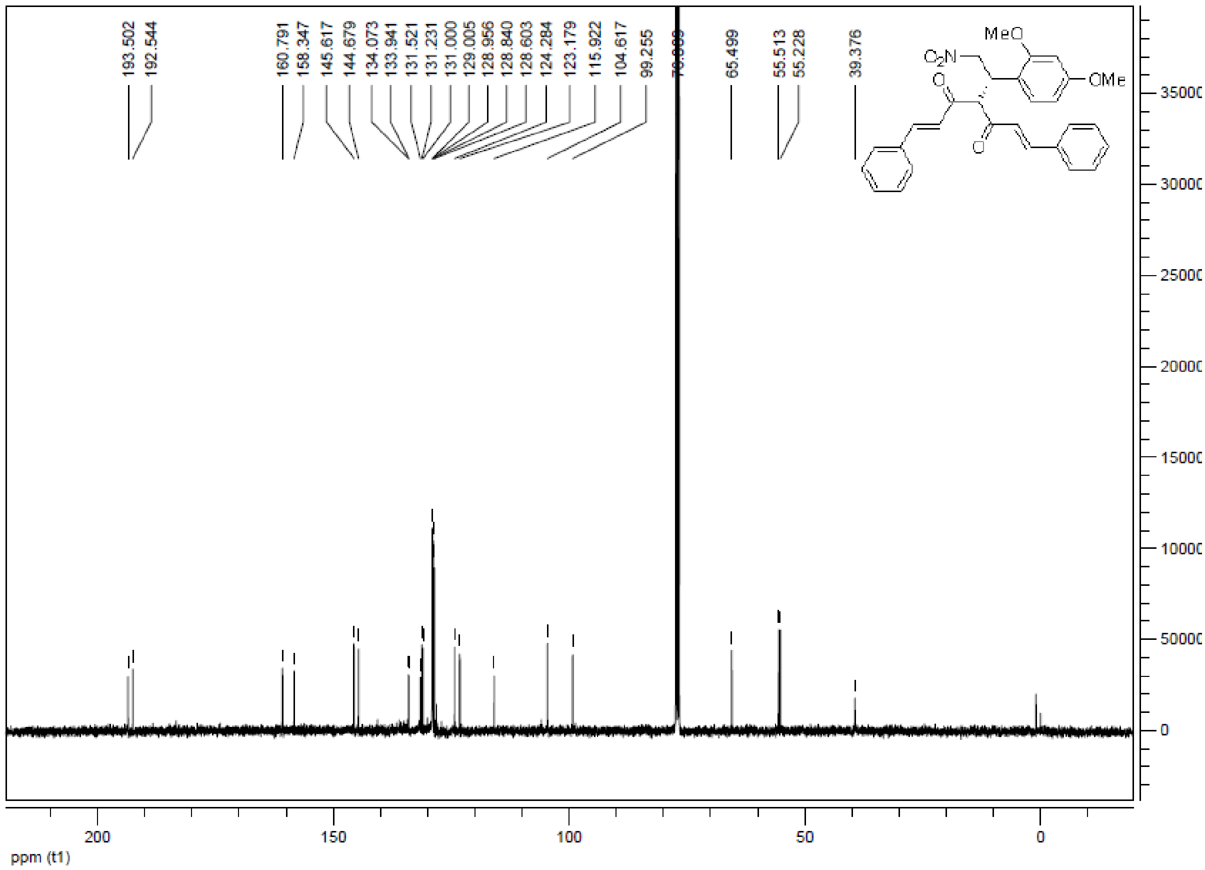
4-(1-(2,3-dimethoxyphenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ja)



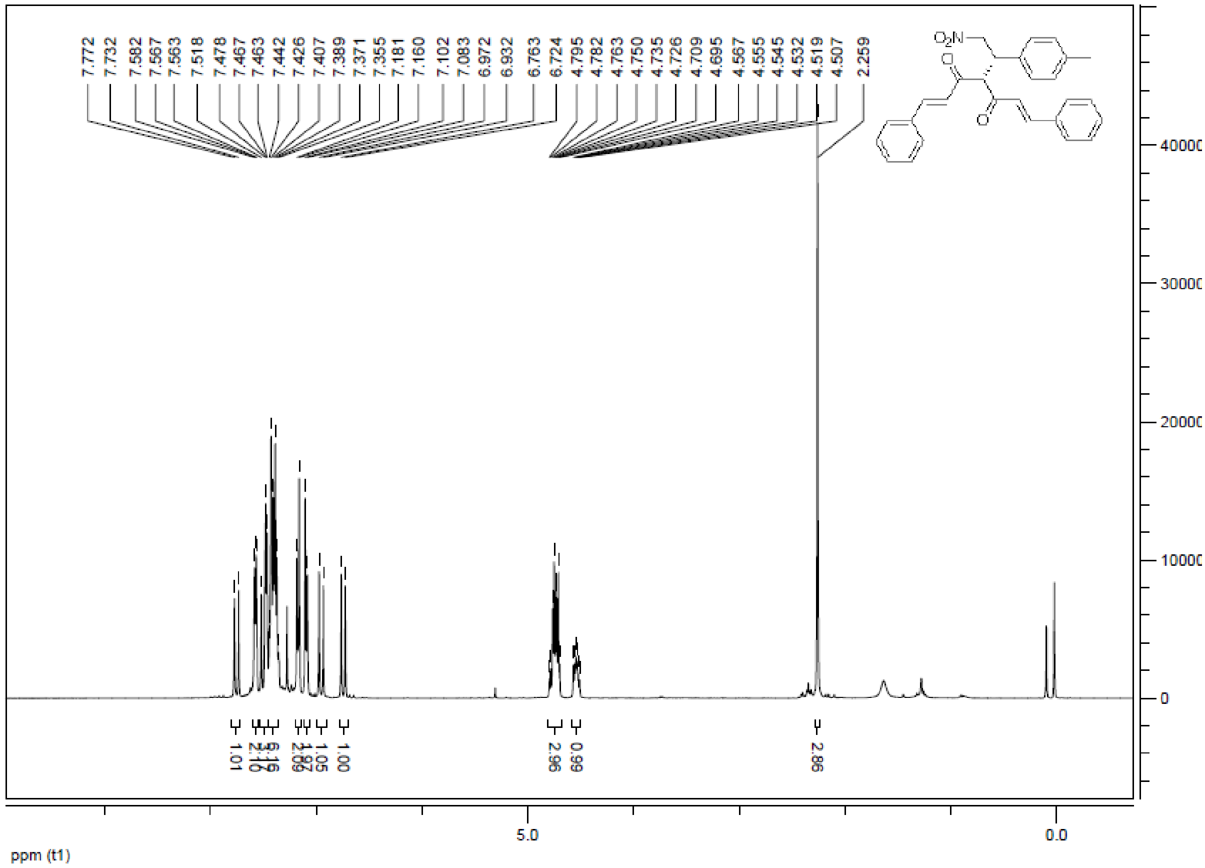


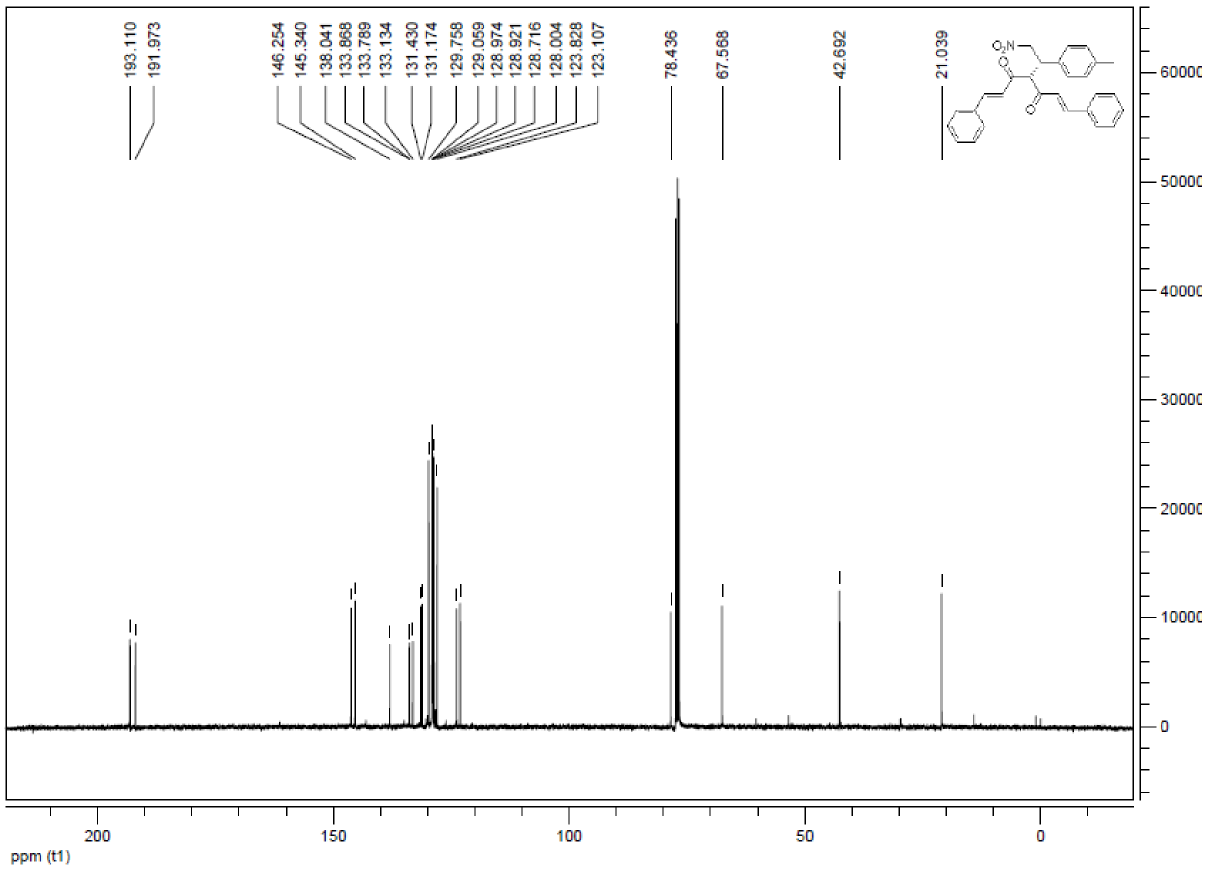
4-(1-(2,4-dimethoxyphenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ka)



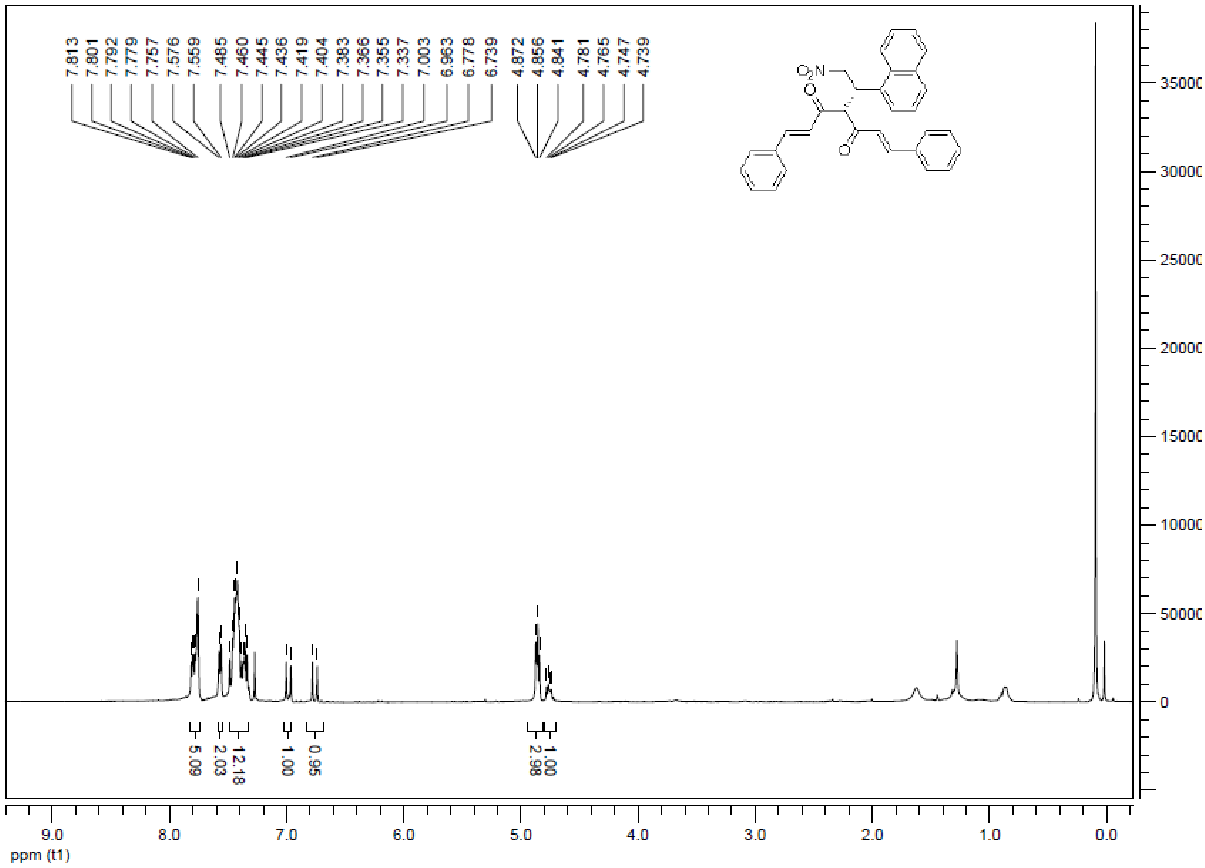


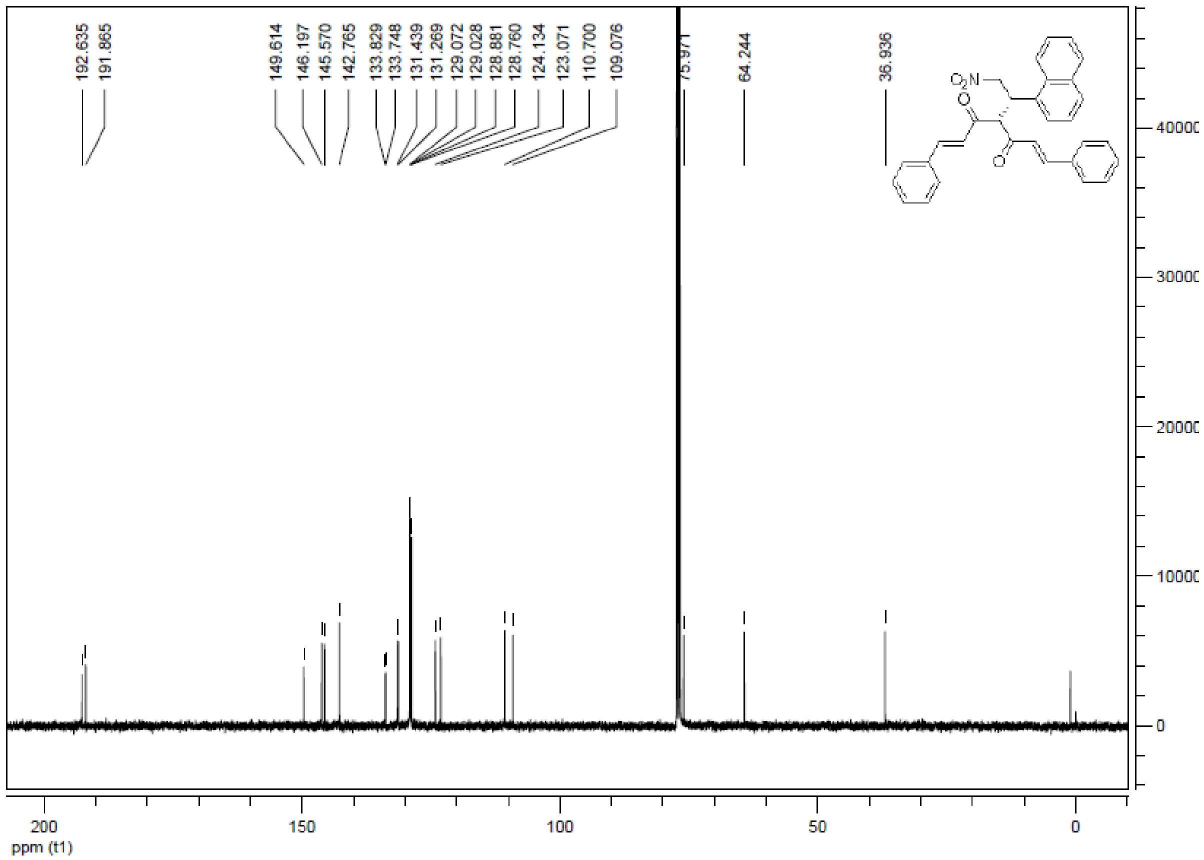
4-(2-nitro-1-p-tolylethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4la)



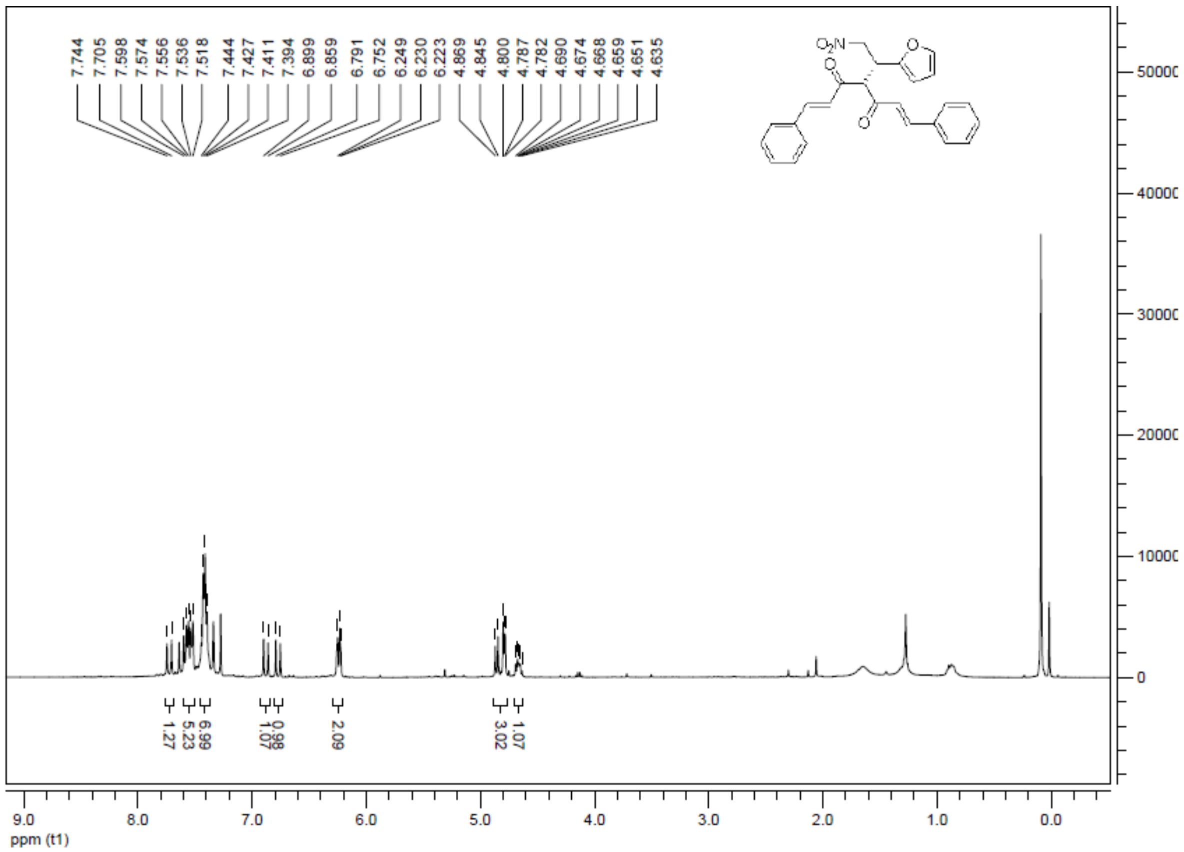


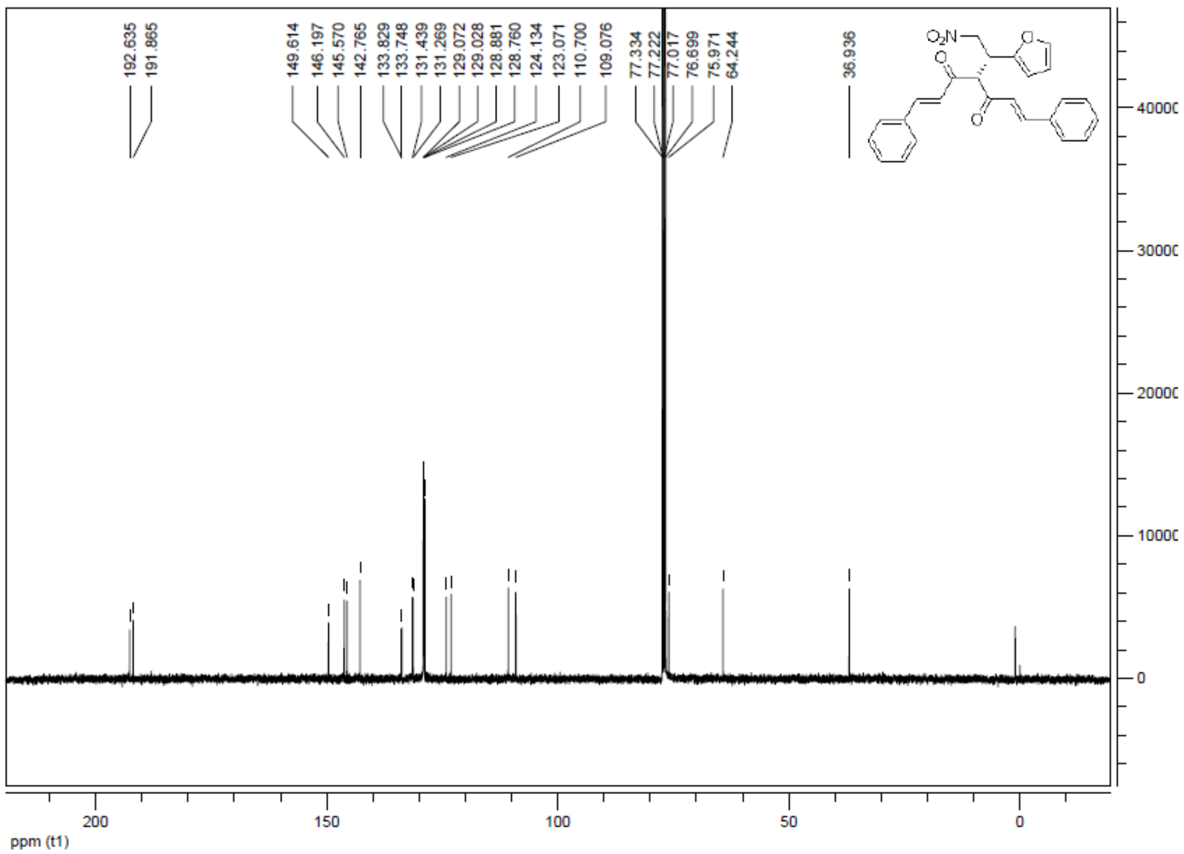
4-(1-(naphthalen-1-yl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ma)



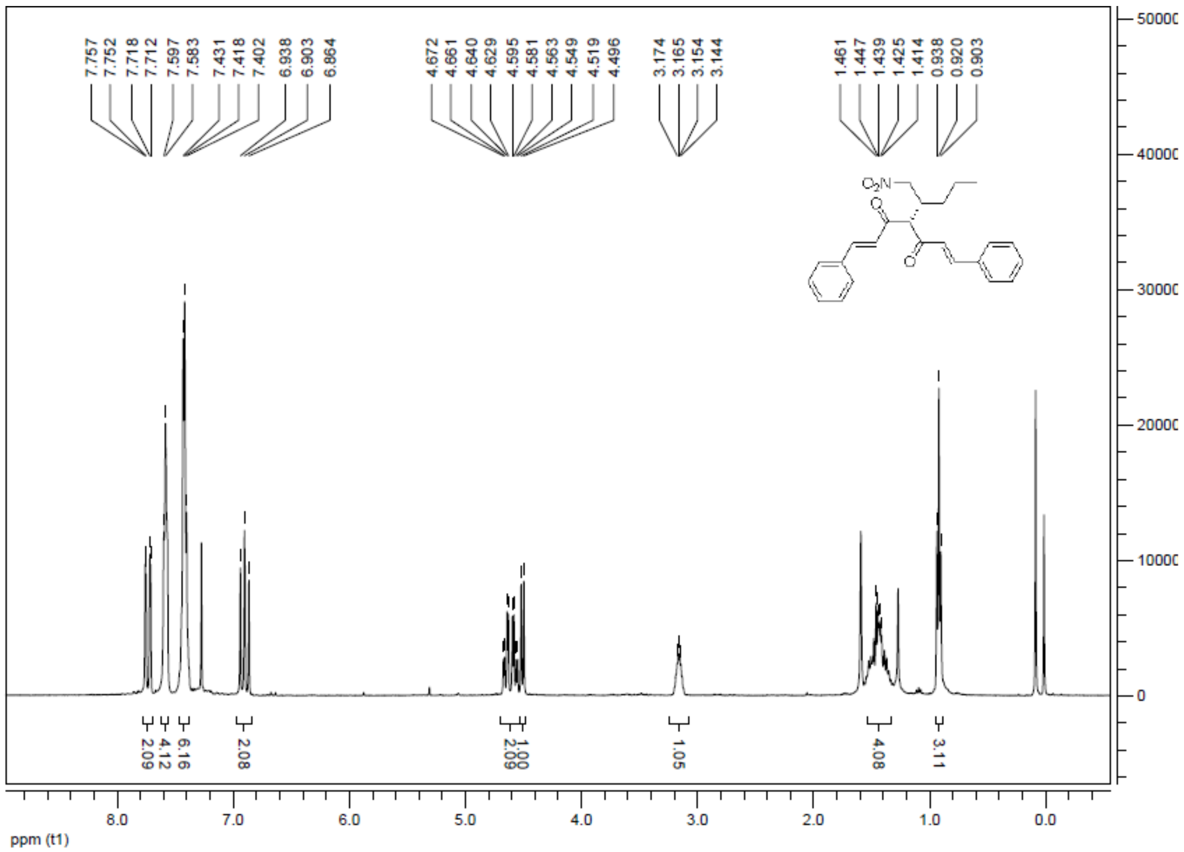


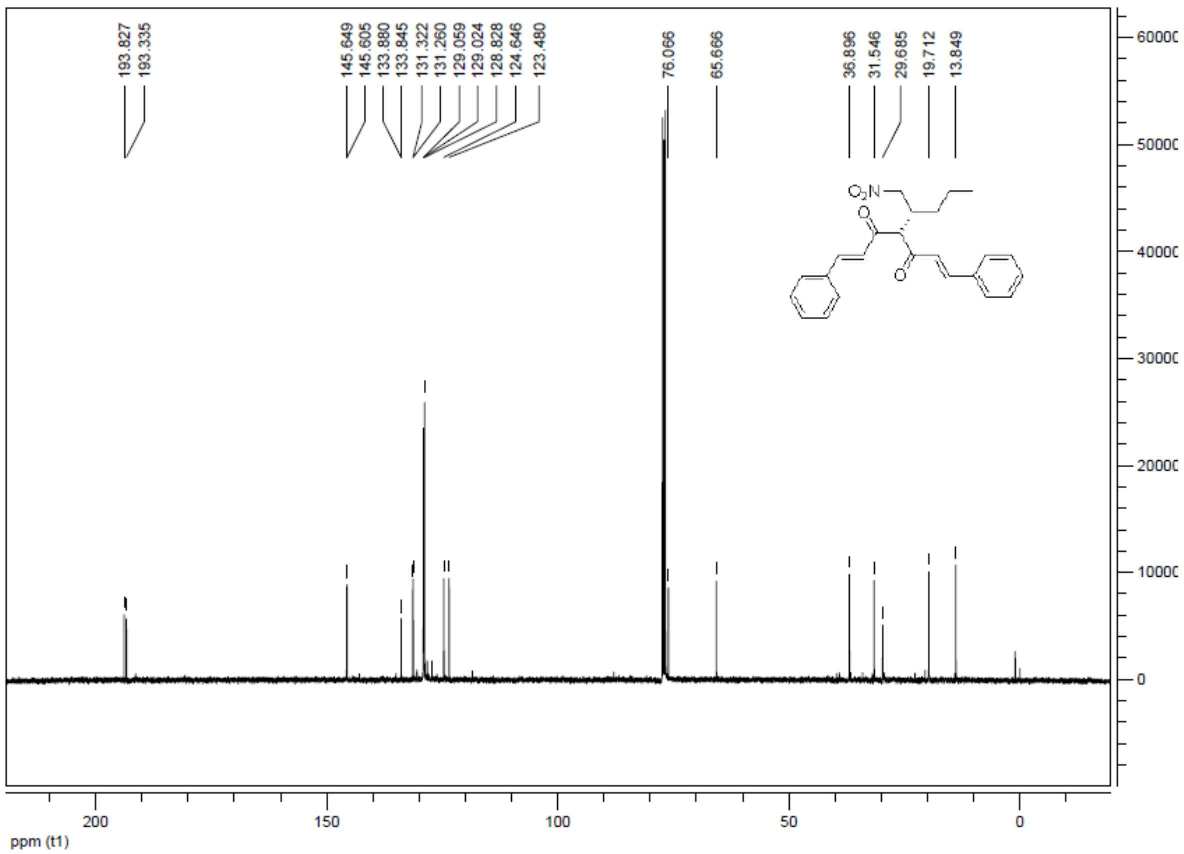
4-(1-(furan-2-yl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4na)



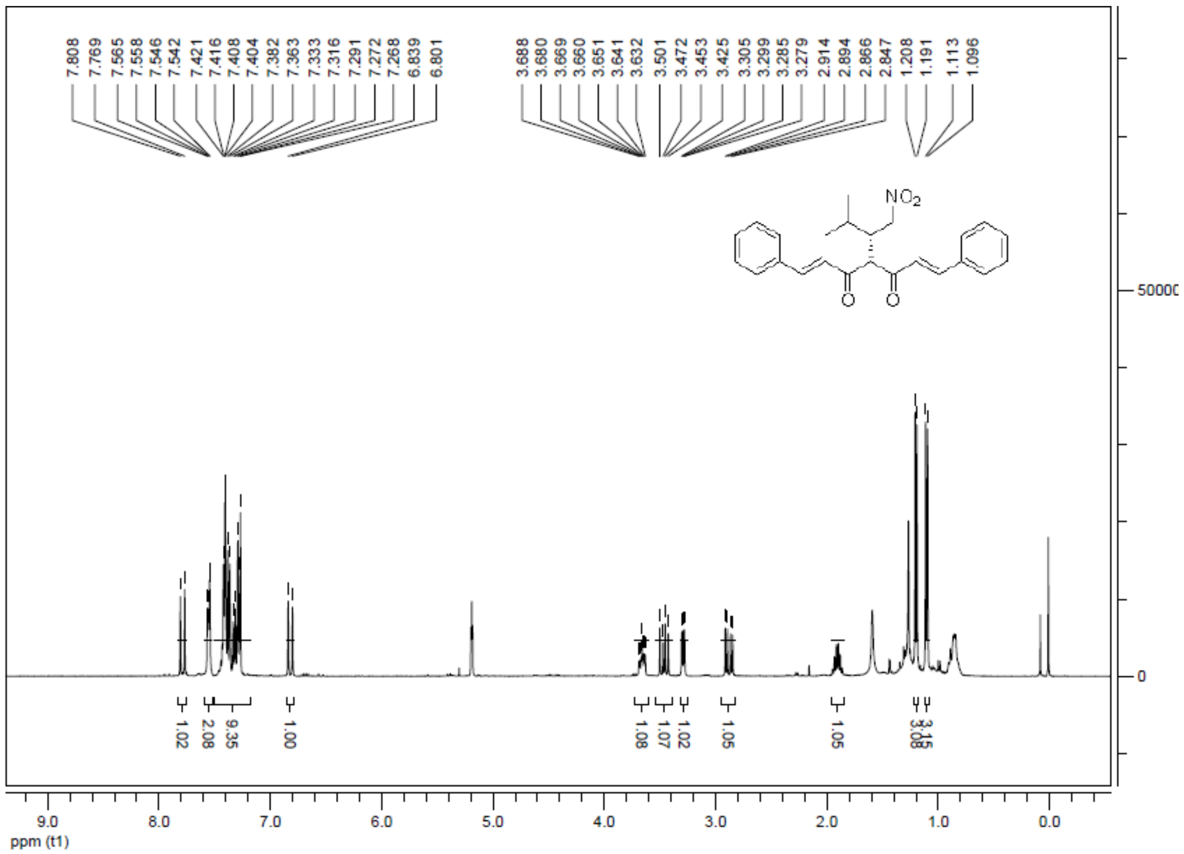


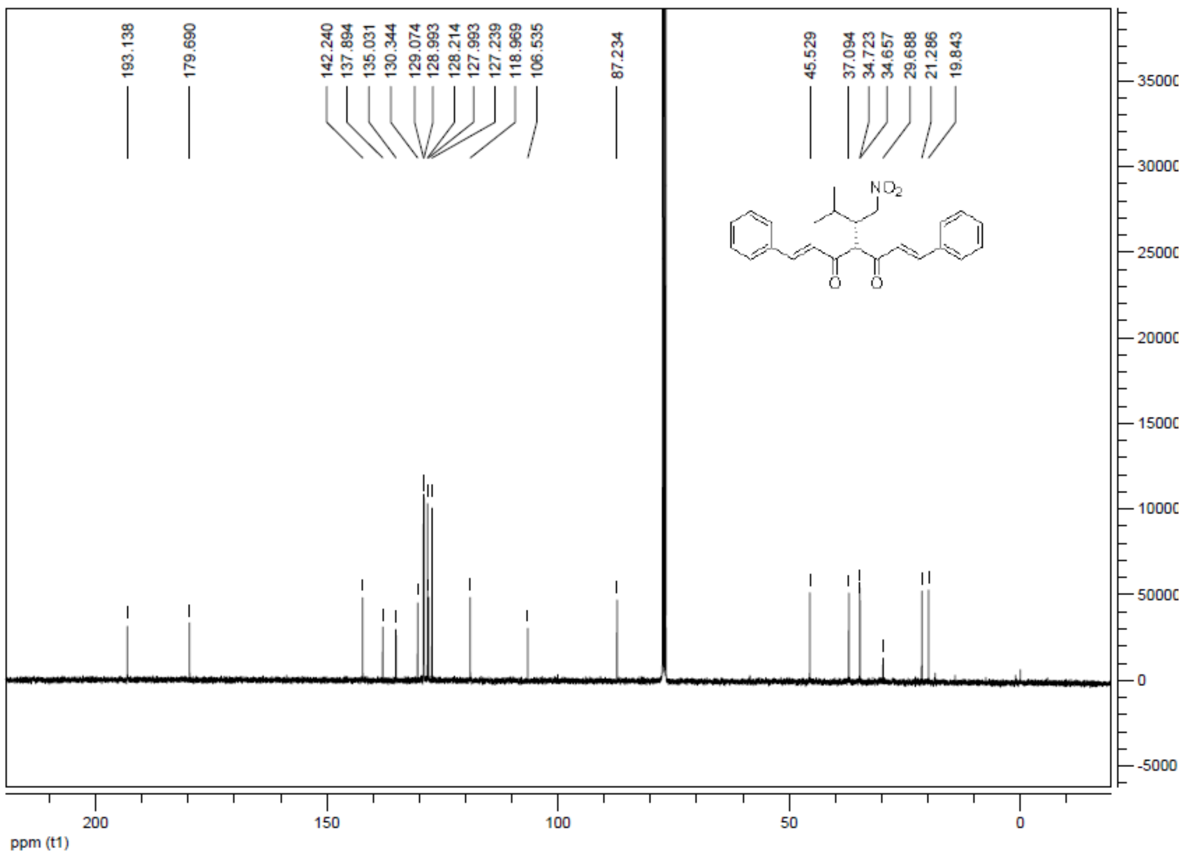
4-(1-nitropentan-2-yl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4oa)



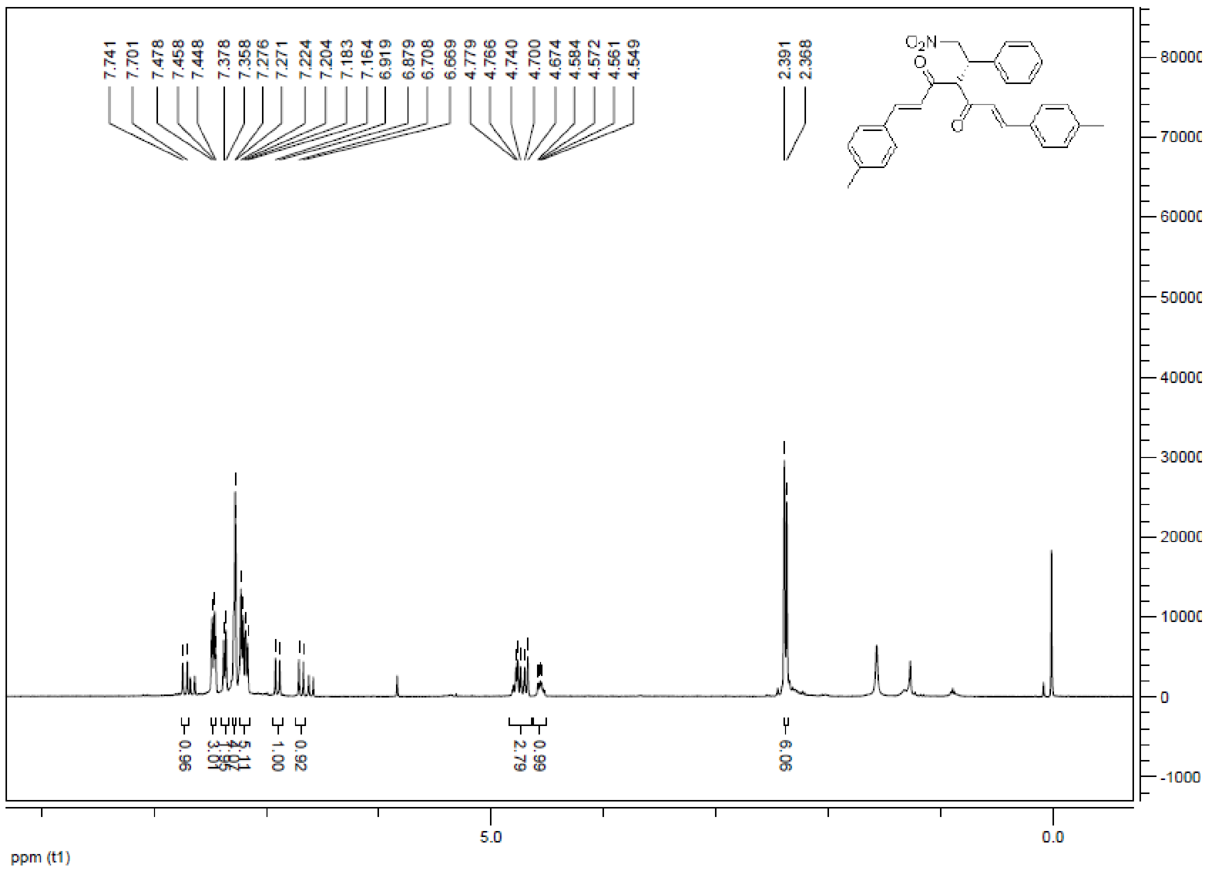


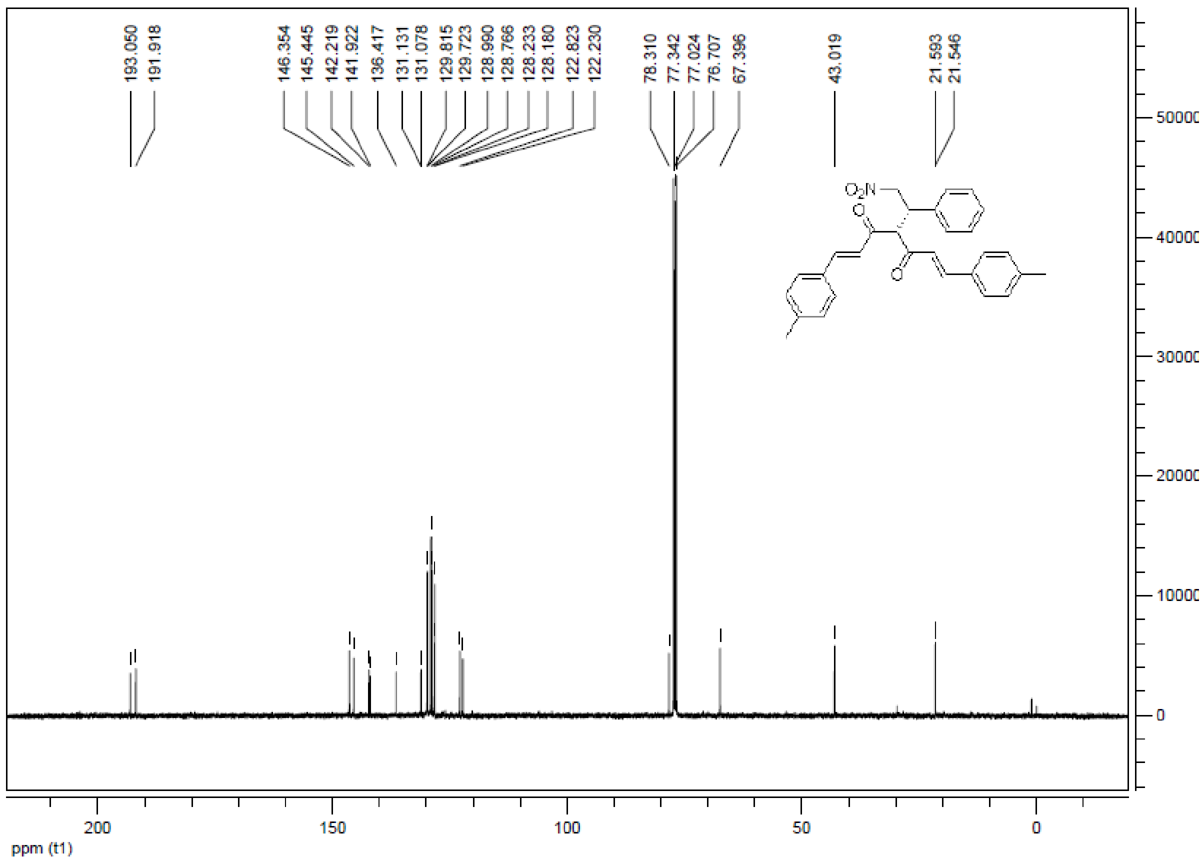
4-(3-methyl-1-nitrobutan-2-yl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4pa)



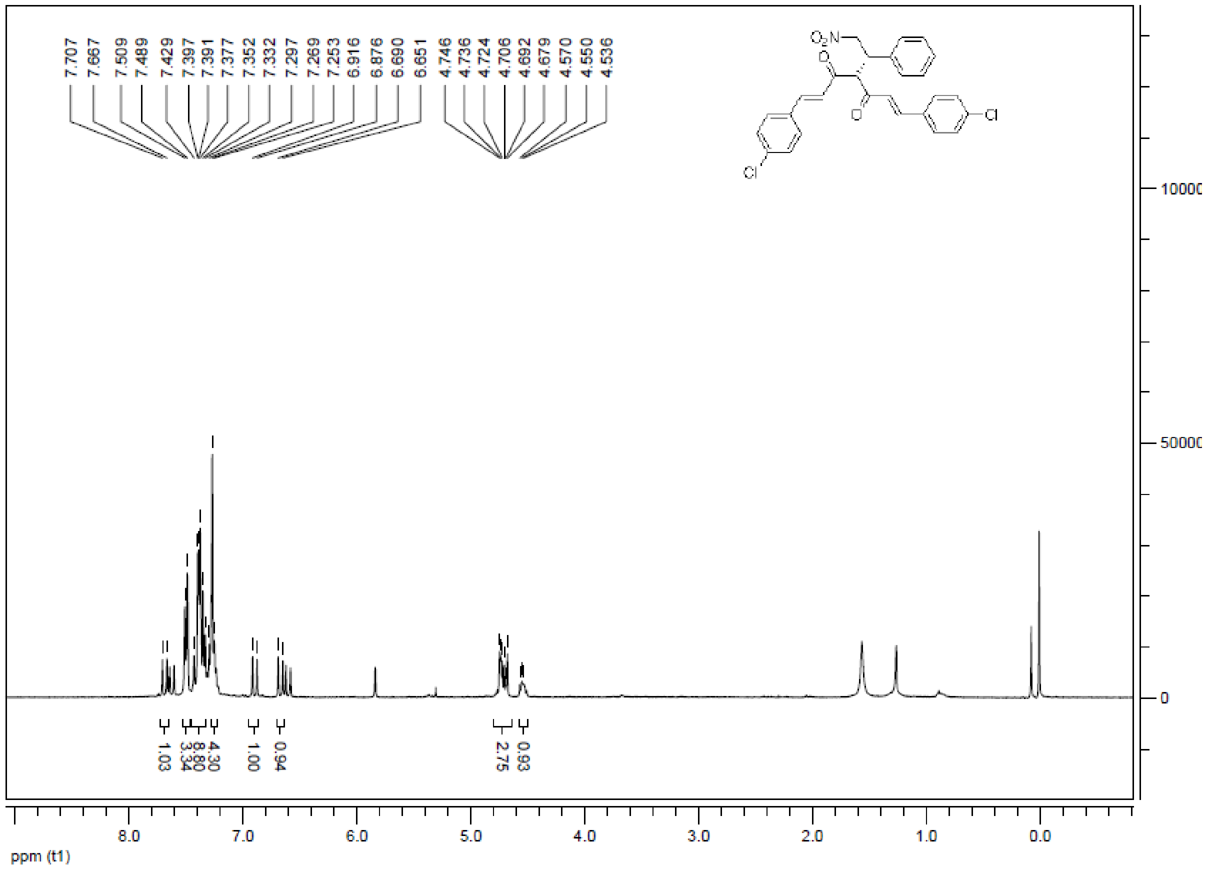


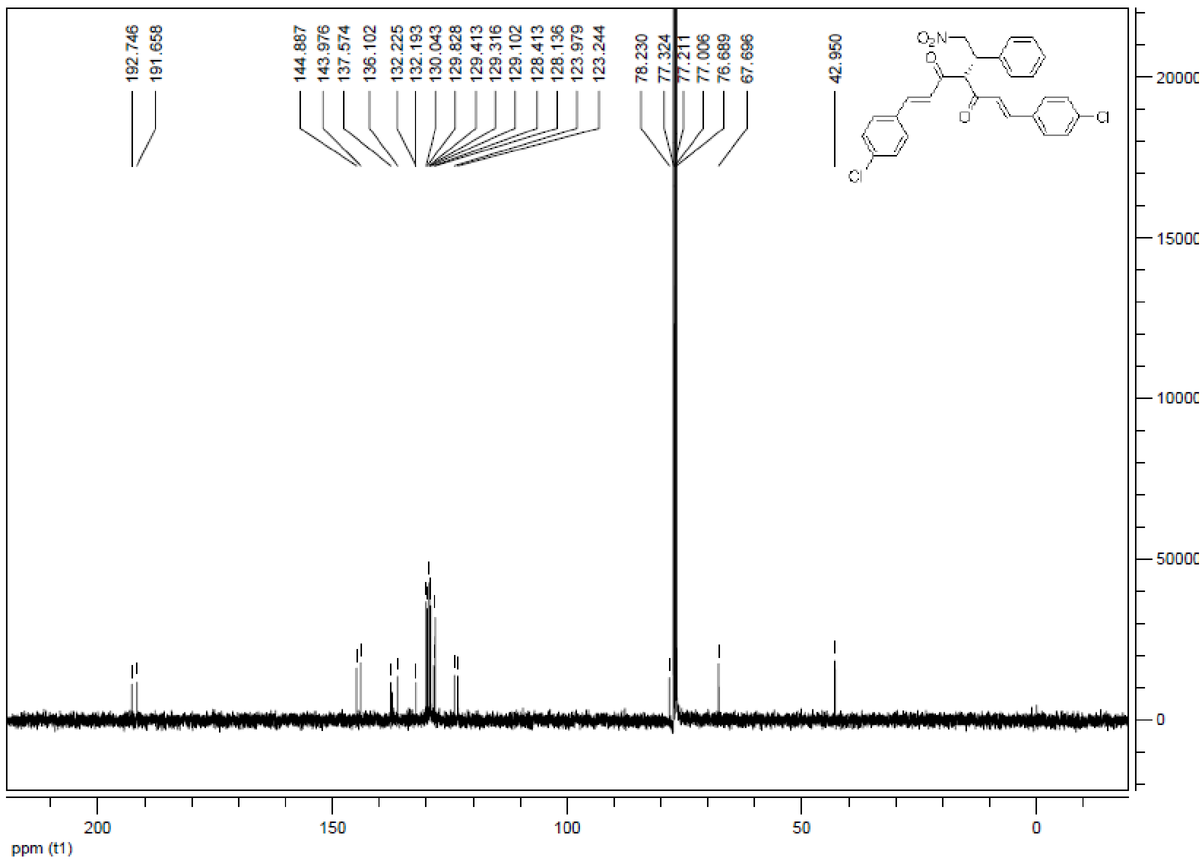
4-(2-nitro-1-phenylethyl)-1,7-dip-tolylhepta-1,6-diene-3,5-dione (4ab)



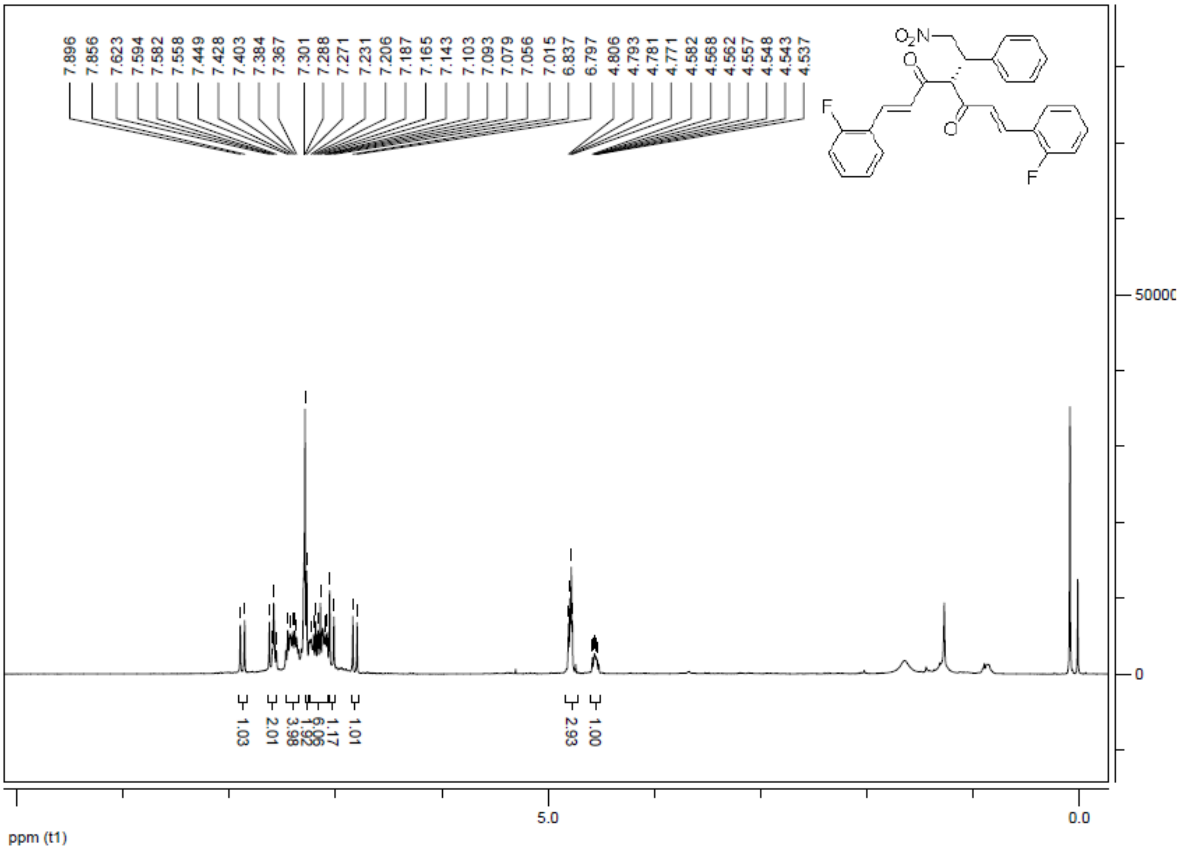


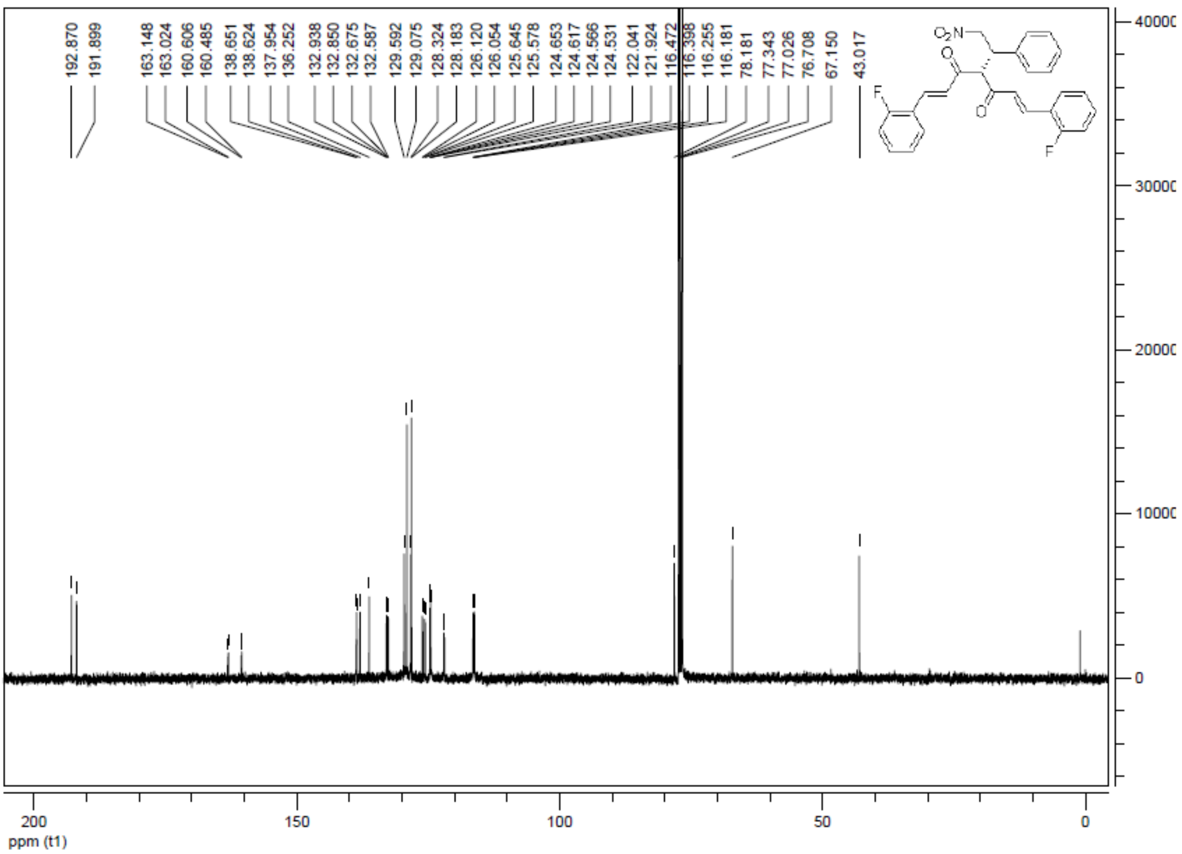
1,7-bis(4-chlorophenyl)-4-(2-nitro-1-phenylethyl)hepta-1,6-diene-3,5-dione (4ac)



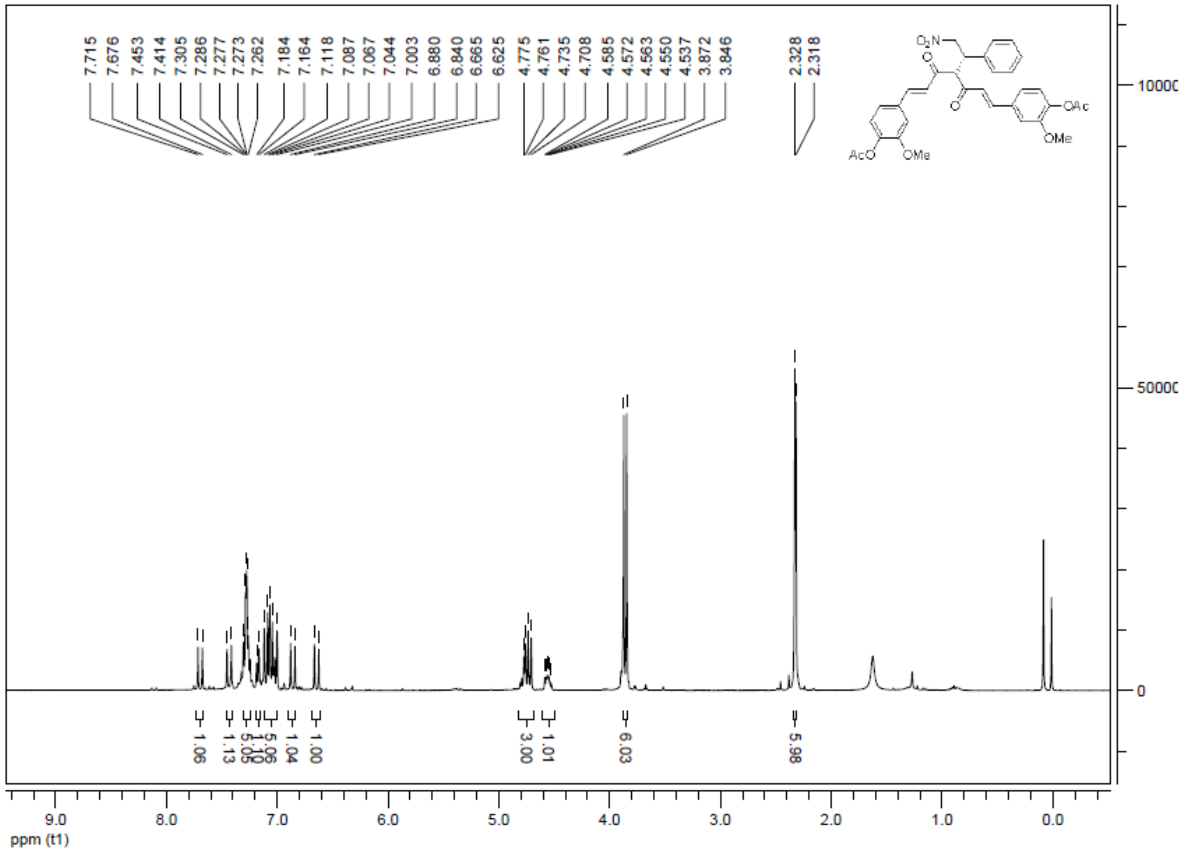


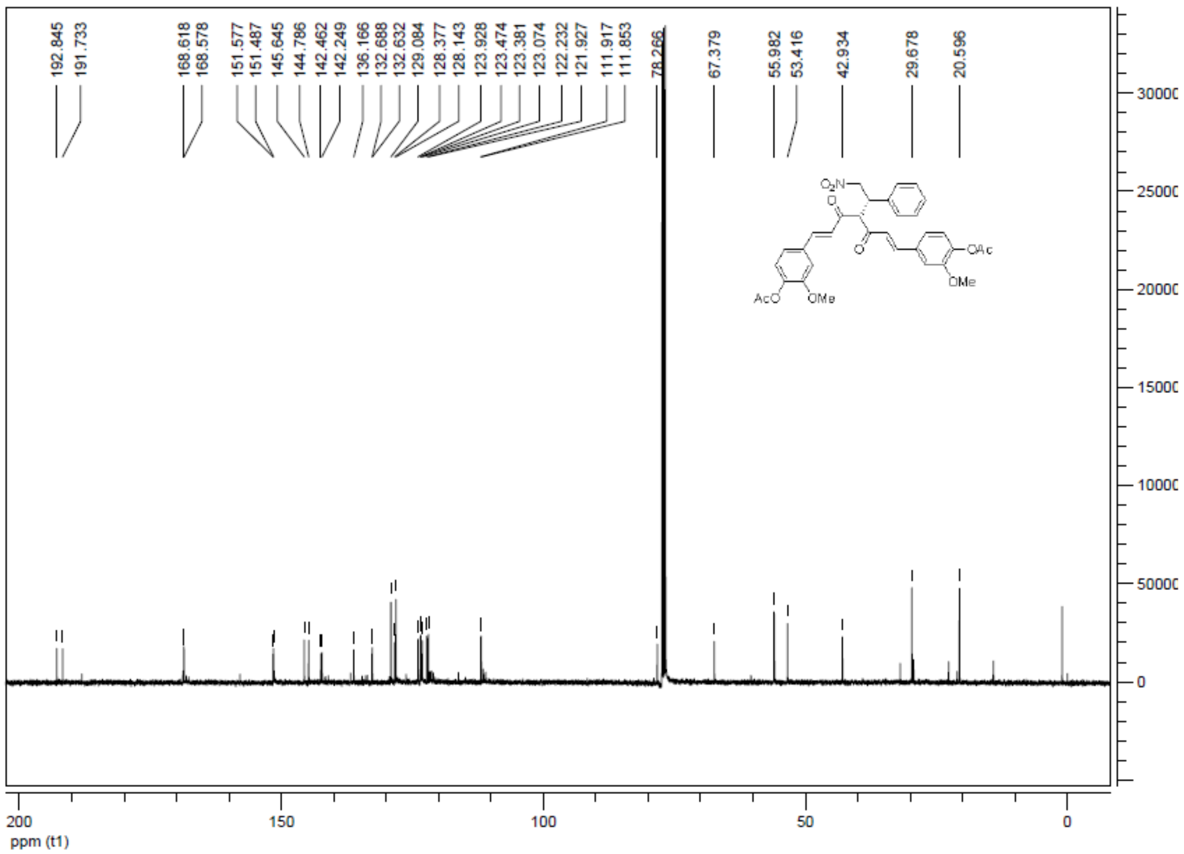
1,7-bis(2-fluorophenyl)-4-(2-nitro-1-phenylethyl)hepta-1,6-diene-3,5-dione (4ad)





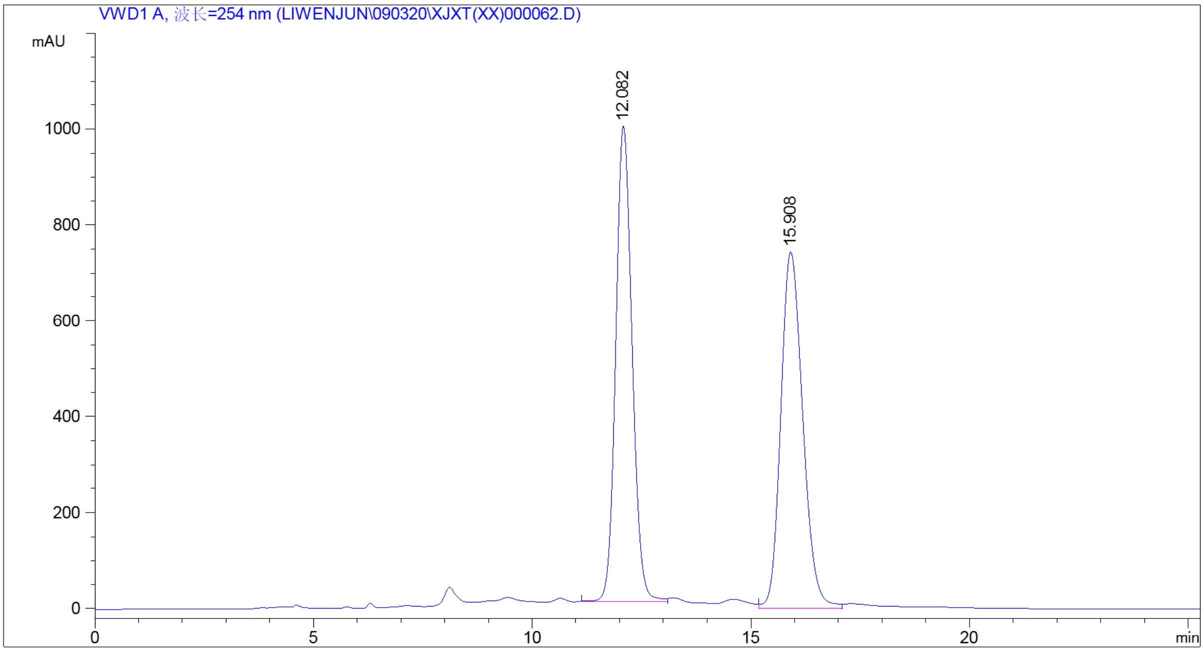
1,7-bis(4-hydroxy-3-methoxyphenyl)-4-(2-nitro-1-phenylethyl)hepta-1,6-diene-3,5-dione (4ae)



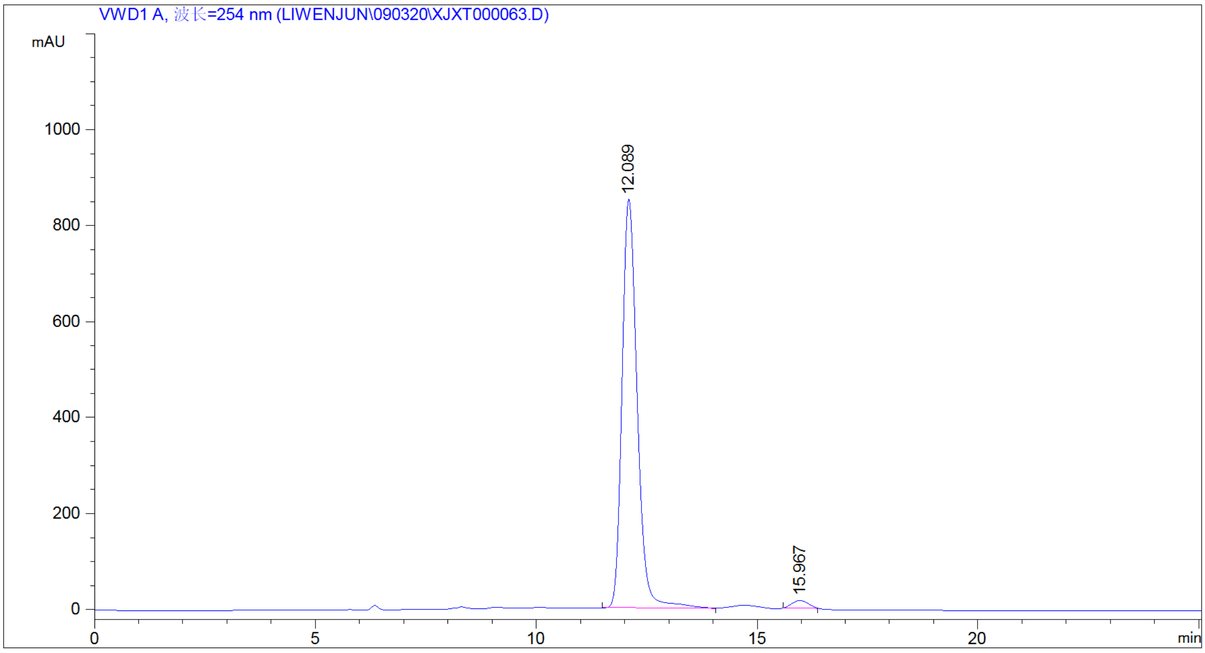


E: Chiral Analysis of Michael Addition Products

4-(2-nitro-1-phenylethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4aa)

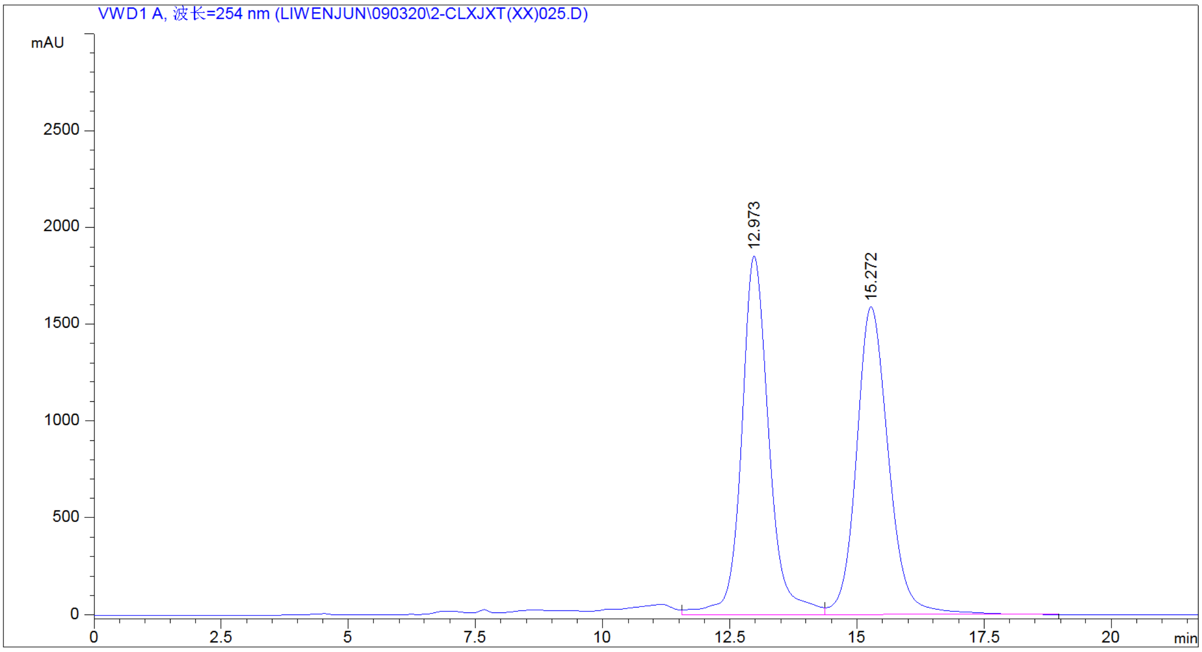


#	Time	Area	Height	Width	Symmetry	Area/%
1	12.082	25805.3	991.4	0.4338	0.851	49.858
2	15.908	25952.6	743.2	0.5457	0.781	50.142

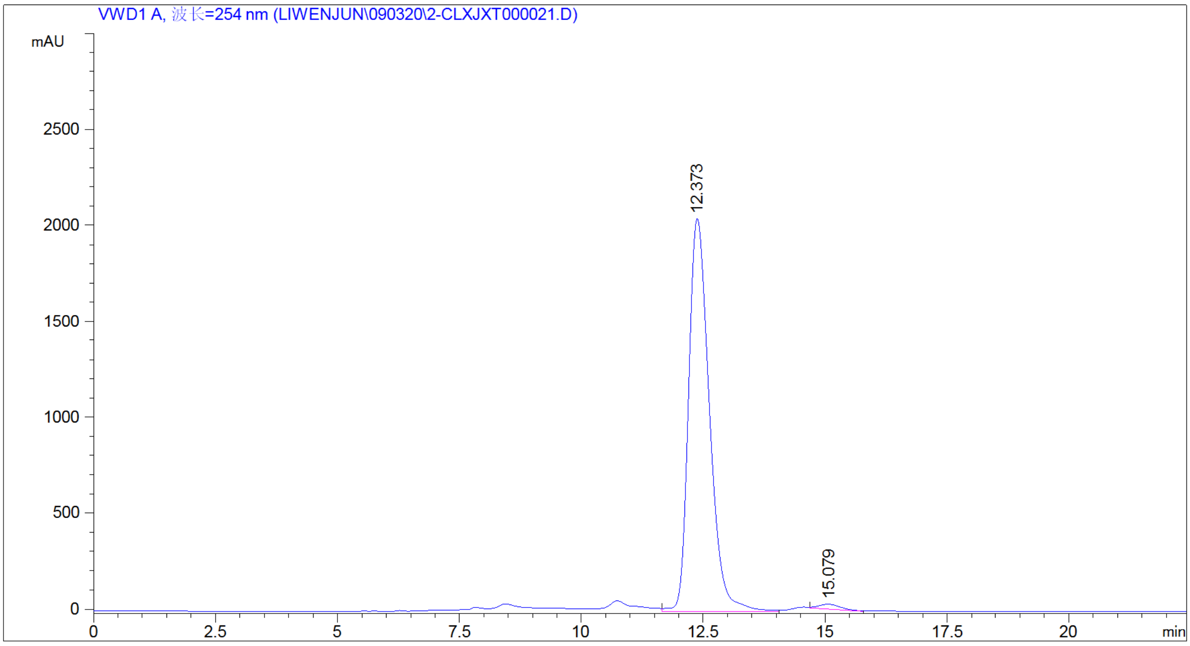


#	Time	Area	Height	Width	Symmetry	Area/%
1	12.089	20413.2	851.7	0.3699	0.729	97.999
2	15.967	416.9	16	0.4157	0	2.001

4-(1-(2-chlorophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ba)

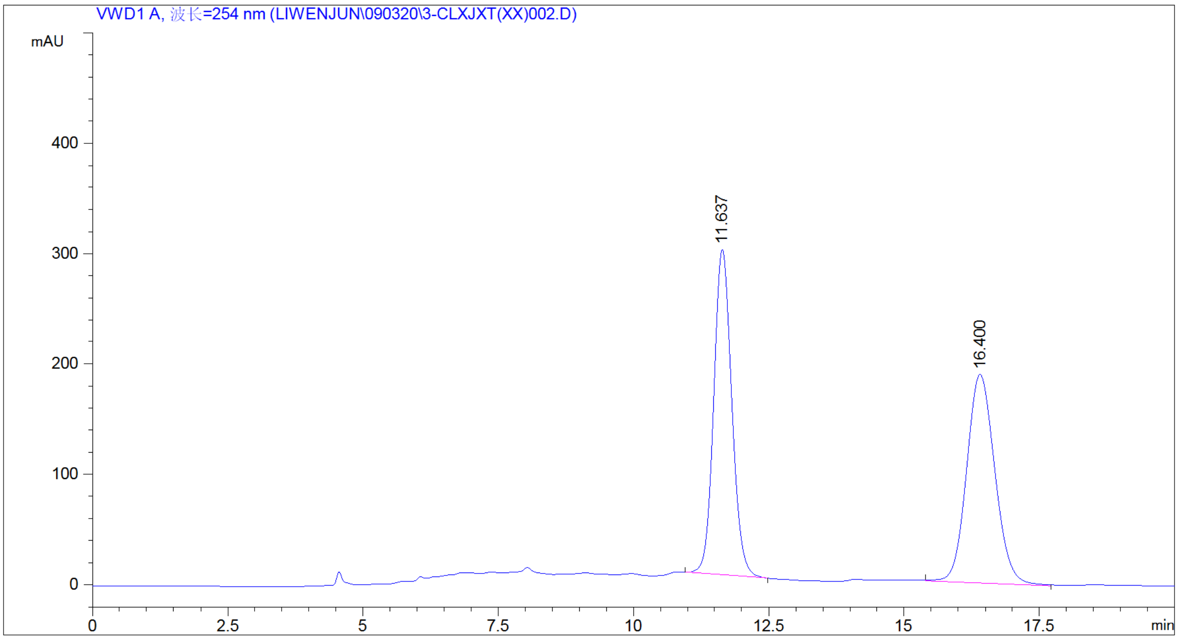


#	Time	Area	Height	Width	Symmetry	Area/%
1	12.973	69536	1850.6	0.5651	0.831	49.896
2	15.272	69826.5	1588.3	0.6716	0.785	50.104

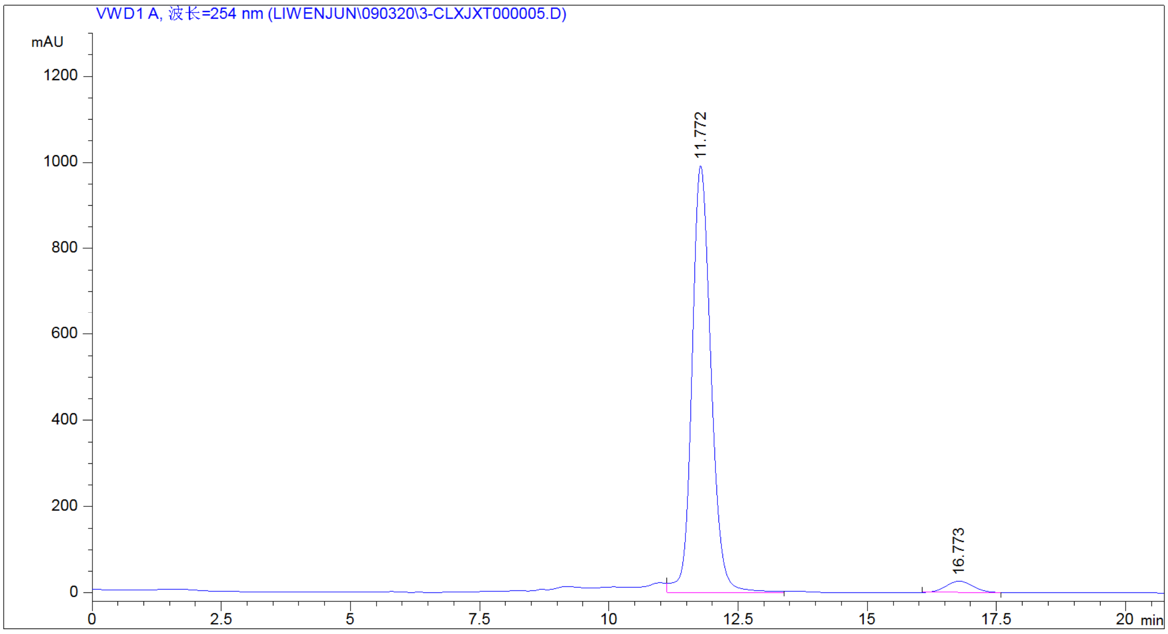


#	Time	Area	Height	Width	Symmetry	Area/%
1	12.373	60757.6	2047	0.4598	0.673	98.600
2	15.079	862.6	26	0.552	0.611	1.400

4-(1-(3-chlorophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ca)

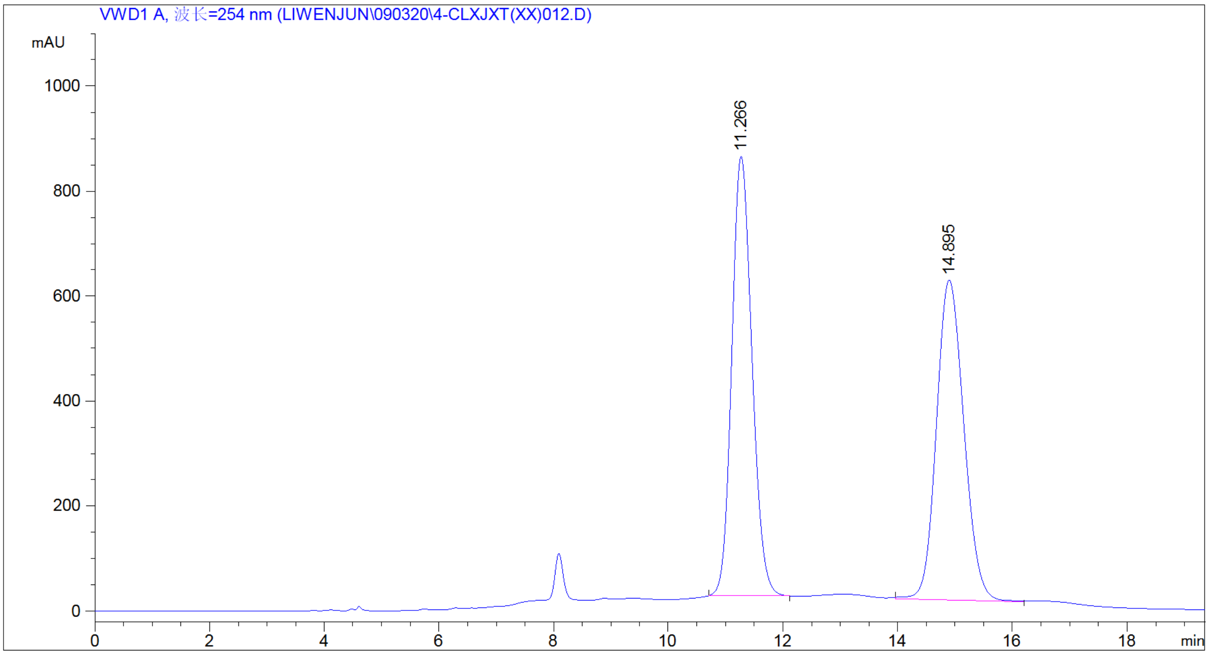


#	Time	Area	Height	Width	Symmetry	Area/%
1	11.637	6837.4	295.2	0.3171	0	49.905
2	16.4	6863.6	188.8	0.4978	0	50.095

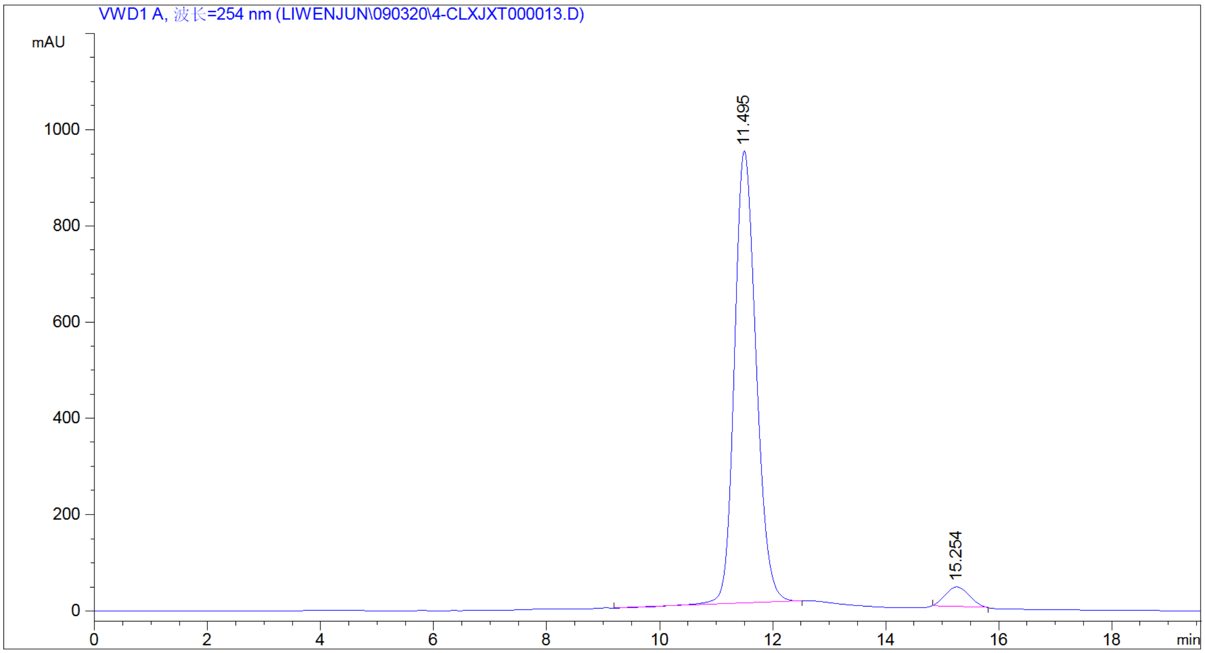


#	Time	Area	Height	Width	Symmetry	Area/%
1	11.772	25397.8	991.3	0.395	0.801	96.288
2	16.773	979	26.4	0.618	0.872	3.712

4-(1-(4-chlorophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4da)

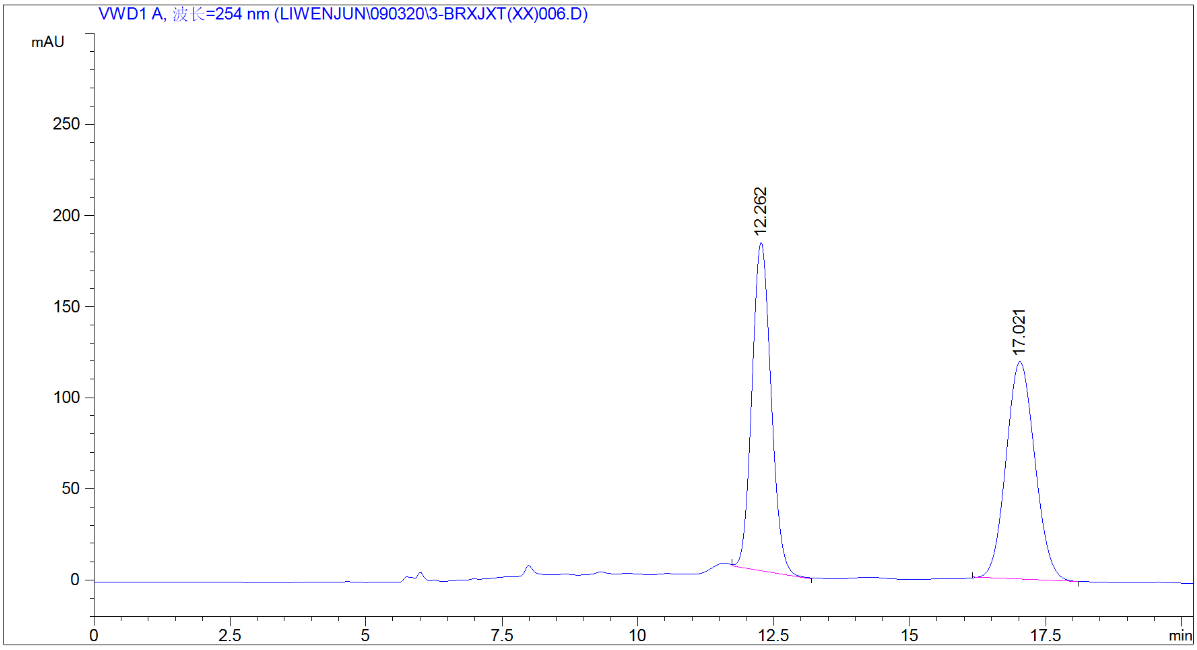


#	Time	Area	Height	Width	Symmetry	Area/%
1	11.266	20508.1	837.9	0.3827	0	50.278
2	14.895	20281.6	609.8	0.5381	0	49.722

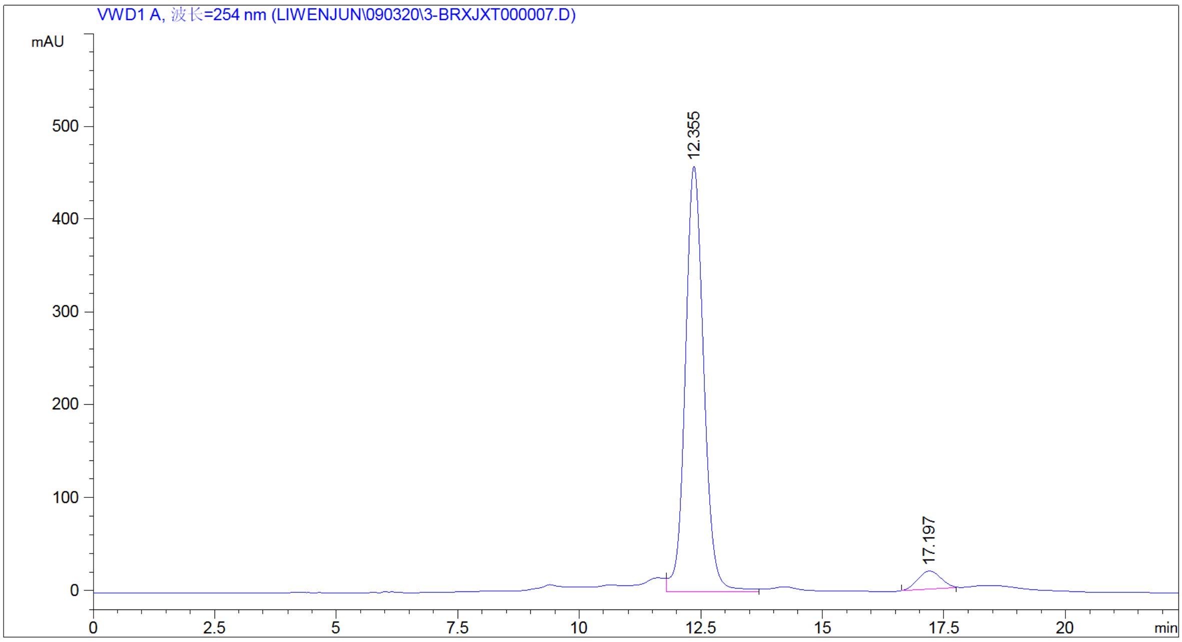


#	Time	Area	Height	Width	Symmetry	Area/%
1	11.495	25031.1	940.2	0.414	0.803	95.426
2	15.254	1199.9	41	0.4883	0.896	4.574

4-(1-(3-bromophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ea)

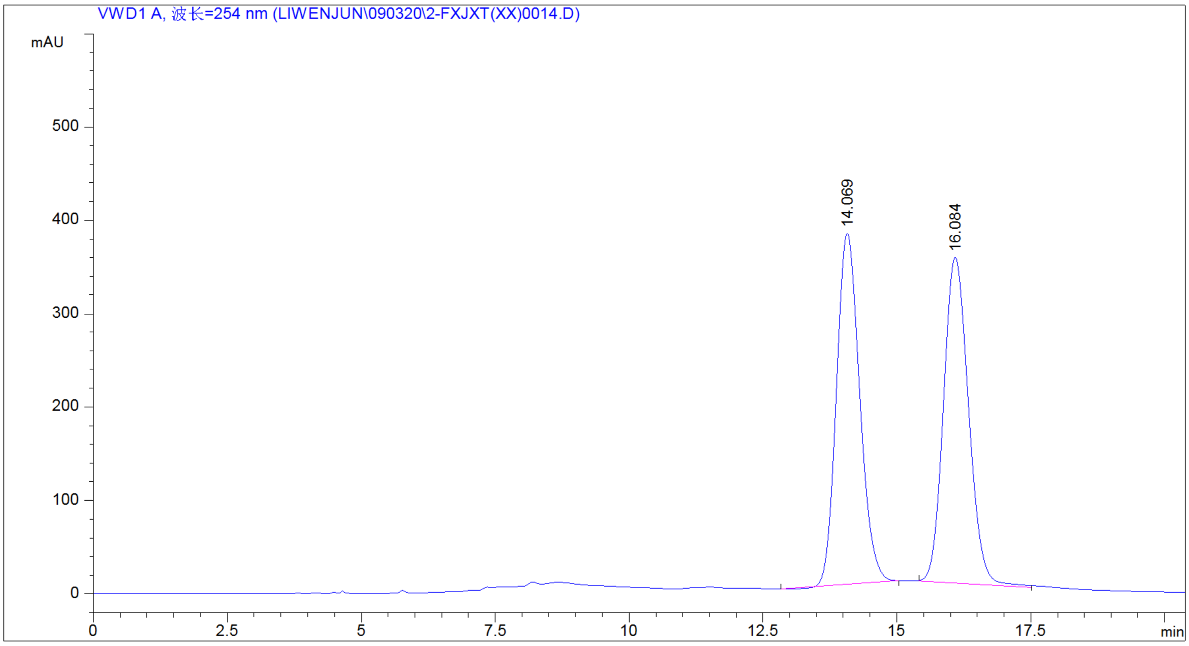


#	Time	Area	Height	Width	Symmetry	Area/%
1	12.262	4420.3	180.4	0.3213	0	50.137
2	17.021	4396.1	119.3	0.4472	0	49.863

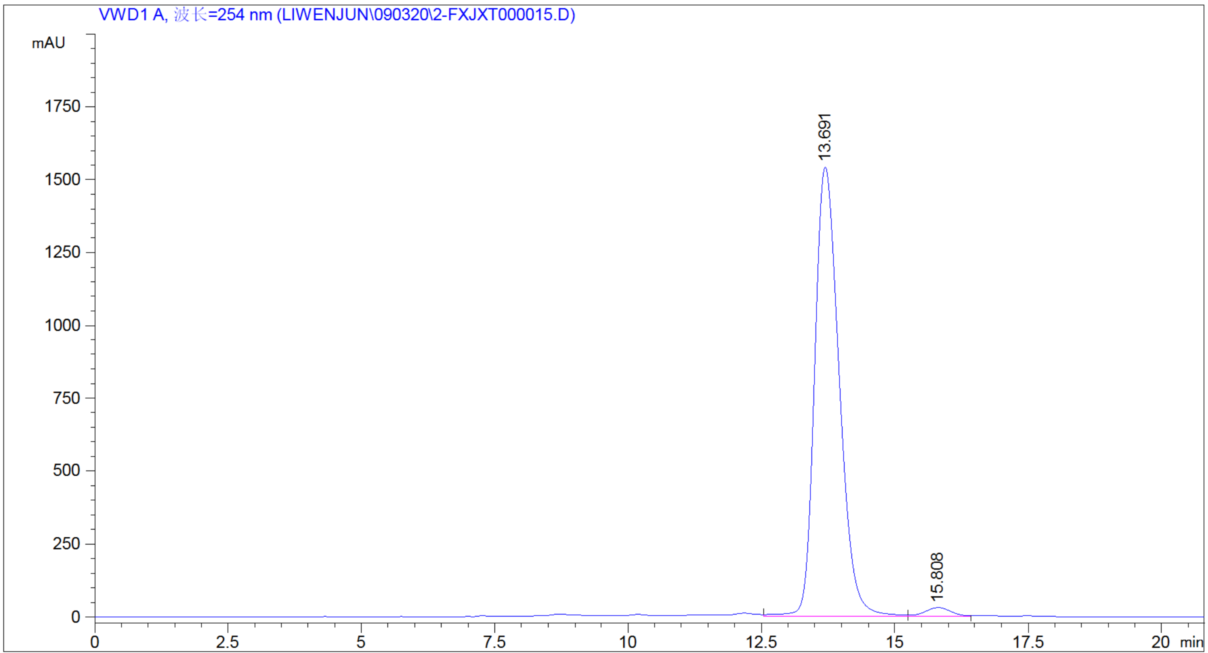


#	Time	Area	Height	Width	Symmetry	Area/%
1	12.355	12077.4	458.3	0.4065	0.855	94.901
2	17.197	649	19.5	0.5308	0	5.099

4-(1-(2-fluorophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4fa)



#	Time	Area	Height	Width	Symmetry	Area/%
1	14.069	11312.2	375.7	0.4677	0.821	49.968
2	16.084	11326.5	348.9	0.4617	0	50.032



#	Time	Area	Height	Width	Symmetry	Area/%
1	13.691	49547.6	1542.4	0.5015	0.716	97.752
2	15.808	1139.3	31.8	0.5443	0.986	2.248

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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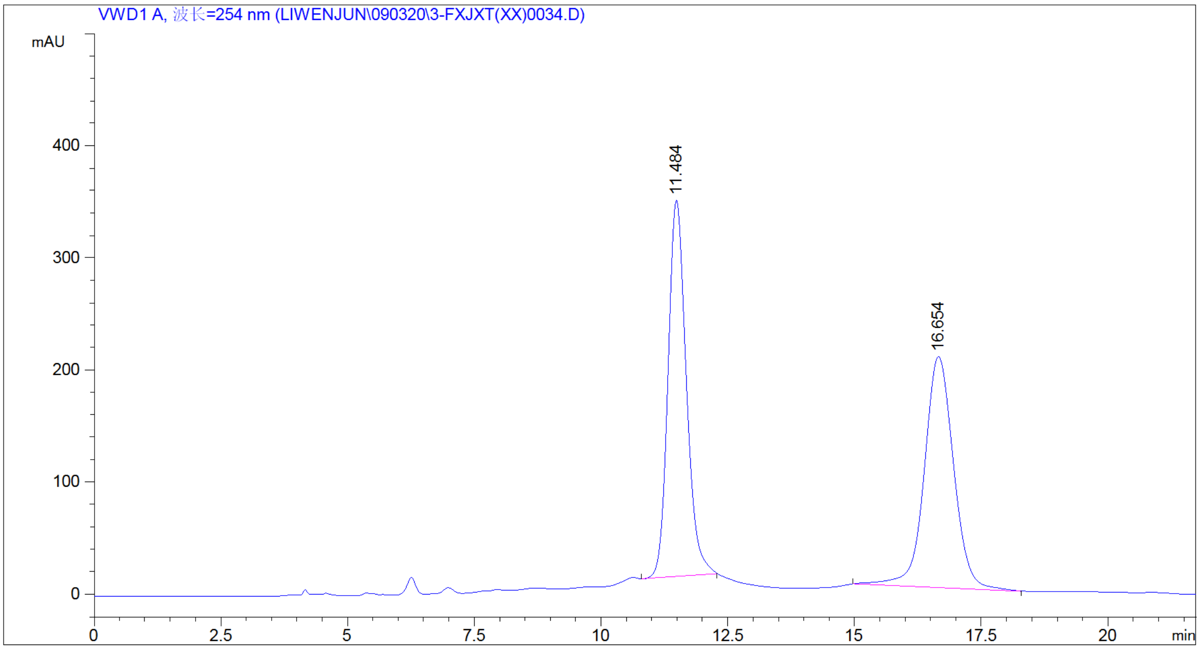
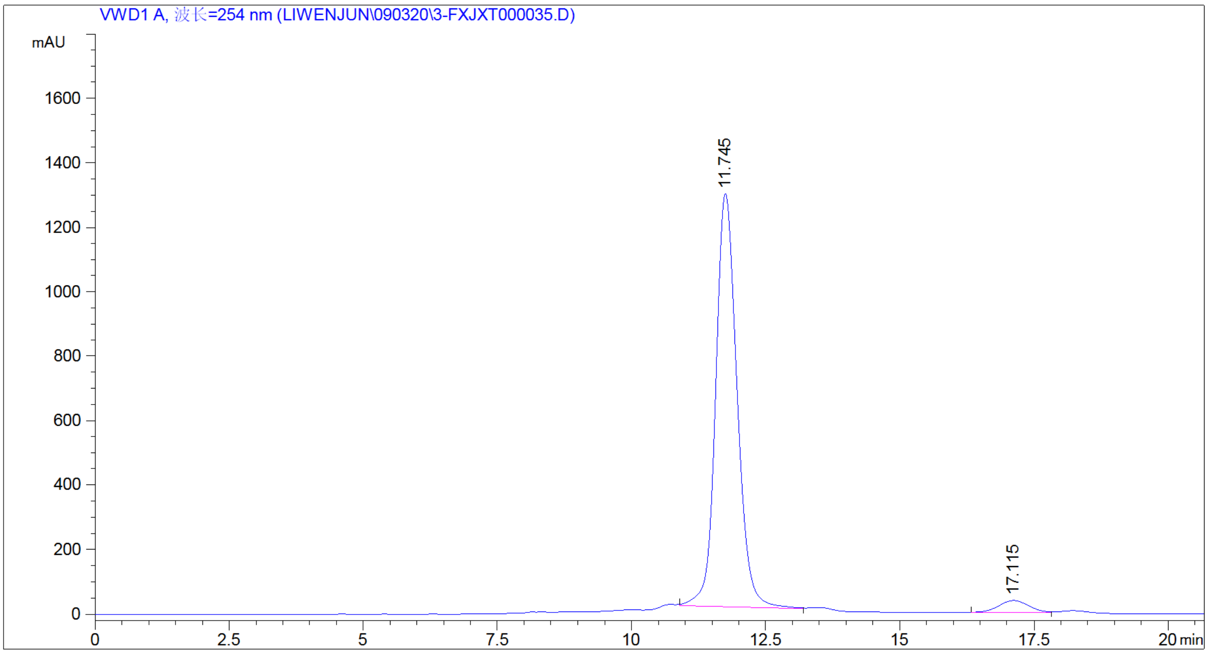
4-(1-(3-fluorophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ga)

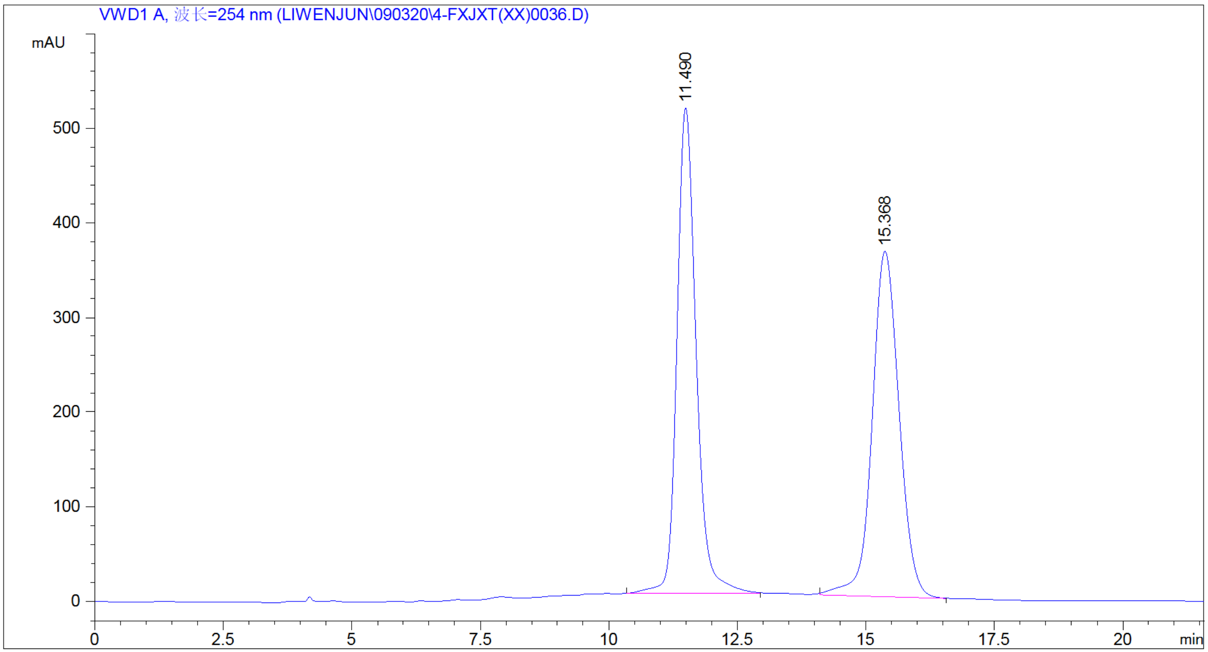


#	Time	Area	Height	Width	Symmetry	Area/%
1	11.484	8399.4	335.6	0.4058	0	50.194
2	16.654	8334.3	206.1	0.57	0	49.806

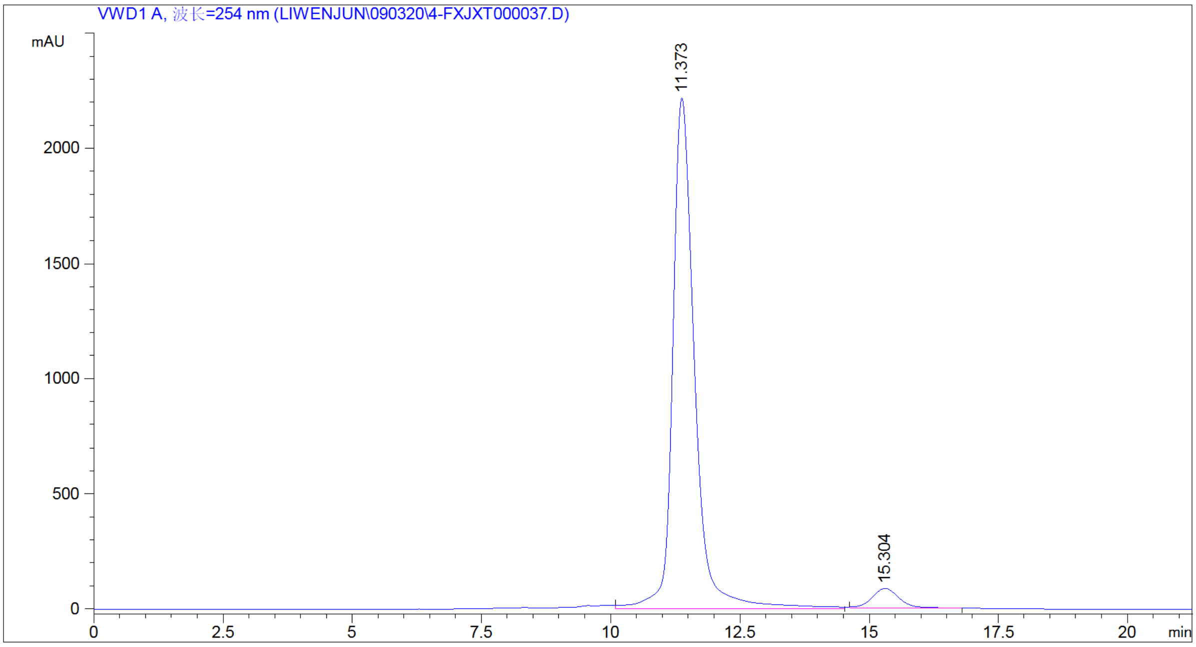


#	Time	Area	Height	Width	Symmetry	Area/%
1	11.745	35582.6	1283.3	0.4267	0	95.919
2	17.115	1513.8	37.8	0.6668	1.011	4.081

4-(1-(4-fluorophenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ha)

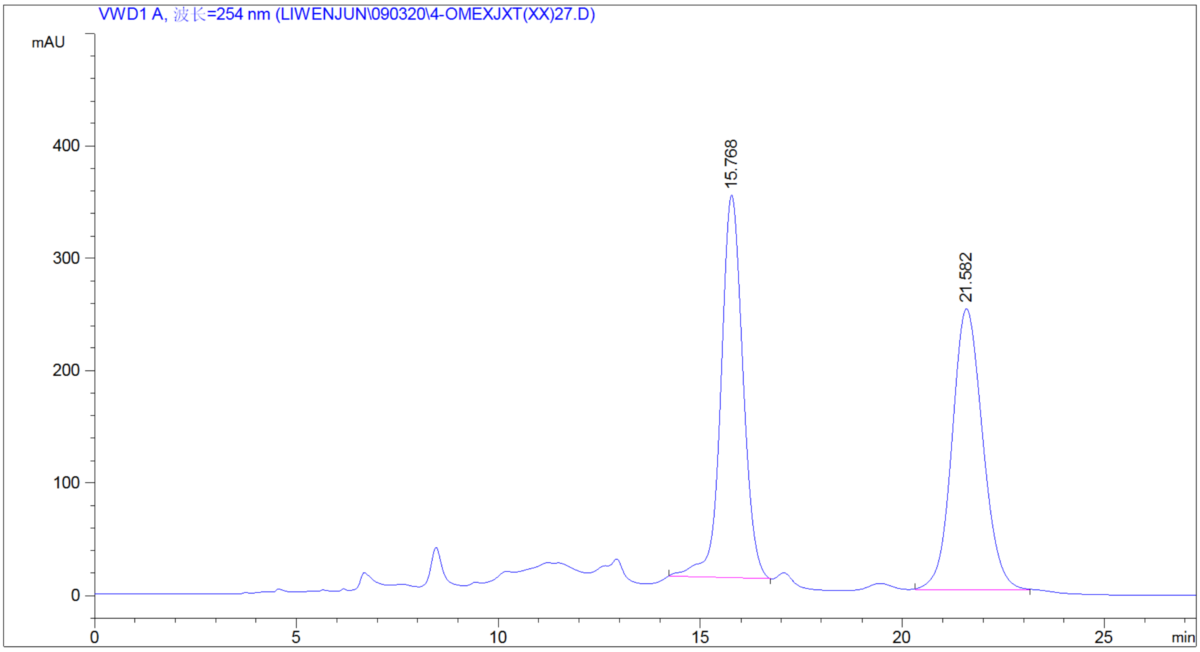


#	Time	Area	Height	Width	Symmetry	Area/%
1	11.49	13349.7	513.4	0.4334	0.798	50.009
2	15.368	13344.9	365.5	0.6085	0.898	49.991

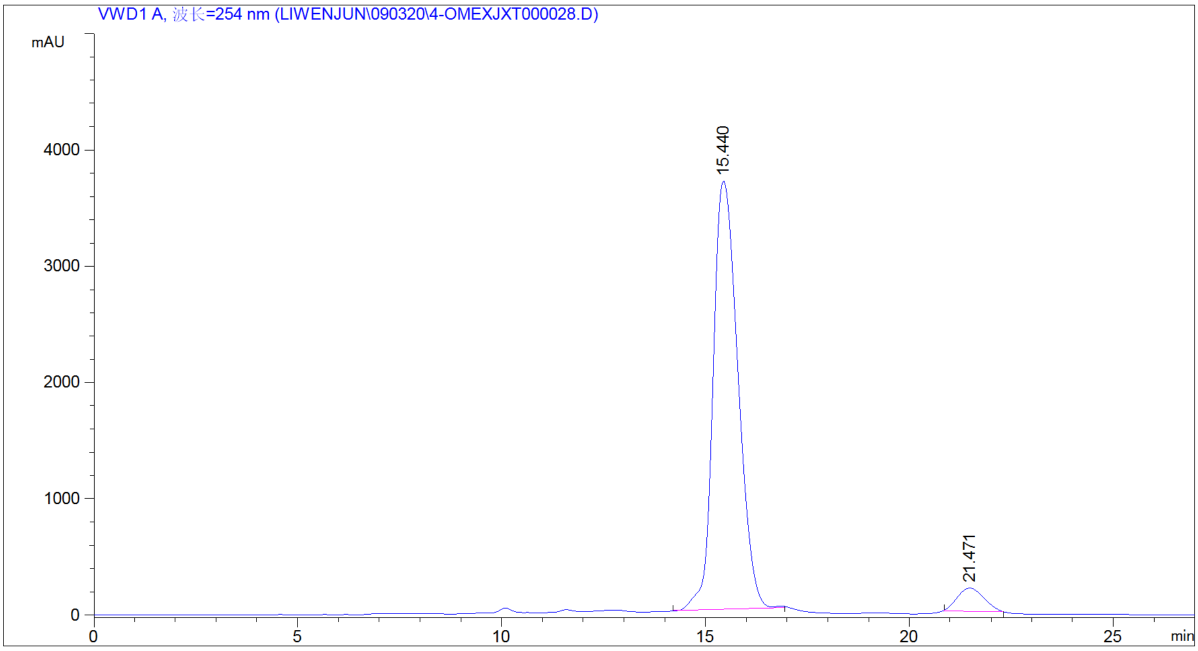


#	Time	Area	Height	Width	Symmetry	Area/%
1	11.373	66082.6	2218.9	0.4494	0.676	95.324
2	15.304	3241.4	85.5	0.5212	0	4.676

4-(1-(4-methoxyphenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ia)

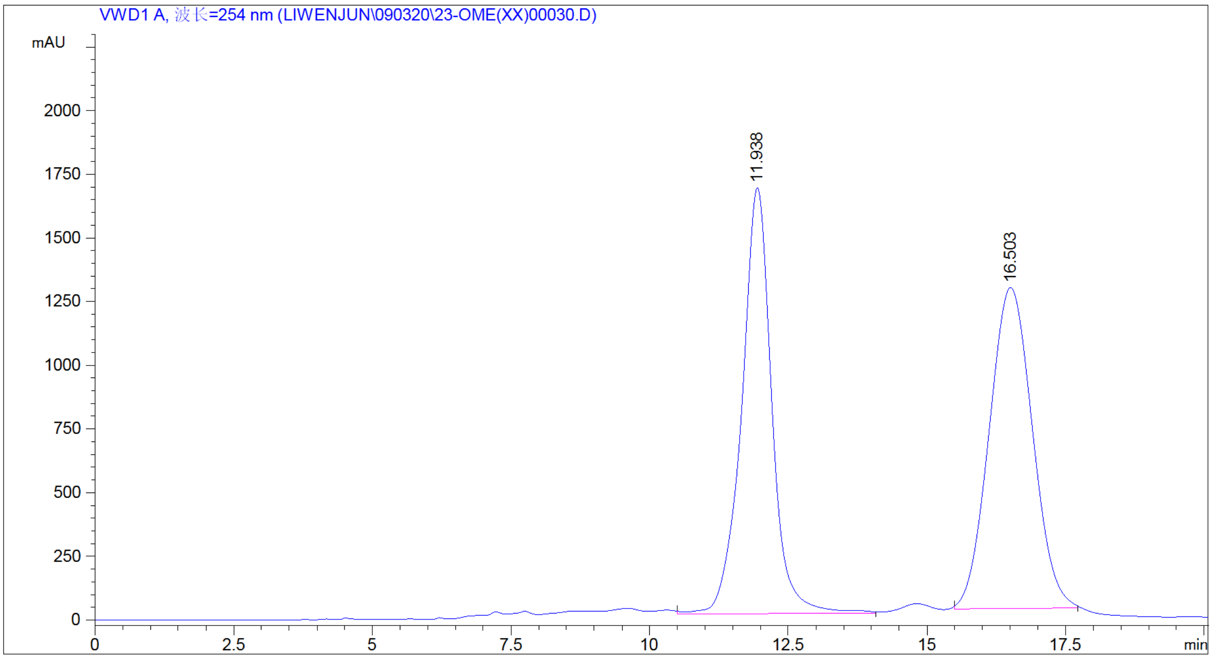


#	Time	Area	Height	Width	Symmetry	Area/%
1	15.768	12907.9	340.6	0.6316	0.939	49.385
2	21.582	13229.3	250.6	0.88	0.861	50.615

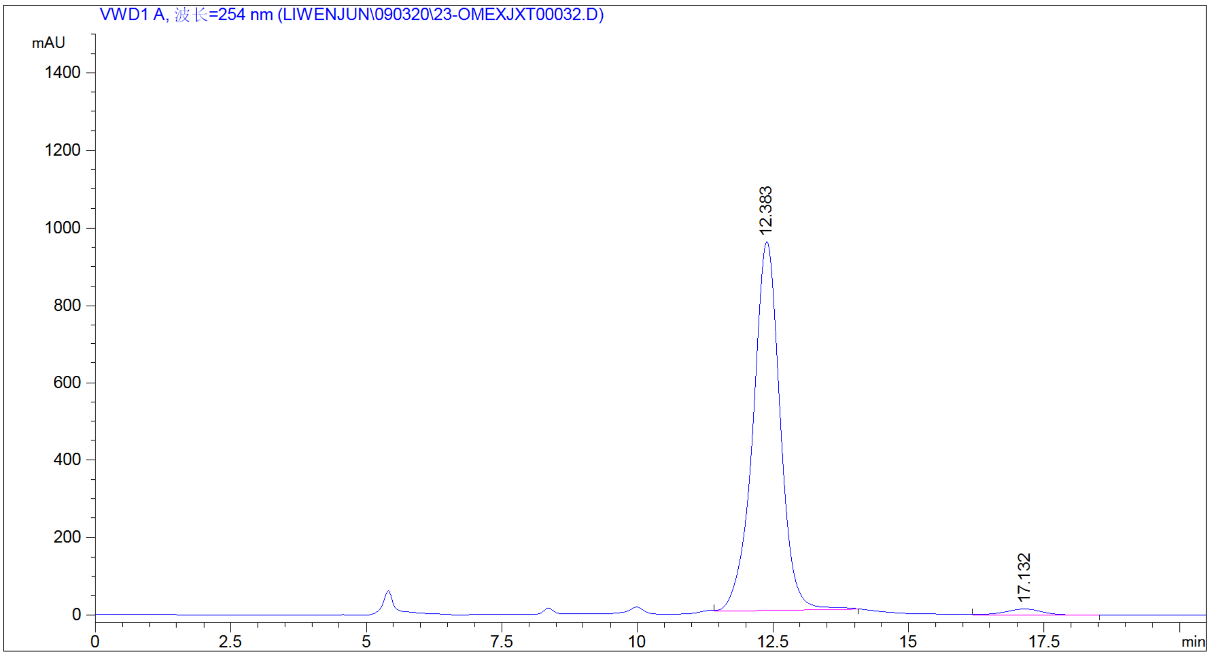


#	Time	Area	Height	Width	Symmetry	Area/%
1	15.44	156395.2	3683.9	0.633	0	94.509
2	21.471	9086.6	199.6	0.7589	0.846	5.491

4-(1-(2,3-dimethoxyphenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ja)

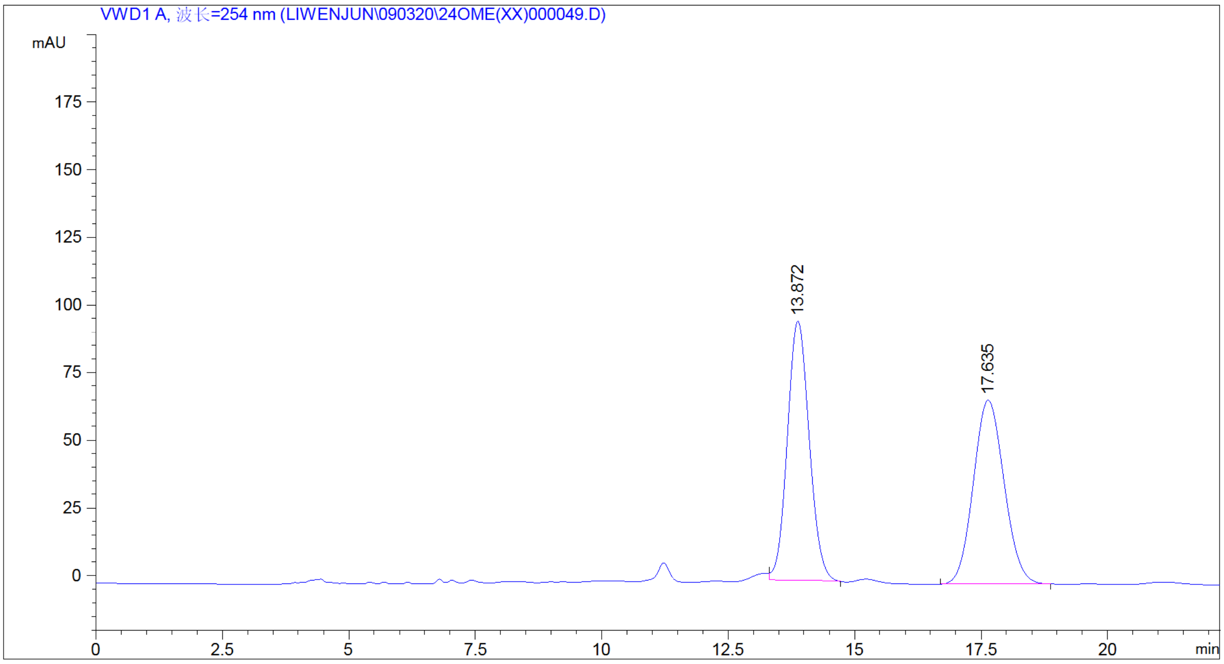


#	Time	Area	Height	Width	Symmetry	Area/%
1	11.938	63156.9	1671.7	0.6297	1.044	48.126
2	16.503	68074.3	1259.4	0.767	0	51.874

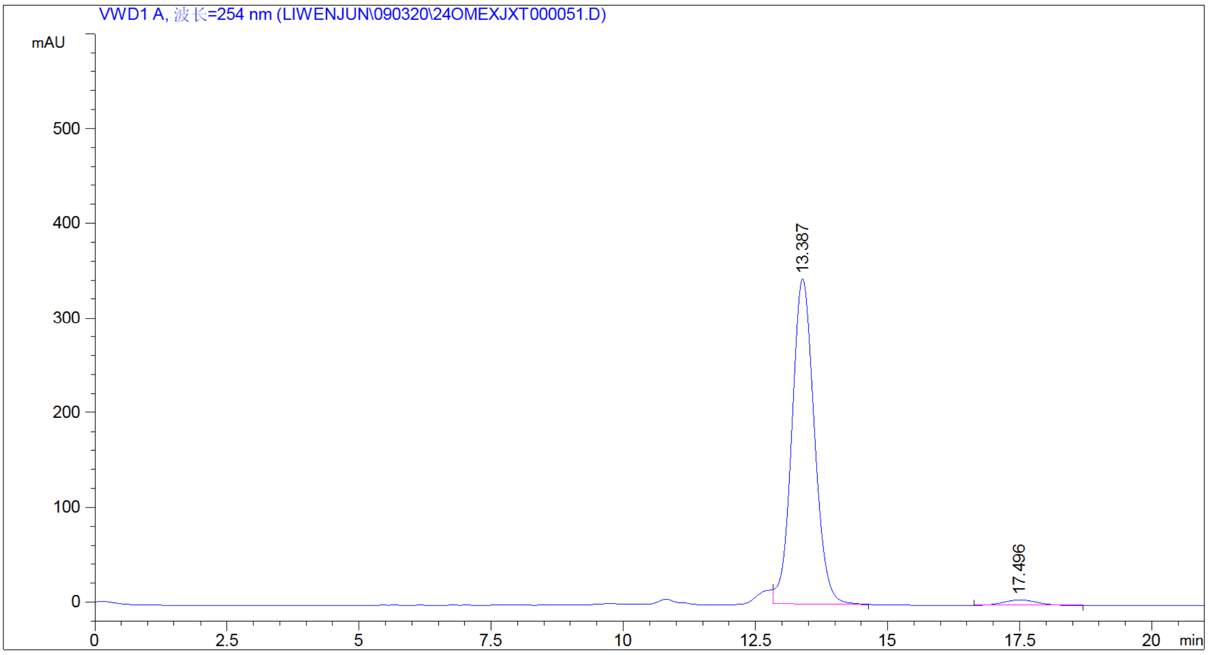


#	Time	Area	Height	Width	Symmetry	Area/%
1	12.383	33246.1	953.5	0.5527	0	97.963
2	17.132	691.4	15.3	0.6959	1.077	2.037

4-(1-(2,4-dimethoxyphenyl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ka)

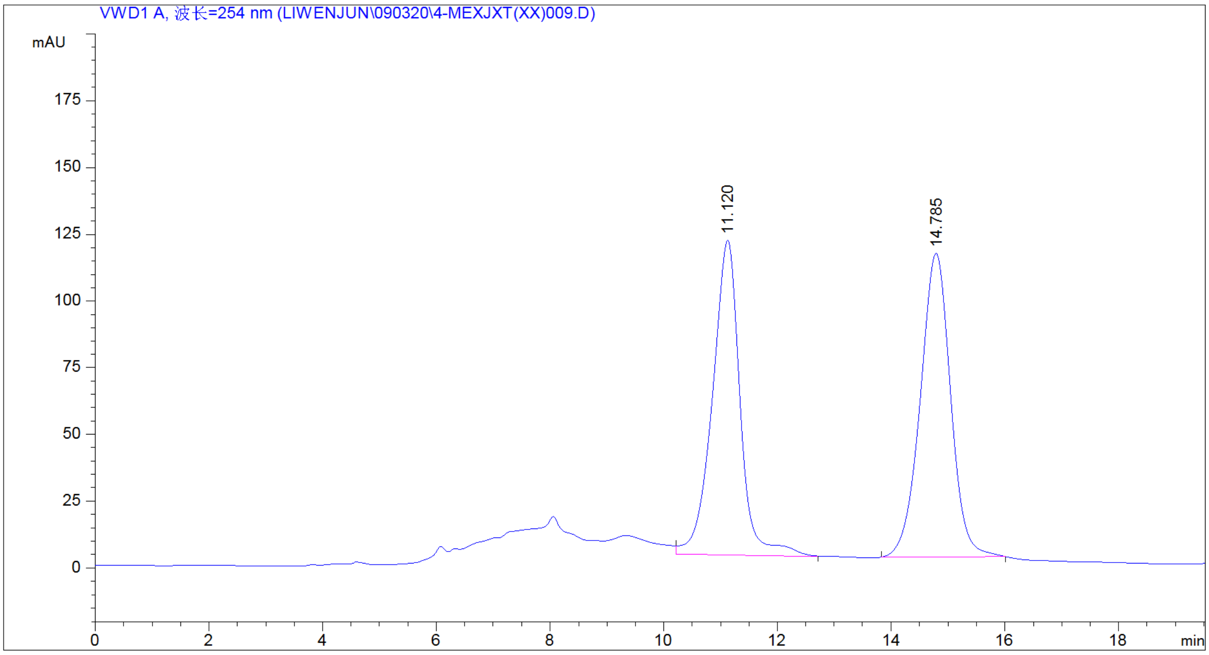


#	Time	Area	Height	Width	Symmetry	Area/%
1	13.872	2883.3	95.9	0.4558	0	50.061
2	17.635	2876.3	67.9	0.6632	0.889	49.939

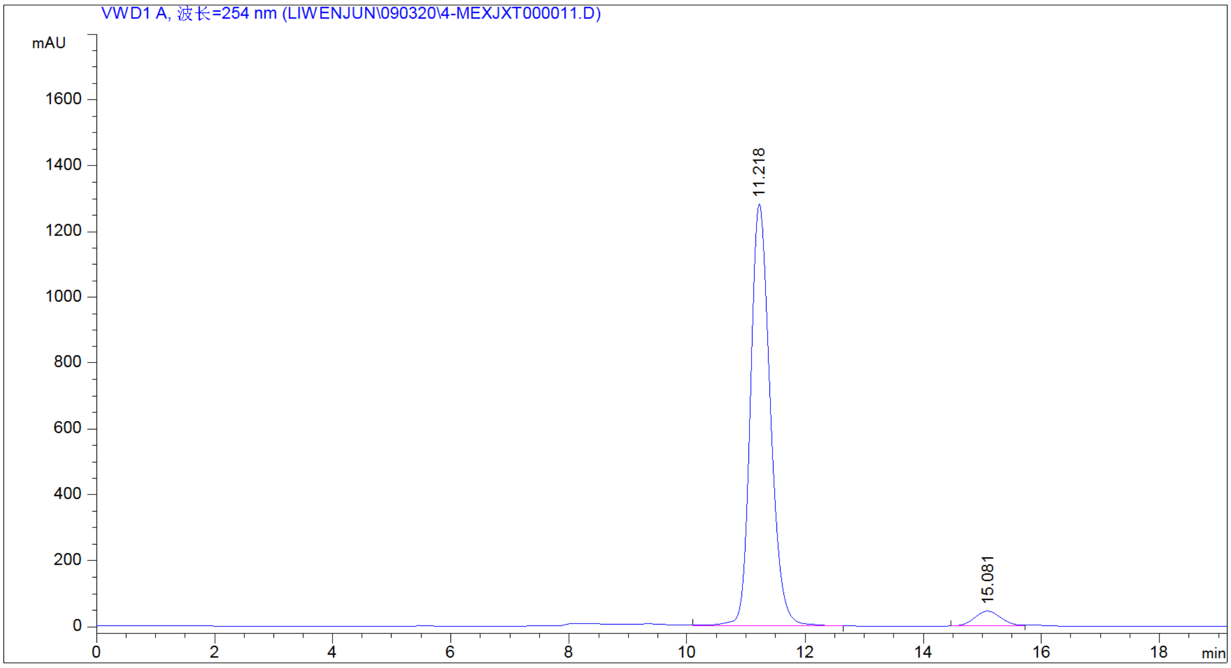


#	Time	Area	Height	Width	Symmetry	Area/%
1	13.387	10164.2	343.5	0.4614	0	97.453
2	17.496	265.7	5.8	0.7083	0.906	2.547

4-(2-nitro-1-p-tolylethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4la)

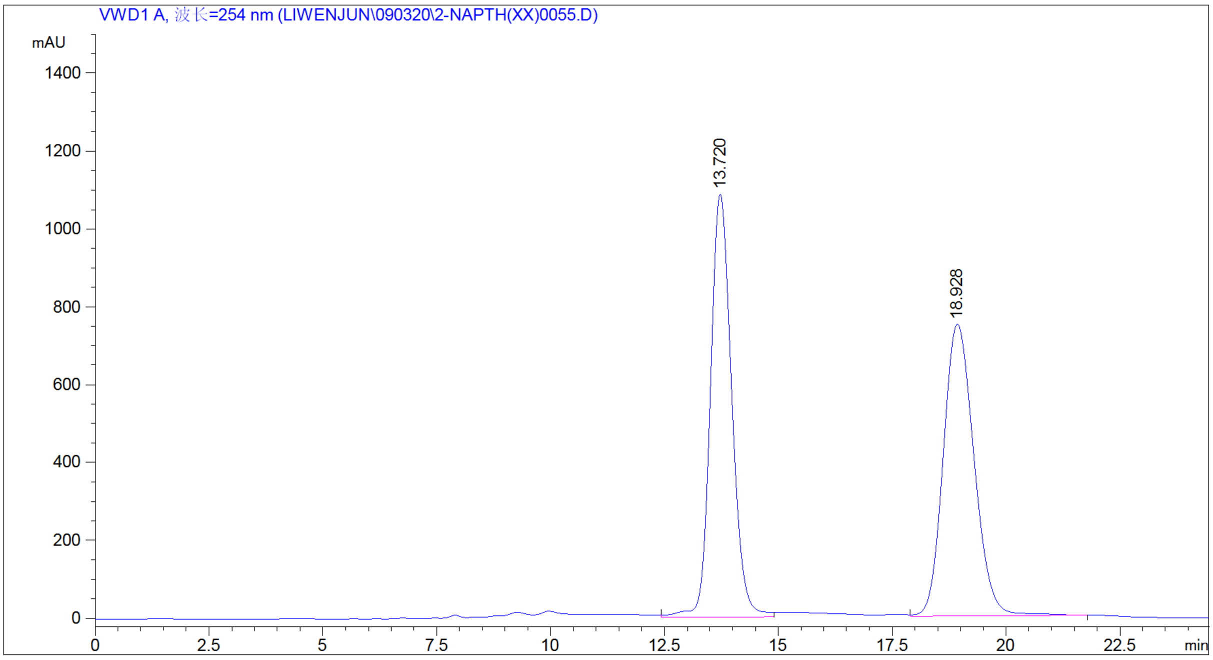


#	Time	Area	Height	Width	Symmetry	Area/%
1	11.12	3998.7	117.8	0.5656	1.163	48.763
2	14.785	4201.6	113.7	0.6161	1.045	51.237

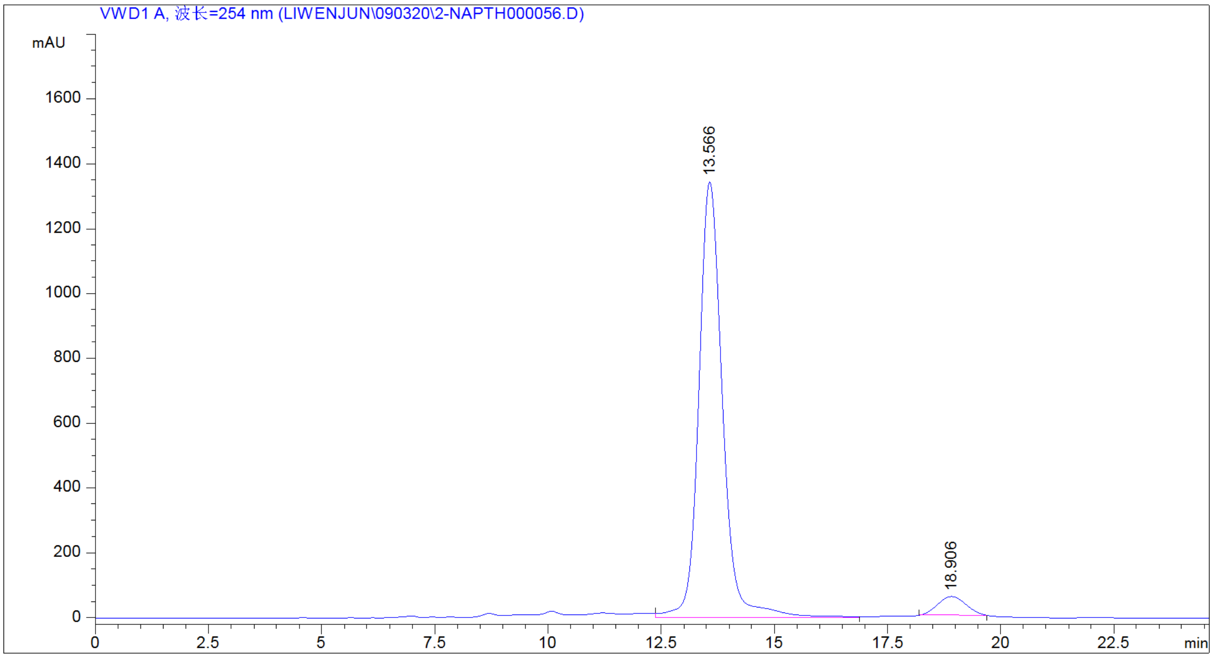


#	Time	Area	Height	Width	Symmetry	Area/%
1	11.218	29982.3	1281.2	0.3604	0.776	95.557
2	15.081	1394.1	45	0.5164	0.945	4.443

4-(1-(naphthalen-1-yl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4ma)

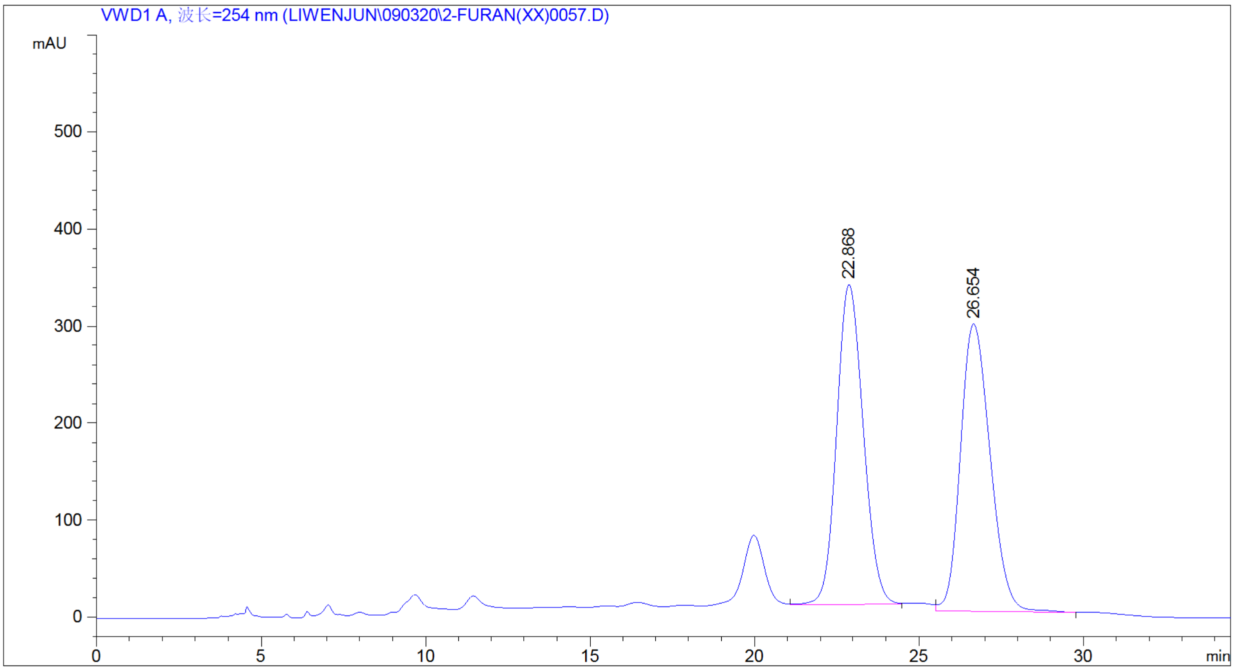


#	Time	Area	Height	Width	Symmetry	Area/%
1	13.72	35442.2	1086.2	0.503	0.827	50.154
2	18.928	35224.5	749	0.7365	0.8	49.846

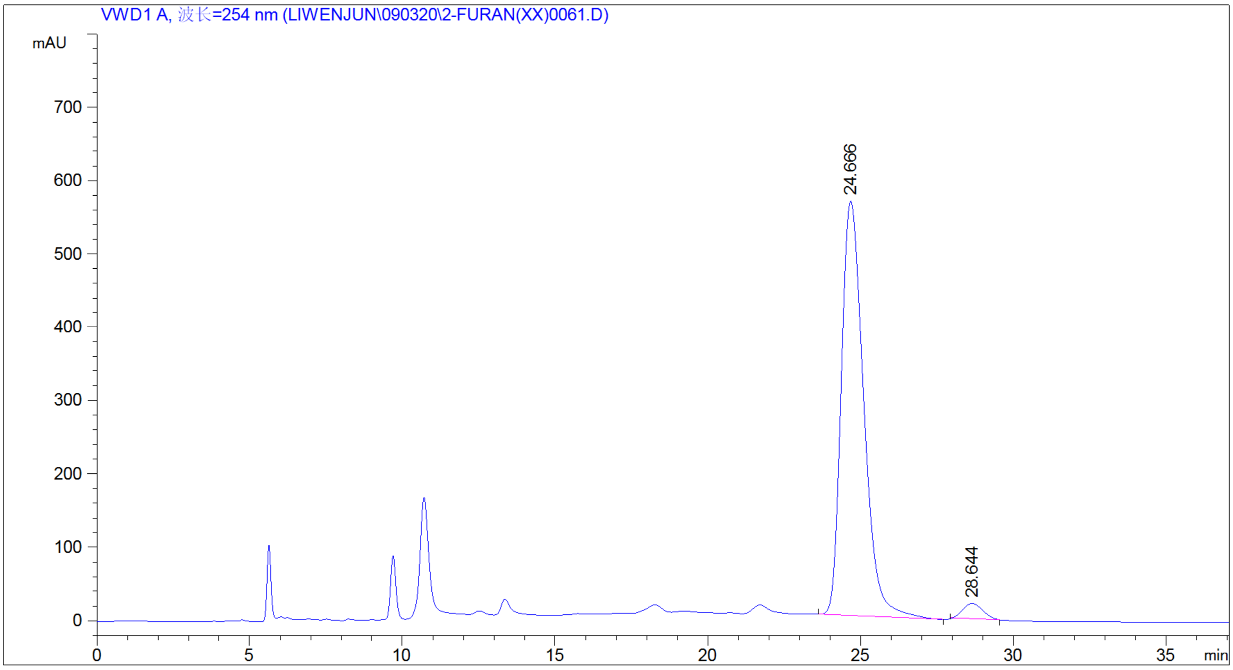


#	Time	Area	Height	Width	Symmetry	Area/%
1	13.566	49377.6	1345	0.5579	0.797	95.154
2	18.906	2514.9	57.9	0.7237	0.937	4.846

4-(1-(furan-2-yl)-2-nitroethyl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4na)

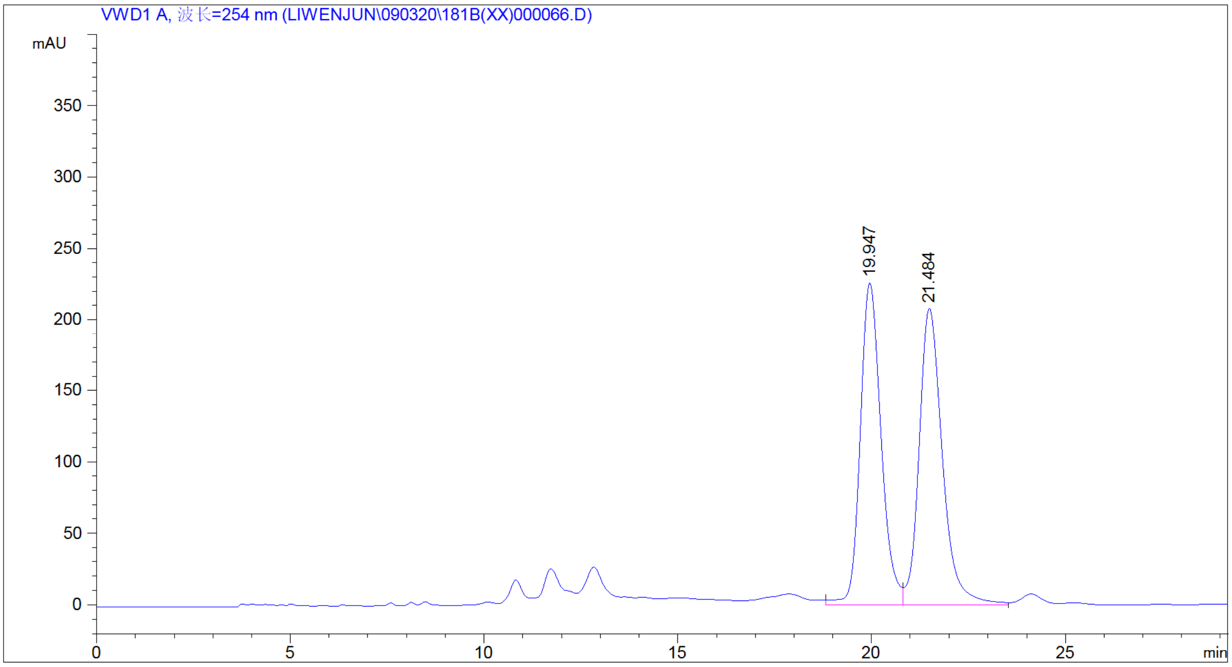


#	Time	Area	Height	Width	Symmetry	Area/%
1	22.868	18528.9	329.8	0.8007	0	49.797
2	26.654	18679.9	296.9	0.9685	0.755	50.203

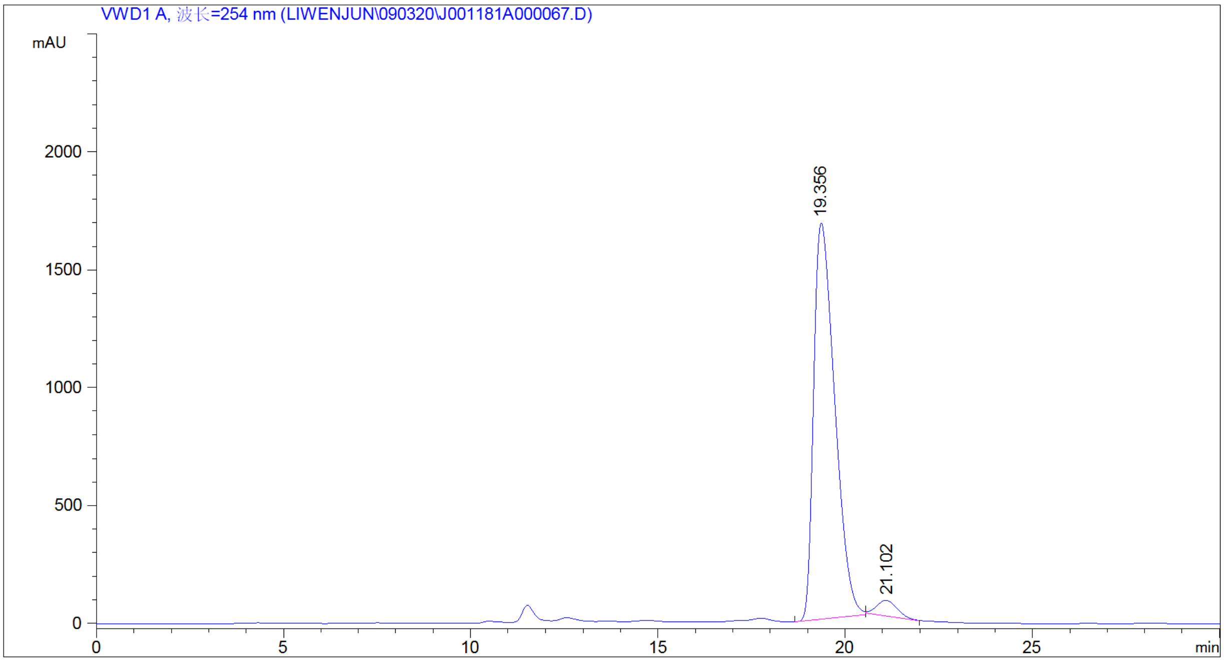


#	Time	Area	Height	Width	Symmetry	Area/%
1	24.666	28733.7	564.9	0.7914	0.674	96.716
2	28.644	975.7	21.1	0.7692	0.807	3.284

4-(1-nitropentan-2-yl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4oa)

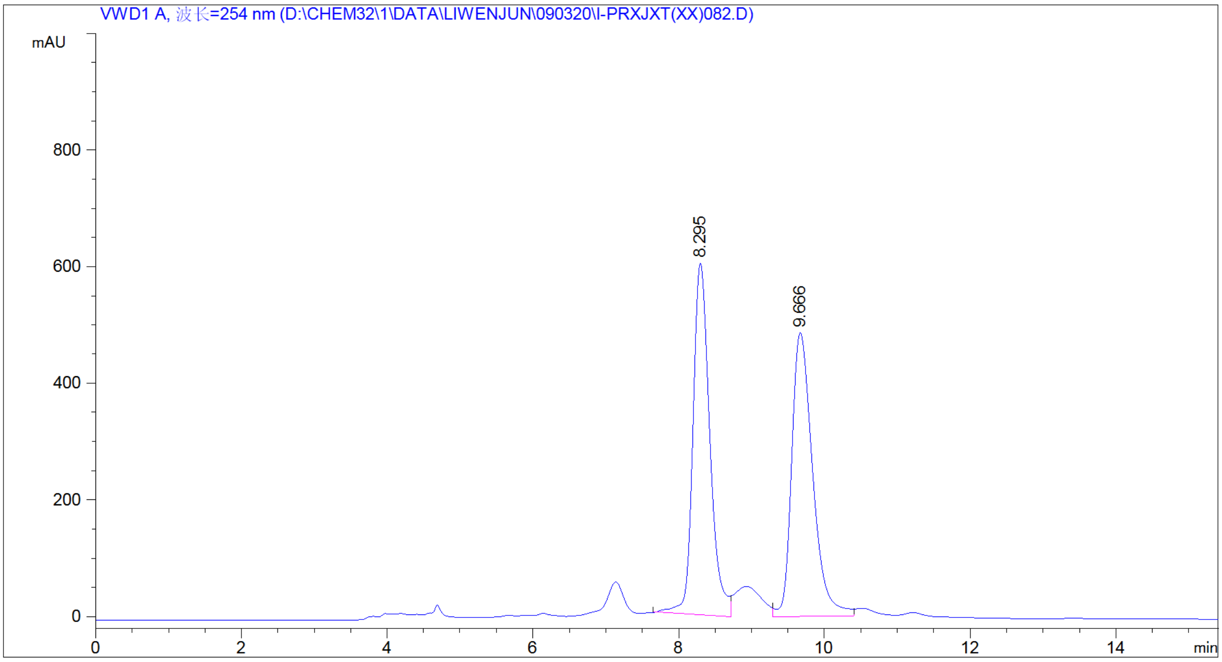


#	Time	Area	Height	Width	Symmetry	Area/%
1	19.947	8474.3	226	0.5744	0.811	49.305
2	21.484	8713.2	208.1	0.6369	0.723	50.695

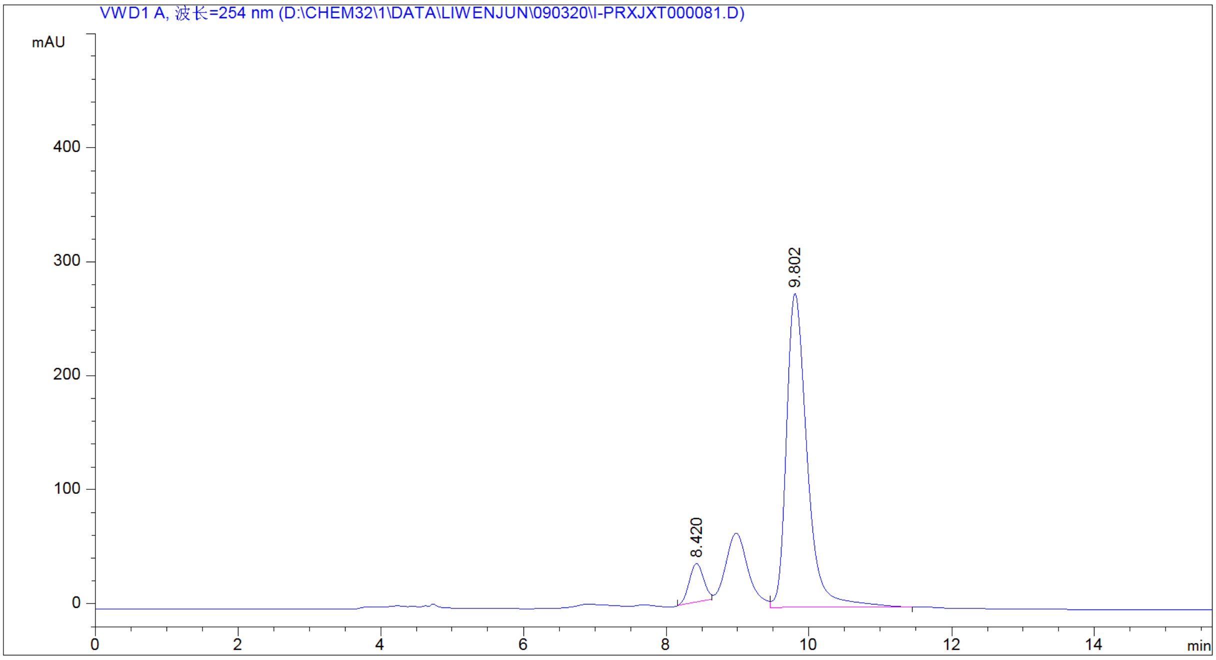


#	Time	Area	Height	Width	Symmetry	Area/%
1	19.356	65700.5	1681.3	0.6018	0	96.205
2	21.102	2591.7	66.8	0.6336	0	3.795

4-(3-methyl-1-nitrobutan-2-yl)-1,7-diphenylhepta-1,6-diene-3,5-dione (4pa)

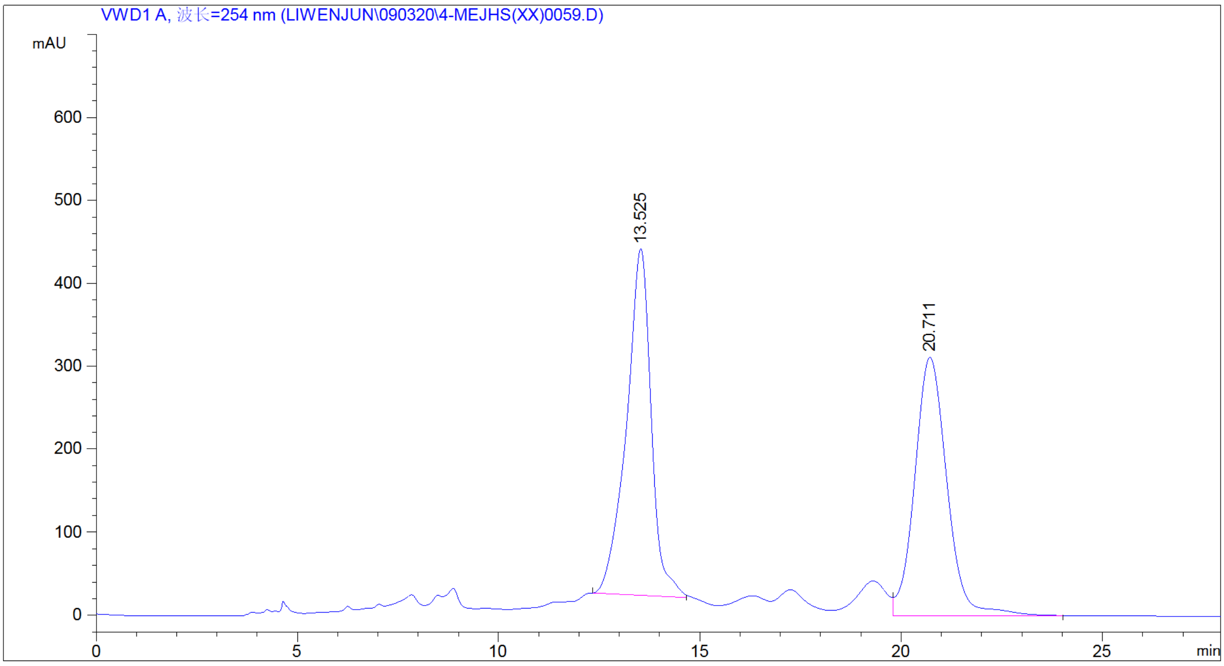


#	Time	Area	Height	Width	Symmetry	Area/%
1	8.295	9726.2	603.2	0.2687	0.767	49.900
2	9.666	9765.1	486.2	0.3347	0.668	50.100

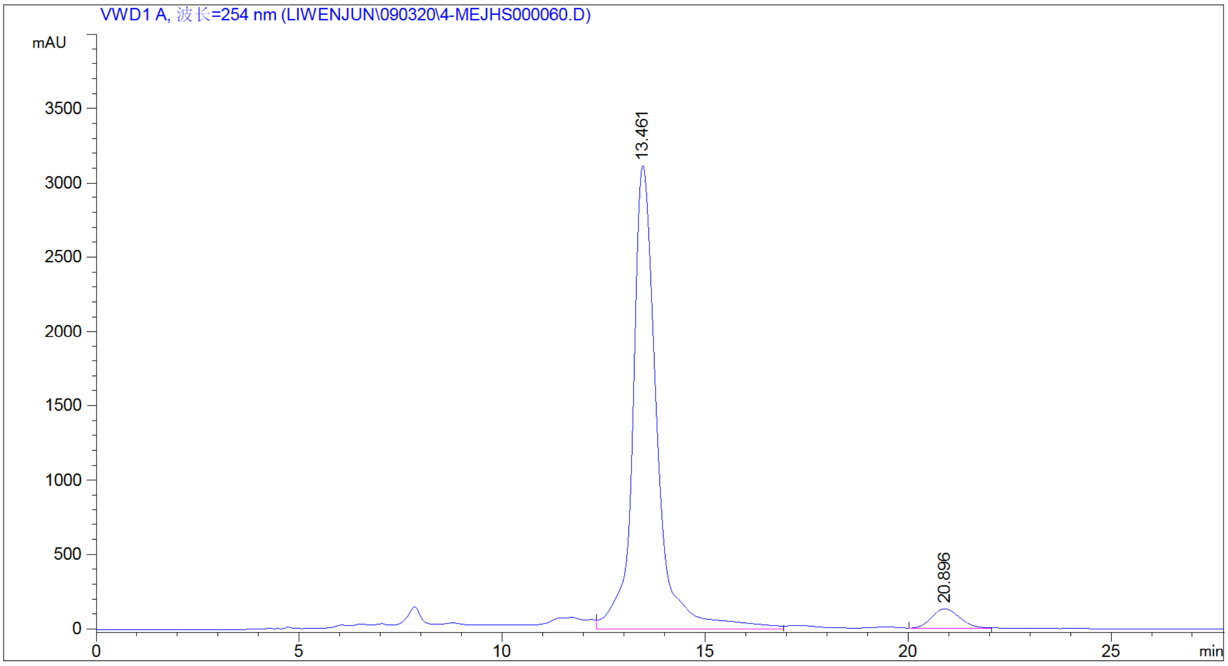


#	Time	Area	Height	Width	Symmetry	Area/%
1	8.42	478.3	34.1	0.2339	0.978	7.900
2	9.802	5575.2	275.8	0.3086	0.647	92.100

4-(2-nitro-1-phenylethyl)-1,7-dip-tolylhepta-1,6-diene-3,5-dione (4ab)

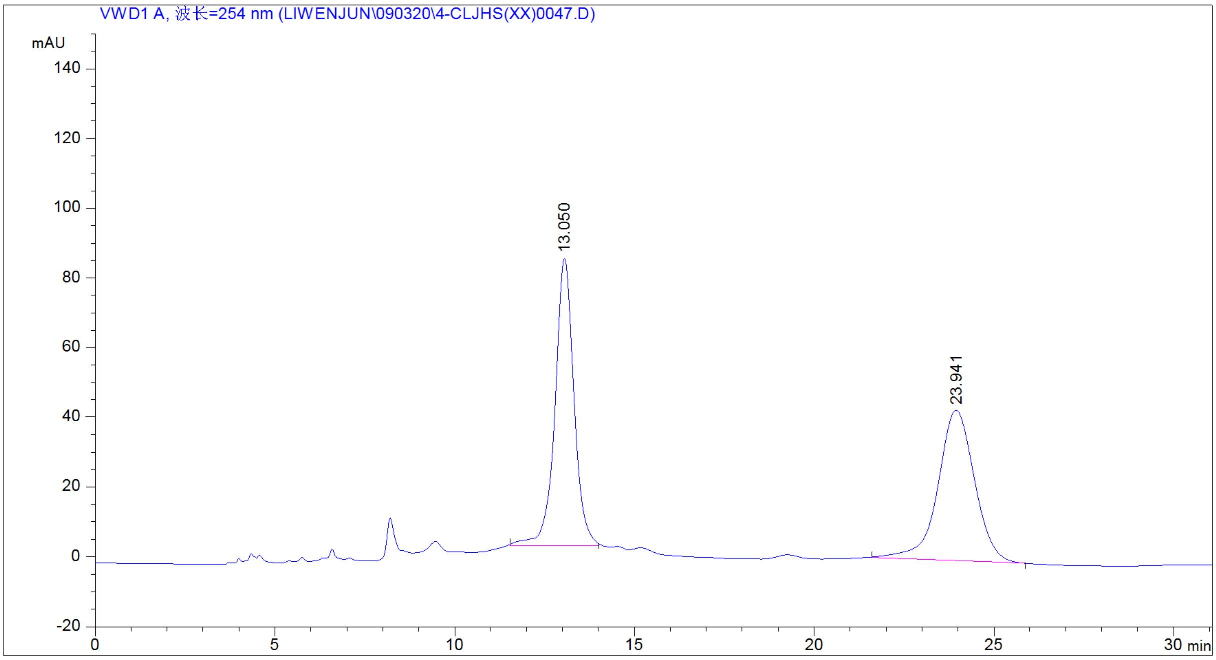


#	Time	Area	Height	Width	Symmetry	Area/%
1	13.525	17897.4	418.1	0.7134	1.297	50.803
2	20.711	17331.7	310.9	0.8484	0.842	49.197

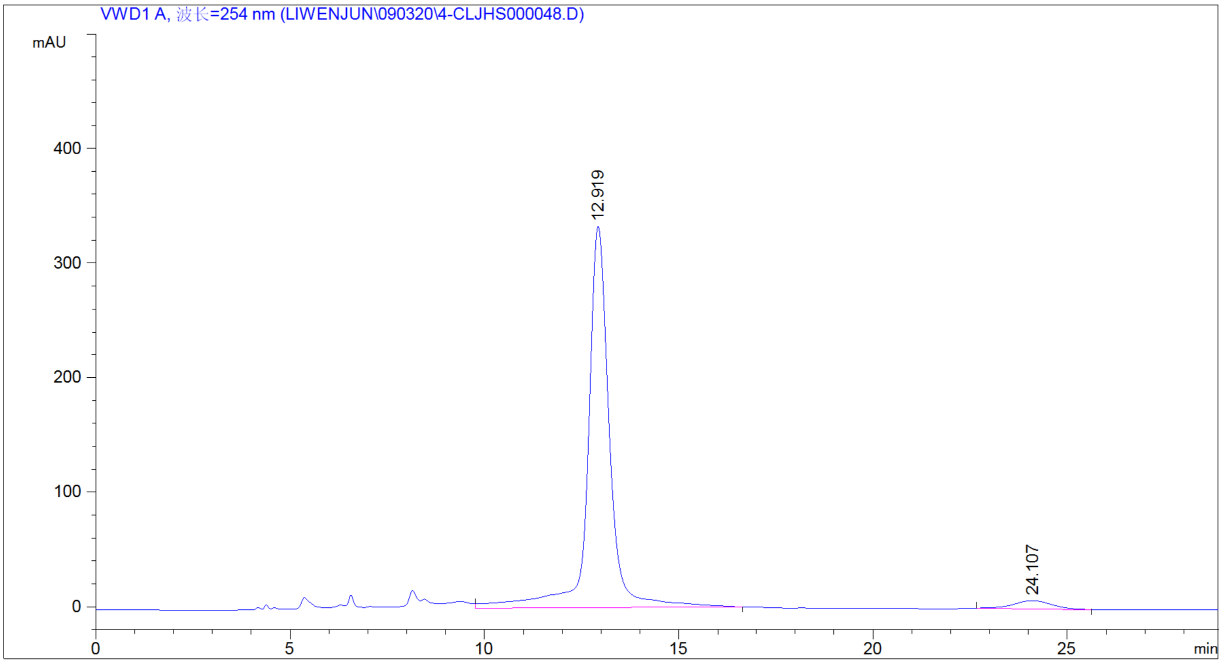


#	Time	Area	Height	Width	Symmetry	Area/%
1	13.461	129018.6	3118.4	0.621	0.68	94.945
2	20.896	6868.5	135.3	0.8463	0.837	5.055

1,7-bis(4-chlorophenyl)-4-(2-nitro-1-phenylethyl)hepta-1,6-diene-3,5-dione (4ac)

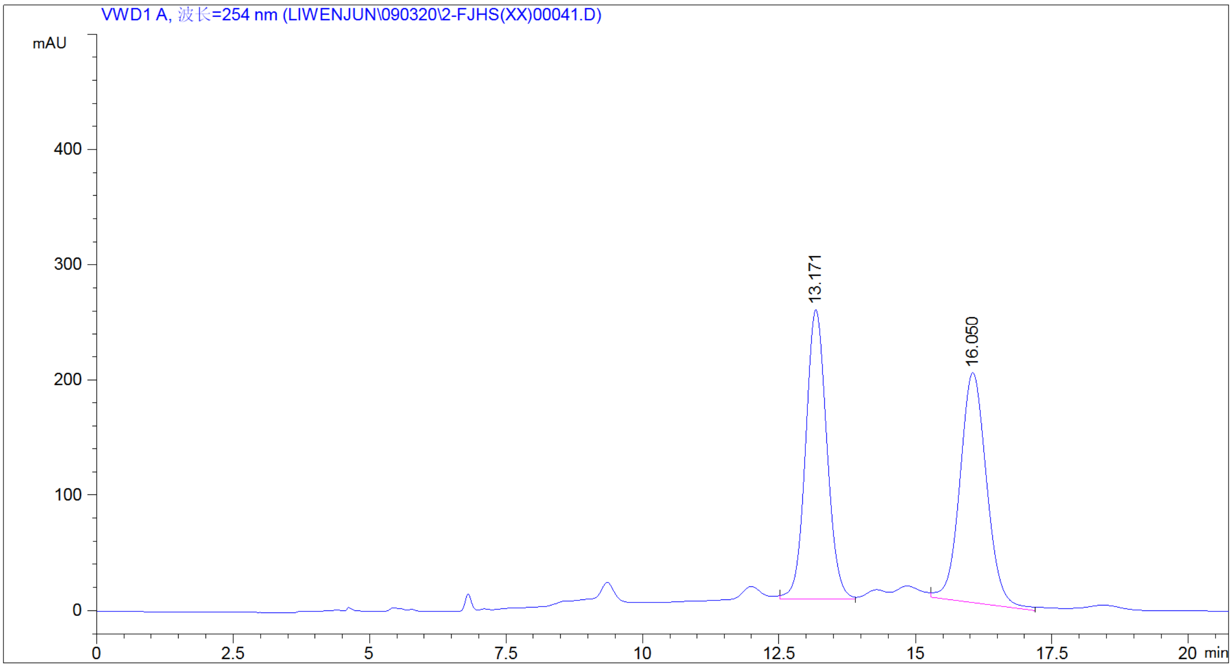


#	Time	Area	Height	Width	Symmetry	Area/%
1	13.05	3033.4	82.4	0.6132	0.998	49.723
2	23.941	3067.1	43.2	1.0703	0.981	50.277

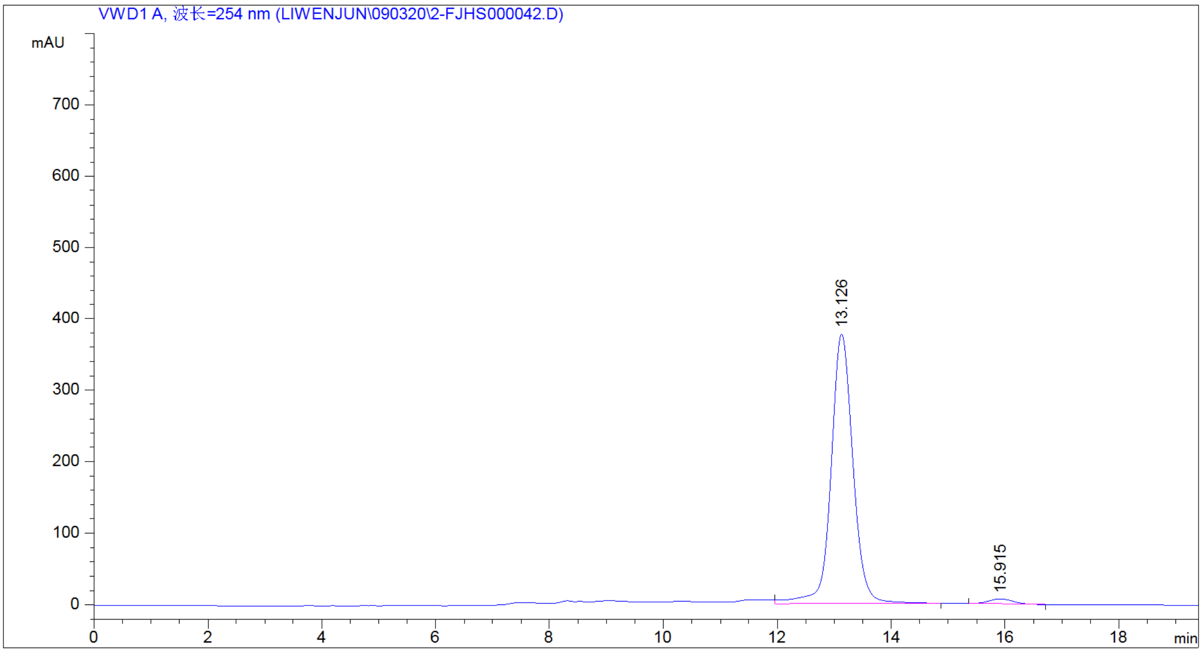


#	Time	Area	Height	Width	Symmetry	Area/%
1	12.919	13163	333.2	0.5832	0.943	96.065
2	24.107	539.1	7.5	1.2058	0.965	3.935

1,7-bis(2-fluorophenyl)-4-(2-nitro-1-phenylethyl)hepta-1,6-diene-3,5-dione (4ad)

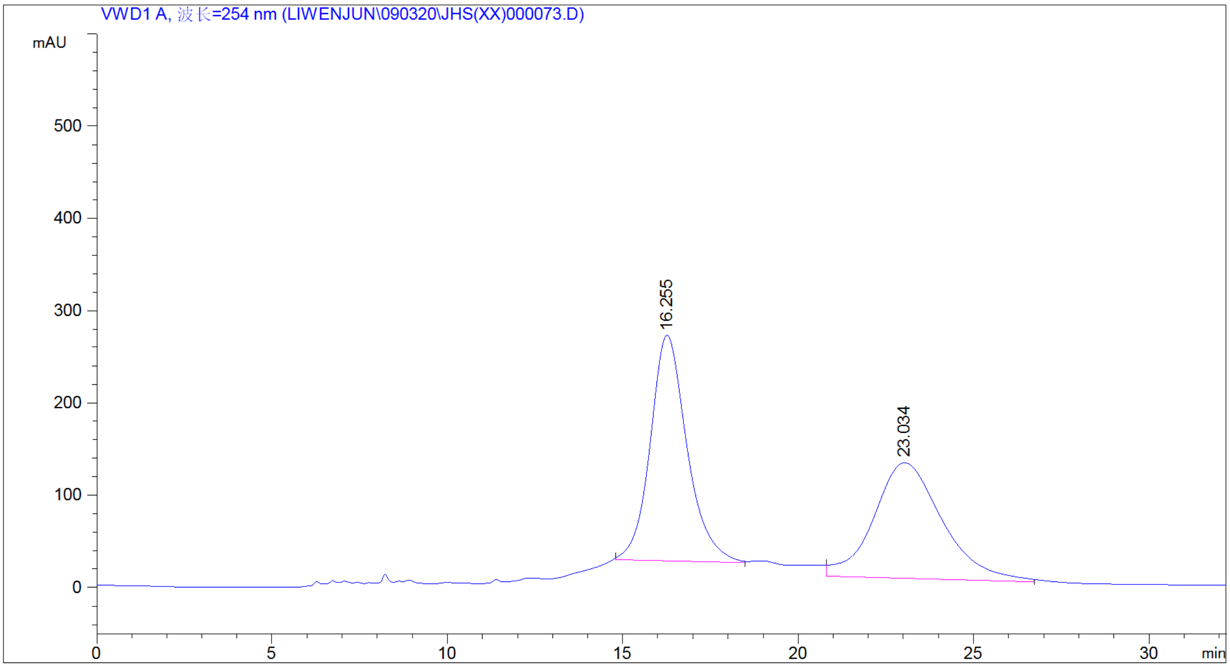


#	Time	Area	Height	Width	Symmetry	Area/%
1	13.171	6800.6	251.6	0.4504	0.91	50.085
2	16.05	6777.6	199.5	0.5466	0	49.915

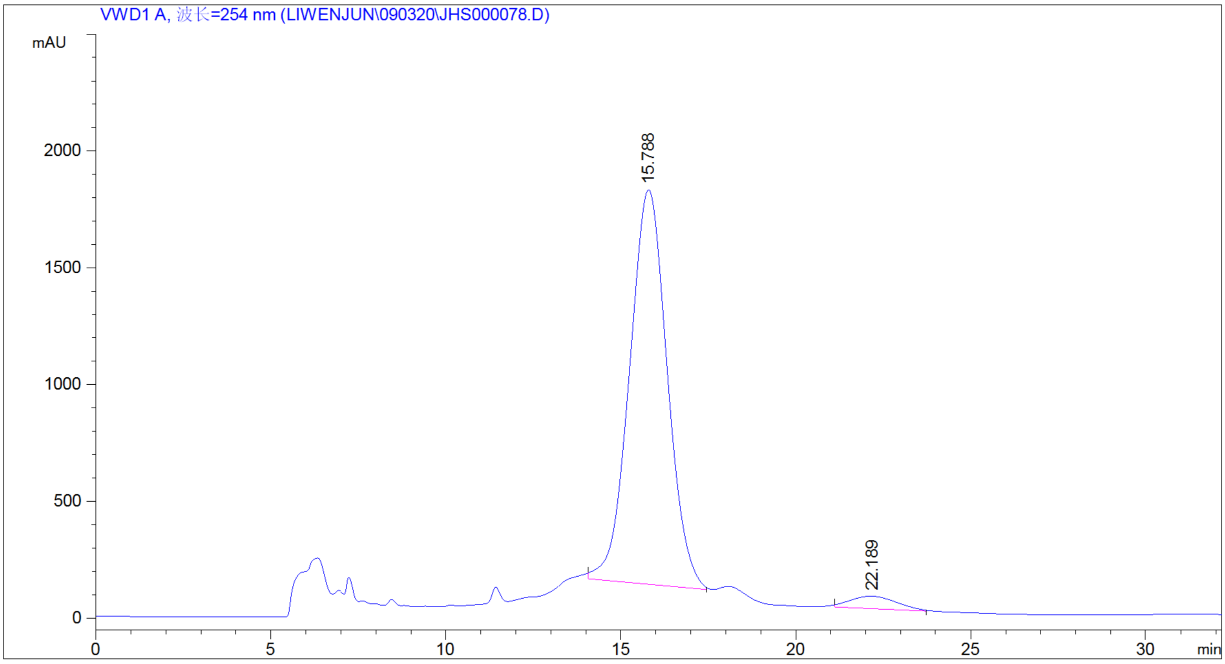


#	Time	Area	Height	Width	Symmetry	Area/%
1	13.126	10170.7	377	0.4123	0.928	98.043
2	15.915	203	7	0.4581	0.908	1.957

1,7-bis(4-hydroxy-3-methoxyphenyl)-4-(2-nitro-1-phenylethyl)hepta-1,6-diene-3,5-dione (4ae)

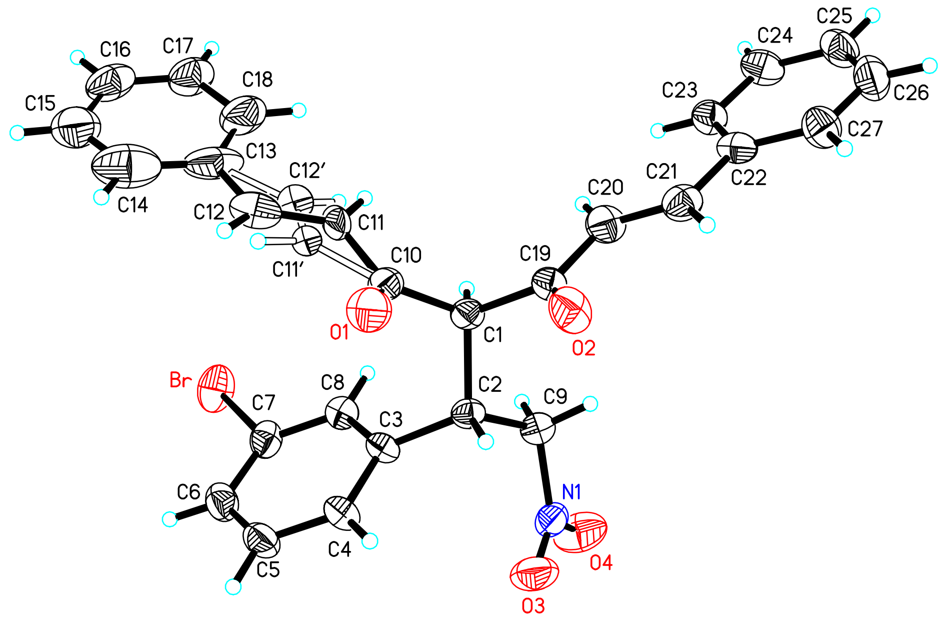


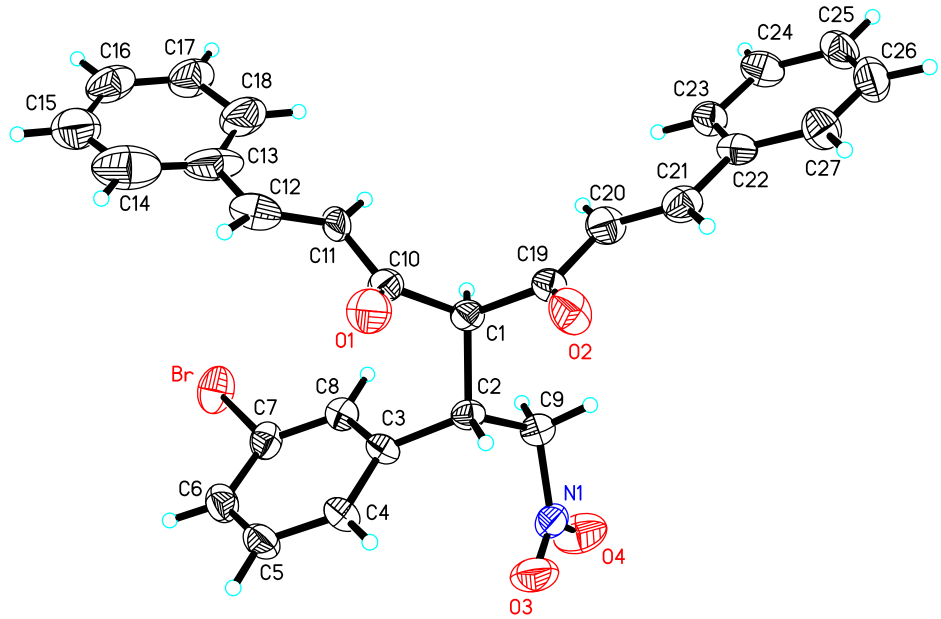
#	Time	Area	Height	Width	Symmetry	Area/%
1	16.255	17847.2	244.5	1.1292	0	51.053
2	23.034	17110.9	125.3	2.224	0	48.947

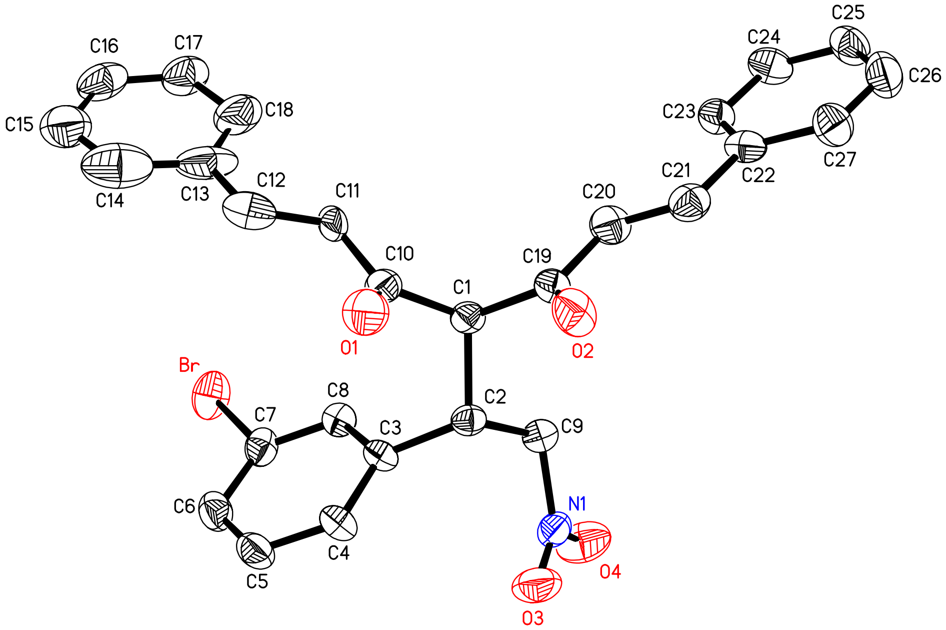


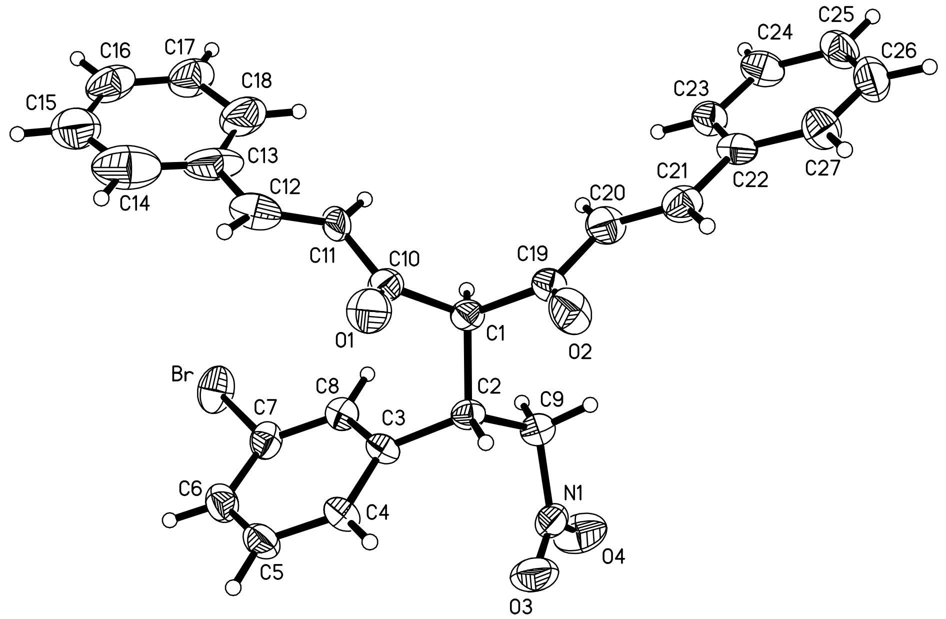
#	Time	Area	Height	Width	Symmetry	Area/%
1	15.788	126710.9	1690.6	1.1487	0	96.179
2	22.189	5033.3	54.2	1.5484	0.761	3.821

F: X-Ray Analysis Data and Absolute Configuration






C16
C17
C25
C24
C26
C15
C18
C23
C21
C22
C27
C14
C13
C12
C11
C20
C10
C19
C1
O1
O2
Br
C8
C2
C7
C3
C9
C6
N1
C4
O4
C5
O3


C16
C17
C18
C15
C24
C25
C26
C23
C13
C12
C14
C21
C22
C27
C20
C11
C10
C19
O1
C1
O2
Br
C8
C2
C9
C7
C3
C6
N1
C4
O4
C5
O3

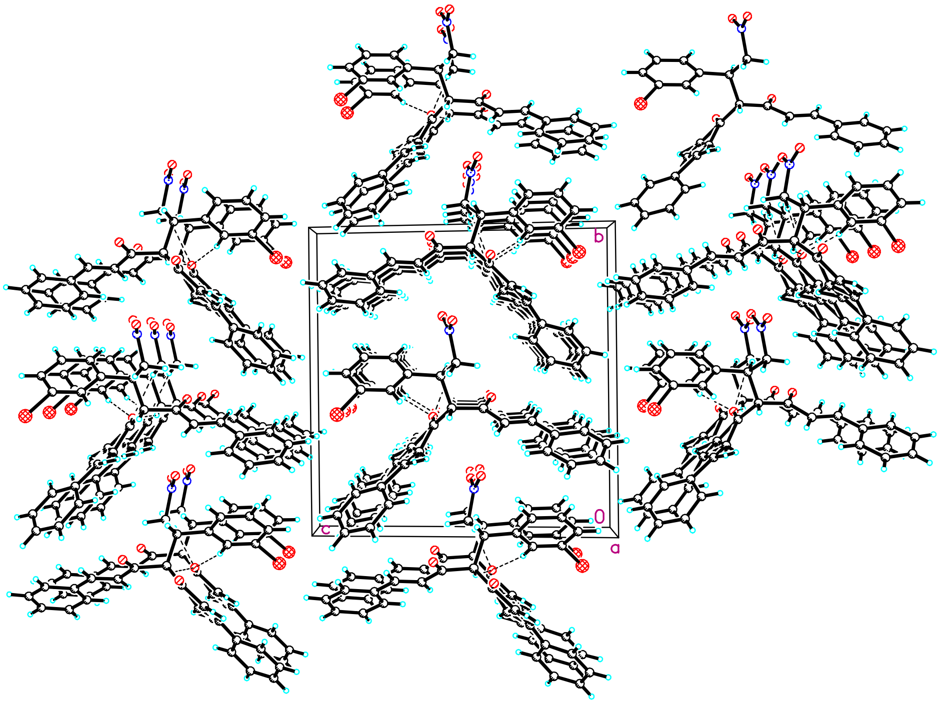


Table 1. Crystal data and structure refinement for 794851.

Identification code	794851
Empirical formula	C27 H22 Br N O4
Formula weight	504.37
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 5.4962(10) A alpha = 90 deg. b = 14.702(3) A beta = 100.037(3) deg. c = 14.657(3) A gamma = 90 deg.
Volume	1166.3(4) A^3
Z, Calculated density	2, 1.436 Mg/m^3

Absorption coefficient	1.796 mm^-1
F(000)	516
Crystal size	0.412 x 0.309 x 0.125 mm
Theta range for data collection	1.98 to 25.99 deg.
Limiting indices	-6<=h<=5, -16<=k<=18, -17<=l<=18
Reflections collected / unique	6407 / 4047 [R(int) = 0.0766]
Completeness to theta = 25.99	99.6 %
Absorption correction	Empirical
Max. and min. transmission	1.0000 and 0.3343
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4047 / 3 / 316
Goodness-of-fit on F^2	0.938
Final R indices [I>2sigma(I)]	R1 = 0.0590, wR2 = 0.1375
R indices (all data)	R1 = 0.0803, wR2 = 0.1467
Absolute structure parameter	0.041(14)
Largest diff. peak and hole	0.487 and -0.405 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 794851.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Br(1)	-1067(1)	3185(1)	6144(1)	78(1)
N(1)	1773(11)	5704(4)	9630(3)	54(1)
O(1)	8169(8)	2999(4)	9067(3)	71(1)
O(2)	7742(9)	3605(3)	10951(3)	69(1)
O(3)	-178(11)	6009(4)	9734(4)	93(2)
O(4)	3406(11)	6163(3)	9419(4)	80(2)
C(1)	4245(10)	4301(4)	9348(4)	40(1)
C(2)	2208(11)	4712(4)	9822(4)	50(1)
C(3)	4534(9)	3312(4)	9682(3)	43(1)
C(4)	6098(12)	2761(4)	9107(4)	53(2)
C(5)	4330(30)	1945(10)	8677(9)	44(3)
C(6)	5100(30)	1570(9)	7919(10)	57(3)
C(6')	3470(50)	1617(13)	8276(14)	68(7)
C(5')	5360(40)	2081(12)	8444(14)	40(4)
C(7)	5743(10)	3269(5)	10696(3)	52(1)
C(8)	4160(11)	2855(4)	11326(4)	59(2)
C(9)	4710(12)	2885(4)	12207(4)	60(2)
C(10)	3709(11)	4380(4)	8293(4)	42(1)
C(11)	1763(10)	3895(4)	7779(4)	46(1)
C(12)	1449(10)	3933(4)	6828(4)	52(1)
C(13)	2947(12)	4417(5)	6360(4)	59(2)
C(14)	4858(12)	4907(5)	6889(4)	62(2)
C(15)	5221(11)	4891(5)	7836(5)	49(2)
C(16)	3250(20)	877(6)	7459(8)	111(4)
C(17)	1310(20)	394(6)	7701(6)	103(3)
C(18)	139(18)	-279(6)	7135(7)	89(3)
C(19)	832(18)	-450(6)	6310(7)	91(3)
C(20)	2680(20)	23(7)	6043(7)	102(3)
C(21)	3930(20)	670(8)	6622(10)	128(4)
C(22)	3384(11)	2498(4)	12887(5)	55(2)
C(23)	4299(13)	2579(5)	13821(5)	71(2)
C(24)	3113(15)	2218(6)	14468(5)	79(2)
C(25)	964(14)	1746(5)	14215(6)	72(2)
C(26)	-20(14)	1645(5)	13285(5)	66(2)
C(27)	1138(12)	2020(5)	12626(5)	60(2)

Table 3. Bond lengths [A] and angles [deg] for 794851.

Br(1)-C(12)	1.908(6)
N(1)-O(3)	1.197(7)
N(1)-O(4)	1.205(7)
N(1)-C(2)	1.496(8)
O(1)-C(4)	1.202(7)
O(2)-C(7)	1.203(7)
C(1)-C(10)	1.527(7)
C(1)-C(3)	1.533(8)
C(1)-C(2)	1.540(8)
C(1)-H(1)	0.9800
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(7)	1.519(7)
C(3)-C(4)	1.536(8)
C(3)-H(3)	0.9800
C(4)-C(5')	1.404(19)
C(4)-C(5)	1.603(18)
C(5)-C(6)	1.37(2)
C(5)-H(5)	0.9300
C(6)-C(16)	1.510(18)
C(6)-H(6)	0.9300
C(6')-C(5')	1.23(3)
C(6')-C(16)	1.607(17)
C(6')-H(6')	0.9300
C(5')-H(5')	0.9300
C(7)-C(8)	1.504(8)
C(8)-C(9)	1.275(8)
C(8)-H(8)	0.9300
C(9)-C(22)	1.449(8)
C(9)-H(9)	0.9300
C(10)-C(15)	1.378(8)
C(10)-C(11)	1.392(8)
C(11)-C(12)	1.377(8)
C(11)-H(11)	0.9300
C(12)-C(13)	1.360(9)
C(13)-C(14)	1.393(9)
C(13)-H(13)	0.9300
C(14)-C(15)	1.367(9)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
C(16)-C(21)	1.376(17)

C(16)-C(17)	1.380(16)
C(17)-C(18)	1.376(12)
C(17)-H(17)	0.9300
C(18)-C(19)	1.353(12)
C(18)-H(18)	0.9300
C(19)-C(20)	1.343(13)
C(19)-H(19)	0.9300
C(20)-C(21)	1.378(15)
C(20)-H(20)	0.9300
C(21)-H(21)	0.9300
C(22)-C(23)	1.379(10)
C(22)-C(27)	1.415(10)
C(23)-C(24)	1.350(10)
C(23)-H(23)	0.9300
C(24)-C(25)	1.364(11)
C(24)-H(24)	0.9300
C(25)-C(26)	1.384(11)
C(25)-H(25)	0.9300
C(26)-C(27)	1.362(10)
C(26)-H(26)	0.9300
C(27)-H(27)	0.9300

O(3)-N(1)-O(4)	123.1(6)
O(3)-N(1)-C(2)	117.3(6)
O(4)-N(1)-C(2)	119.5(5)
C(10)-C(1)-C(3)	112.7(4)
C(10)-C(1)-C(2)	113.6(5)
C(3)-C(1)-C(2)	105.7(4)
C(10)-C(1)-H(1)	108.2
C(3)-C(1)-H(1)	108.2
C(2)-C(1)-H(1)	108.2
N(1)-C(2)-C(1)	113.7(5)
N(1)-C(2)-H(2A)	108.8
C(1)-C(2)-H(2A)	108.8
N(1)-C(2)-H(2B)	108.8
C(1)-C(2)-H(2B)	108.8
H(2A)-C(2)-H(2B)	107.7
C(7)-C(3)-C(1)	110.8(5)
C(7)-C(3)-C(4)	108.9(4)
C(1)-C(3)-C(4)	111.2(4)
C(7)-C(3)-H(3)	108.6
C(1)-C(3)-H(3)	108.6
C(4)-C(3)-H(3)	108.6
O(1)-C(4)-C(5')	109.5(11)

O(1)-C(4)-C(3)	119.9(6)
C(5')-C(4)-C(3)	129.4(11)
O(1)-C(4)-C(5)	135.4(7)
C(5')-C(4)-C(5)	27.4(8)
C(3)-C(4)-C(5)	104.6(7)
C(6)-C(5)-C(4)	111.7(14)
C(6)-C(5)-H(5)	124.1
C(4)-C(5)-H(5)	124.1
C(5)-C(6)-C(16)	110.9(13)
C(5)-C(6)-H(6)	124.5
C(16)-C(6)-H(6)	124.5
C(5')-C(6')-C(16)	118(2)
C(5')-C(6')-H(6')	120.8
C(16)-C(6')-H(6')	120.8
C(6')-C(5')-C(4)	132(2)
C(6')-C(5')-H(5')	114.2
C(4)-C(5')-H(5')	114.2
O(2)-C(7)-C(8)	124.7(5)
O(2)-C(7)-C(3)	120.5(5)
C(8)-C(7)-C(3)	114.6(5)
C(9)-C(8)-C(7)	123.2(6)
C(9)-C(8)-H(8)	118.4
C(7)-C(8)-H(8)	118.4
C(8)-C(9)-C(22)	128.6(7)
C(8)-C(9)-H(9)	115.7
C(22)-C(9)-H(9)	115.7
C(15)-C(10)-C(11)	119.1(5)
C(15)-C(10)-C(1)	120.5(5)
C(11)-C(10)-C(1)	120.2(5)
C(12)-C(11)-C(10)	118.5(5)
C(12)-C(11)-H(11)	120.8
C(10)-C(11)-H(11)	120.8
C(13)-C(12)-C(11)	123.5(6)
C(13)-C(12)-Br(1)	118.9(4)
C(11)-C(12)-Br(1)	117.4(5)
C(12)-C(13)-C(14)	117.0(5)
C(12)-C(13)-H(13)	121.5
C(14)-C(13)-H(13)	121.5
C(15)-C(14)-C(13)	121.2(6)
C(15)-C(14)-H(14)	119.4
C(13)-C(14)-H(14)	119.4
C(14)-C(15)-C(10)	120.7(6)
C(14)-C(15)-H(15)	119.7
C(10)-C(15)-H(15)	119.6

C(21)-C(16)-C(17)	117.2(9)
C(21)-C(16)-C(6)	106.4(12)
C(17)-C(16)-C(6)	136.1(12)
C(21)-C(16)-C(6')	144.7(14)
C(17)-C(16)-C(6')	96.8(13)
C(6)-C(16)-C(6')	41.6(10)
C(18)-C(17)-C(16)	121.1(10)
C(18)-C(17)-H(17)	119.5
C(16)-C(17)-H(17)	119.4
C(19)-C(18)-C(17)	119.8(10)
C(19)-C(18)-H(18)	120.1
C(17)-C(18)-H(18)	120.1
C(20)-C(19)-C(18)	120.6(9)
C(20)-C(19)-H(19)	119.7
C(18)-C(19)-H(19)	119.7
C(19)-C(20)-C(21)	120.0(11)
C(19)-C(20)-H(20)	120.0
C(21)-C(20)-H(20)	120.0
C(16)-C(21)-C(20)	121.2(11)
C(16)-C(21)-H(21)	119.4
C(20)-C(21)-H(21)	119.4
C(23)-C(22)-C(27)	117.5(6)
C(23)-C(22)-C(9)	120.6(6)
C(27)-C(22)-C(9)	122.0(6)
C(24)-C(23)-C(22)	121.8(7)
C(24)-C(23)-H(23)	119.1
C(22)-C(23)-H(23)	119.1
C(23)-C(24)-C(25)	120.7(7)
C(23)-C(24)-H(24)	119.6
C(25)-C(24)-H(24)	119.6
C(24)-C(25)-C(26)	119.5(7)
C(24)-C(25)-H(25)	120.2
C(26)-C(25)-H(25)	120.2
C(27)-C(26)-C(25)	120.3(7)
C(27)-C(26)-H(26)	119.8
C(25)-C(26)-H(26)	119.8
C(26)-C(27)-C(22)	120.2(7)
C(26)-C(27)-H(27)	119.9
C(22)-C(27)-H(27)	119.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 794851.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Br(1)	74(1)	104(1)	53(1)	-22(1)	1(1)	-8(1)
N(1)	74(4)	52(3)	37(3)	-6(2)	9(3)	2(3)
O(1)	67(3)	83(4)	70(3)	3(3)	34(2)	5(3)
O(2)	68(3)	88(4)	44(2)	5(2)	-7(2)	-17(2)
O(3)	81(4)	72(4)	129(5)	3(3)	29(4)	26(3)
O(4)	108(4)	47(3)	94(4)	1(3)	42(3)	-6(3)
C(1)	45(3)	42(3)	33(3)	3(2)	7(2)	-4(2)
C(2)	61(4)	46(3)	44(3)	1(3)	15(3)	4(3)
C(3)	43(3)	45(3)	40(2)	5(3)	6(2)	-9(3)
C(4)	71(4)	47(3)	38(3)	6(3)	2(3)	5(3)
C(5)	50(9)	50(8)	42(9)	4(6)	31(6)	12(6)
C(6)	62(8)	55(8)	62(9)	18(7)	32(7)	13(6)
C(6')	81(16)	60(13)	50(12)	-3(9)	-24(12)	-17(11)

C(5')	55(12)	39(10)	29(9)	-15(8)	16(8)	15(8)
C(7)	63(3)	54(3)	40(3)	-1(3)	13(2)	11(4)
C(8)	64(4)	56(4)	54(4)	1(3)	3(3)	8(3)
C(9)	66(4)	63(5)	53(4)	4(3)	17(3)	9(3)
C(10)	49(4)	47(3)	29(3)	5(3)	6(3)	5(3)
C(11)	45(3)	53(4)	42(3)	4(3)	12(3)	0(3)
C(12)	50(3)	64(4)	37(3)	-9(3)	0(3)	6(3)
C(13)	69(4)	78(5)	29(3)	5(3)	8(3)	8(4)
C(14)	71(4)	72(5)	50(4)	12(3)	25(3)	-3(3)
C(15)	48(4)	59(4)	42(4)	2(3)	10(3)	-6(3)
C(16)	162(10)	42(4)	96(7)	12(5)	-72(7)	-13(5)
C(17)	169(9)	57(5)	73(5)	-14(4)	-9(6)	-5(6)
C(18)	110(7)	54(5)	94(7)	-10(5)	-8(5)	-4(4)
C(19)	111(7)	61(5)	83(6)	0(5)	-32(5)	-8(5)
C(20)	128(8)	83(7)	90(7)	4(5)	6(6)	7(6)
C(21)	122(8)	90(8)	145(10)	34(8)	-49(8)	-22(6)
C(22)	55(4)	50(4)	67(4)	17(3)	31(3)	7(3)
C(23)	64(4)	87(5)	63(5)	1(4)	12(4)	0(4)
C(24)	89(6)	101(6)	50(4)	3(4)	21(4)	11(5)
C(25)	71(5)	85(5)	68(5)	14(4)	39(4)	9(4)
C(26)	57(4)	72(5)	71(5)	13(4)	18(4)	0(4)
C(27)	69(4)	66(4)	47(4)	5(3)	15(3)	7(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 794851.

	x	y	z	U(eq)
H(1)	5793	4623	9577	48
H(2A)	678	4385	9614	60
H(2B)	2656	4624	10486	60
H(3)	2890	3035	9615	51
H(5)	2956	1749	8913	53
H(6)	6554	1722	7715	68
H(6')	2204	1693	8613	81
H(5')	6510	1959	8063	48
H(8)	2708	2562	11060	71
H(9)	6153	3197	12446	72
H(11)	700	3554	8072	55
H(13)	2707	4420	5716	71
H(14)	5907	5252	6593	75

H(15)	6500	5228	8174	59
H(17)	781	525	8255	124
H(18)	-1124	-615	7319	107
H(19)	22	-898	5925	109
H(20)	3108	-87	5467	122
H(21)	5262	972	6445	153
H(23)	5773	2891	14010	85
H(24)	3767	2292	15093	95
H(25)	166	1494	14665	86
H(26)	-1478	1320	13109	79
H(27)	449	1961	12003	72

Table 6. Torsion angles [deg] for 794851.

O(3)-N(1)-C(2)-C(1)	158.7(6)
O(4)-N(1)-C(2)-C(1)	-24.2(7)
C(10)-C(1)-C(2)-N(1)	-59.9(7)
C(3)-C(1)-C(2)-N(1)	176.0(4)
C(10)-C(1)-C(3)-C(7)	164.3(5)
C(2)-C(1)-C(3)-C(7)	-71.1(5)
C(10)-C(1)-C(3)-C(4)	43.1(6)
C(2)-C(1)-C(3)-C(4)	167.7(4)
C(7)-C(3)-C(4)-O(1)	-64.2(7)
C(1)-C(3)-C(4)-O(1)	58.2(7)
C(7)-C(3)-C(4)-C(5')	129.6(12)
C(1)-C(3)-C(4)-C(5')	-108.1(12)
C(7)-C(3)-C(4)-C(5)	116.1(7)
C(1)-C(3)-C(4)-C(5)	-121.5(6)
O(1)-C(4)-C(5)-C(6)	-19.8(15)
C(5')-C(4)-C(5)-C(6)	2.8(17)
C(3)-C(4)-C(5)-C(6)	159.9(9)
C(4)-C(5)-C(6)-C(16)	-173.5(8)

C(16)-C(6')-C(5')-C(4)	-179.2(14)
O(1)-C(4)-C(5')-C(6')	176(2)
C(3)-C(4)-C(5')-C(6')	-17(3)
C(5)-C(4)-C(5')-C(6')	12.3(18)
C(1)-C(3)-C(7)-O(2)	-57.6(7)
C(4)-C(3)-C(7)-O(2)	65.0(8)
C(1)-C(3)-C(7)-C(8)	117.6(6)
C(4)-C(3)-C(7)-C(8)	-119.8(6)
O(2)-C(7)-C(8)-C(9)	5.8(11)
C(3)-C(7)-C(8)-C(9)	-169.2(6)
C(7)-C(8)-C(9)-C(22)	-178.4(6)
C(3)-C(1)-C(10)-C(15)	-123.5(6)
C(2)-C(1)-C(10)-C(15)	116.3(6)
C(3)-C(1)-C(10)-C(11)	53.0(7)
C(2)-C(1)-C(10)-C(11)	-67.2(7)
C(15)-C(10)-C(11)-C(12)	1.1(9)
C(1)-C(10)-C(11)-C(12)	-175.4(5)
C(10)-C(11)-C(12)-C(13)	0.2(9)
C(10)-C(11)-C(12)-Br(1)	175.1(4)
C(11)-C(12)-C(13)-C(14)	-1.2(10)
Br(1)-C(12)-C(13)-C(14)	-176.0(5)
C(12)-C(13)-C(14)-C(15)	0.8(10)

C(13)-C(14)-C(15)-C(10)	0.5(10)
C(11)-C(10)-C(15)-C(14)	-1.5(9)
C(1)-C(10)-C(15)-C(14)	175.0(6)
C(5)-C(6)-C(16)-C(21)	168.9(10)
C(5)-C(6)-C(16)-C(17)	-16.6(18)
C(5)-C(6)-C(16)-C(6')	7.1(14)
C(5')-C(6')-C(16)-C(21)	-30(3)
C(5')-C(6')-C(16)-C(17)	164.5(18)
C(5')-C(6')-C(16)-C(6)	0.8(14)
C(21)-C(16)-C(17)-C(18)	1.4(15)
C(6)-C(16)-C(17)-C(18)	-172.7(10)
C(6')-C(16)-C(17)-C(18)	171.7(11)
C(16)-C(17)-C(18)-C(19)	-2.6(14)
C(17)-C(18)-C(19)-C(20)	1.0(13)
C(18)-C(19)-C(20)-C(21)	1.9(14)
C(17)-C(16)-C(21)-C(20)	1.5(15)
C(6)-C(16)-C(21)-C(20)	177.2(9)
C(6')-C(16)-C(21)-C(20)	-161.7(17)
C(19)-C(20)-C(21)-C(16)	-3.2(15)
C(8)-C(9)-C(22)-C(23)	178.3(7)
C(8)-C(9)-C(22)-C(27)	-1.2(11)
C(27)-C(22)-C(23)-C(24)	0.0(10)

C(9)-C(22)-C(23)-C(24)	-179.4(7)
C(22)-C(23)-C(24)-C(25)	0.9(12)
C(23)-C(24)-C(25)-C(26)	-0.7(12)
C(24)-C(25)-C(26)-C(27)	-0.5(11)
C(25)-C(26)-C(27)-C(22)	1.4(11)
C(23)-C(22)-C(27)-C(26)	-1.2(10)
C(9)-C(22)-C(27)-C(26)	178.3(6)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 794851 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(11)-H(11)...O(1)#1	0.93	2.33	3.240(7)	165.7
C(3)-H(3)...O(1)#1	0.98	2.58	3.488(7)	154.1
C(2)-H(2A)...O(1)#1	0.97	2.51	3.411(8)	154.1

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z

G: References

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