Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Synthesis, structures, fullerene-binding and resolution of C_3-symmetric cavitands with rigid and deeper cavities

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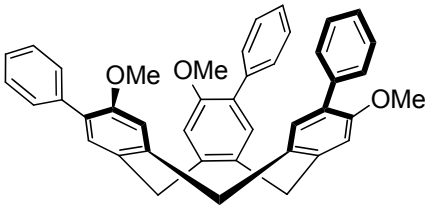
1. Characterization data for compounds 5a-5i, 6 and diastereoisomers

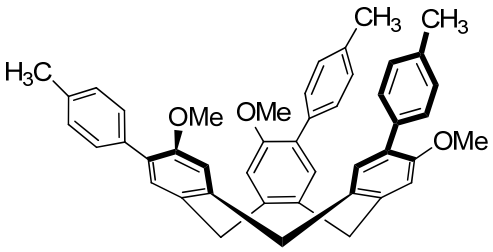
(±)-2,7,12-trimethoxy-3,8,13-triphenyl-10,15-dihydro-5*H*-tribenzo[a,d,g]cyclonoene (5a):



(±)-5a

Mp 282-283 °C; yield: 76%; IR (KBr) *v* 3020, 2935, 1609, 1511, 1486, 1463, 1441, 1390, 1235, 1044, 698 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 7.2, 6H, Ph-*H*), 7.42-7.34 (m, 9H, Ph-*H*), 7.31 (t, J = 7.2, 3H, Ph-*H*), 6.98 (s, 3H, Ar_{CTV}-*H*), 4.92 (d, J = 13.6, 3H, C*H*$_2$), 3.79 (d, J = 13.7, 3H, C*H*$_2$), 3.73 (s, 9H, OC*H*$_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.5, 140.3, 138.5, 132.6, 131.6, 129.7, 129.6, 128.1, 126.9, 113.0 (Ar*C*), 56.0 (O*C*H$_3$), 36.8 (*C*H$_2$); MS (positive APCI): *m*/*z* 589.44 ($[M+H]^+$). Anal. calcd. for $C_{42}H_{36}O_3 \cdot 0.9CHCl_3$: C, 74.01; H, 5.34. Found: C, 74.30; H, 5.38.

(±)-2,7,12-trimethoxy-3,8,13-tri(*p*-tolyl)-10,15-dihydro-5*H*-tribenzo[a,d,g]cyclonoene (5b):

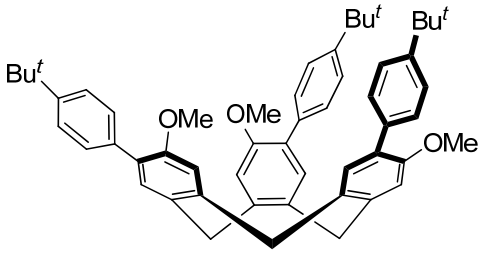


(±)-5b

Mp 158-159°C; yield: 67%; IR (KBr) *v* 3013, 2938, 1608, 1519, 1493, 1464, 1386, 1235, 1043, 816 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, J = 8.0, 6H, Tol-*H*), 7.33 (s, 3H, Ar_{CTV}-*H*), 7.19 (d, J = 8.0, 6H, Tol-*H*), 6.95 (s, 3H, Ar_{CTV}-*H*), 4.90 (d, J = 13.6, 3H, C*H*$_2$), 3.78 (d, J = 13.6, 3H, C*H*$_2$), 3.73 (s, 9H, OC*H*$_3$), 2.37 (s, 9H, Tol-C*H*$_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.5, 140.1, 136.6, 135.6, 132.5, 131.6, 129.7, 129.4, 128.8, 113.0 (Ar*C*), 56.0 (O*C*H$_3$), 36.8 (*C*H$_2$), 21.3 (Tol-*C*H$_3$); MS

(positive APCI): *m*/*z* 631.57 ([M+H]$^+$). Anal. calcd. for $C_{45}H_{42}O_3 \cdot 0.25CHCl_3$: C, 82.26; H, 6.45. Found: C, 82.11; H, 6.48.

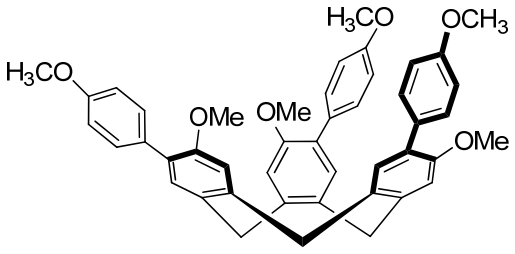
(±)-3,8,13-tri(4-*tert*-butylphenyl)-2,7,12-trimethoxy-10,15-dihydro-5*H*-tribenzo[a, d,g]cyclonoene (5c):



(±)-5c

Mp 193-194 ^{o}C; yield: 46%; IR (KBr) *v* 2959, 1610, 1494, 1462, 1385, 1238, 1044, 836 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (m, 12H, ^{t}BuPh-*H*), 7.37 (s, 3H, Ar_{CTV}-*H*), 6.97 (s, 3H, Ar_{CTV}-*H*), 4.90 (d, *J* = 13.6, 3H, C*H*$_2$), 3.78 (s, 9H, OC*H*$_3$), 3.76 (d, *J* = 13.6, 3H, C*H*$_2$), 12H), 1.35 (s, 27H, C(C*H*$_3$)$_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 149.7, 140.1, 135.6, 132.6, 131.6, 129.6, 129.2, 125.1, 113.1 (Ar*C*), 56.1 (O*C*H$_3$), 36.9 (*C*H$_2$), 34.7 (*C*(CH$_3$)$_3$), 31.6 (C(*C*H$_3$)$_3$); MS (positive APCI): *m*/*z* 757.67 ([M+H]$^+$). Anal. calcd. for $C_{54}H_{60}O_3 \cdot 0.1CHCl_3$: C, 84.50; H, 7.88. Found: C, 84.81; H,8.02.

(±)-2,7,12-trimethoxy-3,8,13-tri(4-methoxyphenyl)-10,15-dihydro-5*H*-tribenzo[a, d,g]cyclonoene (5d):

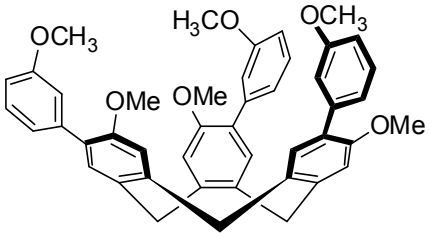


(±)-5d

Mp 177-179^{o}C; yield: 65%; IR (KBr) *v* 2934, 2835, 1607, 1558, 1495, 1458, 1245, 901, 836 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.4, 6H, *p*Anisole-*H*), 7.33 (s, 3H, Ar_{CTV}-*H*), 6.94 (d, *J* = 8.4, 6H, *p*Anisole-*H*), 6.91 (s, 3H, Ar_{CTV}-*H*), 4.90 (d, *J* = 13.6, 3H, C*H*$_2$), 3.83 (s, 9H, OC*H*$_3$), 3.76 (d, *J* = 13.6, 3H, C*H*$_2$), 3.74 (s, 9H,

OC*H*$_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 155.5, 139.9, 132.4, 131.6, 130.9, 130.6, 129.4, 113.6, 113.0 (Ar*C*), 56.0, 55.4 (O*C*H$_3$), 36.8 (*C*H$_2$); MS (positive APCI): *m*/*z* 679.40 ([M+H]$^+$). Anal. calcd. for $C_{45}H_{42}O_6$: C, 79.62; H, 6.24. Found: C, 79.65; H, 6.44.

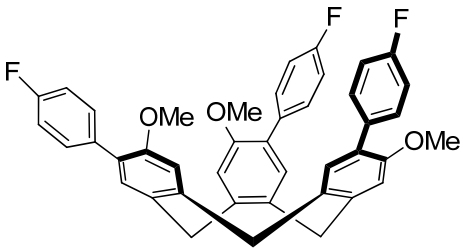
(±)-2,7,12-trimethoxy-3,8,13-tri(3-methoxyphenyl)-10,15-dihydro-5*H*-tribenzo[a, d,g] cyclonoene (5e):



(±)-**5e**

Mp 187-188 ^{o}C; yield: 67%; IR (KBr) *v* 2992, 2933, 2827, 1597, 1585, 1477, 1464, 1390, 1251, 1038, 850, 699 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (s, 3H, Ar$_{CTV}$-*H*), 7.30 (t, *J* = 7.9, 3H, *m*Anisole-*H*), 7.05-6.98 (m, 6H, *m*Anisole-*H*), 6.97 (s, 3H, Ar$_{CTV}$-*H*), 6.86 (dd, *J* = 8.2, 2.5, 3H, *m*Anisole-*H*), 4.91 (d, *J* = 13.6, 3H, C*H*$_2$), 3.81 (s, 9H, OC*H*$_3$), 3.79 (d, *J* = 13.6, 3H, C*H*$_2$), 3.75 (s, 9H, OC*H*$_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 155.5, 140.4, 139.9, 132.5, 131.5, 129.6, 129.0, 122.1, 115.4, 113.0, 112.6 (Ar*C*), 56.0, 55.3 (O*C*H$_3$), 36.8 (*C*H$_2$); MS (positive APCI): *m*/*z* 679.40 ([M+H]$^+$). Anal. calcd. for $C_{45}H_{42}O_6$: C, 79.62; H, 6.24. Found: C, 79.43; H, 6.25.

(±)-3,8,13-tri(4-fluorophenyl)-2,7,12-trimethoxy-10,15-dihydro-5*H*-tribenzo[a,d,g]cyclonoene (5f):

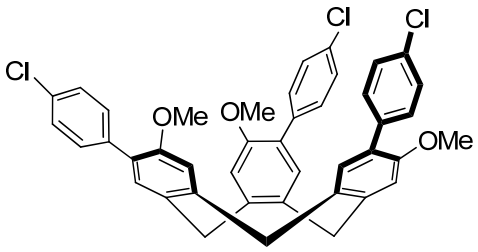


(±)-**5f**

Mp 248-249 ^{o}C; yield: 73%; IR (KBr) *v* 2933, 2840, 1604, 1518, 1494, 1385, 1158,

1042, 836 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.41 (dd, J = 8.6, 5.6, 6H, FPh-*H*), 7.32 (s, 3H, Ar_{CTV}-*H*), 7.07 (t, J = 8.6, 6H, FPh-*H*), 6.96 (s, 3H, Ar_{CTV}-*H*), 4.91 (d, J = 13.6, 3H, CH_2), 3.78 (d, J = 13.8, 3H, CH_2), 3.75 (s, 9H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3, 160.9, 155.4, 140.4, 134.3, 134.3, 132.5, 131.6, 131.1, 131.0, 128.8, 115.1, 114.9, 113.0 (Ar*C*), 56.0 (OCH_3), 36.8 (CH_2); MS (positive APCI): *m*/*z* 643.53 ($[M+H]^+$). Anal. calcd. for $C_{42}H_{33}F_3O_3$: C, 78.49; H, 5.18. Found: C, 78.59; H, 5.32.

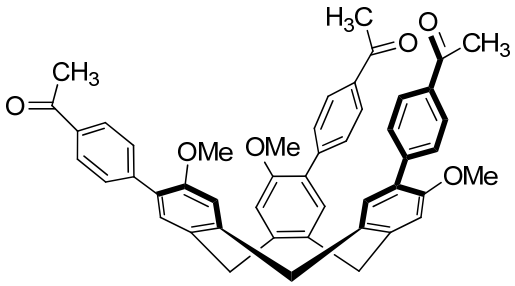
(±)-3,8,13-tri(4-chlorophenyl)-2,7,12-trimethoxy-10,15-dihydro-5*H*-tribenzo[a,d,g]cyclonoene (5g):



(±)-5g

Mp 273-275°C; yield: 5%; IR (KBr) *v* 2931, 2837, 1606, 1508, 1485, 1462, 1382, 1278, 1092, 830 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.40-7.32 (m, 12H, ClPh-*H*), 7.31 (s, 3H, Ar_{CTV}-*H*), 6.95 (s, 3H, Ar_{CTV}-*H*), 4.90 (d, J = 13.6, 3H, CH_2), 3.78 (d, J = 13.6, 3H, CH_2), 3.74 (s, 9H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.5, 140.6, 136.8, 133.0, 132.4, 131.6, 130.8, 128.6, 128.3, 113.0 (Ar*C*), 56.0 (OCH_3), 36.8 (CH_2); MS (negative APCI): *m*/*z* 690.43 (M^-). Anal. calcd. for $C_{42}H_{33}Cl_3O_3$: C, 72.89; H, 4.81. Found: C, 72.97; H, 4.88.

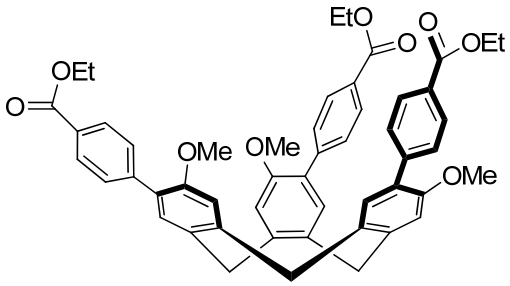
(±)-3,8,13-tri(4-acetylphenyl)-2,7,12-trimethoxy-10,15-dihydro-5*H*-tribenzo[a,d,g]cyclonoene (5h):



(±)-5h

Mp 201-204 ^{o}C; yield: 68%; IR (KBr) ν 2995, 2912, 2840, 1675, 1604, 1573, 1518, 1493, 1461, 1386, 1043, 957 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 8.2, 6H, actPh-*H*), 7.55 (d, J = 8.2, 6H, actPh-*H*), 7.37 (s, 3H, Ar_{CTV}-*H*), 6.98 (s, 3H, Ar_{CTV}-*H*), 4.93 (d, J = 13.6, 3H, CH_2), 3.81 (d, J = 13.6, 3H, CH_2), 3.75 (s, 9H, OCH_3), 2.62 (s, 9H, COCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.8 (*C*O), 155.5, 143.3, 141.1, 135.6, 132.4, 131.6, 129.6, 128.5, 128.2, 112.9 (Ar*C*), 55.9 (O*C*H$_3$), 36.7 (*C*H$_2$), 26.6 (CO*C*H$_3$); MS (positive APCI): *m*/*z* 715.54 ([M+H]$^+$). Anal. calcd. for $C_{48}H_{42}O_6$: C, 80.65; H, 5.92. Found: C, 80.19; H, 6.19.

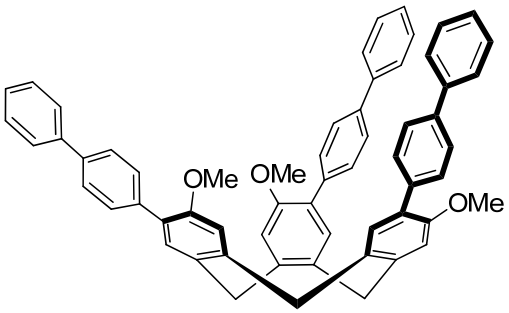
(±)-3,8,13-tri(4-(ethoxycarbonyl)phenyl)-2,7,12-trimethoxy-10,15-dihydro-5*H*-tribenzo[a,d,g]cyclonoene (5i):



(±)–5i

Mp 241-242 ^{o}C; yield: 42%; IR (KBr) ν 2931, 1713, 1609, 1494, 1464, 1387, 1278, 1103, 859 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 8.3, 6H, ECPh-*H*), 7.53 (d, J = 8.3, 6H, ECPh-*H*), 7.37 (s, 3H, Ar_{CTV}-*H*), 6.98 (s, 3H, Ar_{CTV}-*H*), 4.92 (d, J = 13.6, 3H, CTV-CH_2), 4.39 (q, J = 7.1, 6H, CH_2CH$_3$), 3.80 (d, J = 13.7, 3H, CTV-CH_2), 3.75 (s, 9H, OCH_3), 1.40 (t, J = 7.1, 9H, CH$_2$CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7 (*C*O$_2$), 155.6, 143.1, 141.1, 132.5, 131.6, 129.5, 129.4, 129.4, 129.0, 128.9 (Ar*C*), 61.0 (*C*H$_2$CH$_3$), 56.0 (O*C*H$_3$), 36.8 (CTV-*C*H$_2$), 14.5 (CH$_2$*C*H$_3$); MS (positive APCI) : *m*/*z* 805.53 ([M+H]$^+$). Anal. calcd. for $C_{51}H_{48}O_9$: C, 76.10; H, 6.01. Found: C,75.64; H, 6.04.

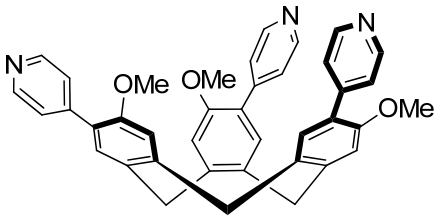
(±)-3,8,13-tri(biphenyl-4-yl)-2,7,12-trimethoxy-10,15-dihydro-5*H*-tribenzo[a,d,g]cyclonoene (5j):



(±)-5j

Mp 193-195 °C; yield: 45%; IR (KBr) *v* 3025, 2837, 1609, 1498, 1483, 1463, 1045, 840 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.63-7.58 (m, 12H, Biph-*H*), 7.55 (d, $J = 8.2$, 6H, Biph-*H*), 7.49-7.40 (m, 6H, Biph-*H*), 7.43 (s, 3H, Ar_{CTV}-*H*), 7.34 (t, $J = 7.3$, 3H, Biph-*H*), 7.03 (s, 3H, Ar_{CTV}-*H*), 4.95 (d, $J = 13.6$, 3H, CH_2), 3.83 (d, $J = 13.6$, 3H, CH_2), 3.80 (s, 9H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 141.1, 140.4, 139.8, 137.5, 132.5, 131.7, 130.0, 129.3, 128.9, 127.3, 127.2, 126.9, 113.1 (Ar*C*), 56.1 (OCH_3), 36.9 (CH_2); MS (positive APCI): *m/z* 817.34 ($[M+H]^+$). Anal. calcd. for $C_{60}H_{48}O_3$: C, 88.20; H, 5.92. Found: C, 87.64; H, 5.93.

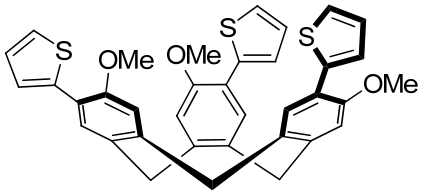
(±)-2,7,12-trimethoxy-3,8,13-tri(pyridin-4-yl)-10,15-dihydro-5*H*-tribenzo[a,d,g]cyclonoene (5k):



(±)-5k

Mp >320 °C; yield: 23%; IR (KBr) *v* 2962, 1595, 1508, 1486, 1456, 1390, 1240, 1040, 993, 830 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, $J = 5.2$, 6H, Py-*H*), 7.39 (d, $J = 5.2$, 6H, Py-*H*), 7.36 (s, 3H, Ar_{CTV}-*H*), 6.98 (s, 3H, Ar_{CTV}-*H*), 4.92 (d, $J = 13.6$, 3H, CH_2), 3.81 (d, $J = 13.8$, 3H, CH_2), 3.78 (s, 9H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 149.7, 146.1, 141.8, 132.2, 131.6, 127.0, 124.3, 113.0 (Ar*C*), 56.0 (OCH_3), 36.8 (CH_2); MS (positive APCI): *m/z* 592.49 ($[M+H]^+$). Anal. calcd. for $C_{39}H_{33}N_3O_3$: C, 79.16; H, 5.62; N, 7.10. Found: C, 79.33; H, 5.76; N, 7.12.

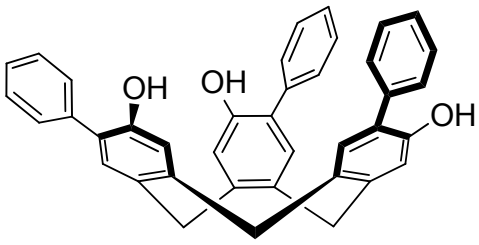
(±)-2,7,12-trimethoxy-3,8,13-tri(thiophen-2-yl)-10,15-dihydro-5*H*-tribenzo[a,d,g] cyclonoene (5l):



(±)-5l

Mp: 160 °C (decomp.); yield: 21%; IR (KBr) *v* 3100, 2956, 2931, 1604, 1567, 1492, 1463, 1392, 1267, 1209, 1020, 847 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) *δ* 7.60 (s, 3H, Ar_{CTV}-*H*), 7.40 (d, *J* = 3.2, 3H, Tp-*H*), 7.25 (d, *J* = 5.2, 3H, Tp-*H*), 7.04 (dd, *J* = 5.2, 3.2, 3H, Tp-*H*), 6.99 (s, 3H, Ar_{CTV}-*H*), 4.82 (d, *J* = 13.6, 3H, C*H*$_2$), 3.88 (s, 9H, OC*H*$_3$), 3.73 (d, *J* = 13.6, 3H, C*H*$_2$); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 154.8, 140.1, 139.7, 131.5, 130.5, 127.2, 125.5, 124.9, 122.4, 113.2 (Ar*C*), 56.0 (O*C*H$_3$), 36.7 (*C*H$_2$); MS (positive APCI) : *m*/*z* 607.38 ($[M+H]^+$). Anal. calcd. for $C_{36}H_{30}O_3S_3 \cdot 0.1CHCl_3$: C, 70.07; H, 4.90. Found: C,70.01; H, 4.95.

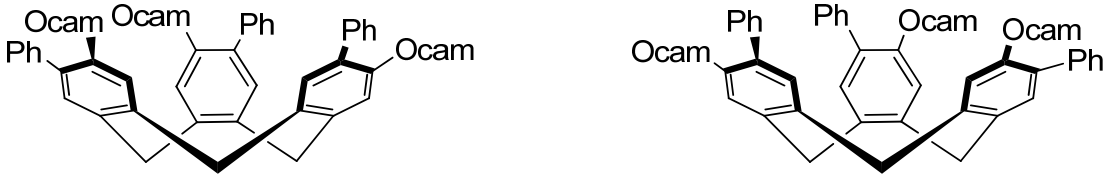
2,7,12-trihydroxy-3,8,13-triphenyl-10,15-dihydro-5*H* –tribenzo[a,d,g] cyclonoene (+)/(-)-6:



(±) – 6

Mp >220°C, decompose; IR (KBr) *v* 3640~3164(br), 3053, 3029, 2914, 2855, 1621, 1578, 1507, 1484, 1447, 1385, 899, 762, 744, 699cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.43 (m, 6H), 7.42 (s, 3H), 7.41 – 7.35 (m, 6H), 7.28 (s, 3H), 6.98 (s, 3H), 5.00 (s, 3H), 4.84 (d, *J* = 13.5, 3H), 3.73 (d, *J* = 13.6, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.3, 141.1, 137.0, 132.0, 131.7, 129.5, 129.2, 128.0, 127.2, 117.0, 36.4; MS (APCI) : *m*/*z* 545.45 $[M-H]^+$; Anal. Calcd for $C_{39}H_{30}O_3$: C, 85.69; H, 5.53. Found: C, 84.19; H, 5.57 (**6** + 0.5 H_2O).

2,7,12-tricamphananic ester-3,8,13-triphenyl-10,15-dihydro-5*H* –tribenzo[a,d,g] cyclonoene diastereoisomers part A and part B:

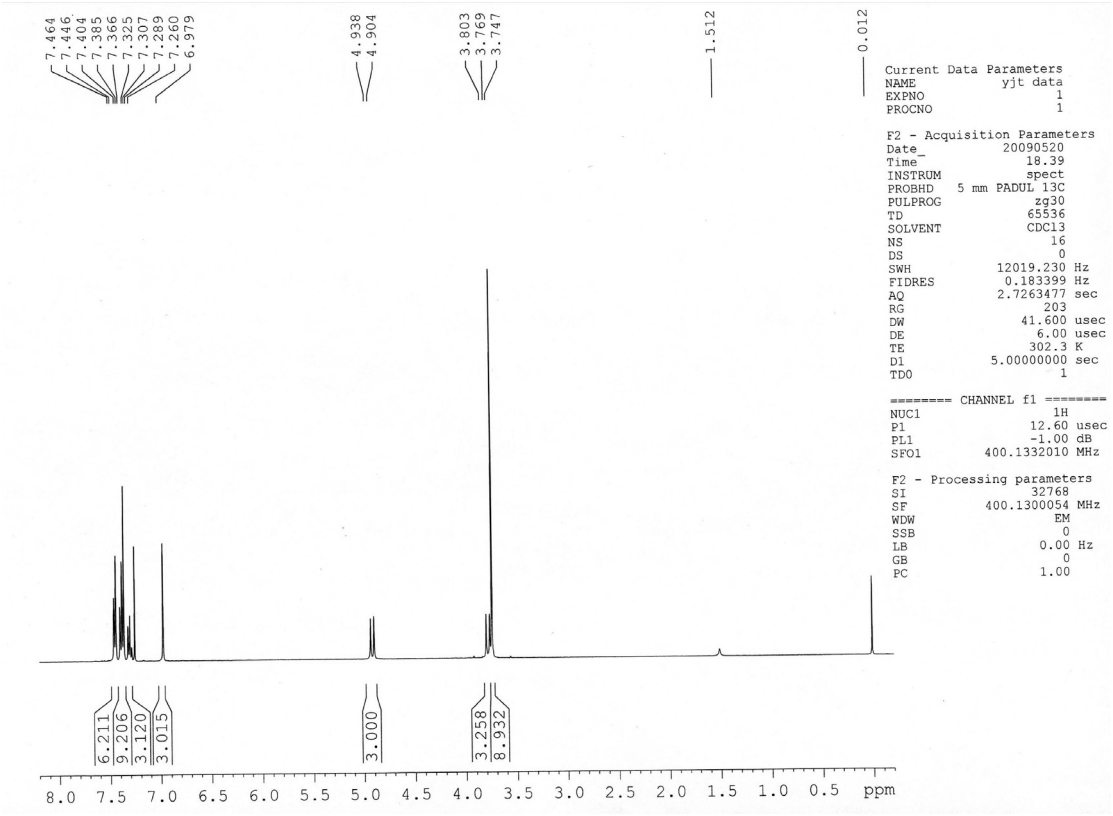


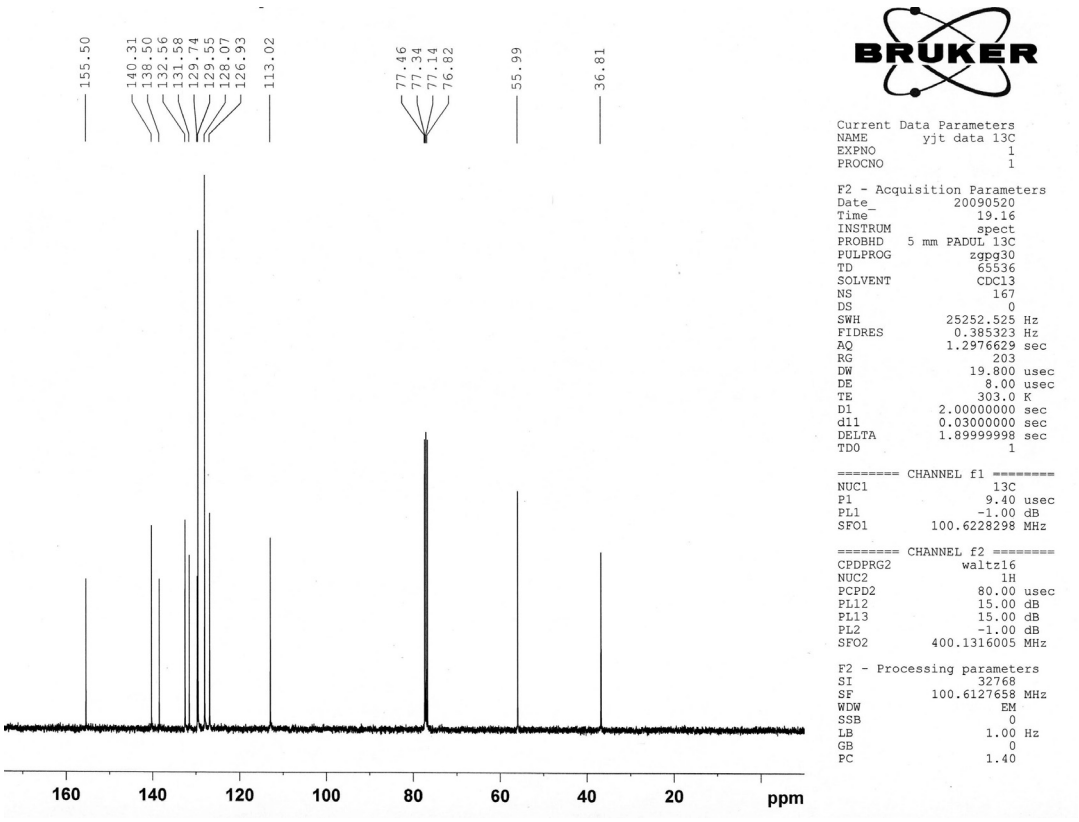
Part **A** and **B**

A: Mp 218-219°C; IR (KBr) *v* 3056, 3028, 2968, 2875, 1793, 1755, 1617, 1508, 1484, 1446, 1260, 1046, 903, 839, 764, 701; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (s, 3H), 7.40 – 7.27 (m, 15H), 7.16 (s, 3H), 4.94 (d, *J* = 13.6, 3H), 3.87 (d, *J* = 13.7, 3H), 2.23 – 2.10 (m, 3H), 1.96 – 1.76 (m, 6H), 1.62 (ddd, *J* = 13.3, 9.3, 4.2, 3H), 1.05 (s, 9H), 0.85 (s, 9H), 0.66 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.0, 166.1, 146.1, 140.0, 137.5, 137.0, 134.2, 132.9, 129.3, 128.4, 127.8, 123.8, 90.8, 54.9, 54.4, 36.5, 31.0, 29.0, 16.7, 16.3, 9.7; **B:** Mp 225°C; IR (KBr) *v* 3056, 3028, 2967, 2929, 2874, 1793, 1755, 1617, 1508, 1484, 1446, 1259, 1167, 1046, 903, 838, 764, 702cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (s, 3H), 7.40 – 7.28 (m, 15H), 7.14 (s, 3H), 4.94 (d, *J* = 13.6, 3H), 3.87 (d, *J* = 13.7, 3H), 2.11 (ddd, *J* = 28.9, 16.6, 10.0, 3H), 1.90 – 1.74 (m, 6H), 1.68 – 1.56 (m, 3H), 1.04 (s, 9H), 0.82 (s, 9H), 0.72 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.0, 166.0, 146.2, 139.9, 137.4, 137.0, 134.3, 132.9, 129.5, 128.5, 127.8, 123.8, 90.8, 54.9, 54.3, 36.6, 31.0, 29.0, 16.5, 16.4, 9.7; MS (APCI) : *m*/*z* 1046.81 $[M+H]^+$; Anal. Calcd for $C_{66}H_{60}O_{12}$: C, 75.84; H, 5.79. Found: C, 75.29; H, 6.03 (**A**/**B** + 0.5 H_2O).

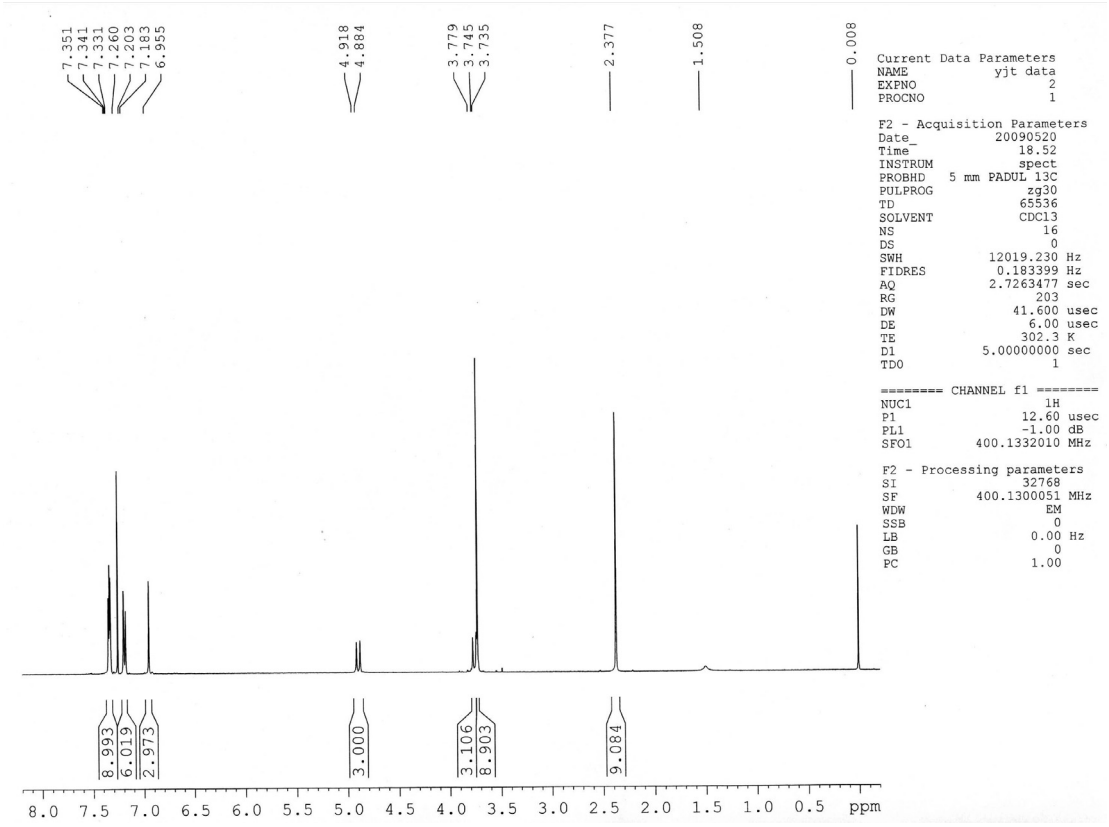
2. NMR spectra of compound 5a-5l, 6 and diastereoisomers

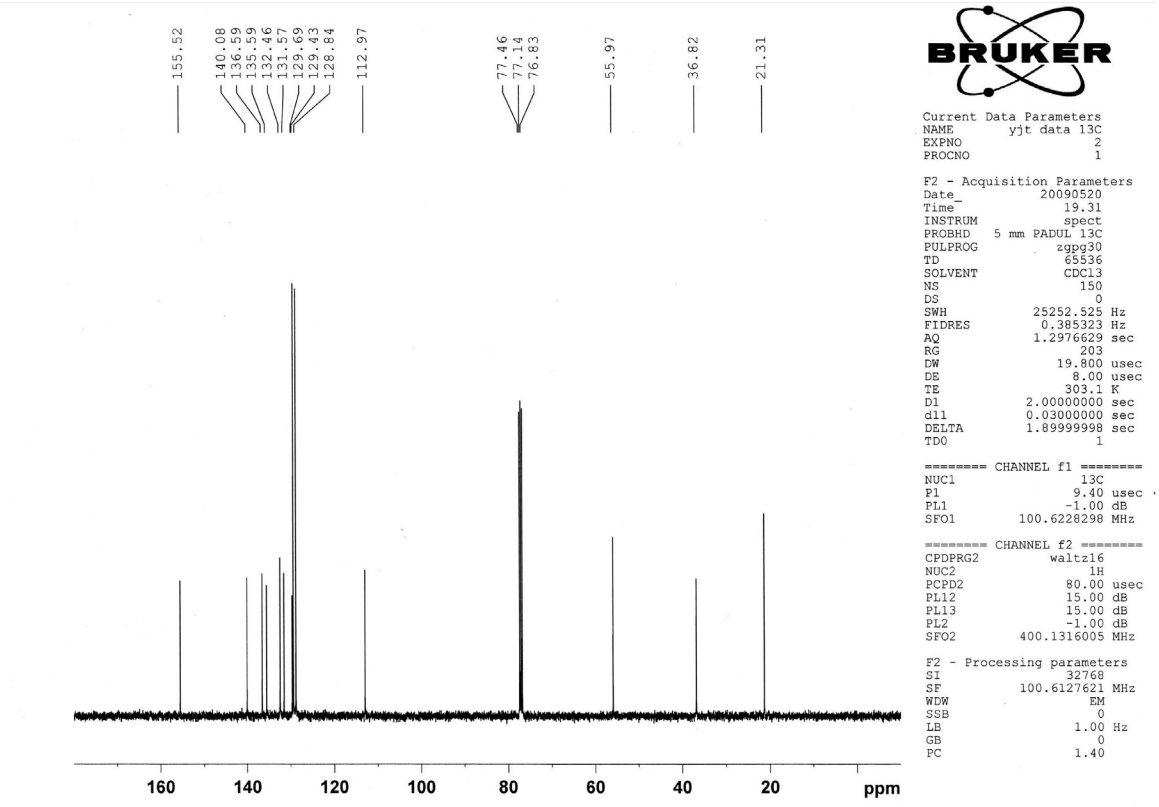
^{1}H and ^{13}C NMR of **(±)-5a**



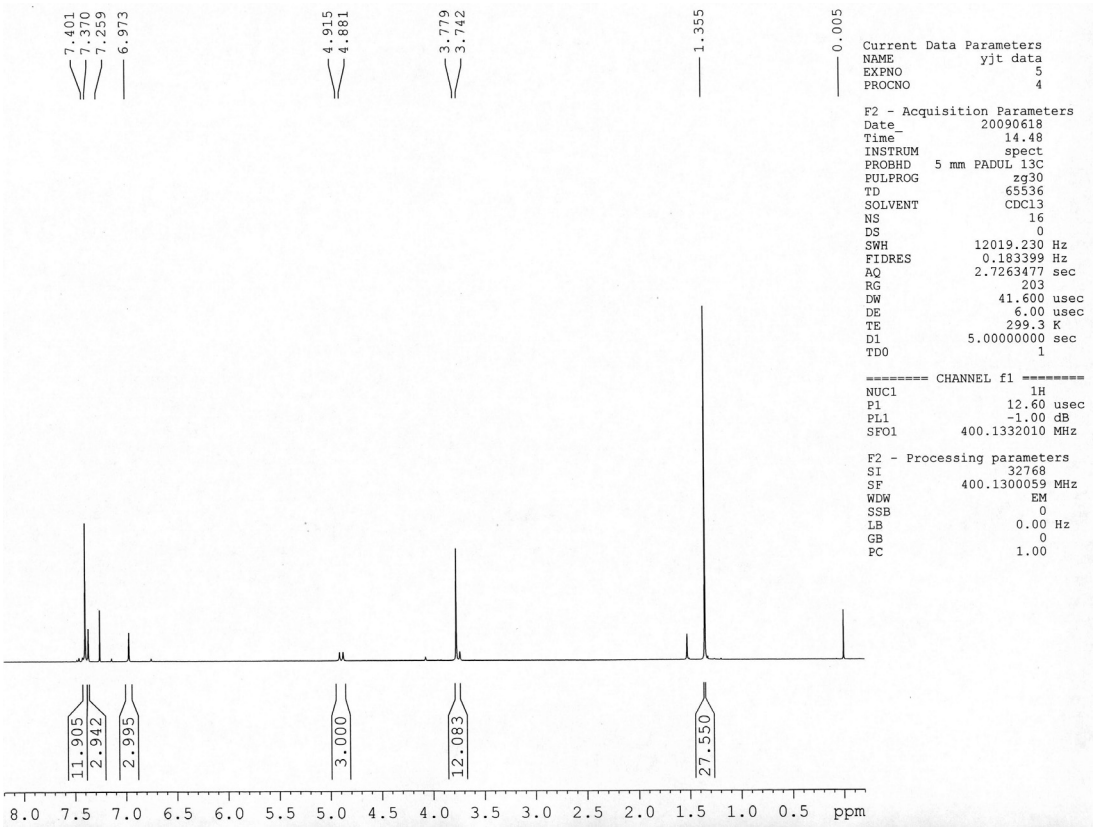


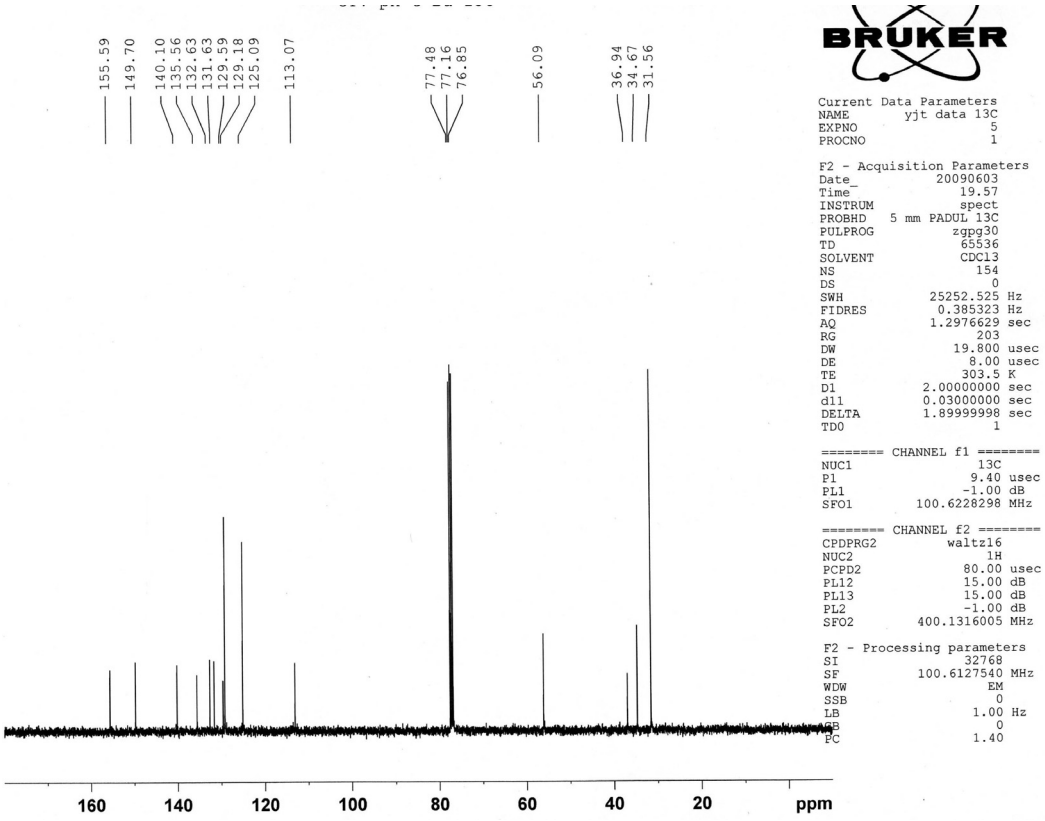
^{1}H and ^{13}C NMR of **(±)-5b**



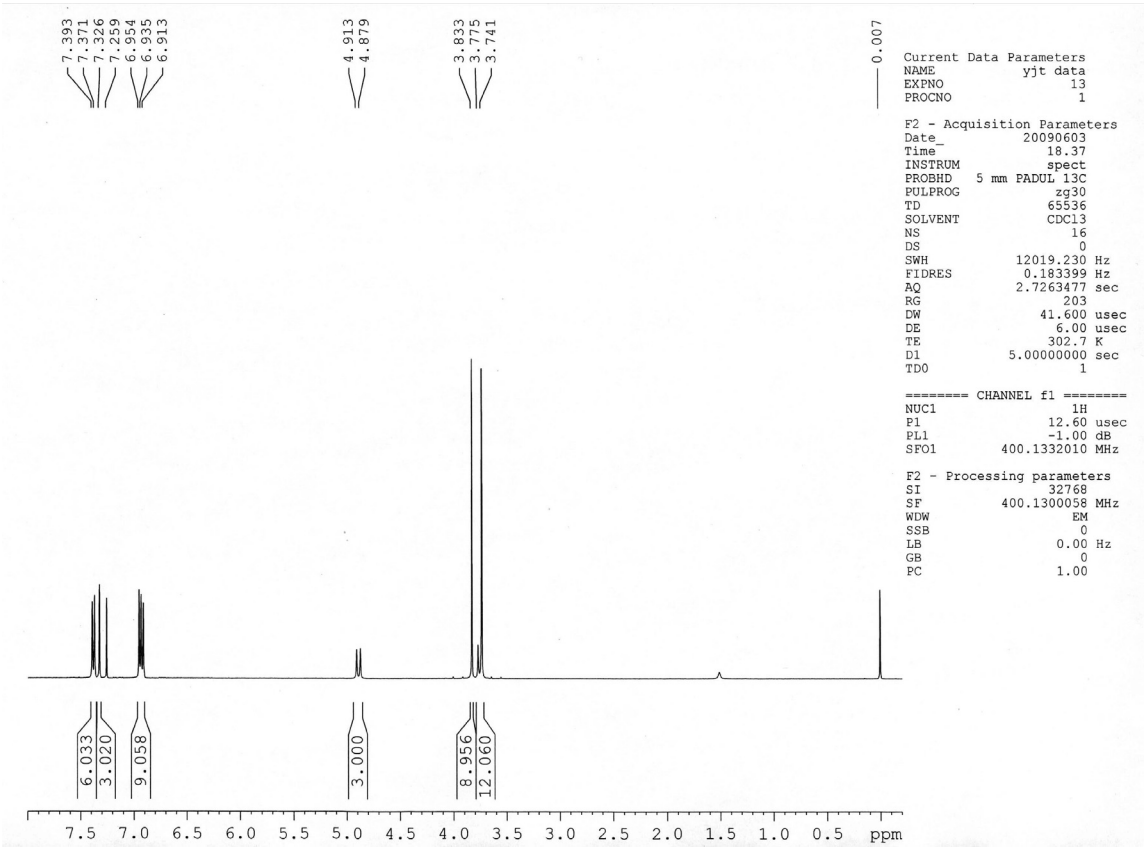


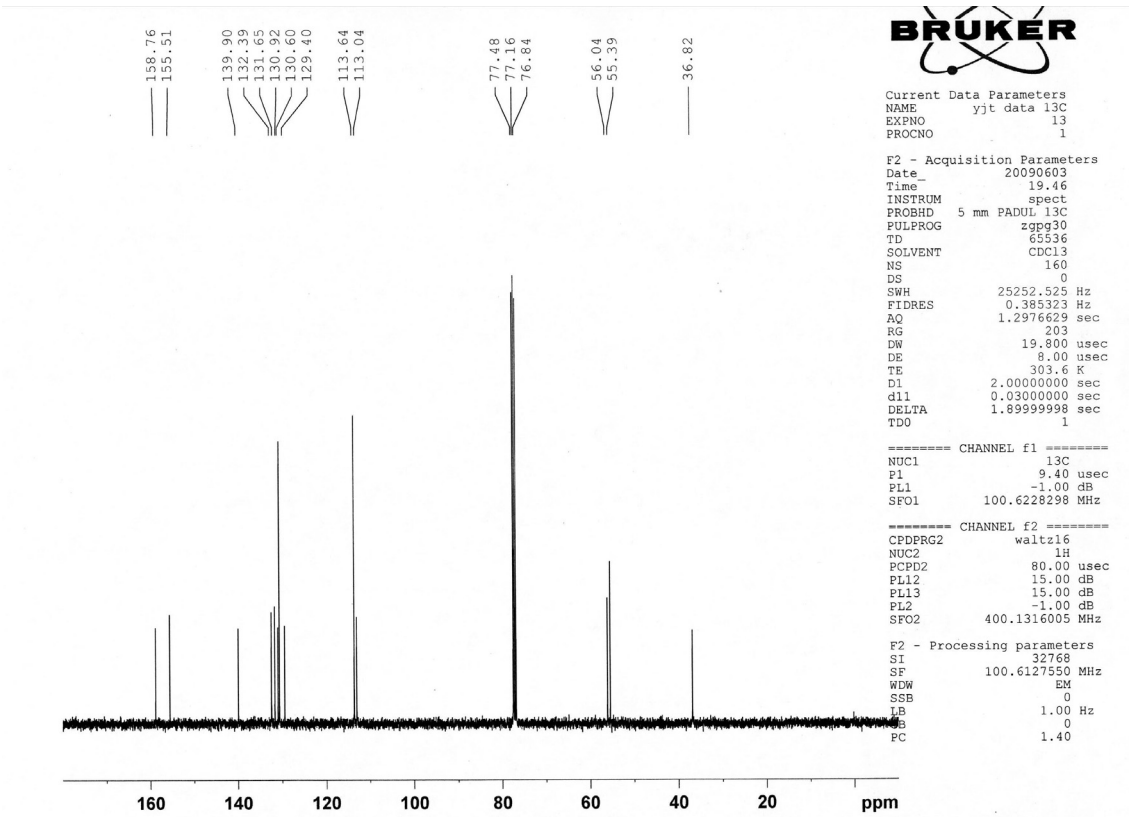
^{1}H and ^{13}C NMR of **(±)-5c**



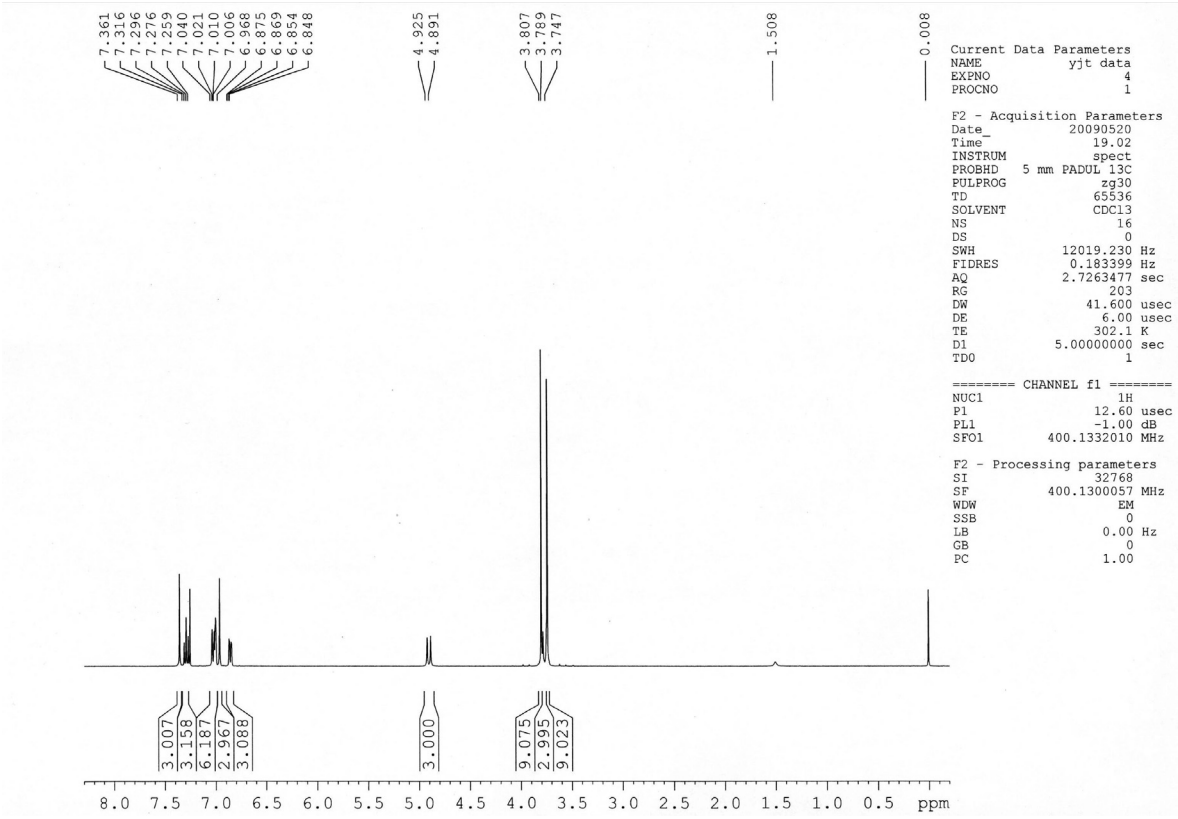


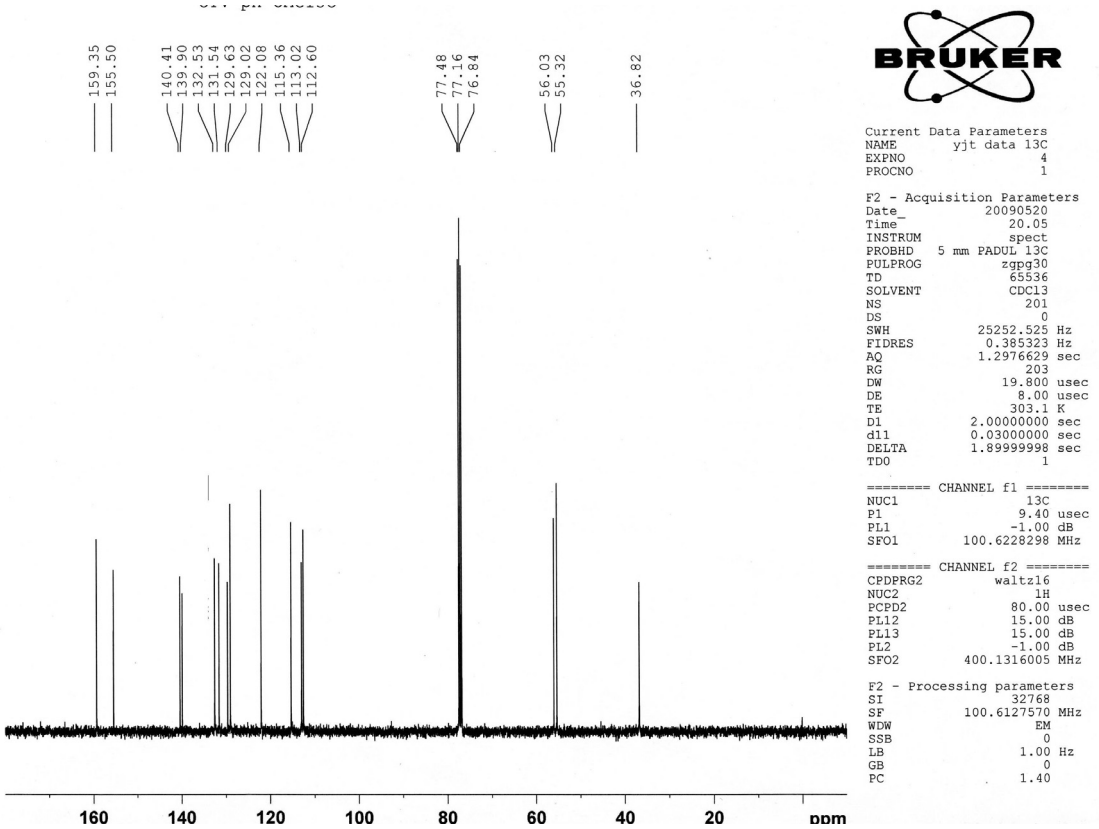
^{1}H and ^{13}C NMR of **(±)-5d**



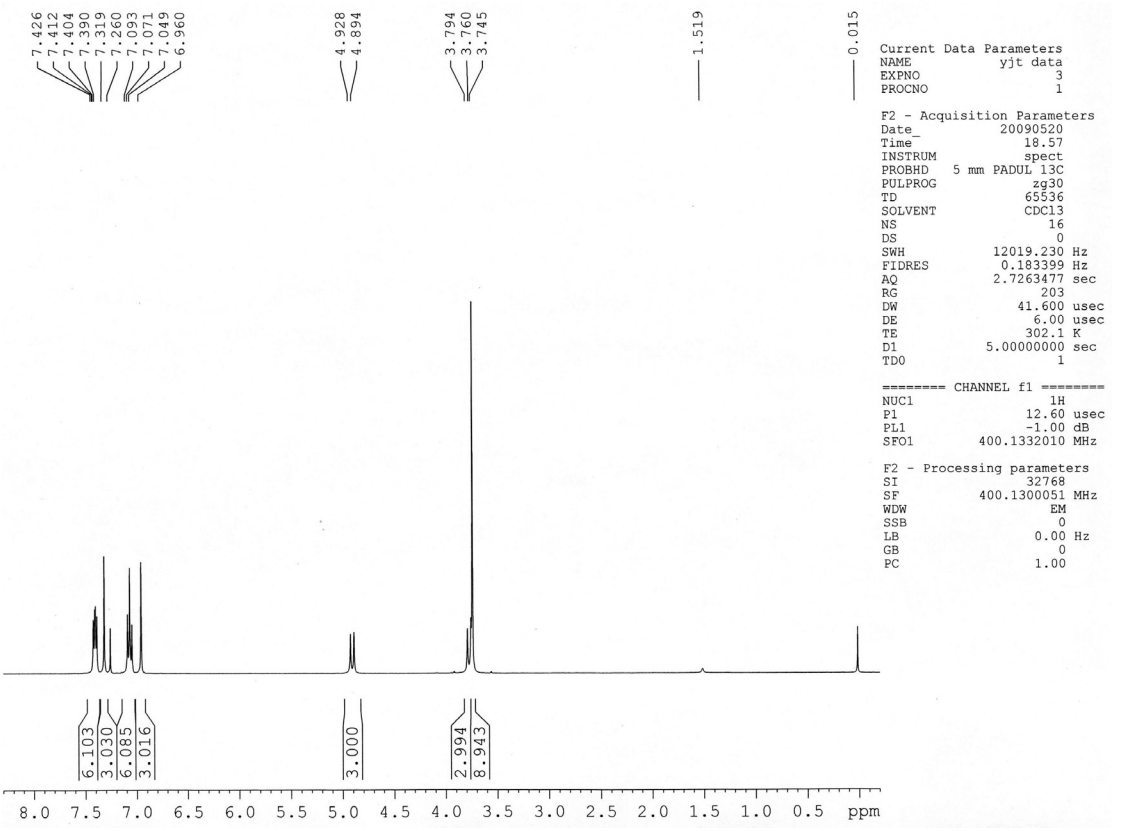


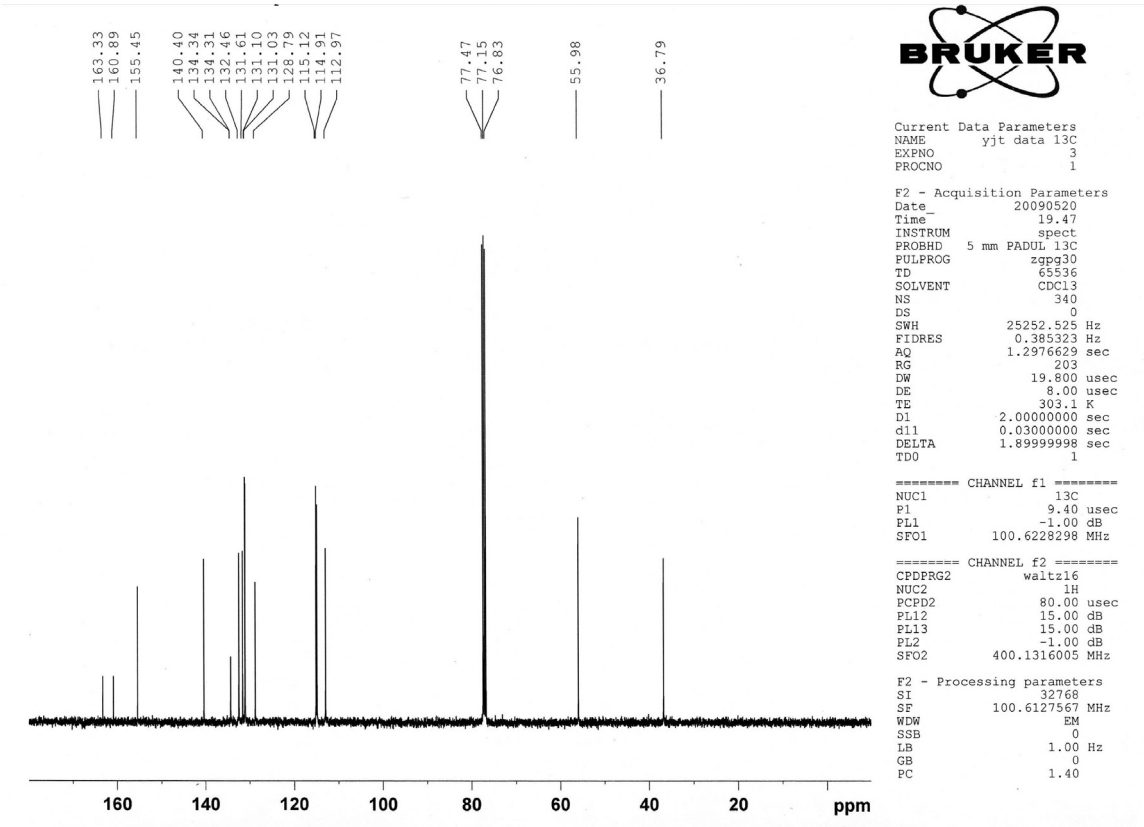
^{1}H and ^{13}C NMR of **(±)-5e**



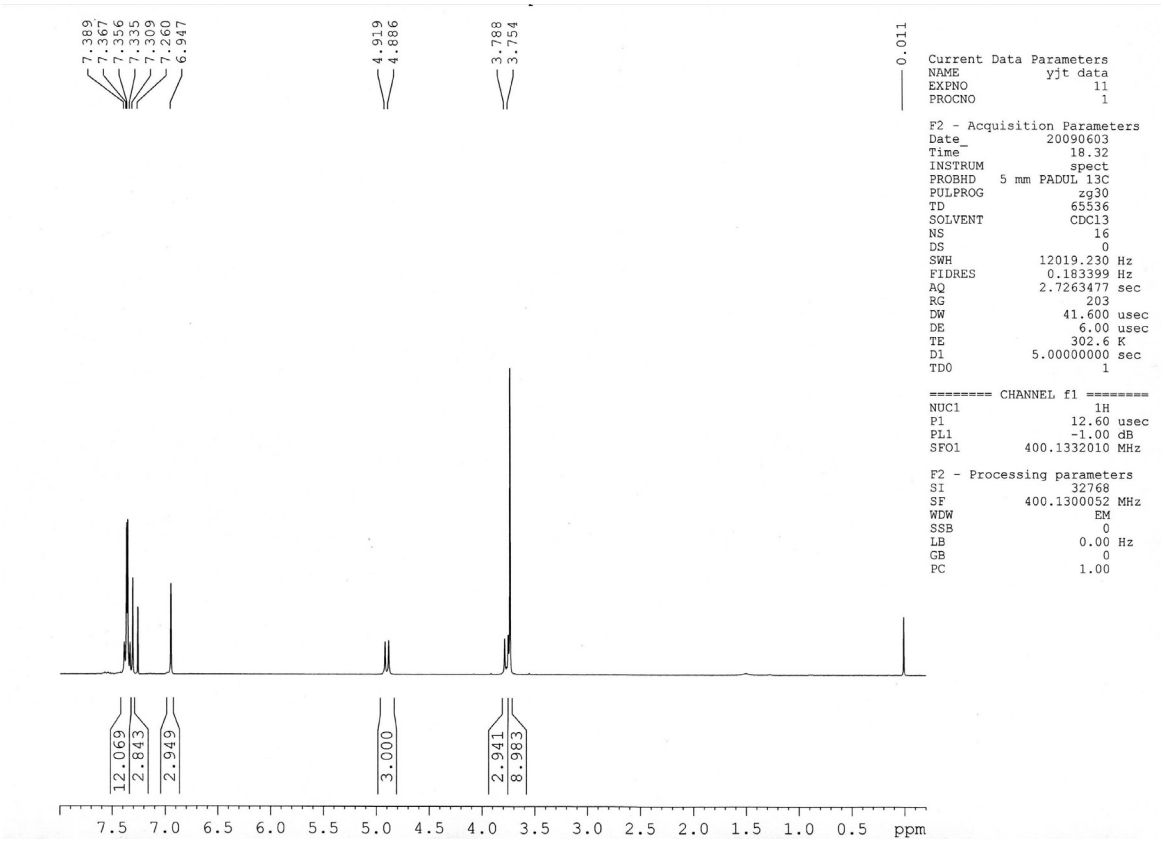


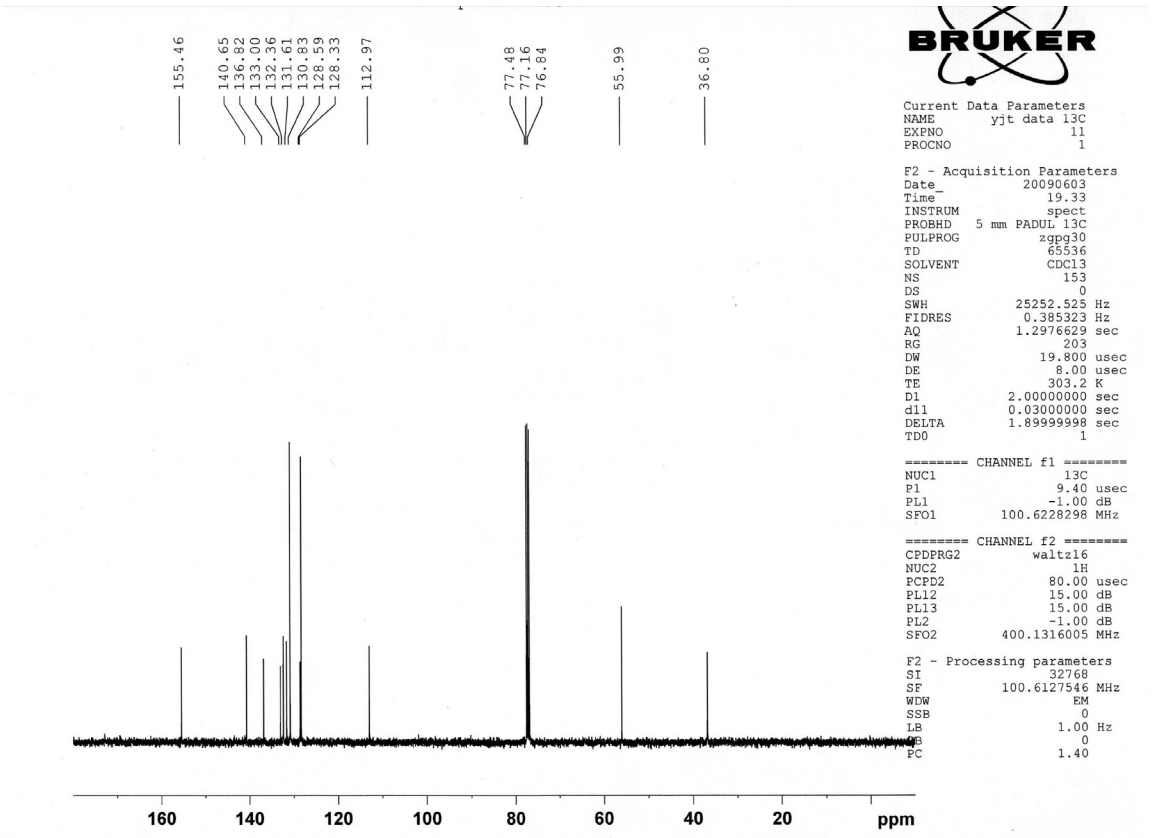
^{1}H and ^{13}C NMR of **(±)-5f**



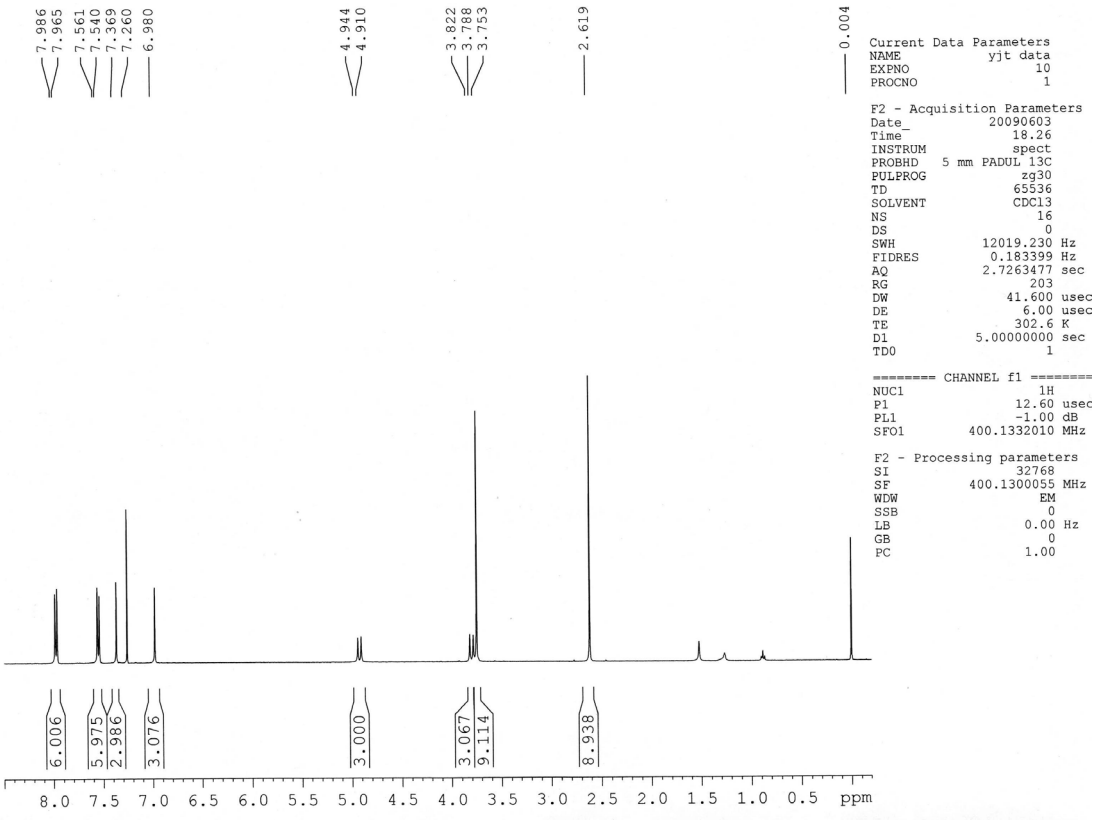


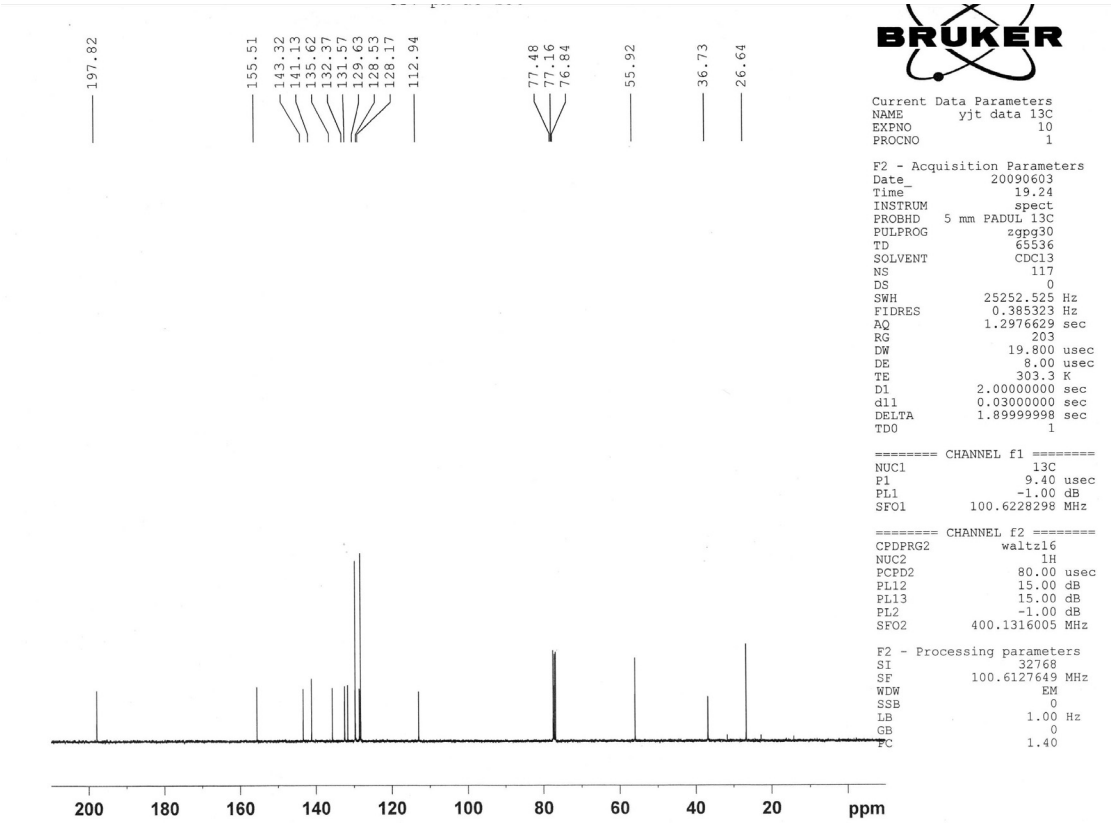
^{1}H and ^{13}C NMR of **(±)-5g**



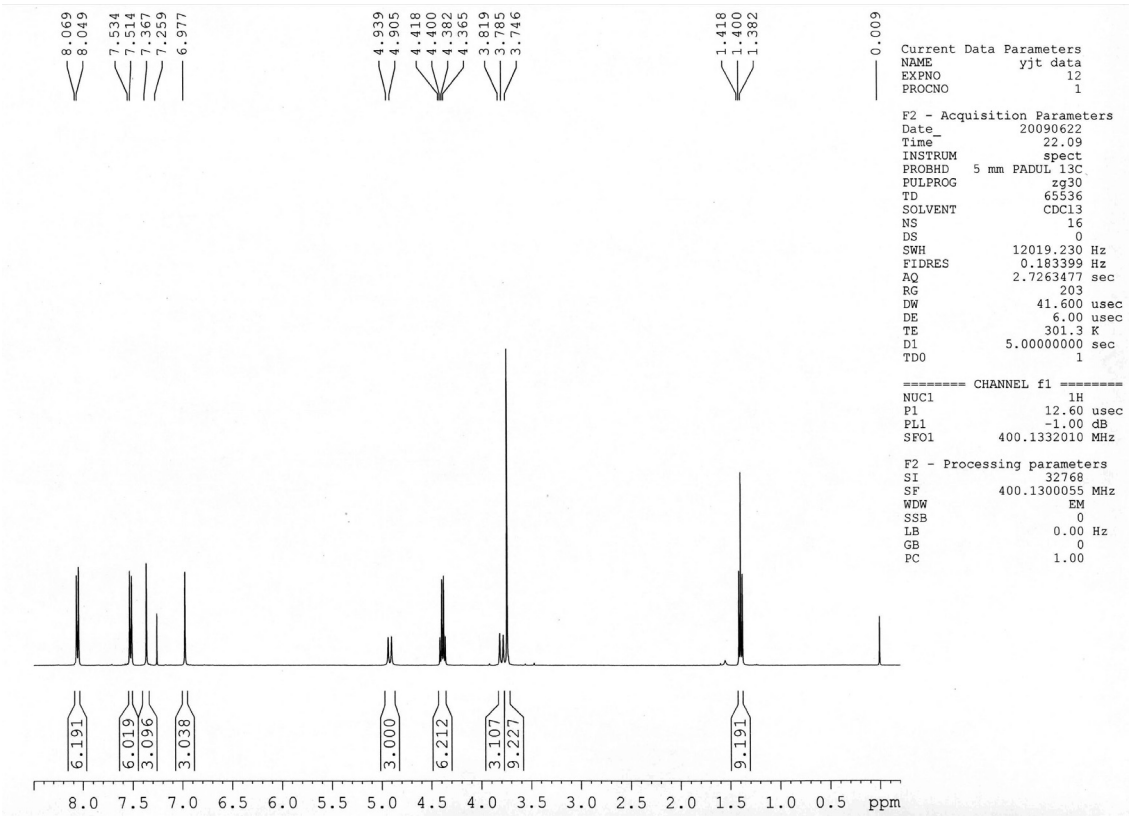


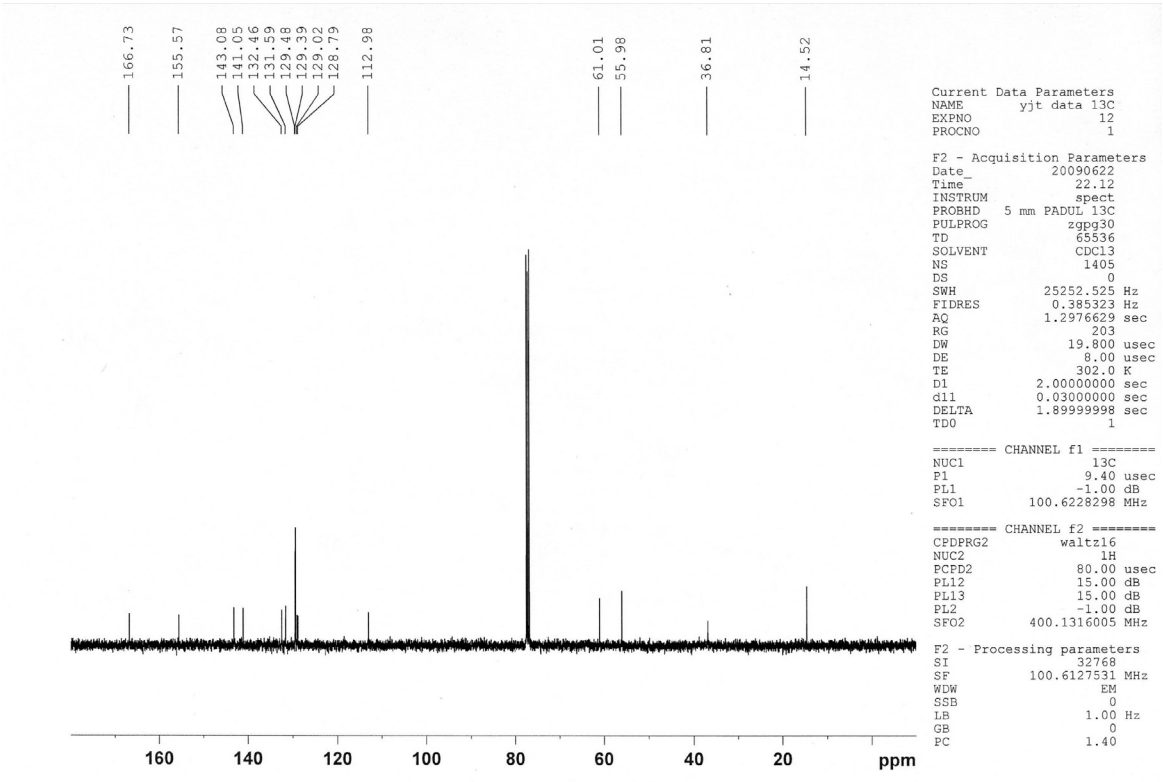
^{1}H and ^{13}C NMR of **(±)-5h**



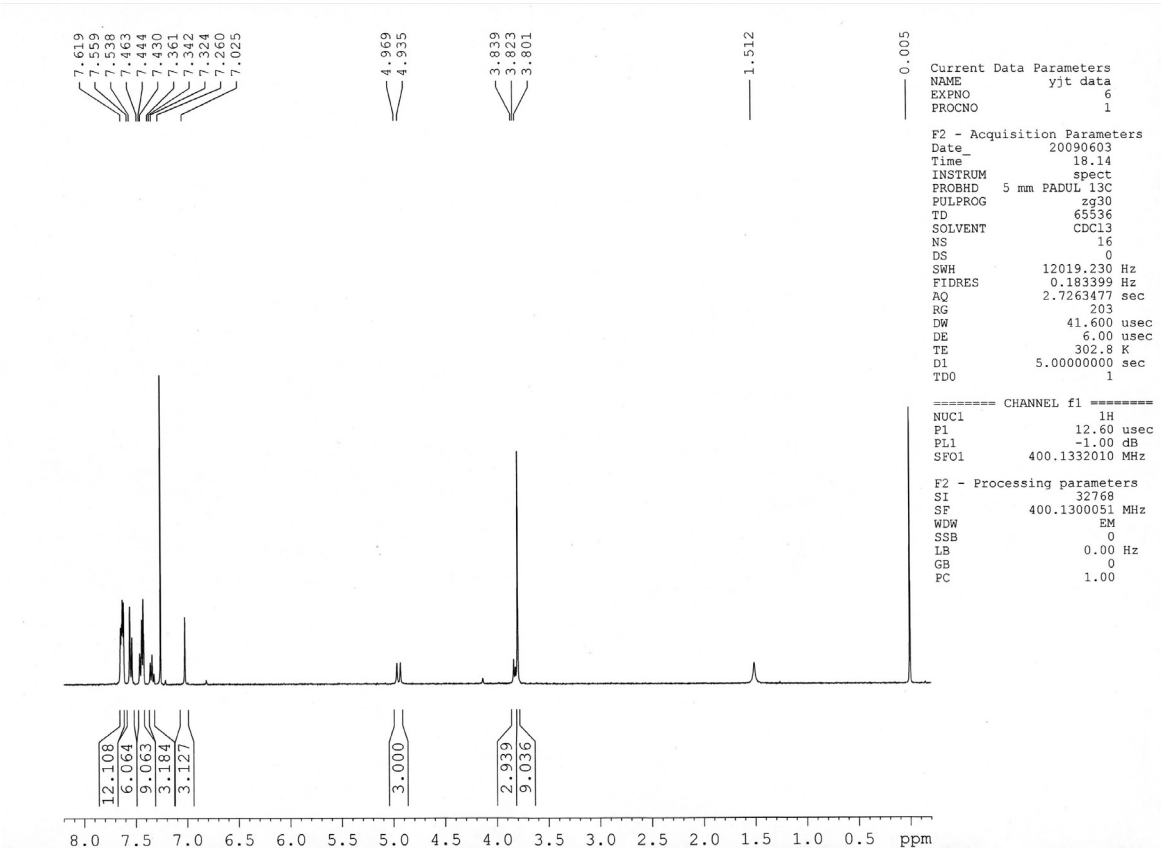


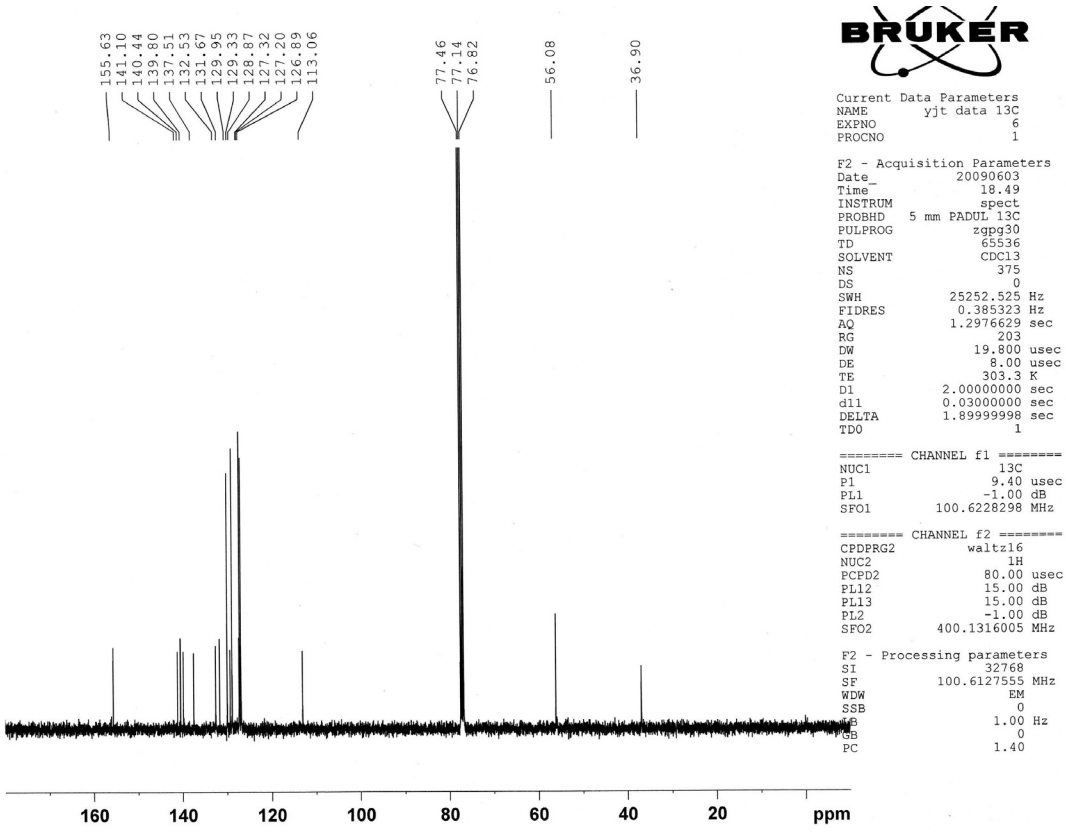
^{1}H and ^{13}C NMR of **(±)-5i**



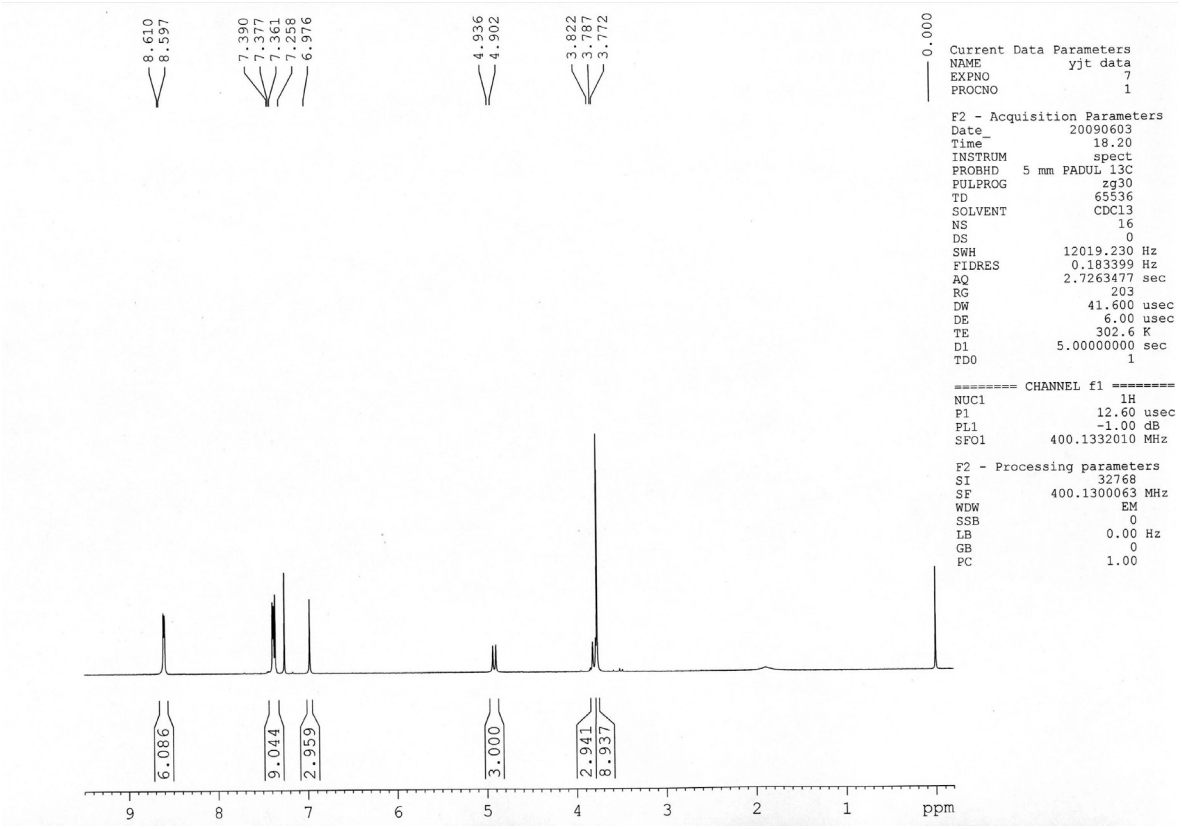


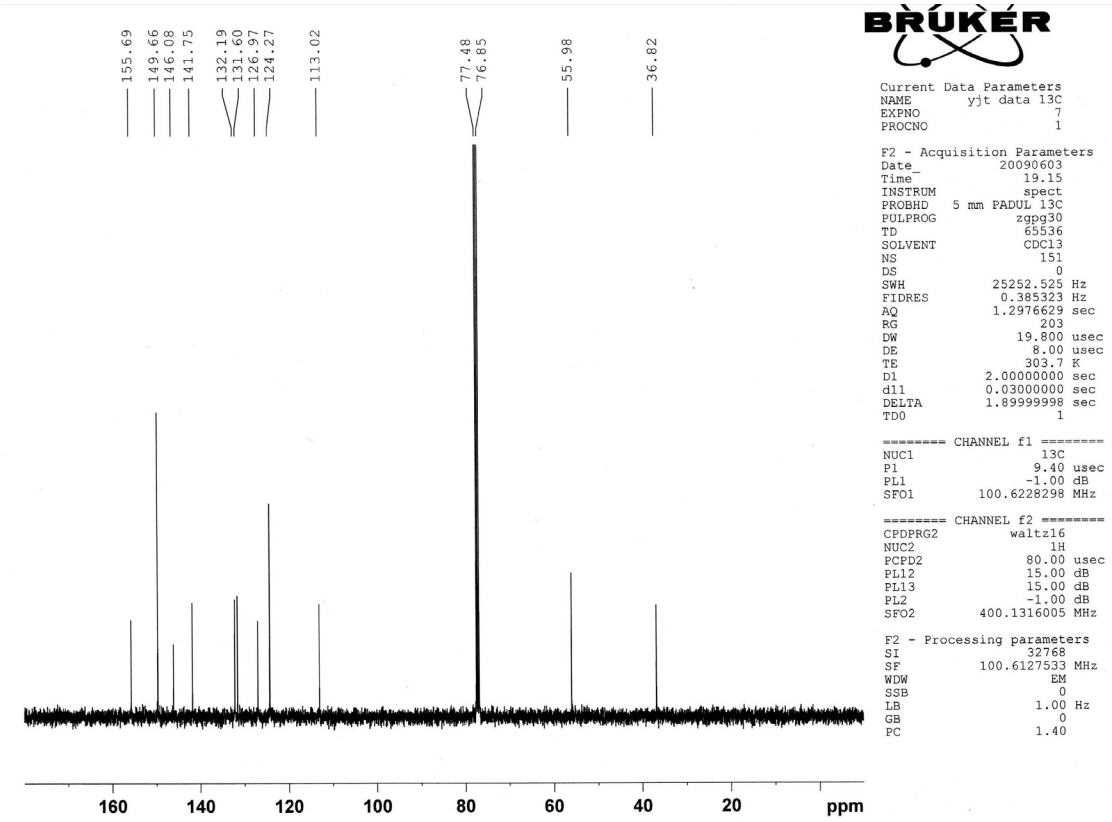
^{1}H and ^{13}C NMR of **(±)-5j**



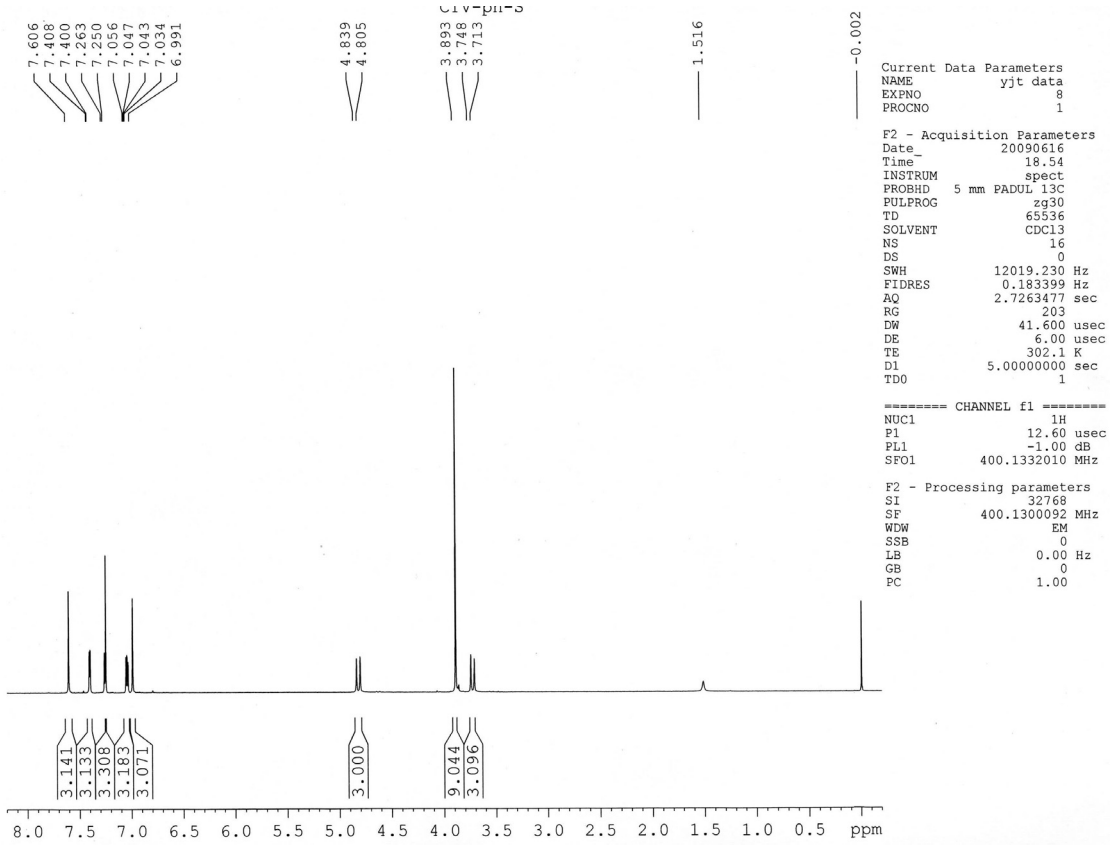


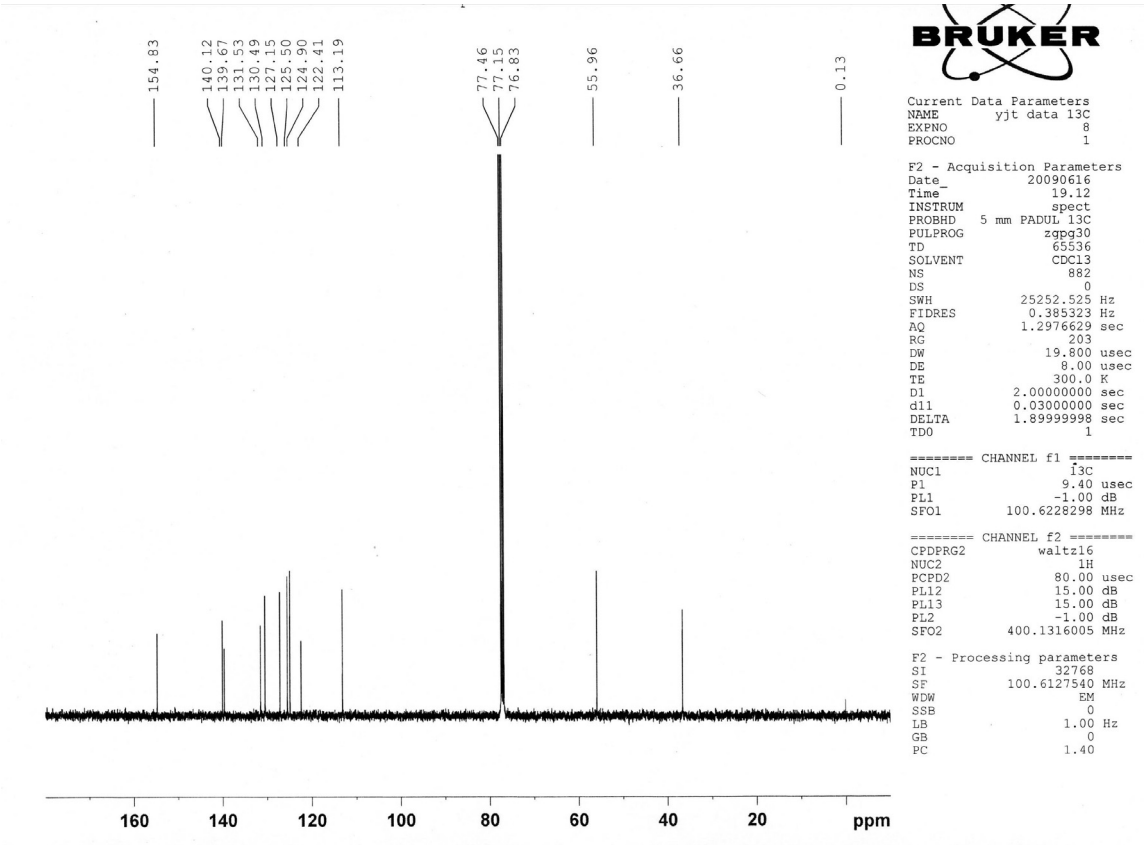
^{1}H and ^{13}C NMR of **(±)-5k**



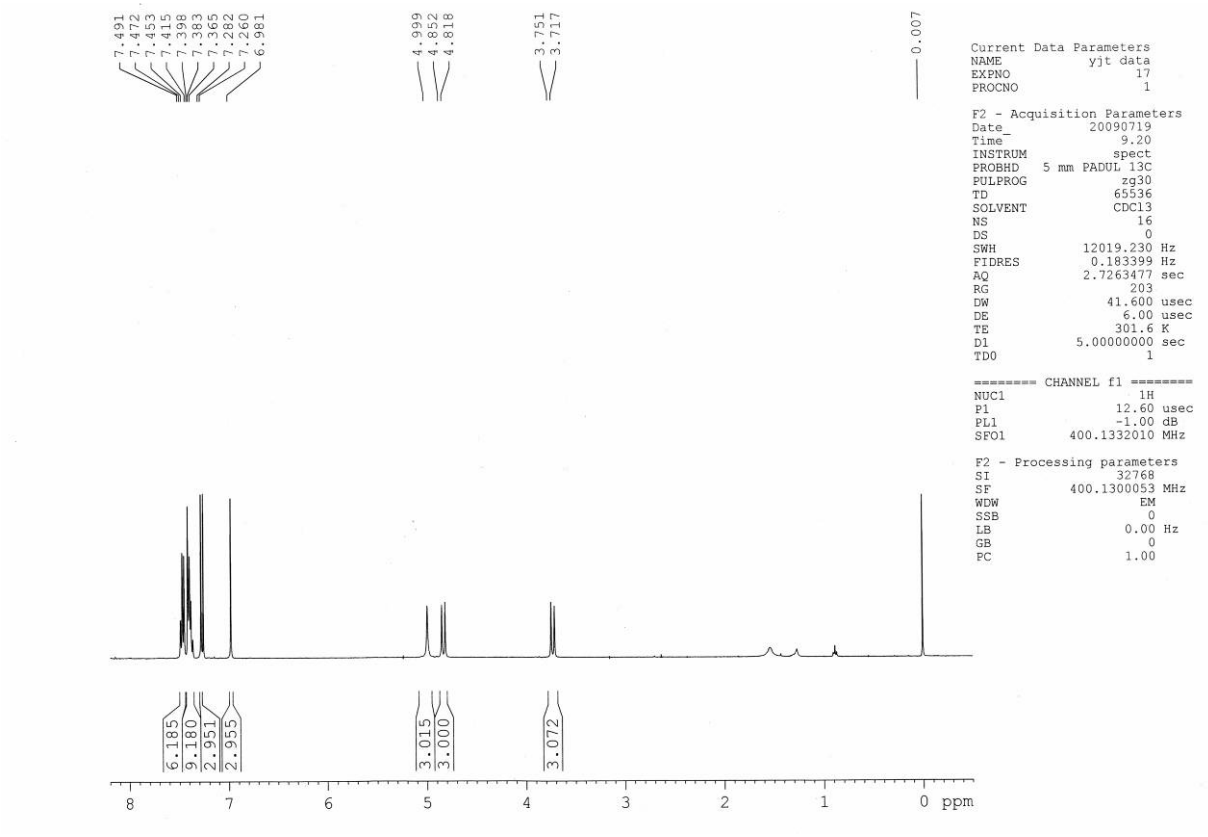


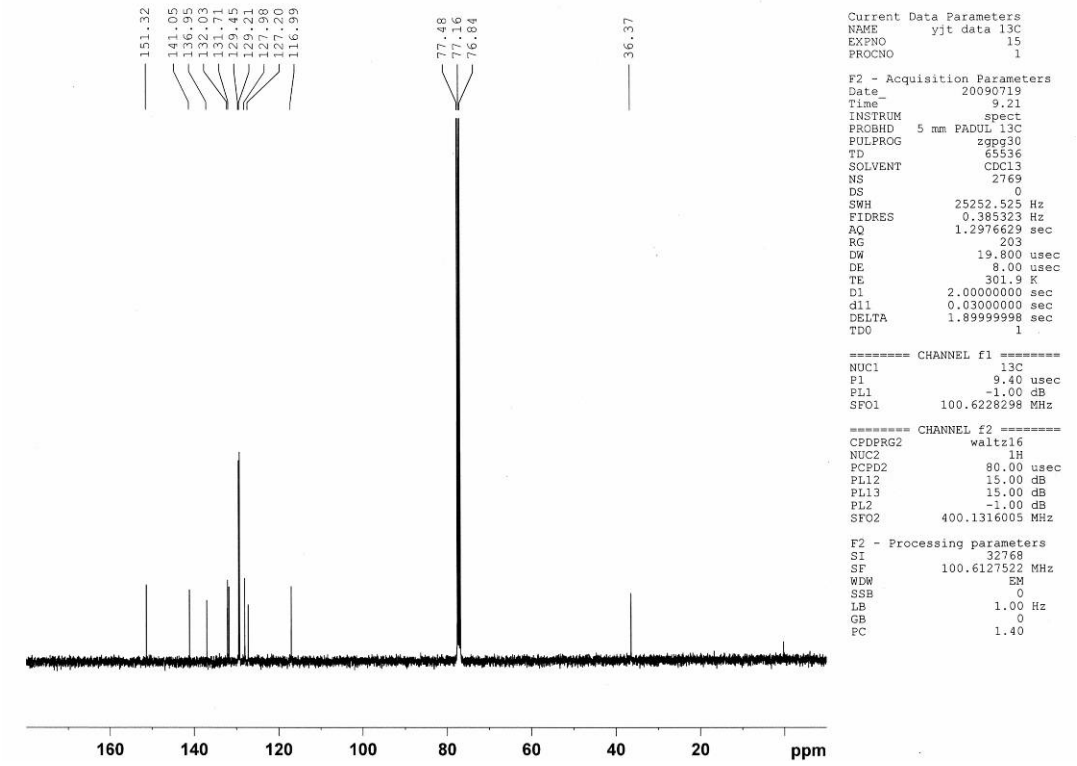
^{1}H and ^{13}C NMR of **(±)-5l**



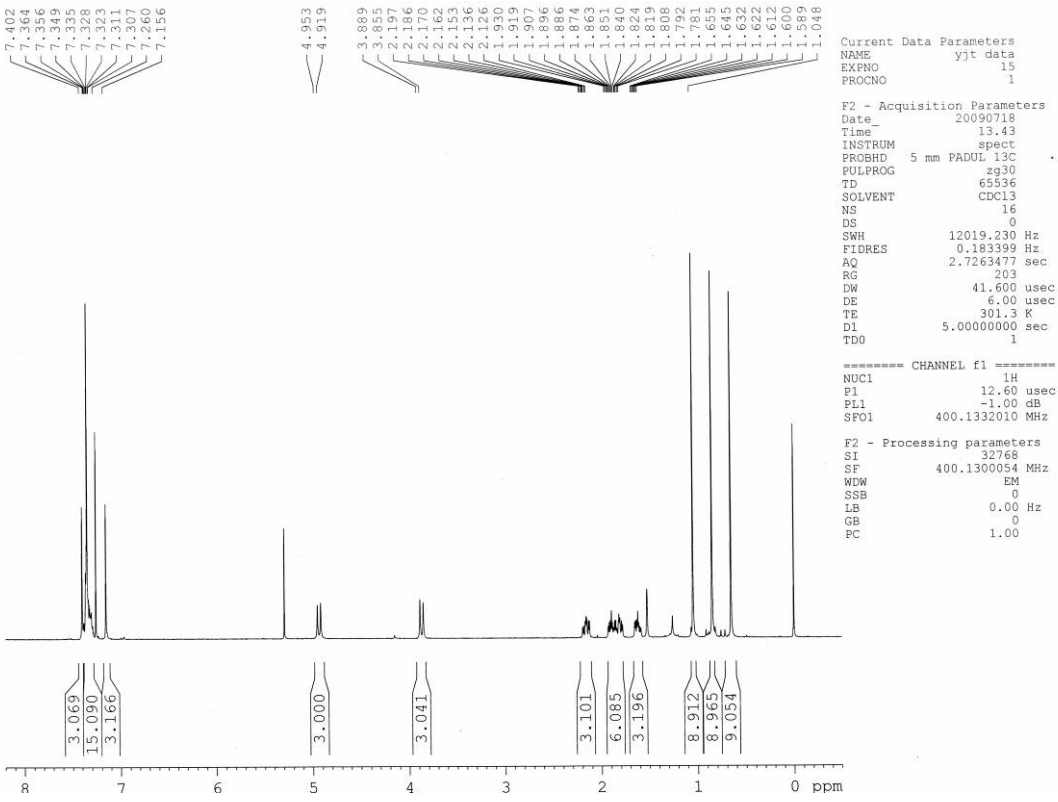


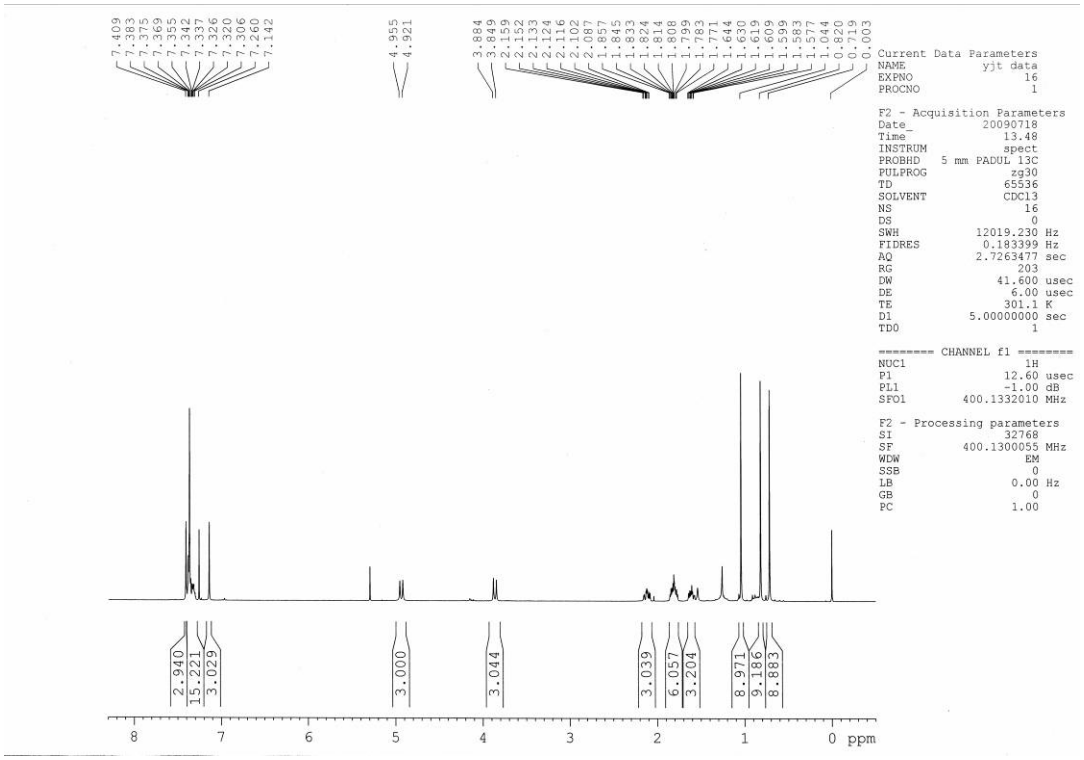
^{1}H and ^{13}C NMR of **(±)-6**



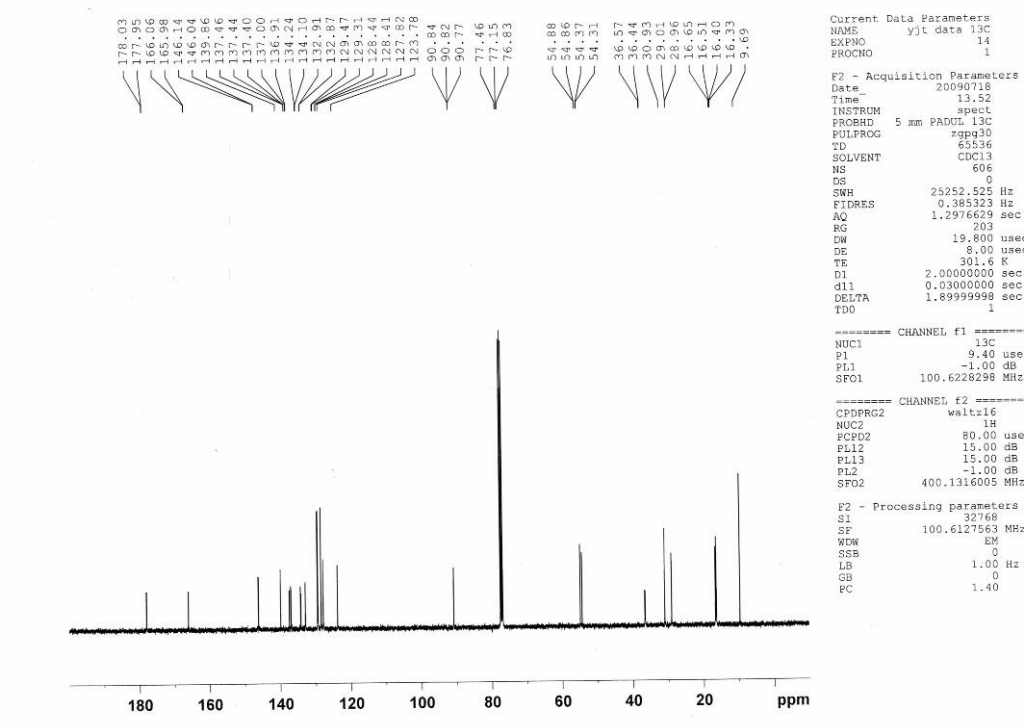


^{1}H NMR spectra of part **A** and part **B**





^{13}C NMR spectrum of the diastereoisomers



3. Titration experiment between fullerene and hosts

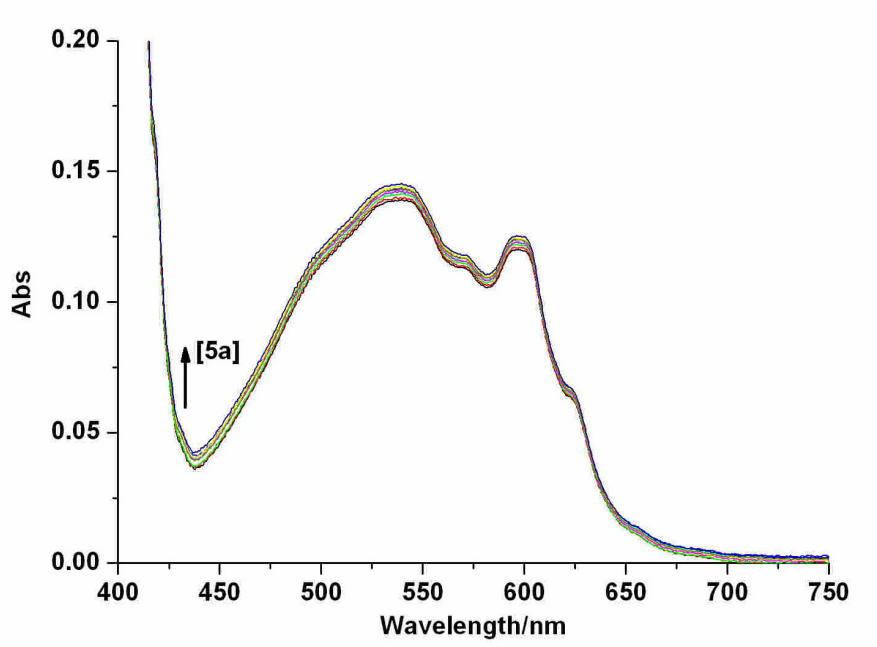


Fig. S1 Absorption spectra of C_{60} (1.60×10^{-4} mol·dm^{-3}) in the presence of **5a** in toluene at 25 °C. The concentrations of **5a** for the curves (from bottom to top) are: 0, 0.16, 0.32, 0.64, 0.96, 1.28, 1.60, 1.92, 2.40 × 10^{-4} mol·dm^{-3} .

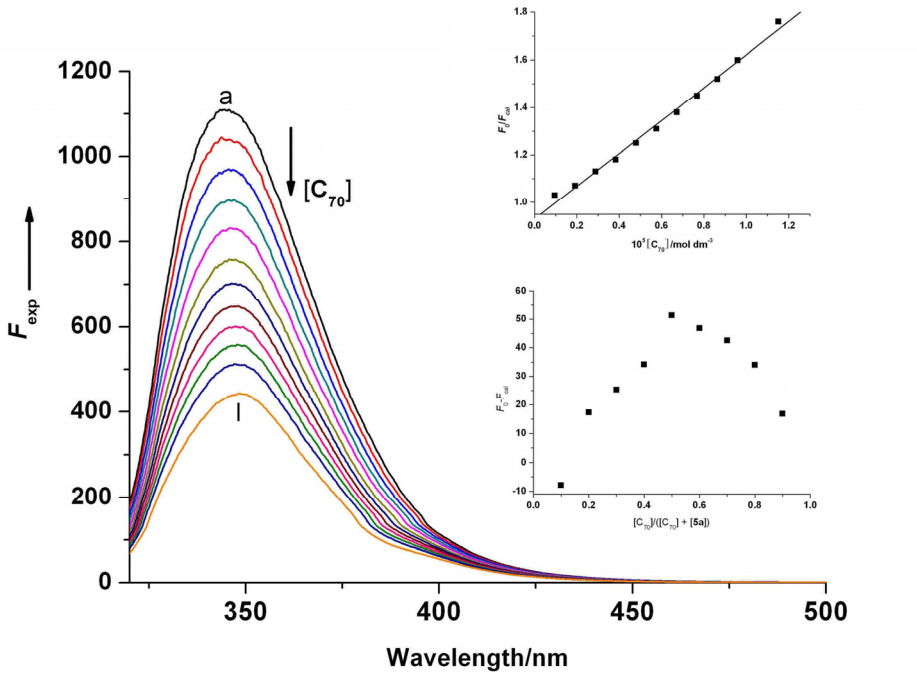


Fig. S2 Emission spectra (λ_{ex}= 305 nm, λ_{em} = 346 nm.) of **5a** (3.2×10^{-6} mol•dm^{-3}) in the presence of C_{70} in toluene at 25 °C. The concentrations of C_{70} for curves a-l (from top to bottom) were 0, 0.096, 0.192, 0.288, 0.384, 0.480, 0.576, 0.672, 0.768, 0.864, 0.960, 1.152 (× 10^{-5} mol•dm^{-3}). Insets: The up inset was the variation of fluorescence intensity F_0/F_{cal} of **5a** with increasing of C_{70} concentration. The down inset was the Job's plot for **5a**-C_{70} complex in toluene solution ([**5a**] + [C_{70}] = 6.4×10^{-6} mol•dm^{-1}).

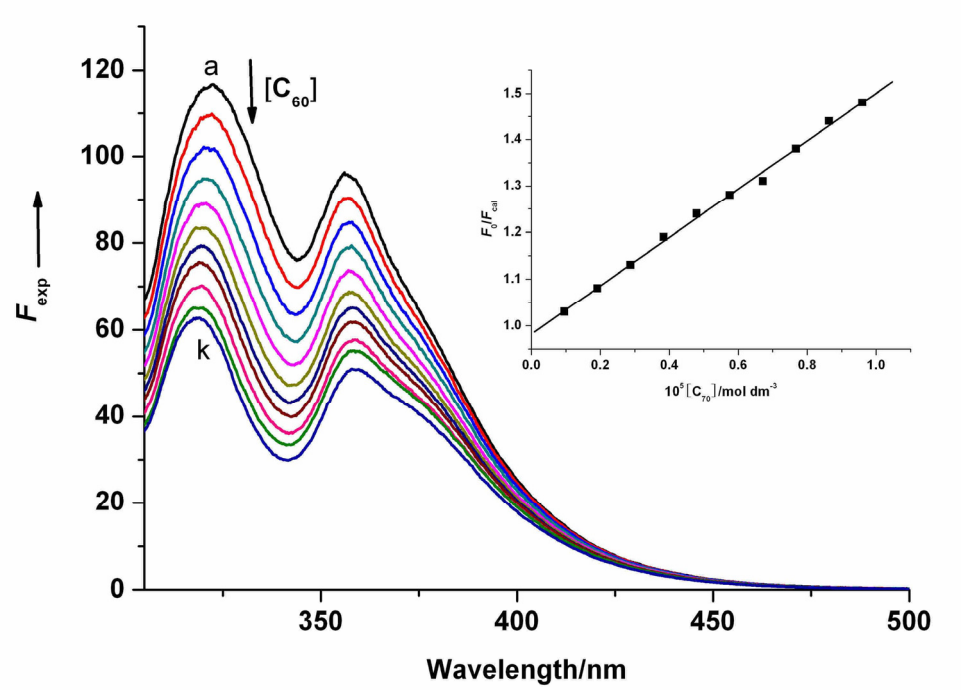


Fig. S3 Emission spectra (λ_{ex}= 296 nm, λ_{em} = 322 nm.) of CTV (**1**) (3.2×10^{-6} mol•dm^{-3}) in the presence of C_{60} in toluene at 25 ^{o}C. The concentrations of C_{60} for curves a-k (from top to bottom) were 0, 0.096, 0.192, 0.288, 0.384, 0.480, 0.576, 0.672, 0.768, 0.864, 0.960 ($\times 10^{-5}$ mol•dm^{-3}). The inset was the variation of fluorescence intensity F_0/F_{cal} of CTV with increasing of C_{60} concentration.

4. Molecular modeling of 5a-C_{60}

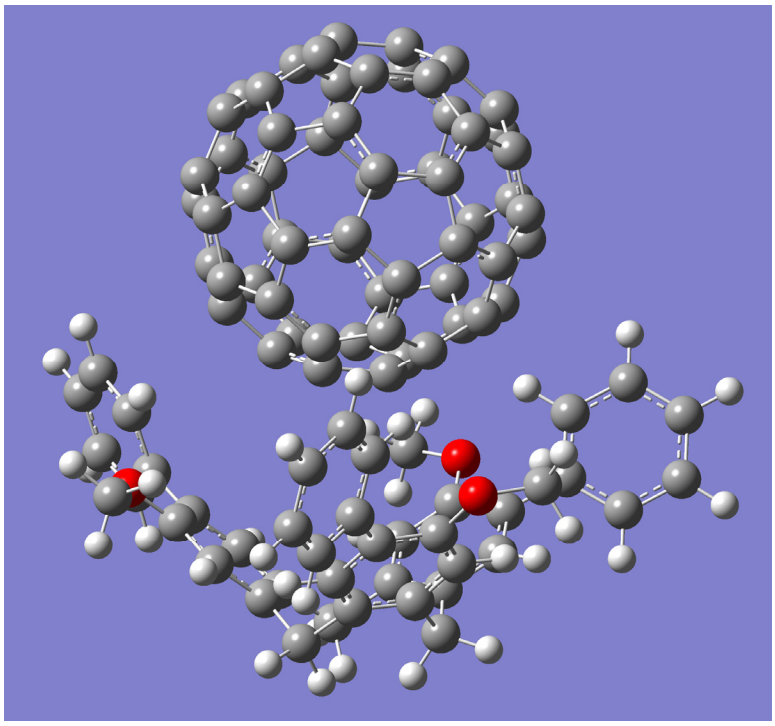


Fig. S4 Molecular modeling of complex **5a** and C_{60}. Based on the DFT(B3LYP, 3-21G) calculation results with Gaussian 09 software.

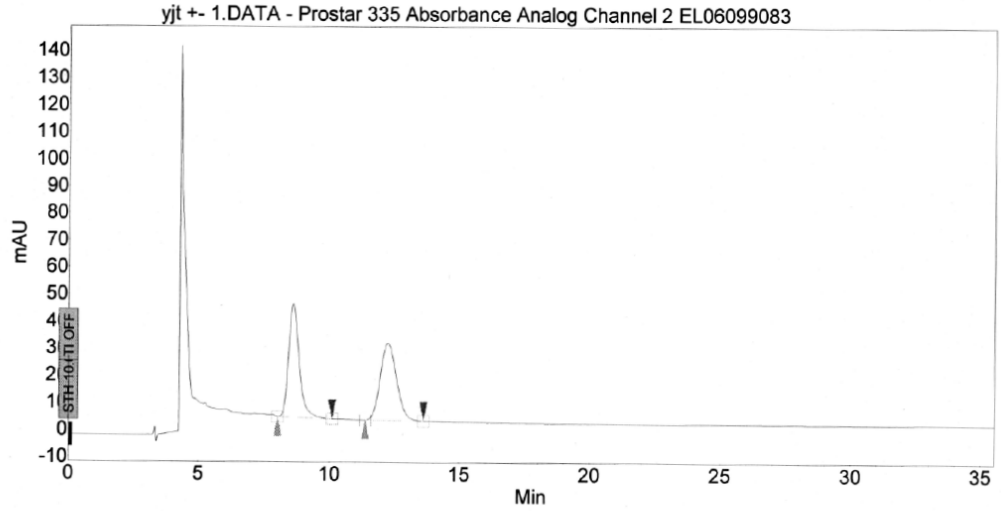
Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

5. Chiral HPLC trace of compound 6

Chromatogram : yjt +- 1_channel2

System : HPLC
Method : 1-75-25
User : Tian Hua

Acquired : 2008-10-21 12:50:18
Processed : 2008-10-21 13:30:56
Printed : 2009-7-10 20:01:08



Peak results :

Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	8.61	48.97	41.9	19.7	48.967
2	UNKNOWN	12.24	51.03	28.4	20.5	51.033
Total			100.00	70.3	40.1	100.000

Chromatogram : yjt +1_channel2

System : HPLC
Method : 1-75-25
User : Tian Hua

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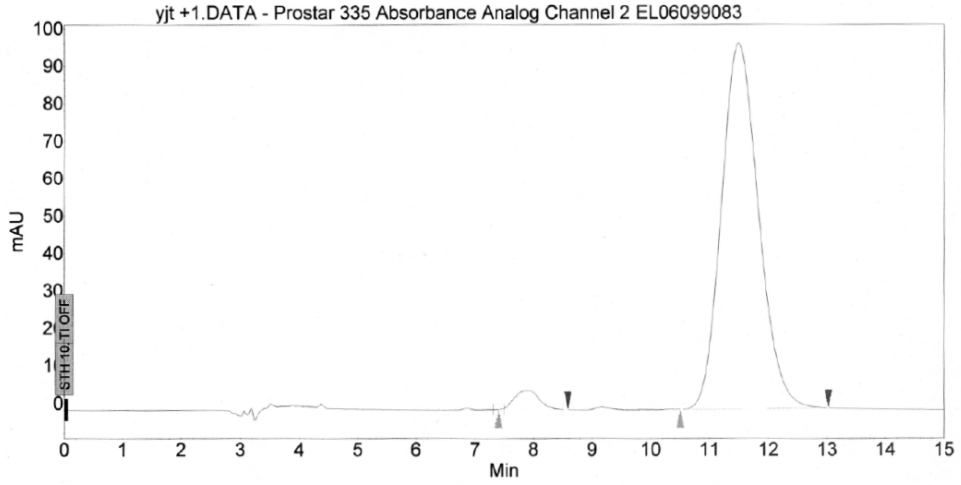

Peak results :

Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	7.92	3.38	5.0	2.5	3.383
2	UNKNOWN	11.49	96.62	97.5	71.4	96.617
Total			100.00	102.5	73.9	100.000

Chromatogram : yjt -1_channel1

System : HPLC
Method : 1-75-25
User : Tian Hua

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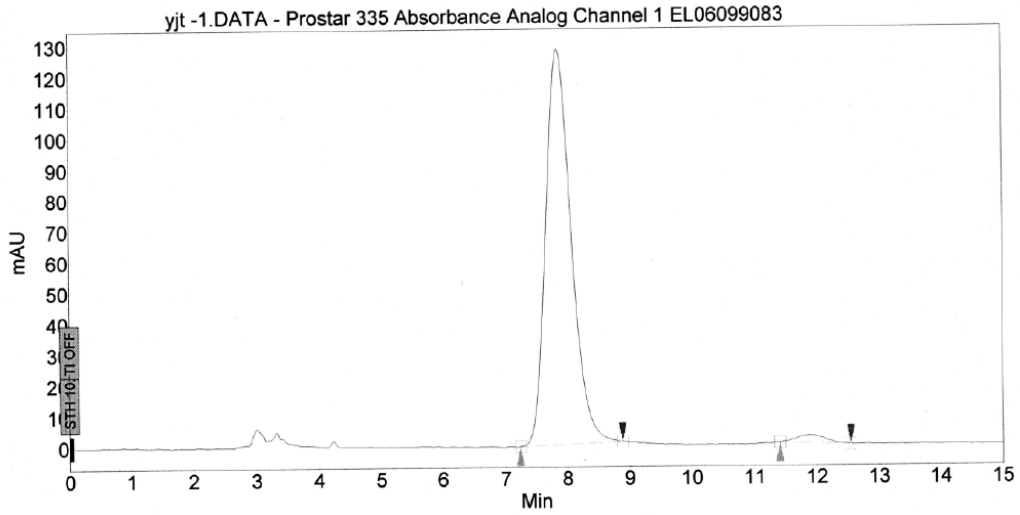

Peak results :

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2	UNKNOWN	11.91	2.05	2.4	1.3	2.048
Total			100.00	130.6	62.1	100.000