Supplementary Material for Organic & Biomolecular Chemistry

Supplementary data

Carbolithiation of *gem*-Aryl Disubstituted Methylenecyclopropanes

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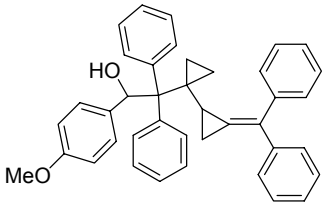
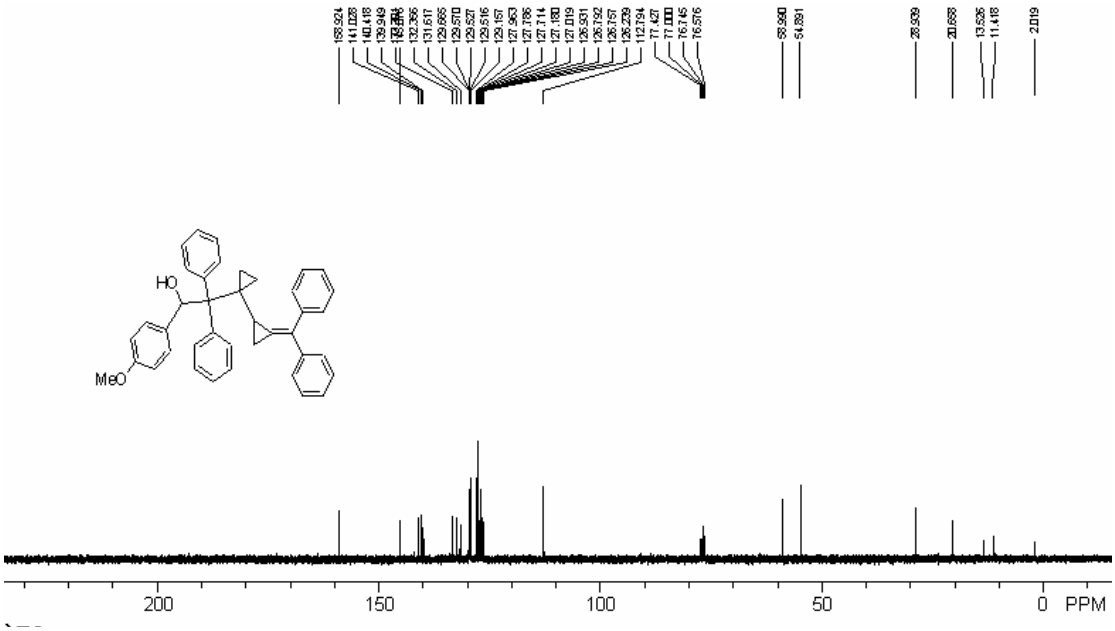
General Remarks. ^{1}H NMR spectra were recorded on a Bruker AM-300 spectrometer for solution in $CDCl_3$ with tetramethylsilane (TMS) as an internal standard; *J*-values are in Hz. Mass spectra were recorded with a HP-5989 instrument. Part of the solid compounds reported in this paper gave satisfactory CHN microanalyses with a Carlo-Erba 1106 analyzer. Commercially obtained reagents were used without further purification. All reactions were monitored by TLC with Huanghai GF_{254} silica gel coated plates. Flash column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

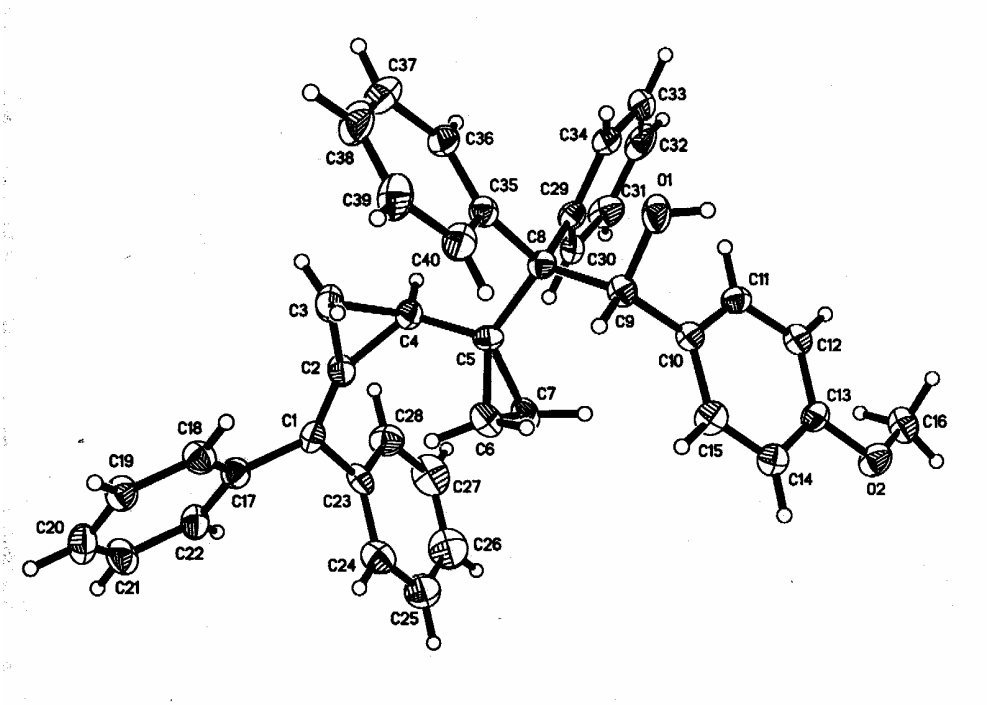
Typical Procedure for Carbolithiation of *gem*-Aryl Disubstituted Methylenecyclopropanes
Under an argon atmosphere, to the solution of MCP **1a** (284 mg, 1.4 mmol) in THF (5.0 mL) was added BuLi (1.6 M in hexane, 1.0 mL, 1.60 mmol), the resulting reaction mixture was stirred at -78 ^{o}C for about five hours, then *p*-anisaldehyde (191 mg, 1.4 mmol) was added and the reaction solution was further stirred for 1 hour at the same temperature. After reaction complete (monitored by TLC), the reaction mixture was quench by the addition of MeOH and warmed to room temperature. The reaction solution was diluted with ether (20 mL) and washed with water, saturated $NaHCO_3$ aqueous solution, brine and water. The organic layers were dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (petroleum ether/ethyl acetate = 10/1 to 2/1) to give **3d** as a colorless solid, 370 mg, yield 99%.

2-(2'-Benzhydrylidene-bicyclopropyl-1-yl)-1-(4-methoxyphenyl)-2,2-diphenylethanol (3d).



a white solid, yield: 99%. mp: 216-218 ^{o}C; IR (thin film): ν 3450, 2931, 1610, 1512, 1494, 1443, 1303, 1248, 1178, 1034 cm^{-1}; ^{1}H NMR ($CDCl_3$, TMS, 300 MHz): δ 0-0.11 (m, 2H, CH_2), 0.33-0.45 (m, 2H, CH_2), 0.65 (t, *J* = 9.0 Hz, 1H, CH_2), 1.08 (dd, *J* = 9.6, 4.2 Hz, 1H, CH_2), 2.12 (d, *J* = 3.0 Hz, 1H, OH), 2.28 (dd, *J* = 8.4, 4.8 Hz, 1H, CH), 3.85 (s, 3H, OCH_3), 5.56 (d, *J* = 3.0 Hz, 1H, CH), 6.44 (d, *J* = 8.1 Hz, 2H, ArH), 6.67 (d, *J* = 9.0 Hz, 2H, ArH), 7.34-7.62 (m, 16H, ArH), 7.86 (d, *J* = 7.2 Hz, 2H, ArH), 8.01-8.04 (m, 2H, ArH); ^{13}C NMR ($CDCl_3$, TMS, 75 MHz): δ 2.0, 11.4, 13.5, 20.7, 28.9, 54.9, 59.0, 76.7, 112.8, 126.2, 126.76, 126.80, 126.9, 127.0, 127.2, 127.7, 127.8, 128.0, 129.2, 129.6, 129.7, 131.6, 132.4, 133.3, 140.0, 140.4, 141.0, 145.1, 158.9; MS (EI) m/z: 411 (M^+-$C_8H_8O_2$) (7), 325 (7), 219 (14), 165 (16), 137 (100), 91 (29); HRMS (MALDI): calcd for $C_{40}H_{36}O_2Na$ (M^++Na) requires 571.2608, found: 571.2617.





The crystal data of *anti*-**3d** has been deposited in CCDC with number 246793. Empirical Formula: $C_{40}H_{36}O_2$; Formula Weight: 548.69; Crystal Color, Habit: colorless, prismatic; Crystal Dimensions: 0.398 x 0.217 x 0.071 mm; Crystal System: Orthorhombic; Lattice Type: Primitive; Lattice Parameters: a= 10.113(2)Å, b= 10.206(2)Å, c= 29.277(7)Å, α= 90°, β= 90°, γ= 90°, V= 3021.7(12)Å^3; Space group: P2(1)2(1)2(1); Z= 4; D_{calc}= 1.206 g/cm^3; F_{000}= 1168; Diffractometer: Rigaku AFC7R; Residuals: R; Rw: 0.0555, 0.0742.

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Table 1. Crystal data and structure refinement for cd2493.

Identification code	cd2493
Empirical formula	C40 H36 O2
Formula weight	548.69
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 10.113(2) A alpha = 90 deg. b = 10.206(2) A beta = 90 deg. c = 29.277(7) A gamma = 90 deg.
Volume	3021.7(12) A^3
Z, Calculated density	4, 1.206 Mg/m^3
Absorption coefficient	0.072 mm^-1
F(000)	1168
Crystal size	0.398 x 0.217 x 0.071 mm
Theta range for data collection	2.11 to 28.13 deg.
Limiting indices	-12<=h<=12, -13<=k<=12, -32<=l<=37
Reflections collected / unique	18167 / 6835 [R(int) = 0.1626]
Completeness to theta = 28.13	95.3 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.81329
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6835 / 6 / 413
Goodness-of-fit on F^2	0.635
Final R indices [I>2sigma(I)]	R1 = 0.0555, wR2 = 0.0742
R indices (all data)	R1 = 0.2113, wR2 = 0.1046
Absolute structure parameter	-1(2)
Extinction coefficient	0.0019(3)
Largest diff. peak and hole	0.158 and -0.159 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for cd2493.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	823(2)	5656(3)	409(1)	54(1)
O(2)	6772(3)	7495(3)	419(1)	52(1)
C(1)	1679(4)	3851(4)	2826(2)	40(1)
C(2)	1134(4)	3622(5)	2425(2)	42(1)
C(3)	-115(5)	3525(6)	2164(2)	53(2)
C(4)	1253(5)	3478(5)	1926(2)	42(1)
C(5)	1696(4)	4611(5)	1625(2)	37(1)
C(6)	1748(6)	5943(6)	1864(2)	56(2)
C(7)	3026(5)	5215(5)	1770(2)	50(1)
C(8)	1270(4)	4504(4)	1115(2)	35(1)
C(9)	1558(5)	5783(5)	831(2)	38(1)
C(10)	2967(4)	6163(4)	730(1)	35(1)
C(11)	3770(4)	5467(4)	440(1)	39(1)
C(12)	5051(4)	5863(4)	329(1)	39(1)
C(13)	5524(4)	6988(5)	514(2)	40(1)
C(14)	4766(4)	7737(4)	811(1)	44(1)
C(15)	3492(4)	7323(4)	904(2)	44(1)
C(16)	7689(4)	6611(4)	202(2)	54(1)
C(17)	918(4)	4135(4)	3241(2)	43(1)
C(18)	-375(4)	4653(4)	3209(2)	48(1)
C(19)	-1097(4)	4920(4)	3601(2)	50(1)
C(20)	-575(5)	4689(5)	4027(2)	58(2)
C(21)	705(5)	4174(5)	4060(2)	57(2)
C(22)	1417(4)	3917(4)	3674(2)	50(1)
C(23)	3179(5)	3869(5)	2861(2)	41(1)
C(24)	3838(5)	4927(5)	3049(2)	55(2)
C(25)	5201(6)	4963(6)	3060(2)	74(2)
C(26)	5932(6)	3943(7)	2880(2)	85(2)
C(27)	5288(5)	2878(6)	2699(2)	74(2)
C(28)	3905(5)	2850(5)	2693(2)	57(2)
C(29)	1985(4)	3353(4)	872(2)	37(1)
C(30)	3147(4)	2814(4)	1047(2)	43(1)
C(31)	3869(5)	1914(5)	798(2)	58(2)
C(32)	3466(5)	1523(5)	373(2)	63(2)
C(33)	2314(5)	2027(5)	198(2)	58(2)
C(34)	1579(4)	2927(5)	450(2)	48(1)
C(35)	-244(4)	4295(5)	1132(1)	38(1)
C(36)	-837(4)	3085(5)	1080(1)	47(1)
C(37)	-2214(5)	2941(6)	1138(2)	70(2)
C(38)	-2970(5)	3951(6)	1267(2)	70(2)
C(39)	-2421(5)	5159(6)	1325(2)	61(2)
C(40)	-1075(5)	5349(5)	1261(2)	53(1)

Table 3. Bond lengths [A] and angles [deg] for cd2493.

O(1)-C(9)	1.447(5)
O(1)-H(1)	0.8200
O(2)-C(13)	1.393(5)
O(2)-C(16)	1.442(4)
C(1)-C(2)	1.320(6)
C(1)-C(17)	1.468(6)
C(1)-C(23)	1.521(5)
C(2)-C(4)	1.470(6)
C(2)-C(3)	1.478(7)
C(3)-C(4)	1.549(6)
C(3)-H(1)	0.92(3)
C(3)-H(2)	0.986(18)
C(4)-C(5)	1.521(6)
C(4)-H(3)	0.96(3)
C(5)-C(6)	1.530(6)
C(5)-C(7)	1.539(6)
C(5)-C(8)	1.560(5)
C(6)-C(7)	1.515(7)
C(6)-H(4)	0.939(18)
C(6)-H(5)	0.970(18)
C(7)-H(6)	0.999(18)
C(7)-H(7)	0.988(17)
C(8)-C(35)	1.547(5)
C(8)-C(29)	1.552(6)
C(8)-C(9)	1.574(6)
C(9)-C(10)	1.507(6)
C(9)-H(8)	0.957(17)
C(10)-C(11)	1.373(5)
C(10)-C(15)	1.393(5)
C(11)-C(12)	1.395(5)
C(11)-H(11)	0.9300
C(12)-C(13)	1.357(5)
C(12)-H(12)	0.9300
C(13)-C(14)	1.388(5)
C(14)-C(15)	1.383(5)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-C(22)	1.380(6)
C(17)-C(18)	1.414(5)
C(18)-C(19)	1.387(5)
C(18)-H(18)	0.9300
C(19)-C(20)	1.376(5)
C(19)-H(19)	0.9300
C(20)-C(21)	1.400(6)
C(20)-H(20)	0.9300
C(21)-C(22)	1.365(5)
C(21)-H(21)	0.9300
C(22)-H(22)	0.9300
C(23)-C(28)	1.365(6)
C(23)-C(24)	1.383(6)
C(24)-C(25)	1.379(6)
C(24)-H(24)	0.9300
C(25)-C(26)	1.381(7)
C(25)-H(25)	0.9300
C(26)-C(27)	1.374(7)
C(26)-H(26)	0.9300
C(27)-C(28)	1.400(6)
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300
C(29)-C(34)	1.372(5)
C(29)-C(30)	1.395(6)

C(30)-C(31)	1.382(5)
C(30)-H(30)	0.9300
C(31)-C(32)	1.369(6)
C(31)-H(31)	0.9300
C(32)-C(33)	1.372(6)
C(32)-H(32)	0.9300
C(33)-C(34)	1.393(6)
C(33)-H(33)	0.9300
C(34)-H(34)	0.9300
C(35)-C(36)	1.381(5)
C(35)-C(40)	1.417(6)
C(36)-C(37)	1.411(6)
C(36)-H(36)	0.9300
C(37)-C(38)	1.338(7)
C(37)-H(37)	0.9300
C(38)-C(39)	1.361(6)
C(38)-H(38)	0.9300
C(39)-C(40)	1.388(6)
C(39)-H(39)	0.9300
C(40)-H(40)	0.9300

C(9)-O(1)-H(1)	109.5
C(13)-O(2)-C(16)	116.0(3)
C(2)-C(1)-C(17)	123.7(4)
C(2)-C(1)-C(23)	118.6(4)
C(17)-C(1)-C(23)	117.7(4)
C(1)-C(2)-C(4)	150.1(5)
C(1)-C(2)-C(3)	145.9(5)
C(4)-C(2)-C(3)	63.4(3)
C(2)-C(3)-C(4)	58.1(3)
C(2)-C(3)-H(1)	111(2)
C(4)-C(3)-H(1)	107(2)
C(2)-C(3)-H(2)	119(3)
C(4)-C(3)-H(2)	112(2)
H(1)-C(3)-H(2)	128(3)
C(2)-C(4)-C(5)	121.5(4)
C(2)-C(4)-C(3)	58.6(3)
C(5)-C(4)-C(3)	120.0(5)
C(2)-C(4)-H(3)	116(2)
C(5)-C(4)-H(3)	113(2)
C(3)-C(4)-H(3)	117(2)
C(4)-C(5)-C(6)	114.9(4)
C(4)-C(5)-C(7)	113.7(4)
C(6)-C(5)-C(7)	59.2(3)
C(4)-C(5)-C(8)	114.9(4)
C(6)-C(5)-C(8)	120.6(4)
C(7)-C(5)-C(8)	122.2(4)
C(7)-C(6)-C(5)	60.7(3)
C(7)-C(6)-H(4)	112(2)
C(5)-C(6)-H(4)	108(2)
C(7)-C(6)-H(5)	114(3)
C(5)-C(6)-H(5)	117(3)
H(4)-C(6)-H(5)	127(4)
C(6)-C(7)-C(5)	60.1(3)
C(6)-C(7)-H(6)	118(3)
C(5)-C(7)-H(6)	111(3)
C(6)-C(7)-H(7)	108.0(19)
C(5)-C(7)-H(7)	110.0(19)
H(6)-C(7)-H(7)	130(3)
C(35)-C(8)-C(29)	111.8(4)
C(35)-C(8)-C(5)	104.6(3)
C(29)-C(8)-C(5)	111.3(4)
C(35)-C(8)-C(9)	108.3(4)
C(29)-C(8)-C(9)	107.5(3)
C(5)-C(8)-C(9)	113.3(4)
O(1)-C(9)-C(10)	109.9(4)
O(1)-C(9)-C(8)	106.3(4)
C(10)-C(9)-C(8)	119.5(4)

O(1)-C(9)-H(8)	107.6(18)
C(10)-C(9)-H(8)	110.2(18)
C(8)-C(9)-H(8)	102.5(18)
C(11)-C(10)-C(15)	116.2(4)
C(11)-C(10)-C(9)	123.2(4)
C(15)-C(10)-C(9)	120.4(4)
C(10)-C(11)-C(12)	122.8(4)
C(10)-C(11)-H(11)	118.6
C(12)-C(11)-H(11)	118.6
C(13)-C(12)-C(11)	118.7(4)
C(13)-C(12)-H(12)	120.7
C(11)-C(12)-H(12)	120.7
C(12)-C(13)-O(2)	123.7(4)
C(12)-C(13)-C(14)	121.4(4)
O(2)-C(13)-C(14)	114.9(4)
C(15)-C(14)-C(13)	118.0(5)
C(15)-C(14)-H(14)	121.0
C(13)-C(14)-H(14)	121.0
C(14)-C(15)-C(10)	122.8(5)
C(14)-C(15)-H(15)	118.6
C(10)-C(15)-H(15)	118.6
O(2)-C(16)-H(16A)	109.5
O(2)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
O(2)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(22)-C(17)-C(18)	117.4(4)
C(22)-C(17)-C(1)	122.4(4)
C(18)-C(17)-C(1)	120.2(4)
C(19)-C(18)-C(17)	120.4(4)
C(19)-C(18)-H(18)	119.8
C(17)-C(18)-H(18)	119.8
C(20)-C(19)-C(18)	121.0(5)
C(20)-C(19)-H(19)	119.5
C(18)-C(19)-H(19)	119.5
C(19)-C(20)-C(21)	118.7(5)
C(19)-C(20)-H(20)	120.6
C(21)-C(20)-H(20)	120.6
C(22)-C(21)-C(20)	120.2(5)
C(22)-C(21)-H(21)	119.9
C(20)-C(21)-H(21)	119.9
C(21)-C(22)-C(17)	122.4(5)
C(21)-C(22)-H(22)	118.8
C(17)-C(22)-H(22)	118.8
C(28)-C(23)-C(24)	118.7(5)
C(28)-C(23)-C(1)	120.2(5)
C(24)-C(23)-C(1)	121.1(5)
C(25)-C(24)-C(23)	120.8(5)
C(25)-C(24)-H(24)	119.6
C(23)-C(24)-H(24)	119.6
C(24)-C(25)-C(26)	120.4(6)
C(24)-C(25)-H(25)	119.8
C(26)-C(25)-H(25)	119.8
C(27)-C(26)-C(25)	119.3(6)
C(27)-C(26)-H(26)	120.3
C(25)-C(26)-H(26)	120.3
C(26)-C(27)-C(28)	119.7(6)
C(26)-C(27)-H(27)	120.2
C(28)-C(27)-H(27)	120.2
C(23)-C(28)-C(27)	121.1(5)
C(23)-C(28)-H(28)	119.4
C(27)-C(28)-H(28)	119.4
C(34)-C(29)-C(30)	117.3(4)
C(34)-C(29)-C(8)	120.8(4)
C(30)-C(29)-C(8)	121.4(4)
C(31)-C(30)-C(29)	120.9(5)
C(31)-C(30)-H(30)	119.6

C(29)-C(30)-H(30)	119.6
C(32)-C(31)-C(30)	121.0(5)
C(32)-C(31)-H(31)	119.5
C(30)-C(31)-H(31)	119.5
C(31)-C(32)-C(33)	118.9(5)
C(31)-C(32)-H(32)	120.6
C(33)-C(32)-H(32)	120.6
C(32)-C(33)-C(34)	120.2(5)
C(32)-C(33)-H(33)	119.9
C(34)-C(33)-H(33)	119.9
C(29)-C(34)-C(33)	121.7(5)
C(29)-C(34)-H(34)	119.2
C(33)-C(34)-H(34)	119.2
C(36)-C(35)-C(40)	116.7(4)
C(36)-C(35)-C(8)	123.3(4)
C(40)-C(35)-C(8)	119.5(4)
C(35)-C(36)-C(37)	120.6(5)
C(35)-C(36)-H(36)	119.7
C(37)-C(36)-H(36)	119.7
C(38)-C(37)-C(36)	121.1(6)
C(38)-C(37)-H(37)	119.4
C(36)-C(37)-H(37)	119.4
C(37)-C(38)-C(39)	120.0(5)
C(37)-C(38)-H(38)	120.0
C(39)-C(38)-H(38)	120.0
C(38)-C(39)-C(40)	120.7(5)
C(38)-C(39)-H(39)	119.7
C(40)-C(39)-H(39)	119.7
C(39)-C(40)-C(35)	120.8(5)
C(39)-C(40)-H(40)	119.6
C(35)-C(40)-H(40)	119.6

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for cd2493.
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
O(1)	31(2)	88(3)	44(2)	18(2)	0(2)	-9(2)
O(2)	35(2)	54(2)	67(2)	-6(2)	11(2)	-5(2)
C(1)	37(3)	35(3)	47(3)	6(3)	9(3)	-1(3)
C(2)	34(3)	58(4)	35(3)	5(3)	-1(3)	1(3)
C(3)	45(4)	67(5)	46(3)	12(4)	5(3)	-7(4)
C(4)	35(3)	53(4)	40(3)	0(3)	3(3)	-6(3)
C(5)	33(3)	41(3)	38(3)	-3(2)	-8(2)	-2(3)
C(6)	64(4)	66(4)	37(4)	-4(3)	4(3)	-2(4)
C(7)	57(4)	65(4)	30(3)	6(3)	-1(3)	-3(3)
C(8)	26(3)	39(3)	40(3)	-1(2)	0(2)	1(2)
C(9)	34(3)	42(3)	39(3)	-1(3)	3(3)	5(3)
C(10)	31(3)	36(3)	36(3)	-1(2)	1(2)	4(2)
C(11)	43(3)	34(3)	41(3)	-3(3)	-3(3)	-2(3)
C(12)	34(3)	46(4)	37(3)	1(3)	2(2)	7(3)
C(13)	31(3)	43(3)	46(3)	2(3)	1(3)	-4(3)
C(14)	44(3)	41(3)	47(3)	1(3)	2(3)	3(3)
C(15)	40(3)	37(3)	55(3)	-1(3)	4(3)	8(3)
C(16)	35(3)	79(4)	47(3)	6(3)	1(3)	3(3)
C(17)	44(3)	47(3)	40(3)	4(3)	-1(3)	-2(3)
C(18)	45(3)	55(4)	44(3)	-1(3)	-4(3)	3(3)
C(19)	38(3)	62(4)	50(3)	1(3)	0(3)	2(3)
C(20)	57(4)	52(4)	63(4)	5(3)	23(3)	3(3)
C(21)	74(4)	62(4)	35(3)	8(3)	0(3)	0(3)
C(22)	44(3)	60(4)	46(3)	5(3)	7(3)	-1(3)
C(23)	42(3)	57(4)	26(3)	0(3)	1(2)	11(3)
C(24)	49(4)	66(4)	50(3)	-4(3)	-7(3)	9(3)
C(25)	62(5)	91(5)	67(4)	-7(4)	-5(3)	-15(4)
C(26)	50(4)	127(7)	77(5)	5(4)	-19(4)	0(5)
C(27)	47(4)	102(6)	74(5)	6(4)	-7(3)	28(4)
C(28)	49(3)	61(4)	61(4)	-4(3)	-7(3)	2(3)
C(29)	26(3)	40(3)	44(3)	1(2)	2(2)	-1(2)
C(30)	39(3)	53(3)	37(3)	2(3)	8(3)	-11(3)
C(31)	34(3)	57(4)	81(4)	-13(3)	7(3)	3(3)
C(32)	51(4)	51(4)	88(5)	-19(3)	37(4)	-11(3)
C(33)	65(4)	66(4)	42(3)	-14(3)	20(3)	-21(3)
C(34)	38(3)	62(4)	43(3)	1(3)	-3(3)	-18(3)
C(35)	39(3)	41(3)	36(3)	5(3)	-1(2)	1(3)
C(36)	37(3)	58(4)	46(3)	3(3)	-4(2)	-8(3)
C(37)	50(4)	75(5)	84(5)	-3(4)	4(3)	-24(4)
C(38)	34(4)	102(6)	75(4)	11(4)	6(3)	-12(4)
C(39)	38(4)	77(5)	69(4)	17(3)	7(3)	11(3)
C(40)	45(3)	63(4)	51(3)	12(3)	-6(3)	-2(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for cd2493.

	x	y	z	U(eq)
H(1)	1312	5812	192	82
H(11)	3446	4698	311	47
H(12)	5571	5365	133	47
H(14)	5104	8494	943	53
H(15)	2962	7840	1091	53
H(16A)	7733	5809	373	80
H(16B)	8550	7007	192	80
H(16C)	7395	6427	-103	80
H(18)	-744	4815	2924	58
H(19)	-1947	5261	3575	60
H(20)	-1063	4870	4289	69
H(21)	1072	4007	4345	69
H(22)	2269	3584	3703	60
H(24)	3357	5623	3169	66
H(25)	5630	5679	3189	88
H(26)	6851	3976	2883	102
H(27)	5769	2179	2581	89
H(28)	3472	2124	2572	68
H(30)	3439	3065	1335	52
H(31)	4641	1567	922	69
H(32)	3964	927	206	76
H(33)	2024	1767	-89	70
H(34)	793	3248	329	57
H(36)	-324	2359	1007	57
H(37)	-2604	2129	1085	83
H(38)	-3869	3829	1318	84
H(39)	-2954	5862	1408	74
H(40)	-715	6179	1304	63
H(1)	-430(30)	2680(30)	2167(12)	26(12)
H(2)	-600(40)	4340(30)	2092(13)	66(17)
H(3)	1550(30)	2640(30)	1822(11)	30(12)
H(4)	1460(30)	5830(30)	2166(7)	36(12)
H(5)	1630(40)	6710(30)	1674(12)	60(16)
H(6)	3420(40)	4710(40)	2027(11)	82(18)
H(7)	3460(30)	5630(30)	1504(8)	21(11)
H(8)	1140(30)	6450(20)	1010(9)	1(9)

Table 6. Torsion angles [deg] for cd2493.

C(17)-C(1)-C(2)-C(4)	166.7(8)
C(23)-C(1)-C(2)-C(4)	-11.3(12)
C(17)-C(1)-C(2)-C(3)	1.5(12)
C(23)-C(1)-C(2)-C(3)	-176.5(7)
C(1)-C(2)-C(3)-C(4)	171.8(9)
C(1)-C(2)-C(4)-C(5)	-62.6(11)
C(3)-C(2)-C(4)-C(5)	108.2(6)
C(1)-C(2)-C(4)-C(3)	-170.8(10)
C(2)-C(3)-C(4)-C(5)	-110.8(5)
C(2)-C(4)-C(5)-C(6)	-11.0(7)
C(3)-C(4)-C(5)-C(6)	58.3(6)
C(2)-C(4)-C(5)-C(7)	54.6(6)
C(3)-C(4)-C(5)-C(7)	123.9(5)
C(2)-C(4)-C(5)-C(8)	-157.6(4)
C(3)-C(4)-C(5)-C(8)	-88.3(5)
C(4)-C(5)-C(6)-C(7)	103.9(5)
C(8)-C(5)-C(6)-C(7)	-111.6(5)
C(4)-C(5)-C(7)-C(6)	-105.9(5)
C(8)-C(5)-C(7)-C(6)	109.0(5)
C(4)-C(5)-C(8)-C(35)	53.6(5)
C(6)-C(5)-C(8)-C(35)	-90.9(5)
C(7)-C(5)-C(8)-C(35)	-161.6(4)
C(4)-C(5)-C(8)-C(29)	-67.4(5)
C(6)-C(5)-C(8)-C(29)	148.1(4)
C(7)-C(5)-C(8)-C(29)	77.4(5)
C(4)-C(5)-C(8)-C(9)	171.4(4)
C(6)-C(5)-C(8)-C(9)	26.8(6)
C(7)-C(5)-C(8)-C(9)	-43.9(6)
C(35)-C(8)-C(9)-O(1)	-50.4(4)
C(29)-C(8)-C(9)-O(1)	70.6(4)
C(5)-C(8)-C(9)-O(1)	-165.9(3)
C(35)-C(8)-C(9)-C(10)	-175.4(4)
C(29)-C(8)-C(9)-C(10)	-54.4(5)
C(5)-C(8)-C(9)-C(10)	69.1(5)
O(1)-C(9)-C(10)-C(11)	-54.4(6)
C(8)-C(9)-C(10)-C(11)	68.8(6)
O(1)-C(9)-C(10)-C(15)	120.5(4)
C(8)-C(9)-C(10)-C(15)	-116.3(5)
C(15)-C(10)-C(11)-C(12)	1.5(7)
C(9)-C(10)-C(11)-C(12)	176.6(4)
C(10)-C(11)-C(12)-C(13)	-0.4(7)
C(11)-C(12)-C(13)-O(2)	-178.3(4)
C(11)-C(12)-C(13)-C(14)	0.5(7)
C(16)-O(2)-C(13)-C(12)	-15.0(6)
C(16)-O(2)-C(13)-C(14)	166.1(4)
C(12)-C(13)-C(14)-C(15)	-1.8(7)
O(2)-C(13)-C(14)-C(15)	177.1(4)
C(13)-C(14)-C(15)-C(10)	3.0(7)
C(11)-C(10)-C(15)-C(14)	-2.8(7)
C(9)-C(10)-C(15)-C(14)	-178.1(4)
C(2)-C(1)-C(17)-C(22)	156.4(5)
C(23)-C(1)-C(17)-C(22)	-25.6(7)
C(2)-C(1)-C(17)-C(18)	-23.7(7)
C(23)-C(1)-C(17)-C(18)	154.3(4)
C(22)-C(17)-C(18)-C(19)	-0.2(7)
C(1)-C(17)-C(18)-C(19)	179.9(4)
C(17)-C(18)-C(19)-C(20)	0.0(7)
C(18)-C(19)-C(20)-C(21)	-0.1(7)
C(19)-C(20)-C(21)-C(22)	0.4(8)
C(20)-C(21)-C(22)-C(17)	-0.6(8)
C(18)-C(17)-C(22)-C(21)	0.5(7)
C(1)-C(17)-C(22)-C(21)	-179.6(4)
C(2)-C(1)-C(23)-C(28)	-51.4(7)
C(17)-C(1)-C(23)-C(28)	130.6(5)

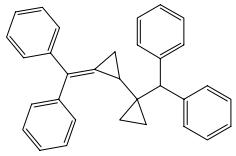
C(2)-C(1)-C(23)-C(24)	126.4(5)
C(17)-C(1)-C(23)-C(24)	-51.6(7)
C(28)-C(23)-C(24)-C(25)	0.9(8)
C(1)-C(23)-C(24)-C(25)	-176.9(4)
C(23)-C(24)-C(25)-C(26)	0.4(9)
C(24)-C(25)-C(26)-C(27)	-1.3(9)
C(25)-C(26)-C(27)-C(28)	0.8(9)
C(24)-C(23)-C(28)-C(27)	-1.4(8)
C(1)-C(23)-C(28)-C(27)	176.5(4)
C(26)-C(27)-C(28)-C(23)	0.5(9)
C(35)-C(8)-C(29)-C(34)	51.0(5)
C(5)-C(8)-C(29)-C(34)	167.6(4)
C(9)-C(8)-C(29)-C(34)	-67.7(5)
C(35)-C(8)-C(29)-C(30)	-136.4(4)
C(5)-C(8)-C(29)-C(30)	-19.8(5)
C(9)-C(8)-C(29)-C(30)	104.9(4)
C(34)-C(29)-C(30)-C(31)	1.6(6)
C(8)-C(29)-C(30)-C(31)	-171.3(4)
C(29)-C(30)-C(31)-C(32)	-0.1(7)
C(30)-C(31)-C(32)-C(33)	-1.0(8)
C(31)-C(32)-C(33)-C(34)	0.5(7)
C(30)-C(29)-C(34)-C(33)	-2.1(7)
C(8)-C(29)-C(34)-C(33)	170.8(4)
C(32)-C(33)-C(34)-C(29)	1.1(7)
C(29)-C(8)-C(35)-C(36)	20.0(6)
C(5)-C(8)-C(35)-C(36)	-100.6(5)
C(9)-C(8)-C(35)-C(36)	138.2(4)
C(29)-C(8)-C(35)-C(40)	-168.0(4)
C(5)-C(8)-C(35)-C(40)	71.4(5)
C(9)-C(8)-C(35)-C(40)	-49.8(5)
C(40)-C(35)-C(36)-C(37)	2.4(7)
C(8)-C(35)-C(36)-C(37)	174.5(5)
C(35)-C(36)-C(37)-C(38)	-3.5(8)
C(36)-C(37)-C(38)-C(39)	3.0(9)
C(37)-C(38)-C(39)-C(40)	-1.5(9)
C(38)-C(39)-C(40)-C(35)	0.4(8)
C(36)-C(35)-C(40)-C(39)	-0.9(7)
C(8)-C(35)-C(40)-C(39)	-173.4(4)

Symmetry transformations used to generate equivalent atoms:

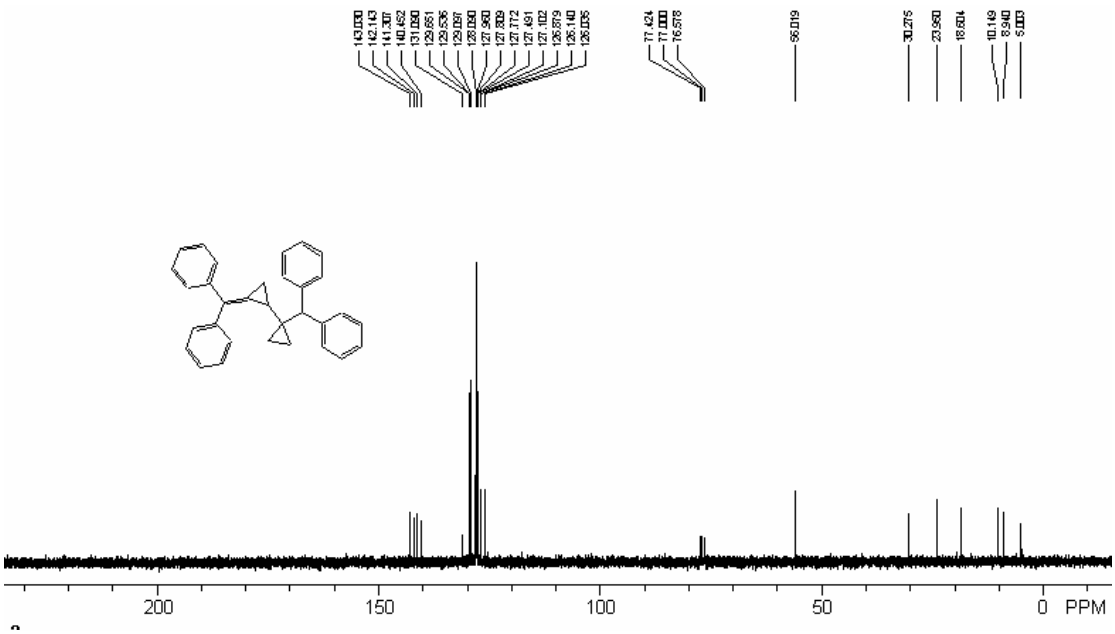
Table 7. Hydrogen bonds for cd2493 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

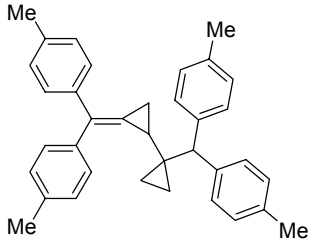
1-Benzhydryl-2'-benzhydrylidene-bicyclopropyl (2a).



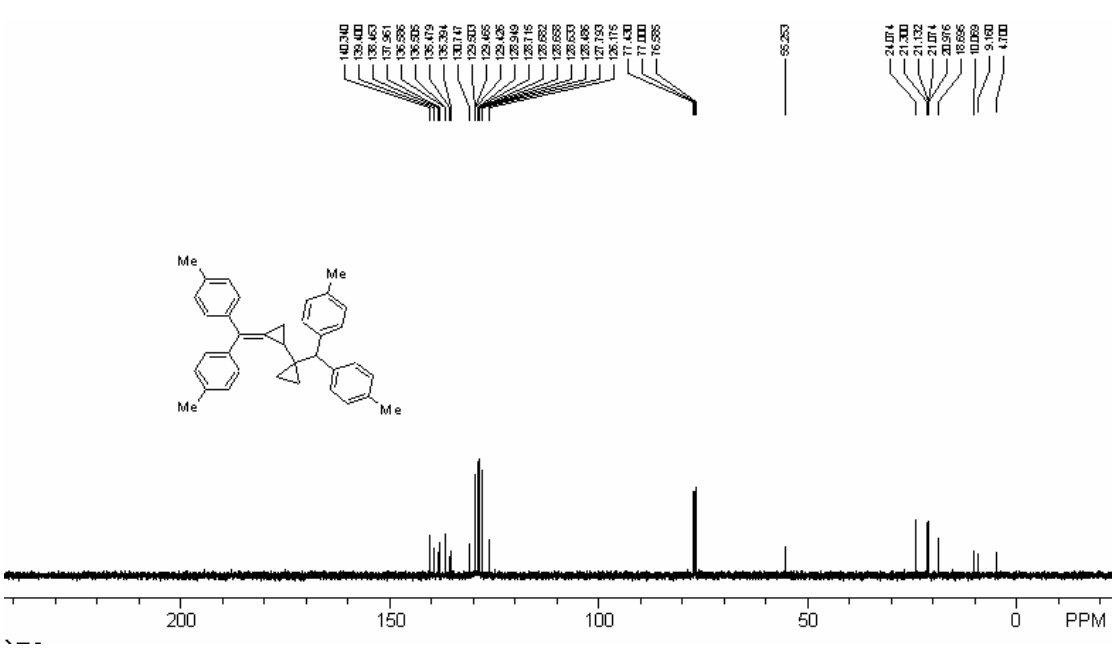
a white solid, yield: 99%. mp: 104-106 ^{o}C; IR (thin film): ν 3021, 1598, 1493, 1447, 1077, 1032 cm^{-1}; ^{1}H NMR ($CDCl_3$, TMS, 300 MHz): δ 0-0.08 (m, 2H, CH_2), 0.18-0.27 (m, 2H, CH_2), 1.18 (dd, J = 8.7, 5.1 Hz, 1H, CH_2), 1.34-1.40 (m, 1H, CH_2), 2.37 (dd, J = 8.4, 5.1 Hz, 1H, CH), 4.16 (s, 1H, C=CH), 7.22-7.53 (m, 20H, ArH); ^{13}C NMR ($CDCl_3$, TMS, 75 MHz): δ 5.0, 8.9, 10.1, 18.6, 24.0, 56.0, 126.1, 126.2, 126.9, 127.1, 127.5, 127.80, 127.83, 128.0, 128.1, 129.1, 129.6, 129.7, 131.1, 140.5, 141.3, 142.2, 143.1; MS (EI) m/z: 412 (M^+) (38), 383 (16), 321 (39), 245 (83), 217 (62), 205 (74), 167 (100), 152 (42), 115 (41), 91 (73); HRMS (EI): calcd. for $C_{32}H_{28}$ requires 412.2191, found: 412.2176.



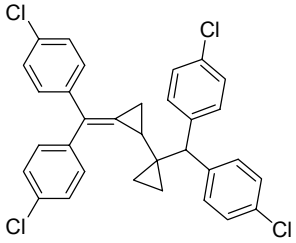
1-Di-p-tolylmethyl-2'-di-p-tolylmethylene-bicyclopropyl (2b).



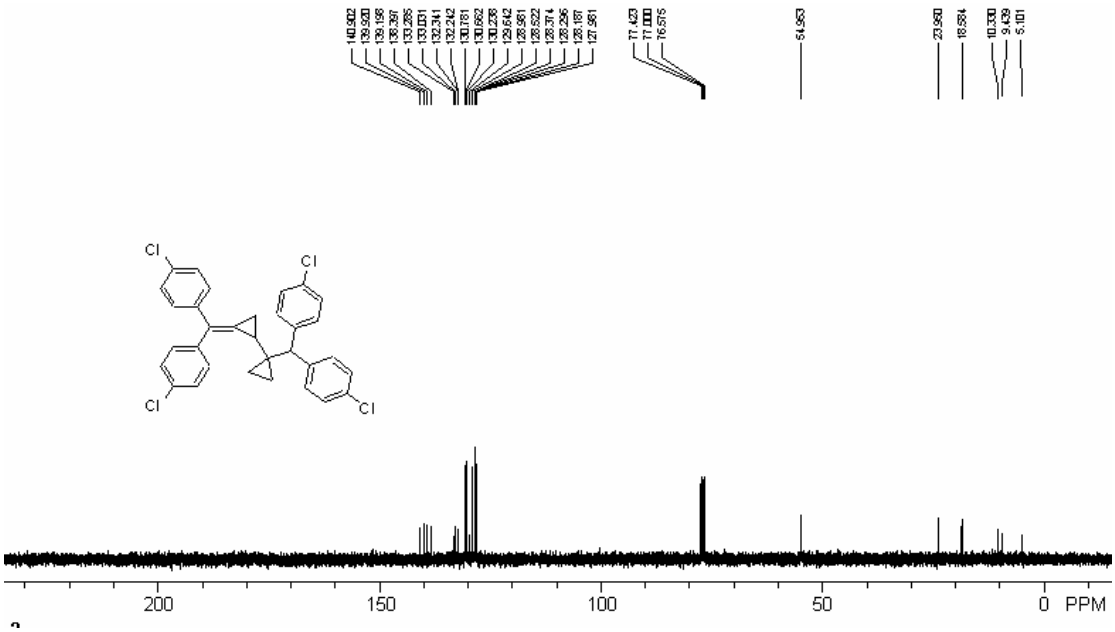
a white solid, yield: 32%. IR (thin film): ν 2921, 1511, 1454, 1418, 1265, 1182, 1111, 1022 cm^{-1}; ^1H NMR ($CDCl_3$, TMS, 300 MHz): δ 0-0.12 (m, 2H, CH_2), 0.19-0.31 (m, 2H, CH_2), 1.21 (dd, J = 9.3, 4.8 Hz, 1H, CH_2), 1.36-1.41 (m, 1H, CH_2), 2.41 (dd, J = 8.4, 4.5 Hz, 1H, CH), 2.44 (s, 3H, CH_3), 2.49 (s, 6H, CH_3), 2.56 (s, 3H, CH_3), 4.15 (s, 1H, CH), 7.17-7.46 (m, 16H, ArH); ^{13}C NMR ($CDCl_3$, TMS, 75 MHz): δ 4.7, 9.2, 10.1, 18.7, 20.96, 21.06, 21.12, 21.3, 24.1, 55.3, 126.2, 127.8, 128.5, 128.63, 128.68, 128.72, 129.0, 129.4, 129.5, 130.7, 135.4, 135.5, 136.5, 136.6, 138.0, 138.5, 139.4, 140.3; MS (EI) m/z: 468 (M^+) (7), 376 (9), 363 (12), 273 (25), 247 (27), 219 (26), 195 (75), 165 (45), 105 (100); HRMS (MALDI): calcd for $C_{36}H_{37}$ (M^++1) requires 469.2890, found: 469.2872.



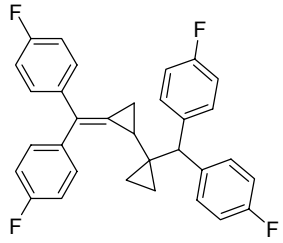
1-[Bis(4-chlorophenyl)methyl]-2'-[bis(4-chlorophenyl)methylene]bicyclopropyl (2c).



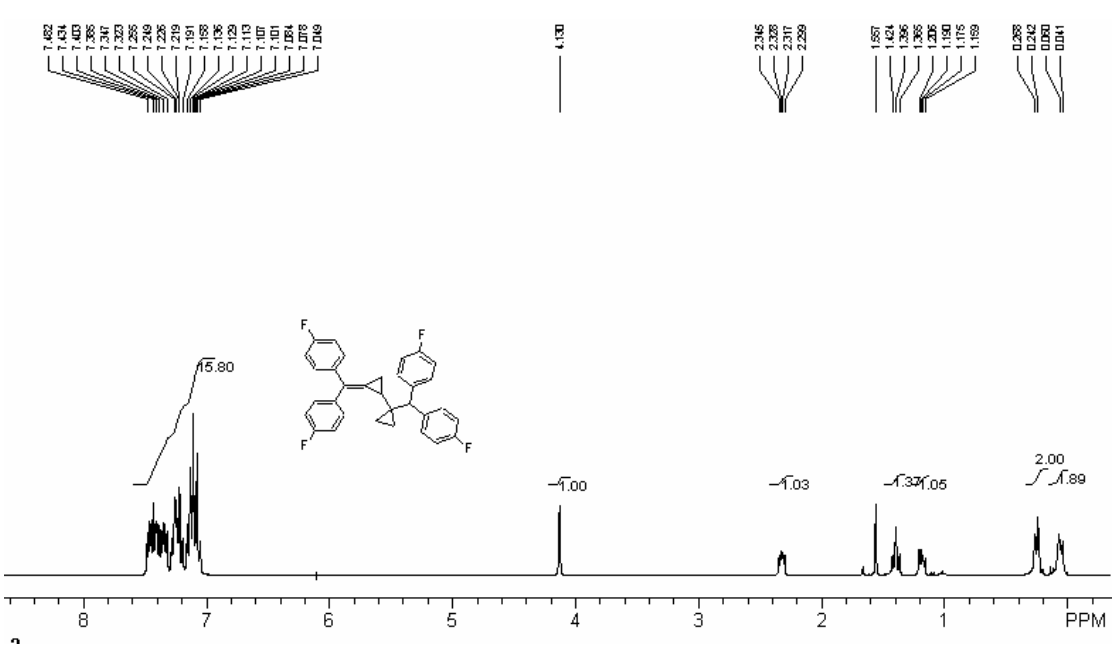
a white solid , yield: 92%. mp: 157-159 ^{o}C; IR (thin film): ν 2930, 1592, 1490, 1398, 1091, 1014 cm^{-1}; ^{1}H NMR ($CDCl_3$, TMS, 300 MHz): δ 0-0.05 (m, 2H, CH_2), 0.14-0.22 (m, 2H, CH_2), 1.33 (dd, J = 9.6, 5.1 Hz, 1H, CH_2), 1.33 (t, J = 8.4 Hz, 1H, CH_2), 2.25 (dd, J = 8.4, 5.1 Hz, 1H, CH), 4.04 (s, 1H, CH), 7.16 (d, J = 8.4 Hz, 2H, ArH), 7.23-7.44 (m, 12H, ArH), 7.44 (d, J = 8.4 Hz, 2H, ArH); ^{13}C NMR ($CDCl_3$, TMS, 75 MHz): δ 5.1, 9.4, 10.3, 18.6, 23.9, 54.9, 128.0, 128.2, 128.3, 128.4, 128.5, 129.0, 129.7, 130.2, 130.7, 130.8, 132.3, 132.4, 133.0, 133.3, 138.4, 139.2, 139.9, 140.9; MS (EI) m/z: 548 (M^+) (1), 484 (5), 388 (8), 375 (8), 251 (24, 239 (28), 227 (33), 201 (67), 183 (60), 165 (62), 125 (43), 109 (100); HRMS (MALDI): calcd for $C_{32}H_{25}Cl_4$ (M^++1) requires 549.0705, found: 549.0680.



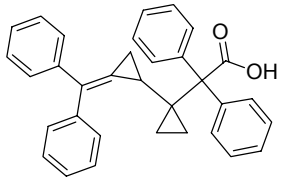
1-[Bis(4-fluorophenyl)methyl]-2'-[bis(4-fluorophenyl)methylene]bicyclopropyl (2d).



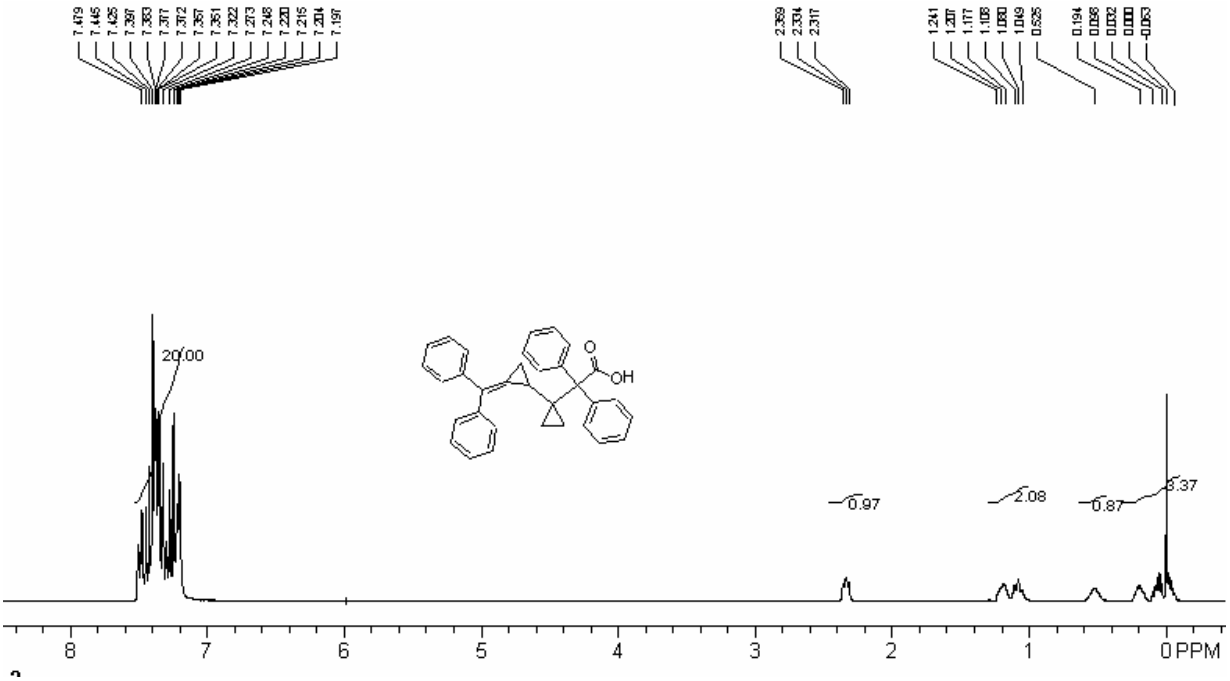
a white solid, yield: 81%. IR (thin film): ν 3060, 1603, 1508, 1225, 1157, 1096, 1015 cm^{-1}; ^1H NMR ($CDCl_3$, TMS, 300 MHz): δ 0-0.10 (m, 2H, CH_2), 0.21-0.29 (m, 2H, CH_2), 1.18 (dd, *J* = 9.0, 4.5 Hz, 1H, CH_2), 1.39 (t, *J* = 9.0 Hz, 1H, CH_2), 2.32 (dd, *J* = 8.4, 5.4 Hz, 1H, CH), 4.13 (s, 1H, CH), 7.03-7.50 (m, 16H, ArH); ^{13}C NMR ($CDCl_3$, TMS, 75 MHz): δ 5.1, 9.2, 10.2, 18.5, 24.1, 26.9, 54.6, 114.7, 114.8, 114.9, 115.05, 115.11, 115.3, 126.8, 129.2, 129.3, 129.6, 130.6, 130.7, 130.79, 130.81, 130.9, 138.5 (d, *J* = 12.3 Hz), 137.1 (d, *J* = 14.1 Hz), 136.3 (d, *J* = 12.0 Hz), 161.3 (d, *J* = 243.9 Hz), 161.5 (d, *J* = 243.9 Hz), 162.0 (d, *J* = 245.0 Hz), 162.1 (d, *J* = 245.0 Hz); MS (EI) m/z: 484 (M^+) (5), 388 (8), 281 (17), 253 (18), 227 (24), 203 (51), 183 (40), 133 (28), 109 (100); HRMS (EI): calcd.for $C_{32}H_{25}F_4$ (M^++1) requires 485.1887, found: 1485.1878.



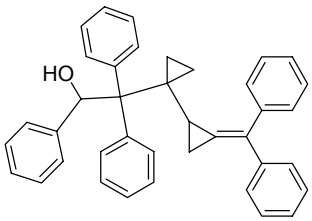
(2'-Benzhydrylidene-bicyclopropyl-1-yl)diphenyl acetic acid (3a).



a white solid, yield: 96%. mp: 190-192 ^{o}C; IR (thin film): ν 3057, 3023, 1698, 1494, 1445, 1264, 1032 cm^{-1}; ^{1}H NMR ($CDCl_3$, TMS, 300 MHz): δ -0.06-0.02 (m, 2H, CH_2), 0.03-0.10 (m, 1H, CH_2), 0.13-0.26 (m, 1H, CH_2), 0.44-0.61 (m, 1H, CH_2), 1.14-1.25 (m, 1H, CH), 2.29-2.38 (m, 1H, CH), 7.15-7.54 (m, 20H, ArH); ^{13}C NMR ($CDCl_3$, TMS, 75 MHz): δ 3.9, 11.4, 11.9, 18.7, 26.6, 26.9, 64.3, 125.9, 126.9, 127.10, 127.12, 127.3, 127.5, 127.9, 128.0, 128.1, 129.4, 130.2, 131.0, 132.3, 179.5; MS (EI) m/z: 451 (M^+) (1), 411 (8), 245 (32), 215 (39), 205 (44), 191 (49), 165 (88), 115 (45), 91 (100); HRMS (EI): calcd for $C_{33}H_{28}O_2Na$ (M□□Na) requires 1479.1982, found: 479.2009.

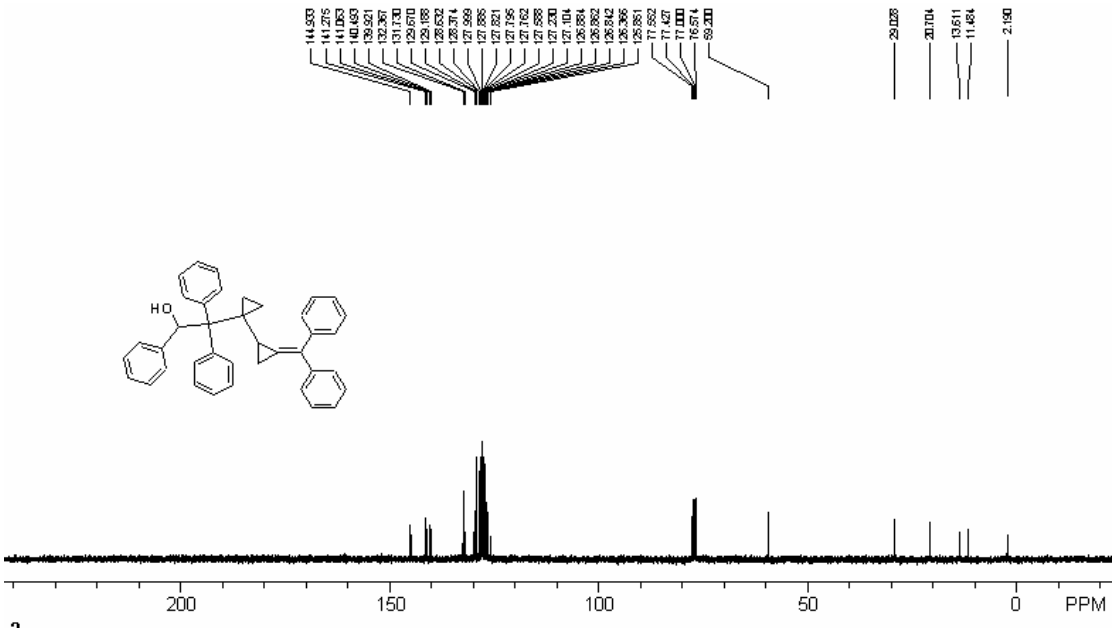


2-(2'-Benzhydrylidene-bicyclopropyl-1-yl)-1,2,2-triphenylethanol (3b).

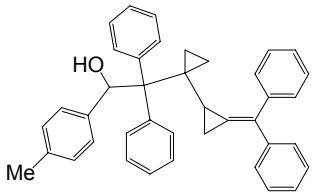


a white solid, yield: 92%. mp: 200-202 ^{o}C; IR (thin film): ν 3422, 2928, 1598, 1494, 1446, 1186,

1031 cm^{-1}; ^1H NMR ($CDCl_3$, TMS, 300 MHz): δ 0-0.11 (m, 2H, CH_2), 0.32-0.44 (m, 2H, CH_2), 0.64 (t, *J* = 9.0 Hz, 1H, CH_2), 1.02-1.11 (m, 1H, CH_2), 2.20 (1H, s, OH), 2.24-2.32 (m, 1H, CH), 5.55 (s, 1H, CH), 6.53 (d, *J* = 7.2, 2H, ArH), 7.07-7.15 (m, 2H, ArH), 7.20-7.28 (m, 1H, ArH), 7.31-7.62 (m, 16H, ArH), 7.83-7.90 (m, 2H, ArH), 7.95-8.03 (m, 2H, ArH); ^{13}C NMR ($CDCl_3$, TMS, 75 MHz): δ 2.2, 11.5, 13.6, 20.7, 29.0, 59.2, 77.6, 126.4, 126.84, 126.85, 126.89, 127.1, 127.2, 127.4, 127.6, 127.77, 127.79, 127.82, 127.9, 128.0, 128.6, 129.2, 129.7, 131.7, 139.9, 140.5, 141.1, 141.3, 145.0; MS (EI) m/z: 411 (M^+-C_7H_7O) (6), 295 (12), 219 (58), 205 (35), 191 (33), 167 (49), 107 (47), 91 (100); HRMS (MALDI): calcd for $C_{39}H_{34}ONa$ (M^++Na) requires 541.2502, found: 541.2517.

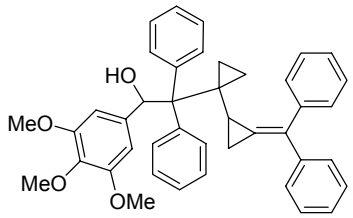


2-(2'-Benzhydrylidene-bicyclopropyl-1-yl)-2,2-diphenyl-1-p-tolyl-ethanol (3c).

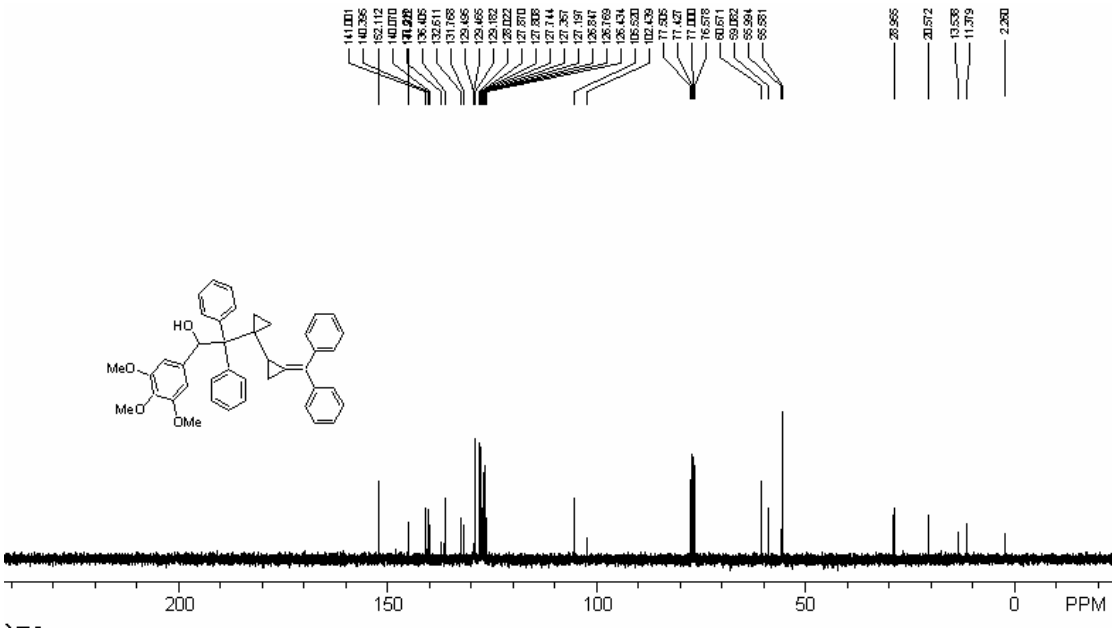


a white solid, yield: 77%. IR (thin film): ν 3427, 2956, 2929, 2860, 1598, 1513, 1494, 1446, 1379, 1266, 1188, 1032 cm^{-1}; ^1H NMR ($CDCl_3$, TMS, 300 MHz): δ 0-0.13 (m, 2H, CH_2), 0.30-0.47 (m, 2H, CH_2), 0.64 (t, J = 9.0 Hz, 1H, CH_2), 1.02-1.15 (m, 1H, CH_2), 2.25-2.32 (m, 1H, CH), 2.44 (s, 3H, CH_3), 5.52 (s, 1H, CH), 6.40 (d, J = 8.7 Hz, 2H, ArH), 7.29-7.61 (m, 20H, ArH), 7.85 (d, J = 8.7 Hz, 2H, ArH); MS (ESI) m/z: 555 (M^++Na); HRMS (MALDI): calcd. for $C_{40}H_{36}ONa$ (M^++Na) requires 555.2658, found: 555.2646.

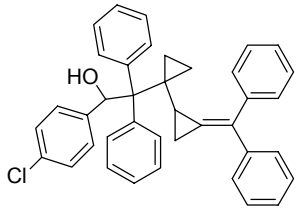
2-(2'-Benzhydrylidene-bicyclopropyl-1-yl)-2,2-diphenyl-1-(3,4,5-trimethoxyphenyl)ethanol (3e).



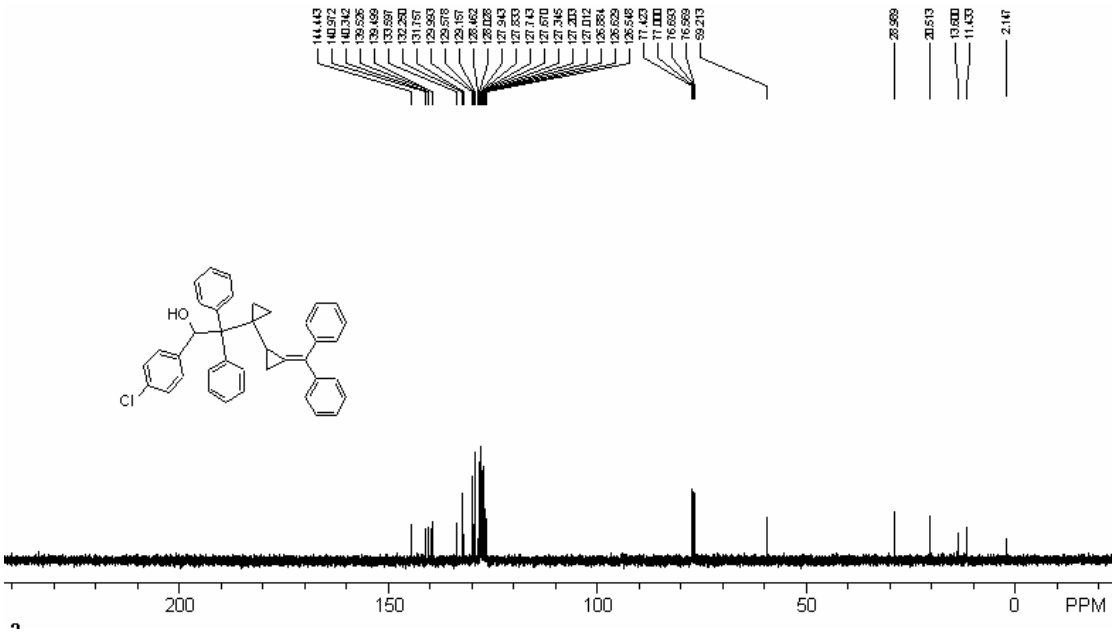
a white solid, yield: 78%. mp: 199-201 ^{o}C; IR (thin film): ν 3478, 2933, 1592, 1507, 1462, 1420, 1326, 1234, 1128, 1008 cm^{-1}; ^{1}H NMR ($CDCl_3$, TMS, 300 MHz): δ 0-0.08 (m, 2H, CH_2), 0.36-0.47 (m, 2H, CH_2), 0.63 (t, J = 9.0 Hz, 1H), 1.02-1.11 (m, 1H, CH_2), 2.20-2.28 (m, 1H, CH), 2.21 (s, 1H, OH), 3.64 (s, 6H, OCH_3), 3.88 (s, 3H, OCH_3), 5.49 (d, J = 2.7 Hz, 1H, CH), 5.87 (s, 2H, ArH), 7.34-7.62 (m, 20H); ^{13}C NMR ($CDCl_3$, TMS, 75 MHz): δ 2.3, 11.4, 13.5, 20.6, 29.0, 55.9, 56.0, 59.1, 60.7, 77.5, 102.4, 105.5, 126.4, 126.77, 126.85, 127.2, 127.4, 127.7, 127.8, 127.9, 128.0, 129.2, 131.8, 132.6, 136.4, 137.2, 140.1, 140.4, 144.9, 162.1; MS (ESI) m/z: 591 (M^{+}-H_2O), 631 (M^{+}+Na); Anal. calcd. for $C_{42}H_{40}O_4$ requires C, 82.86; H, 6.62; found: C, 82.71; H, 6.64%.



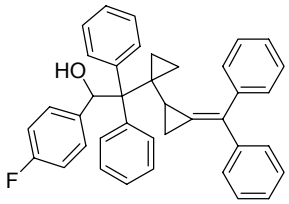
2-(2'-Benzhydrylidene-bicyclopropyl-1-yl)-1-(4-chlorophenyl)-2,2-diphenylethanol (3f).



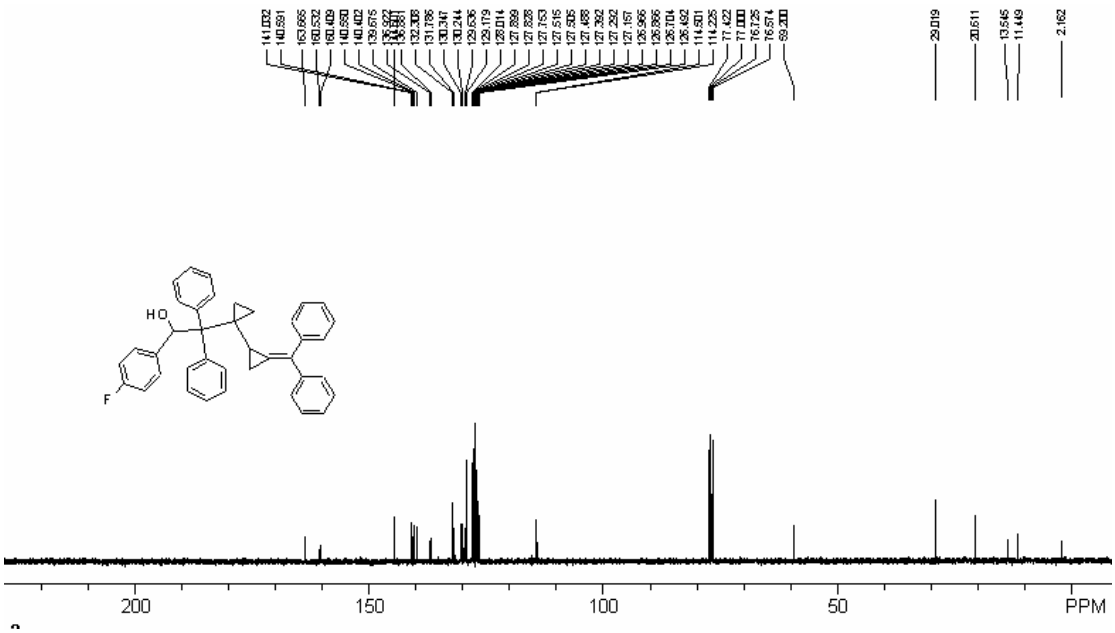
a white solid, yield: 94%. mp: 183-185 ^{o}C; IR (thin film): ν 3398, 2957, 2928, 1597, 1492, 1446, 1090, 1032, 1014 cm^{-1}; ^{1}H NMR ($CDCl_3$, TMS, 300 MHz): δ 0-0.14 (m, 2H, CH_2), 0.29-0.47 (m, 2H, CH_2), 0.67 (t, J = 9.0 Hz, 1H, CH_2), 1.01-1.10 (m, 1H, CH_2), 2.24-2.31 (m, 1H, CH), 2.21 (s, 1H, OH), 5.53 (s, 1H, CH), 6.46 (d, J = 8.7 Hz, 2H, ArH), 7.10 (d, J = 8.4 Hz, 2H, ArH), 7.33-7.64 (m, 16H, ArH), 7.86 (d, J = 7.5 Hz, 2H, ArH), 7.95-7.99 (m, 2H, ArH); ^{13}C NMR ($CDCl_3$, TMS, 300 MHz): δ 2.2, 11.4, 13.6, 20.6, 29.0, 59.2, 76.7, 126.5, 126.6, 126.9, 127.0, 127.2, 127.3, 127.67, 127.74, 127.8, 127.9, 128.0, 128.5, 129.2, 129.6, 130.0, 131.7, 132.3, 133.6, 139.5, 140.3, 141.0, 144.4; MS (ESI) m/z: 535 (M^+-H_2O+1), 575 (M^++Na); Anal. calcd. for $C_{39}H_{33}ClO$ requires C, 84.68; H, 6.01; found: C, 84.44; H, 6.04%.



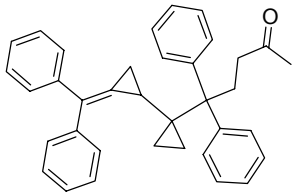
2-(2'-Benzhydrylidene-bicyclopropyl-1-yl)-1-(4-fluorophenyl)-2,2-diphenylethanol (3g).



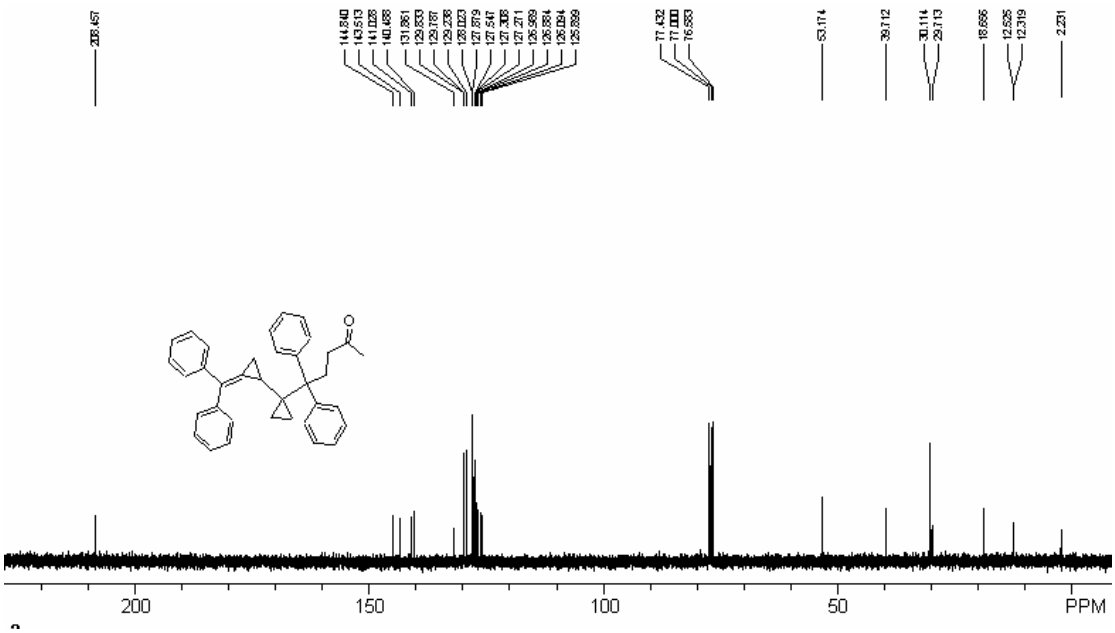
a white solid, yield: 70%. mp: 172-174 ^{o}C; IR (thin film): ν 3423, 2927, 1602, 1508, 1494, 1446, 1225, 1160, 1030 cm^{-1}; ^{1}H NMR ($CDCl_3$, TMS, 300 MHz): δ 0-0.14 (m, 2H, CH_2), 0.31-0.37 (m, 1H, CH_2), 0.44-0.46 (m, 1H, CH_2), 0.67 (t, J = 9.0 Hz, 1H, CH_2), 1.05-1.16 (m, 1H, CH_2), 2.22 (s, 1H, OH), 2.24-2.31 (m, 1H, CH), 5.59 (s, 1H, CH), 6.48 (m, 2H, ArH), 6.80 (m, 2H, ArH), 7.38-7.63 (m, 16H, ArH), 7.86-7.89 (m, 2H, ArH), 7.89-8.01 (m, 2H, ArH); ^{13}C NMR ($CDCl_3$, TMS, 75 MHz): δ 2.1, 11.4, 13.6, 20.6, 22.5, 29.0, 59.2, 76.7, 114.4 (d, J_{C-F} = 21.3 Hz), 126.6, 126.7, 126.9, 127.2, 127.3, 127.8, 127.9, 127.97, 128.04, 129.6, 130.3, 130.4, 131.8, 132.3, 136.8, 136.9, 139.6, 140.4, 141.0, 144.6, 162.2 (d, J_{C-F} = 245.0 Hz); MS (ESI) m/z: 519 (M^+-H_2O), 559 (M^++Na); HRMS (ESI): calcd. for $C_{39}H_{33}FONa$ requires 559.2408, found: 559.2422.



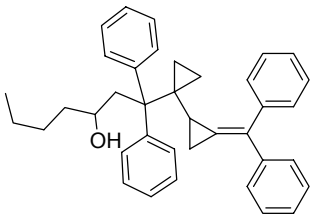
5-(2'-Benzhydrylidene-bicyclopropyl-1-yl)-5,5-diphenylpentan-2-one (3h).



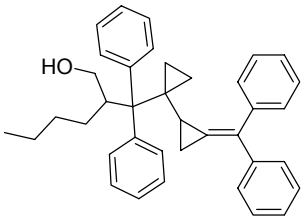
a white solid, yield: 95%. IR (thin film): ν 3055, 3021, 2964, 1715, 1598, 1494, 1446, 1362, 1266, 1158, 1030 cm^{-1}; ^{1}H NMR ($CDCl_3$, TMS, 300 MHz): δ -0.26-0.19 (m, 1H, CH_2), 0.31-0.41 (m, 1H, CH_2), 0.47 (dd, J = 9.9, 4.8 Hz, 1H, CH_2), 0.67-0.77 (m, 1H, CH_2), 0.90 (t, J = 9.0 Hz, 1H, CH_2), 1.60-1.74 (m, 1H, CH_2), 1.94 (s, 3H), 2.0-2.15 (m, 1H, CH), 2.16-2.47 (m, 4H, CH, CH_2), 7.15-7.57 (m, 20H, ArH); ^{13}C NMR ($CDCl_3$, TMS, 75 MHz): δ 2.2, 12.3, 12.5, 18.7, 29.7, 30.1, 39.7, 53.2, 125.9, 126.1, 126.9, 127.0, 127.27, 127.30, 127.5, 127.9, 128.0, 129.2, 129.79, 129.83, 131.9, 140.5, 141.0, 143.5, 144.8, 208.5; MS (EI) m/z: 482 (M^+) (1), 411 (5), 321 (23), 293 (16), 219 (67), 205 (62), 191 (35), 167 (45), 91 (100); HRMS (MALDI): calcd. for $C_{36}H_{34}ONa$ (M^++Na) requires 505.2502, found: 505.2513.



1-(2'-Benzhydrylidene-bicyclopropyl-1-yl)-1,1-diphenyl-heptan-3-ol (3i).



3i-1



3i-2

for **3i-1**: a white solid, yield: 26%. mp: 167-169 ^{o}C; IR (thin film): ν 3590, 2956, 2928, 1598, 1494, 1446, 1301 cm^{-1}; ^{1}H NMR ($CDCl_3$, TMS, 300 MHz): δ 0-0.06 (m, 1H, CH_2), 0.29-0.35 (m, 1H, CH_2), 0.52-0.56 (m, 1H, CH_2), 0.70 (dd, *J* = 9.4, 5.1 Hz, 1H, CH_2), 1.12 (t, *J* = 7.2 Hz, 3H, CH_3), 1.20-1.30 (m, 1H, CH_2), 1.40-1.56 (m, 8H, CH_2), 1.80-1.89 (m, 1H, CH_2), 2.44-2.47 (br. s, OH), 2.58 (dd, *J* = 8.1, 5.1 Hz, 1H, CH_2), 3.88-3.93 (m, 1H, CHO), 7.48-7.72 (m, 18H, ArH), 8.02-8.05 (m, 2H, ArH); ^{13}C NMR ($CDCl_3$, TMS, 75 MHz): δ 2.0, 12.5, 12.6, 14.0, 18.2, 22.6, 27.6, 30.1, 38.3, 45.3, 53.4, 68.0, 126.0, 126.7, 126.9, 127.0, 127.2, 127.3, 127.9, 128.0, 128.6, 129.2, 129.3, 129.9, 131.9, 140.5, 141.0, 143.6, 145.8; ESI-MS (m/z): 513 (M^++1), 535 (M^++Na); HRMS (ESI): calcd. for $C_{38}H_{40}ONa$ requires 535.2971, found: 535.2993.

for **3i-2**: a white solid, yield: 16%. mp: 117-119 ^{o}C; IR (thin film): ν 3592, 2931, 1598, 1494, 1446, 1030 cm^{-1}; ^{1}H NMR ($CDCl_3$, TMS, 300 MHz): δ 0-0.07 (m, 1H, CH_2), 0.24-0.30 (m, 1H, CH_2), 0.58-0.68 (m, 2H, CH_2), 0.84-0.91 (m, 1H, CH_2), 0.98 (t, *J* = 6.9 Hz, 3H, CH_3), 1.04-1.15 (m, 4H, CH_2), 1.26-1.42 (m, 4H, CH_2), 1.60 (br. s, OH), 1.84 (dd, *J* = 13.5, 2.0 Hz, 1H, CH), 2.30 (dd, *J* = 14.7, 6.6 Hz, 1H, CH), 2.51 (dd, *J* = 8.4, 5.1 Hz, 1H, OCH_2), 3.60-3.65 (m, 1H, OCH_2), 7.43-7.65 (m, 16H, ArH), 7.65-7.80 (m, 2H, ArH), 7.80-7.96 (m, 2H, ArH); ^{13}C NMR ($CDCl_3$, TMS, 75 MHz): δ 2.2, 12.2, 12.6, 13.9, 18.4, 22.5, 27.7, 29.9, 38.3, 44.6, 53.2, 69.3, 126.1, 126.4, 126.9, 127.0, 127.26, 127.29, 127.88, 127.90, 128.1, 129.3, 129.8, 130.0, 131.8, 140.5, 141.1, 144.1, 144.9; MS (ESI) m/z: 513 (M^++1), 536(M^++Na+1); HRMS (ESI): for $C_{38}H_{40}ONa$ requires 535.2971, found: 535.2996.