

Electronic Supplementary Information

Synthesis and Properties of Aggregation-Induced Emission Enhancement Compounds Derived from Triarylcyclopentadiene

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S1 Structural characterization of 1-7

1) The ^1H NMR, ^{13}C NMR and HRMS spectra of 1

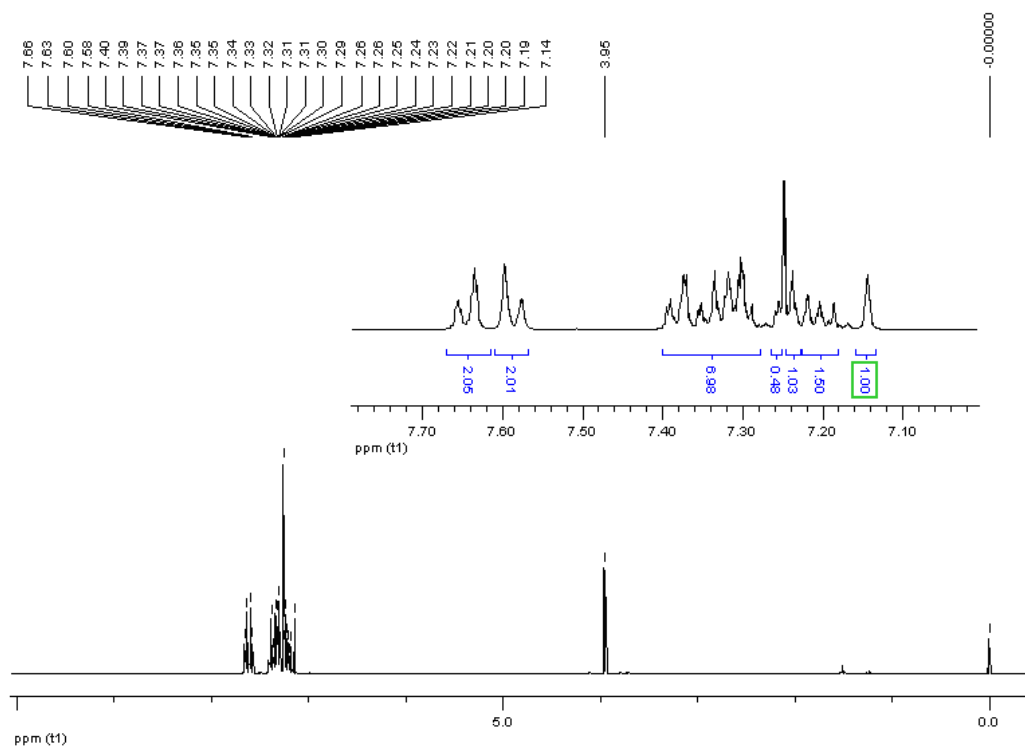


Fig. S1 The ^1H NMR spectrum of 1.

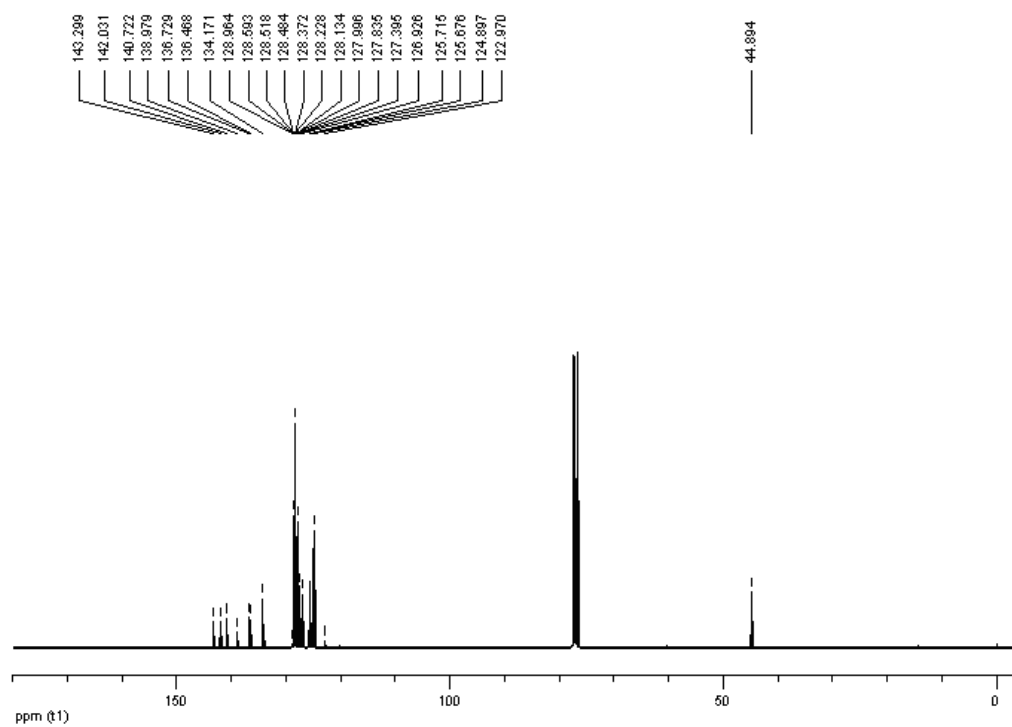


Fig. S2 The ^{13}C NMR spectrum of **1**.

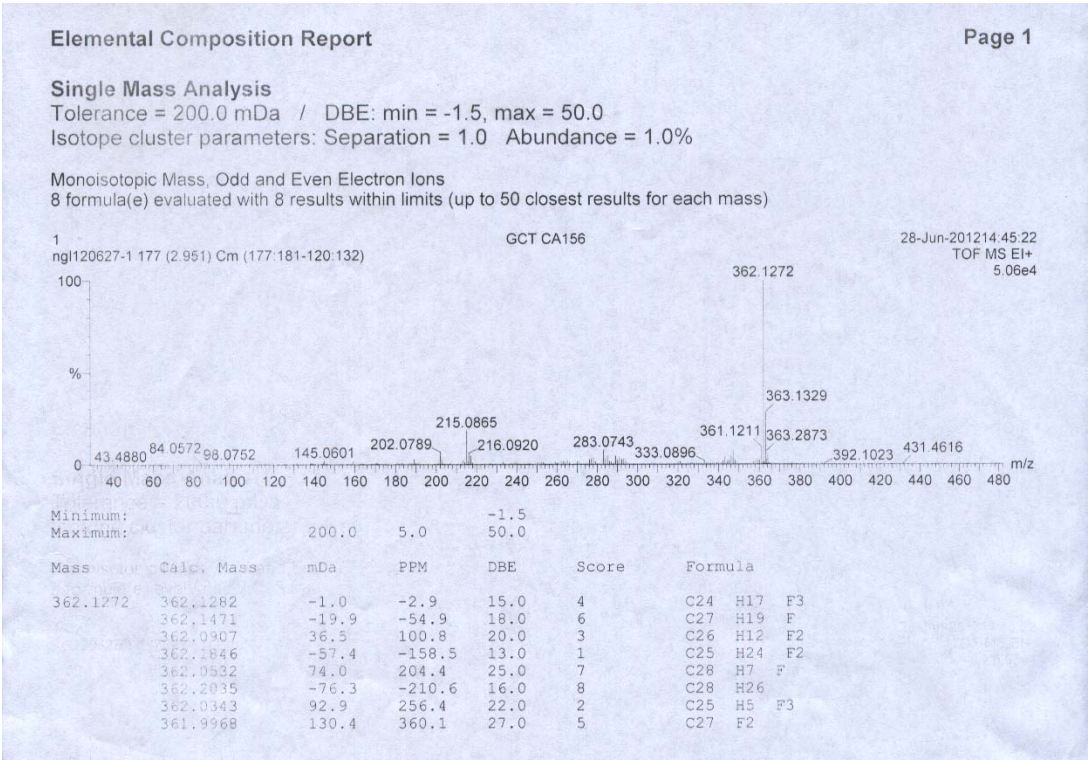


Fig. S3 The HRMS spectrum of **1**.

2) The ^1H NMR, ^{13}C NMR and HRMS spectra of **2**

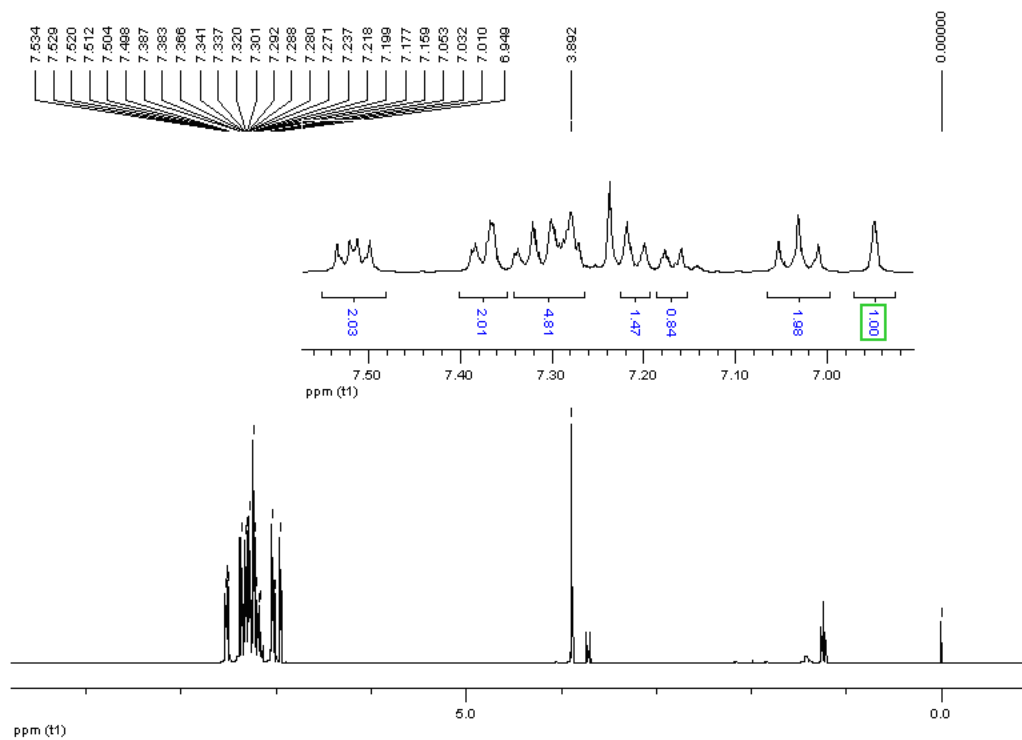


Fig. S4 The ^1H NMR spectrum of **2**.

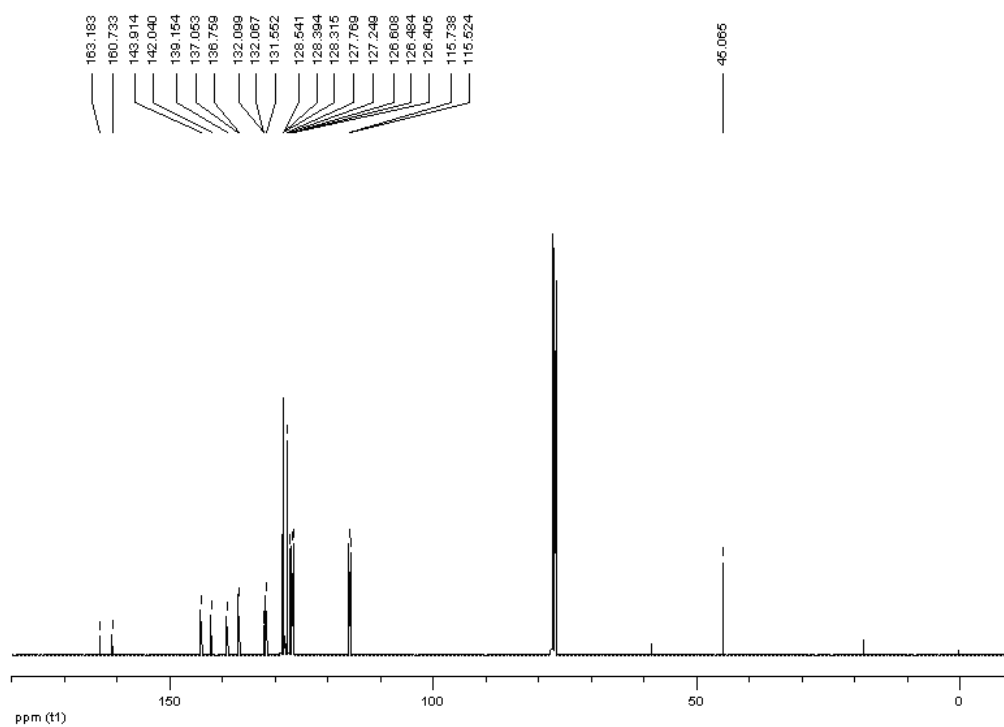


Fig. S5 The ^{13}C NMR spectrum of **2**.

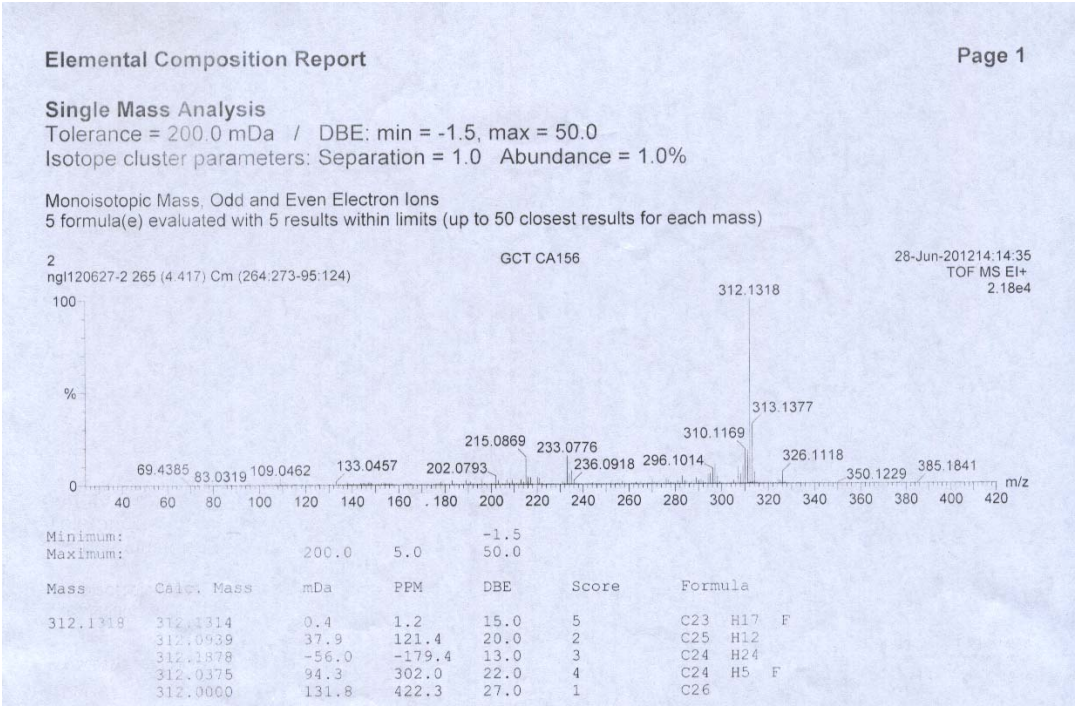


Fig. S6 The HRMS spectrum of **2**.

3) The ^1H NMR, ^{13}C NMR and MS spectra of **3**

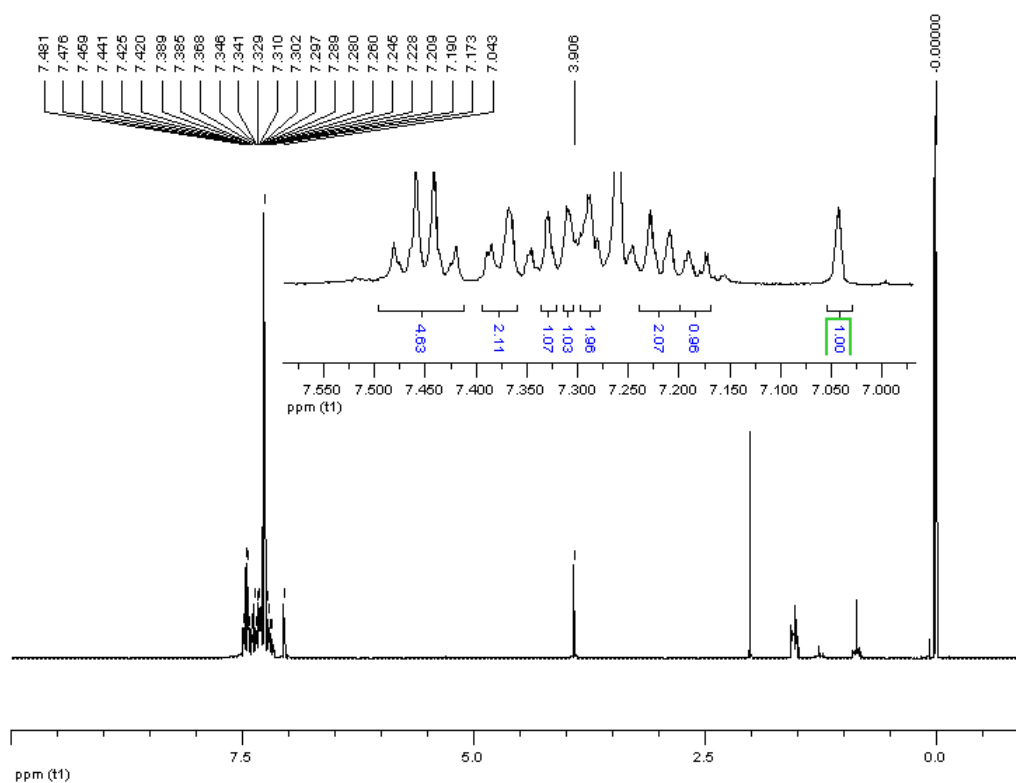


Fig. S7 The ^1H NMR spectrum of **3**.

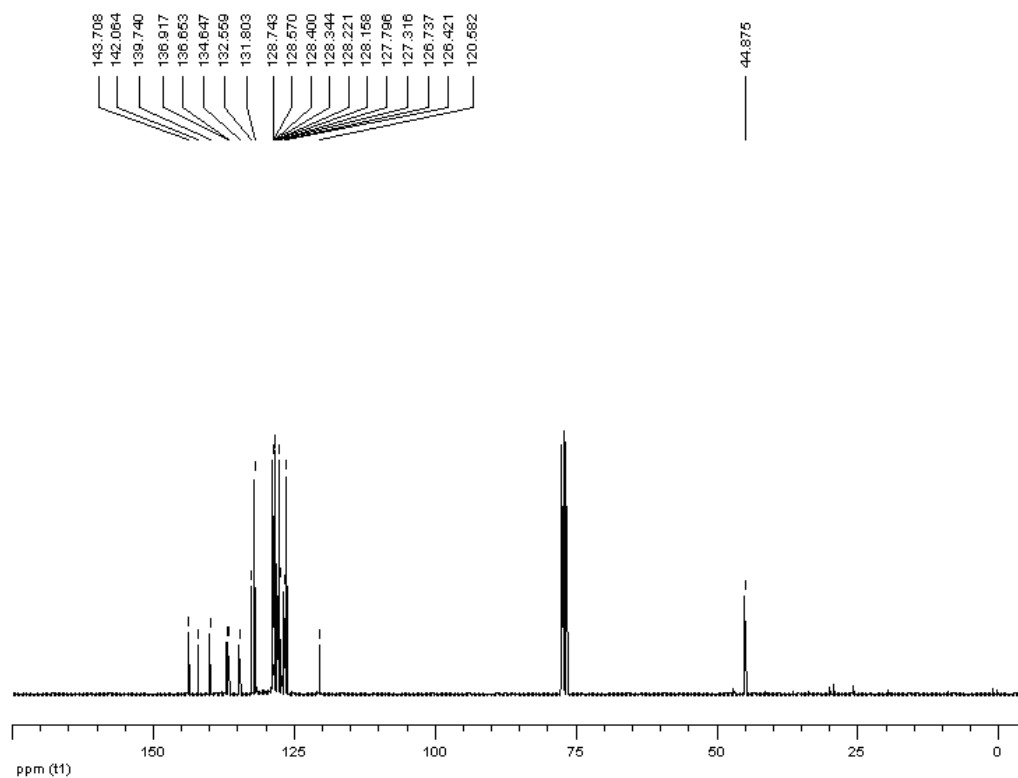


Fig. S8 The ^{13}C NMR spectrum of **3**.

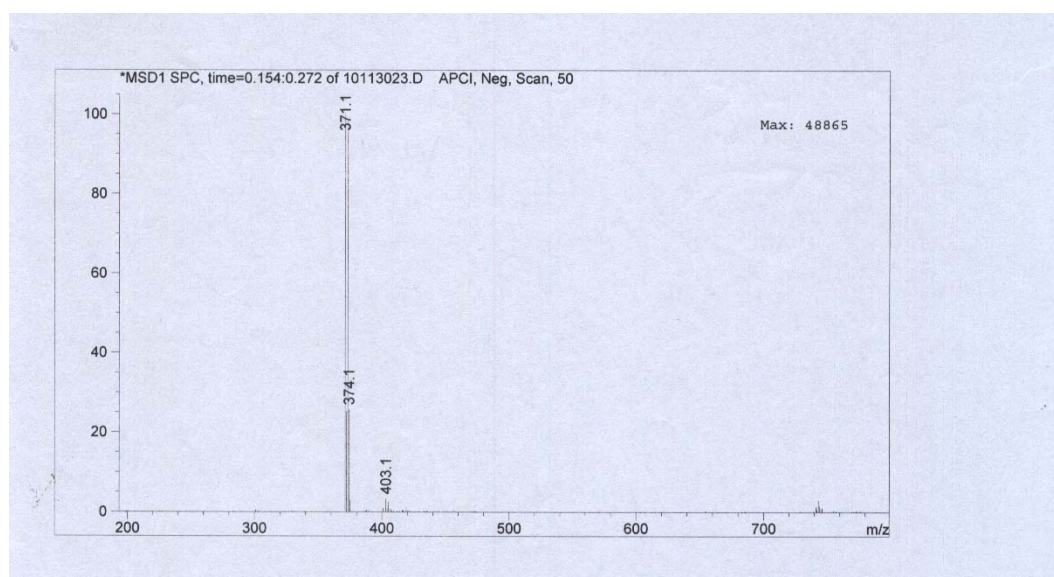


Fig. S9 The MS spectrum of **3**.

4) The ^1H NMR, ^{13}C NMR and HRMS spectra of 4

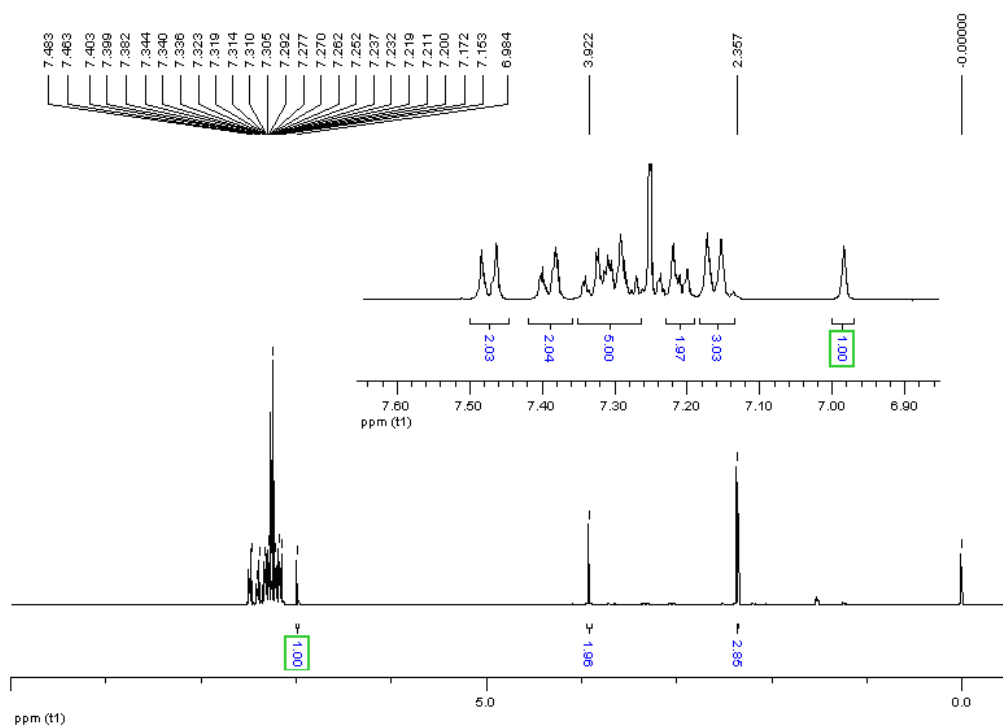


Fig. S10 The ^1H NMR spectrum of 4.

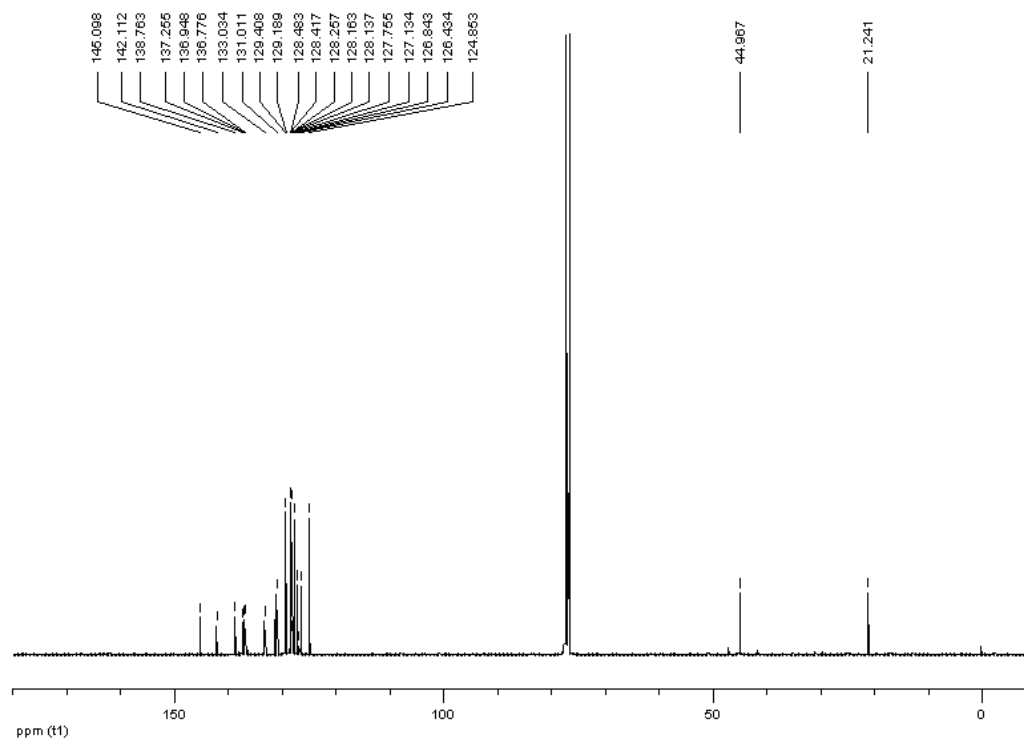


Fig. S11 The ^{13}C NMR spectrum of **4**.

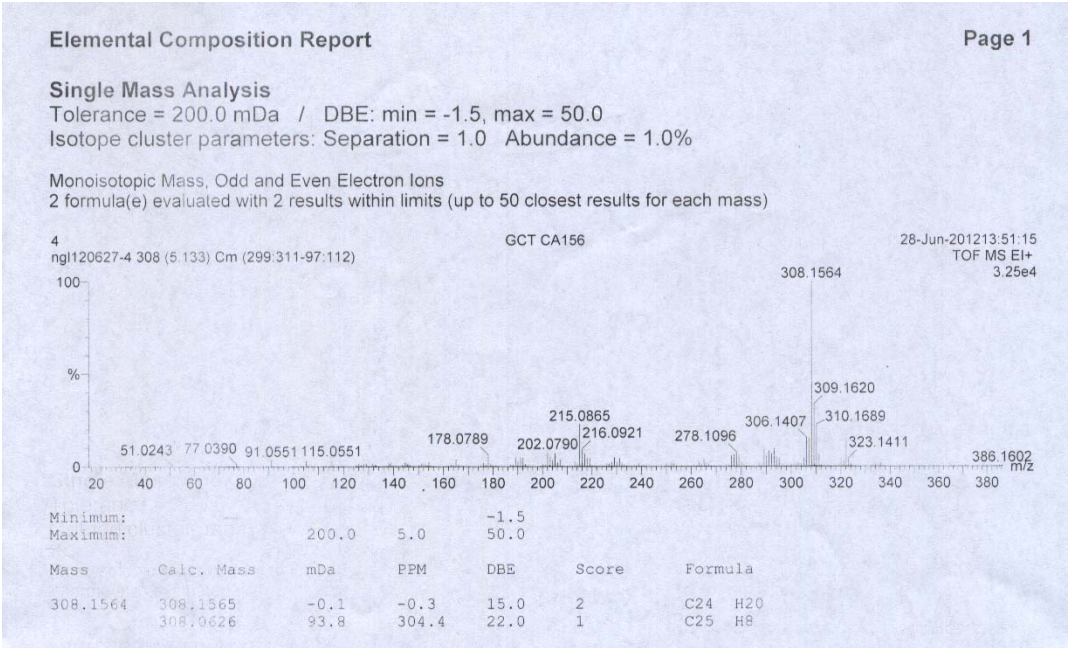


Fig. S12 The HRMS spectrum of **4**.

5) The ^1H NMR, ^{13}C NMR and HRMS spectra of **5**

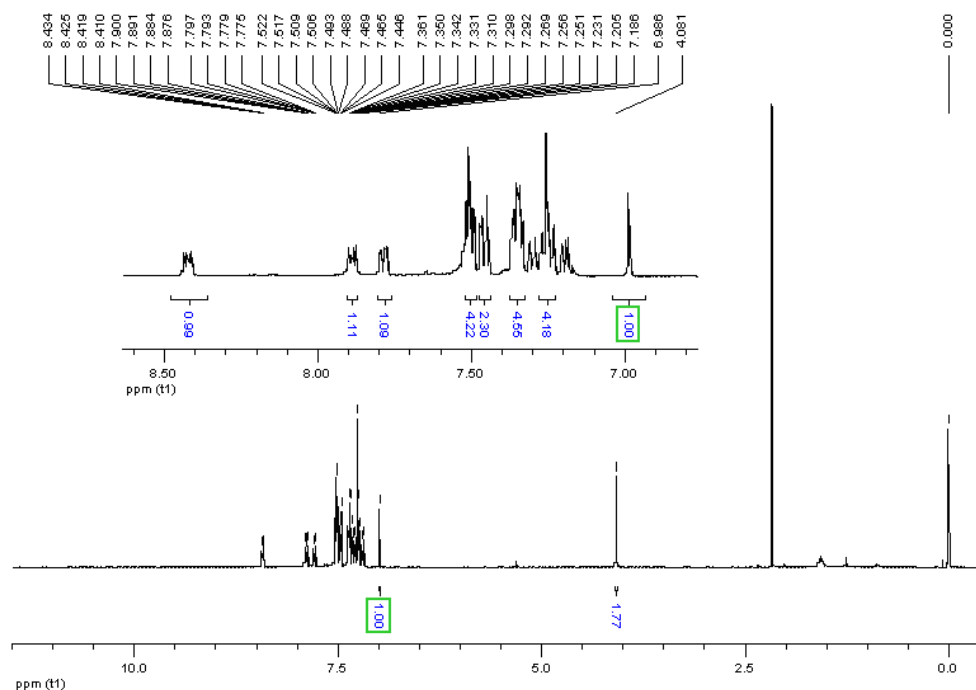


Fig. S13 The ^1H NMR spectrum of **5**.

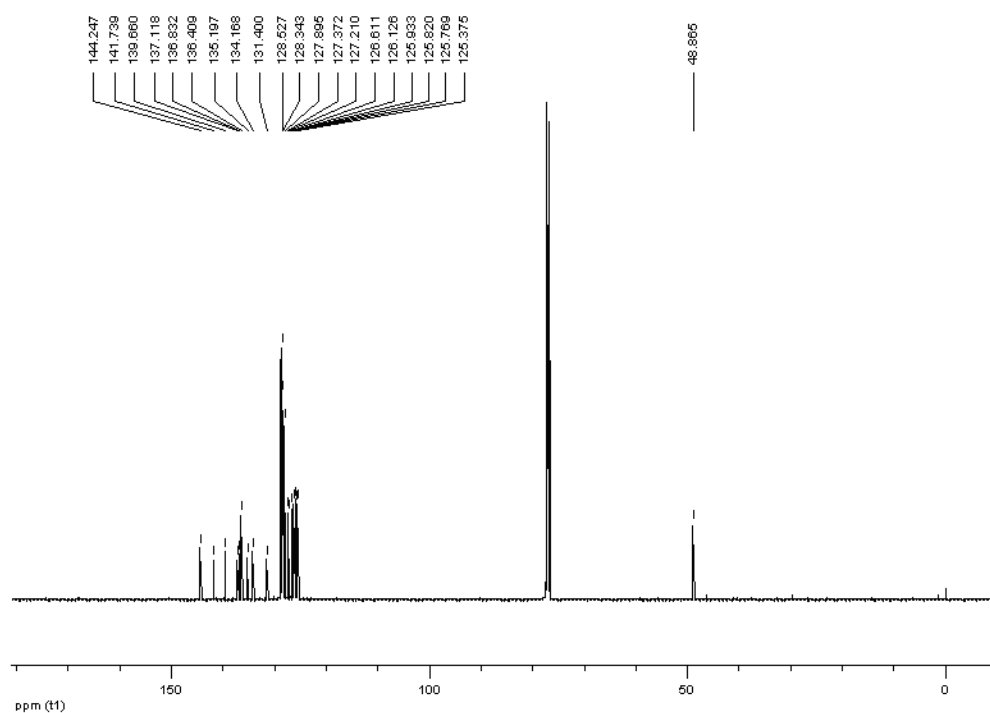


Fig. S14 The ^{13}C NMR spectrum of **5**.

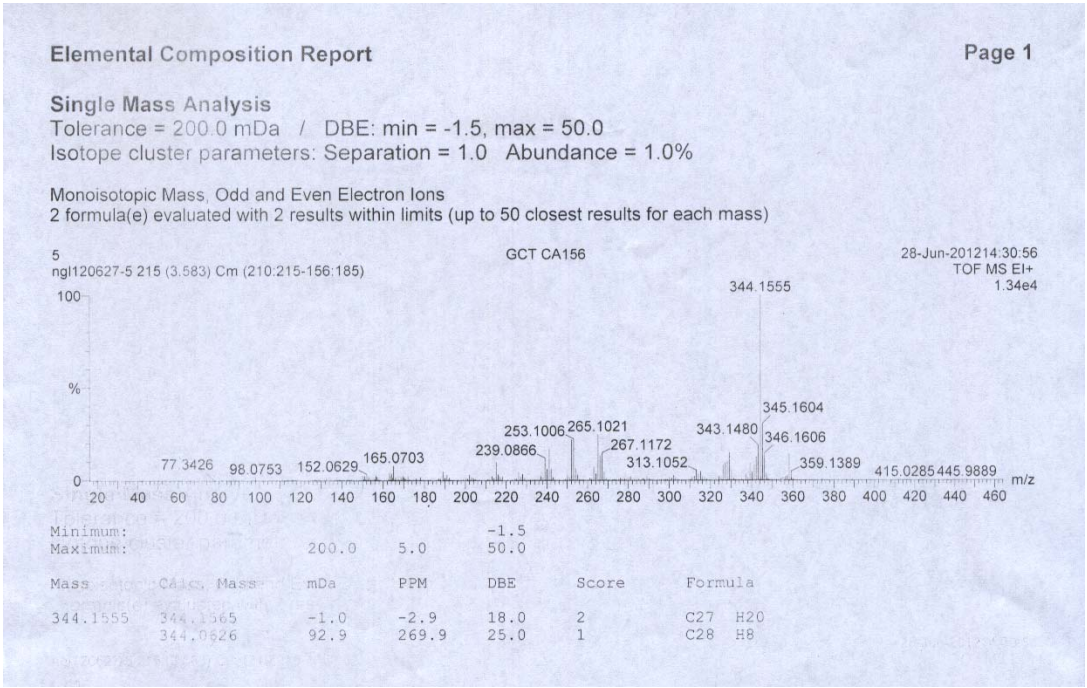


Fig. S15 The HRMS spectrum of 5.

6) The ^1H NMR, ^{13}C NMR and HRMS spectra of 6

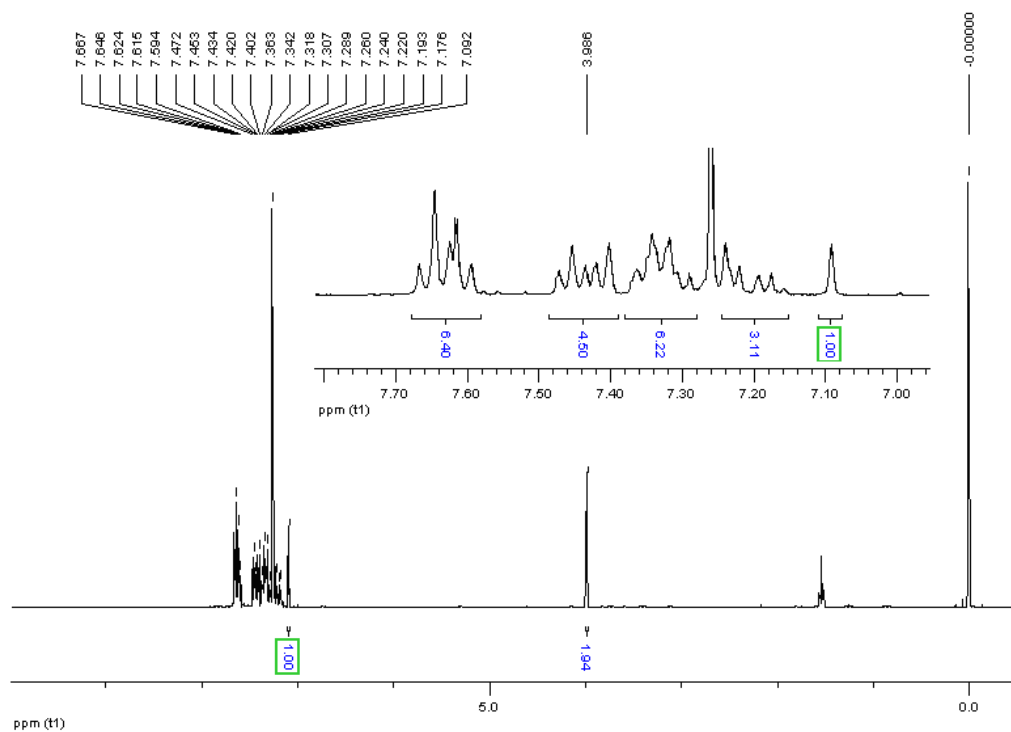


Fig. S16 The ^1H NMR spectrum of 6.

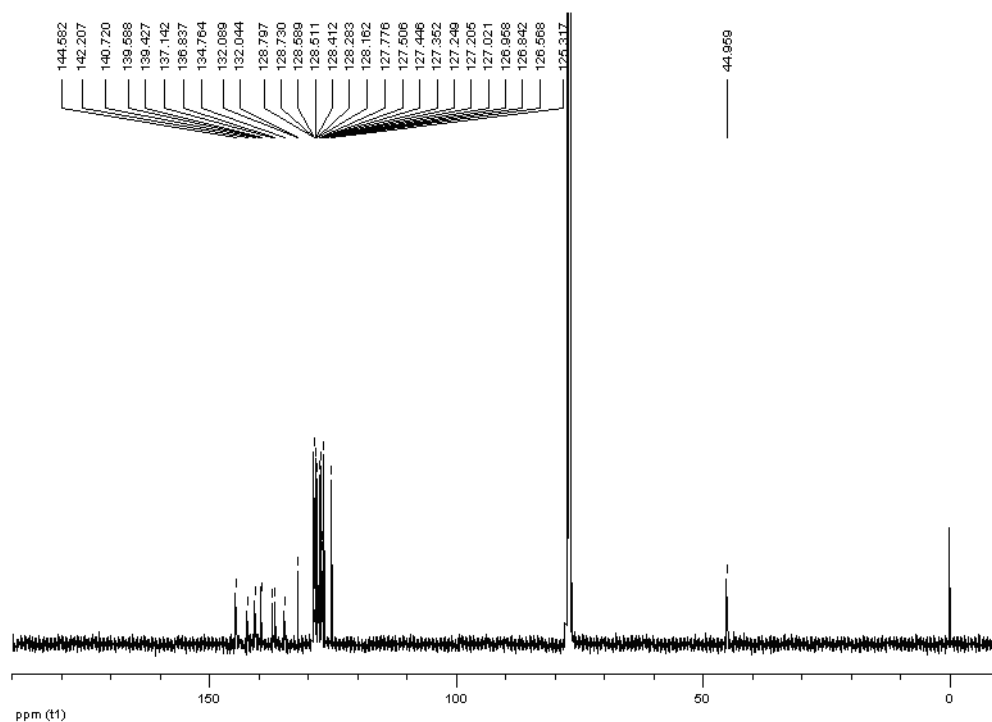


Fig. S17 The ^{13}C NMR spectrum of **6**.

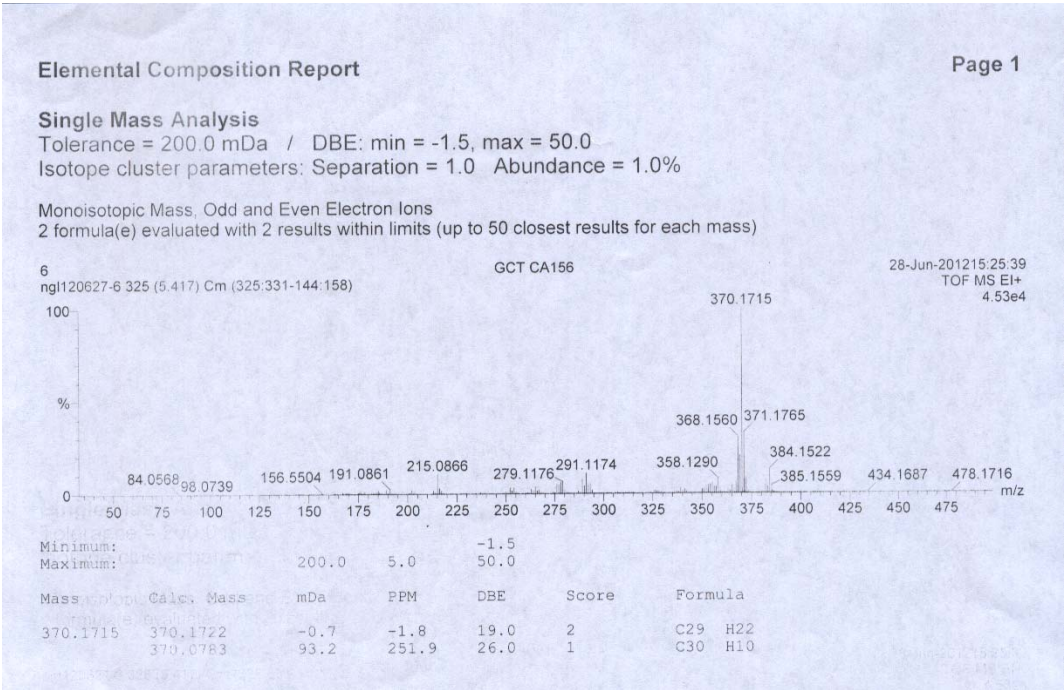


Fig. S18 The HRMS spectrum of 6.

7) The ^1H NMR, ^{13}C NMR and HRMS spectra of 7

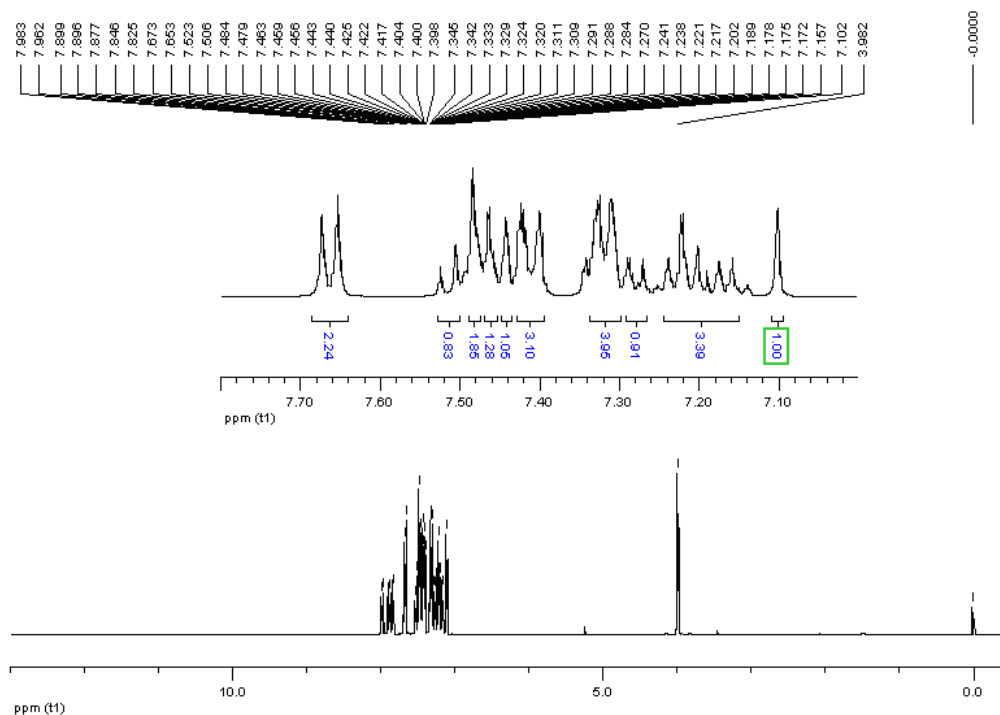


Fig. S19 The ^1H NMR spectrum of 7.

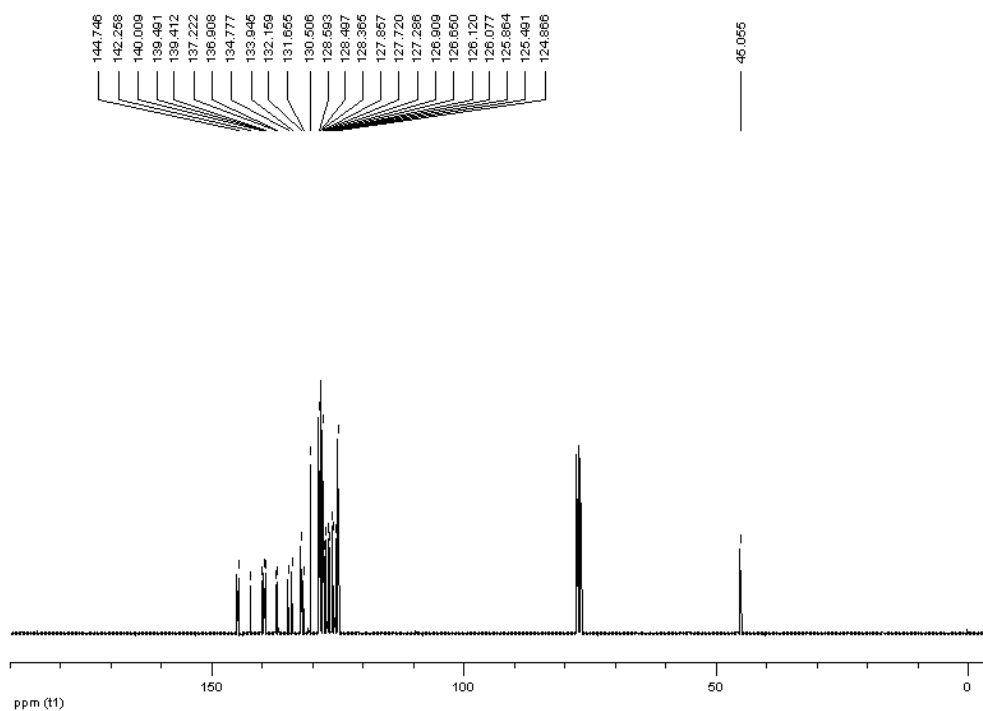


Fig. S20 The ^{13}C NMR spectrum of **7**.

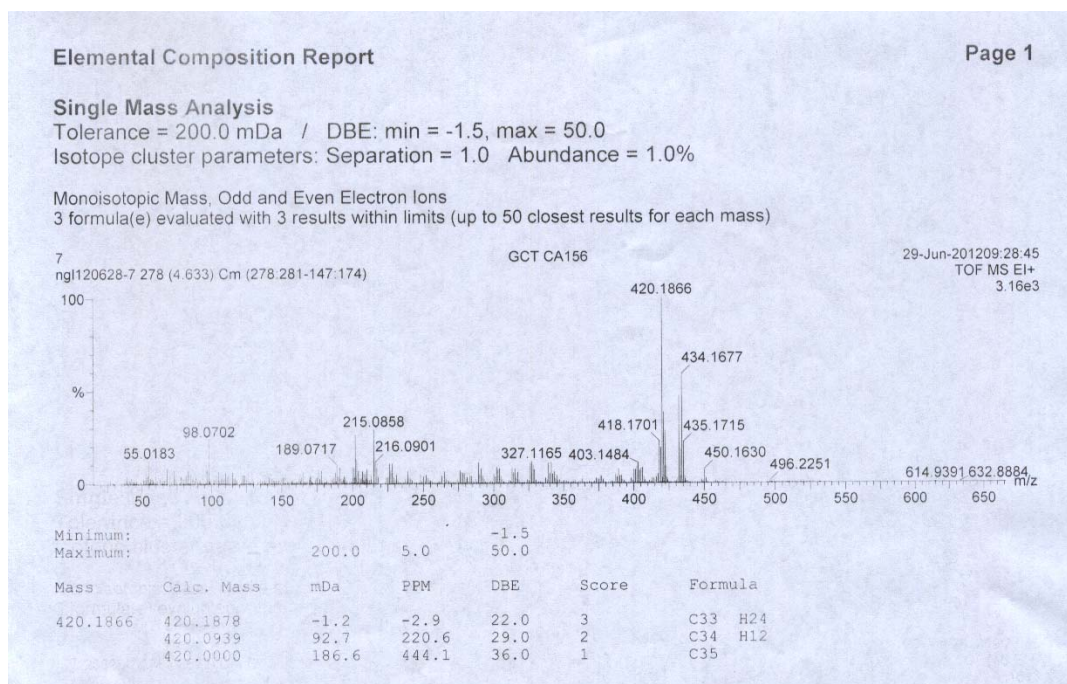


Fig. S21 The HRMS spectrum of **7**.

S2. UV-vis absorption spectroscopy of 1-7

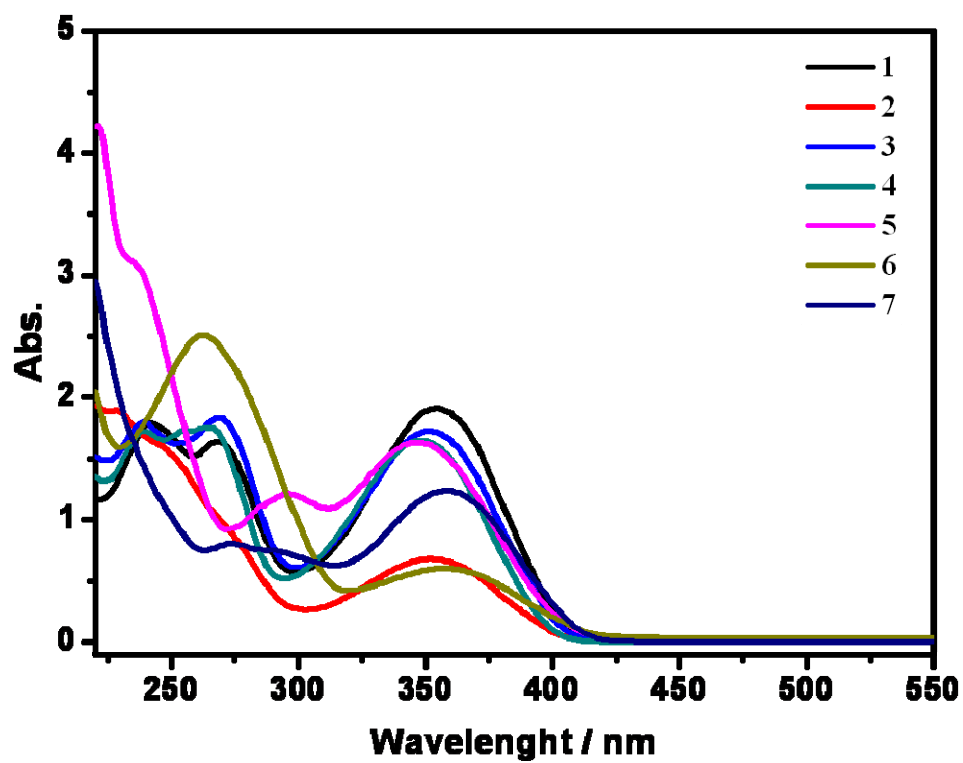


Fig. S22 UV-vis absorption spectra of the compounds in CH_3CN solution ($100\ \mu\text{M}$).

S3. PL spectroscopy of 1-7 in solution

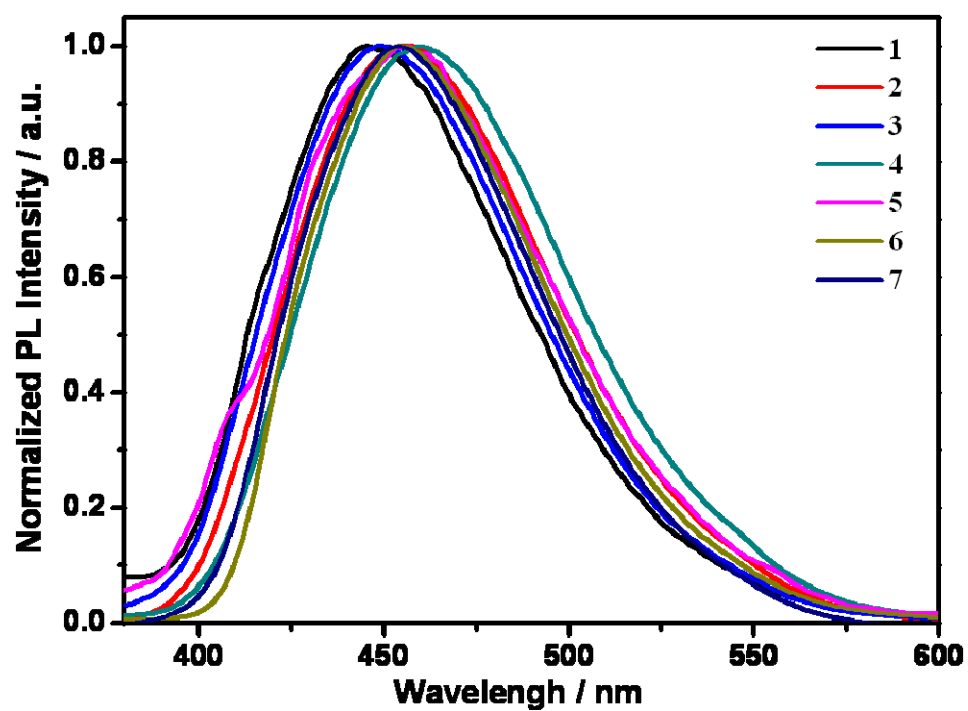


Fig. S23 PL spectra of the compounds in CH_3CN solution ($100\ \mu\text{M}$).

S4. PL spectroscopy of 1-7 in solid state

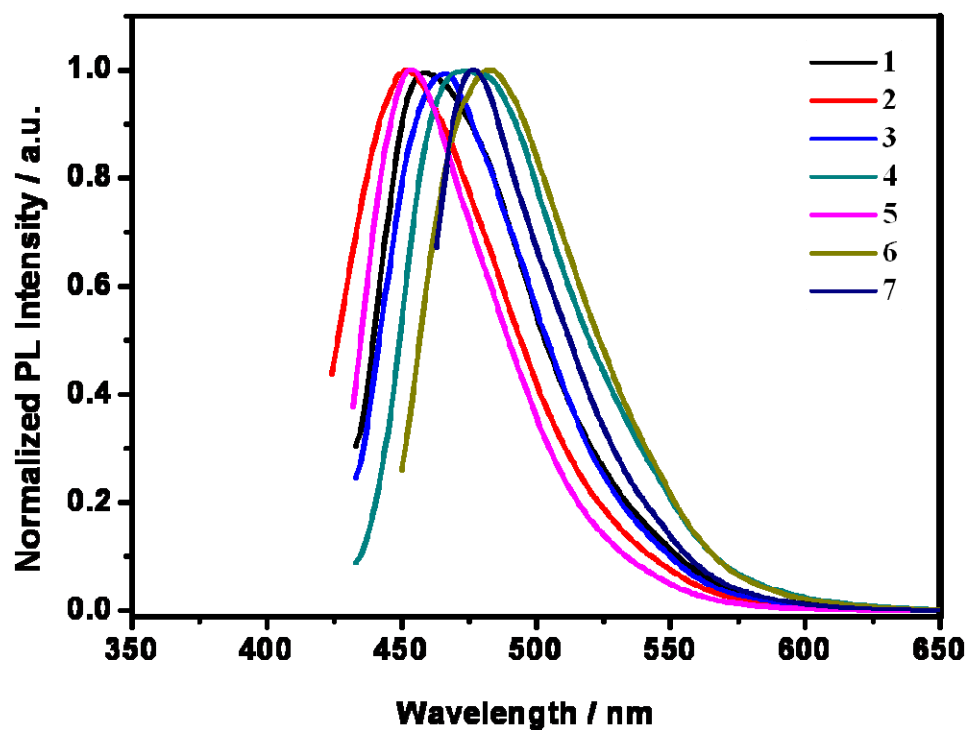


Fig. S24 PL spectra of the compounds in solid state.

S5. UV spectroscopy of compound 1, 2, 4 and 5 (in water / CH₃CN)

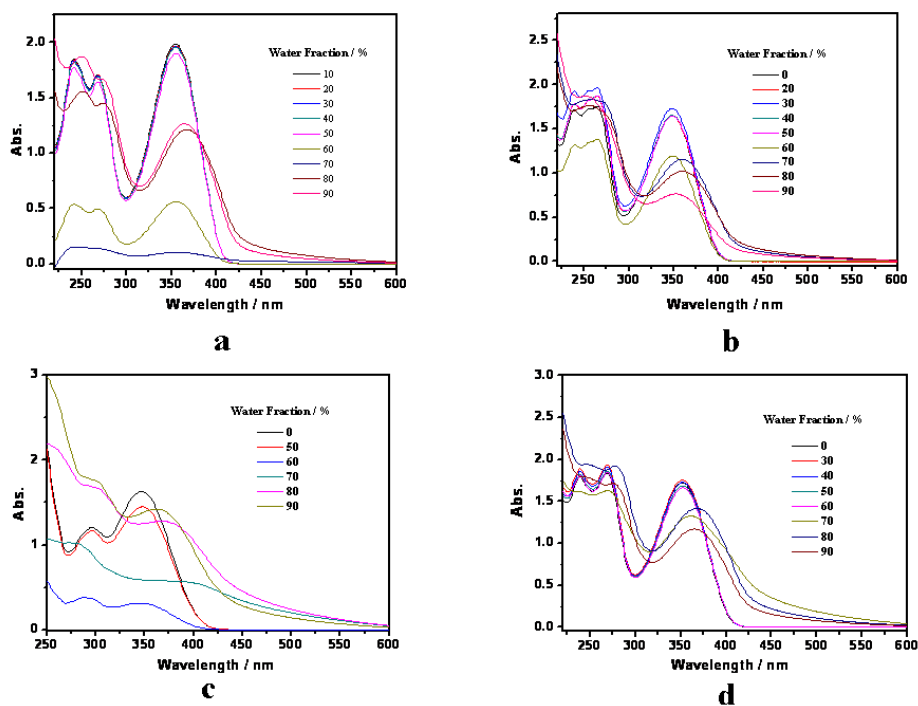


Fig. S25 UV spectra of compounds 1 (a), 2 (b), 4 (c) and 5 (d) in water/CH₃CN mixtures with different water fraction.

S6. DSC curves of 1-7

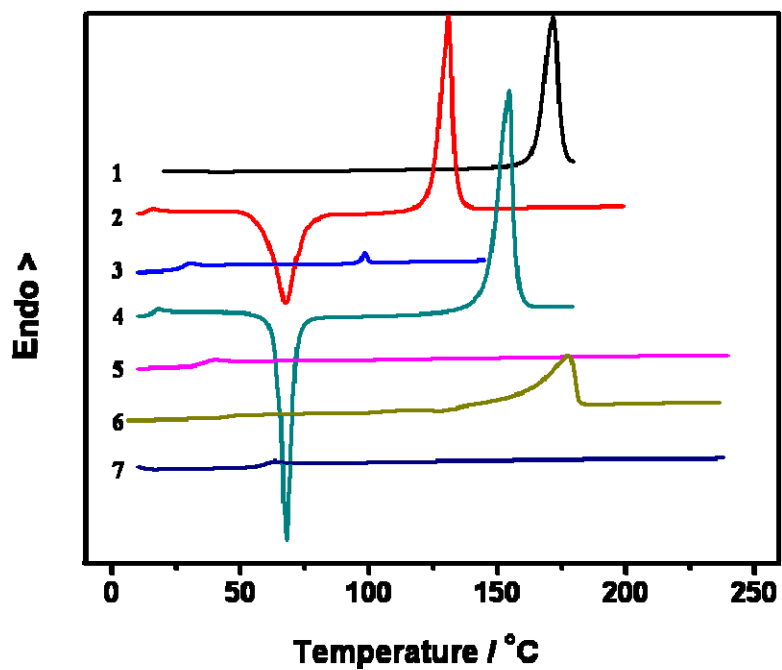


Fig. S26 DSC curves upon second heating of the compounds after a 10 °C/min cooling rate from the melts.

S7. TGA curves of 1-7

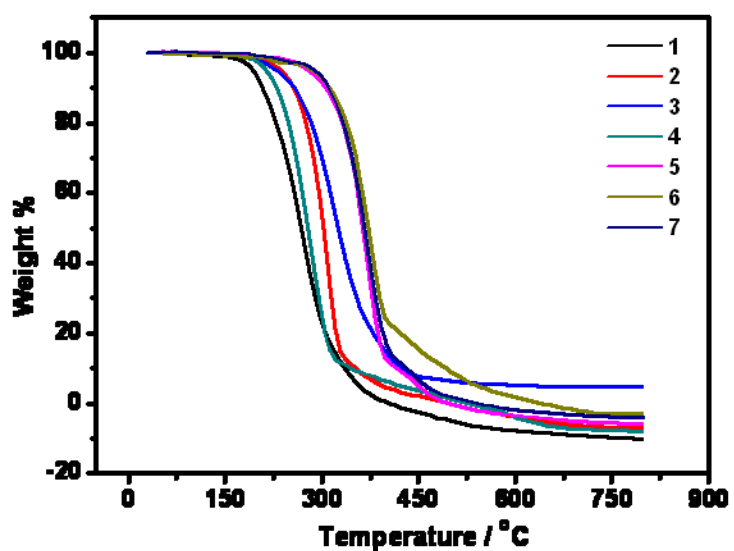


Fig. S27 TGA curves of the compounds.

S8. CV curves of 1-7

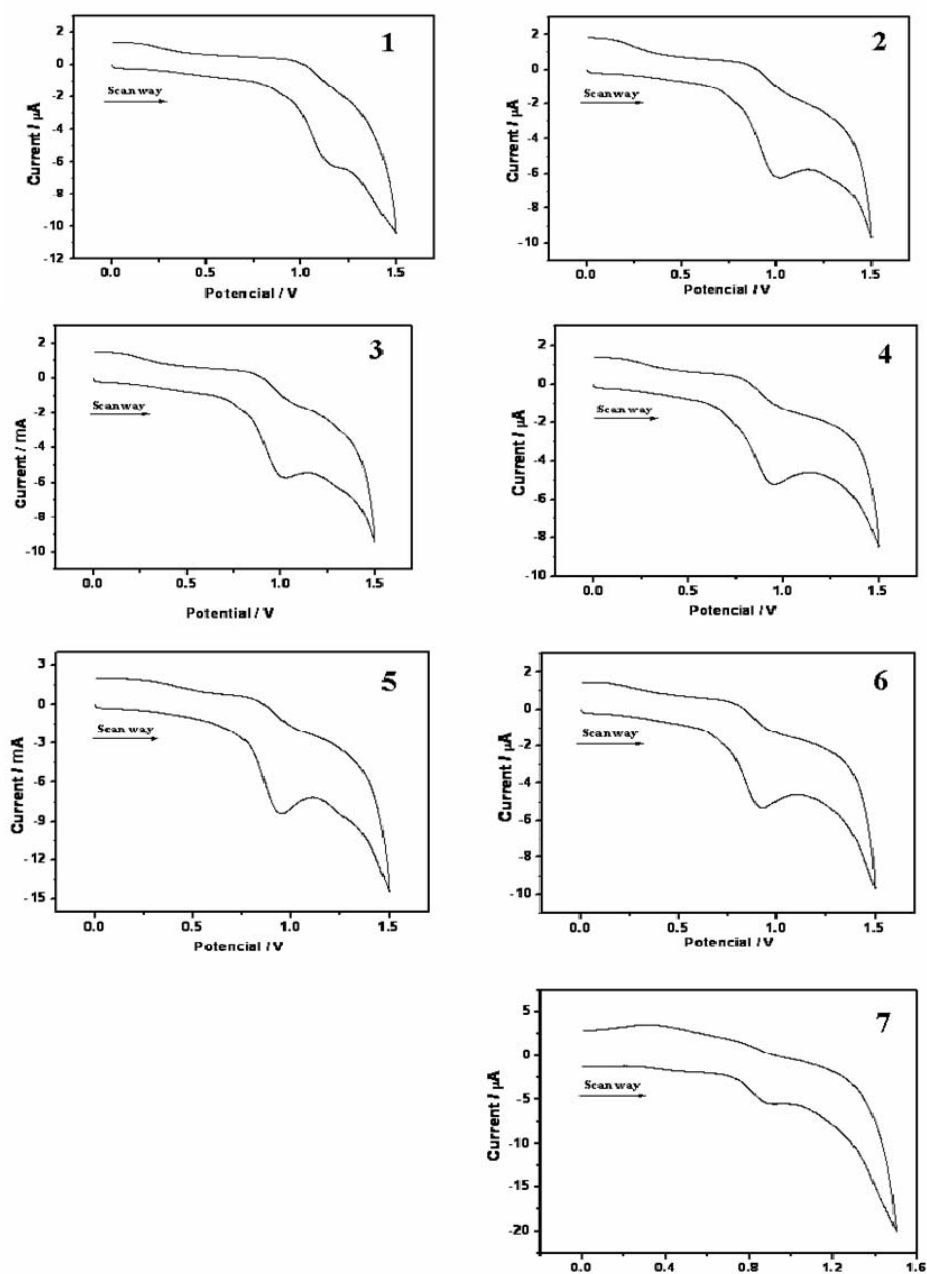


Fig. S28 CV curves of the compounds in CH_3CN solution (100 μM).

S9. HOMO and LUMO levels of 1-7

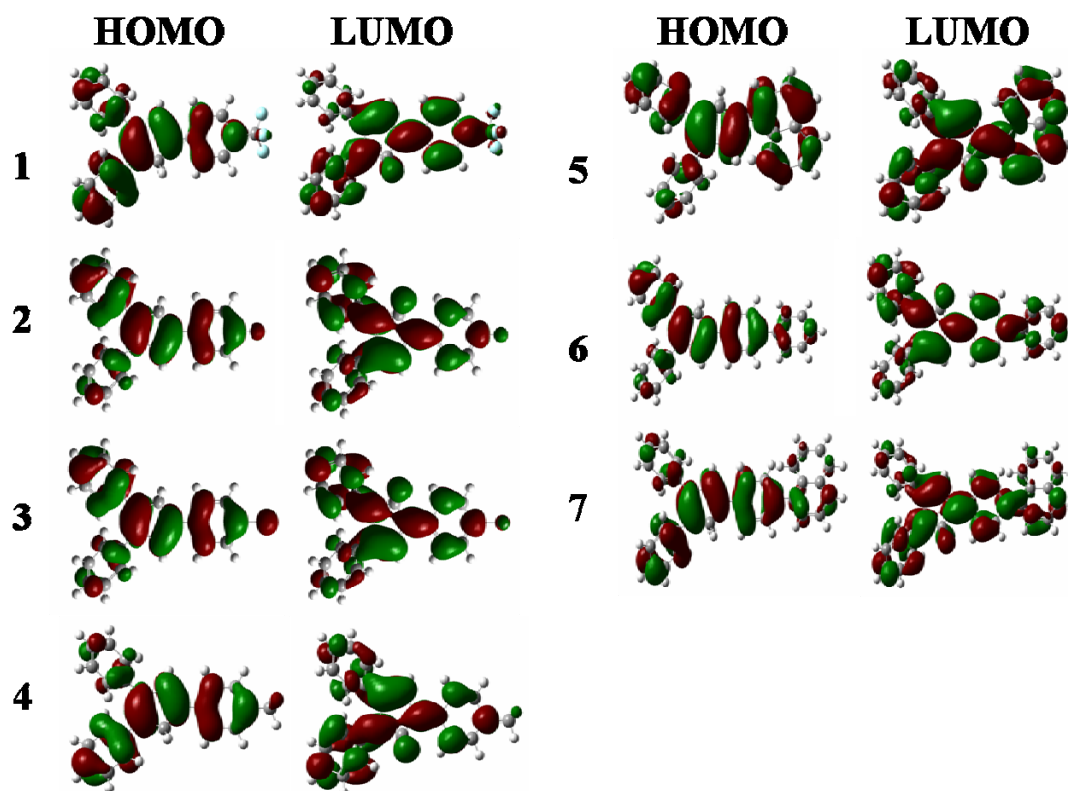


Figure S29 Calculated molecular orbital amplitude plots of HOMO and LUMO levels.

S10 Energy levels and band gaps of 1-7

Table S1 Energy levels of the molecular orbitals and band gaps of the compounds.

Compounds	HOMO/eV	LUMO /eV	ΔE_g /eV
1	5.53	2.45	3.08
2	5.41	2.29	3.12
3	5.42	2.35	3.07
4	5.34	2.25	3.09
5	5.38	2.31	3.07
6	5.35	2.35	3.00
7	5.37	2.33	3.04

S11 Selected bond lengths [$\text{\AA}$] and angles [$^\circ$] for 1, 4, 5 and 6

Table S2. Selected bond lengths [$\text{\AA}$] and angles [$^\circ$] for 1.

F(1)-C(24)	1.311(6)	C(10)-C(11)	1.377(5)
F(2)-C(24)	1.266(5)	C(9)-C(10)	1.371(6)
F(3)-C(24)	1.221(5)	C(12)-C(13)	1.386(4)
C(1)-C(2)	1.359(4)	C(12)-C(17)	1.388(4)
C(1)-C(6)	1.475(4)	C(13)-C(14)	1.383(5)
C(1)-C(5)	1.500(4)	C(14)-C(15)	1.367(6)
C(2)-C(3)	1.471(4)	C(15)-C(16)	1.363(5)
C(2)-C(12)	1.476(4)	C(16)-C(17)	1.381(5)
C(3)-C(4)	1.380(4)	C(18)-C(19)	1.384(4)
C(4)-C(5)	1.458(4)	C(18)-C(23)	1.392(4)
C(4)-C(18)	1.460(4)	C(19)-C(20)	1.379(4)
C(6)-C(11)	1.385(4)	C(20)-C(21)	1.372(5)
C(6)-C(7)	1.391(4)	C(21)-C(22)	1.370(5)
C(7)-C(8)	1.381(5)	C(21)-C(24)	1.461(5)
C(8)-C(9)	1.366(6)	C(22)-C(23)	1.371(5)
C(9)-C(10)	1.371(6)		
C(2)-C(1)-C(6)	130.8(3)	C(14)-C(13)-C(12)	120.7(4)
C(2)-C(1)-C(5)	108.4(2)	C(15)-C(14)-C(13)	121.0(4)
C(6)-C(1)-C(5)	120.8(2)	C(16)-C(15)-C(14)	119.1(4)
C(1)-C(2)-C(3)	108.3(3)	C(15)-C(16)-C(17)	120.4(4)
C(1)-C(2)-C(12)	130.4(3)	C(16)-C(17)-C(12)	121.5(3)
C(3)-C(2)-C(12)	121.3(2)	C(19)-C(18)-C(23)	116.7(3)
C(4)-C(3)-C(2)	109.5(2)	C(19)-C(18)-C(4)	121.4(3)
C(3)-C(4)-C(5)	107.9(2)	C(23)-C(18)-C(4)	121.9(3)
C(3)-C(4)-C(18)	126.8(2)	C(20)-C(19)-C(18)	121.5(3)
C(5)-C(4)-C(18)	125.2(3)	C(21)-C(20)-C(19)	120.9(3)
C(4)-C(5)-C(1)	105.8(2)	C(22)-C(21)-C(20)	118.2(3)
C(11)-C(6)-C(7)	117.3(3)	C(22)-C(21)-C(24)	121.2(4)
C(11)-C(6)-C(1)	122.0(3)	C(20)-C(21)-C(24)	120.5(3)
C(7)-C(6)-C(1)	120.6(3)	C(21)-C(22)-C(23)	121.3(3)
C(8)-C(7)-C(6)	120.9(4)	C(22)-C(23)-C(18)	121.4(3)
C(9)-C(8)-C(7)	120.6(4)	F(3)-C(24)-F(2)	107.1(5)
C(8)-C(9)-C(10)	119.4(4)	F(3)-C(24)-F(1)	102.8(5)
C(9)-C(10)-C(11)	120.3(4)	F(2)-C(24)-F(1)	98.8(4)
C(10)-C(11)-C(6)	121.4(4)	F(3)-C(24)-C(21)	117.1(4)
C(13)-C(12)-C(17)	117.2(3)	F(2)-C(24)-C(21)	115.4(4)
C(13)-C(12)-C(2)	122.5(3)	F(1)-C(24)-C(21)	113.3(4)
C(17)-C(12)-C(2)	120.3(3)		

Table S3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **4**.

C(1)-C(2)	1.3582(17)	C(12)-C(17)	1.3875(19)
C(1)-C(6)	1.4706(17)	C(12)-C(13)	1.3933(18)
C(1)-C(5)	1.5055(16)	C(13)-C(14)	1.380(2)
C(2)-C(3)	1.4627(18)	C(14)-C(15)	1.378(3)
C(2)-C(12)	1.4854(17)	C(15)-C(16)	1.372(2)
C(3)-C(4)	1.3623(17)	C(16)-C(17)	1.381(2)
C(4)-C(18)	1.4653(16)	C(18)-C(23)	1.3939(17)
C(4)-C(5)	1.4884(17)	C(18)-C(19)	1.3950(18)
C(6)-C(7)	1.3891(19)	C(19)-C(20)	1.3768(18)
C(6)-C(11)	1.3976(18)	C(20)-C(21)	1.3891(19)
C(7)-C(8)	1.381(2)	C(21)-C(22)	1.379(2)
C(8)-C(9)	1.371(2)	C(21)-C(24)	1.5085(19)
C(9)-C(10)	1.370(2)	C(22)-C(23)	1.3859(18)
C(10)-C(11)	1.381(2)		
C(2)-C(1)-C(6)	130.59(11)	C(17)-C(12)-C(13)	118.46(12)
C(2)-C(1)-C(5)	108.33(11)	C(17)-C(12)-C(2)	120.00(12)
C(6)-C(1)-C(5)	121.06(11)	C(13)-C(12)-C(2)	121.48(12)
C(1)-C(2)-C(3)	108.86(11)	C(14)-C(13)-C(12)	120.37(14)
C(1)-C(2)-C(12)	130.28(12)	C(15)-C(14)-C(13)	120.31(15)
C(3)-C(2)-C(12)	120.79(11)	C(16)-C(15)-C(14)	119.84(14)
C(4)-C(3)-C(2)	110.16(11)	C(15)-C(16)-C(17)	120.21(15)
C(3)-C(4)-C(18)	127.26(11)	C(16)-C(17)-C(12)	120.71(14)
C(3)-C(4)-C(5)	107.85(11)	C(23)-C(18)-C(19)	116.93(11)
C(18)-C(4)-C(5)	124.79(10)	C(23)-C(18)-C(4)	121.91(11)
C(4)-C(5)-C(1)	104.77(10)	C(19)-C(18)-C(4)	121.12(11)
C(7)-C(6)-C(11)	116.82(12)	C(20)-C(19)-C(18)	121.46(12)
C(7)-C(6)-C(1)	120.21(12)	C(19)-C(20)-C(21)	121.49(12)
C(11)-C(6)-C(1)	122.91(12)	C(22)-C(21)-C(20)	117.27(12)
C(8)-C(7)-C(6)	121.78(14)	C(22)-C(21)-C(24)	122.09(13)
C(9)-C(8)-C(7)	120.41(15)	C(20)-C(21)-C(24)	120.62(13)
C(10)-C(9)-C(8)	118.97(14)	C(21)-C(22)-C(23)	121.74(12)
C(9)-C(10)-C(11)	121.11(14)	C(22)-C(23)-C(18)	121.04(12)
C(10)-C(11)-C(6)	120.89(14)		

Table S4. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **5**.

C(1)-C(2)	1.352(3)	C(13)-C(14)	1.387(4)
C(1)-C(6)	1.462(4)	C(14)-C(15)	1.373(5)
C(1)-C(5)	1.514(3)	C(15)-C(16)	1.354(5)
C(2)-C(3)	1.460(4)	C(16)-C(17)	1.383(4)
C(2)-C(12)	1.481(4)	C(18)-C(27)	1.366(4)
C(3)-C(4)	1.358(4)	C(18)-C(19)	1.433(4)
C(4)-C(18)	1.473(4)	C(19)-C(20)	1.401(4)

C(4)-C(5)	1.481(3)	C(19)-C(24)	1.420(4)
C(6)-C(11)	1.376(4)	C(20)-C(21)	1.371(4)
C(6)-C(7)	1.383(4)	C(21)-C(22)	1.396(5)
C(7)-C(8)	1.373(4)	C(22)-C(23)	1.337(4)
C(8)-C(9)	1.359(5)	C(23)-C(24)	1.406(5)
C(9)-C(10)	1.363(6)	C(24)-C(25)	1.392(5)
C(10)-C(11)	1.375(4)	C(25)-C(26)	1.357(5)
C(12)-C(17)	1.379(4)	C(26)-C(27)	1.414(4)
C(12)-C(13)	1.381(4)		
C(15)-C(14)-C(13)	119.9(4)	C(12)-C(13)-C(14)	120.4(4)
C(2)-C(1)-C(6)	130.4(3)	C(15)-C(14)-C(13)	119.9(4)
C(2)-C(1)-C(5)	107.7(2)	C(15)-C(14)-C(13)	119.9(4)
C(6)-C(1)-C(5)	121.9(3)	C(16)-C(15)-C(14)	120.0(4)
C(1)-C(2)-C(3)	109.1(2)	C(15)-C(16)-C(17)	120.6(4)
C(1)-C(2)-C(12)	129.9(3)	C(12)-C(17)-C(16)	120.4(4)
C(3)-C(2)-C(12)	120.9(3)	C(27)-C(18)-C(19)	119.5(3)
C(4)-C(3)-C(2)	110.5(3)	C(27)-C(18)-C(4)	118.4(3)
C(3)-C(4)-C(18)	128.9(3)	C(19)-C(18)-C(4)	122.0(3)
C(3)-C(4)-C(5)	107.5(3)	C(20)-C(19)-C(24)	117.9(3)
C(18)-C(4)-C(5)	123.4(3)	C(20)-C(19)-C(18)	123.5(3)
C(4)-C(5)-C(1)	105.2(2)	C(24)-C(19)-C(18)	118.6(3)
C(11)-C(6)-C(7)	117.5(3)	C(21)-C(20)-C(19)	121.0(3)
C(11)-C(6)-C(1)	121.8(3)	C(20)-C(21)-C(22)	120.3(4)
C(7)-C(6)-C(1)	120.8(3)	C(23)-C(22)-C(21)	120.0(4)
C(8)-C(7)-C(6)	121.4(4)	C(22)-C(23)-C(24)	121.8(4)
C(9)-C(8)-C(7)	120.2(4)	C(25)-C(24)-C(23)	122.0(4)
C(10)-C(9)-C(8)	119.4(4)	C(25)-C(24)-C(19)	119.2(4)
C(9)-C(10)-C(11)	120.8(4)	C(23)-C(24)-C(19)	118.7(4)
C(6)-C(11)-C(10)	120.8(4)	C(26)-C(25)-C(24)	122.1(4)
C(17)-C(12)-C(13)	118.7(3)	C(25)-C(26)-C(27)	119.1(4)
C(17)-C(12)-C(2)	119.6(3)	C(18)-C(27)-C(26)	121.4(3)
C(13)-C(12)-C(2)	121.7(3)		

Table S5. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **6**.

C(1)-C(2)	1.356(5)	C(30)-C(31)	1.358(5)
C(1)-C(6)	1.472(5)	C(30)-C(34)	1.458(5)
C(1)-C(5)	1.498(5)	C(30)-C(35)	1.485(5)
C(2)-C(12)	1.478(5)	C(31)-C(41)	1.486(5)
C(2)-C(3)	1.479(5)	C(31)-C(32)	1.509(5)
C(3)-C(4)	1.365(5)	C(32)-C(33)	1.466(5)
C(4)-C(18)	1.462(6)	C(33)-C(34)	1.393(5)
C(4)-C(5)	1.465(5)	C(33)-C(47)	1.468(5)
C(6)-C(7)	1.391(5)	C(35)-C(40)	1.383(5)

C(6)-C(11)	1.399(5)	C(35)-C(36)	1.392(5)
C(7)-C(8)	1.372(5)	C(36)-C(37)	1.384(5)
C(8)-C(9)	1.377(6)	C(37)-C(38)	1.369(6)
C(9)-C(10)	1.379(6)	C(38)-C(39)	1.367(6)
C(10)-C(11)	1.377(5)	C(39)-C(40)	1.382(5)
C(12)-C(17)	1.388(5)	C(41)-C(46)	1.383(5)
C(12)-C(13)	1.396(5)	C(41)-C(42)	1.389(5)
C(13)-C(14)	1.369(5)	C(42)-C(43)	1.383(5)
C(14)-C(15)	1.386(6)	C(43)-C(44)	1.365(6)
C(15)-C(16)	1.375(6)	C(44)-C(45)	1.377(6)
C(16)-C(17)	1.371(5)	C(45)-C(46)	1.393(5)
C(18)-C(23)	1.383(5)	C(47)-C(48)	1.393(5)
C(18)-C(19)	1.397(5)	C(47)-C(52)	1.394(5)
C(19)-C(20)	1.388(4)	C(48)-C(49)	1.377(5)
C(20)-C(21)	1.397(5)	C(49)-C(50)	1.395(5)
C(21)-C(22)	1.372(5)	C(50)-C(51)	1.394(4)
C(21)-C(24)	1.488(5)	C(50)-C(53)	1.486(5)
C(22)-C(23)	1.380(5)	C(51)-C(52)	1.380(4)
C(24)-C(29)	1.374(5)	C(53)-C(54)	1.393(5)
C(24)-C(25)	1.401(5)	C(53)-C(58)	1.398(5)
C(25)-C(26)	1.385(4)	C(54)-C(55)	1.380(4)
C(26)-C(27)	1.377(6)	C(55)-C(56)	1.366(5)
C(27)-C(28)	1.366(6)	C(56)-C(57)	1.390(5)
C(28)-C(29)	1.391(5)	C(57)-C(58)	1.370(4)
C(59)-C(60)	1.353(5)	C(88)-C(89)	1.370(5)
C(59)-C(64)	1.478(5)	C(88)-C(92)	1.465(5)
C(59)-C(63)	1.502(5)	C(88)-C(93)	1.474(5)
C(60)-C(61)	1.475(5)	C(89)-C(99)	1.476(5)
C(60)-C(70)	1.478(5)	C(89)-C(90)	1.492(5)
C(61)-C(62)	1.385(5)	C(90)-C(91)	1.469(5)
C(64)-C(69)	1.388(5)	C(91)-C(92)	1.372(5)
C(64)-C(65)	1.401(5)	C(91)-C(105)	1.472(5)
C(65)-C(66)	1.382(5)	C(93)-C(94)	1.400(5)
C(66)-C(67)	1.363(6)	C(93)-C(98)	1.407(5)
C(67)-C(68)	1.377(6)	C(94)-C(95)	1.388(5)
C(68)-C(69)	1.379(5)	C(95)-C(96)	1.379(6)
C(70)-C(71)	1.367(5)	C(96)-C(97)	1.377(6)
C(70)-C(75)	1.387(5)	C(97)-C(98)	1.379(5)
C(71)-C(72)	1.383(5)	C(99)-C(104)	1.394(5)
C(72)-C(73)	1.366(6)	C(99)-C(100)	1.400(5)
C(73)-C(74)	1.370(6)	C(100)-C(101)	1.386(5)
C(74)-C(75)	1.385(5)	C(101)-C(102)	1.387(6)
C(76)-C(81)	1.383(5)	C(102)-C(103)	1.368(6)
C(76)-C(77)	1.390(5)	C(103)-C(104)	1.367(5)

C(77)-C(78)	1.393(4)	C(105)-C(106)	1.385(5)
C(78)-C(79)	1.396(5)	C(105)-C(110)	1.387(5)
C(79)-C(80)	1.379(5)	C(106)-C(107)	1.371(5)
C(79)-C(82)	1.489(5)	C(107)-C(108)	1.390(5)
C(80)-C(81)	1.387(5)	C(108)-C(109)	1.391(5)
C(82)-C(87)	1.390(5)	C(108)-C(111)	1.492(5)
C(82)-C(83)	1.395(5)	C(109)-C(110)	1.387(4)
C(83)-C(84)	1.382(4)	C(111)-C(112)	1.375(5)
C(84)-C(85)	1.382(5)	C(111)-C(116)	1.401(5)
C(85)-C(86)	1.366(5)	C(112)-C(113)	1.390(5)
C(86)-C(87)	1.381(5)	C(113)-C(114)	1.361(5)
C(115)-C(116)	1.389(4)	C(114)-C(115)	1.377(5)
C(2)-C(1)-C(6)	130.9(4)	C(31)-C(30)-C(34)	108.6(4)
C(2)-C(1)-C(5)	108.0(3)	C(31)-C(30)-C(35)	129.4(4)
C(6)-C(1)-C(5)	120.9(3)	C(34)-C(30)-C(35)	121.9(3)
C(1)-C(2)-C(12)	130.2(4)	C(30)-C(31)-C(41)	130.7(4)
C(1)-C(2)-C(3)	108.7(4)	C(30)-C(31)-C(32)	108.4(3)
C(12)-C(2)-C(3)	121.1(3)	C(41)-C(31)-C(32)	120.8(3)
C(4)-C(3)-C(2)	109.2(4)	C(33)-C(32)-C(31)	105.7(3)
C(3)-C(4)-C(18)	126.4(4)	C(34)-C(33)-C(32)	107.2(3)
C(3)-C(4)-C(5)	108.2(4)	C(34)-C(33)-C(47)	126.6(4)
C(18)-C(4)-C(5)	125.4(4)	C(32)-C(33)-C(47)	126.2(4)
C(4)-C(5)-C(1)	105.8(3)	C(33)-C(34)-C(30)	110.1(4)
C(7)-C(6)-C(11)	116.9(4)	C(40)-C(35)-C(36)	116.9(4)
C(7)-C(6)-C(1)	121.3(3)	C(40)-C(35)-C(30)	123.3(3)
C(11)-C(6)-C(1)	121.7(3)	C(36)-C(35)-C(30)	119.8(4)
C(8)-C(7)-C(6)	121.6(4)	C(37)-C(36)-C(35)	122.2(4)
C(7)-C(8)-C(9)	120.5(4)	C(38)-C(37)-C(36)	119.4(4)
C(8)-C(9)-C(10)	119.1(4)	C(39)-C(38)-C(37)	119.6(4)
C(11)-C(10)-C(9)	120.4(4)	C(38)-C(39)-C(40)	121.0(4)
C(10)-C(11)-C(6)	121.3(4)	C(39)-C(40)-C(35)	120.9(4)
C(17)-C(12)-C(13)	117.1(4)	C(46)-C(41)-C(42)	118.4(4)
C(17)-C(12)-C(2)	120.3(4)	C(46)-C(41)-C(31)	120.7(3)
C(13)-C(12)-C(2)	122.5(4)	C(42)-C(41)-C(31)	120.9(3)
C(14)-C(13)-C(12)	121.0(4)	C(43)-C(42)-C(41)	120.5(4)
C(13)-C(14)-C(15)	120.7(4)	C(44)-C(43)-C(42)	120.6(4)
C(16)-C(15)-C(14)	118.9(4)	C(43)-C(44)-C(45)	120.1(4)
C(17)-C(16)-C(15)	120.3(4)	C(44)-C(45)-C(46)	119.4(4)
C(16)-C(17)-C(12)	121.8(4)	C(41)-C(46)-C(45)	121.0(4)
C(23)-C(18)-C(19)	116.0(4)	C(48)-C(47)-C(52)	117.0(3)
C(23)-C(18)-C(4)	121.2(4)	C(48)-C(47)-C(33)	121.5(4)
C(19)-C(18)-C(4)	122.8(4)	C(52)-C(47)-C(33)	121.4(3)
C(20)-C(19)-C(18)	121.8(4)	C(49)-C(48)-C(47)	121.4(4)

C(19)-C(20)-C(21)	120.8(3)	C(48)-C(49)-C(50)	122.0(3)
C(22)-C(21)-C(20)	117.5(3)	C(51)-C(50)-C(49)	116.4(3)
C(22)-C(21)-C(24)	121.3(4)	C(51)-C(50)-C(53)	121.5(3)
C(20)-C(21)-C(24)	121.3(4)	C(49)-C(50)-C(53)	122.1(3)
C(21)-C(22)-C(23)	121.3(4)	C(52)-C(51)-C(50)	121.8(3)
C(22)-C(23)-C(18)	122.6(4)	C(51)-C(52)-C(47)	121.3(3)
C(29)-C(24)-C(25)	117.4(4)	C(54)-C(53)-C(58)	116.2(3)
C(29)-C(24)-C(21)	121.4(4)	C(54)-C(53)-C(50)	121.6(4)
C(25)-C(24)-C(21)	121.2(4)	C(58)-C(53)-C(50)	122.1(3)
C(26)-C(25)-C(24)	120.7(4)	C(55)-C(54)-C(53)	122.0(3)
C(27)-C(26)-C(25)	120.5(4)	C(56)-C(55)-C(54)	120.5(4)
C(28)-C(27)-C(26)	119.6(4)	C(55)-C(56)-C(57)	118.9(4)
C(27)-C(28)-C(29)	120.0(4)	C(58)-C(57)-C(56)	120.5(4)
C(24)-C(29)-C(28)	121.9(4)	C(57)-C(58)-C(53)	121.8(3)
C(60)-C(59)-C(64)	130.3(3)	C(89)-C(88)-C(92)	108.6(4)
C(60)-C(59)-C(63)	108.9(3)	C(89)-C(88)-C(93)	129.9(4)
C(64)-C(59)-C(63)	120.8(3)	C(92)-C(88)-C(93)	121.4(3)
C(59)-C(60)-C(61)	108.5(3)	C(88)-C(89)-C(99)	130.9(4)
C(59)-C(60)-C(70)	130.2(3)	C(88)-C(89)-C(90)	108.1(3)
C(61)-C(60)-C(70)	121.3(3)	C(99)-C(89)-C(90)	120.8(3)
C(62)-C(61)-C(60)	109.5(3)	C(91)-C(90)-C(89)	105.6(3)
C(61)-C(62)-C(76)	126.4(4)	C(92)-C(91)-C(90)	108.2(4)
C(61)-C(62)-C(63)	107.7(3)	C(92)-C(91)-C(105)	126.2(4)
C(76)-C(62)-C(63)	125.8(4)	C(90)-C(91)-C(105)	125.6(4)
C(62)-C(63)-C(59)	105.4(3)	C(91)-C(92)-C(88)	109.4(4)
C(69)-C(64)-C(65)	117.0(4)	C(94)-C(93)-C(98)	117.4(4)
C(69)-C(64)-C(59)	122.7(3)	C(94)-C(93)-C(88)	120.2(4)
C(65)-C(64)-C(59)	120.3(3)	C(98)-C(93)-C(88)	122.3(4)
C(66)-C(65)-C(64)	121.6(4)	C(95)-C(94)-C(93)	120.9(4)
C(67)-C(66)-C(65)	120.1(4)	C(96)-C(95)-C(94)	120.7(4)
C(66)-C(67)-C(68)	119.3(4)	C(95)-C(96)-C(97)	119.1(4)
C(67)-C(68)-C(69)	121.1(4)	C(96)-C(97)-C(98)	121.1(4)
C(68)-C(69)-C(64)	120.7(4)	C(97)-C(98)-C(93)	120.7(4)
C(71)-C(70)-C(75)	117.1(4)	C(104)-C(99)-C(100)	117.4(4)
C(71)-C(70)-C(60)	122.8(3)	C(104)-C(99)-C(89)	120.4(3)
C(75)-C(70)-C(60)	120.0(3)	C(100)-C(99)-C(89)	122.1(3)
C(70)-C(71)-C(72)	121.5(4)	C(101)-C(100)-C(99)	121.2(4)
C(73)-C(72)-C(71)	120.2(4)	C(100)-C(101)-C(102)	119.4(4)
C(72)-C(73)-C(74)	120.3(4)	C(103)-C(102)-C(101)	119.8(4)
C(73)-C(74)-C(75)	118.6(4)	C(104)-C(103)-C(102)	120.9(4)
C(74)-C(75)-C(70)	122.3(4)	C(103)-C(104)-C(99)	121.2(4)
C(81)-C(76)-C(77)	116.5(3)	C(106)-C(105)-C(110)	116.7(4)
C(81)-C(76)-C(62)	121.3(4)	C(106)-C(105)-C(91)	120.9(4)
C(77)-C(76)-C(62)	122.1(4)	C(110)-C(105)-C(91)	122.4(4)

C(76)-C(77)-C(78)	121.6(3)	C(107)-C(106)-C(105)	122.2(3)
C(77)-C(78)-C(79)	121.2(3)	C(106)-C(107)-C(108)	121.4(4)
C(80)-C(79)-C(78)	116.9(3)	C(107)-C(108)-C(109)	116.8(3)
C(80)-C(79)-C(82)	122.0(4)	C(107)-C(108)-C(111)	120.9(4)
C(78)-C(79)-C(82)	121.1(4)	C(109)-C(108)-C(111)	122.3(4)
C(79)-C(80)-C(81)	121.5(4)	C(110)-C(109)-C(108)	121.4(3)
C(76)-C(81)-C(80)	122.2(4)	C(109)-C(110)-C(105)	121.4(3)
C(87)-C(82)-C(83)	116.6(3)	C(112)-C(111)-C(116)	117.6(3)
C(87)-C(82)-C(79)	121.3(4)	C(112)-C(111)-C(108)	121.5(3)
C(83)-C(82)-C(79)	122.1(3)	C(116)-C(111)-C(108)	120.9(3)
C(84)-C(83)-C(82)	121.4(3)	C(111)-C(112)-C(113)	121.4(4)
C(85)-C(84)-C(83)	120.4(4)	C(114)-C(113)-C(112)	120.4(4)
C(86)-C(85)-C(84)	119.2(4)	C(113)-C(114)-C(115)	119.8(4)
C(85)-C(86)-C(87)	120.4(4)	C(114)-C(115)-C(116)	120.0(4)
C(86)-C(87)-C(82)	122.0(4)	C(115)-C(116)-C(111)	120.8(3)