

Electronic supplemental information

Phenothiazine-azaBODIPY-fullerene supramolecules: syntheses, structural characterization, and photochemical studies

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Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1b**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
S(1)	-6586(2)	3443(1)	277(1)	36(1)
F(1)	2311(4)	6016(2)	3501(1)	24(1)
O(1)	-4962(5)	6352(2)	1677(2)	27(1)
N(1)	1450(5)	6914(3)	4463(2)	20(1)
C(1)	-158(6)	7155(3)	4315(2)	19(1)
B(1)	2352(7)	6043(4)	4126(3)	21(1)
S(2)	7726(2)	-460(1)	1209(1)	24(1)
F(2)	1537(4)	5214(2)	4141(1)	23(1)
O(2)	-5469(4)	5345(2)	2210(2)	25(1)
N(2)	3925(5)	7656(3)	5273(2)	20(1)
C(2)	-337(6)	8014(3)	4779(2)	21(1)
O(3)	6732(5)	2744(2)	2022(2)	25(1)
N(3)	4221(5)	6175(3)	4499(2)	18(1)
C(3)	1192(6)	8318(3)	5222(2)	21(1)
O(4)	5538(5)	2008(2)	2606(2)	22(1)
C(4)	2305(7)	7624(3)	5011(2)	20(1)
C(5)	5480(6)	5580(3)	4447(2)	18(1)
C(6)	6891(6)	6012(3)	4948(2)	20(1)
C(7)	6528(6)	6867(3)	5320(2)	20(1)
C(8)	4833(6)	6976(3)	5035(2)	20(1)
C(9)	-1480(6)	6649(3)	3762(2)	20(1)
C(10)	-2865(7)	7139(4)	3618(3)	26(1)
C(11)	-4181(7)	6730(4)	3099(3)	26(1)
C(12)	-4123(6)	5816(4)	2715(2)	22(1)
C(13)	-2806(7)	5303(4)	2838(3)	25(1)
C(14)	-1494(7)	5714(4)	3361(2)	24(1)
C(15)	-5782(7)	5694(4)	1717(2)	23(1)
N(4)	-7177(5)	5169(3)	1279(2)	23(1)
C(16)	-7953(7)	4308(4)	1317(3)	25(1)
C(17)	-8901(7)	4339(4)	1785(3)	31(1)
C(18)	-9669(7)	3508(5)	1806(3)	38(2)

C(19)	-9501(8)	2653(4)	1358(3)	41(2)
C(20)	-8577(8)	2624(4)	890(3)	43(2)
C(21)	-7781(7)	3464(4)	865(3)	29(1)
C(22)	-7117(7)	4501(4)	147(3)	27(1)
C(23)	-7194(8)	4600(4)	-446(3)	34(1)
C(24)	-7669(8)	5424(4)	-548(3)	37(2)
C(25)	-8107(7)	6139(4)	-58(3)	36(2)
C(26)	-7977(7)	6070(4)	549(3)	27(1)
C(27)	-7429(7)	5258(4)	655(3)	24(1)
C(28)	1571(7)	9180(3)	5785(2)	21(1)
C(29)	557(7)	9924(4)	5826(3)	26(1)
C(30)	914(8)	10741(4)	6356(3)	30(1)
C(31)	2270(8)	10829(4)	6852(3)	35(1)
C(32)	3278(8)	10100(4)	6812(3)	30(1)
C(33)	2934(7)	9285(4)	6288(3)	24(1)
C(34)	5403(6)	4657(3)	3960(2)	19(1)
C(35)	6621(7)	4052(3)	4069(2)	22(1)
C(36)	6681(6)	3189(3)	3626(2)	21(1)
C(37)	5516(6)	2909(3)	3058(2)	20(1)
C(38)	4298(7)	3472(3)	2930(2)	23(1)
C(39)	4244(7)	4340(4)	3380(2)	23(1)
C(40)	6063(6)	2043(3)	2070(2)	20(1)
N(5)	5765(5)	1170(3)	1600(2)	19(1)
C(41)	4970(6)	326(3)	1654(2)	20(1)
C(42)	3404(7)	300(4)	1841(2)	24(1)
C(43)	2697(7)	-537(4)	1877(2)	25(1)
C(44)	3520(7)	-1349(4)	1721(2)	25(1)
C(45)	5048(7)	-1332(4)	1509(2)	24(1)
C(46)	5778(6)	-492(3)	1479(2)	20(1)
C(47)	7263(6)	335(3)	784(2)	22(1)
C(48)	7844(7)	216(4)	215(3)	26(1)
C(49)	7479(7)	853(4)	-109(3)	30(1)
C(50)	6491(7)	1577(4)	115(3)	29(1)
C(51)	5927(7)	1686(4)	675(2)	24(1)
C(52)	6322(6)	1073(3)	1013(2)	19(1)
C(53)	7563(6)	7518(3)	5916(2)	20(1)

C(54)	7377(7)	8486(4)	6125(2)	24(1)
C(55)	8339(7)	9076(4)	6694(3)	28(1)
C(56)	9496(7)	8728(4)	7072(3)	29(1)
C(57)	9685(7)	7768(4)	6870(3)	28(1)
C(58)	8734(7)	7170(4)	6295(3)	24(1)
Cl(1)	9122(2)	7637(1)	1568(1)	38(1)
Cl(2)	11134(2)	7153(1)	2602(1)	43(1)
C(1A)	9331(7)	6832(4)	1997(3)	24(1)
C(2A)	5148(7)	9558(3)	4748(2)	24(1)
Cl(3)	3525(6)	8933(4)	4043(3)	177(2)

Table S2. Bond lengths [Å] and angles [°] for **1b**

S(1)-C(21)	1.753(6)
S(1)-C(22)	1.763(6)
F(1)-B(1)	1.390(7)
O(1)-C(15)	1.196(6)
N(1)-C(1)	1.368(6)
N(1)-C(4)	1.391(6)
N(1)-B(1)	1.567(7)
C(1)-C(2)	1.411(7)
C(1)-C(9)	1.457(7)
B(1)-F(2)	1.388(6)
B(1)-N(3)	1.556(7)
S(2)-C(47)	1.769(5)
S(2)-C(46)	1.770(5)
O(2)-C(15)	1.364(6)
O(2)-C(12)	1.398(6)
N(2)-C(8)	1.309(6)
N(2)-C(4)	1.322(6)
C(2)-C(3)	1.395(7)
C(2)-H(2A)	0.9500
O(3)-C(40)	1.202(6)
N(3)-C(5)	1.373(6)
N(3)-C(8)	1.402(6)
C(3)-C(4)	1.421(7)
C(3)-C(28)	1.471(7)
O(4)-C(40)	1.358(6)
O(4)-C(37)	1.415(6)
C(5)-C(6)	1.415(7)
C(5)-C(34)	1.460(7)
C(6)-C(7)	1.367(7)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.439(7)
C(7)-C(53)	1.468(7)
C(9)-C(14)	1.406(7)
C(9)-C(10)	1.407(7)

C(10)-C(11)	1.386(7)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.378(7)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.375(7)
C(13)-C(14)	1.389(7)
C(13)-H(13A)	0.9500
C(14)-H(14A)	0.9500
C(15)-N(4)	1.375(6)
N(4)-C(27)	1.435(7)
N(4)-C(16)	1.439(6)
C(16)-C(21)	1.381(8)
C(16)-C(17)	1.391(8)
C(17)-C(18)	1.381(8)
C(17)-H(17A)	0.9500
C(18)-C(19)	1.387(9)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.378(10)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.407(8)
C(20)-H(20A)	0.9500
C(22)-C(23)	1.383(8)
C(22)-C(27)	1.400(8)
C(23)-C(24)	1.386(8)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.381(9)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.391(8)
C(25)-H(25A)	0.9500
C(26)-C(27)	1.393(7)
C(26)-H(26A)	0.9500
C(28)-C(33)	1.398(7)
C(28)-C(29)	1.401(7)
C(29)-C(30)	1.390(7)
C(29)-H(29A)	0.9500
C(30)-C(31)	1.387(8)

C(30)-H(30A)	0.9500
C(31)-C(32)	1.380(8)
C(31)-H(31A)	0.9500
C(32)-C(33)	1.380(7)
C(32)-H(32A)	0.9500
C(33)-H(33A)	0.9500
C(34)-C(39)	1.396(7)
C(34)-C(35)	1.408(7)
C(35)-C(36)	1.370(7)
C(35)-H(35A)	0.9500
C(36)-C(37)	1.378(7)
C(36)-H(36A)	0.9500
C(37)-C(38)	1.373(7)
C(38)-C(39)	1.381(7)
C(38)-H(38A)	0.9500
C(39)-H(39A)	0.9500
C(40)-N(5)	1.378(6)
N(5)-C(52)	1.433(6)
N(5)-C(41)	1.439(6)
C(41)-C(42)	1.390(7)
C(41)-C(46)	1.391(7)
C(42)-C(43)	1.385(7)
C(42)-H(42A)	0.9500
C(43)-C(44)	1.387(8)
C(43)-H(43A)	0.9500
C(44)-C(45)	1.388(8)
C(44)-H(44A)	0.9500
C(45)-C(46)	1.390(7)
C(45)-H(45A)	0.9500
C(47)-C(52)	1.381(7)
C(47)-C(48)	1.398(7)
C(48)-C(49)	1.390(8)
C(48)-H(48A)	0.9500
C(49)-C(50)	1.389(8)
C(49)-H(49A)	0.9500
C(50)-C(51)	1.376(8)

C(50)-H(50A)	0.9500
C(51)-C(52)	1.384(7)
C(51)-H(51A)	0.9500
C(53)-C(58)	1.392(7)
C(53)-C(54)	1.402(7)
C(54)-C(55)	1.379(7)
C(54)-H(54A)	0.9500
C(55)-C(56)	1.385(8)
C(55)-H(55A)	0.9500
C(56)-C(57)	1.391(8)
C(56)-H(56A)	0.9500
C(57)-C(58)	1.386(7)
C(57)-H(57A)	0.9500
C(58)-H(58A)	0.9500
Cl(1)-C(1A)	1.769(5)
Cl(2)-C(1A)	1.738(5)
C(1A)-H(1AA)	0.9900
C(1A)-H(1AB)	0.9900
C(2A)-C(2A)#1	1.506(11)
C(2A)-Cl(3)	1.824(7)
C(2A)-H(2AA)	0.9900
C(2A)-H(2AB)	0.9900
C(21)-S(1)-C(22)	98.8(3)
C(1)-N(1)-C(4)	107.6(4)
C(1)-N(1)-B(1)	131.3(4)
C(4)-N(1)-B(1)	121.1(4)
N(1)-C(1)-C(2)	108.7(4)
N(1)-C(1)-C(9)	127.2(4)
C(2)-C(1)-C(9)	124.1(5)
F(2)-B(1)-F(1)	110.9(4)
F(2)-B(1)-N(3)	108.5(4)
F(1)-B(1)-N(3)	111.1(4)
F(2)-B(1)-N(1)	110.4(4)
F(1)-B(1)-N(1)	107.9(4)
N(3)-B(1)-N(1)	108.0(4)

C(47)-S(2)-C(46)	98.0(2)
C(15)-O(2)-C(12)	117.1(4)
C(8)-N(2)-C(4)	120.7(4)
C(3)-C(2)-C(1)	108.7(4)
C(3)-C(2)-H(2A)	125.6
C(1)-C(2)-H(2A)	125.6
C(5)-N(3)-C(8)	107.1(4)
C(5)-N(3)-B(1)	131.6(4)
C(8)-N(3)-B(1)	121.0(4)
C(2)-C(3)-C(4)	105.4(4)
C(2)-C(3)-C(28)	127.1(5)
C(4)-C(3)-C(28)	127.5(5)
C(40)-O(4)-C(37)	113.6(4)
N(2)-C(4)-N(1)	124.4(5)
N(2)-C(4)-C(3)	126.0(4)
N(1)-C(4)-C(3)	109.5(4)
N(3)-C(5)-C(6)	108.5(4)
N(3)-C(5)-C(34)	126.4(4)
C(6)-C(5)-C(34)	125.0(5)
C(7)-C(6)-C(5)	109.7(5)
C(7)-C(6)-H(6A)	125.1
C(5)-C(6)-H(6A)	125.1
C(6)-C(7)-C(8)	105.6(4)
C(6)-C(7)-C(53)	128.3(5)
C(8)-C(7)-C(53)	126.0(4)
N(2)-C(8)-N(3)	124.7(4)
N(2)-C(8)-C(7)	125.8(5)
N(3)-C(8)-C(7)	109.0(4)
C(14)-C(9)-C(10)	117.2(5)
C(14)-C(9)-C(1)	125.6(5)
C(10)-C(9)-C(1)	117.1(4)
C(11)-C(10)-C(9)	122.0(5)
C(11)-C(10)-H(10A)	119.0
C(9)-C(10)-H(10A)	119.0
C(12)-C(11)-C(10)	118.5(5)
C(12)-C(11)-H(11A)	120.7

C(10)-C(11)-H(11A)	120.7
C(13)-C(12)-C(11)	121.8(5)
C(13)-C(12)-O(2)	117.0(5)
C(11)-C(12)-O(2)	121.1(5)
C(12)-C(13)-C(14)	119.5(5)
C(12)-C(13)-H(13A)	120.3
C(14)-C(13)-H(13A)	120.3
C(13)-C(14)-C(9)	121.0(5)
C(13)-C(14)-H(14A)	119.5
C(9)-C(14)-H(14A)	119.5
O(1)-C(15)-O(2)	124.9(5)
O(1)-C(15)-N(4)	125.9(5)
O(2)-C(15)-N(4)	109.2(4)
C(15)-N(4)-C(27)	117.1(4)
C(15)-N(4)-C(16)	122.5(4)
C(27)-N(4)-C(16)	115.8(4)
C(21)-C(16)-C(17)	121.3(5)
C(21)-C(16)-N(4)	118.3(5)
C(17)-C(16)-N(4)	120.3(5)
C(18)-C(17)-C(16)	119.6(6)
C(18)-C(17)-H(17A)	120.2
C(16)-C(17)-H(17A)	120.2
C(17)-C(18)-C(19)	119.9(6)
C(17)-C(18)-H(18A)	120.1
C(19)-C(18)-H(18A)	120.1
C(20)-C(19)-C(18)	120.6(5)
C(20)-C(19)-H(19A)	119.7
C(18)-C(19)-H(19A)	119.7
C(19)-C(20)-C(21)	120.1(6)
C(19)-C(20)-H(20A)	119.9
C(21)-C(20)-H(20A)	119.9
C(16)-C(21)-C(20)	118.5(6)
C(16)-C(21)-S(1)	120.6(4)
C(20)-C(21)-S(1)	120.9(5)
C(23)-C(22)-C(27)	119.6(5)
C(23)-C(22)-S(1)	120.9(4)

C(27)-C(22)-S(1)	119.5(4)
C(22)-C(23)-C(24)	120.4(6)
C(22)-C(23)-H(23A)	119.8
C(24)-C(23)-H(23A)	119.8
C(25)-C(24)-C(23)	119.8(6)
C(25)-C(24)-H(24A)	120.1
C(23)-C(24)-H(24A)	120.1
C(24)-C(25)-C(26)	120.9(6)
C(24)-C(25)-H(25A)	119.6
C(26)-C(25)-H(25A)	119.6
C(25)-C(26)-C(27)	119.0(5)
C(25)-C(26)-H(26A)	120.5
C(27)-C(26)-H(26A)	120.5
C(26)-C(27)-C(22)	120.1(5)
C(26)-C(27)-N(4)	121.5(5)
C(22)-C(27)-N(4)	118.4(5)
C(33)-C(28)-C(29)	118.2(5)
C(33)-C(28)-C(3)	121.7(5)
C(29)-C(28)-C(3)	120.1(5)
C(30)-C(29)-C(28)	120.2(5)
C(30)-C(29)-H(29A)	119.9
C(28)-C(29)-H(29A)	119.9
C(31)-C(30)-C(29)	120.6(5)
C(31)-C(30)-H(30A)	119.7
C(29)-C(30)-H(30A)	119.7
C(32)-C(31)-C(30)	119.4(5)
C(32)-C(31)-H(31A)	120.3
C(30)-C(31)-H(31A)	120.3
C(33)-C(32)-C(31)	120.5(5)
C(33)-C(32)-H(32A)	119.8
C(31)-C(32)-H(32A)	119.8
C(32)-C(33)-C(28)	121.1(5)
C(32)-C(33)-H(33A)	119.5
C(28)-C(33)-H(33A)	119.5
C(39)-C(34)-C(35)	117.2(5)
C(39)-C(34)-C(5)	124.7(5)

C(35)-C(34)-C(5)	118.0(4)
C(36)-C(35)-C(34)	121.8(5)
C(36)-C(35)-H(35A)	119.1
C(34)-C(35)-H(35A)	119.1
C(35)-C(36)-C(37)	118.9(5)
C(35)-C(36)-H(36A)	120.6
C(37)-C(36)-H(36A)	120.6
C(38)-C(37)-C(36)	121.5(5)
C(38)-C(37)-O(4)	119.2(4)
C(36)-C(37)-O(4)	119.3(4)
C(37)-C(38)-C(39)	119.3(5)
C(37)-C(38)-H(38A)	120.4
C(39)-C(38)-H(38A)	120.4
C(38)-C(39)-C(34)	121.3(5)
C(38)-C(39)-H(39A)	119.3
C(34)-C(39)-H(39A)	119.3
O(3)-C(40)-O(4)	123.9(4)
O(3)-C(40)-N(5)	124.8(5)
O(4)-C(40)-N(5)	111.3(4)
C(40)-N(5)-C(52)	118.4(4)
C(40)-N(5)-C(41)	125.2(4)
C(52)-N(5)-C(41)	116.4(4)
C(42)-C(41)-C(46)	120.1(5)
C(42)-C(41)-N(5)	122.1(5)
C(46)-C(41)-N(5)	117.8(4)
C(43)-C(42)-C(41)	119.3(5)
C(43)-C(42)-H(42A)	120.3
C(41)-C(42)-H(42A)	120.3
C(42)-C(43)-C(44)	120.8(5)
C(42)-C(43)-H(43A)	119.6
C(44)-C(43)-H(43A)	119.6
C(45)-C(44)-C(43)	119.8(5)
C(45)-C(44)-H(44A)	120.1
C(43)-C(44)-H(44A)	120.1
C(44)-C(45)-C(46)	119.7(5)
C(44)-C(45)-H(45A)	120.1

C(46)-C(45)-H(45A)	120.1
C(41)-C(46)-C(45)	120.2(5)
C(41)-C(46)-S(2)	119.6(4)
C(45)-C(46)-S(2)	120.2(4)
C(52)-C(47)-C(48)	119.9(5)
C(52)-C(47)-S(2)	120.1(4)
C(48)-C(47)-S(2)	120.1(4)
C(49)-C(48)-C(47)	119.2(5)
C(49)-C(48)-H(48A)	120.4
C(47)-C(48)-H(48A)	120.4
C(50)-C(49)-C(48)	120.5(5)
C(50)-C(49)-H(49A)	119.8
C(48)-C(49)-H(49A)	119.8
C(51)-C(50)-C(49)	119.7(5)
C(51)-C(50)-H(50A)	120.2
C(49)-C(50)-H(50A)	120.2
C(50)-C(51)-C(52)	120.4(5)
C(50)-C(51)-H(51A)	119.8
C(52)-C(51)-H(51A)	119.8
C(47)-C(52)-C(51)	120.3(5)
C(47)-C(52)-N(5)	117.9(4)
C(51)-C(52)-N(5)	121.8(5)
C(58)-C(53)-C(54)	118.6(5)
C(58)-C(53)-C(7)	119.8(4)
C(54)-C(53)-C(7)	121.6(5)
C(55)-C(54)-C(53)	120.3(5)
C(55)-C(54)-H(54A)	119.8
C(53)-C(54)-H(54A)	119.8
C(54)-C(55)-C(56)	121.0(5)
C(54)-C(55)-H(55A)	119.5
C(56)-C(55)-H(55A)	119.5
C(55)-C(56)-C(57)	119.1(5)
C(55)-C(56)-H(56A)	120.4
C(57)-C(56)-H(56A)	120.4
C(58)-C(57)-C(56)	120.3(5)
C(58)-C(57)-H(57A)	119.9

C(56)-C(57)-H(57A)	119.9
C(57)-C(58)-C(53)	120.7(5)
C(57)-C(58)-H(58A)	119.6
C(53)-C(58)-H(58A)	119.6
Cl(2)-C(1A)-Cl(1)	112.1(3)
Cl(2)-C(1A)-H(1AA)	109.2
Cl(1)-C(1A)-H(1AA)	109.2
Cl(2)-C(1A)-H(1AB)	109.2
Cl(1)-C(1A)-H(1AB)	109.2
H(1AA)-C(1A)-H(1AB)	107.9
C(2A)#1-C(2A)-Cl(3)	122.6(5)
C(2A)#1-C(2A)-H(2AA)	106.7
Cl(3)-C(2A)-H(2AA)	106.7
C(2A)#1-C(2A)-H(2AB)	106.7
Cl(3)-C(2A)-H(2AB)	106.7
H(2AA)-C(2A)-H(2AB)	106.6

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1

Table S3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	42(1)	25(1)	38(1)	8(1)	4(1)	8(1)
F(1)	26(2)	22(2)	20(2)	6(1)	1(1)	2(1)
O(1)	28(2)	19(2)	30(2)	8(2)	-2(2)	-10(2)
N(1)	20(2)	15(2)	20(2)	4(2)	0(2)	-2(2)
C(1)	18(2)	15(2)	21(3)	5(2)	0(2)	0(2)
B(1)	20(3)	19(3)	21(3)	5(2)	-1(2)	-1(2)
S(2)	24(1)	19(1)	31(1)	8(1)	4(1)	2(1)
F(2)	24(2)	16(1)	28(2)	8(1)	0(1)	-4(1)
O(2)	24(2)	22(2)	28(2)	12(2)	-6(2)	-9(2)
N(2)	19(2)	16(2)	22(2)	5(2)	1(2)	-2(2)
C(2)	18(3)	18(3)	27(3)	8(2)	3(2)	-2(2)
O(3)	30(2)	15(2)	27(2)	5(2)	5(2)	-6(2)
N(3)	21(2)	16(2)	17(2)	4(2)	2(2)	0(2)
C(3)	24(3)	15(2)	23(3)	6(2)	3(2)	0(2)
O(4)	32(2)	13(2)	18(2)	3(1)	6(2)	0(2)
C(4)	28(3)	13(2)	18(3)	6(2)	-1(2)	-4(2)
C(5)	21(3)	16(2)	18(3)	6(2)	5(2)	-1(2)
C(6)	20(3)	20(3)	16(2)	5(2)	2(2)	-3(2)
C(7)	21(3)	14(2)	25(3)	8(2)	2(2)	-5(2)
C(8)	22(3)	18(2)	18(3)	6(2)	1(2)	-4(2)
C(9)	22(3)	18(2)	22(3)	10(2)	6(2)	0(2)
C(10)	27(3)	17(3)	29(3)	5(2)	2(2)	-2(2)
C(11)	20(3)	27(3)	29(3)	10(2)	1(2)	1(2)
C(12)	20(3)	23(3)	23(3)	11(2)	-2(2)	-7(2)
C(13)	26(3)	17(3)	28(3)	8(2)	-1(2)	-2(2)
C(14)	26(3)	19(3)	26(3)	7(2)	5(2)	1(2)
C(15)	23(3)	21(3)	23(3)	8(2)	1(2)	3(2)
N(4)	22(2)	20(2)	26(2)	10(2)	-5(2)	-5(2)
C(16)	19(3)	24(3)	28(3)	11(2)	-7(2)	-8(2)
C(17)	23(3)	32(3)	37(3)	17(3)	-2(3)	-1(2)
C(18)	21(3)	45(4)	57(4)	35(3)	-2(3)	-6(3)

C(19)	29(3)	33(4)	63(5)	31(3)	-11(3)	-14(3)
C(20)	37(4)	24(3)	57(4)	11(3)	-11(3)	-2(3)
C(21)	26(3)	20(3)	36(3)	9(2)	-5(2)	-3(2)
C(22)	24(3)	24(3)	30(3)	8(2)	-1(2)	-3(2)
C(23)	34(3)	37(3)	26(3)	6(3)	1(3)	-1(3)
C(24)	33(3)	45(4)	32(3)	20(3)	-3(3)	-9(3)
C(25)	27(3)	30(3)	50(4)	22(3)	-5(3)	-8(3)
C(26)	25(3)	20(3)	36(3)	12(2)	1(2)	-5(2)
C(27)	22(3)	23(3)	26(3)	10(2)	-2(2)	-5(2)
C(28)	24(3)	15(2)	23(3)	6(2)	3(2)	-3(2)
C(29)	29(3)	23(3)	24(3)	7(2)	3(2)	3(2)
C(30)	40(3)	18(3)	31(3)	7(2)	7(3)	5(2)
C(31)	56(4)	21(3)	25(3)	3(2)	6(3)	1(3)
C(32)	37(3)	21(3)	25(3)	5(2)	-1(3)	-2(2)
C(33)	29(3)	15(2)	26(3)	5(2)	4(2)	0(2)
C(34)	20(3)	19(3)	18(3)	7(2)	2(2)	-3(2)
C(35)	24(3)	20(3)	21(3)	8(2)	4(2)	1(2)
C(36)	19(3)	17(2)	27(3)	8(2)	5(2)	1(2)
C(37)	24(3)	18(3)	20(3)	5(2)	7(2)	0(2)
C(38)	23(3)	20(3)	20(3)	3(2)	-1(2)	-3(2)
C(39)	21(3)	20(3)	27(3)	8(2)	6(2)	3(2)
C(40)	17(2)	19(3)	20(3)	3(2)	-1(2)	1(2)
N(5)	23(2)	13(2)	19(2)	4(2)	2(2)	-2(2)
C(41)	24(3)	18(3)	18(3)	5(2)	4(2)	-3(2)
C(42)	25(3)	21(3)	22(3)	5(2)	1(2)	-2(2)
C(43)	26(3)	25(3)	21(3)	6(2)	3(2)	-8(2)
C(44)	33(3)	20(3)	20(3)	7(2)	0(2)	-9(2)
C(45)	31(3)	15(2)	20(3)	5(2)	-5(2)	-4(2)
C(46)	24(3)	19(3)	14(2)	1(2)	1(2)	-3(2)
C(47)	21(3)	17(2)	23(3)	5(2)	2(2)	-5(2)
C(48)	26(3)	19(3)	28(3)	0(2)	6(2)	-7(2)
C(49)	36(3)	26(3)	23(3)	4(2)	3(2)	-16(2)
C(50)	35(3)	23(3)	25(3)	10(2)	-5(2)	-10(2)
C(51)	27(3)	19(3)	25(3)	9(2)	-2(2)	-4(2)
C(52)	21(3)	15(2)	17(2)	5(2)	-3(2)	-8(2)
C(53)	19(3)	19(3)	20(3)	5(2)	2(2)	-4(2)

C(54)	25(3)	23(3)	23(3)	7(2)	5(2)	-3(2)
C(55)	27(3)	20(3)	27(3)	-1(2)	4(2)	-4(2)
C(56)	25(3)	31(3)	23(3)	2(2)	2(2)	-5(2)
C(57)	24(3)	33(3)	24(3)	10(2)	-2(2)	-3(2)
C(58)	24(3)	20(3)	25(3)	3(2)	2(2)	-2(2)
Cl(1)	34(1)	31(1)	52(1)	22(1)	3(1)	3(1)
Cl(2)	43(1)	47(1)	39(1)	19(1)	1(1)	7(1)
C(1A)	25(2)	21(2)	29(2)	19(2)	-3(2)	-10(2)
C(2A)	25(2)	21(2)	29(2)	19(2)	-3(2)	-10(2)
Cl(3)	124(3)	219(5)	208(5)	104(4)	23(3)	10(3)

Table S4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **1b**.

	x	y	z	U(eq)
H(2A)	-1335	8333	4788	25
H(6A)	7933	5748	5016	23
H(10A)	-2899	7768	3886	31
H(11A)	-5104	7073	3009	31
H(13A)	-2795	4674	2567	30
H(14A)	-593	5357	3449	28
H(17A)	-9019	4927	2089	37
H(18A)	-10312	3523	2127	46
H(19A)	-10027	2083	1375	49
H(20A)	-8476	2035	583	51
H(23A)	-6921	4101	-786	41
H(24A)	-7692	5496	-953	44
H(25A)	-8502	6686	-137	43
H(26A)	-8259	6570	886	33
H(29A)	-379	9870	5490	31
H(30A)	224	11244	6379	36
H(31A)	2503	11387	7215	42
H(32A)	4215	10159	7149	35
H(33A)	3635	8788	6270	29
H(35A)	7423	4247	4461	26
H(36A)	7511	2789	3709	25
H(38A)	3502	3267	2537	27
H(39A)	3400	4730	3292	27
H(42A)	2824	850	1942	28
H(43A)	1635	-556	2011	30
H(44A)	3040	-1914	1760	30
H(45A)	5592	-1892	1384	28
H(48A)	8482	-293	52	32
H(49A)	7908	793	-487	36
H(50A)	6206	1995	-118	35

H(51A)	5263	2186	832	29
H(54A)	6585	8736	5873	29
H(55A)	8207	9732	6829	33
H(56A)	10150	9139	7465	35
H(57A)	10470	7520	7126	34
H(58A)	8883	6517	6159	29
H(1AA)	8305	6803	2185	28
H(1AB)	9398	6194	1699	28
H(2AA)	5464	9097	4966	28
H(2AB)	6168	9721	4592	28

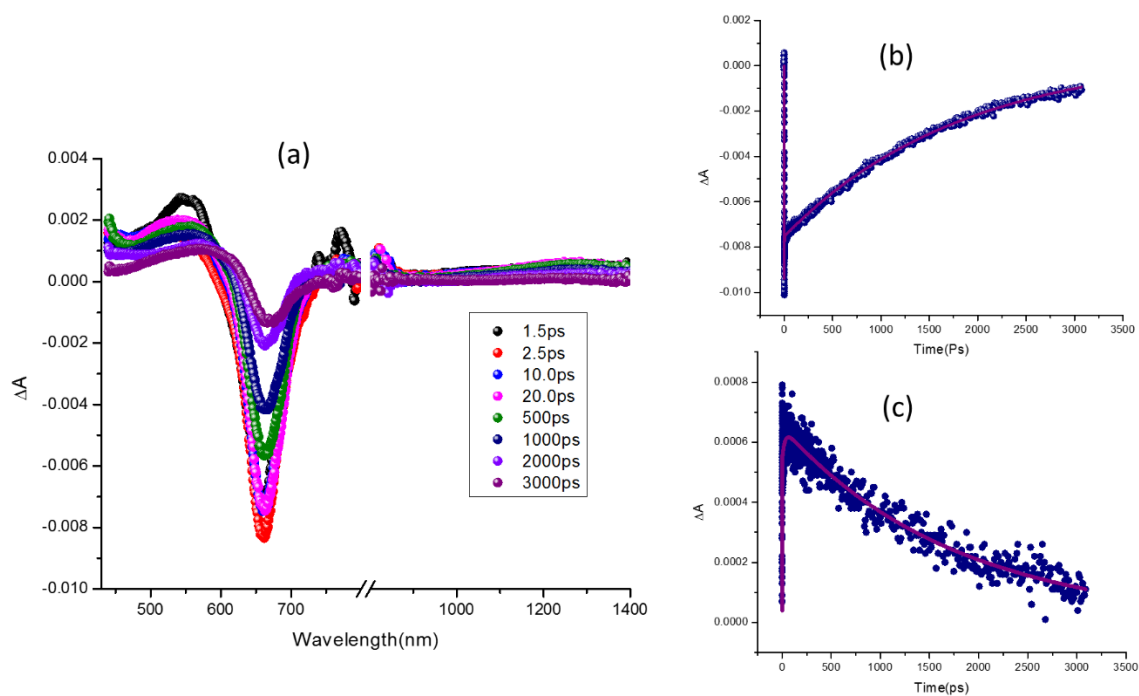


Fig. S1. (a) Femtosecond transient absorption spectra of azaBODIPY in benzonitrile at the excitation wavelength of 400 nm of 100 fs laser pulses. The time profiles of the 667 nm band (b) and 1267 nm band (c) are also shown.

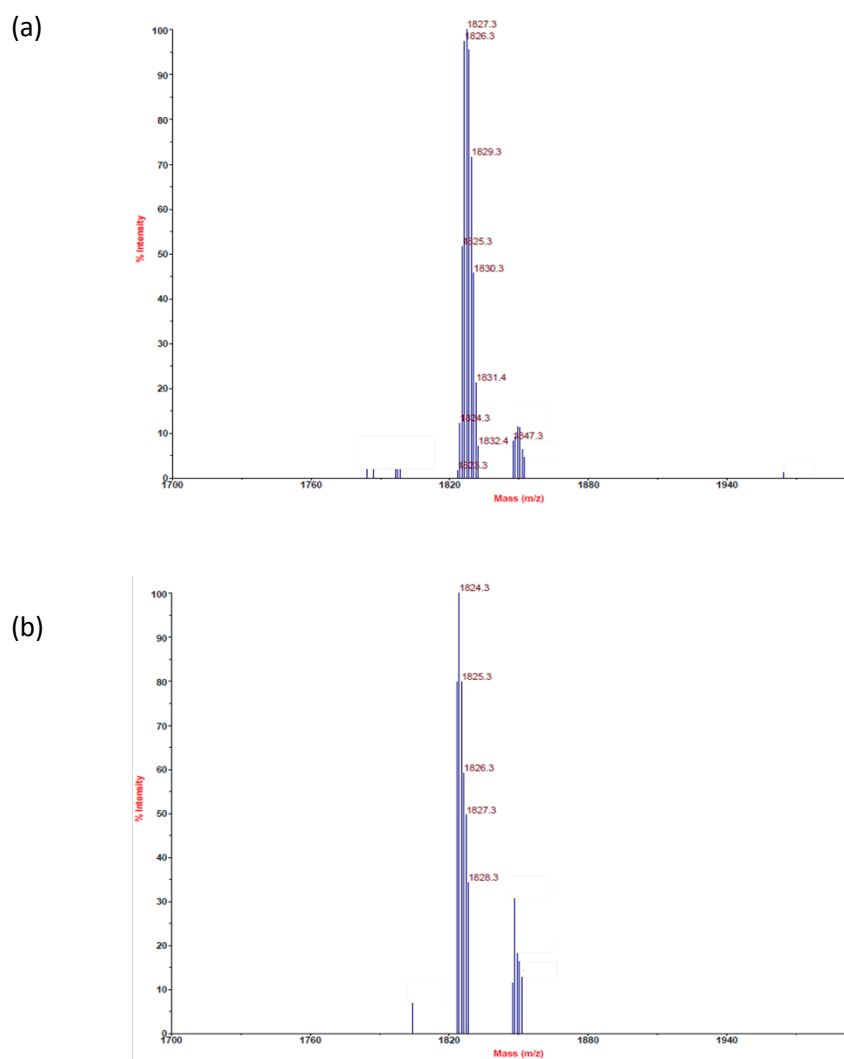


Fig. S2. Maldi-Mass of compounds **1** and **2**.

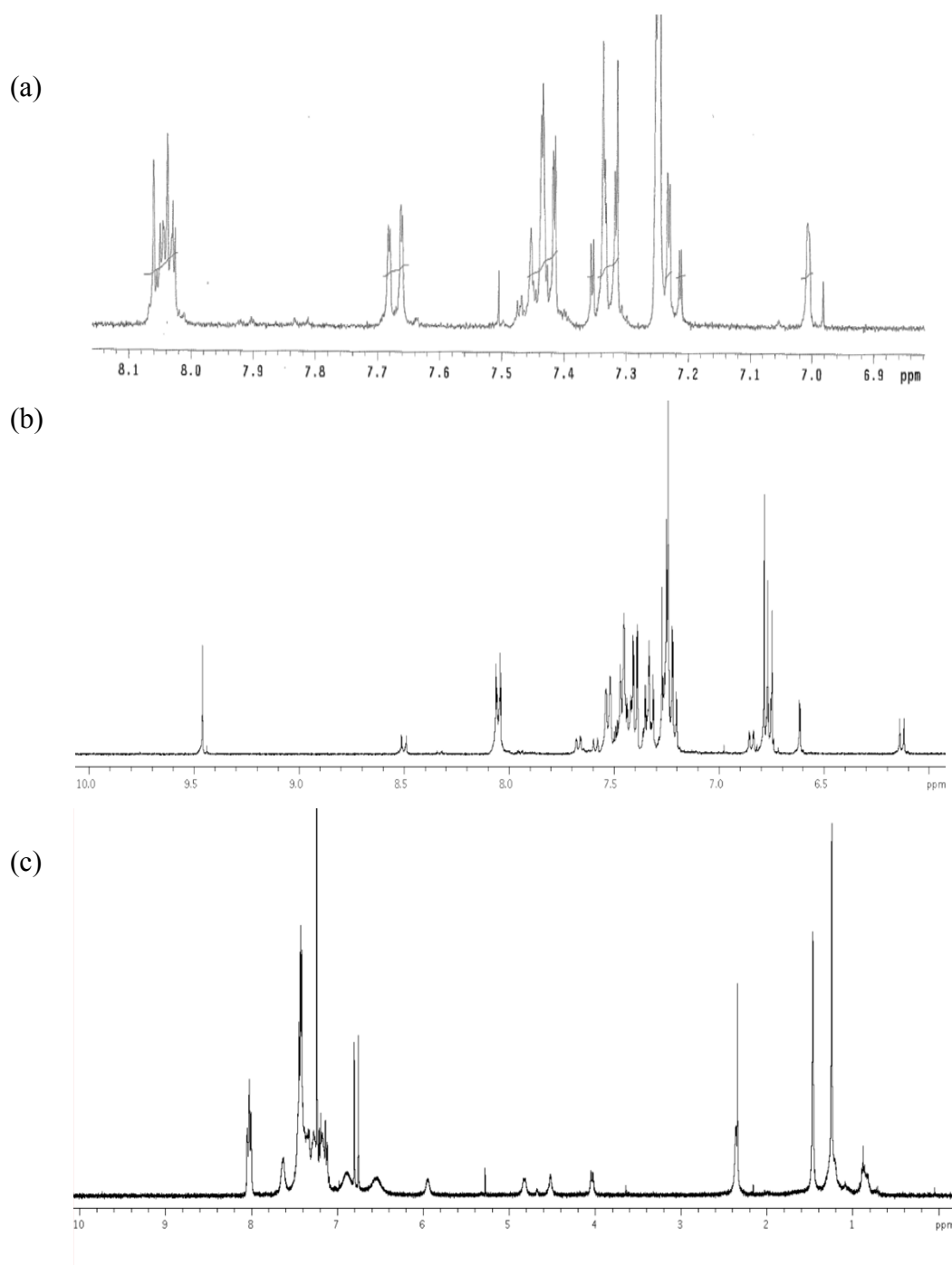


Fig. S3. ^1H NMR spectrum of (a) **1b**, (b) **1c** and (c) **1**.

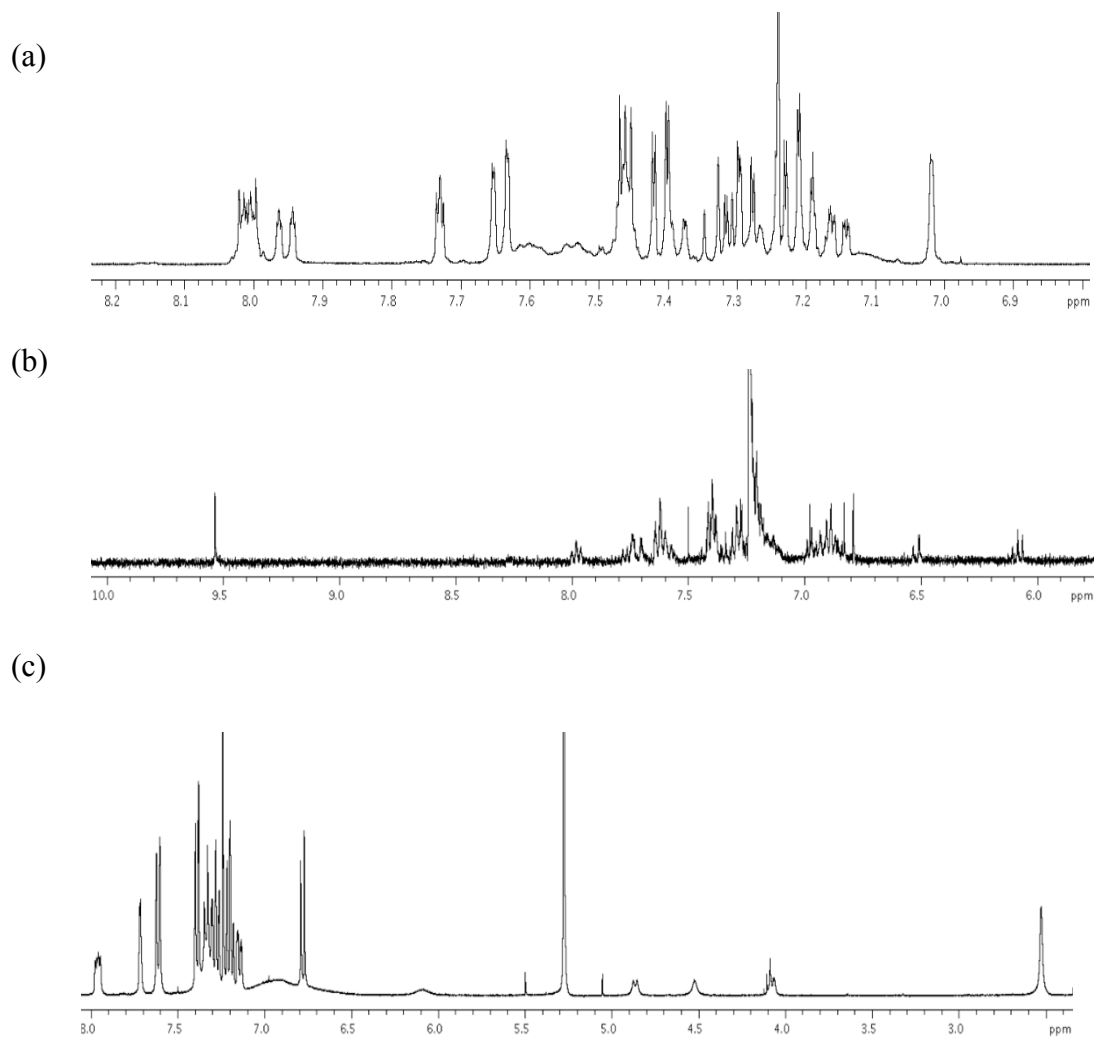


Fig. S4. ^1H NMR spectrum of (a) **2b**, (b) **2c** and (c) **2**.

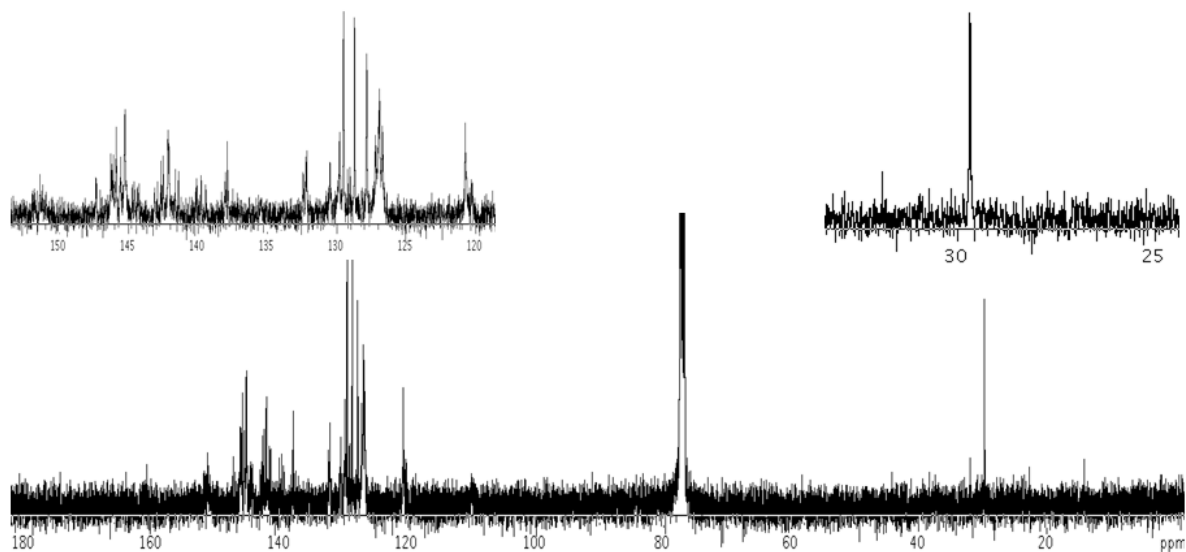


Fig. S5. ^{13}C NMR spectra of compound **1** in CDCl_3 .

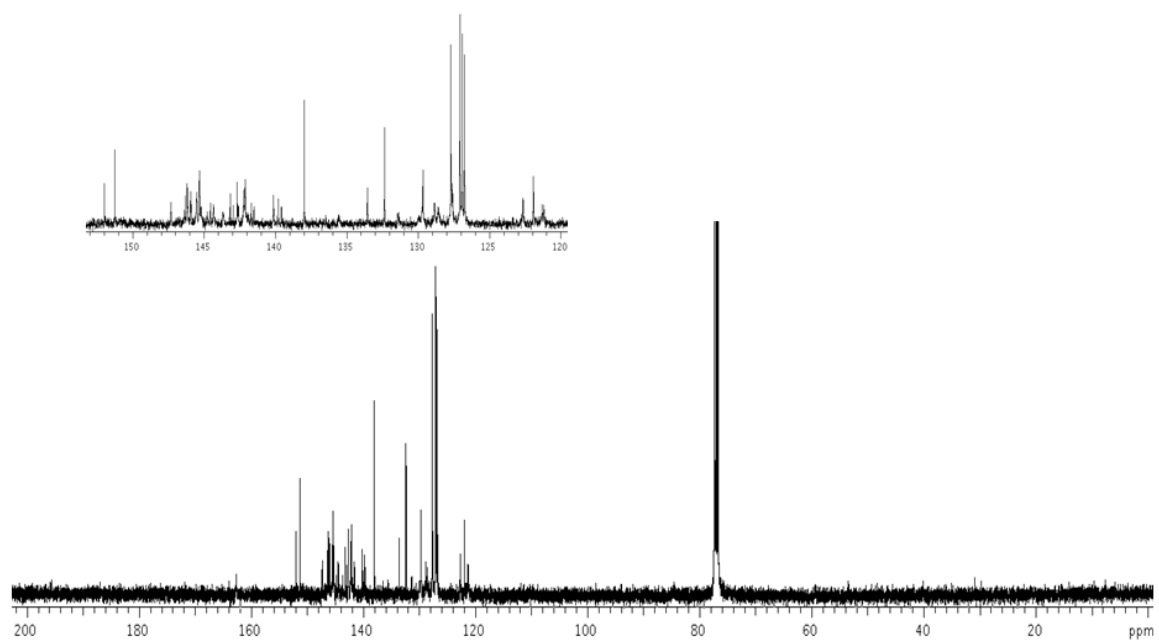


Fig. S6. ^{13}C NMR spectra of compound **2** in CDCl_3 .

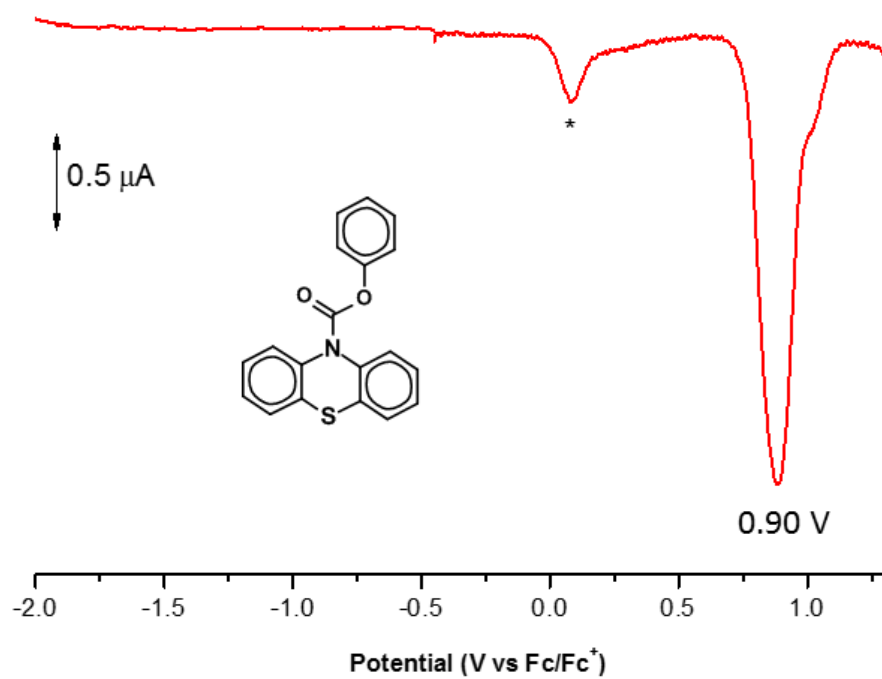


Fig. S7. Differential pulse voltammogram (DPV) of phenyl carbamoyl phenothiazine (control compound) in benzonitrile containing 0.1 M (*t*-Bu₄N)ClO₄. Scan rate = 5 mV/s, pulse width = 0.25 s, pulse height = 0.025 V.