Electronic supplementary information

Effects of alkyl group in (dialkylamino)perfluorophenazines on melting point and solid-state fluorescence

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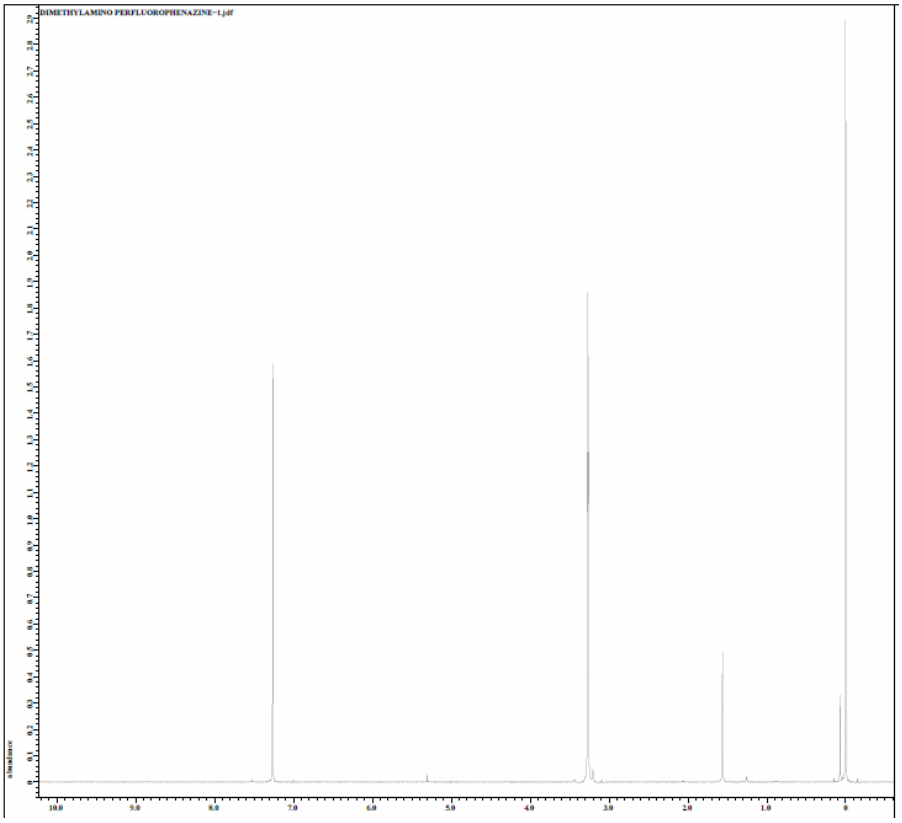


Figure S1. ^{1}H-NMR spectrum of 2-(dimethylamino)perfluorophenazine (**3a**).

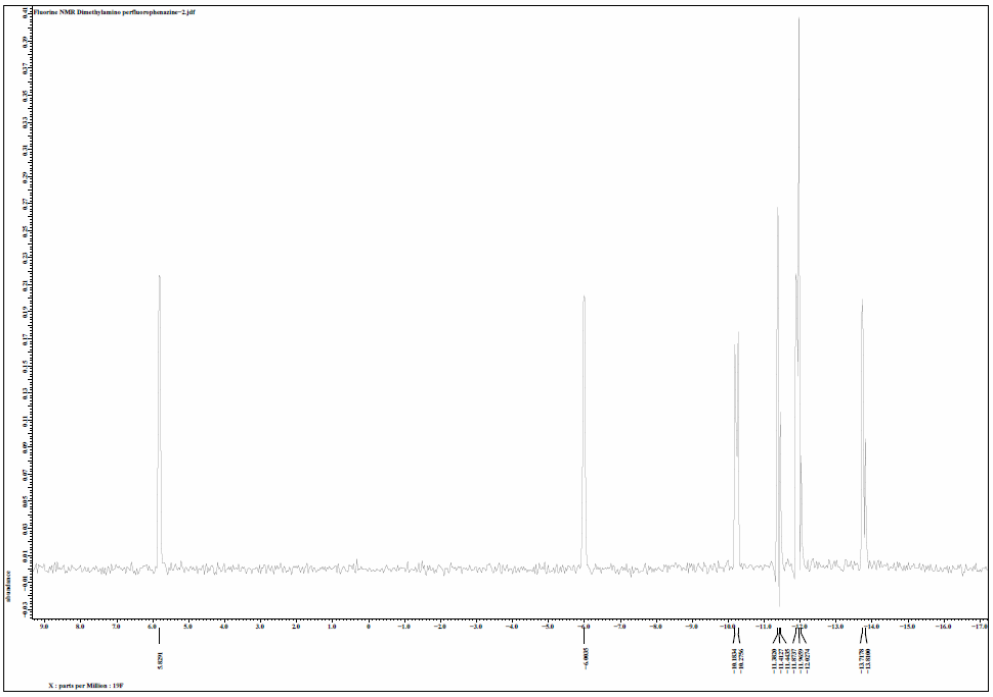


Figure S2. ^{19}F-NMR spectrum of 2-(dimethylamino)perfluorophenazine (**3a**).

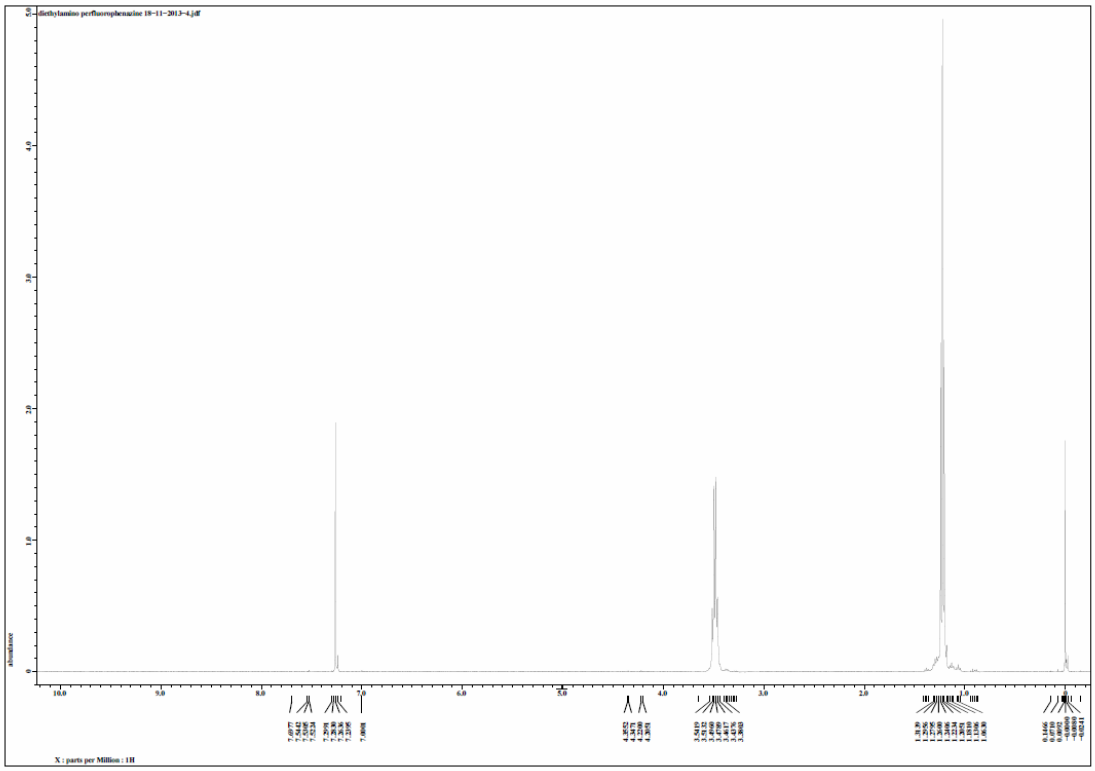


Figure S3. ^{1}H-NMR spectrum of 2-(diethylamino)perfluorophenazine (**3b**).

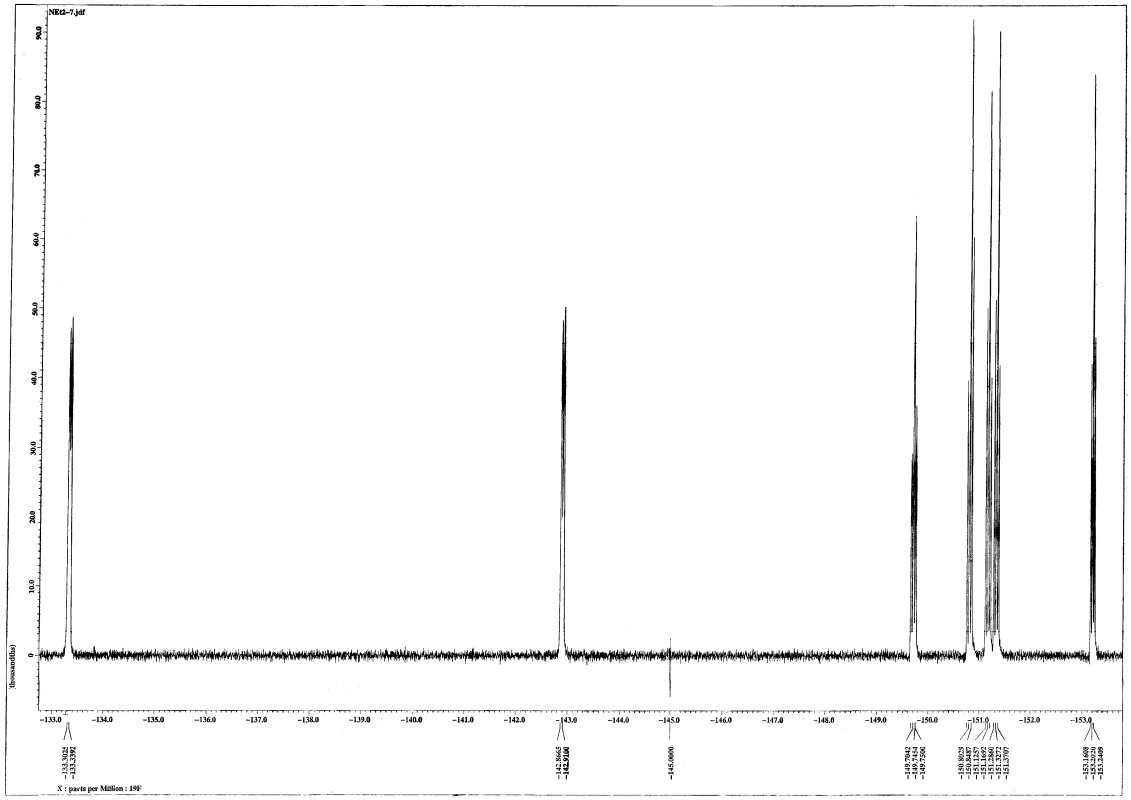


Figure S4. ^{19}F-NMR spectrum of 2-(diethylamino)perfluorophenazine (**3b**).

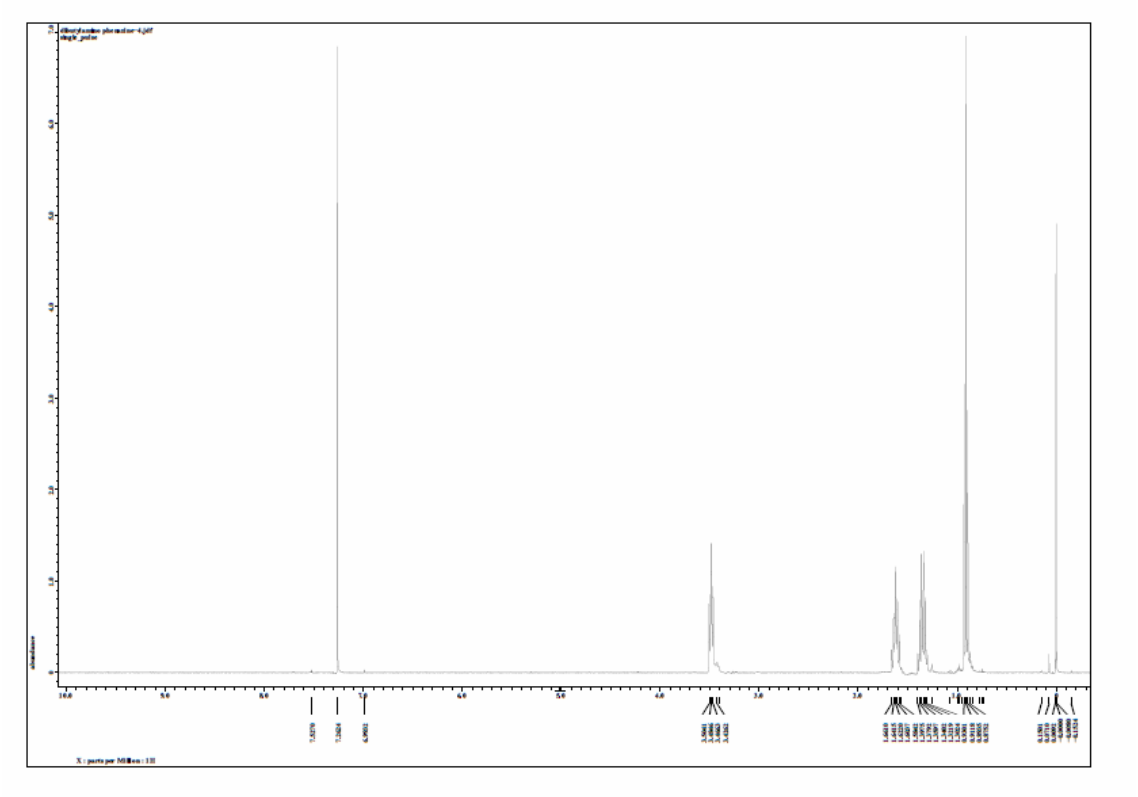


Figure S5. ^{1}H-NMR spectrum of 2-(dibutylamino)perfluorophenazine (**3c**).

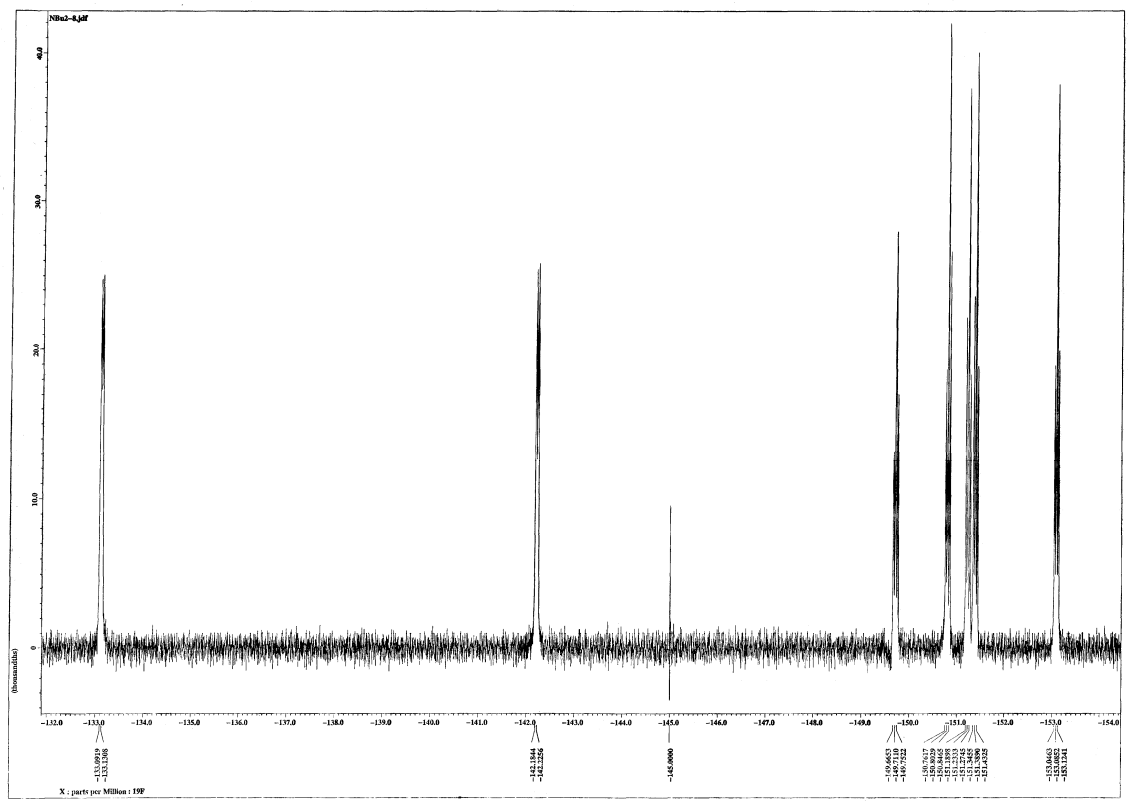


Figure S6. ^{19}F-NMR spectrum of 2-(dibutylamino)perfluorophenazine (**3c**).

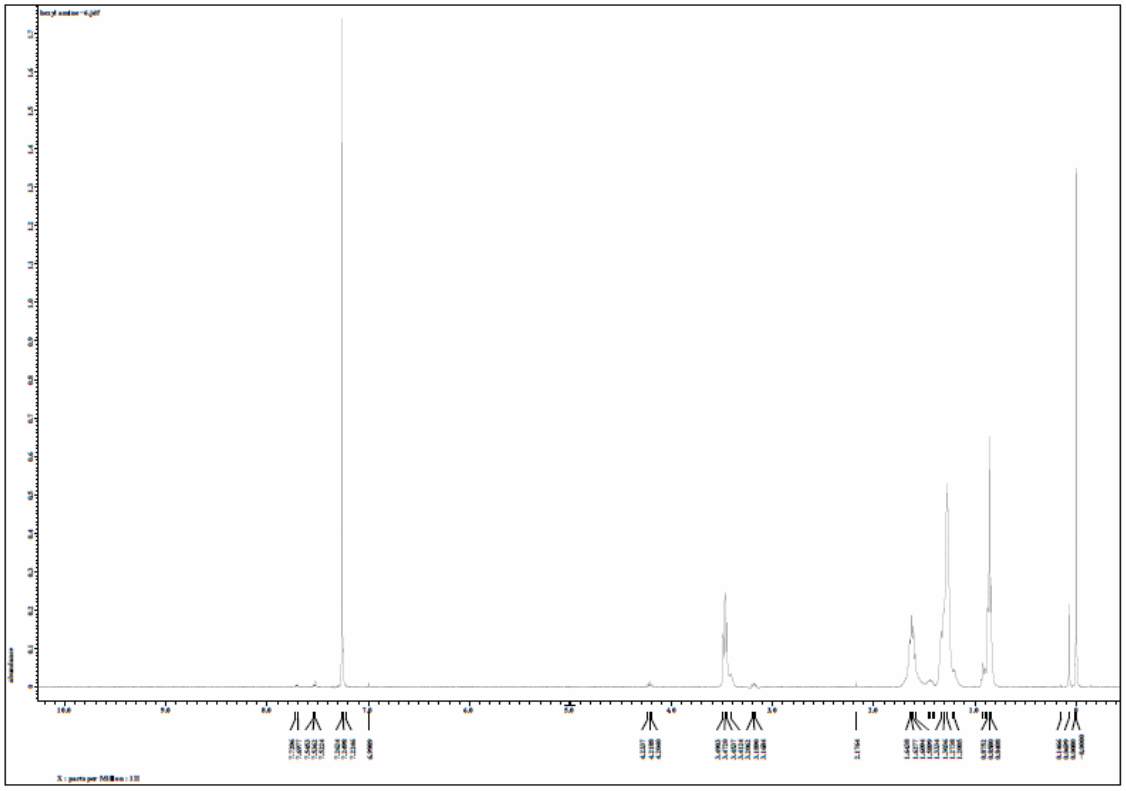


Figure S7. ^{1}H-NMR spectrum of 2-(dihexylamino)perfluorophenazine (**3d**).

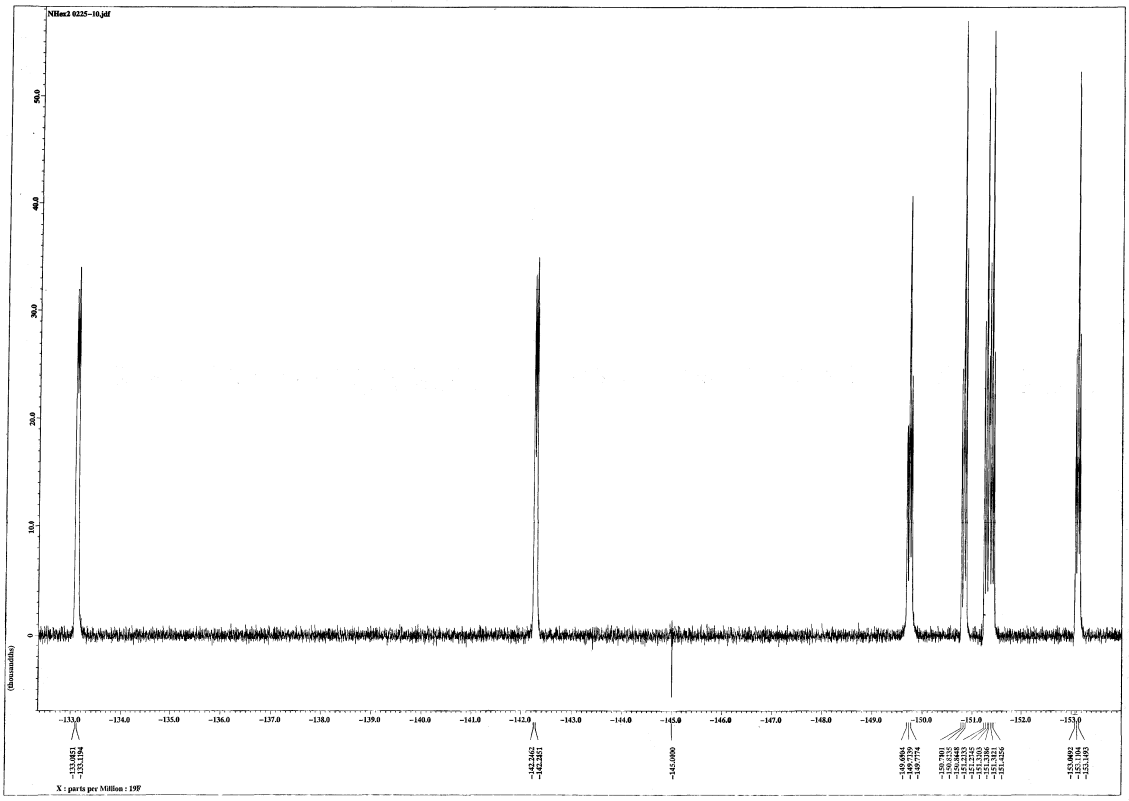


Figure S8. ^{19}F-NMR spectrum of 2-(dihexylamino)perfluorophenazine (**3d**).

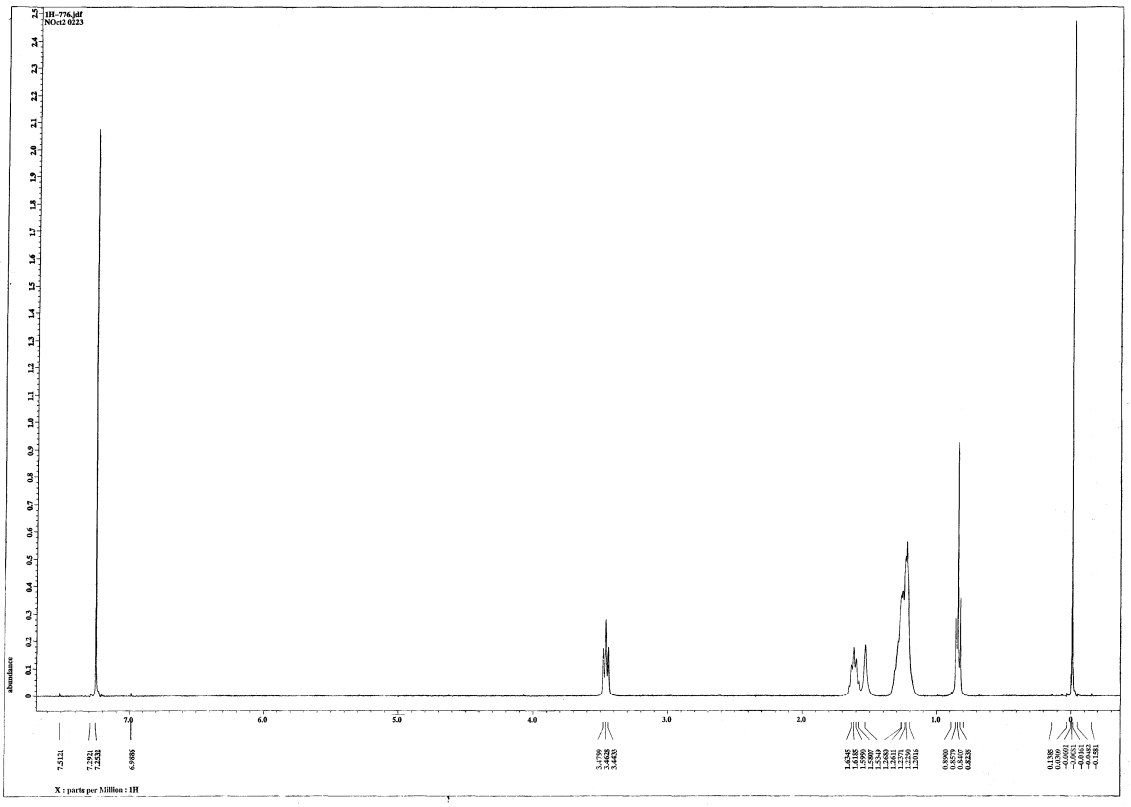


Figure S9. ^{1}H-NMR spectrum of 2-(dioctylamino)perfluorophenazine (**3e**).

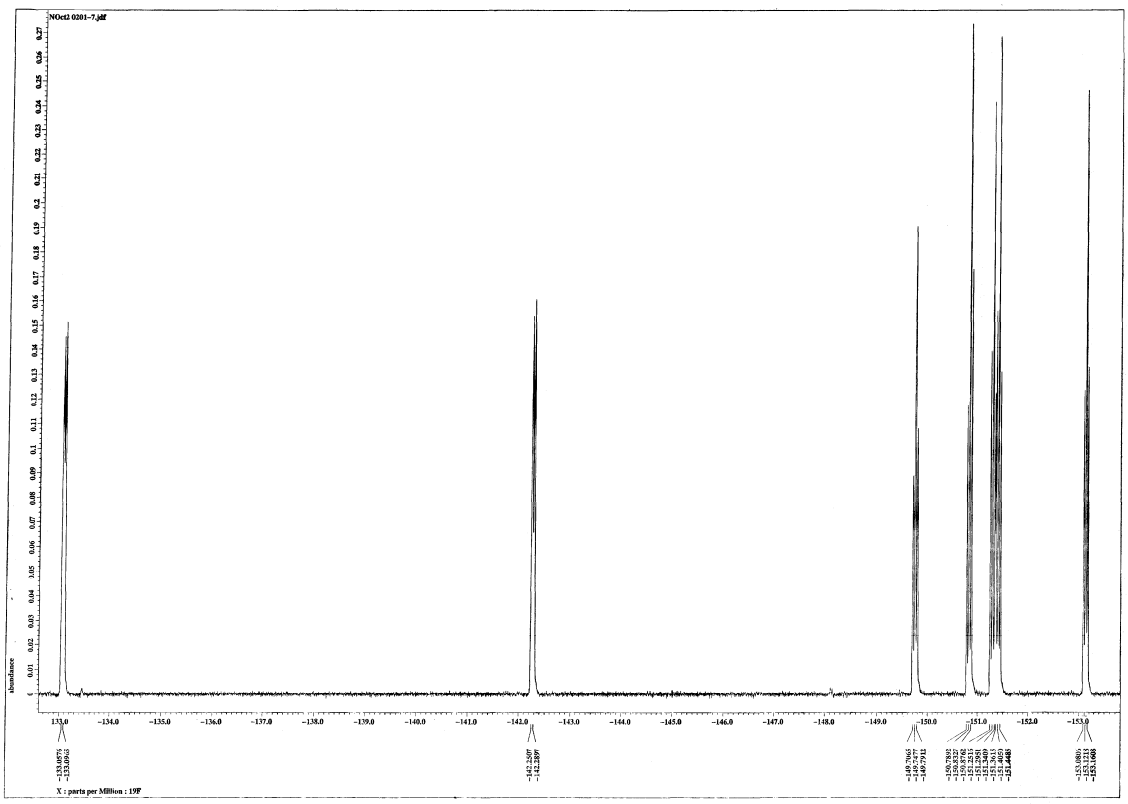


Figure S10. ^{19}F-NMR spectrum of 2-(dioctylamino)perfluorophenazine (**3e**).

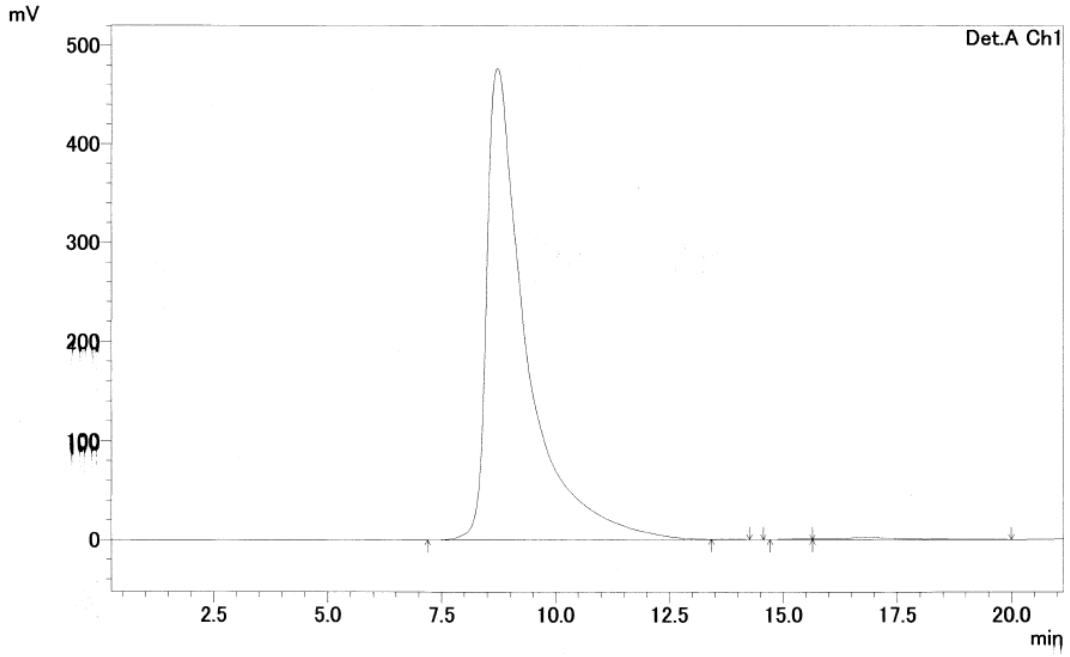


Figure S11. HPLC chart of **3e**. Column: Mightysil Si60 (Kanto Chemical Co., Lnc.), 250 mm x 4.6 mm, Eluent: chloroform : hexane = 2 : 8, Flow: 0.5 mL min^{-1}, Detection: 254 nm.

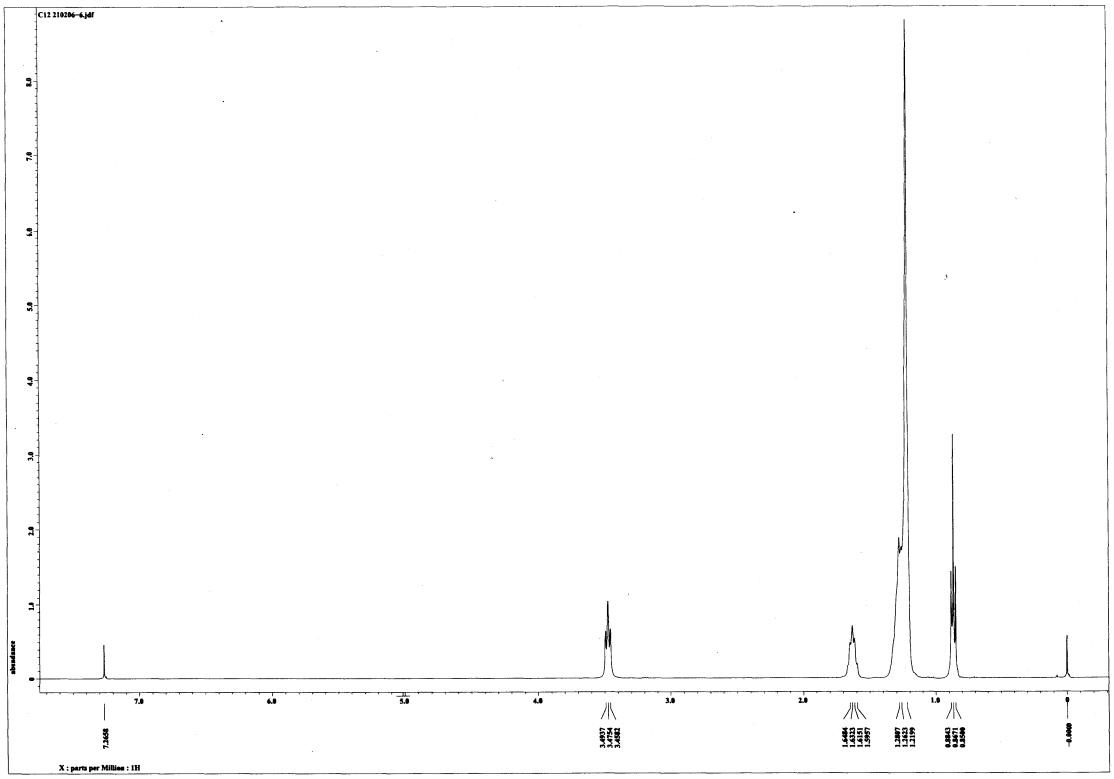


Figure S12. ^{1}H-NMR spectrum of 2-(didodecylamino)perfluorophenazine (**3f**).

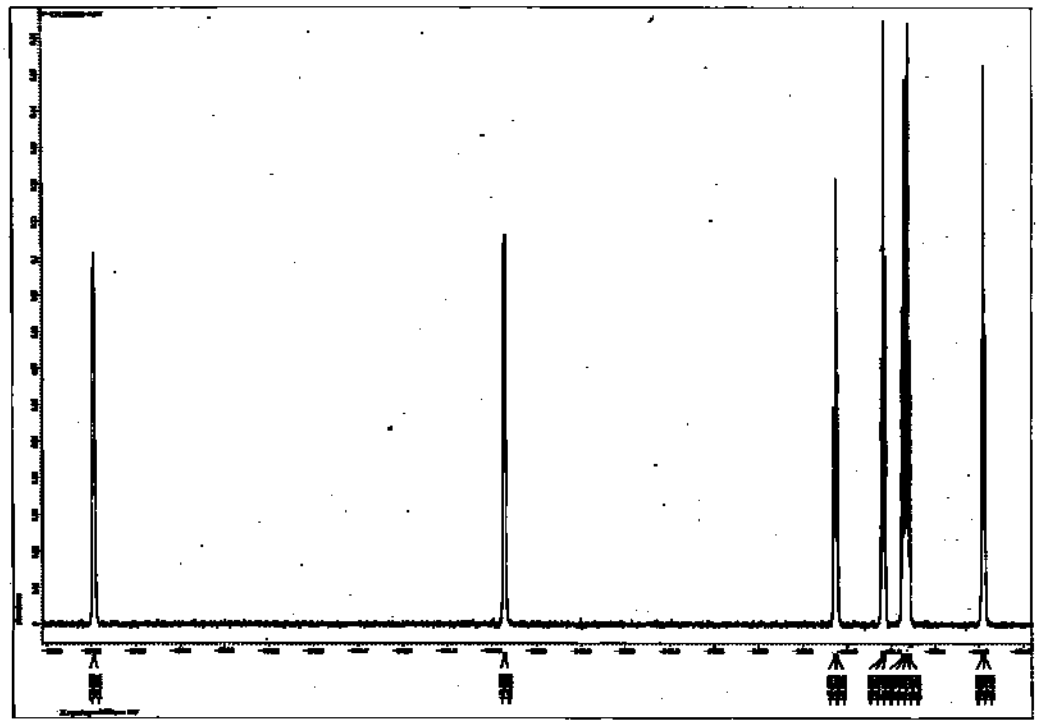


Figure S13. ^{19}F-NMR spectrum of 2-(didodecylamino)perfluorophenazine (**3f**).

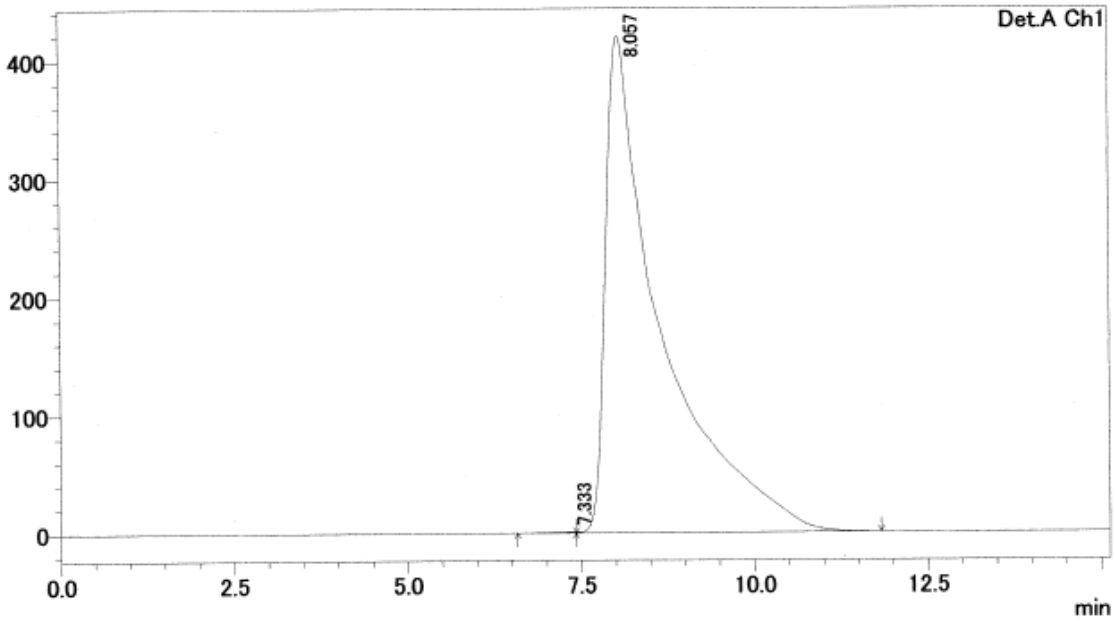


Figure S14. HPLC chart of 2-(didodecylamino)perfluorophenazine (**3f**). Column: Mightysil Si60 (Kanto Chemical Co., Lnc.), 250 mm x 4.6 mm, Eluent: chloroform : hexane = 2 : 8, Flow: 0.5 mL min^{-1}, Detection: 254 nm.

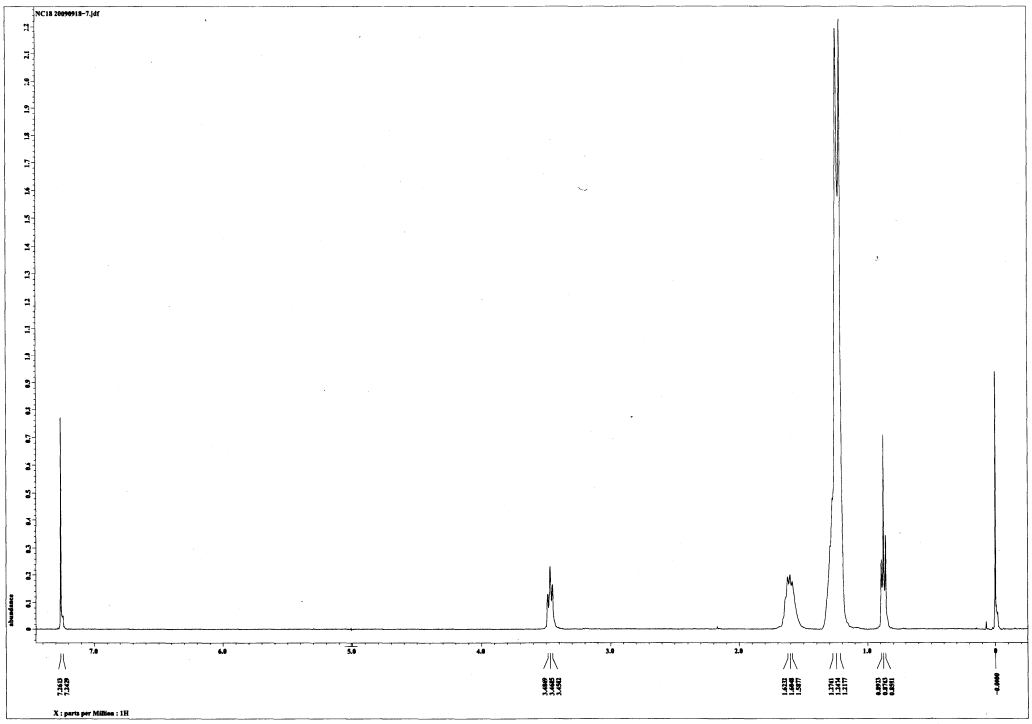


Figure S15. ^{1}H-NMR spectrum of 2-(dioctadecylamino)perfluorophenazine (**3g**).

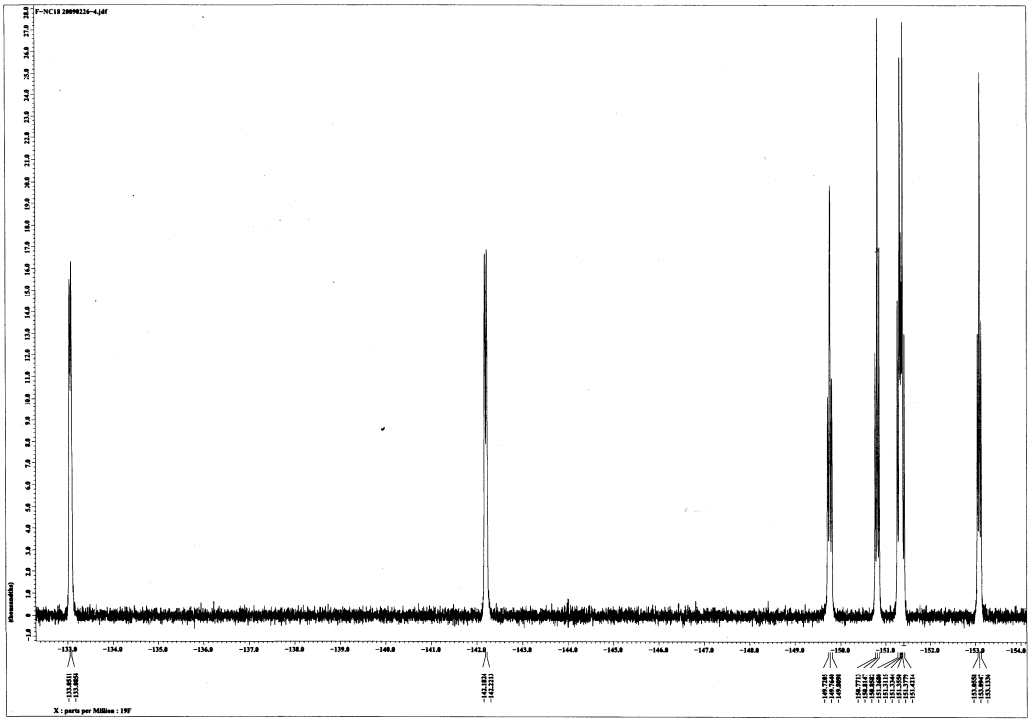


Figure S16. ^{19}F-NMR spectrum of 2-(dioctadecylamino)perfluorophenazine (**3g**).

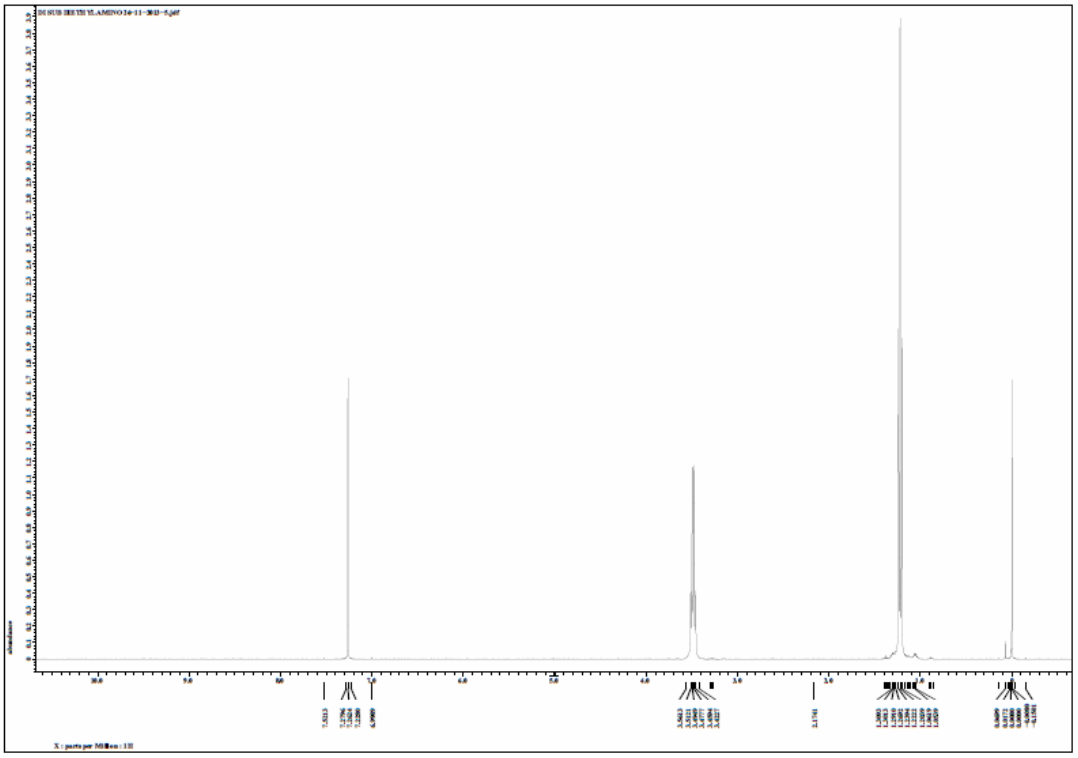


Figure S17. ^{1}H-NMR spectrum of 2,7-bis(diethylamino)perfluorophenazine (**4b**).

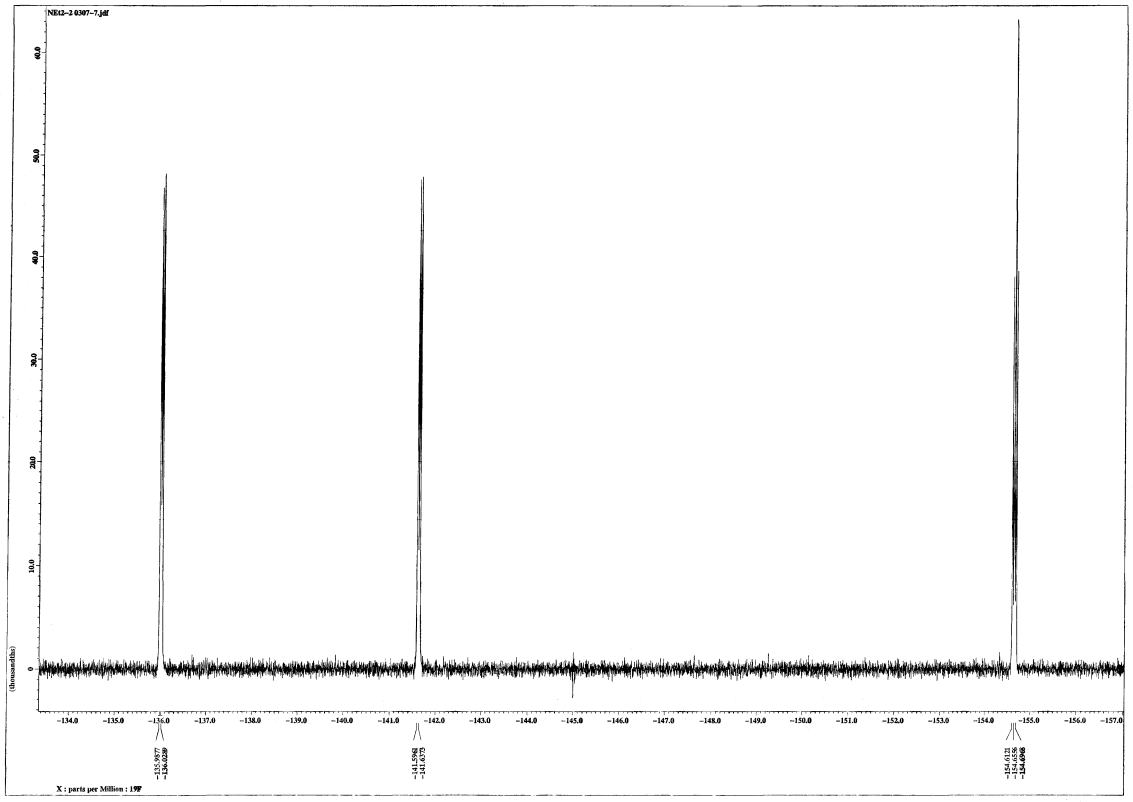


Figure S18. ^{19}F-NMR spectrum of 2,7-bis(diethylamino)perfluorophenazine (**4b**).

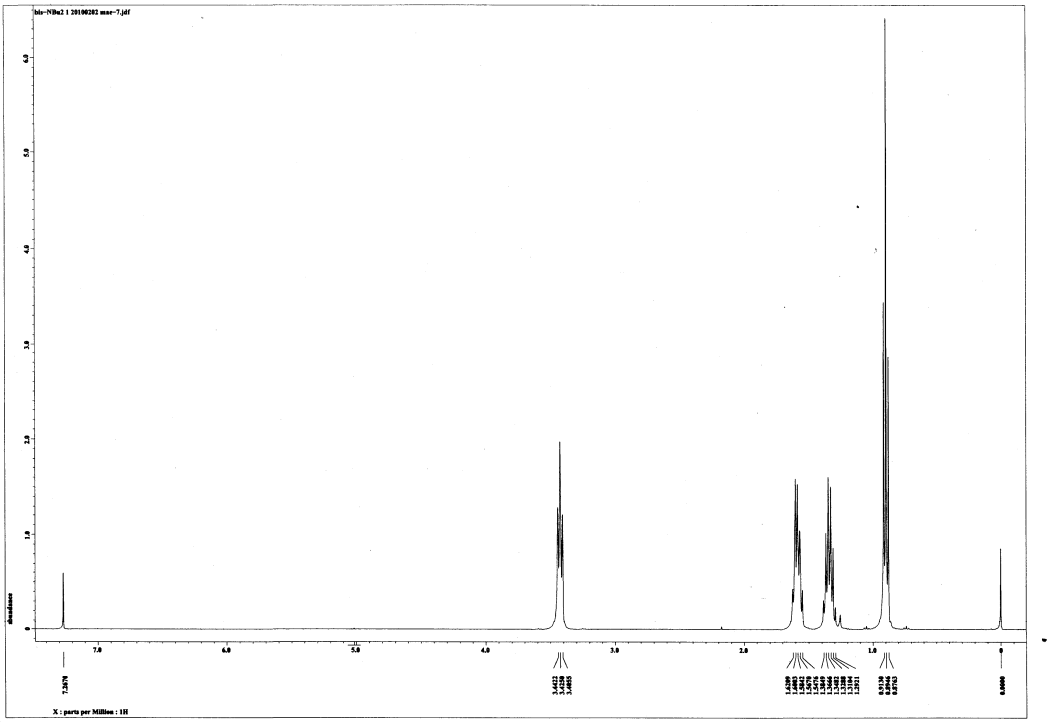


Figure S19. ^{1}H-NMR spectrum of 2,7-bis(dibutylamino)perfluorophenazine (**4c**).

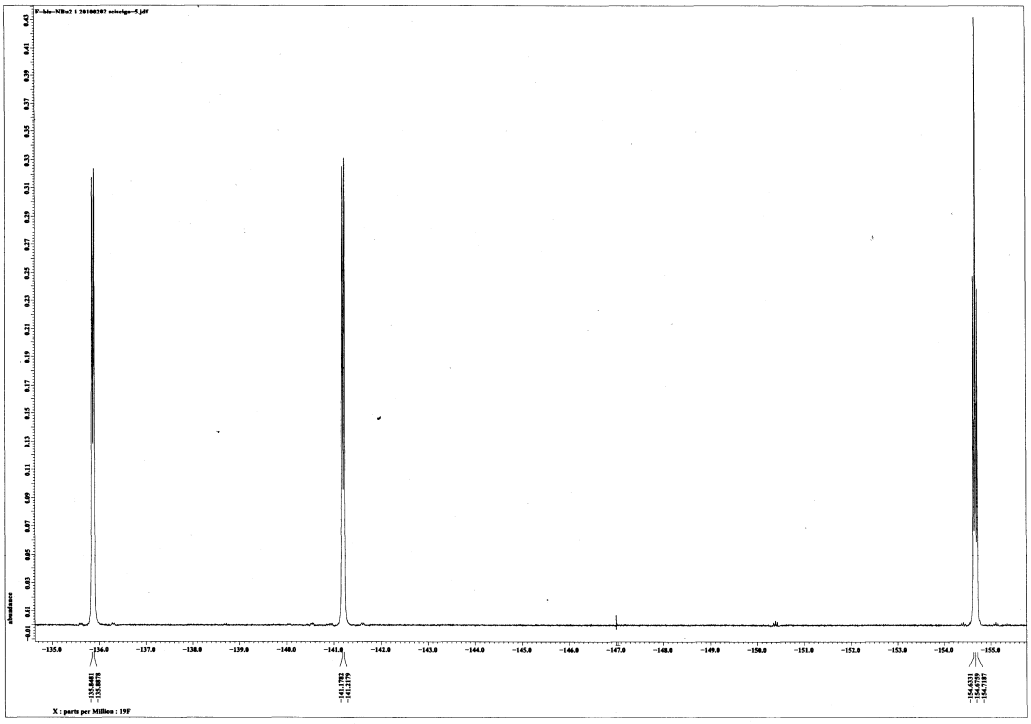


Figure S20. ^{19}F-NMR spectrum of 2,7-bis(dibutylamino)perfluorophenazine (**4c**)

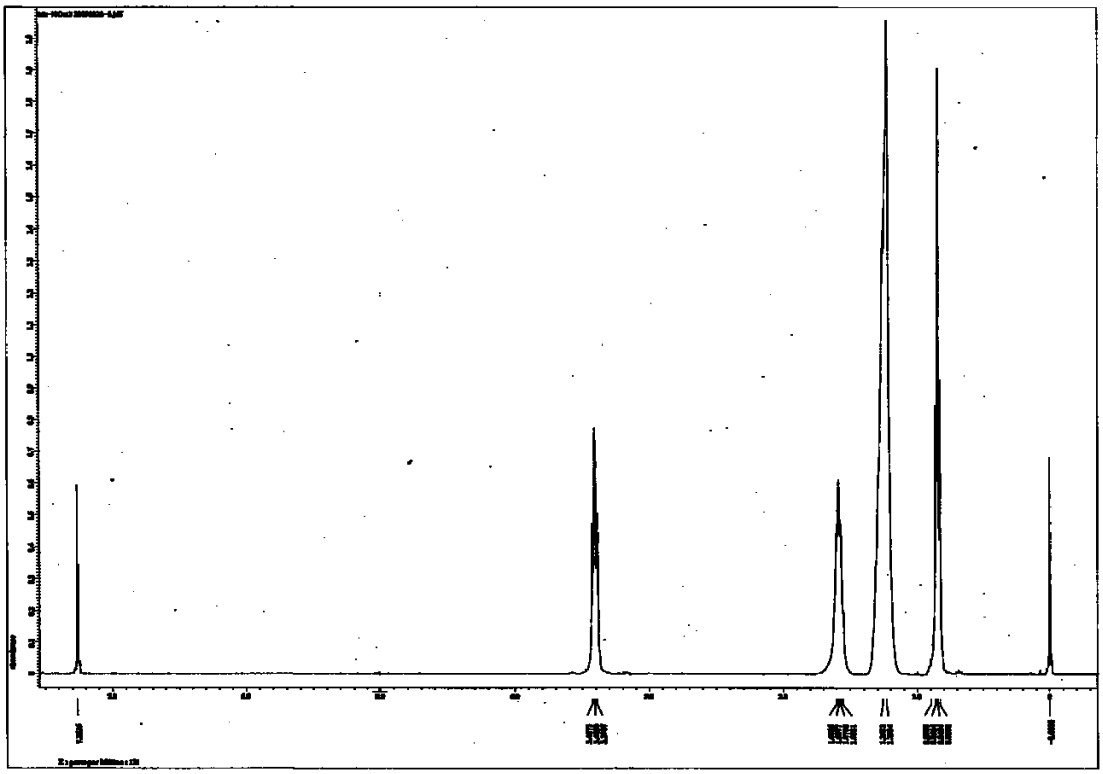


Figure S21. ^{1}H-NMR spectrum of 2,7-bis(dioctylamino)perfluorophenazine (**4e**).

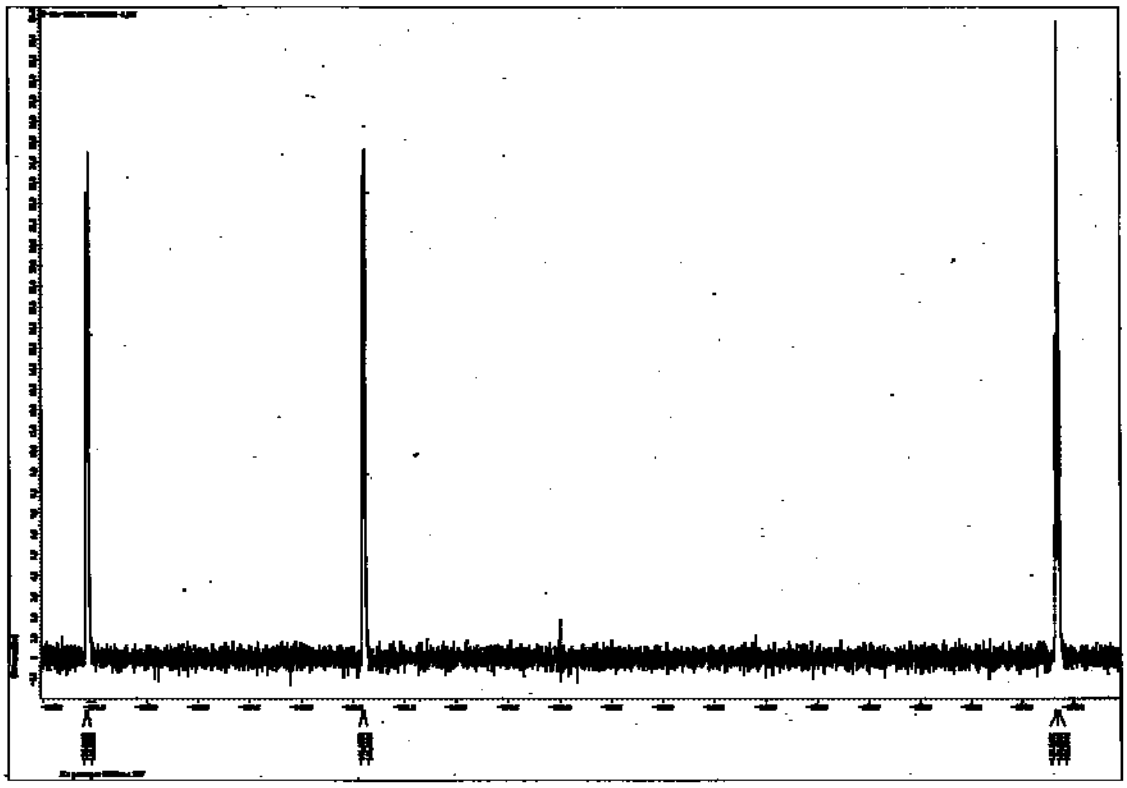


Figure S22. ^{19}F-NMR spectrum of 2,7-bis(dioctylamino)perfluorophenazine (**4e**).

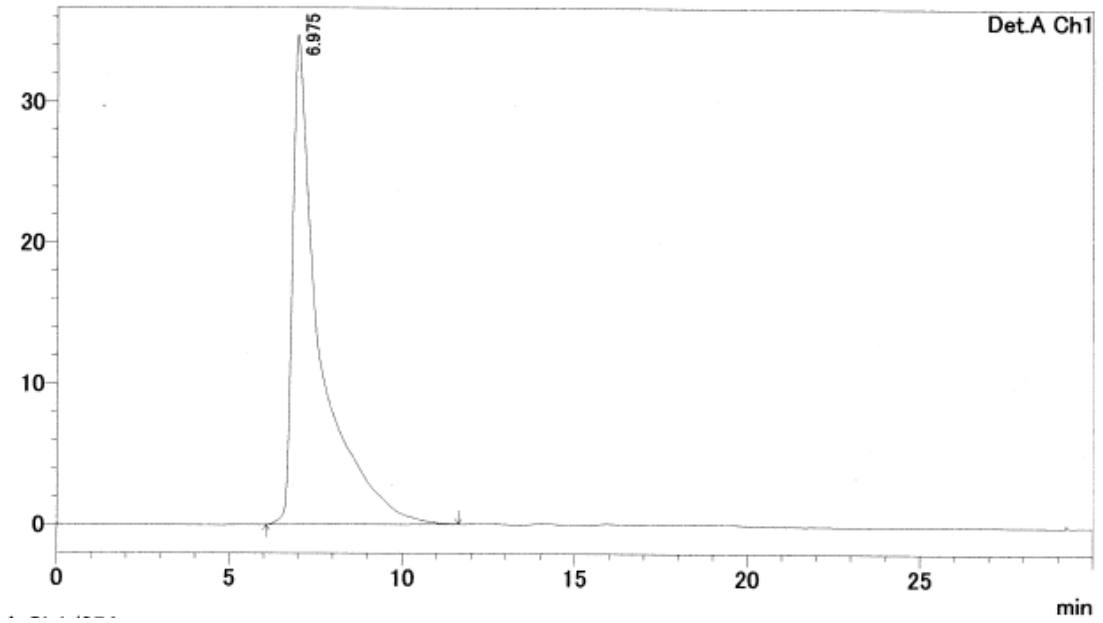


Figure S23. HPLC chart of 2,7-bis(dioctylamino)perfluorophenazine (**4e**). Column: Mightysil Si60 (Kanto Chemical Co., Lnc.), 250 mm x 4.6 mm, Eluent: chloroform : hexane = 2 : 8, Flow: 0.5 mL min^{-1}, Detection: 254 nm.

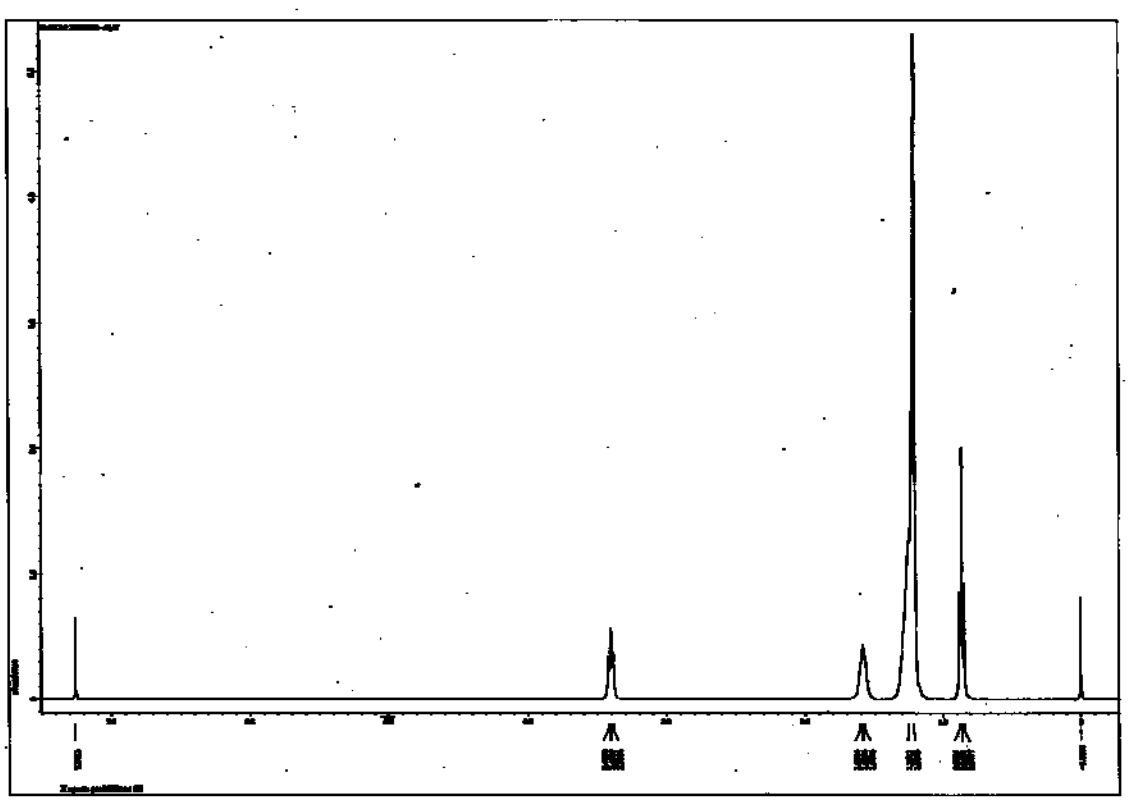


Figure S24. ^{1}H-NMR spectrum of 2,7-bis(didodecylamino)perfluorophenazine (**4f**).

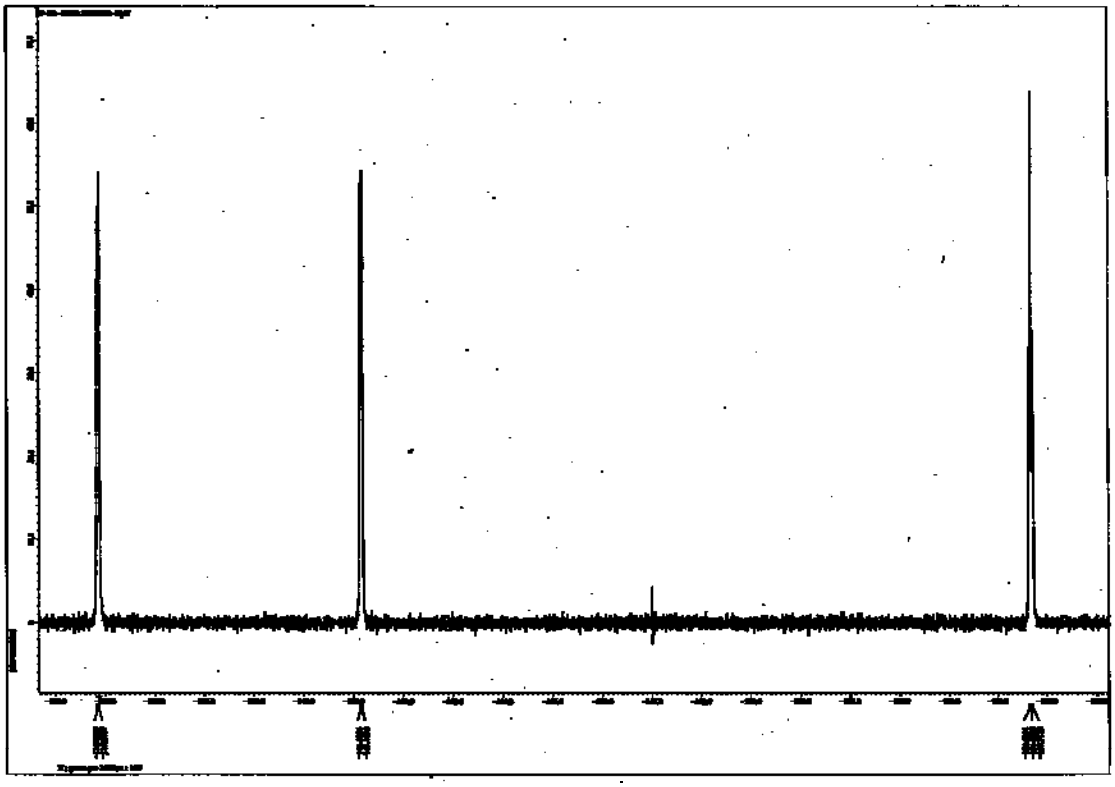


Figure S25. ^{19}F-NMR spectrum of 2,7-bis(didodecylamino)perfluorophenazine (**4f**).

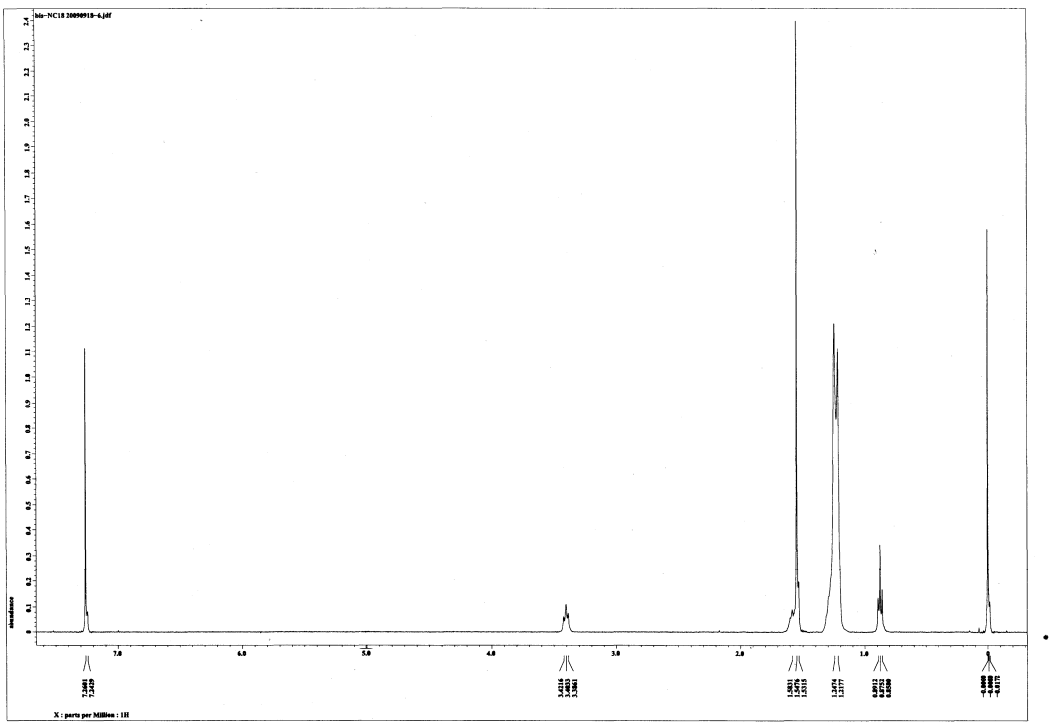


Figure S26. ^{1}H-NMR spectrum of 2,7-bis(otadecylamino)perfluorophenazine (**4g**).

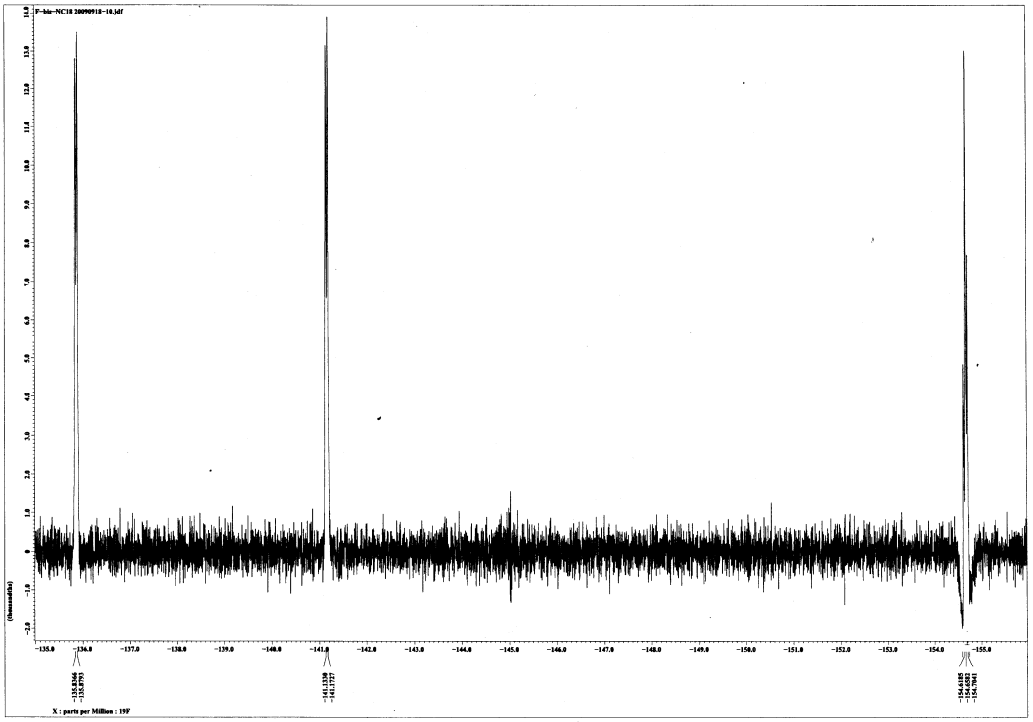


Figure S27. ^{19}F-NMR spectrum of 2,7-bis(otadecylamino)perfluorophenazine (**4g**).

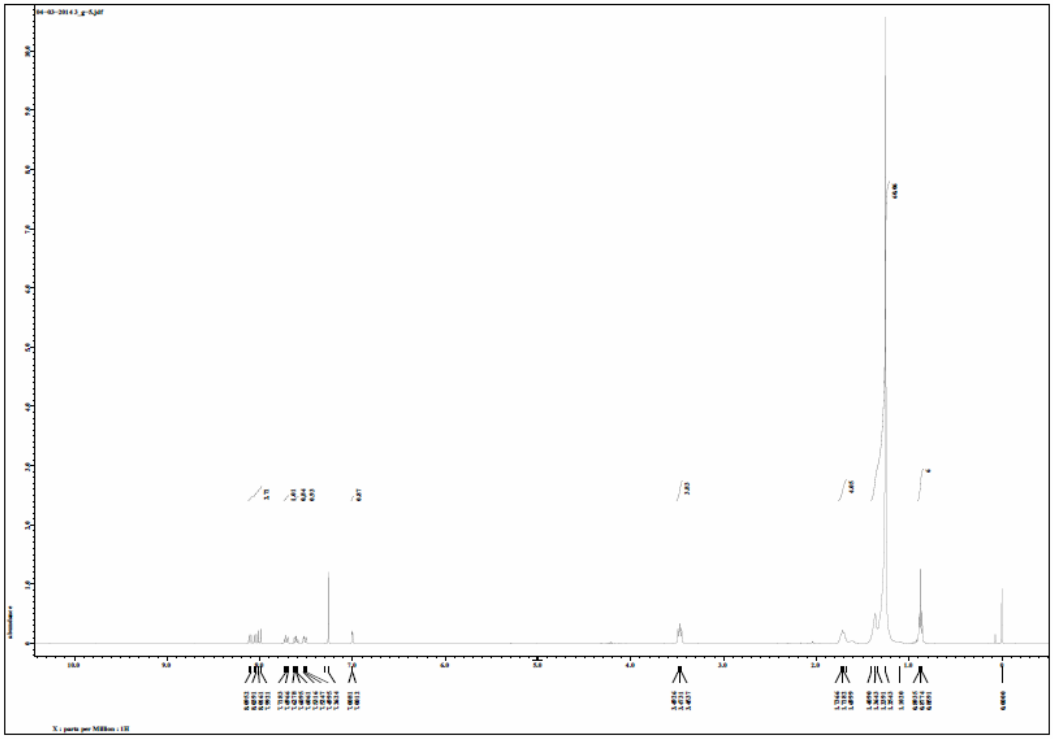


Figure S28. ^{1}H-NMR spectrum of 2-(otadecylamino)phenazine (**3'g**).

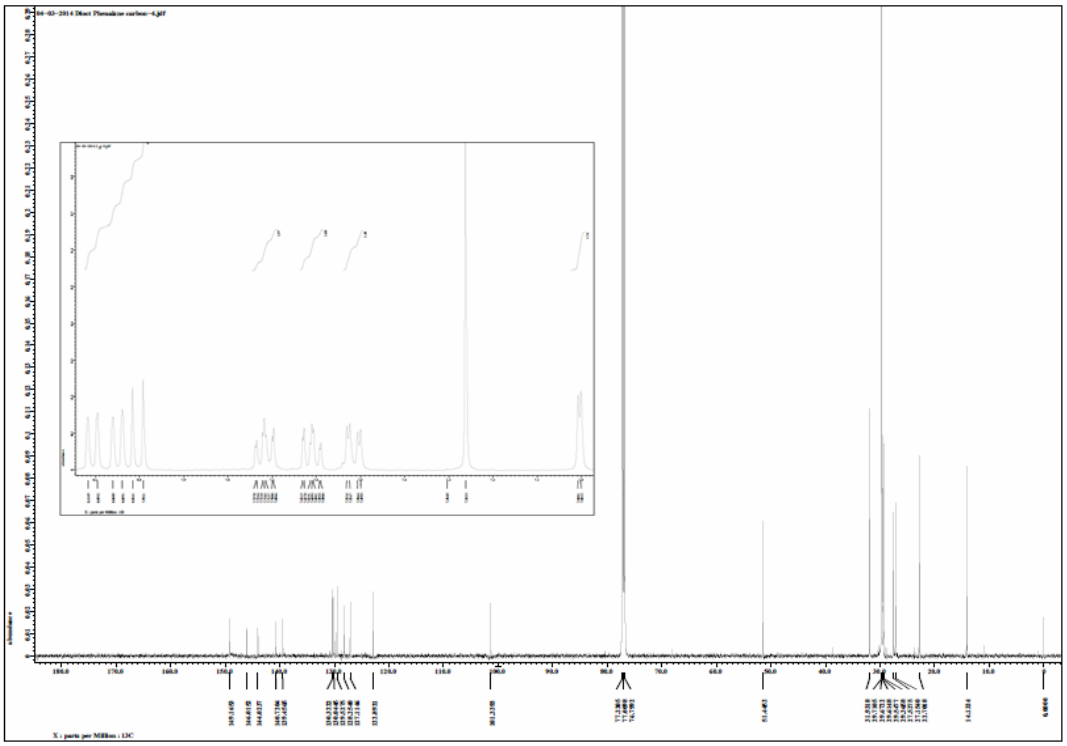
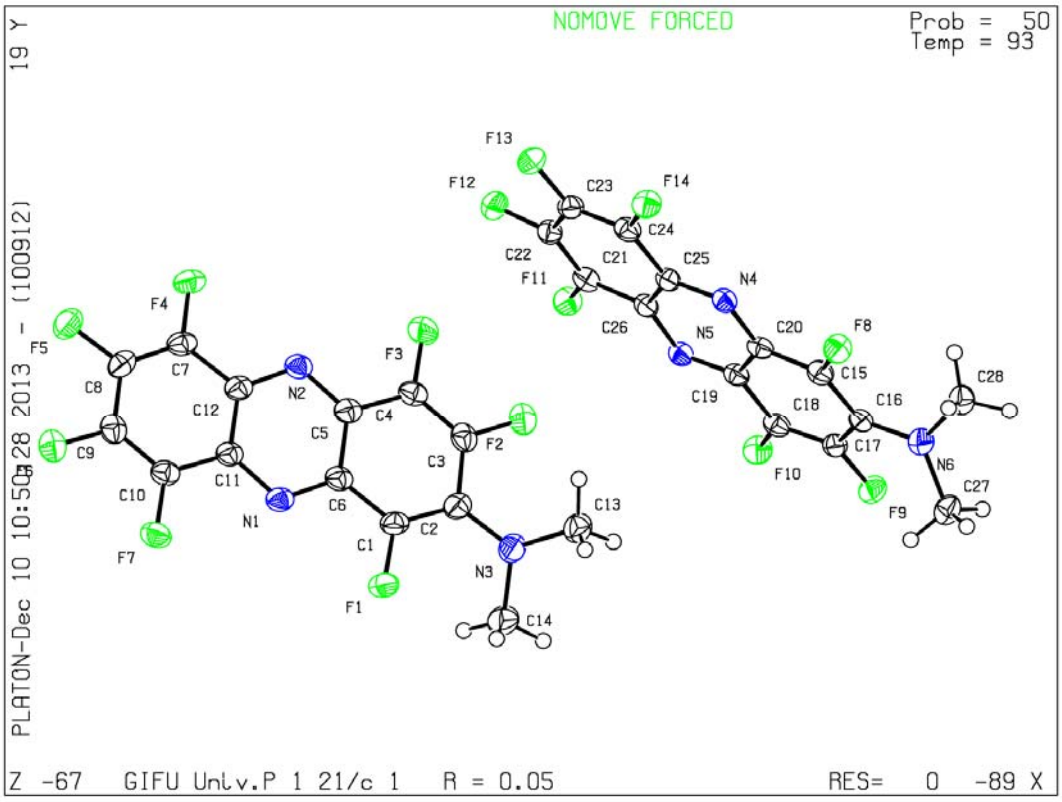


Figure S29. ^{13}C-NMR spectrum of 2-(otadecylamino)phenazine (**3'g**).

Table S1. UV-vis absorption and fluorescence spectra of **3a** in various solvents

Solvent	$\triangle f$	λ_{max} / nm	F_{max} / nm
Hexane	0	466	548
Cyclohexane	0	470	551
Toluene	0.02	479	597
Ethyl acetate	0.19	480	643
THF	0.21	481	647
Acetone	0.28	481	664

X-ray data for **3a**



Figur S29. Compound **3a**.

Table S2. Crystal Data for **3a**

Empirical Formula	$C_{14}H_6F_7N_3$
Formula Weight	349.21
Crystal Color, Habit	red, needle
Crystal Dimensions	0.340 X 0.080 X 0.010 mm
Crystal System	monoclinic
Lattice Parameters	*a* = 21.7935(6) Å
	b = 4.37356(11) Å
	c = 26.8772(7) Å
	β = 94.408(7)°
	V = 2554.23(11) Å^3
Space Group	$P2_1/c$ (#14)
Z value	8
D_{calc}	1.816 g cm^{-3}
F_{000}	1392.00
μ(Cu*K*α)	16.510 cm^{-1}
Temperature	-180.0°C
No. of Reflections Measured	Total: 26719
	Absorption (trans. factors: 0.650 - 0.984)
	Unique: 4664 (R_{int} = 0.0450)
No. Observations (All reflections)	4664
No. Variables	437
Reflection/Parameter Ratio	10.67
Residuals: R1 (I>2.00σ(I))	0.0542
Residuals: R (All reflections)	0.0625
Residuals: wR2 (All reflections)	0.1728
Goodness of Fit Indicator	1.100

Table S3. Atomic coordinates and B_{iso}/B_{eq} for **3a**

atom	x	y	z	B_{eq}
F1	0.56043(10)	1.2755(6)	0.00075(8)	2.98(5)
F2	0.71329(10)	0.5318(6)	0.04539(8)	2.92(4)
F3	0.74218(10)	0.4933(5)	-0.04863(8)	2.94(4)
F4	0.69806(10)	0.7631(5)	-0.22159(8)	2.73(4)
F5	0.63156(11)	1.1005(6)	-0.29154(8)	3.19(5)
F6	0.54715(10)	1.5012(6)	-0.26524(8)	2.93(4)
F7	0.52118(10)	1.5604(5)	-0.16865(8)	2.82(4)
F8	0.94549(9)	0.9528(5)	0.23970(8)	2.47(4)
F9	0.79419(10)	0.3098(5)	0.30389(7)	2.50(4)
F10	0.76171(9)	0.1026(5)	0.21369(8)	2.50(4)
F11	0.79954(9)	0.0290(5)	0.04032(8)	2.44(4)
F12	0.86230(10)	0.2211(5)	-0.03712(7)	2.59(4)
F13	0.94842(10)	0.6587(5)	-0.02425(7)	2.55(4)
F14	0.97968(9)	0.8967(5)	0.06720(8)	2.44(4)
N1	0.58383(13)	1.2235(8)	-0.09525(11)	2.25(6)
N2	0.67880(13)	0.8236(8)	-0.12245(11)	2.21(5)
N3	0.62425(15)	0.9111(9)	0.07670(12)	2.99(7)
N4	0.91945(13)	0.7174(7)	0.14816(11)	1.88(5)
N5	0.82281(13)	0.2765(7)	0.13332(11)	1.88(5)
N6	0.88730(14)	0.7363(8)	0.32360(11)	2.60(6)
C1	0.60424(16)	1.0726(10)	-0.01037(14)	2.36(7)
C2	0.63595(16)	0.9123(10)	0.02714(14)	2.44(7)
C3	0.68368(17)	0.7132(9)	0.01106(14)	2.40(7)
C4	0.69771(16)	0.6891(9)	-0.03684(14)	2.24(6)
C5	0.66488(16)	0.8545(9)	-0.07560(14)	2.16(6)
C6	0.61611(16)	1.0515(9)	-0.06145(14)	2.16(6)
C7	0.65578(16)	0.9610(9)	-0.20828(14)	2.30(7)
C8	0.62290(17)	1.1263(10)	-0.24297(13)	2.43(7)
C9	0.57723(17)	1.3330(10)	-0.22913(14)	2.43(7)
C10	0.56503(16)	1.3642(9)	-0.18088(14)	2.31(6)
C11	0.59805(16)	1.1934(9)	-0.14292(13)	2.11(6)

C12	0.64527(16)	0.9913(9)	-0.15660(13)	2.17(6)
C13	0.67439(18)	0.9577(11)	0.11555(14)	2.95(8)
C14	0.56428(19)	0.9978(14)	0.09191(16)	4.03(11)
C15	0.90170(16)	0.7319(9)	0.23457(13)	2.06(6)
C16	0.87193(16)	0.6412(9)	0.27623(13)	2.01(6)
C17	0.82315(16)	0.4221(9)	0.26550(13)	2.01(6)
C18	0.80674(15)	0.3108(9)	0.21974(13)	1.99(6)
C19	0.83853(15)	0.3991(8)	0.17745(13)	1.87(6)
C20	0.88803(15)	0.6184(8)	0.18618(13)	1.88(6)
C21	0.84238(16)	0.2483(9)	0.04706(14)	2.04(6)
C22	0.87308(16)	0.3428(9)	0.00850(13)	2.02(6)
C23	0.91992(16)	0.5683(9)	0.01578(13)	2.10(6)
C24	0.93475(16)	0.6879(9)	0.06125(13)	2.06(6)
C25	0.90334(15)	0.5939(8)	0.10336(13)	1.86(6)
C26	0.85539(15)	0.3718(9)	0.09560(13)	1.86(6)
C27	0.84285(18)	0.7706(10)	0.36163(14)	2.69(7)
C28	0.94975(17)	0.8448(11)	0.33908(14)	2.77(7)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S4. Bond lengths (Å) for **3a**

atom	atom	distance	atom	atom	distance
F1	C1	1.354(5)	F2	C3	1.344(4)
F3	C4	1.349(4)	F4	C7	1.333(4)
F5	C8	1.338(4)	F6	C9	1.347(4)
F7	C10	1.344(4)	F8	C15	1.358(4)
F9	C17	1.343(4)	F10	C18	1.340(4)
F11	C21	1.341(4)	F12	C22	1.341(4)
F13	C23	1.343(4)	F14	C24	1.339(4)
N1	C6	1.337(5)	N1	C11	1.348(5)
N2	C5	1.325(5)	N2	C12	1.346(5)
N3	C2	1.375(5)	N3	C13	1.467(5)
N3	C14	1.450(6)	N4	C20	1.345(5)
N4	C25	1.342(5)	N5	C19	1.323(5)
N5	C26	1.348(5)	N6	C16	1.357(5)
N6	C27	1.469(5)	N6	C28	1.471(5)
C1	C2	1.371(5)	C1	C6	1.419(5)
C2	C3	1.448(6)	C3	C4	1.350(5)
C4	C5	1.416(5)	C5	C6	1.442(5)
C7	C8	1.343(5)	C7	C12	1.431(5)
C8	C9	1.415(6)	C9	C10	1.351(5)
C10	C11	1.416(5)	C11	C12	1.426(5)
C15	C16	1.394(5)	C15	C20	1.403(5)
C16	C17	1.443(5)	C17	C18	1.345(5)
C18	C19	1.429(5)	C19	C20	1.449(5)
C21	C22	1.341(5)	C21	C26	1.420(5)
C22	C23	1.422(5)	C23	C24	1.346(5)
C24	C25	1.427(5)	C25	C26	1.430(5)

Table S5. Bond angles (°) for **3a**

atom	atom	atom	angle	atom	atom	atom	angle
C6	N1	C11	116.3(3)	C5	N2	C12	116.1(3)
C2	N3	C13	120.4(3)	C2	N3	C14	120.7(3)
C13	N3	C14	113.7(3)	C20	N4	C25	116.0(3)
C19	N5	C26	115.7(3)	C16	N6	C27	123.8(3)
C16	N6	C28	121.4(3)	C27	N6	C28	114.6(3)
F1	C1	C2	119.8(3)	F1	C1	C6	116.1(3)
C2	C1	C6	124.0(4)	N3	C2	C1	126.4(4)
N3	C2	C3	118.5(3)	C1	C2	C3	114.9(3)
F2	C3	C2	117.9(3)	F2	C3	C4	118.5(3)
C2	C3	C4	123.5(3)	F3	C4	C3	119.5(3)
F3	C4	C5	118.9(3)	C3	C4	C5	121.5(3)
N2	C5	C4	120.5(3)	N2	C5	C6	122.6(3)
C4	C5	C6	116.9(3)	N1	C6	C1	119.7(3)
N1	C6	C5	121.1(3)	C1	C6	C5	119.1(3)
F4	C7	C8	120.4(3)	F4	C7	C12	119.1(3)
C8	C7	C12	120.5(4)	F5	C8	C7	121.6(4)
F5	C8	C9	117.7(3)	C7	C8	C9	120.7(3)
F6	C9	C8	118.2(3)	F6	C9	C10	121.0(3)
C8	C9	C10	120.8(3)	F7	C10	C9	119.7(3)
F7	C10	C11	119.5(3)	C9	C10	C11	120.8(4)
N1	C11	C10	119.5(3)	N1	C11	C12	121.9(3)
C10	C11	C12	118.6(3)	N2	C12	C7	119.5(3)
N2	C12	C11	121.8(3)	C7	C12	C11	118.7(3)
F8	C15	C16	119.2(3)	F8	C15	C20	116.3(3)
C16	C15	C20	124.4(3)	N6	C16	C15	124.7(3)
N6	C16	C17	121.1(3)	C15	C16	C17	114.2(3)
F9	C17	C16	118.1(3)	F9	C17	C18	117.5(3)
C16	C17	C18	124.2(3)	F10	C18	C17	119.9(3)
F10	C18	C19	118.9(3)	C17	C18	C19	121.2(3)
N5	C19	C18	119.7(3)	N5	C19	C20	123.5(3)
C18	C19	C20	116.8(3)	N4	C20	C15	120.4(3)
N4	C20	C19	120.4(3)	C15	C20	C19	119.1(3)

F11	C21	C22	120.0(3)	F11	C21	C26	118.9(3)
C22	C21	C26	121.1(3)	F12	C22	C21	121.4(3)
F12	C22	C23	118.3(3)	C21	C22	C23	120.2(3)
F13	C23	C22	117.7(3)	F13	C23	C24	121.3(3)
C22	C23	C24	121.0(3)	F14	C24	C23	119.7(3)
F14	C24	C25	119.5(3)	C23	C24	C25	120.8(3)
N4	C25	C24	119.2(3)	N4	C25	C26	122.8(3)
C24	C25	C26	118.0(3)	N5	C26	C21	119.6(3)
N5	C26	C25	121.4(3)	C21	C26	C25	119.0(3)

X-ray data for **3g**

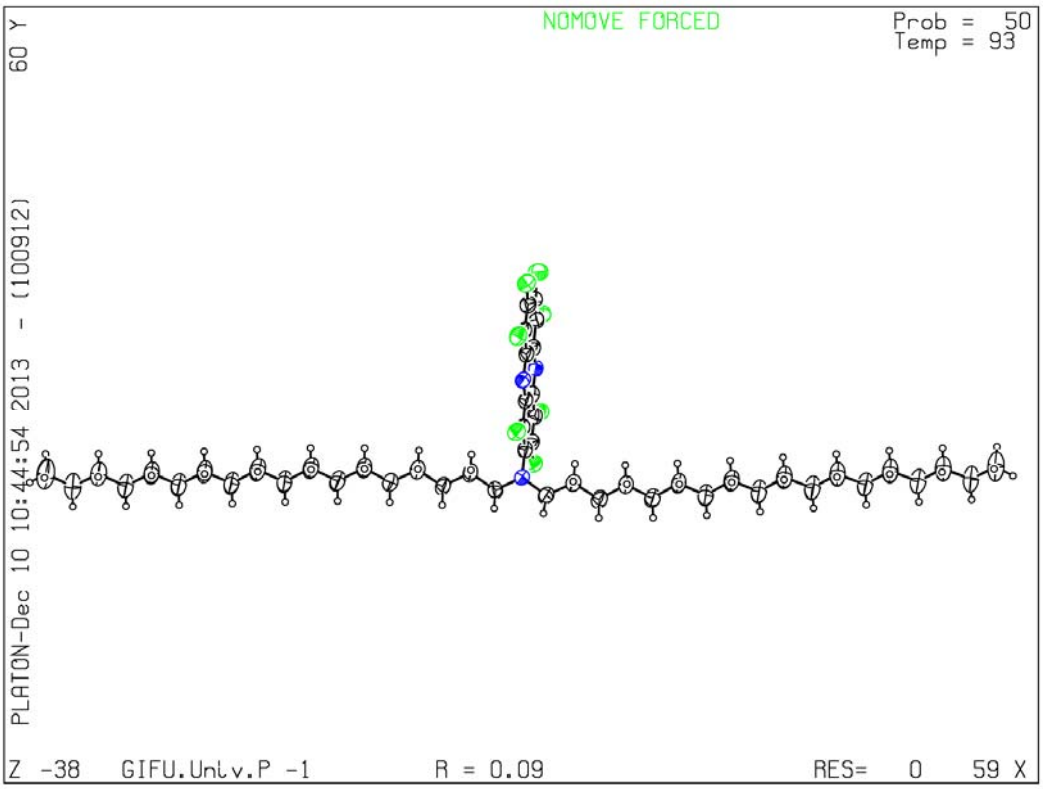


Figure S30. Compound **3g**.

Table S6. Crystal Data for **3g**

Empirical Formula	$C_{48}H_{74}F_7N_3$
Formula Weight	826.12
Crystal Color, Habit	orange, needle
Crystal Dimensions	0.110 X 0.005 X 0.005 mm
Crystal System	triclinic
Lattice Parameters	*a* = 5.5096(9) Å
	b = 16.029(3) Å
	c = 25.975(4) Å
	α = 89.460(6)°
	β = 84.761(6)°
	γ = 87.863(6)°
	V = 2282.7(7) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.202 g/cm^3
μ(Cu*K*α)	7.337 cm^{-1}
Temperature	-180.0°C
No. of Reflections Measured	Total: 26462
	Unique: 8116 (R_{int} = 0.1018)
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.583 - 0.996)
No. Observations (All reflections)	8116
No. Variables	525
Reflection/Parameter Ratio	15.46
Residuals: R1 (I>2.00σ(I))	0.0939
Residuals: R (All reflections)	0.1756
Residuals: wR2 (All reflections)	0.2985
Goodness of Fit Indicator	0.919

Table S7. Atomic coordinates and B_{iso}/B_{eq} **for 3g**

atom	x	y	z	B_{eq}
F1	1.1826(4)	0.19200(14)	0.07133(8)	5.80(5)
F2	0.5021(4)	0.24293(14)	-0.02396(9)	5.81(6)
F3	0.5103(4)	0.40572(14)	-0.00535(8)	5.51(5)
F4	0.8711(4)	0.63398(14)	0.07473(8)	5.78(5)
F5	1.2276(5)	0.68939(15)	0.13106(9)	6.83(6)
F6	1.5540(5)	0.58252(15)	0.16789(9)	6.27(6)
F7	1.5417(4)	0.41649(15)	0.15091(8)	5.92(6)
N1	1.1993(7)	0.3546(2)	0.09257(12)	5.16(7)
N2	0.8528(6)	0.4687(2)	0.05272(12)	4.84(7)
N3	0.8502(6)	0.1244(2)	0.01173(12)	4.98(7)
C1	1.0232(8)	0.3296(3)	0.06386(14)	4.76(9)
C2	1.0125(8)	0.2430(3)	0.05127(15)	5.11(9)
C3	0.8438(8)	0.2118(3)	0.02230(15)	4.81(9)
C4	0.6760(8)	0.2711(3)	0.00385(15)	5.26(9)
C5	0.6790(8)	0.3540(3)	0.01401(15)	4.90(9)
C6	0.8532(8)	0.3866(3)	0.04359(14)	4.69(8)
C7	1.0271(8)	0.4945(3)	0.08156(15)	4.85(8)
C8	1.0405(8)	0.5808(3)	0.09394(16)	5.14(8)
C9	1.2129(8)	0.6077(3)	0.12110(16)	5.18(8)
C10	1.3822(8)	0.5520(3)	0.14081(16)	5.25(8)
C11	1.3775(8)	0.4690(3)	0.13131(15)	5.09(8)
C12	1.1998(8)	0.4372(3)	0.10194(15)	4.95(8)
C13	0.8695(8)	0.1049(3)	-0.04399(15)	5.51(9)
C14	1.0764(8)	0.1468(3)	-0.07468(14)	5.28(9)
C15	1.0848(8)	0.1370(3)	-0.13323(15)	5.70(10)
C16	1.2889(8)	0.1853(3)	-0.16173(14)	5.41(9)
C17	1.2882(8)	0.1864(3)	-0.22024(15)	5.92(10)
C18	1.5004(8)	0.2328(3)	-0.24714(15)	6.15(10)
C19	1.5017(9)	0.2391(3)	-0.30564(16)	6.86(11)
C20	1.7198(9)	0.2835(3)	-0.33153(16)	6.89(12)
C21	1.7251(9)	0.2922(4)	-0.38994(17)	7.50(13)

C22	1.9480(9)	0.3340(4)	-0.41500(17)	7.50(13)
C23	1.9596(10)	0.3440(4)	-0.47379(17)	8.01(14)
C24	2.1848(9)	0.3834(4)	-0.49866(17)	7.77(13)
C25	2.1977(9)	0.3935(4)	-0.55657(17)	7.72(13)
C26	2.4251(9)	0.4316(4)	-0.58142(17)	7.77(13)
C27	2.4372(9)	0.4419(4)	-0.63959(17)	7.84(14)
C28	2.6695(10)	0.4771(4)	-0.66440(18)	8.26(14)
C29	2.6839(10)	0.4859(4)	-0.72264(18)	8.32(14)
C30	2.9198(10)	0.5202(4)	-0.7470(2)	10.20(18)
C31	0.6653(7)	0.0785(3)	0.04270(14)	5.04(9)
C32	0.6638(8)	0.0911(3)	0.10057(14)	5.66(10)
C33	0.4665(8)	0.0445(3)	0.13171(14)	5.42(9)
C34	0.4729(8)	0.0528(3)	0.18998(14)	5.71(10)
C35	0.2645(8)	0.0103(3)	0.22084(15)	5.86(10)
C36	0.2713(8)	0.0116(3)	0.27931(15)	6.29(11)
C37	0.0578(9)	-0.0303(3)	0.30839(15)	6.64(11)
C38	0.0619(9)	-0.0335(3)	0.36702(16)	6.93(12)
C39	-0.1576(9)	-0.0761(3)	0.39442(16)	7.17(12)
C40	-0.1570(9)	-0.0819(4)	0.45277(16)	7.60(13)
C41	-0.3767(9)	-0.1235(4)	0.47965(16)	7.48(13)
C42	-0.3784(10)	-0.1300(4)	0.53791(17)	7.73(13)
C43	-0.5992(10)	-0.1701(4)	0.56475(16)	7.67(13)
C44	-0.6007(9)	-0.1762(4)	0.62315(17)	7.51(13)
C45	-0.8232(10)	-0.2153(4)	0.65029(17)	7.74(13)
C46	-0.8242(10)	-0.2211(4)	0.70873(17)	7.98(13)
C47	-1.0490(11)	-0.2579(4)	0.73573(19)	8.72(15)
C48	-1.0471(13)	-0.2632(4)	0.7948(2)	11.6(2)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S8. Bond lengths (Å) for **3g**

atom	atom	distance	atom	atom	distance
F1	C2	1.357(5)	F2	C4	1.345(5)
F3	C5	1.351(5)	F4	C8	1.365(5)
F5	C9	1.345(5)	F6	C10	1.339(5)
F7	C11	1.344(5)	N1	C1	1.351(6)
N1	C12	1.350(6)	N2	C6	1.339(5)
N2	C7	1.350(5)	N3	C3	1.429(5)
N3	C13	1.477(5)	N3	C31	1.456(5)
C1	C2	1.433(6)	C1	C6	1.417(6)
C2	C3	1.360(6)	C3	C4	1.412(6)
C4	C5	1.357(7)	C5	C6	1.402(6)
C7	C8	1.430(6)	C7	C12	1.430(6)
C8	C9	1.320(7)	C9	C10	1.394(6)
C10	C11	1.357(7)	C11	C12	1.408(6)
C13	C14	1.506(6)	C14	C15	1.527(5)
C15	C16	1.521(6)	C16	C17	1.520(5)
C17	C18	1.521(6)	C18	C19	1.521(6)
C19	C20	1.520(7)	C20	C21	1.520(6)
C21	C22	1.513(7)	C22	C23	1.530(6)
C23	C24	1.503(7)	C24	C25	1.507(6)
C25	C26	1.504(7)	C26	C27	1.514(6)
C27	C28	1.506(7)	C28	C29	1.513(7)
C29	C30	1.512(8)	C31	C32	1.518(5)
C32	C33	1.511(6)	C33	C34	1.524(5)
C34	C35	1.519(6)	C35	C36	1.523(6)
C36	C37	1.513(6)	C37	C38	1.526(6)
C38	C39	1.527(7)	C39	C40	1.518(6)
C40	C41	1.515(7)	C41	C42	1.515(6)
C42	C43	1.508(7)	C43	C44	1.518(6)
C44	C45	1.511(7)	C45	C46	1.519(6)
C46	C47	1.504(8)	C47	C48	1.538(7)

Table S9. Bond angles (°) for **3g**

atom	atom	atom	angle	atom	atom	atom	angle
C1	N1	C12	115.9(4)	C6	N2	C7	116.2(3)
C3	N3	C13	113.6(3)	C3	N3	C31	114.0(3)
C13	N3	C31	114.3(3)	N1	C1	C2	119.5(4)
N1	C1	C6	122.3(4)	C2	C1	C6	118.2(4)
F1	C2	C1	115.1(4)	F1	C2	C3	120.9(4)
C1	C2	C3	123.9(4)	N3	C3	C2	119.4(4)
N3	C3	C4	125.0(4)	C2	C3	C4	115.5(4)
F2	C4	C3	117.7(4)	F2	C4	C5	119.1(4)
C3	C4	C5	123.2(4)	F3	C5	C4	118.7(4)
F3	C5	C6	119.7(4)	C4	C5	C6	121.6(4)
N2	C6	C1	122.2(4)	N2	C6	C5	120.3(4)
C1	C6	C5	117.6(4)	N2	C7	C8	120.5(4)
N2	C7	C12	121.9(4)	C8	C7	C12	117.6(4)
F4	C8	C7	116.4(4)	F4	C8	C9	122.0(4)
C7	C8	C9	121.5(4)	F5	C9	C8	120.8(4)
F5	C9	C10	118.2(4)	C8	C9	C10	121.0(4)
F6	C10	C9	118.6(4)	F6	C10	C11	120.8(4)
C9	C10	C11	120.6(4)	F7	C11	C10	119.6(4)
F7	C11	C12	119.7(4)	C10	C11	C12	120.7(4)
N1	C12	C7	121.6(4)	N1	C12	C11	119.8(4)
C7	C12	C11	118.5(4)	N3	C13	C14	113.6(3)
C13	C14	C15	115.4(4)	C14	C15	C16	112.3(4)
C15	C16	C17	114.7(4)	C16	C17	C18	112.9(4)
C17	C18	C19	114.9(4)	C18	C19	C20	113.7(4)
C19	C20	C21	115.2(4)	C20	C21	C22	114.2(4)
C21	C22	C23	115.7(4)	C22	C23	C24	115.5(4)
C23	C24	C25	115.8(4)	C24	C25	C26	115.7(4)
C25	C26	C27	115.6(4)	C26	C27	C28	115.2(4)
C27	C28	C29	115.3(4)	C28	C29	C30	114.6(5)
N3	C31	C32	114.4(3)	C31	C32	C33	113.3(4)
C32	C33	C34	113.6(4)	C33	C34	C35	113.2(4)

C34	C35	C36	115.4(4)	C35	C36	C37	113.5(4)
C36	C37	C38	115.4(4)	C37	C38	C39	113.2(4)
C38	C39	C40	114.6(4)	C39	C40	C41	114.2(4)
C40	C41	C42	114.8(4)	C41	C42	C43	114.8(4)
C42	C43	C44	114.7(4)	C43	C44	C45	114.9(4)
C44	C45	C46	114.7(4)	C45	C46	C47	114.6(4)
C46	C47	C48	113.8(5)				