Electronic Supplementary Material (ESI) for RSC Advances.

Targeting chemorefractory COLO205 (B-Raf V600E) cell lines using substituted benzo[α]phenoxazines

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Supplementary information

Figure Legends

Table legends

Table S1 Bond lengths [Å] and angles [°] for **2B**

Table S2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **2B**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

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

Table S4 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) For **2B**

Table S5 Bond lengths [Å] and angles [°] for **3B**

Table S5 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **3B**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

Table S6 Anisotropic displacement parameters (Å^{2}x 10^3) for **3B**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Table S7 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **3B**

Table S8 Torsion angles [°] for **3B**

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Analysis Info

Analysis Name	D:\Data\DR.SALUNKE\DATTATRAY CHADAR\1B_BA6_01_471.d	Acquisition Date	3/10/2015 1:35:41 PM
Method	hplc-ms600mz.m	Operator	CIF
Sample Name	1B	Instrument	impact HD 1819696.00184
Comment			

Acquisition Parameter

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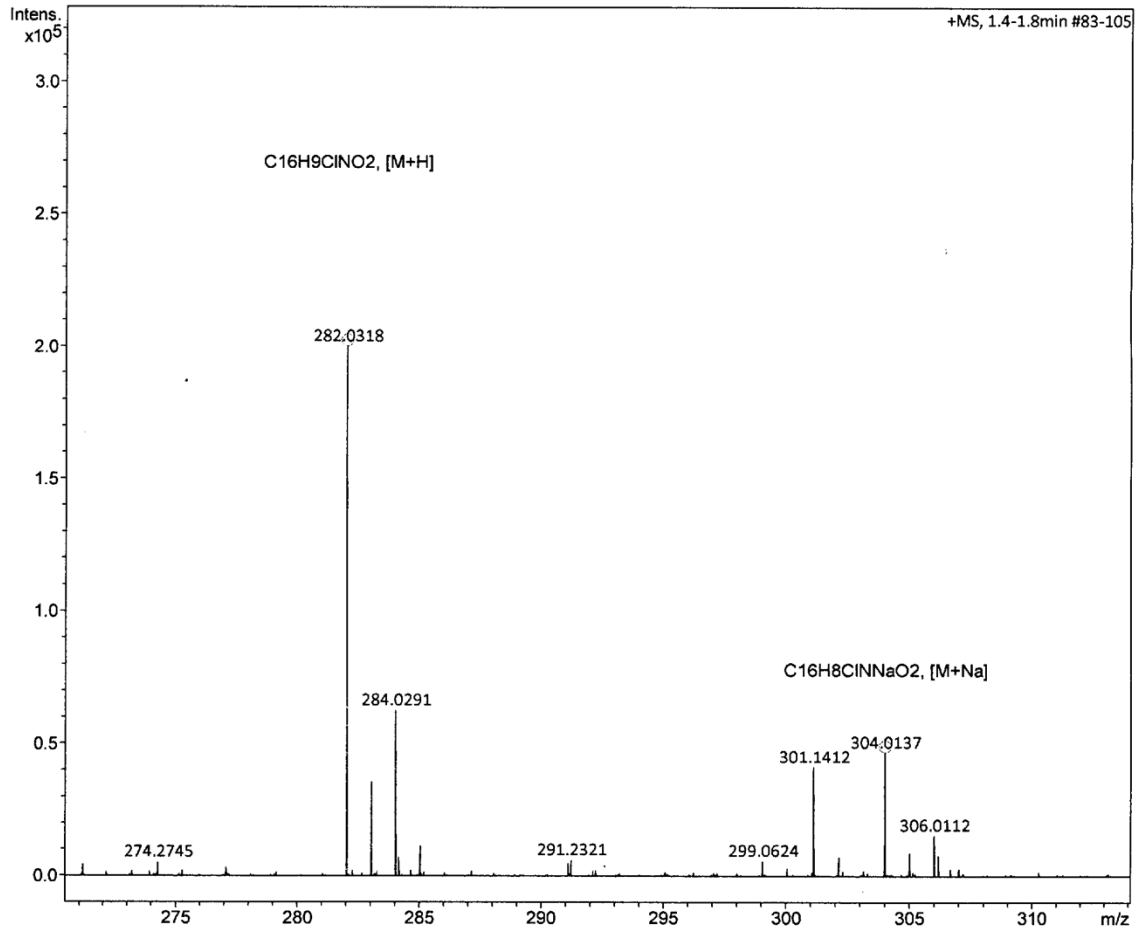

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304.0137	1	C16H8ClNNaO2	304.0136	-0.5	6.2	1	100.00	12.5	even	ok	M+Na

1B_BA6_01_471.d

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Fig. S1 HR-MS spectra of 1B

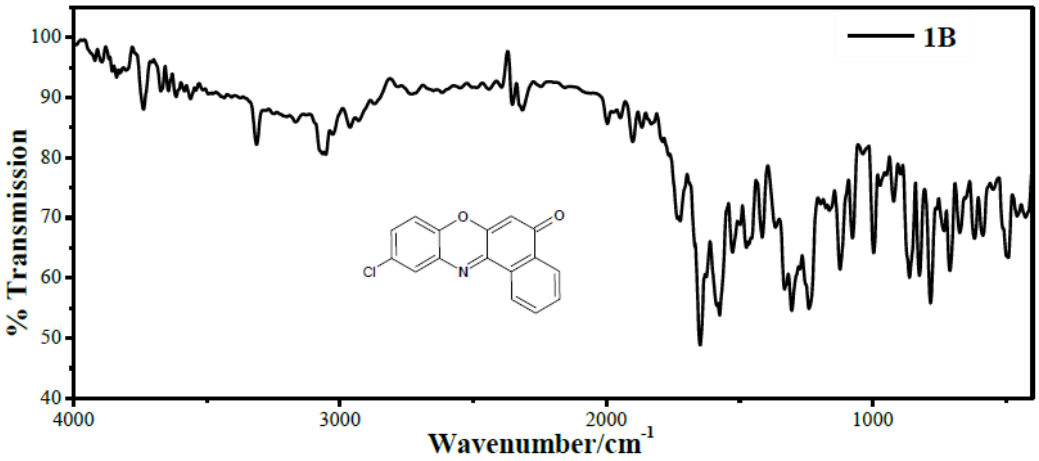

Fig.S2 FT-IR spectrums of **1B** in region 400 cm^{-1} to 4000 cm^{-1}

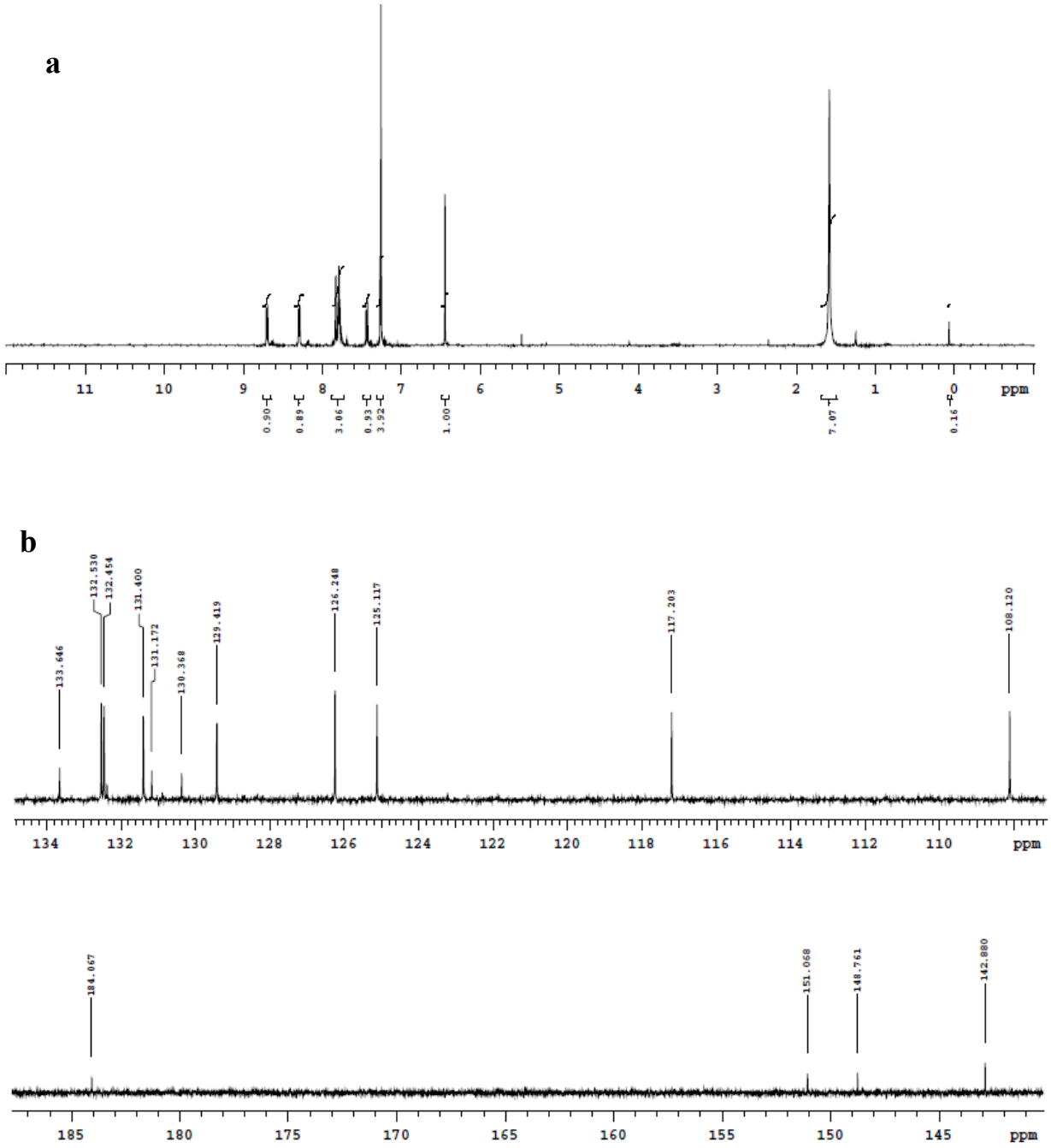

Fig. S3 a) ^{1}H, b) ^{13}C NMR spectra of **1B**

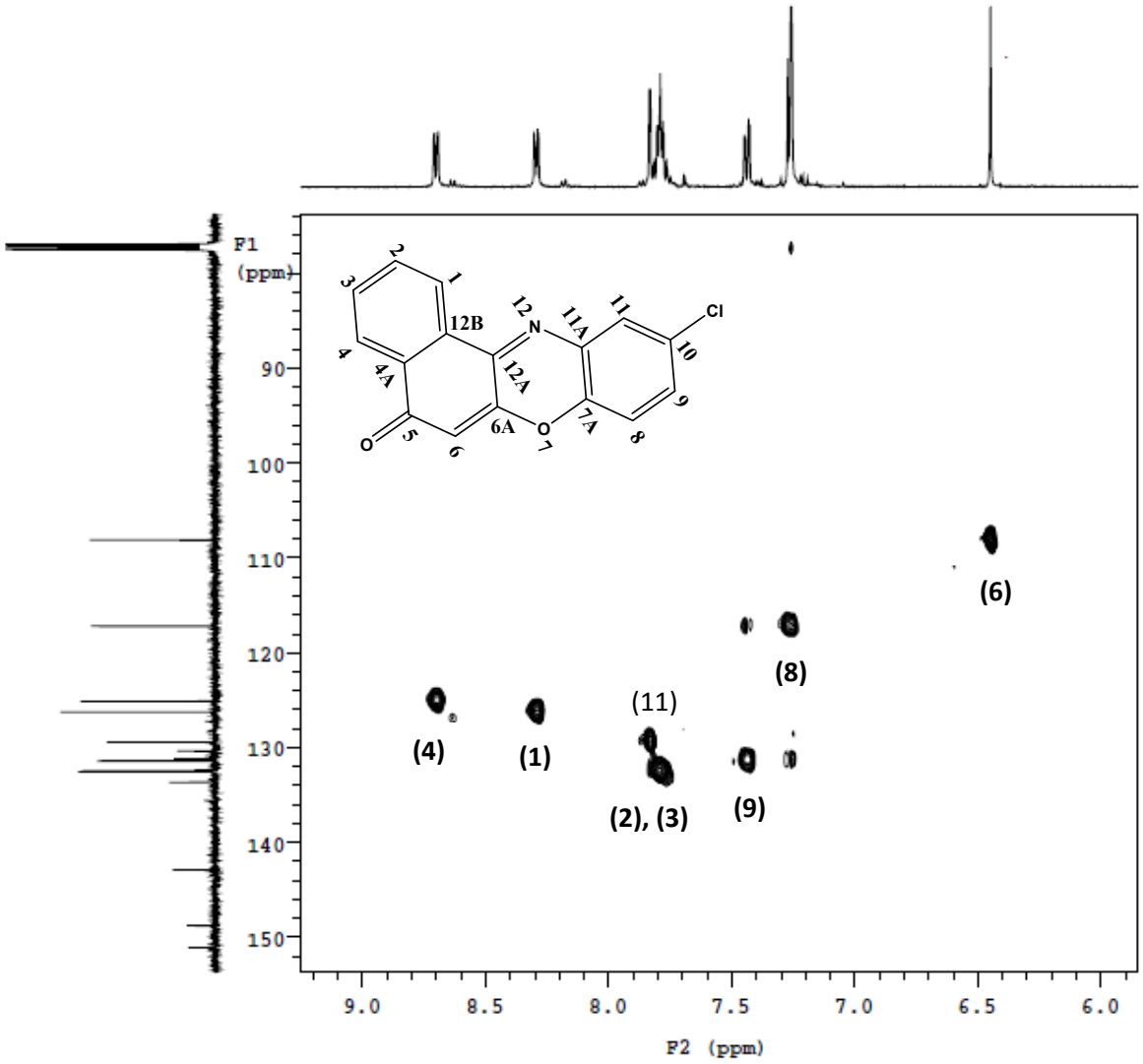

Fig. S4 2D gHSQCAD NMR spectra of **1B**

Interpretation of the 2D gHSQCAD NMR of 1B that shows the correlation between the Carbon and Proton

Spot (6) show the correlation between the proton i.e. observed at 6.449 ppm (C6-H) in proton NMR and the carbon observed at 108.12 ppm in carbon NMR.

Spot (8) show the correlation between the proton i.e. observed at 7.265 ppm (C8-H) in proton NMR and the carbons observed at 117.2 ppm in carbon NMR.

Spot (4) show the correlation between the proton i.e. observed at 8.295 ppm (C4-H) in proton NMR and the carbon observed at 126.24 ppm in carbon NMR.

Spot (1) show the correlation between the proton i.e. observed at 8.701 ppm (C1-H) in proton NMR and the carbon observed at 125.11 ppm in carbon NMR.

Spot (2, 3) show the correlation between the protons i.e. observed multiplate at 7.796 ppm (C2-H, C3-H) in proton NMR and the carbon observed at 132.45 (C2) ppm and 132.53 (C3) ppm carbons NMR.

Spot (11) show the correlation between the proton i.e. observed at 7.835 ppm (C11-H) in proton NMR and the carbon observed at 129.41 ppm in carbon NMR

Spot (9) show the correlation between the proton i.e. observed at 7.437 ppm (C9-H) in proton NMR and the carbon observed at 131.40 ppm in carbon NMR.

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Analysis Info

Analysis Name	D:\Data\DR.SALUNKE\DATTATRAY CHADAR\2B_BA5_01_468.d	Acquisition Date	3/10/2015 11:22:12 AM
Method	hplc-ms600mz.m	Operator	CIF
Sample Name	2B	Instrument	impact HD 1819696.00184
Comment			

Acquisition Parameter

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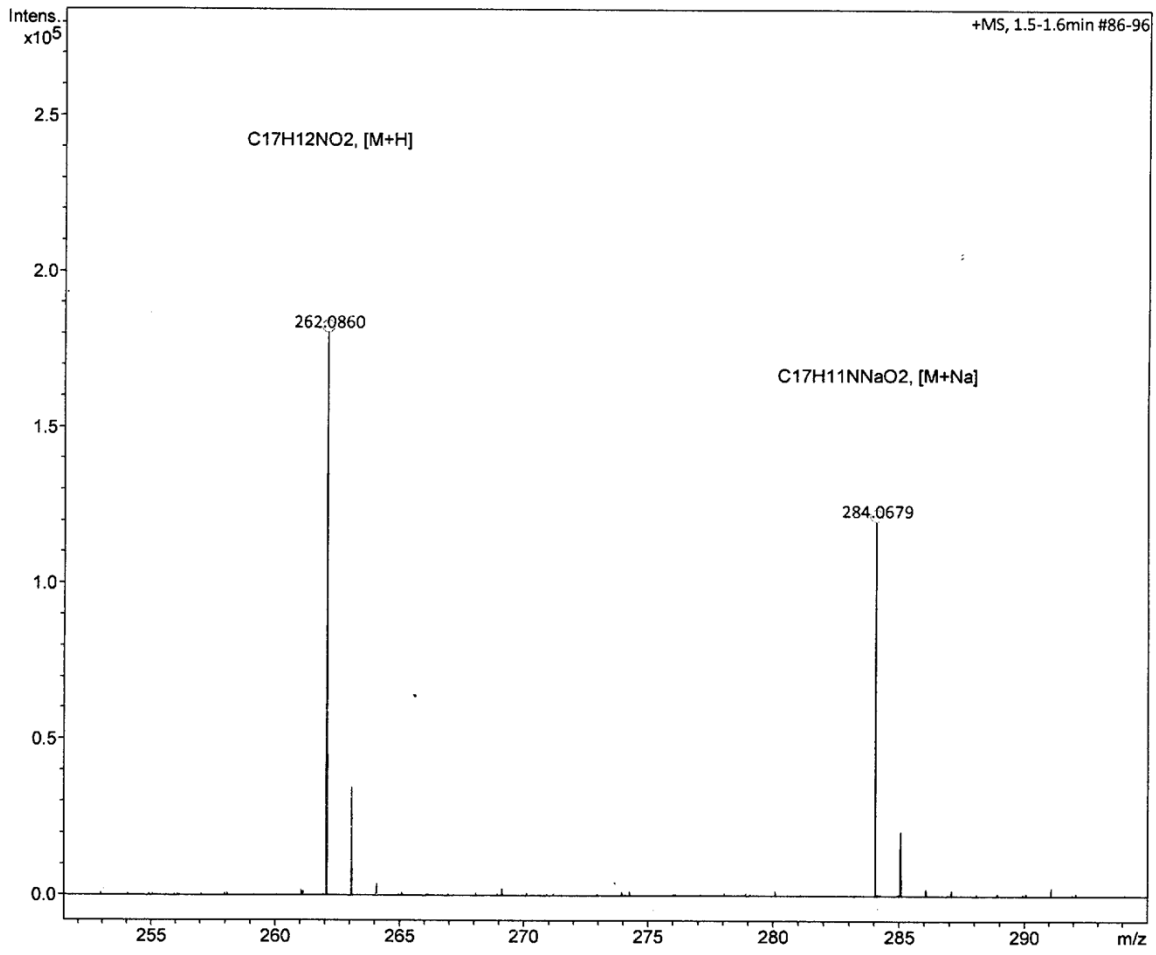

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
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284.0679	1	C17H11NNaO2	284.0682	1.1	10.3	1	100.00	12.5	even	ok	M+Na

Fig. S5 HR-MS spectra of **1B**

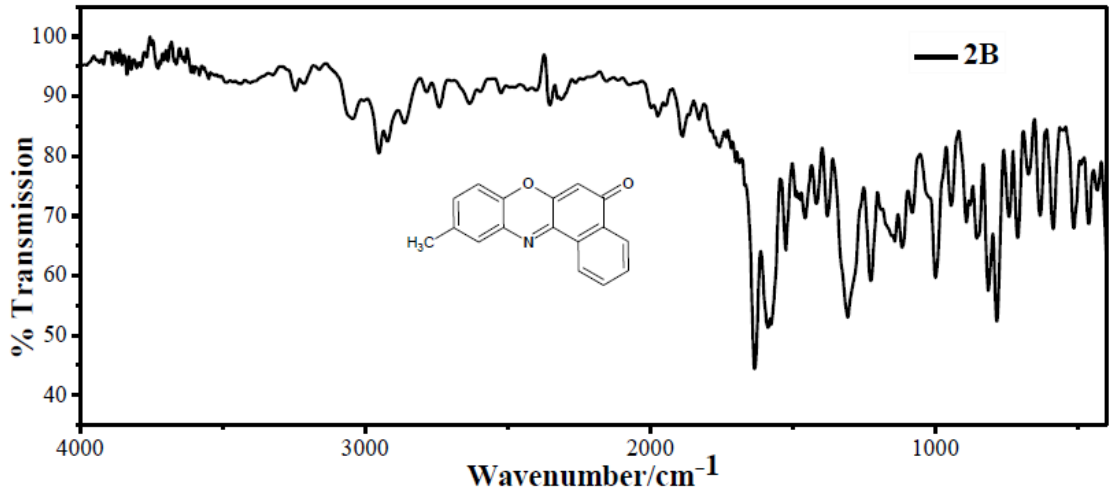

Fig. S6 FT-IR spectrums of **2B** in region 400 cm^{-1} to 4000 cm^{-1}

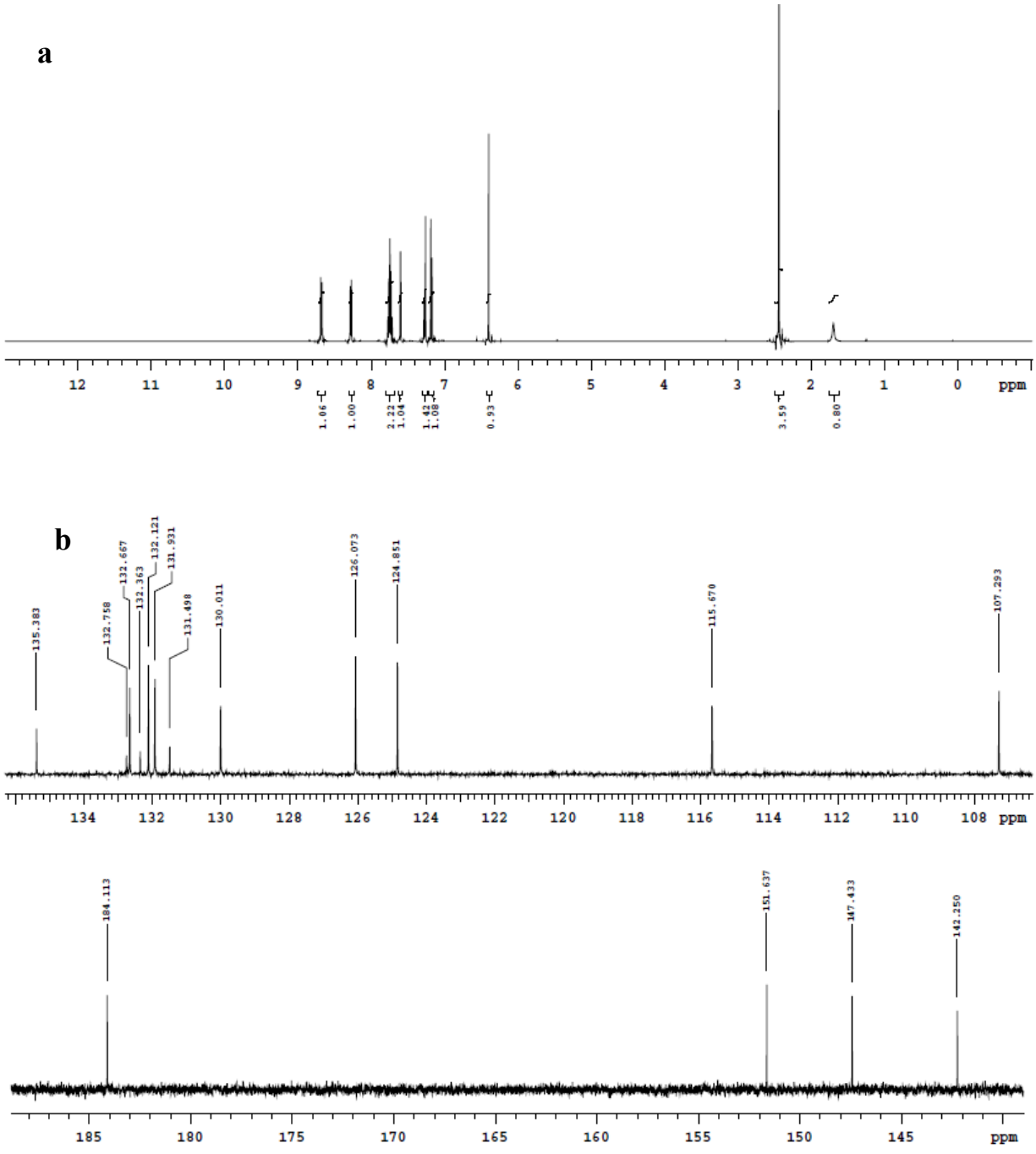

Fig. S7 a) ^{1}H, b) ^{13}C NMR spectra of **2B**

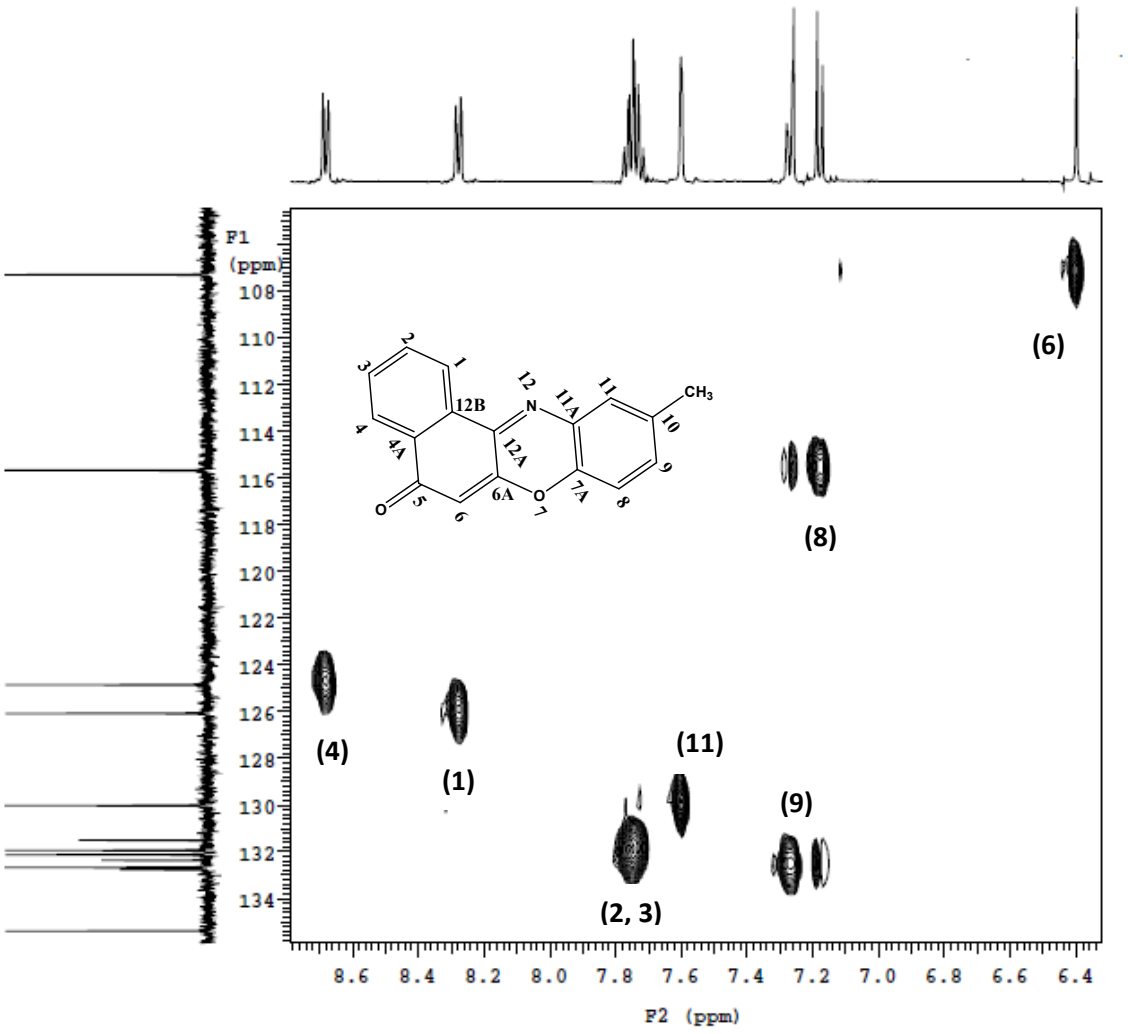

Fig. S82D gHSQCAD NMR spectra of **2B**

Interpretation of the 2D gHSQCAD NMR of 2B that shows the correlation between the Carbon and Proton

Spot (6) show the correlation between the proton i.e. observed at 6.399 ppm (C6-H) in proton NMR and the carbon observed at 107.29 ppm in carbon NMR.

Spot (8) show the correlation between the proton i.e. observed at 7.179 ppm (C8-H) in proton NMR and the carbon observed at 115.67 ppm in carbon NMR.

Spot (4) show the correlation between the proton i.e. observed at 8.276 ppm (C4-H) in proton NMR and the carbon observed at 126.07 ppm in carbon NMR.

Spot (1) show the correlation between the protons i.e. observes at 8.680 ppm (C1-H) in proton NMR and the carbon observed at 124.85 ppm in carbon NMR.
Spot (11) show the correlation between the proton i.e. observed at 7.601 ppm (C11-H) in proton NMR and the carbon observed at 130.01 ppm in carbon NMR.
Spot (2, 3) show the correlation between the proton i.e. observed multiplate for 2H at 7.731 ppm (C-2, 3) in proton NMR and the carbon observed at 131.93 (C2-H) and 132.12 (C3-H) ppm in carbon NMR.
Spot (9) show the correlation between the proton i.e. observed at 7.269 ppm (C9-H) in proton NMR and the carbon observed at 132.66 ppm in carbon NMR.

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Analysis Info

Analysis Name	D:\Data\DR.SALUNKE\DATTATRAY CHADAR\3B_BA4_01_467.d	Acquisition Date	3/10/2015 11:18:00 AM
Method	hplc-ms600mz.m	Operator	CIF
Sample Name	3B	Instrument	impact HD 1819696.00184
Comment			

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
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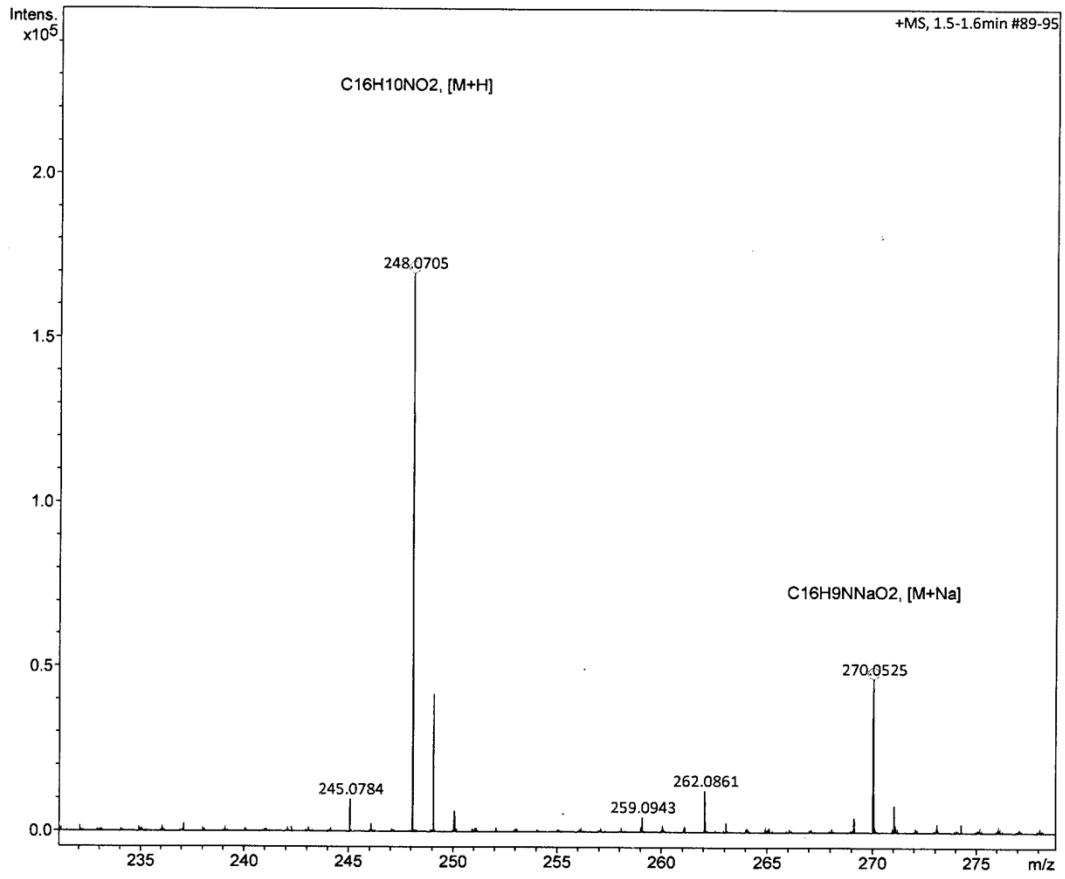
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
248.0705	1	C16H10NO2	248.0706	0.2	39.9	1	100.00	12.5	even	ok	M+H
270.0525	1	C16H9NNaO2	270.0525	0.1	3.3	1	100.00	12.5	even	ok	M+Na

3B_BA4_01_467.d

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Fig. S9 HR-MS spectra of **3B**

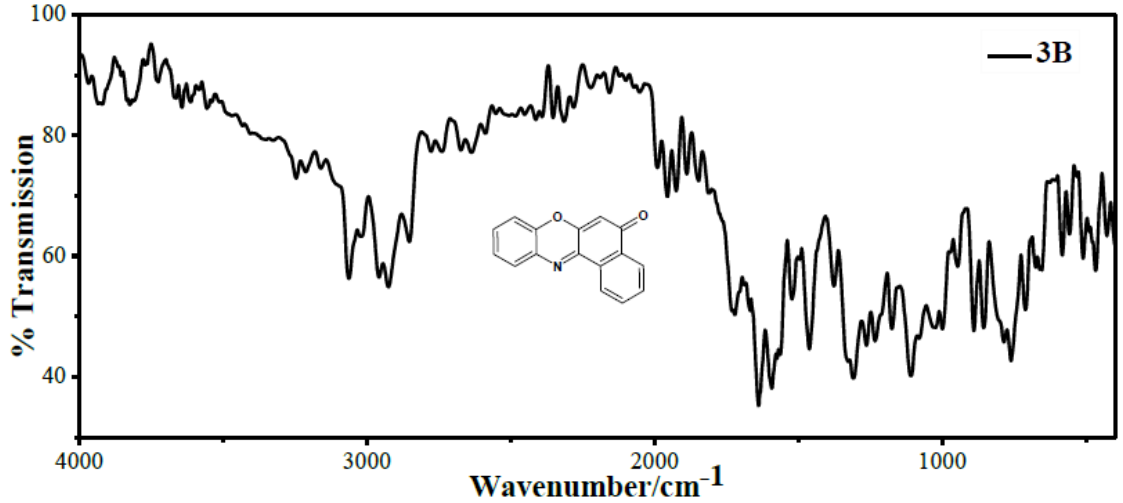


Fig. S10 FT-IR spectrums of **3B** in region 400 cm^{-1} to 4000 cm^{-1}

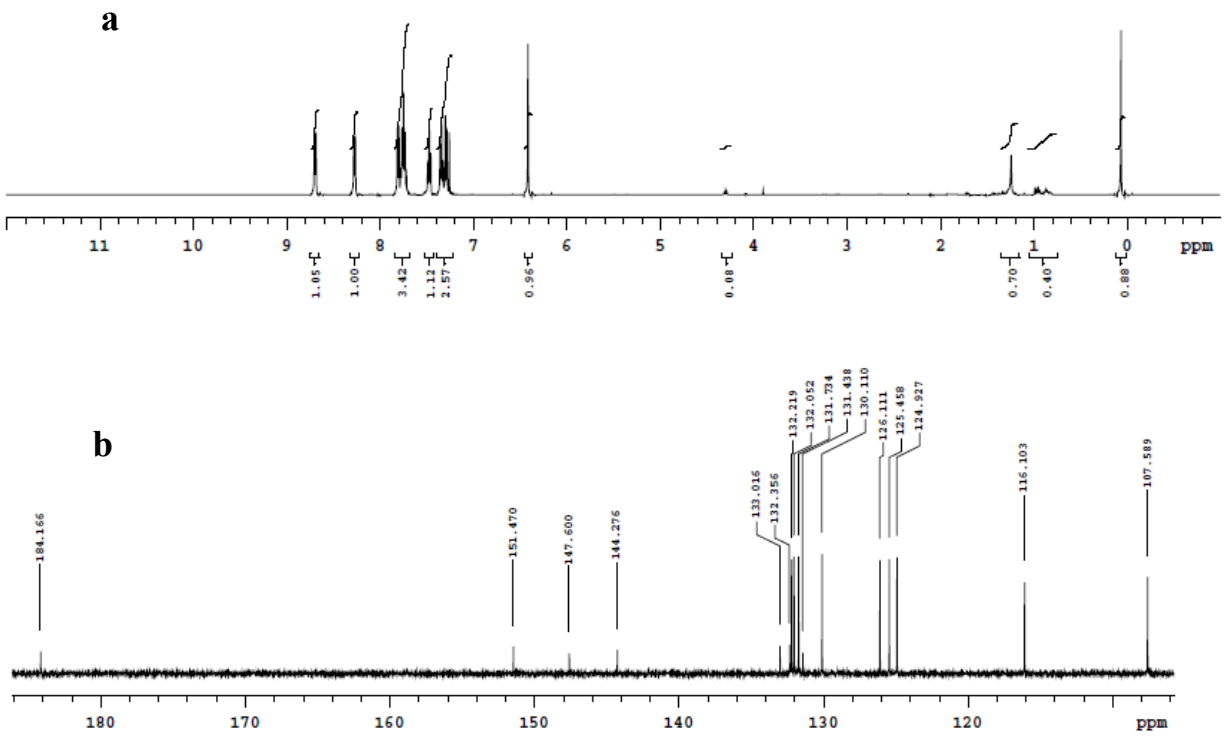


Fig. S11 a) ^{1}H, b) ^{13}C NMR spectra of **3B**

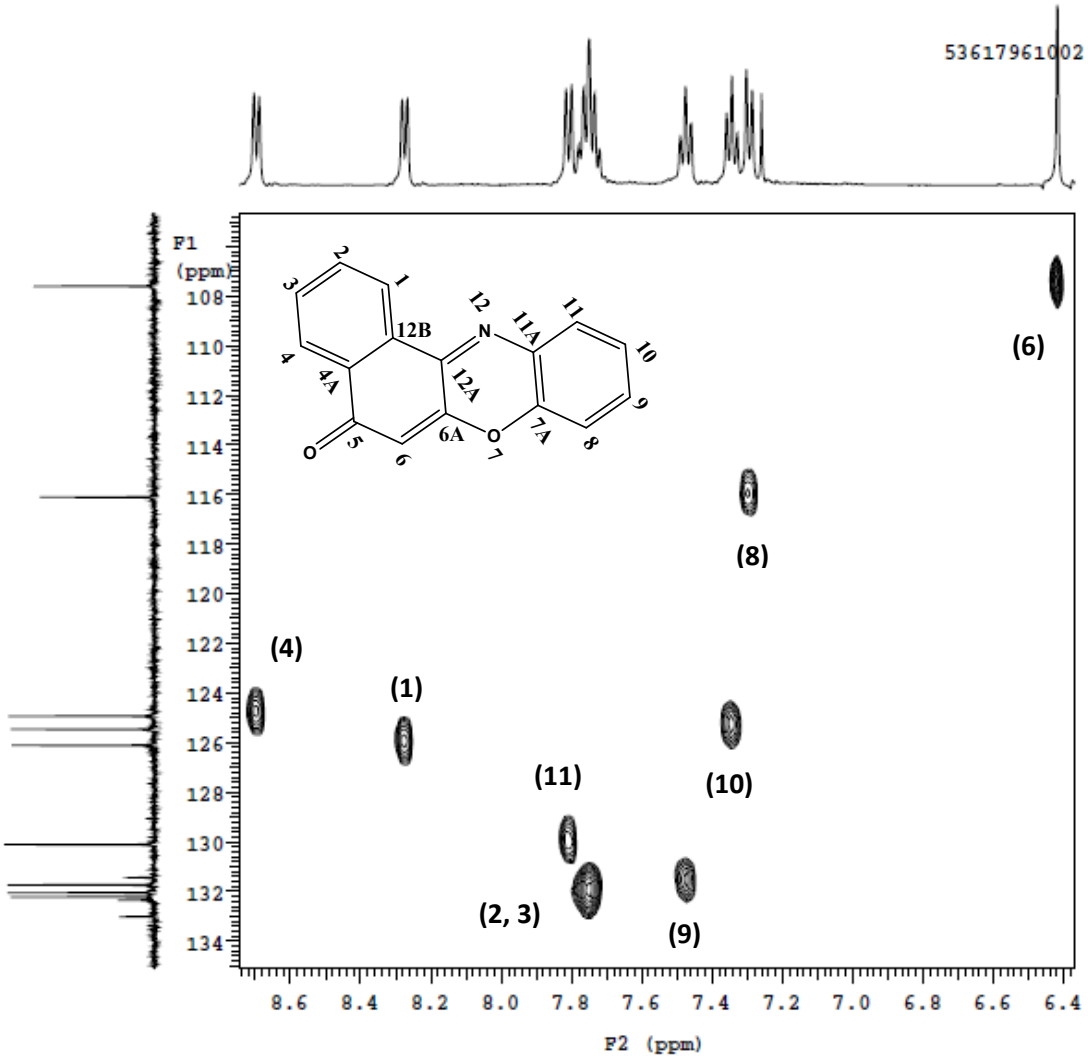


Fig. S12 2D gHSQCAD NMR spectra of **3B**

Interpretation of the 2D gHSQCAD NMR of 3B that shows the correlation between the Carbon and Proton.

Spot (6) show the correlation between the proton i.e. observed at 6.419 ppm (C6-H) in proton NMR and the carbon observed at 107.58 ppm in carbon NMR.

Spot (8) show the correlation between the proton i.e. observed at 7.260 ppm (C8-H) in proton NMR and the carbon observed at 116.10 ppm in carbon NMR.

Spot (1) show the correlation between the proton i.e. observed at 8.696 ppm (C1-H) in proton NMR and the carbon observed at 124.11 ppm in carbon NMR.

Spot (4) show the correlation between the proton i.e. observed at 8.274 ppm (C4-H) in proton NMR and the carbon observed at 126.11 ppm in carbon NMR.

Spot (10) show the correlation between the proton i.e. observed at 7.475 ppm (C10-H) in proton NMR and the carbon observed at 125.45 ppm in carbon NMR.

Spot (11) show the correlation between the proton i.e. observed at 7.808 ppm (C11-H) in proton NMR and the carbon observed at 130.11 ppm in carbon NMR.

Spot (2, 3) show the correlation between the proton i.e. observed multiplate for 2H at 7.766 ppm (C-2, 3) in proton NMR and the carbon observed at 132.05 (C2-H) and 132.21 (C3-H) ppm in carbon NMR.

Spot (9) show the correlation between the proton i.e. observed at 7.344 ppm (C9-H) in proton NMR and the carbon observed at 131.73 ppm in carbon NMR.

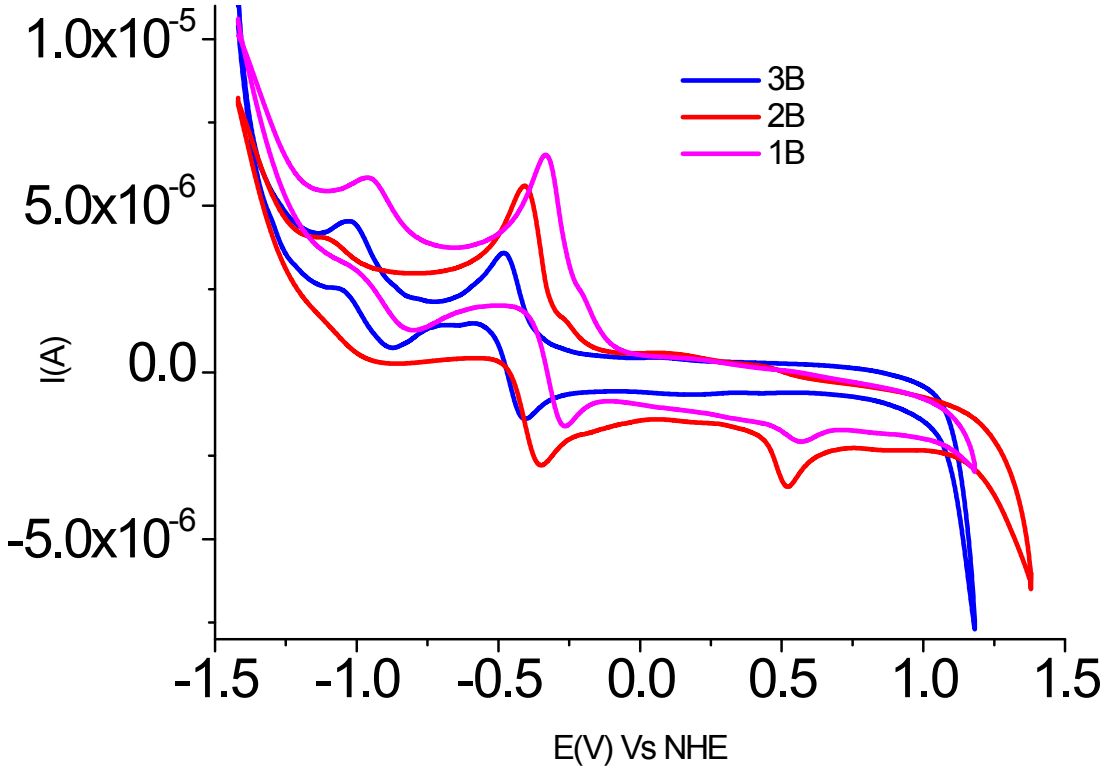


Fig.S13Cyclic voltammogram of **1B**, **2B** and **3B**

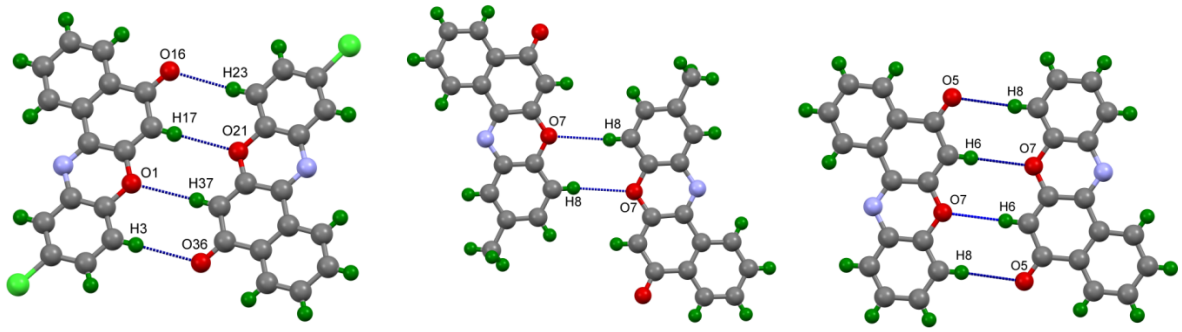


Fig.S14 Hydrogen bonding of oppositely oriented molecules of **1B** to **3B**

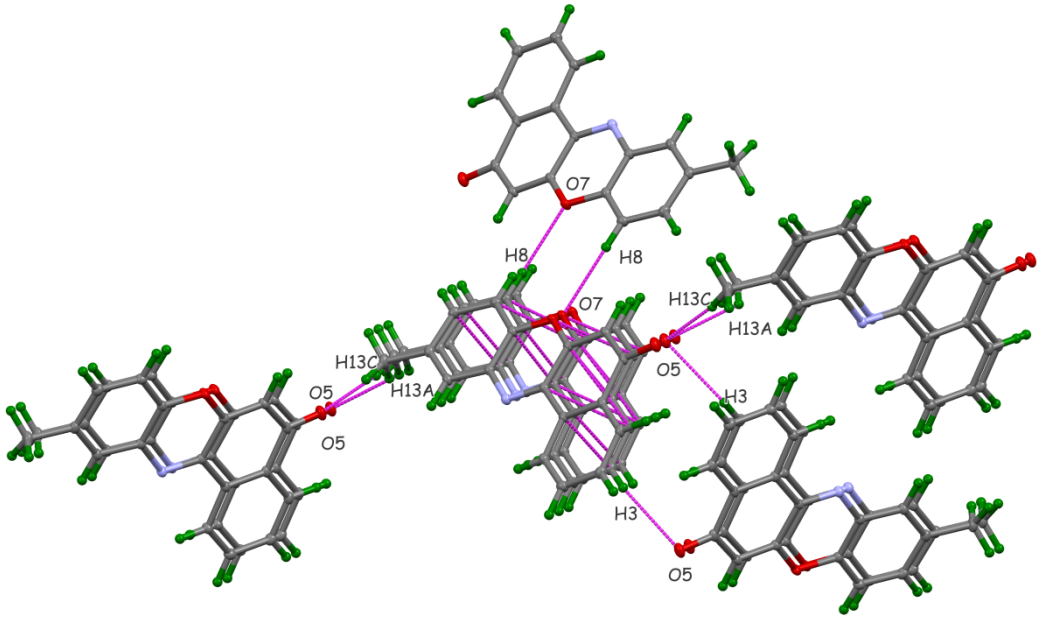


Fig.S15 Hydrogen bonding interactions to neighboring molecules of **2B**

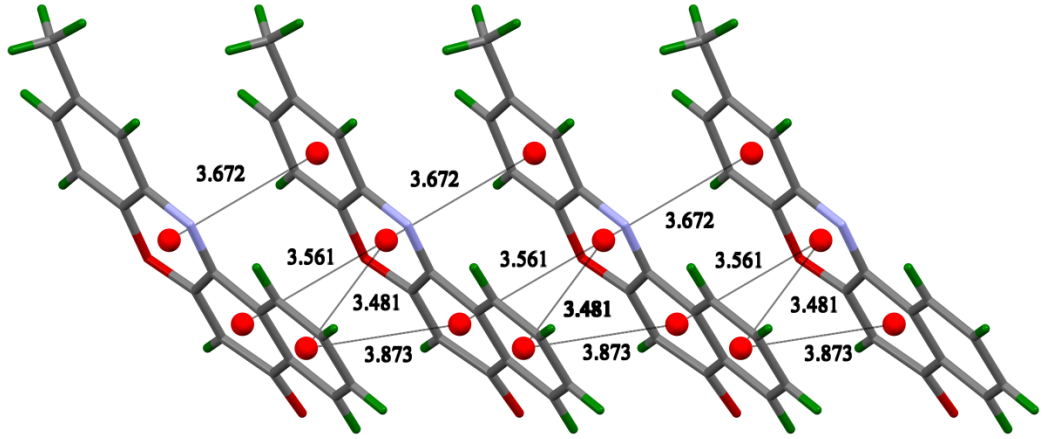
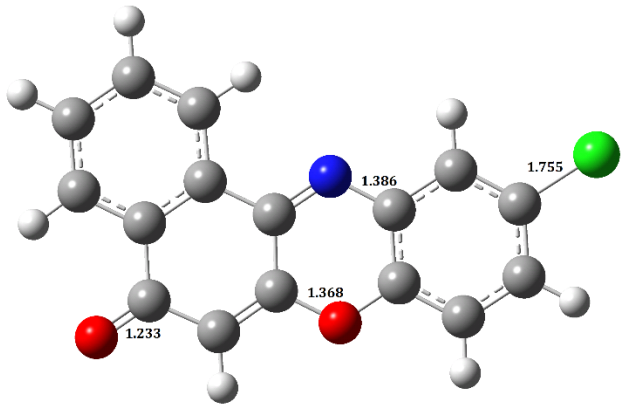
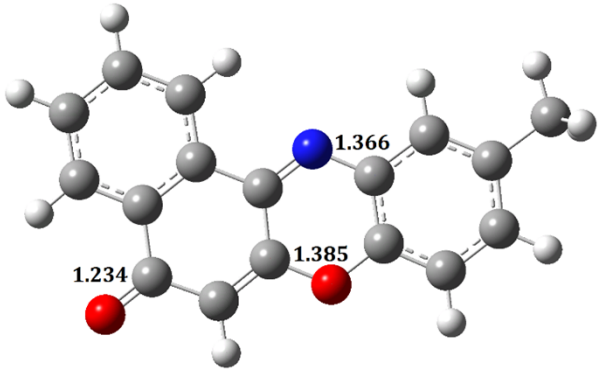


Fig.S16 Slipped π-πstacked interaction in **2B**

a)



b)



c)

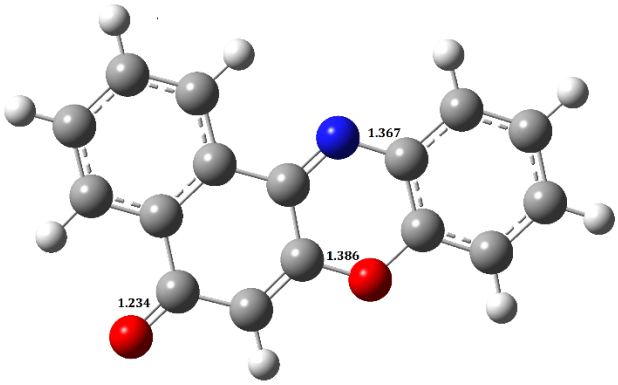


Fig.S17 Optimized structures of **1B**, **2B** and **3B** from the M06-2x theory.

Table S1 Bond lengths [Å] and angles [°] for 2B.

O(1)-C(2)	1.2337(12)
C(2)-C(19)	1.4522(14)
C(2)-C(3)	1.4894(14)
C(3)-C(4)	1.3998(14)
C(3)-C(8)	1.4042(14)
C(4)-C(5)	1.3869(14)
C(5)-C(6)	1.3967(15)
C(6)-C(7)	1.3890(14)
C(7)-C(8)	1.3985(14)
C(8)-C(9)	1.4676(14)
C(9)-N(10)	1.3008(13)
C(9)-C(18)	1.4609(13)
N(10)-C(11)	1.3934(13)
C(11)-C(16)	1.3937(13)
C(11)-C(12)	1.4002(14)
C(12)-C(13)	1.3920(14)
C(13)-C(14)	1.4006(15)
C(13)-C(20)	1.5074(15)
C(14)-C(15)	1.3895(14)
C(15)-C(16)	1.3870(14)
C(16)-O(17)	1.3789(12)
O(17)-C(18)	1.3666(12)
C(18)-C(19)	1.3505(14)

O(1)-C(2)-C(19)	121.63(9)
O(1)-C(2)-C(3)	121.03(10)
C(19)-C(2)-C(3)	117.34(9)
C(4)-C(3)-C(8)	119.79(9)
C(4)-C(3)-C(2)	119.47(9)
C(8)-C(3)-C(2)	120.74(9)
C(5)-C(4)-C(3)	120.27(9)
C(4)-C(5)-C(6)	119.88(10)
C(7)-C(6)-C(5)	120.38(9)

C(6)-C(7)-C(8)	120.09(9)
C(7)-C(8)-C(3)	119.59(9)
C(7)-C(8)-C(9)	120.31(9)
C(3)-C(8)-C(9)	120.11(9)
N(10)-C(9)-C(18)	123.28(9)
N(10)-C(9)-C(8)	119.71(9)
C(18)-C(9)-C(8)	117.00(8)
C(9)-N(10)-C(11)	117.07(8)
N(10)-C(11)-C(16)	121.92(9)
N(10)-C(11)-C(12)	119.40(9)
C(16)-C(11)-C(12)	118.68(9)
C(13)-C(12)-C(11)	121.08(9)
C(12)-C(13)-C(14)	118.34(9)
C(12)-C(13)-C(20)	120.80(9)
C(14)-C(13)-C(20)	120.85(9)
C(15)-C(14)-C(13)	121.81(10)
C(16)-C(15)-C(14)	118.40(9)
O(17)-C(16)-C(15)	117.82(9)
O(17)-C(16)-C(11)	120.53(9)
C(15)-C(16)-C(11)	121.65(9)
C(18)-O(17)-C(16)	118.36(8)
C(19)-C(18)-O(17)	118.11(9)
C(19)-C(18)-C(9)	123.38(9)
O(17)-C(18)-C(9)	118.51(8)
C(18)-C(19)-C(2)	120.97(9)

Table S2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2B**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
O(1)	9532(1)	15519(2)	1964(1)	17(1)
C(2)	8909(1)	14203(2)	1518(1)	12(1)
C(3)	7798(1)	14974(2)	1370(1)	11(1)
C(4)	7443(1)	17076(2)	1778(1)	13(1)
C(5)	6410(1)	17805(2)	1650(1)	14(1)
C(6)	5721(1)	16450(2)	1110(1)	14(1)
C(7)	6064(1)	14357(2)	702(1)	13(1)
C(8)	7105(1)	13614(2)	826(1)	10(1)
C(9)	7474(1)	11432(2)	391(1)	10(1)
N(10)	6844(1)	10356(2)	-147(1)	11(1)
C(11)	7239(1)	8298(2)	-541(1)	11(1)
C(12)	6611(1)	7187(2)	-1148(1)	12(1)
C(13)	6978(1)	5132(2)	-1556(1)	13(1)
C(14)	7991(1)	4162(2)	-1339(1)	14(1)
C(15)	8629(1)	5209(2)	-736(1)	13(1)
C(16)	8247(1)	7304(2)	-350(1)	11(1)
O(17)	8901(1)	8409(2)	231(1)	12(1)
C(18)	8552(1)	10588(2)	592(1)	10(1)
C(19)	9224(1)	11840(2)	1122(1)	12(1)
C(20)	6299(1)	3956(3)	-2210(1)	17(1)

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	16(1)	17(1)	15(1)	-2(1)	-3(1)	-2(1)
C(2)	12(1)	11(1)	10(1)	3(1)	-1(1)	-2(1)
C(3)	12(1)	10(1)	10(1)	2(1)	0(1)	-1(1)
C(4)	16(1)	12(1)	10(1)	0(1)	1(1)	-1(1)
C(5)	17(1)	12(1)	13(1)	0(1)	4(1)	1(1)
C(6)	13(1)	14(1)	16(1)	1(1)	3(1)	2(1)
C(7)	11(1)	13(1)	13(1)	0(1)	1(1)	0(1)
C(8)	11(1)	9(1)	10(1)	1(1)	1(1)	0(1)
C(9)	10(1)	9(1)	10(1)	2(1)	1(1)	0(1)
N(10)	11(1)	10(1)	11(1)	0(1)	1(1)	0(1)
C(11)	11(1)	10(1)	11(1)	1(1)	2(1)	0(1)
C(12)	12(1)	12(1)	12(1)	1(1)	0(1)	0(1)
C(13)	15(1)	12(1)	11(1)	1(1)	2(1)	-2(1)
C(14)	16(1)	12(1)	13(1)	-1(1)	5(1)	0(1)
C(15)	12(1)	13(1)	15(1)	1(1)	3(1)	1(1)
C(16)	11(1)	11(1)	11(1)	1(1)	1(1)	-1(1)
O(17)	9(1)	13(1)	13(1)	-2(1)	-1(1)	2(1)
C(18)	10(1)	9(1)	11(1)	2(1)	2(1)	1(1)
C(19)	9(1)	12(1)	14(1)	1(1)	-1(1)	0(1)
C(20)	20(1)	18(1)	12(1)	-3(1)	0(1)	-1(1)

Table S4 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)

For **2B**

	x	y	z	U(eq)
H(4)	7912	18006	2143	16
H(5)	6171	19224	1930	17
H(6)	5015	16963	1020	17
H(7)	5591	13429	338	15
H(12)	5922	7848	-1284	14
H(14)	8248	2750	-1611	17
H(15)	9311	4507	-591	16
H(19)	9913	11164	1236	15
H(20A)	5967	2183	-2097	26
H(20B)	6716	3537	-2560	26
H(20C)	5772	5382	-2400	26

Table S5 Bond lengths [Å] and angles [°] for 3B

C(1)-C(2)	1.374(2)
C(1)-C(12B)	1.395(2)
C(1)-H(1)	0.968(17)
C(2)-C(3)	1.381(2)
C(2)-H(2)	0.976(18)
C(3)-C(4)	1.380(2)
C(3)-H(3)	0.979(18)
C(4)-C(4A)	1.388(2)
C(4)-H(4)	0.989(18)
C(4A)-C(12B)	1.404(2)
C(4A)-C(5)	1.486(2)
C(5)-O(5)	1.2350(18)
C(5)-C(6)	1.440(2)
C(6)-C(6A)	1.343(2)
C(6)-H(6)	0.949(17)
C(6A)-O(7)	1.3605(18)
C(6A)-C(12A)	1.462(2)
C(7)-C(8)	1.373(2)
C(7)-O(7)	1.3802(18)
C(7)-C(11A)	1.393(2)
C(8)-C(9)	1.374(2)
C(8)-H(8)	0.926(16)
C(9)-C(10)	1.385(2)
C(9)-H(9)	0.965(16)
C(10)-C(11)	1.370(2)
C(10)-H(10)	0.961(19)
C(11)-C(11A)	1.396(2)
C(11)-H(11)	0.982(17)
C(11A)-N(12)	1.3928(19)
C(12A)-N(12)	1.2988(18)
C(12A)-C(12B)	1.460(2)
C(2)-C(1)-C(12B)	120.43(15)
C(2)-C(1)-H(1)	122.5(10)

C(12B)-C(1)-H(1)	117.0(10)
C(1)-C(2)-C(3)	120.55(16)
C(1)-C(2)-H(2)	119.3(11)
C(3)-C(2)-H(2)	120.2(11)
C(4)-C(3)-C(2)	119.83(16)
C(4)-C(3)-H(3)	120.9(10)
C(2)-C(3)-H(3)	119.3(10)
C(3)-C(4)-C(4A)	120.56(17)
C(3)-C(4)-H(4)	121.2(10)
C(4A)-C(4)-H(4)	118.3(10)
C(4)-C(4A)-C(12B)	119.59(15)
C(4)-C(4A)-C(5)	120.12(15)
C(12B)-C(4A)-C(5)	120.28(14)
O(5)-C(5)-C(6)	121.29(15)
O(5)-C(5)-C(4A)	121.00(15)
C(6)-C(5)-C(4A)	117.70(14)
C(6A)-C(6)-C(5)	121.34(15)
C(6A)-C(6)-H(6)	120.9(10)
C(5)-C(6)-H(6)	117.8(10)
C(6)-C(6A)-O(7)	118.38(13)
C(6)-C(6A)-C(12A)	123.27(14)
O(7)-C(6A)-C(12A)	118.35(13)
C(8)-C(7)-O(7)	117.88(14)
C(8)-C(7)-C(11A)	122.14(15)
O(7)-C(7)-C(11A)	119.98(13)
C(6A)-O(7)-C(7)	119.23(12)
C(7)-C(8)-C(9)	118.44(16)
C(7)-C(8)-H(8)	118.4(10)
C(9)-C(8)-H(8)	123.1(10)
C(8)-C(9)-C(10)	120.90(17)
C(8)-C(9)-H(9)	118.7(9)
C(10)-C(9)-H(9)	120.4(9)
C(11)-C(10)-C(9)	120.34(17)
C(11)-C(10)-H(10)	120.0(11)
C(9)-C(10)-H(10)	119.6(11)
C(10)-C(11)-C(11A)	120.02(16)

C(10)-C(11)-H(11)	120.8(9)
C(11A)-C(11)-H(11)	119.2(9)
N(12)-C(11A)-C(7)	121.82(13)
N(12)-C(11A)-C(11)	120.02(14)
C(7)-C(11A)-C(11)	118.15(14)
N(12)-C(12A)-C(12B)	120.14(13)
N(12)-C(12A)-C(6A)	123.00(13)
C(12B)-C(12A)-C(6A)	116.86(13)
C(1)-C(12B)-C(4A)	119.04(14)
C(1)-C(12B)-C(12A)	120.46(14)
C(4A)-C(12B)-C(12A)	120.50(13)
C(12A)-N(12)-C(11A)	117.62(12)

Table S5 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3B**, U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	327(4)	1434(1)	5992(1)	42(1)
C(2)	998(5)	1993(1)	5722(2)	48(1)
C(3)	2800(4)	2349(1)	6453(1)	48(1)
C(4)	3934(4)	2143(1)	7463(2)	46(1)
C(4A)	3293(4)	1580(1)	7752(1)	38(1)
C(5)	4608(4)	1358(1)	8831(1)	44(1)
O(5)	6279(4)	1668(1)	9485(1)	65(1)
C(6)	3902(4)	769(1)	9081(1)	42(1)
C(6A)	2051(4)	433(1)	8375(1)	36(1)
C(7)	-501(4)	-468(1)	7959(1)	36(1)
O(7)	1370(3)	-114(1)	8677(1)	43(1)
C(8)	-1112(4)	-1019(1)	8283(1)	42(1)
C(9)	-2961(4)	-1376(1)	7574(2)	46(1)
C(10)	-4169(5)	-1185(1)	6554(2)	48(1)
C(11)	-3559(4)	-633(1)	6238(1)	44(1)
C(11A)	-1699(4)	-261(1)	6943(1)	36(1)
C(12A)	714(4)	627(1)	7301(1)	34(1)
C(12B)	1450(4)	1219(1)	7010(1)	35(1)
N(12)	-1070(3)	300(1)	6621(1)	38(1)

Table S6 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3B**, The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	46(1)	42(1)	38(1)	1(1)	-4(1)	0(1)
C(2)	54(1)	48(1)	41(1)	8(1)	-1(1)	2(1)
C(3)	52(1)	39(1)	53(1)	3(1)	5(1)	1(1)
C(4)	51(1)	42(1)	46(1)	-7(1)	3(1)	-3(1)
C(4A)	39(1)	39(1)	35(1)	-4(1)	2(1)	4(1)
C(5)	45(1)	47(1)	38(1)	-8(1)	-2(1)	2(1)
O(5)	87(1)	57(1)	48(1)	-6(1)	-20(1)	-14(1)
C(6)	48(1)	46(1)	30(1)	0(1)	-3(1)	4(1)
C(6A)	38(1)	37(1)	33(1)	0(1)	3(1)	7(1)
C(7)	36(1)	37(1)	36(1)	-4(1)	3(1)	5(1)
O(7)	55(1)	38(1)	35(1)	2(1)	-5(1)	1(1)
C(8)	46(1)	42(1)	39(1)	5(1)	4(1)	6(1)
C(9)	45(1)	36(1)	56(1)	1(1)	6(1)	1(1)
C(10)	48(1)	43(1)	53(1)	-4(1)	-4(1)	-3(1)
C(11)	47(1)	44(1)	41(1)	0(1)	-4(1)	1(1)
C(11A)	36(1)	37(1)	37(1)	-1(1)	2(1)	4(1)
C(12A)	32(1)	37(1)	31(1)	-3(1)	1(1)	7(1)
C(12B)	34(1)	37(1)	33(1)	-2(1)	4(1)	6(1)
N(12)	43(1)	37(1)	34(1)	0(1)	-1(1)	2(1)

Table S7 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3B**

	x	y	z	U(eq)
H(1)	-940(40)	1175(7)	5500(13)	49(5)
H(2)	210(40)	2135(8)	5003(15)	62(5)
H(3)	3280(40)	2744(8)	6241(13)	54(5)
H(4)	5220(40)	2391(7)	8000(14)	56(5)
H(6)	4750(40)	626(7)	9769(14)	45(5)
H(8)	-200(40)	-1137(7)	8959(13)	45(5)
H(9)	-3420(40)	-1763(7)	7801(12)	46(4)
H(10)	-5510(50)	-1439(8)	6077(14)	62(5)
H(11)	-4400(40)	-496(7)	5515(15)	54(5)

Table S8 Torsion angles [°] for **3B**

C(12B)-C(1)-C(2)-C(3)	0.2(3)
C(1)-C(2)-C(3)-C(4)	-0.1(3)
C(2)-C(3)-C(4)-C(4A)	0.3(3)
C(3)-C(4)-C(4A)-C(12B)	-0.5(2)
C(3)-C(4)-C(4A)-C(5)	178.32(14)
C(4)-C(4A)-C(5)-O(5)	0.0(2)
C(12B)-C(4A)-C(5)-O(5)	178.85(15)
C(4)-C(4A)-C(5)-C(6)	-179.25(15)
C(12B)-C(4A)-C(5)-C(6)	-0.4(2)
O(5)-C(5)-C(6)-C(6A)	179.22(15)
C(4A)-C(5)-C(6)-C(6A)	-1.5(2)
C(5)-C(6)-C(6A)-O(7)	-177.62(14)
C(5)-C(6)-C(6A)-C(12A)	2.0(2)
C(6)-C(6A)-O(7)-C(7)	-179.40(13)
C(12A)-C(6A)-O(7)-C(7)	1.0(2)
C(8)-C(7)-O(7)-C(6A)	179.24(13)
C(11A)-C(7)-O(7)-C(6A)	-0.7(2)
O(7)-C(7)-C(8)-C(9)	-179.77(13)
C(11A)-C(7)-C(8)-C(9)	0.2(2)
C(7)-C(8)-C(9)-C(10)	0.3(2)
C(8)-C(9)-C(10)-C(11)	-0.5(3)
C(9)-C(10)-C(11)-C(11A)	0.2(3)
C(8)-C(7)-C(11A)-N(12)	179.98(14)
O(7)-C(7)-C(11A)-N(12)	-0.1(2)
C(8)-C(7)-C(11A)-C(11)	-0.4(2)
O(7)-C(7)-C(11A)-C(11)	179.51(13)
C(10)-C(11)-C(11A)-N(12)	179.82(15)
C(10)-C(11)-C(11A)-C(7)	0.2(2)
C(6)-C(6A)-C(12A)-N(12)	179.89(14)
O(7)-C(6A)-C(12A)-N(12)	-0.5(2)
C(6)-C(6A)-C(12A)-C(12B)	-0.5(2)
O(7)-C(6A)-C(12A)-C(12B)	179.11(12)
C(2)-C(1)-C(12B)-C(4A)	-0.4(2)
C(2)-C(1)-C(12B)-C(12A)	179.48(15)

C(4)-C(4A)-C(12B)-C(1)	0.6(2)
C(5)-C(4A)-C(12B)-C(1)	-178.27(14)
C(4)-C(4A)-C(12B)-C(12A)	-179.30(14)
C(5)-C(4A)-C(12B)-C(12A)	1.9(2)
N(12)-C(12A)-C(12B)-C(1)	-1.7(2)
C(6A)-C(12A)-C(12B)-C(1)	178.69(13)
N(12)-C(12A)-C(12B)-C(4A)	178.17(13)
C(6A)-C(12A)-C(12B)-C(4A)	-1.4(2)
C(12B)-C(12A)-N(12)-C(11A)	-179.86(13)
C(6A)-C(12A)-N(12)-C(11A)	-0.3(2)
C(7)-C(11A)-N(12)-C(12A)	0.6(2)
C(11)-C(11A)-N(12)-C(12A)	-179.02(14)

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