Supplementary Materials

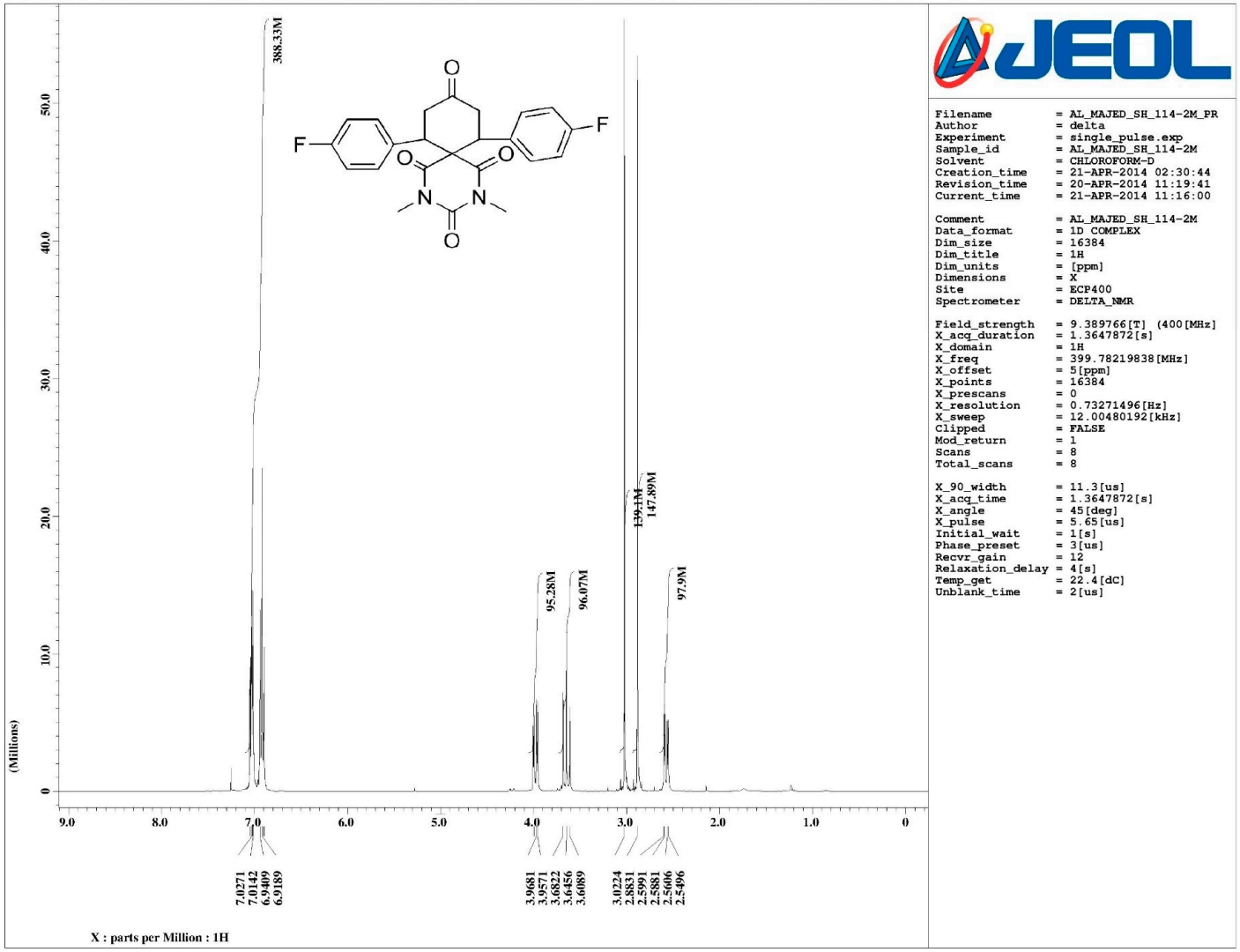

Figure S1. ^{1}H-NMR spectrum of compound **3a**.

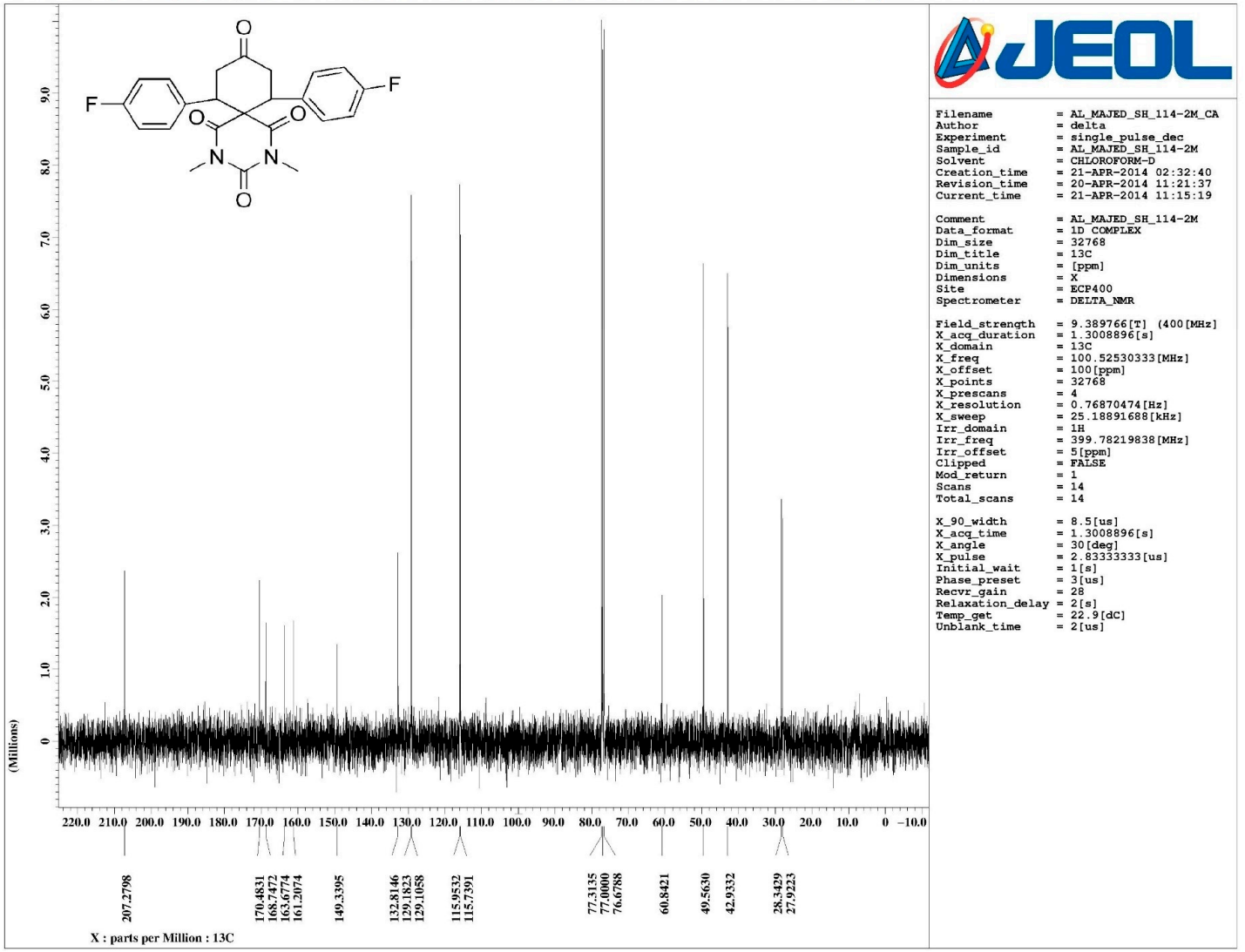

Figure S2. ^{13}C-NMR spectrum of compound **3a**.

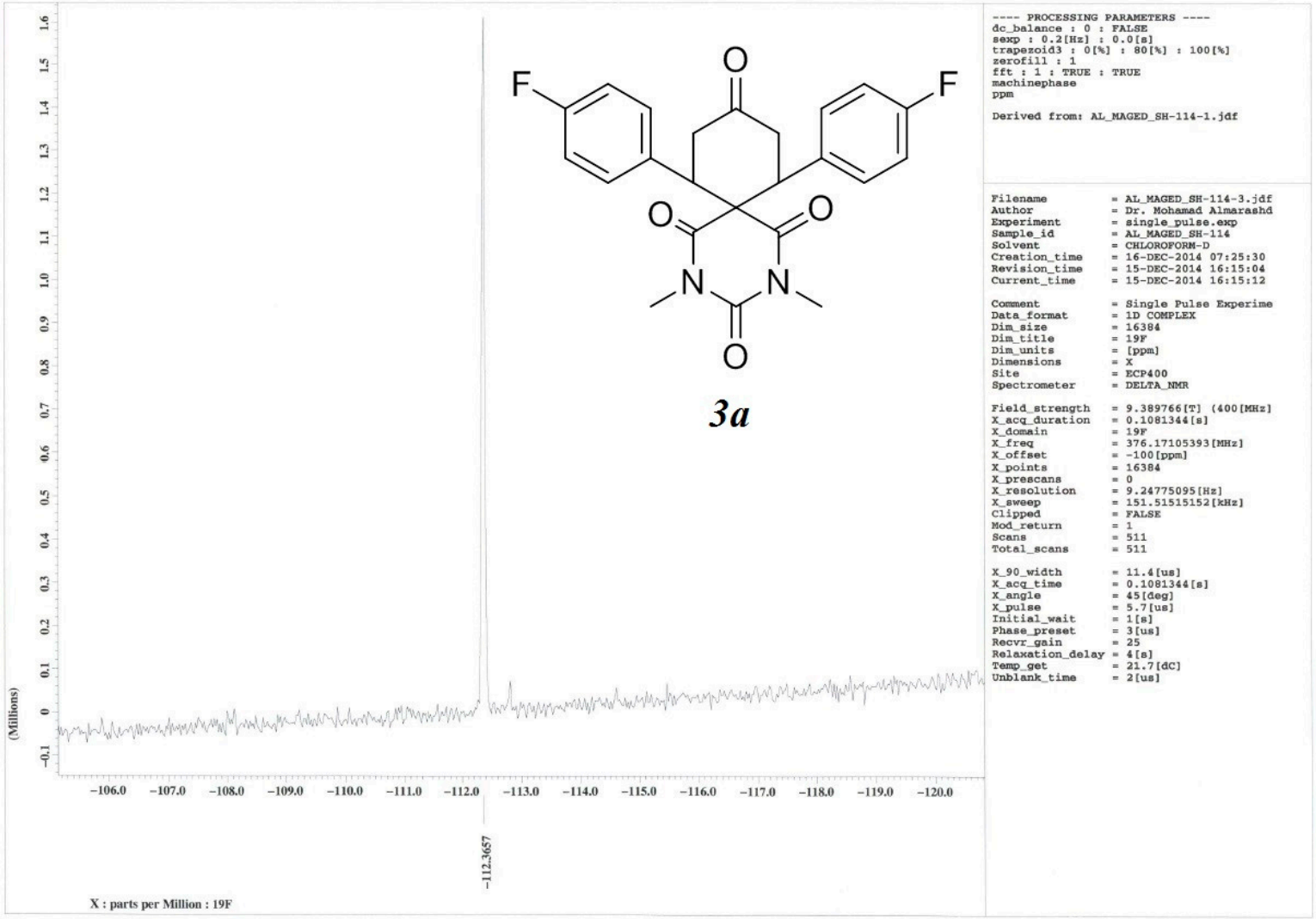

Figure S3. ^{19}F-NMR spectrum of compound **3a**.

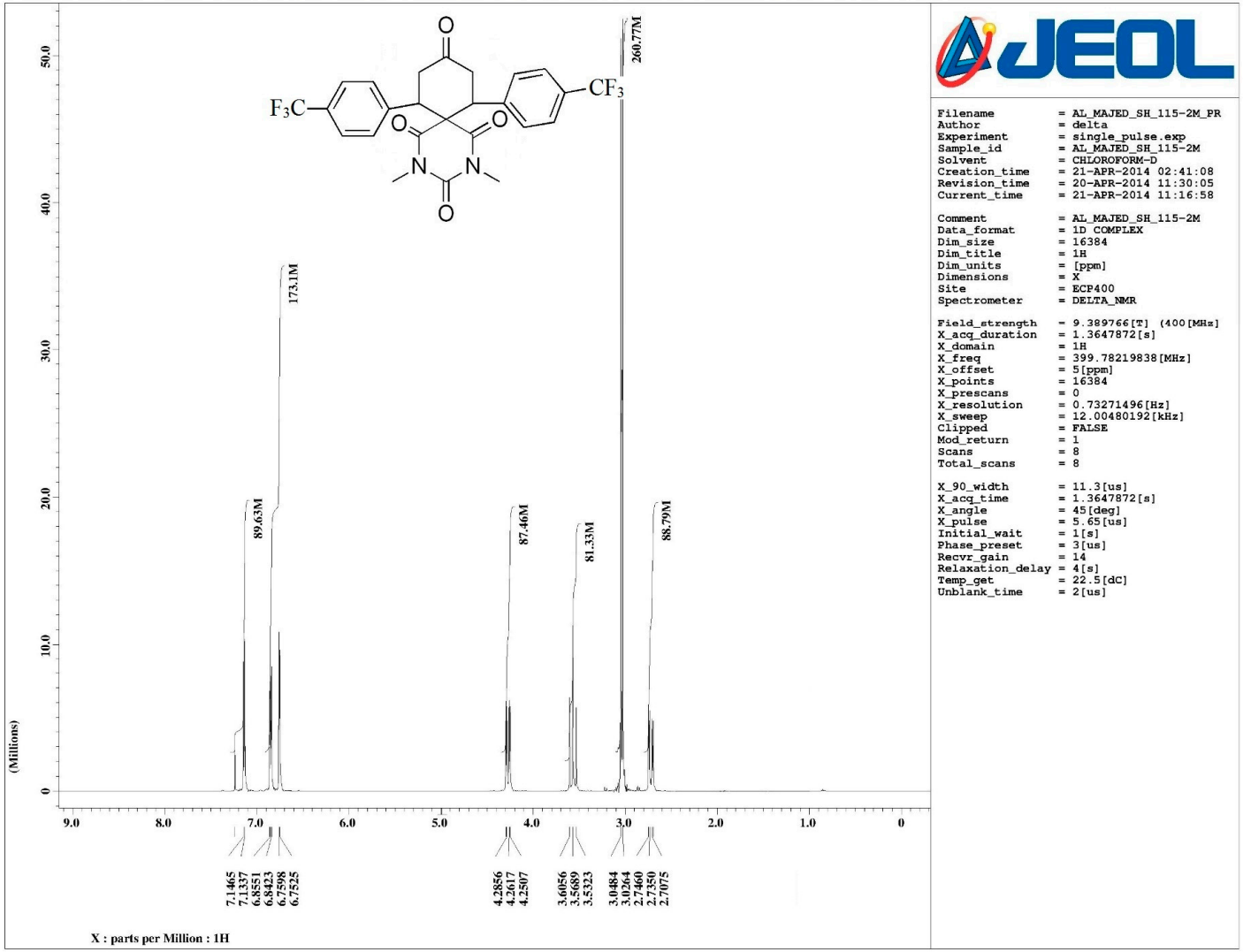

Figure S4. ^{1}H-NMR spectrum of compound **3b**.

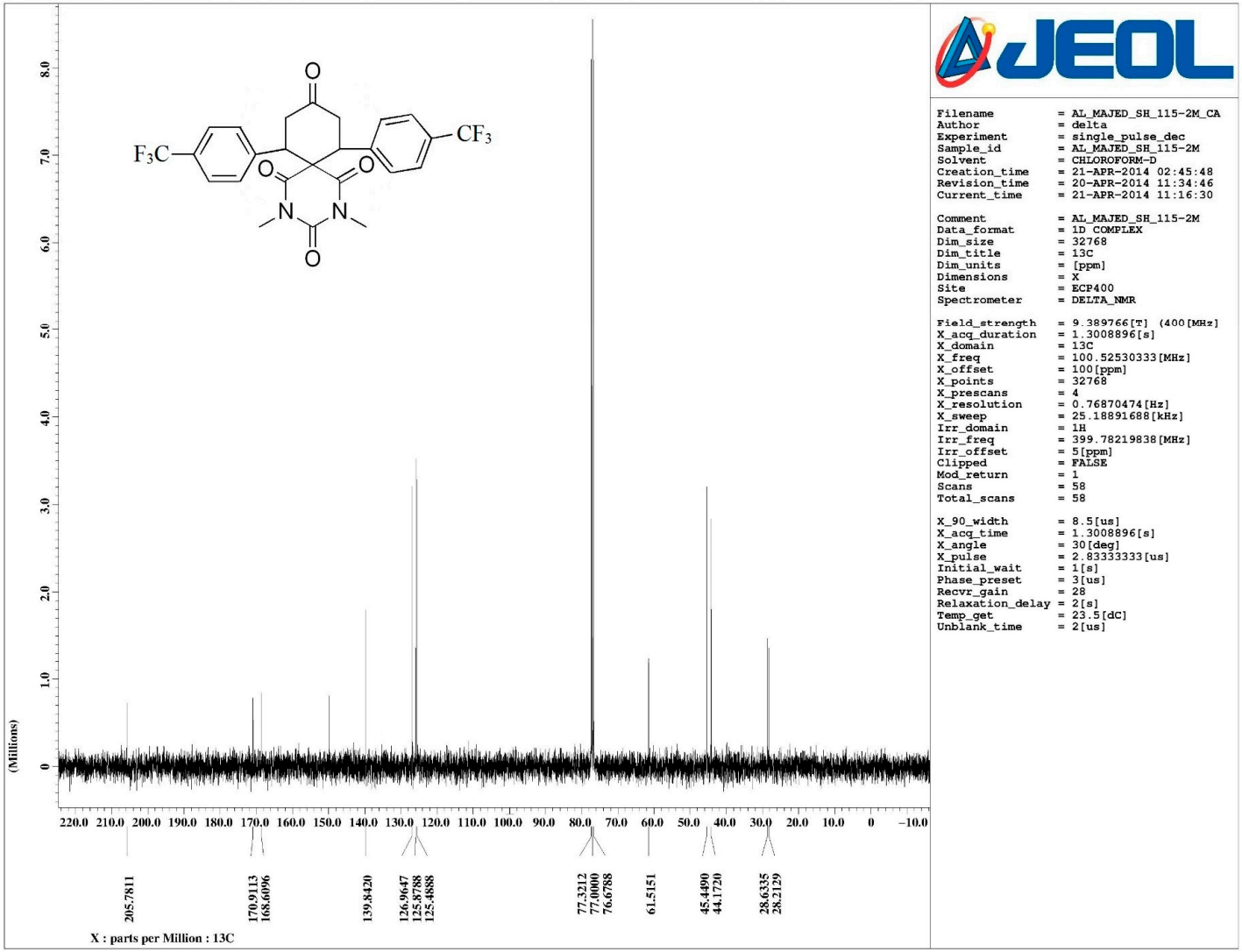

Figure S5. ^{13}C-NMR spectrum of compound **3b**.

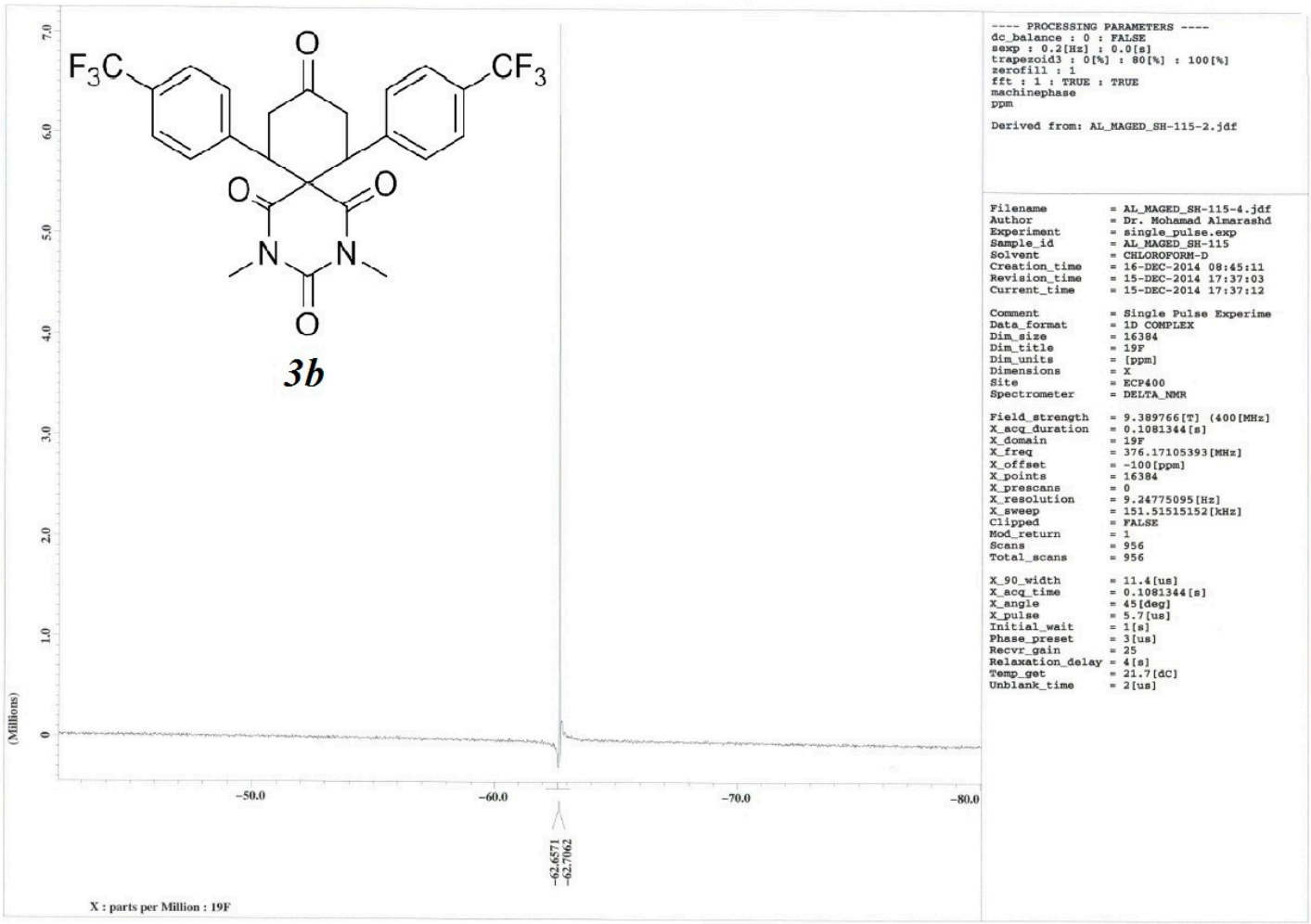

Figure S6. ^{19}F-NMR spectrum of compound **3b**.

Table S1. Geometric parameters (Å, °) of **3a**.

F1-C3	1.3604 (15)	C8-C13	1.5192 (17)
F2-C19	1.3656 (17)	C8-C9	1.5666 (17)
O1-C13	1.2167 (16)	C9-C16	1.5256 (18)
O2-C14	1.2099 (17)	C9-C10	1.5333 (18)
O3-C15	1.2176 (16)	C9-H9A	0.9800
O4-C11	1.2098 (17)	C10-C11	1.506 (2)
N1-C13	1.3770 (16)	C10-H10A	0.9700
N1-C14	1.3898 (17)	C10-H10B	0.9700
N1-C23	1.4691 (18)	C11-C12	1.5076 (19)
N2-C15	1.3793 (17)	C12-H12A	0.9700
N2-C14	1.3856 (18)	C12-H12B	0.9700
N2-C24	1.4710 (17)	C16-C21	1.3922 (19)
C1-C2	1.3835 (19)	C16-C17	1.393 (2)
C1-C6	1.3937 (19)	C17-C18	1.391 (2)
C1-H1A	0.9300	C17-H17A	0.9300
C2-C3	1.3763 (19)	C18-C19	1.370 (3)
C2-H2A	0.9300	C18-H18A	0.9300
C3-C4	1.376 (2)	C19-C20	1.374 (2)
C4-C5	1.3940 (19)	C20-C21	1.395 (2)
C4-H4A	0.9300	C20-H20A	0.9300
C5-C6	1.3967 (18)	C21-H21A	0.9300
C5-H5A	0.9300	C23-H23A	0.9600
C6-C7	1.5210 (17)	C23-H23B	0.9600
C7-C12	1.5311 (18)	C23-H23C	0.9600
C7-C8	1.5799 (18)	C24-H24A	0.9600
C7-H7A	0.9800	C24-H24B	0.9600
C8-C15	1.5134 (18)	C24-H24C	0.9600
C13-N1-C14	125.26 (11)	O4-C11-C10	121.76 (13)
C13-N1-C23	118.08 (12)	O4-C11-C12	121.27 (13)
C14-N1-C23	116.56 (12)	C10-C11-C12	116.79 (12)
C15-N2-C14	124.96 (11)	C11-C12-C7	113.55 (11)
C15-N2-C24	117.62 (12)	C11-C12-H12A	108.9
C14-N2-C24	117.34 (12)	C7-C12-H12A	108.9
C2-C1-C6	121.19 (12)	C11-C12-H12B	108.9
C2-C1-H1A	119.4	C7-C12-H12B	108.9
C6-C1-H1A	119.4	H12A-C12-H12B	107.7
C3-C2-C1	118.23 (12)	O1-C13-N1	120.43 (12)
C3-C2-H2A	120.9	O1-C13-C8	120.88 (11)
C1-C2-H2A	120.9	N1-C13-C8	118.65 (11)
F1-C3-C2	118.33 (12)	O2-C14-N2	121.67 (13)
F1-C3-C4	118.43 (12)	O2-C14-N1	121.09 (13)
C2-C3-C4	123.24 (12)	N2-C14-N1	117.23 (11)
C3-C4-C5	117.53 (12)	O3-C15-N2	120.23 (12)

Table S1. *Cont.*

C3-C4-H4A	121.2	O3-C15-C8	120.68 (12)
C5-C4-H4A	121.2	N2-C15-C8	119.04 (11)
C4-C5-C6	121.32 (12)	C21-C16-C17	118.13 (13)
C4-C5-H5A	119.3	C21-C16-C9	119.20 (12)
C6-C5-H5A	119.3	C17-C16-C9	122.65 (12)
C1-C6-C5	118.48 (12)	C18-C17-C16	121.03 (15)
C1-C6-C7	119.08 (12)	C18-C17-H17A	119.5
C5-C6-C7	122.41 (12)	C16-C17-H17A	119.5
C6-C7-C12	112.60 (11)	C19-C18-C17	118.61 (15)
C6-C7-C8	111.27 (10)	C19-C18-H18A	120.7
C12-C7-C8	112.71 (11)	C17-C18-H18A	120.7
C6-C7-H7A	106.6	F2-C19-C18	118.73 (15)
C12-C7-H7A	106.6	F2-C19-C20	118.49 (15)
C8-C7-H7A	106.6	C18-C19-C20	122.77 (14)
C15-C8-C13	114.46 (10)	C19-C20-C21	117.77 (15)
C15-C8-C9	111.40 (10)	C19-C20-H20A	121.1
C13-C8-C9	107.57 (10)	C21-C20-H20A	121.1
C15-C8-C7	109.94 (10)	C16-C21-C20	121.66 (14)
C13-C8-C7	104.36 (10)	C16-C21-H21A	119.2
C9-C8-C7	108.76 (10)	C20-C21-H21A	119.2
C16-C9-C10	112.42 (11)	N1-C23-H23A	109.5
C16-C9-C8	112.26 (10)	N1-C23-H23B	109.5
C10-C9-C8	112.78 (10)	H23A-C23-H23B	109.5
C16-C9-H9A	106.3	N1-C23-H23C	109.5
C10-C9-H9A	106.3	H23A-C23-H23C	109.5
C8-C9-H9A	106.3	H23B-C23-H23C	109.5
C11-C10-C9	114.33 (11)	N2-C24-H24A	109.5
C11-C10-H10A	108.7	N2-C24-H24B	109.5
C9-C10-H10A	108.7	H24A-C24-H24B	109.5
C11-C10-H10B	108.7	N2-C24-H24C	109.5
C9-C10-H10B	108.7	H24A-C24-H24C	109.5
H10A-C10-H10B	107.6	H24B-C24-H24C	109.5
C6-C1-C2-C3	−0.1 (2)	C15-C8-C13-O1	−176.12 (12)
C1-C2-C3-F1	179.47 (12)	C9-C8-C13-O1	−51.76 (16)
C1-C2-C3-C4	−0.2 (2)	C7-C8-C13-O1	63.66 (15)
F1-C3-C4-C5	−179.25 (12)	C15-C8-C13-N1	5.85 (17)
C2-C3-C4-C5	0.4 (2)	C9-C8-C13-N1	130.22 (12)
C3-C4-C5-C6	−0.3 (2)	C7-C8-C13-N1	−114.37 (12)
C2-C1-C6-C5	0.2 (2)	C15-N2-C14-O2	−178.48 (13)
C2-C1-C6-C7	178.24 (12)	C24-N2-C14-O2	−1.8 (2)
C4-C5-C6-C1	0.0 (2)	C15-N2-C14-N1	2.42 (19)
C4-C5-C6-C7	−177.95 (12)	C24-N2-C14-N1	179.10 (12)
C1-C6-C7-C12	134.22 (13)	C13-N1-C14-O2	177.61 (13)

Table S1. *Cont.*

C5-C6-C7-C12	−47.84 (17)	C23-N1-C14-O2	1.5 (2)
C1-C6-C7-C8	−98.13 (14)	C13-N1-C14-N2	−3.3 (2)
C5-C6-C7-C8	79.81 (15)	C23-N1-C14-N2	−179.42 (13)
C6-C7-C8-C15	−60.41 (13)	C14-N2-C15-O3	−179.81 (13)
C12-C7-C8-C15	67.19 (14)	C24-N2-C15-O3	3.52 (19)
C6-C7-C8-C13	62.79 (13)	C14-N2-C15-C8	2.71 (19)
C12-C7-C8-C13	−169.61 (11)	C24-N2-C15-C8	−173.97 (12)
C6-C7-C8-C9	177.37 (10)	C13-C8-C15-O3	175.90 (12)
C12-C7-C8-C9	−55.03 (14)	C9-C8-C15-O3	53.60 (16)
C15-C8-C9-C16	60.96 (14)	C7-C8-C15-O3	−67.04 (15)
C13-C8-C9-C16	−65.24 (13)	C13-C8-C15-N2	−6.62 (17)
C7-C8-C9-C16	−177.71 (10)	C9-C8-C15-N2	−128.92 (12)
C15-C8-C9-C10	−67.26 (14)	C7-C8-C15-N2	110.44 (13)
C13-C8-C9-C10	166.54 (11)	C10-C9-C16-C21	−145.41 (13)
C7-C8-C9-C10	54.07 (14)	C8-C9-C16-C21	86.18 (15)
C16-C9-C10-C11	−176.88 (11)	C10-C9-C16-C17	32.76 (17)
C8-C9-C10-C11	−48.74 (15)	C8-C9-C16-C17	−95.65 (15)
C9-C10-C11-O4	−141.89 (15)	C21-C16-C17-C18	−1.3 (2)
C9-C10-C11-C12	43.01 (17)	C9-C16-C17-C18	−179.44 (14)
O4-C11-C12-C7	141.24 (15)	C16-C17-C18-C19	−0.1 (3)
C10-C11-C12-C7	−43.63 (18)	C17-C18-C19-F2	−179.47 (15)
C6-C7-C12-C11	176.94 (12)	C17-C18-C19-C20	1.2 (3)
C8-C7-C12-C11	50.05 (16)	F2-C19-C20-C21	179.75 (15)
C14-N1-C13-O1	−179.11 (13)	C18-C19-C20-C21	−0.9 (3)
C23-N1-C13-O1	−3.0 (2)	C17-C16-C21-C20	1.5 (2)
C14-N1-C13-C8	−1.1 (2)	C9-C16-C21-C20	179.80 (14)
C23-N1-C13-C8	175.00 (13)	C19-C20-C21-C16	−0.5 (2)

Table S2. Geometric parameters (Å, °) of **3b** (full molecule disorder).

F1X-C22X	1.343 (7)	F1Y-C22Y	1.330 (15)
F2X-C22X	1.344 (7)	F2Y-C22Y	1.318 (16)
F3X-C22X	1.311 (8)	F3Y-C22Y	1.278 (15)
F4X-C25X	1.346 (8)	F4Y-C25Y	1.345 (16)
F5X-C25X	1.371 (8)	F5Y-C25Y	1.381 (15)
F6X-C25X	1.340 (7)	F6Y-C25Y	1.325 (15)
N1X-C13X	1.384 (8)	N1Y-C14Y	1.385 (16)
N1X-C14X	1.385 (9)	N1Y-C13Y	1.393 (15)
N1X-C23X	1.468 (7)	N1Y-C23Y	1.469 (16)
N2X-C15X	1.350 (8)	N2Y-C15Y	1.345 (14)
N2X-C14X	1.377 (9)	N2Y-C14Y	1.377 (15)
N2X-C24X	1.499 (9)	N2Y-C24Y	1.504 (15)
O1X-C13X	1.223 (6)	O1Y-C13Y	1.222 (15)
O2X-C14X	1.217 (7)	O2Y-C14Y	1.214 (13)
O3X-C15X	1.210 (7)	O3Y-C15Y	1.224 (14)
O4X-C11X	1.200 (6)	O4Y-C11Y	1.198 (13)

Table S2. *Cont.*

C1X-C6X	1.381 (7)	C1Y-C2Y	1.3900
C1X-C2X	1.403 (6)	C1Y-C6Y	1.3900
C1X-H1XA	0.9300	C1Y-H1YA	0.9300
C2X-C3X	1.394 (7)	C2Y-C3Y	1.3900
C2X-H2XA	0.9300	C2Y-H2YA	0.9300
C3X-C4X	1.374 (7)	C3Y-C4Y	1.3900
C3X-C22X	1.474 (8)	C3Y-C22Y	1.454 (14)
C4X-C5X	1.382 (6)	C4Y-C5Y	1.3900
C4X-H4XA	0.9300	C4Y-H4YA	0.9300
C5X-C6X	1.396 (7)	C5Y-C6Y	1.3900
C5X-H5XA	0.9300	C5Y-H5YA	0.9300
C6X-C7X	1.532 (6)	C6Y-C7Y	1.515 (11)
C7X-C12X	1.543 (7)	C7Y-C12Y	1.548 (13)
C7X-C8X	1.552 (7)	C7Y-C8Y	1.560 (14)
C7X-H7XA	0.9800	C7Y-H7YA	0.9800
C8X-C13X	1.510 (7)	C8Y-C13Y	1.512 (14)
C8X-C15X	1.539 (8)	C8Y-C15Y	1.542 (13)
C8X-C9X	1.590 (7)	C8Y-C9Y	1.573 (13)
C9X-C16X	1.525 (7)	C9Y-C10Y	1.520 (14)
C9X-C10X	1.529 (7)	C9Y-C16Y	1.525 (12)
C9X-H9XA	0.9800	C9Y-H9YA	0.9800
C10X-C11X	1.495 (7)	C10Y-C11Y	1.504 (14)
C10X-H10A	0.9700	C10Y-H10C	0.9700
C10X-H10B	0.9700	C10Y-H10D	0.9700
C11X-C12X	1.498 (7)	C11Y-C12Y	1.499 (13)
C12X-H12A	0.9700	C12Y-H12C	0.9700
C12X-H12B	0.9700	C12Y-H12D	0.9700
C16X-C21X	1.381 (7)	C16Y-C17Y	1.3900
C16X-C17X	1.387 (7)	C16Y-C21Y	1.3900
C17X-C18X	1.379 (7)	C17Y-C18Y	1.3900
C17X-H17A	0.9300	C17Y-H17B	0.9300
C18X-C19X	1.383 (7)	C18Y-C19Y	1.3900
C18X-H18A	0.9300	C18Y-H18B	0.9300
C19X-C20X	1.390 (6)	C19Y-C20Y	1.3900
C19X-C25X	1.489 (9)	C19Y-C25Y	1.496 (14)
C20X-C21X	1.377 (7)	C20Y-C21Y	1.3900
C20X-H20A	0.9300	C20Y-H20B	0.9300
C21X-H21A	0.9300	C21Y-H21B	0.9300
C23X-H23A	0.9600	C23Y-H23D	0.9600
C23X-H23B	0.9600	C23Y-H23E	0.9600
C23X-H23C	0.9600	C23Y-H23F	0.9600
C24X-H24A	0.9600	C24Y-H24E	0.9600
C24X-H24B	0.9600	C24Y-H24F	0.9600
C24X-H24C	0.9600	C24Y-H24G	0.9600

Table S3. Bond Angles.

3a		3b	
C13X-N1X-C14X	124.3 (5)	C14Y-N1Y-C13Y	124.3 (18)
C13X-N1X-C23X	118.5 (5)	C14Y-N1Y-C23Y	117 (2)
C14X-N1X-C23X	117.1 (5)	C13Y-N1Y-C23Y	117 (2)
C15X-N2X-C14X	126.1 (6)	C15Y-N2Y-C14Y	126.5 (14)
C15X-N2X-C24X	116.2 (6)	C15Y-N2Y-C24Y	116.3 (14)
C14X-N2X-C24X	117.2 (7)	C14Y-N2Y-C24Y	116.9 (14)
C6X-C1X-C2X	120.9 (5)	C2Y-C1Y-C6Y	120.0
C6X-C1X-H1XA	119.6	C2Y-C1Y-H1YA	120.0
C2X-C1X-H1XA	119.6	C6Y-C1Y-H1YA	120.0
C3X-C2X-C1X	120.0 (5)	C1Y-C2Y-C3Y	120.0
C3X-C2X-H2XA	120.0	C1Y-C2Y-H2YA	120.0
C1X-C2X-H2XA	120.0	C3Y-C2Y-H2YA	120.0
C4X-C3X-C2X	119.1 (5)	C4Y-C3Y-C2Y	120.0
C4X-C3X-C22X	117.6 (6)	C4Y-C3Y-C22Y	113.2 (11)
C2X-C3X-C22X	123.3 (5)	C2Y-C3Y-C22Y	126.3 (11)
C3X-C4X-C5X	120.7 (5)	C3Y-C4Y-C5Y	120.0
C3X-C4X-H4XA	119.7	C3Y-C4Y-H4YA	120.0
C5X-C4X-H4XA	119.7	C5Y-C4Y-H4YA	120.0
C4X-C5X-C6X	121.3 (5)	C6Y-C5Y-C4Y	120.0
C4X-C5X-H5XA	119.3	C6Y-C5Y-H5YA	120.0
C6X-C5X-H5XA	119.3	C4Y-C5Y-H5YA	120.0
C1X-C6X-C5X	118.0 (4)	C5Y-C6Y-C1Y	120.0
C1X-C6X-C7X	122.8 (5)	C5Y-C6Y-C7Y	119.4 (10)
C5X-C6X-C7X	119.1 (4)	C1Y-C6Y-C7Y	120.6 (10)
C6X-C7X-C12X	112.4 (4)	C6Y-C7Y-C12Y	111.6 (10)
C6X-C7X-C8X	110.5 (4)	C6Y-C7Y-C8Y	110.4 (11)
C12X-C7X-C8X	114.7 (4)	C12Y-C7Y-C8Y	113.1 (11)
C6X-C7X-H7XA	106.2	C6Y-C7Y-H7YA	107.1
C12X-C7X-H7XA	106.2	C12Y-C7Y-H7YA	107.1
C8X-C7X-H7XA	106.2	C8Y-C7Y-H7YA	107.1
C13X-C8X-C15X	114.1 (4)	C13Y-C8Y-C15Y	113.6 (10)
C13X-C8X-C7X	112.0 (4)	C13Y-C8Y-C7Y	110.7 (15)
C15X-C8X-C7X	109.2 (4)	C15Y-C8Y-C7Y	107.3 (12)
C13X-C8X-C9X	110.2 (4)	C13Y-C8Y-C9Y	111.1 (14)
C15X-C8X-C9X	103.4 (5)	C15Y-C8Y-C9Y	105.1 (12)
C7X-C8X-C9X	107.5 (4)	C7Y-C8Y-C9Y	108.9 (9)
C16X-C9X-C10X	113.2 (4)	C10Y-C9Y-C16Y	114.0 (12)
C16X-C9X-C8X	111.2 (4)	C10Y-C9Y-C8Y	115.6 (12)
C10X-C9X-C8X	111.7 (4)	C16Y-C9Y-C8Y	112.2 (11)
C16X-C9X-H9XA	106.7	C10Y-C9Y-H9YA	104.5
C10X-C9X-H9XA	106.7	C16Y-C9Y-H9YA	104.5
C8X-C9X-H9XA	106.7	C8Y-C9Y-H9YA	104.5
C11X-C10X-C9X	113.3 (4)	C11Y-C10Y-C9Y	112.6 (12)
C11X-C10X-H10A	108.9	C11Y-C10Y-H10C	109.1
C9X-C10X-H10A	108.9	C9Y-C10Y-H10C	109.1

Table S3. *Cont.*

3a		3b	
C11X-C10X-H10B	108.9	C11Y-C10Y-H10D	109.1
C9X-C10X-H10B	108.9	C9Y-C10Y-H10D	109.1
H10A-C10X-H10B	107.7	H10C-C10Y-H10D	107.8
O4X-C11X-C10X	121.2 (5)	O4Y-C11Y-C12Y	122.2 (14)
O4X-C11X-C12X	122.9 (5)	O4Y-C11Y-C10Y	123.7 (14)
C10X-C11X-C12X	115.5 (4)	C12Y-C11Y-C10Y	114.1 (12)
C11X-C12X-C7X	113.6 (4)	C11Y-C12Y-C7Y	112.1 (11)
C11X-C12X-H12A	108.8	C11Y-C12Y-H12C	109.2
C7X-C12X-H12A	108.8	C7Y-C12Y-H12C	109.2
C11X-C12X-H12B	108.8	C11Y-C12Y-H12D	109.2
C7X-C12X-H12B	108.8	C7Y-C12Y-H12D	109.2
H12A-C12X-H12B	107.7	H12C-C12Y-H12D	107.9
O1X-C13X-N1X	119.7 (5)	O1Y-C13Y-N1Y	117.1 (16)
O1X-C13X-C8X	121.6 (5)	O1Y-C13Y-C8Y	123.0 (16)
N1X-C13X-C8X	118.7 (5)	N1Y-C13Y-C8Y	118.1 (14)
O2X-C14X-N2X	121.4 (7)	O2Y-C14Y-N2Y	121.4 (17)
O2X-C14X-N1X	120.9 (6)	O2Y-C14Y-N1Y	121.4 (17)
N2X-C14X-N1X	117.7 (5)	N2Y-C14Y-N1Y	117.2 (12)
O3X-C15X-N2X	121.9 (6)	O3Y-C15Y-N2Y	121.7 (14)
O3X-C15X-C8X	119.8 (5)	O3Y-C15Y-C8Y	119.7 (13)
N2X-C15X-C8X	118.2 (5)	N2Y-C15Y-C8Y	118.5 (13)
C21X-C16X-C17X	117.2 (5)	C17Y-C16Y-C21Y	120.0
C21X-C16X-C9X	121.9 (5)	C17Y-C16Y-C9Y	117.2 (11)
C17X-C16X-C9X	120.9 (5)	C21Y-C16Y-C9Y	122.7 (11)
C18X-C17X-C16X	122.2 (5)	C16Y-C17Y-C18Y	120.0
C18X-C17X-H17A	118.9	C16Y-C17Y-H17B	120.0
C16X-C17X-H17A	118.9	C18Y-C17Y-H17B	120.0
C17X-C18X-C19X	120.1 (5)	C19Y-C18Y-C17Y	120.0
C17X-C18X-H18A	119.9	C19Y-C18Y-H18B	120.0
C19X-C18X-H18A	119.9	C17Y-C18Y-H18B	120.0
C18X-C19X-C20X	118.2 (5)	C18Y-C19Y-C20Y	120.0
C18X-C19X-C25X	119.1 (5)	C18Y-C19Y-C25Y	113.5 (12)
C20X-C19X-C25X	122.7 (5)	C20Y-C19Y-C25Y	126.4 (12)
C21X-C20X-C19X	121.0 (5)	C19Y-C20Y-C21Y	120.0
C21X-C20X-H20A	119.5	C19Y-C20Y-H20B	120.0
C19X-C20X-H20A	119.5	C21Y-C20Y-H20B	120.0
C20X-C21X-C16X	121.4 (5)	C20Y-C21Y-C16Y	120.0
C20X-C21X-H21A	119.3	C20Y-C21Y-H21B	120.0
C16X-C21X-H21A	119.3	C16Y-C21Y-H21B	120.0
F3X-C22X-F1X	107.2 (6)	F3Y-C22Y-F2Y	111.5 (17)
F3X-C22X-F2X	106.6 (5)	F3Y-C22Y-F1Y	113.4 (19)
F1X-C22X-F2X	105.2 (5)	F2Y-C22Y-F1Y	108.3 (17)
F3X-C22X-C3X	113.9 (5)	F3Y-C22Y-C3Y	111.5 (17)
F1X-C22X-C3X	111.5 (5)	F2Y-C22Y-C3Y	108.8 (17)
F2X-C22X-C3X	112.0 (6)	F1Y-C22Y-C3Y	103.0 (15)

Table S3. *Cont.*

3a		3b	
N1X-C23X-H23A	109.5	N1Y-C23Y-H23D	109.5
N1X-C23X-H23B	109.5	N1Y-C23Y-H23E	109.5
H23A-C23X-H23B	109.5	H23D-C23Y-H23E	109.5
N1X-C23X-H23C	109.5	N1Y-C23Y-H23F	109.5
H23A-C23X-H23C	109.5	H23D-C23Y-H23F	109.5
H23B-C23X-H23C	109.5	H23E-C23Y-H23F	109.5
N2X-C24X-H24A	109.5	N2Y-C24Y-H24E	109.5
N2X-C24X-H24B	109.5	N2Y-C24Y-H24F	109.5
H24A-C24X-H24B	109.5	H24E-C24Y-H24F	109.5
N2X-C24X-H24C	109.5	N2Y-C24Y-H24G	109.5
H24A-C24X-H24C	109.5	H24E-C24Y-H24G	109.5
H24B-C24X-H24C	109.5	H24F-C24Y-H24G	109.5
F6X-C25X-F4X	105.8 (6)	F6Y-C25Y-F4Y	108.4 (16)
F6X-C25X-F5X	103.6 (5)	F6Y-C25Y-F5Y	105.1 (16)
F4X-C25X-F5X	102.3 (6)	F4Y-C25Y-F5Y	103.3 (15)
F6X-C25X-C19X	115.9 (6)	F6Y-C25Y-C19Y	115.3 (16)
F4X-C25X-C19X	115.4 (5)	F4Y-C25Y-C19Y	111.1 (16)
F5X-C25X-C19X	112.3 (5)	F5Y-C25Y-C19Y	112.8 (16)

Table S4. Torsion Angles.

3a		3b	
C6X_a-C1X_a-C2X_a-C3X_a	1.1 (9)	C6Y-C1Y-C2Y-C3Y	0.0
C1X-C2X-C3X-C4X	−1.7 (8)	C1Y-C2Y-C3Y-C4Y	0.0
C1X-C2X-C3X-C22X	177.5 (7)	C1Y-C2Y-C3Y-C22Y	−171 (2)
C2X-C3X-C4X-C5X	1.2 (8)	C2Y-C3Y-C4Y-C5Y	0.0
C22X-C3X-C4X-C5X	−178.0 (7)	C22Y-C3Y-C4Y-C5Y	172.2 (19)
C3X-C4X-C5X-C6X	−0.2 (8)	C3Y-C4Y-C5Y-C6Y	0.0
C2X-C1X-C6X-C5X	−0.1 (8)	C4Y-C5Y-C6Y-C1Y	0.0
C2X-C1X-C6X-C7X	−178.2 (6)	C4Y-C5Y-C6Y-C7Y	−179.4 (16)
C4X-C5X-C6X-C1X	−0.3 (7)	C2Y-C1Y-C6Y-C5Y	0.0
C4X-C5X-C6X-C7X	177.8 (5)	C2Y-C1Y-C6Y-C7Y	179.4 (17)
C1X-C6X-C7X-C12X	−42.6 (7)	C5Y-C6Y-C7Y-C12Y	153.7 (13)
C5X-C6X-C7X-C12X	139.4 (5)	C1Y-C6Y-C7Y-C12Y	−25.7 (18)
C1X-C6X-C7X-C8X	86.9 (6)	C5Y-C6Y-C7Y-C8Y	−79.6 (16)
C5X-C6X-C7X-C8X	−91.2 (6)	C1Y-C6Y-C7Y-C8Y	101.1 (14)
C6X-C7X-C8X-C13X	−59.8 (5)	C6Y-C7Y-C8Y-C13Y	−53.7 (16)
C12X-C7X-C8X-C13X	68.5 (5)	C12Y-C7Y-C8Y-C13Y	72.2 (15)
C6X-C7X-C8X-C15X	67.6 (5)	C6Y-C7Y-C8Y-C15Y	70.8 (15)
C12X-C7X-C8X-C15X	−164.2 (5)	C12Y-C7Y-C8Y-C15Y	−163.3 (13)
C6X-C7X-C8X-C9X	179.1 (4)	C6Y-C7Y-C8Y-C9Y	−176.0 (13)
C12X-C7X-C8X-C9X	−52.6 (5)	C12Y-C7Y-C8Y-C9Y	−50.1 (16)
C13X-C8X-C9X-C16X	60.9 (6)	C13Y-C8Y-C9Y-C10Y	−73.5 (17)
C15X-C8X-C9X-C16X	−61.4 (5)	C15Y-C8Y-C9Y-C10Y	163.2 (15)
C7X-C8X-C9X-C16X	−176.8 (4)	C7Y-C8Y-C9Y-C10Y	48.6 (17)
C13X-C8X-C9X-C10X	−66.6 (6)	C13Y-C8Y-C9Y-C16Y	59.5 (18)
C15X-C8X-C9X-C10X	171.0 (5)	C15Y-C8Y-C9Y-C16Y	−63.8 (16)
C7X-C8X-C9X-C10X	55.6 (5)	C7Y-C8Y-C9Y-C16Y	−178.4 (13)
C16X-C9X-C10X-C11X	178.7 (4)	C16Y-C9Y-C10Y-C11Y	178.7 (15)
C8X-C9X-C10X-C11X	−54.8 (6)	C8Y-C9Y-C10Y-C11Y	−49 (2)
C9X-C10X-C11X-O4X	−138.4 (6)	C9Y-C10Y-C11Y-O4Y	−131 (2)
C9X-C10X-C11X-C12X	48.6 (7)	C9Y-C10Y-C11Y-C12Y	51 (2)
O4X-C11X-C12X-C7X	142.9 (6)	O4Y-C11Y-C12Y-C7Y	128 (2)
C10X-C11X-C12X-C7X	−44.3 (7)	C10Y-C11Y-C12Y-C7Y	−53 (2)
C6X-C7X-C12X-C11X	175.3 (4)	C6Y-C7Y-C12Y-C11Y	179.2 (14)
C8X-C7X-C12X-C11X	48.0 (6)	C8Y-C7Y-C12Y-C11Y	53.9 (18)
C14X-N1X-C13X-O1X	176.2 (7)	C14Y-N1Y-C13Y-O1Y	−180 (7)
C23X-N1X-C13X-O1X	−5.7 (8)	C23Y-N1Y-C13Y-O1Y	−13 (10)
C14X-N1X-C13X-C8X	−6.1 (9)	C14Y-N1Y-C13Y-C8Y	15 (11)
C23X-N1X-C13X-C8X	172.0 (5)	C23Y-N1Y-C13Y-C8Y	−179 (6)
C15X-C8X-C13X-O1X	−171.9 (5)	C15Y-C8Y-C13Y-O1Y	−180 (3)
C7X-C8X-C13X-O1X	−47.3 (7)	C7Y-C8Y-C13Y-O1Y	−59 (3)
C9X-C8X-C13X-O1X	72.2 (6)	C9Y-C8Y-C13Y-O1Y	62 (3)
C15X-C8X-C13X-N1X	10.4 (8)	C15Y-C8Y-C13Y-N1Y	−15 (6)
C7X-C8X-C13X-N1X	135.0 (5)	C7Y-C8Y-C13Y-N1Y	106 (5)
C9X-C8X-C13X-N1X	−105.5 (5)	C9Y-C8Y-C13Y-N1Y	−133 (5)
C15X-N2X-C14X-O2X	−177.2 (16)	C15Y-N2Y-C14Y-O2Y	180 (4)
C24X-N2X-C14X-O2X	−6 (3)	C24Y-N2Y-C14Y-O2Y	6 (6)

Table S4. *Cont.*

3a		3b	
C15X-N2X-C14X-N1X	3 (3)	C15Y-N2Y-C14Y-N1Y	−2 (8)
C24X-N2X-C14X-N1X	174.6 (13)	C24Y-N2Y-C14Y-N1Y	−175 (6)
C13X-N1X-C14X-O2X	179.4 (8)	C13Y-N1Y-C14Y-O2Y	172 (7)
C23X-N1X-C14X-O2X	1.3 (12)	C23Y-N1Y-C14Y-O2Y	6 (11)
C13X-N1X-C14X-N2X	−1.0 (17)	C13Y-N1Y-C14Y-N2Y	−6 (12)
C23X-N1X-C14X-N2X	−179.1 (14)	C23Y-N1Y-C14Y-N2Y	−172 (6)
C14X-N2X-C15X-O3X	−179.7 (16)	C14Y-N2Y-C15Y-O3Y	−175 (4)
C24X-N2X-C15X-O3X	9 (2)	C24Y-N2Y-C15Y-O3Y	−2 (4)
C14X-N2X-C15X-C8X	2 (3)	C14Y-N2Y-C15Y-C8Y	0 (5)
C24X-N2X-C15X-C8X	−169.5 (12)	C24Y-N2Y-C15Y-C8Y	173 (2)
C13X-C8X-C15X-O3X	173.2 (6)	C13Y-C8Y-C15Y-O3Y	−176 (2)
C7X-C8X-C15X-O3X	47.1 (8)	C7Y-C8Y-C15Y-O3Y	61 (2)
C9X-C8X-C15X-O3X	−67.1 (8)	C9Y-C8Y-C15Y-O3Y	−54 (2)
C13X-C8X-C15X-N2X	−8.5 (14)	C13Y-C8Y-C15Y-N2Y	8 (3)
C7X-C8X-C15X-N2X	−134.6 (13)	C7Y-C8Y-C15Y-N2Y	−114 (2)
C9X-C8X-C15X-N2X	111.2 (13)	C9Y-C8Y-C15Y-N2Y	130 (2)
C10X-C9X-C16X-C21X	50.5 (7)	C10Y-C9Y-C16Y-C17Y	−125.9 (17)
C8X-C9X-C16X-C21X	−76.3 (6)	C8Y-C9Y-C16Y-C17Y	100.3 (16)
C10X-C9X-C16X-C17X	−130.8 (5)	C10Y-C9Y-C16Y-C21Y	57 (2)
C8X-C9X-C16X-C17X	102.4 (6)	C8Y-C9Y-C16Y-C21Y	−77.2 (18)
C21X-C16X-C17X-C18X	1.0 (8)	C21Y-C16Y-C17Y-C18Y	0.0
C9X-C16X-C17X-C18X	−177.8 (5)	C9Y-C16Y-C17Y-C18Y	−177.6 (17)
C16X-C17X-C18X-C19X	−0.5 (9)	C16Y-C17Y-C18Y-C19Y	0.0
C17X-C18X-C19X-C20X	−0.4 (8)	C17Y-C18Y-C19Y-C20Y	0.0
C17X-C18X-C19X-C25X	−179.6 (6)	C17Y-C18Y-C19Y-C25Y	176 (2)
C18X-C19X-C20X-C21X	0.8 (8)	C18Y-C19Y-C20Y-C21Y	0.0
C25X-C19X-C20X-C21X	180.0 (6)	C25Y-C19Y-C20Y-C21Y	−175 (3)
C19X-C20X-C21X-C16X	−0.3 (9)	C19Y-C20Y-C21Y-C16Y	0.0
C17X-C16X-C21X-C20X	−0.6 (8)	C17Y-C16Y-C21Y-C20Y	0.0
C9X-C16X-C21X-C20X	178.2 (5)	C9Y-C16Y-C21Y-C20Y	177.5 (18)
C4X-C3X-C22X-F3X	73.4 (7)	C4Y-C3Y-C22Y-F3Y	141.2 (17)
C2X-C3X-C22X-F3X	−105.8 (7)	C2Y-C3Y-C22Y-F3Y	−47 (2)
C4X-C3X-C22X-F1X	−48.0 (8)	C4Y-C3Y-C22Y-F2Y	−95.4 (18)
C2X-C3X-C22X-F1X	132.8 (7)	C2Y-C3Y-C22Y-F2Y	76 (2)
C4X-C3X-C22X-F2X	−165.6 (6)	C4Y-C3Y-C22Y-F1Y	19 (2)
C2X-C3X-C22X-F2X	15.2 (9)	C2Y-C3Y-C22Y-F1Y	−169.0 (15)
C18X-C19X-C25X-F6X	−176.7 (6)	C18Y-C19Y-C25Y-F6Y	165.6 (17)
C20X-C19X-C25X-F6X	4.2 (9)	C20Y-C19Y-C25Y-F6Y	−19 (3)
C18X-C19X-C25X-F4X	−52.3 (8)	C18Y-C19Y-C25Y-F4Y	−71 (2)
C20X-C19X-C25X-F4X	128.6 (7)	C20Y-C19Y-C25Y-F4Y	105 (2)
C18X-C19X-C25X-F5X	64.4 (7)	C18Y-C19Y-C25Y-F5Y	45 (2)
C20X-C19X-C25X-F5X	−114.7 (7)	C20Y-C19Y-C25Y-F5Y	−139.8 (18)

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S5. Hydrogen-bond geometry (Å, °) of **3a**.

D-H···*A*	*D*-H	H···*A*	*D*···*A*	*D*-H···*A*
C2-H2A···O3^{i}	0.9300	2.5700	3.2005 (17)	125.00
C9-H9A···O2^{ii}	0.9800	2.4900	3.2986 (17)	139.00
C21-H21A···O1	0.9300	2.6000	3.2311 (18)	126.00
C24-H24B···F1^{iii}	0.9600	2.5000	3.4021 (19)	156.00
C24-H24C···O4^{iv}	0.9600	2.5300	3.132 (2)	121.00

Symmetry codes: (i) $x, y-1, z$; (ii) $x, -y, z-1/2$; (iii) $-x+1/2, y+1/2, -z+1/2$; (iv) $x, -y+1, z+1/2$

Table S6. Hydrogen-bond geometry (Å, °) of **3b** (full molecule disorder).

D-H···*A*	*D*-H	H···*A*	*D*···*A*	*D*-H···*A*
C4X-H4XA···F5X^{i}	0.9300	2.4800	3.362 (8)	157.00
C10X-H10B···O3X^{ii}	0.9700	2.2300	3.143 (6)	156.00
C23X-H23A···F4X^{iii}	0.9600	2.5300	3.481 (8)	171.00
C23X-H23B···O2X^{iii}	0.9600	2.4700	3.430 (8)	179.00
C24X-H24A···F3X^{iv}	0.9600	2.5200	3.332 (10)	143.00

Symmetry codes: (i) $y, -x+2, -z+1$; (ii) $-y+2, x, -z+1$; (iii) $-y+3/2, -x+3/2, z+1/2$; (iv) $-y+3/2, -x+3/2, z-1/2$.

Table S7. The calculated and experimental geometric parameters of the studied compounds using B3LYP/6-311G(d,p) method.

Parameter [a]	3a					Parameter [a]	3b				
	Calc.	Exp	Parameter [a]	Calc.	Exp		Calc.	Exp	Parameter [a]	Calc.	Exp
R(1-13)	1.350	1.360	A(1-13-11)	119.2	118.3	R(1-30)	1.354	1.343	A(4-47-36)	121.1	120.9
R(2-39)	1.350	1.366	A(1-13-14)	119.1	118.4	R(2-30)	1.352	1.344	A(5-48-34)	121.5	121.9
R(3-31)	1.215	1.217	A(2-39-37)	119.1	118.7	R(3-30)	1.349	1.311	A(5-48-45)	120.0	119.8
R(4-32)	1.209	1.210	A(2-39-40)	119.2	118.5	R(4-21)	1.384	1.384	A(6-18-15)	122.4	122.9
R(5-33)	1.219	1.218	A(3-31-7)	121.3	120.4	R(4-47)	1.399	1.385	A(6-18-19)	122.4	121.2
R(6-27)	1.210	1.210	A(3-31-21)	120.1	120.9	R(4-51)	1.473	1.468	A(9-7-14)	121.2	122.2
R(7-31)	1.384	1.377	A(4-32-7)	120.8	121.1	R(5-48)	1.215	1.210	A(7-9-49)	119.8	120.1
R(7-32)	1.396	1.390	A(4-32-8)	122.1	121.7	R(6-18)	1.209	1.200	A(7-14-12)	118.3	117.2
R(7-44)	1.473	1.469	A(5-33-8)	119.6	120.2	R(7-9)	1.391	1.379	A(7-14-46)	119.5	120.9
R(8-32)	1.401	1.386	A(5-33-21)	121.6	120.7	R(7-14)	1.400	1.387	A(9-49-11)	119.8	118.2
R(8-33)	1.382	1.379	A(6-27-24)	122.4	121.8	R(9-49)	1.393	1.383	A(9-49-55)	120.3	119.1
R(8-48)	1.472	1.471	A(6-27-28)	122.4	121.3	R(11-12)	1.390	1.377	A(12-11-49)	120.1	121.0
R(9-11)	1.392	1.384	A(31-7-32)	125.4	125.3	R(11-49)	1.394	1.390	A(11-12-14)	120.9	121.4
R(9-18)	1.401	1.394	A(31-7-44)	119.1	118.1	R(12-14)	1.401	1.381	A(11-49-55)	119.8	122.7
R(11-13)	1.385	1.376	A(7-31-21)	118.6	118.7	R(14-46)	1.524	1.525	A(12-14-46)	122.2	121.9
R(13-14)	1.386	1.376	A(32-7-44)	115.5	116.6	R(15-18)	1.518	1.498	A(14-46-19)	112.5	113.2
R(14-16)	1.392	1.394	A(7-32-8)	117.1	117.2	R(15-43)	1.542	1.543	A(14-46-45)	113.1	111.2
R(16-18)	1.402	1.397	A(32-8-33)	125.3	125.0	R(18-19)	1.518	1.495	A(18-15-43)	112.5	113.6
R(18-19)	1.524	1.521	A(32-8-48)	117.7	117.3	R(19-46)	1.542	1.529	A(15-18-19)	115.2	115.5
R(19-21)	1.586	1.580	A(33-8-48)	117.0	117.6	R(21-35)	1.219	1.223	A(15-43-42)	112.5	112.4
R(19-28)	1.542	1.531	A(8-33-21)	118.8	119.0	R(21-45)	1.524	1.510	A(15-43-45)	113.4	114.7

Table S7. *Cont.*

Parameter [a]	3a					Parameter [a]	3b				
	Calc.	Exp	Parameter [a]	Calc.	Exp		Calc.	Exp	Parameter [a]	Calc.	Exp
R(21-22)	1.586	1.567	A(11-9-18)	121.4	121.2	R(22-24)	1.389	1.403	A(18-19-46)	112.5	113.3
R(21-31)	1.534	1.519	A(9-11-13)	118.6	118.2	R(22-42)	1.402	1.381	A(19-46-45)	113.4	111.7
R(21-33)	1.521	1.513	A(9-18-16)	118.1	118.5	R(24-37)	1.396	1.394	A(35-21-45)	120.8	121.6
R(22-24)	1.542	1.533	A(9-18-19)	119.5	119.1	R(26-34)	1.473	1.499	A(21-45-43)	110.5	112.0
R(22-34)	1.524	1.526	A(11-13-14)	121.8	123.2	R(30-37)	1.504	1.474	A(21-45-46)	110.6	110.2
R(24-27)	1.517	1.506	A(13-14-16)	118.8	117.5	R(31-55)	1.354	1.346	A(21-45-48)	115.2	114.1
R(27-28)	1.517	1.508	A(14-16-18)	121.2	121.3	R(32-55)	1.350	1.371	A(24-22-42)	120.9	120.9
R(34-35)	1.402	1.393	A(16-18-19)	122.3	122.4	R(33-55)	1.351	1.340	A(22-24-37)	120.1	120.0
R(34-42)	1.401	1.392	A(18-19-21)	113.2	111.3	R(34-47)	1.396	1.350	A(22-42-40)	118.3	118.0
R(35-37)	1.392	1.391	A(18-19-28)	112.7	112.6	R(34-48)	1.382	1.377	A(22-42-43)	122.2	122.8
R(37-39)	1.386	1.371	A(21-19-28)	113.1	112.7	R(36-47)	1.208	1.217	A(24-37-30)	119.1	123.3
R(39-40)	1.385	1.374	A(19-21-22)	108.7	108.8	R(37-38)	1.392	1.374	A(24-37-38)	119.8	119.1
R(40-42)	1.392	1.394	A(19-21-31)	106.0	104.4	R(38-40)	1.393	1.382	A(26-34-47)	115.6	117.2
			A(19-21-33)	110.6	109.9	R(40-42)	1.399	1.396	A(26-34-48)	119.3	116.2
			A(19-28-27)	112.5	113.5	R(42-43)	1.524	1.532	A(30-37-38)	121.1	117.6
			A(22-21-31)	106.0	107.6	R(43-45)	1.586	1.552	A(31-55-32)	106.8	102.3
			A(22-21-33)	110.6	111.4	R(45-46)	1.586	1.590	A(31-55-33)	106.6	105.8
			A(21-22-24)	113.1	112.8	R(45-48)	1.536	1.539	A(31-55-49)	111.6	115.4
			A(21-22-34)	113.2	112.3	R(49-55)	1.504	1.489	A(32-55-33)	107.4	103.6
			A(31-21-33)	114.8	114.5	A(1-30-2)	106.5	105.2	A(32-55-49)	112.2	112.3
			A(24-22-34)	112.7	112.4	A(1-30-3)	107.0	107.2	A(33-55-49)	112.0	115.9
			A(22-24-27)	112.5	114.3	A(1-30-37)	111.6	111.5	A(47-34-48)	125.0	126.1
			A(22-34-35)	122.3	122.6	A(2-30-3)	107.3	106.6	A(34-47-36)	121.3	121.4
			A(22-34-42)	119.5	119.2	A(2-30-37)	111.7	112.0	A(34-48-45)	118.5	118.2
			A(24-27-28)	115.2	116.8	A(3-30-37)	112.5	113.9	A(37-38-40)	119.8	120.7
			A(35-34-42)	118.1	118.1	A(21-4-47)	125.3	124.3	A(38-40-42)	121.2	121.3
			A(34-35-37)	121.2	121.0	A(21-4-51)	119.3	118.5	A(40-42-43)	119.5	119.1
			A(34-42-40)	121.4	121.7	A(4-21-35)	120.8	119.7	A(42-43-45)	113.1	110.5
			A(35-37-39)	118.8	118.6	A(4-21-45)	118.3	118.7	A(43-45-46)	108.3	107.5
			A(37-39-40)	121.8	122.8	A(47-4-51)	115.3	117.1	A(43-45-48)	105.9	109.2
			A(39-40-42)	118.6	117.8	A(4-47-34)	117.6	117.7	A(46-45-48)	105.9	103.4

[a] Atom numbering referred to Figure 5.

Table S8. The calculated electronic transitions using TD-DFT method.

λ_{max} (nm)	f	Major Contributions
		3a
293.2	0.0030	H→L + 2 (45%), H→L + 5 (26%)
282.2	0.0008	H→L (99%)
266.3	0.0001	H-5→L (61%), H-4→L (31%)
258.6	0.0001	H-1→L (98%)
255.7	0.0009	H-2→L (97%)
248.1	0.0077	H→L + 1 (87%)
242.0	0.0000	H-2→L + 1 (11%), H→L + 2 (13%), H→L + 3 (50%)
239.2	0.0087	H-7→L (49%), H-5→L + 1 (18%)
235.3	0.0005	H-3→L (91%)
234.0	0.0001	H-5→L (32%), H-4→L (65%)
233.2	0.0064	H-1→L + 1 (50%)
229.8	0.0002	H-2→L + 1 (32%), H-1→L + 3 (18%), H→L + 2 (14%), H→L + 3 (13%)
228.3	0.1530	H-1→L + 2 (20%), H→L + 2 (22%), H→L + 3 (25%), H→L + 5 (19%)
224.3	0.0110	H-6→L (48%), H-1→L + 1 (17%)
222.5	0.0149	H-2→L + 1 (15%), H-1→L + 2 (52%), H→L + 5 (28%)
222.1	0.0169	H-6→L (42%), H-2→L + 2 (17%), H-1→L + 1 (15%), H→L + 4 (11%)
219.0	0.0151	H-2→L + 1 (30%), H-1→L + 3 (52%)
217.8	0.0235	H-2→L + 2 (49%), H→L + 4 (27%)
217.0	0.0003	H-2→L + 3 (31%), H→L + 4 (40%)
215.6	0.0004	H-9→L (73%)
		3b
296.2	0.0056	H→L + 1 (44%), H→L + 5 (45%)
275.9	0.0004	H→L (99%)
266.2	0.0001	H-5→L (15%), H-4→L (22%), H-2→L (55%)
248.5	0.0363	H→L + 1 (51%), H→L + 5 (35%)
244.4	0.0020	H→L + 2 (65%), H→L + 3 (21%)
241.9	0.0036	H-1→L (70%), H→L + 2 (13%)
240.7	0.0156	H-7→L (21%), H-4→L (15%)
239.7	0.0063	H-1→L (21%), H→L + 2 (16%), H→L + 3 (40%)
239.2	0.0015	H-7→L (13%), H-3→L + 1 (12%), H→L + 4 (23%)
234.2	0.0006	H-3→L (83%)
232.9	0.0008	H-4→L (48%), H-2→L (27%), H→L + 4 (11%)
232.2	0.0073	H-2→L + 1 (16%), H→L + 3 (17%)
232.1	0.0005	H-5→L (64%)
229.3	0.0050	H-3→L + 1 (17%), H-1→L + 4 (13%), H→L + 4 (39%)
225.3	0.0016	H-5→L + 1 (17%), H-4→L + 1 (28%), H-2→L + 1 (47%)
224.2	0.0266	H-6→L (84%)
222.1	0.2486	H-1→L + 1 (81%)
217.0	0.0000	H-9→L (79%)
215.8	0.0129	H-5→L + 1 (36%), H-4→L + 1 (35%)
213.7	0.0040	H→L + 6 (79%)

Table S9. The calculated chemical shifts δ (ppm) of the studied compound using GIAO method.

Atom	δ_{calc} (ppm)	$\delta_{exp.}$(ppm)	Atom	δ_{calc} (ppm)	$\delta_{exp.}$(ppm)
C9	137.96	126.96	C7	136.21	126.96
C11	120.65	125.48	C9	131.79	125.48
C13	172.40	168.6	C11	132.27	125.48
C14	121.17	125.87	C12	132.56	126.96
C16	133.67	126.96	C14	150.40	149.93
C18	142.03	139.84	C15	48.47	44.17
C19	58.58	45.44	C18	208.88	205.78
C21	68.12	61.51	C19	48.53	45.44
C22	58.58	45.44	C21	176.56	170.91
C24	48.84	44.17	C22	132.79	126.96
C27	209.61	205.78	C24	133.09	125.48
C28	48.84	44.17	C26	29.71	28.21
C31	178.19	170.91	C30	134.23	125.87
C32	154.66	149.93	C37	138.63	139.84
C33	177.97	170.91	C38	131.15	125.48
C34	142.03	139.84	C40	135.88	126.96
C35	133.67	126.96	C42	150.34	149.93
C37	121.17	125.87	C43	59.14	61.51
C39	172.40	168.6	C45	67.26	61.51
C40	120.65	125.48	C46	59.21	61.51
C42	137.96	126.96	C47	154.96	168.6
C44	30.03	28.21	C48	177.60	170.91
C48	30.34	28.63	C49	138.58	139.84
			C51	29.20	28.63
			C55	134.24	125.87
H10	7.22	7.04	H8	7.34	6.75
H12	6.95	7.01	H10	7.62	7.14
H15	7.03	7.01	H13	7.48	6.75
H17	7.34	7.04	H16	2.33	2.7
H20	3.83	3.64	H17	3.83	4.25
H23	3.83	3.64	H20	3.83	4.28
H25	3.76	3.95	H23	7.50	6.75
H26	2.28	2.55	H25	7.70	7.14
H29	2.28	2.59	H27	2.20	3.02
H30	3.76	3.99	H28	2.22	3.02
H36	7.34	6.94	H29	4.07	3.02
H38	7.03	6.89	H39	7.63	7.14
H41	6.95	6.89	H41	7.32	6.75
H43	7.21	6.94	H44	3.93	3.56
H45	4.12	3.02	H50	7.70	7.14
H46	2.24	2.88	H52	4.39	3.04
H47	2.25	2.88	H53	2.45	3.04
H49	3.93	3.02	H54	2.45	3.04
H50	2.70	2.88	H56	2.32	2.74
H51	2.70	2.88	H57	3.92	3.56

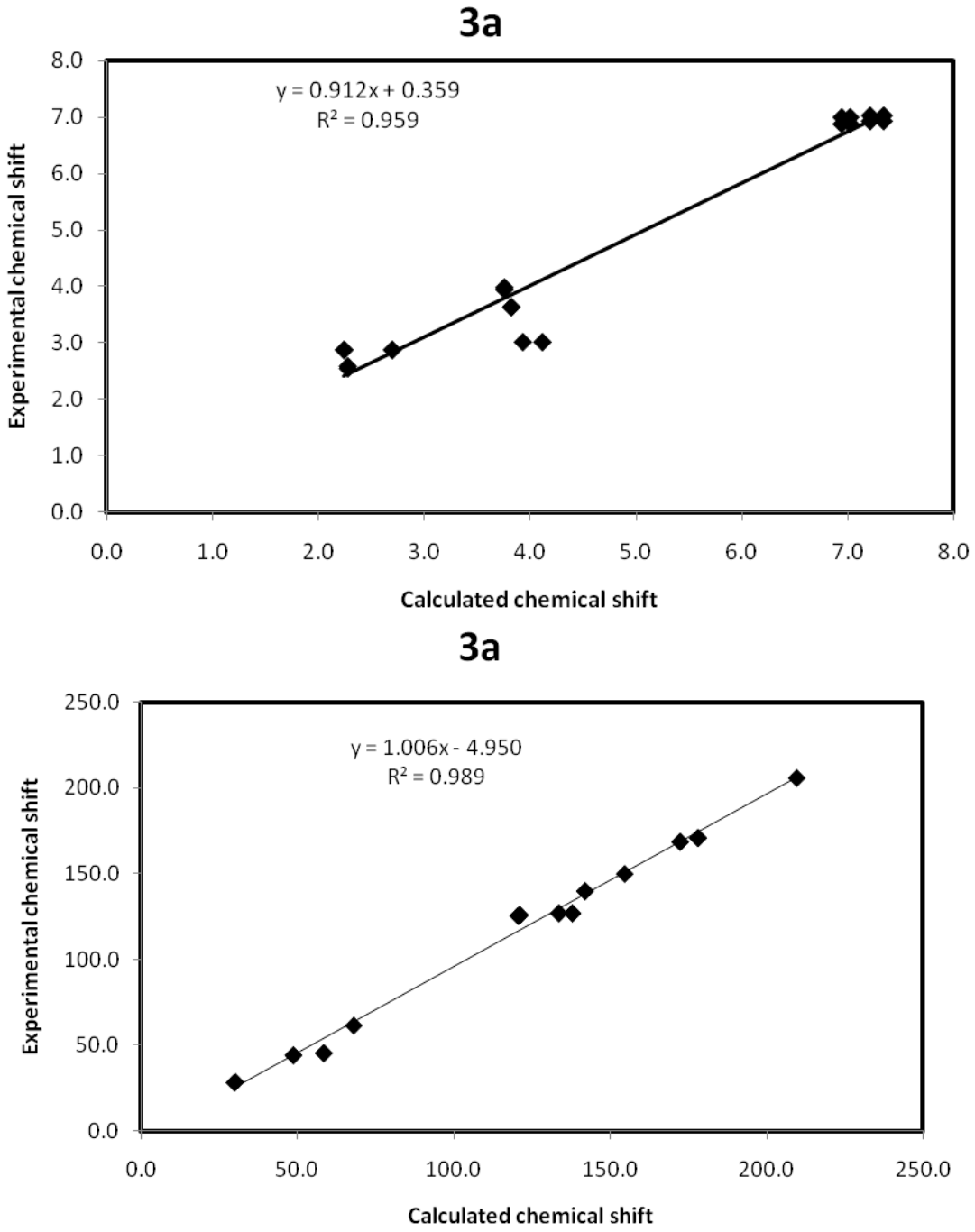

Figure S7. The correlation graphs between the calculated and experimental ^{1}H- and ^{13}C-NMR chemical shifts of **3a**.

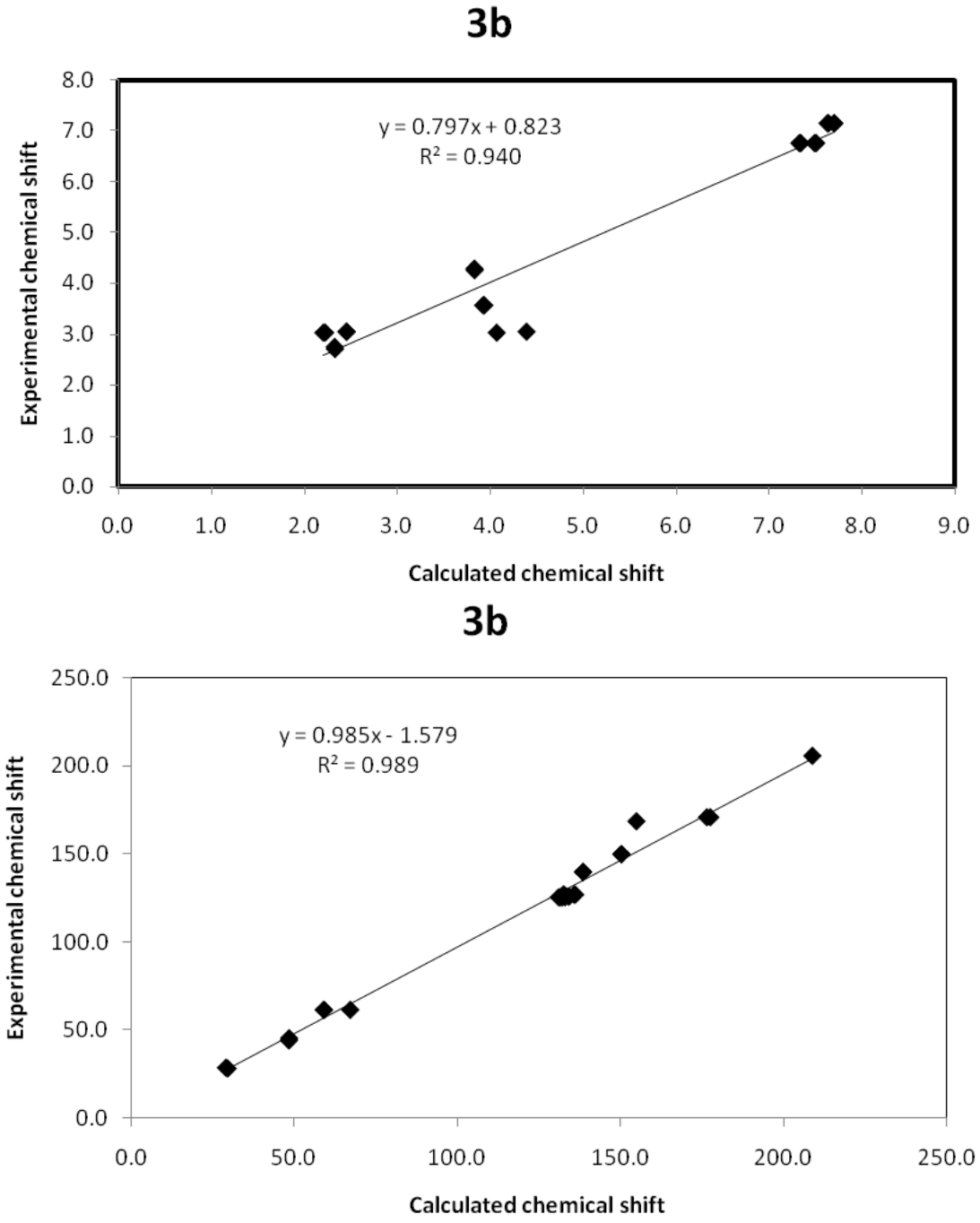

Figure S8. The correlation graphs between the calculated and experimental ^{1}H- and ^{13}C-NMR chemical shifts of **3b**.