Supporting Information for:

Synthesis and Photophysical Properties of BF₂ Complexes of Curcumin Analogues

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1. Photophysical spectra and DPBF degradation plot

1.1 UV-vis and Fluorescence data for all the new compounds



Figure S1. Absorption (a) and emission spectra (b) of curcumin- BF_2 **1a** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 410 nm.



Figure S2. Absorption (a) and emission spectra (b) of curcumin- BF_2 **1b** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 410 nm.



Figure S3. Absorption (a) and emission spectra (b) of curcumin- BF_2 **1c** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 470 nm.



Figure S4. Absorption (a) and emission spectra (b) of curcumin- BF_2 **1d** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 470 nm.



Figure S5. Absorption (a) and emission spectra (b) of curcumin- BF_2 **1e** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 470 nm.



Figure S6. Absorption (a) and emission spectra (b) of curcumin- BF_2 **1f** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 470 nm.



Figure S7. Absorption (a) and emission spectra (b) of curcumin- BF_2 **1g** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 470 nm.



Figure S8. Absorption (a) and emission spectra (b) of curcumin- BF_2 **1h** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 480 nm.



Figure S9. Absorption (a) and emission spectra (b) of curcumin- BF_2 **1i** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 470 nm.



Figure S10. Absorption (a) and emission spectra (b) of curcumin- BF_2 **1j** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 470 nm.



Figure S11. Absorption (a) and emission spectra (b) of curcumin- BF_2 **1k** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 480 nm.



Figure S12. Absorption (a) and emission spectra (b) of curcumin- BF_2 **1** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 480 nm.



Figure S13. Absorption (a) and emission spectra (b) of curcumin- BF_2 **3a** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 420 nm.



Figure S14. Absorption (a) and emission spectra (b) of curcumin- BF_2 **3b** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 480 nm.



Figure S15. Absorption (a) and emission spectra (b) of curcumin- BF_2 **3c** in acetonitrile (black), dichloromethane (red), tetrahydrofuran (blue) and toluene (dark cyan). Excited at 520 nm.



Figure S16. Absorption (a) and emission spectra (b) of curcumin-BF₂ **11** in PBS buffer (including 1% DMSO). Excited at 480 nm.



Figure S17. Absorption (a) and emission spectra (b) of curcumin-BF₂ **1e** in PBS buffer (including 1% DMSO). Excited at 480 nm.

Wavelength (nm)



Figure S18. Absorption (a) and emission spectra (b) of curcumin-BF₂ **1h** in PBS buffer (including 1% DMSO). Excited at 480 nm.



Figure S19. Absorption (a) and emission spectra (b) of curcumin- BF_2 **1i** in PBS buffer (including 1% DMSO). Excited at 480 nm.

1.2 Photooxidation of 1,3-diphenylisobenzofuran (DPBF) with curcumin-BF₂ complexes and Rose Bengal



Figure S16. DPBF (initial concentration at 5×10^{-5} M) degradation profiles in toluene by Rose Bengal (1 $\times 10^{-6}$ M). Filtered light > 455nm used.



Figure S17. DPBF (initial concentration at 5×10^{-5} M) degradation profiles in toluene by curcumin-BF₂ complex **1b** (1×10^{-6} M). Filtered light > 455nm used.



Figure S18. DPBF (initial concentration at 5×10^{-5} M) degradation profiles in toluene by curcumin-BF₂ complex **1c** (1×10^{-6} M). Filtered light > 455nm used.



Figure S19. DPBF (initial concentration at 5×10^{-5} M) degradation profiles in toluene by curcumin-BF₂ complex **1d** (1×10^{-6} M). Filtered light > 455nm used.



Figure S20. DPBF (initial concentration at 5×10^{-5} M) degradation profiles in toluene by curcumin-BF₂ complex **1e** (1×10^{-6} M). Filtered light > 455nm used.



Figure S21. DPBF (initial concentration at 5×10^{-5} M) degradation profiles in toluene by curcumin-BF₂ complex **1f** (1×10^{-6} M). Filtered light > 455nm used.



Figure S22.DPBF (initial concentration at 5×10^{-5} M) degradation profiles in toluene by curcumin-BF₂ complex **1g** (1×10^{-6} M). Filtered light > 455nm used.



Figure S23. DPBF (initial concentration at 5×10^{-5} M) degradation profiles in toluene by curcumin-BF₂ complex **1h** (1×10^{-6} M). Filtered light > 455nm used.



Figure S24. DPBF (initial concentration at 5×10^{-5} M) degradation profiles in toluene by curcumin-BF₂ complex **1i** (1×10^{-6} M). Filtered light > 455nm used.



Figure S25. DPBF (initial concentration at 5×10^{-5} M) degradation profiles in toluene by curcumin-BF₂ complex **1j** (1×10^{-6} M). Filtered light > 455nm used.



Figure S26. DPBF (initial concentration at 5×10^{-5} M) degradation profiles in toluene by curcumin-BF₂ complex **1k** (1×10^{-6} M). Filtered light > 455nm used.



Figure S27. DPBF (initial concentration at 5×10^{-5} M) degradation profiles in acetonitrile by curcumin-BF₂ complex **11** (1 × 10⁻⁶ M). Filtered light > 455nm used.



Figure S28. DPBF (initial concentration at 5×10^{-5} M) degradation profiles in toluene by curcumin-BF₂ complex **3b** (1×10^{-6} M). Filtered light > 455nm used.



Figure S29. DPBF (initial concentration at 5×10^{-5} M) degradation profiles in toluene by curcumin-BF₂ complex **3c** (1×10^{-6} M). Filtered light > 455nm used.

2.Copies of ¹H NMR and ¹³C NMR spectra for all new compounds

¹H NMR compound 1a in CDCl₃







¹H NMR compound **1b** in CDCl₃













	$\frac{7.957}{-7.908}$
	7.533 7.514 -6.945 -6.928
	$\overline{16.597}_{6.547}$
	-6.028
	-4.181

-4.181
-3.885
∼3.743
∖-3.694
1-3.568
L3.387

-2.001





¹³C NMR compound **1f** in CDCl₃





¹H NMR compound **1h** in DMSO-d₆

39

¹H NMR compound **1i** in CDCl₃

¹H NMR compound **1j** in CDCl₃

9.05:8 7.848 7.806 8.0**J**₇7.762 2.31-7.478 7.450 7.5 4.12-7.249 .073 7.023 2.04-<u>⊺</u> 5.68-7.0 -6.917 6.917 -6.855 6.5 -6.802 $\overline{\ }_{6.166}^{6.214}$ -5.866 2.12-6.0 1.00-5.5 5.0 4.5 δ (ppm) 4.0 5.66--3.8423.5 3.02.5 2.0 1.5 H_2O 1.539 1.00.5

 1 H NMR compound **1k** in CDCl₃

¹H NMR compound **3a** in CDCl₃

46

¹H NMR compound **3c** in CDCl₃

3. High resolution mass spectroscopies for all new compounds

1a

m/z	Intensity	Relative	Theo.Mass	Delta(mmu)	Composition
304. 12164	1858299.8	1.55	304. 12294	-1.3	C20 H15 B F2
305.11438	5591580	4.65	305.11436	0.01	C19 H15 O2 B F
306. 11777	1112926.6	0.93	306.11566	2.1	C9 H22 O11
307.12103	112710	0.09	307.1199	1.13	C10 H21 08 F2
310. 31064	3034875.5	2.52	310. 30376	6.88	C19 H39 O2 B
316. 13797	28335092	23.57	316. 1364	1.57	C11 H24 010
317.13434	120207648	100	317.13435	-0.01	C20 H18 O3 B
318. 13727	25581412	21.28	318. 13859	-1.32	C21 H17 B F2
318. 29987	167169.6	0.14	318.29286	7.01	C19 H39 O2 F
319. 14066	2161608.3	1.8	319.13989	0.77	C11 H24 09 F
320. 33069	487092.5	0.41	320. 32491	5.78	C20 H42 F2
325. 12009	150467.7	0.13	325. 12059	-0.51	C19 H16 02 BF2
330. 33624	236563.4	0.2	330. 32925	7	C21 H43 0 F

20111027_APCI+_B1 #9 RT: 0.11 AV: 1 SB: 2 0.04-0.05 NL: 1.20E8 T: FTMS + c APCI corona Full ms [200.00-1200.00]

1b

m/z	Intensity	Relative	Theo. Mass	Delta(mmu)	Composition
362.14346	879514.4	1.16	362.1484	-4.94	C22 H20 O3 B F
363.13977	3541669.5	4.66	363.13983	-0.06	C21 H20 O5 B
364.13913	17820336	23.45	364.14407	-4.94	C22 H19 O2 B F2
365.1355	76004256	100	365.13549	0	C21 H19 O4 B F
366.13849	17036226	22.41	366. 14332	-4.83	C21 H20 O4 B F
367.14194	1498117.5	1.97	367.13516	6.78	C19 H21 O5 F2
371.10088	1226923.8	1.61	371.10853	-7.65	C22 H16 O5 B
372.10037	292889.7	0.39	372.09751	2.86	C19 H15 O5 B F2
373.09769	207066.1	0.27	373.10419	-6.51	C22 H15 O4 B F
374.36261	151229	0.2	374.3526	10.01	C22 H45 O B F2
376.15851	9131629	12.01	376.1652	-6.69	C20 H23 O4 B F2
377.15497	36235996	47.68	377.15548	-0.51	C22 H22 O5 B
378.15817	8735345	11.49	378.16331	-5.13	C22 H23 O5 B
379.16196	649764	0.85	379.17113	-9.17	C22 H24 O5 B
385.14102	133799	0.18	385.14172	-0.7	C21 H20 O4 B F2
388.18024	181798.3	0.24	388. 18518	-4.95	C21 H26 O5 B F

m/z	Intensity	Relative	Theo.Mass	Delta(mmu)	Composition
626.30511	61594440	1.61	626.30569	-0.59	C34 H44 O9 B F
627.2977	249635200	6.52	627.29753	0.17	C32 H45 O10 F2
628.29829	189749344	4.96	628.30136	-3.06	C34 H43 08 B F2
629.29263	603623424	15.77	629.29278	-0.15	C33 H43 O10 B F
630.29503	217307392	5.68	630.30061	-5.58	C33 H44 O10 B F
631.29692	41029376	1.07	631.29244	4.47	C31 H45 O11 F2
632.29122	7645983	0.2	632.29627	-5.06	C33 H43 O9 B F2
640.31914	876877376	22.9	640.32249	-3.35	C32 H47 O10 B F2
641.3124	3.828E+09	100	641.31277	-0.37	C34 H46 O11 B
642.31506	1.394E+09	36.41	642.32059	-5.53	C34 H47 O11 B
643.31869	307709312	8.04	643.30958	9.12	C31 H46 O11 B F2
644. 32378	43824392	1.14	644.3174	6.38	C31 H47 O11 B F2
645.3434	7058135.5	0.18	645.34407	-0.67	C34 H50 O11 B
648.2914	5384291.5	0.14	648.29119	0.21	C33 H43 O10 B F2

1f

20111027_APCH_B15_2 #9 RT: 0.11 AV: 1 SB: 4 0.01-0.05 NL: 3.95E7 T: FTMS + c APCI corona Full ms [200.00-1000.00]

m/z	Intensity	Relative	Theo.Mass	Delta(mmu)	Composition
698.0307	311493.2	0.79	698.03559	-4.89	C28 H30 O3 B F I2
699.02679	1381533.8	3.49	699.02702	-0.22	C27 H30 O5 B I2
700.02637	9409929	23.8	700.03125	-4.89	C28 H29 O2 B F2 I2
701.02283	39544764	100	701.02268	0.15	C27 H29 O4 B F I2
702.02576	10494359	26.54	702.03051	-4.75	C27 H30 O4 B F I2
703.02881	1592926.1	4.03	703.02234	6.47	C25 H31 O5 F2 I2
704.03162	155380.6	0.39	704.03017	1.45	C25 H32 O5 F2 I2
712.0459	4947049	12.51	712.05238	-6.49	C26 H33 O4 B F2 I2
713.04254	20429680	51.66	713.04267	-0.13	C28 H32 O5 B I2
714.04553	5868925	14.84	714.05049	-4.96	C28 H33 O5 B I2
715.04834	852993.3	2.16	715.03947	8.87	C25 H32 O5 B F2 I2
716.05035	87134.9	0.22	716.0473	3.06	C25 H33 O5 B F2 I2
721.0285	66127.5	0.17	721.02891	-0.41	C27 H30 O4 B F2 I2
721.32184	348797.4	0.88	721.23555	86.29	C28 H56 O4 B I2
722.32416	149589.3	0.38	722.24338	80.78	C28 H57 O4 B I2

1h

303.11066

7034259.5

3.22

303.11109

-0.43

C15 H14 O2 N2 B F2

1i

20111027_APCH_B7 #10 RT: 0.12 AV: 1 SB: 1 0.05 NL: 5.74E7 T: FTMS + c APCI corona Full ms [200.00-1200.00]

373.09717

374.36227

377.1514

99894.7

109845.1

125877.5

1j

0.17

0.19

0.22

373.10346

374.35546

377.15189

-6.29

6.81

-0.5

C24 H15 O2 F2 C23 H47 O2 F

C23 H20 O2 B F2

m/z	Intensity	Relative	Theo.Mass	Delta(mmu)	Composition
415.21035	4458394	70.81	415.20866	1.69	C23 H29 O5 B F
416.18961	2519621.3	40.02	416. 19535	-5.75	C26 H26 O3 B F
417.167	6296615.5	100	417.16679	0.21	C25 H23 O4 B F
418.17144	1572638.8	24.98	418.17462	-3.18	C25 H24 O4 B F
419.31507	2327046.5	36.96	419.31559	-0.51	C26 H43 04
420.31836	591822.3	9.4	420. 32056	-2.2	C25 H42 O3 B F
428.25259	130598.2	2.07	428.25287	-0.28	C25 H34 O4 B F
429.16972	798329.9	12.68	429.16794	1.78	C23 H24 O5 B F2
430.17668	203621.6	3.23	430.17576	0.92	C23 H25 O5 B F2
441.26489	234183.2	3.72	441.26184	3.05	C23 H36 O5 B F2

496.7002

523.2019

8902803

5015558

2

1

496.70867

-8.48

C63 H62 O4 B F2 P2

4.38

2.47

3a

20111027_APCH_B13 #9-11 RT: 0.11-0.14 AV: 3 SB: 2 0.04-0.05 NL: 2.01E8 T: FTMS + c APCTcorona Full ms [200.00-1200.00]

m/z	Intensity	Relative	Theo. Mass	Delta(mmu)	Composition
269.15263	409634.6	0.2	269.15189	0.74	C14 H20 O2 B F2
270.11578	5810642.5	2.89	270.11629	-0.51	C16 H15 0 N2 F
271.11834	24186158	12.03	271.11858	-0.24	C12 H16 O3 N B F2
272.1153	12789181	6.36	272.11554	-0.25	C15 H16 O3 N2
273.1095	54276564	26.99	273.10928	0.22	C15 H15 O3 B F
274.11265	8700191	4.33	274.11235	0.3	C12 H16 O3 N2 F2
275.12574	573013.6	0.28	275.12607	-0.33	C12 H18 O4 B F2
279.1118	2566085.5	1.28	279.11109	0.71	C13 H14 O2 N2 B F2
280. 26227	277256.5	0.14	280.26349	-1.22	C18 H34 O N
282.27721	2741554.5	1.36	282.27629	0.93	C17 H34 N B F
283.25921	668345.6	0.33	283.25916	0.06	C20 H32 B
284.13486	47011224	23.38	284.13382	1.04	C12 H18 O4 N2 B F
285.12926	201116384	100	285.12927	-0.01	C16 H18 O4 B
286.13217	32801288	16.31	286.13234	-0.16	C13 H19 O4 N2 F
287.15406	3352016.8	1.67	287.15428	-0.22	C20 H19 N2
288.1747	295934	0.15	288.17468	0.02	C21 H22 N
292.14514	257151.9	0.13	292.14578	-0.64	C20 H20 O2
293.17404	227932	0.11	293.17456	-0.52	C19 H21 N B F
297.27918	342860.9	0.17	297.27881	0.37	C19 H37 O2

3b

m/z	Intensity	Relative	Theo.Mass	Delta(mmu)	Composition
313.17883	22238156	23.91	313.17848	0.35	C18 H23 O2 N3
314.17238	93009536	100	314.17221	0.16	C18 H22 O2 N B F
315.17155	18318092	19.69	315.17149	0.06	C22 H21 B F
316.17139	1492305.8	1.6	316.17188	-0.48	C16 H24 O3 N F2
326.19207	1284773.5	1.38	326.1922	-0.13	C19 H25 O3 N B
327.21273	278473.8	0.3	327.2126	0.13	C20 H28 O3 B
333.18454	947868.1	1.02	333. 18471	-0.16	C18 H24 O2 N3 F
334.17851	3566797.3	3.83	334.17844	0.06	C18 H23 O2 N B F2
335.19041	637959.7	0.69	335.18912	1.28	C19 H26 O3 N F
338.3415	1181849	1.27	338.34174	-0.24	C22 H44 O N