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## Meso-Salicylaldehyde Substituted BODIPY as Chemodosimetric Sensor

# for Cyanide Anion

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Fig. S1 Comparison of <sup>1</sup>H NMR spectra of I, 5, 6 and compound 3.





Fig. S2 Sections of <sup>1</sup>H-<sup>1</sup>H COSY NMR spectra of BODIPY 3.











Fig. S5 Comparison of <sup>1</sup>H NMR spectra of i, 7, 8, 9 and compound 4.



Fig. S6 <sup>11</sup>B NMR spectrum of BODIPY 9.



Fig. S7 <sup>19</sup>F NMR spectrum of BODIPY 9.



Fig. S8 <sup>13</sup>C NMR spectrum of BODIPY 9.



Fig. S9 <sup>11</sup>B NMR spectrum of BODIPY 4.



Fig. S10 <sup>13</sup>C NMR spectrum of BODIPY 4.



### **Elemental Composition Report**

Page 1

Single Mass Analysis Tolerance = 10.0 PPM / Selected filters: None	DBE: min = -1.5,	max = 50.0		
Monoisotopic Mass, Even Electi 33 formula(e) evaluated with 1 r Elements Used: C: 0-20 H: 0-23 N: 0-2 O: 1 Q-Tof MICROMASS (YA-105)	on lons esults within limits (up )-2 S: 0-2 DEPARTM	o to 6 closest results for e	each mass)	07-Nov-201416:04:48
C20H22N2O2 MR-AD-6 57 (1.058) AM (Med,5, Ht,500 100 256	0.0,556.28,1.00); Sm (Md .1264 	, 4.00); Sb (8,40.00 ); Cm (57:	32)	TOF MS ES+ 1.12e4
%- 216.1610221.1494 246.2110 210 220 230 240 250	257.1361 279.1651286 260 270 280 294	323.1761 321.1620 .1485 302.1447 0 300 310 320 330	7.1540 338.1625 355.1714 340 350 360 3	376.2084 391.2900 Innihingangangangang m/z 70 380 390 400
Minimum: Maximum:	5.0 10.0	-1.5 50.0		
Mass Calc. Mass	mDa PPM	DBE i-FIT	Formula	<b>,</b>

Fig. S11 HR-MS of compound 6.



Element	tal Comp	oositic	on Repor	t									Page 1
Single M Tolerand Selected	<b>lass An</b> a ce = 10.0 I filters: N	alysis PPM Ione	/ DBE:	min = -1	.5, max	= 50.0							•
Monoisoto 485 formu	pic Mass, ia(e) evalu	Even E ated wi	lectron lons th 1 results	within limi	ts (up to (	3 closest	results fo	or each	mass)				
C: 0-20	Used: H: 0-19 E	B: 0-1	N: 0-2 O:	0-2 F:0	-2 K: 0-	1 Cu: (	)-1 Br: (	0-1					
Q-Tof MICRO C20H19BF2I MR- AD- BO	OMASS (YA- N2O2 DIPY 3 123 (	105) (2.282) Al	M (Med,4, Ht,	DEPA	RTMENT O 8,1.00); Sm 349 13	F CHEMIS (Mn, 2x4.(	TRY, I.I.T.( )0); Sb (5,4	(B) 0.00 ); C	im (118:21	6)	31	1-Oct-2 T	201416:35:10
100 		,					391.1	1337					3.0004
242	.2820 26	6.1290	301.1413	321.1606 3	48.1524 31 47.1552	50.1530 369.1588	390.1436	407.	1125 408.1189	4	48.1331		477.1620
240	260	280	300	320	340	360	380	400	420	440		460	480
Minimum: Maximum:			5.0	10.0	-1.5 50.0								
Mass	Calc.	Mass	mDa	PPM	DBE	<b>i</b> -1	FIT	Form	ula				
407.1125	407.11	45	-2.0	-4.9	11.5	3.	3	C20.	H19 B	N2 0	2 F2	ĸ	

Fig. S12 HR-MS of compound 3.



## **Elemental Composition Report**

Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

Monoisotopia 4 formula(e) Elements Us	c Mass, ( evaluate ed:	Odd an ed with	nd Even El 1 results v	ectron lons vithin limits (u	p to 6 clos	sest resul	ts for (	each	mass)					
C: 0-16 H: Q-Tof MICRON	0-17 N IASS (YA-	ł: 0-2 105)	O: 0-1	DEPART	MENT OF O	CHEMISTR	Y. I.I.T.	(B)				16-Dec-2	01412:20	3:39
C16H16N2O MR-AD-8 22 (0	).409) Sm	(Md, 4.0 186.	0); Sb (5,40.0 0784	00 ); Cm (15:40)								т	OF MS E 6.1	S+ 7e3
%- 0	168.	0748 	187.0846	25 251.115	3.1338 2 254.1384	292.18	13 11	mţm	سينسبه		<b>1</b>	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	,	m/z
140	160	180	200	220 240	260	280 3	00	320	340	360	380	400	420	
Minimum: Maximum:			5.0	10.0	-1.5 50.0									
Mass	Calc.	Mass	mDa	PPM	DBE	Form	ula							
253.1338	253.13	41	-0.3	-1.2	9.5	C16	H17	N2	0					

Fig. S13 HR-MS of compound 8.



#### **Elemental Composition Report**

Page 1

#### Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

Monoisotopic Mass, Even Electron Ions 62 formula(e) evaluated with 1 results within limits (up to 6 closest results for each mass) Elements Used: C: 0-16 H: 0-13 B: 0-1 N: 0-2 O: 0-1 F: 0-2 Na: 0-1 C: 0-16 H: 0-13 D. 0-1 H. 0-Q-Tof MICROMASS (YA-105) DEPARTMENT OF CHEMISTRY, C16H138F2N2O MR-AD-BODPY-9 16 (0.271) AM (Top,4, Ht,5000.0,0.00,1.00); Sb (8,40.00 ); Cm (15:39) 279.0987 DEPARTMENT OF CHEMISTRY, I.I.T.(B) 04-Nov-201412:05:07 TOF MS ES+ 2.96e3 321.0993 % 278.1101 280.0972 322.1011 533.5167 556.2660 571.5079 m/z 228,9520 198.0499 79.0192 102.1307 337.0667 413.2834451.4330 0-100 125 150 175 200 225 250 275 300÷325 350 375 400 425 450 475 500 525 550 575 600 50 75 Minimum: -1.5 10.0 50.0 Maximum: 5.0 Mass Calc. Mass mDa PPM DBE i-FIT Formula 321.0993 321.0987 C16 H13 B N2 O F2 Na 1.9 10.5 5.5 0.6

Fig. S14 HR-MS of compound 9.



Elemental	Composition	Report					Page 1
Single Ma Tolerance Selected fi	<b>ss Analysis</b> = 100.0 PPM Iters: None	/ DBE: n	nin = -1.5	, max = 5	60.0		
Monoisotopic 61 formula(e) Elements Us	: Mass, Odd and E ) evaluated with 1 ed: 0-11 B: 0-1 N:	iven Electro results with	n Ions in limits (up 1 F <sup>.</sup> 0-2	to 6 close: Na: 0-1	st results for e	ach mass)	· .
Q-Tof MICROM	ASS (YA-105)	0-2 0.0-	DEPARTM	ENT OF CHE	MISTRY, I.I.T.(B)	)	31-Oct-201417:59:35
C16H11BF2N20 MR- AD- BODIF 100 	0 PY42 53 (0.984) AM (C 02.1270 146.05 100 120 140	en,4, 80.00, H 64 180.018 160 180	1t,5000.0,556. 24: 9 207.0796 200 220	28,1.00); Sm 2.2813 276 243.28 243.28 243.28 240 26	(Mn, 2x4.00); Sb 277.0889 .0956 278.0957 46 0 280 300	(5,40.00 ); Cm (46:65) 319.0816 320.0869 352.1118 320 340 360 380	TOF MS ES+ 8.82e3 415.2127 400 420
Minimum: Maximum:		5.0	100.0	-1.5 50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
319.08167	319.0830	-1.4	-4.4	11.5	10.2	C16 H11 B N2 O F	'2 Na

Fig. S15 HR-MS of compound 4.



**Fig. 16** Fluorescence responses of chemodosimeter **3** ( $1x10^{-5}$  M) in the presence of 10 eqv. of different anions and 4 eqv. of CN<sup>-</sup> ion under uv lamp in CH<sub>3</sub>CN: (a) F<sup>-</sup>, (b) Cl<sup>-</sup>, (c) Br<sup>-</sup> (d) I<sup>-</sup>, (e) HSO<sub>4</sub><sup>-</sup>, (f)ClO<sub>4</sub><sup>-</sup>, (g) NO<sub>3</sub><sup>-</sup>, (h), NO<sub>2</sub><sup>-</sup>, (i) N<sub>3</sub><sup>-</sup>, (j) CO<sub>3</sub><sup>--</sup>, (k) H<sub>2</sub>PO<sub>4</sub><sup>-</sup>, (l) CN<sup>-</sup>



**Fig. S17** Absorption spectra of BODIPY **3** (1x10<sup>-5</sup> M) in presence of various anions (10 eqv.) and 4 eqv. of CN<sup>-</sup> ion in CH<sub>3</sub>CN solution.



**Fig. S18** Fluorescence spectra of BODIPY **3** ( $1x10^{-5}$  M) in presence of various anions (10 eqv.) and 4 eqv. of CN<sup>-</sup> ion in CH<sub>3</sub>CN solution.