

Electronic Supplementary Information (ESI)

D–A– π –A featured sensitizers containing auxiliary acceptor of benzoxadiazole: molecular engineering and co-sensitization

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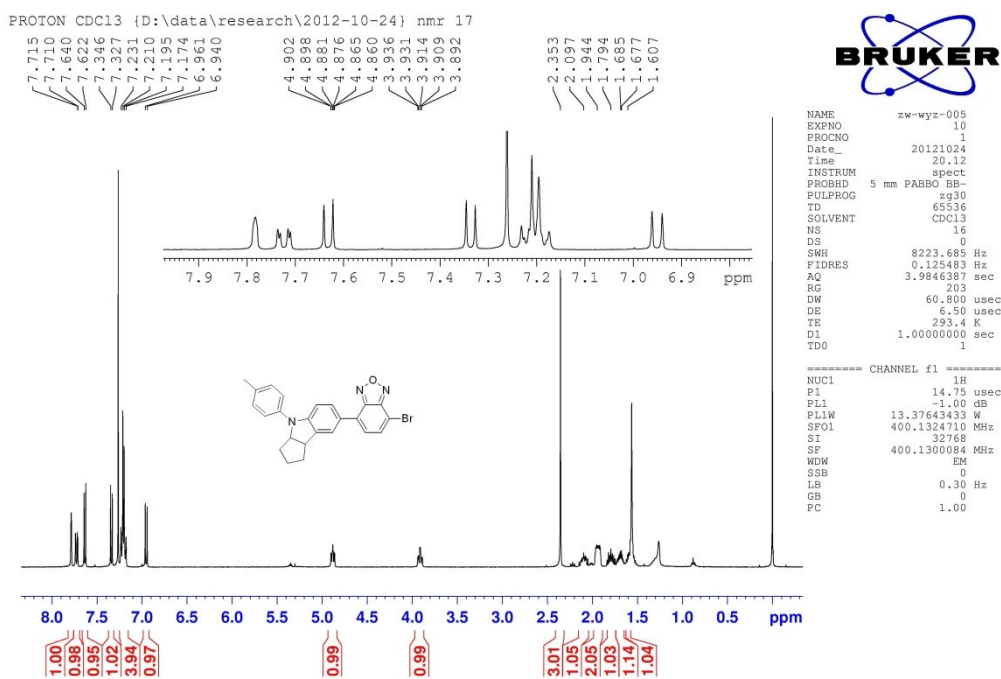


Fig. S1 ^1H NMR of compound 1 in CDCl_3

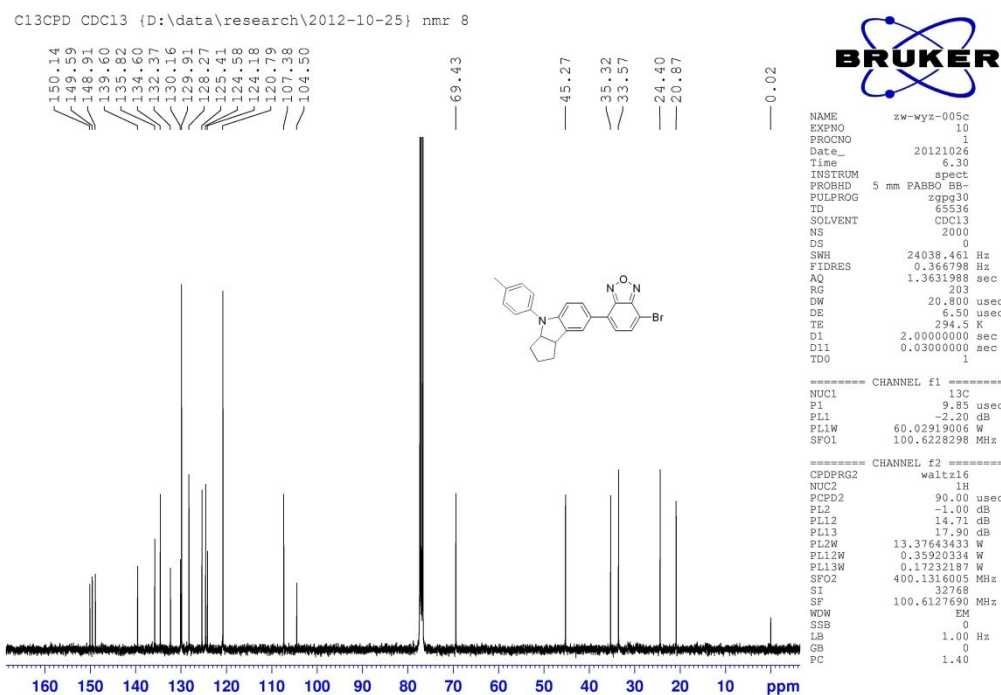


Fig. S2 ^{13}C NMR of compound 1 in CDCl_3

Single Mass Analysis

Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Odd and Even Electron Ions

112 formula(e) evaluated with 35 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-40 H: 0-40 N: 0-3 O: 0-3 Br: 0-1

WH-ZHU

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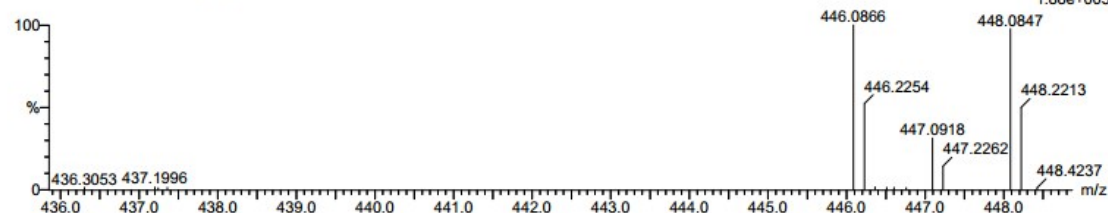
26-Oct-2012

16:50:50

ZWH-ZHB-02 52 (1.675) Cm (47:52)

1: TOF MS ES+

1.88e+003

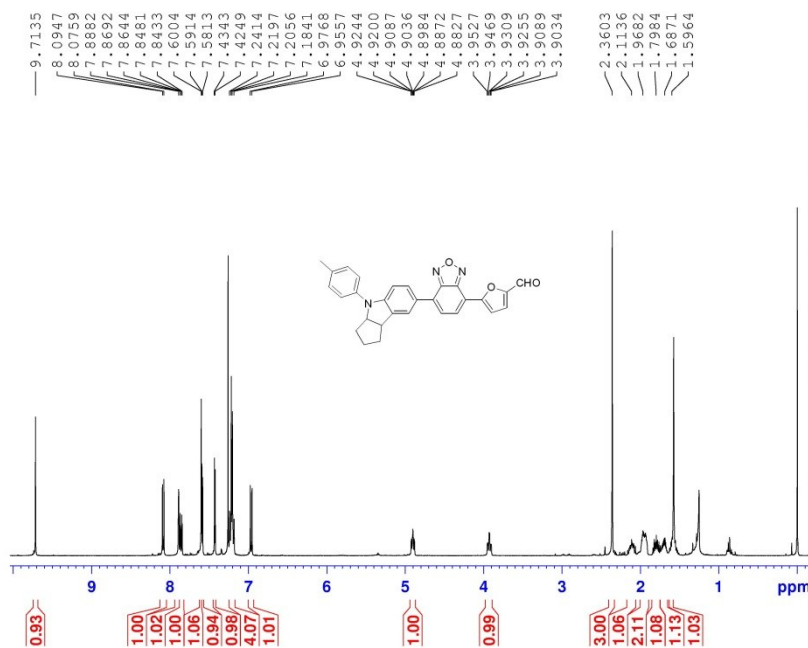


Minimum: -1.5
Maximum: 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
446.0866	446.0868	-0.2	-0.4	15.5	60.4	0.0	C ₂₄ H ₂₁ N ₃ O Br

Fig. S3 HRMS of compound 1

PROTON CDC13 {D:\data\research\2012-10-29} nmr 29



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NAME zw-wyz-006
EXPNO 10
PROCNO 1
Date_ 20121029
Time 17.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 293.5 K
D1 1.00000000 sec
TDO 1
===== CHANNEL f1 =====
NUC1 1H
P1 14.75 usec
PL1 -1.00 dB
PL1W 13.37643433 W
SF01 400.1324710 MHz
SI 32768
SE 400.1300087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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Fig. S4 ¹H NMR of compound 2 in CDCl₃

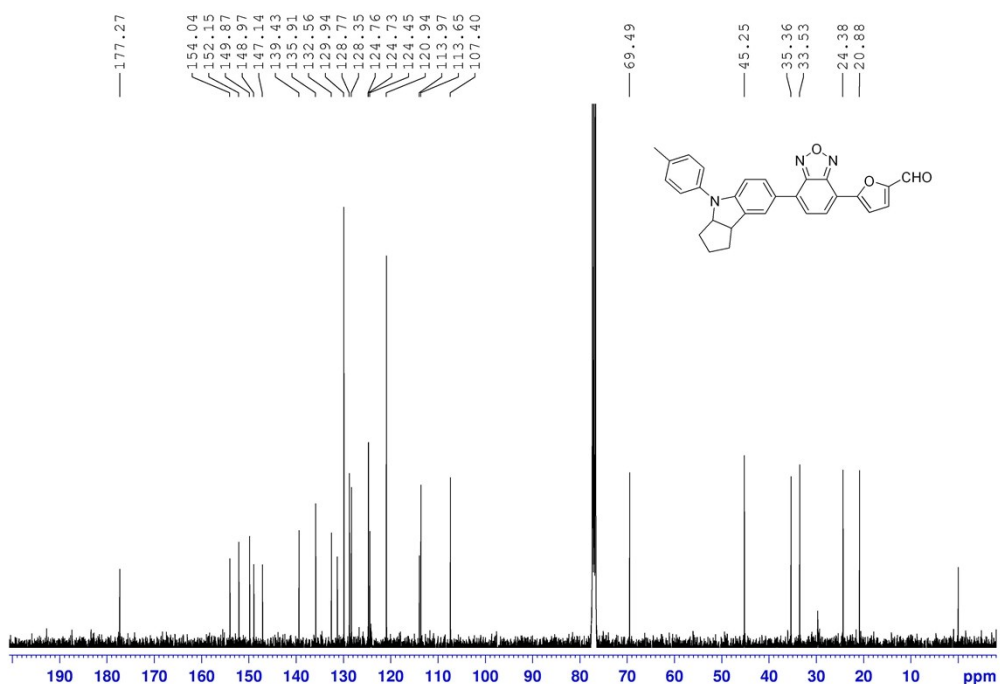


Fig. S5 ^{13}C NMR of compound **2** in CDCl_3

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-29 H: 0-70 N: 0-3 O: 0-3

WH-ZHU

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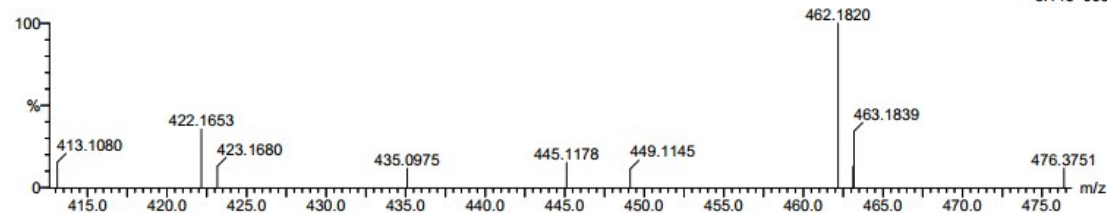
01-Nov-2012

20:19:08

1: TOF MS ES+

5.14e+003

ZW-WYZ-4 28 (0.937) Cm (24:30)



Minimum: -1.5
Maximum: 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
462.1820	462.1818	0.2	0.4	19.5	21.0	0.0	C ₂₉ H ₂₄ N ₃ O ₃

Fig. S6 HRMS of compound **2**

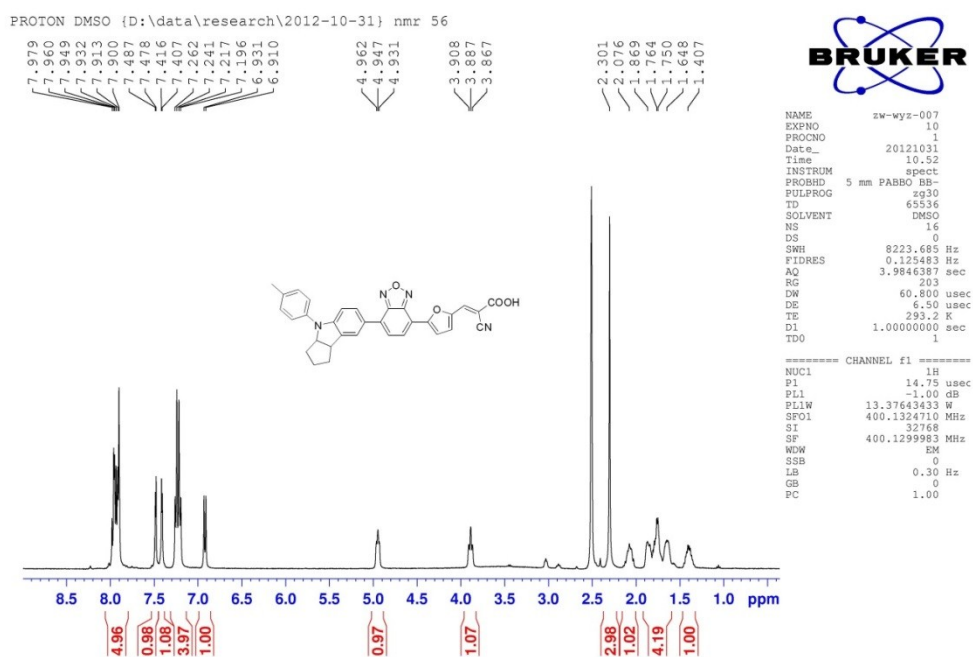


Fig. S7 ^1H NMR of WS-24 in $\text{DMSO-}d_6$

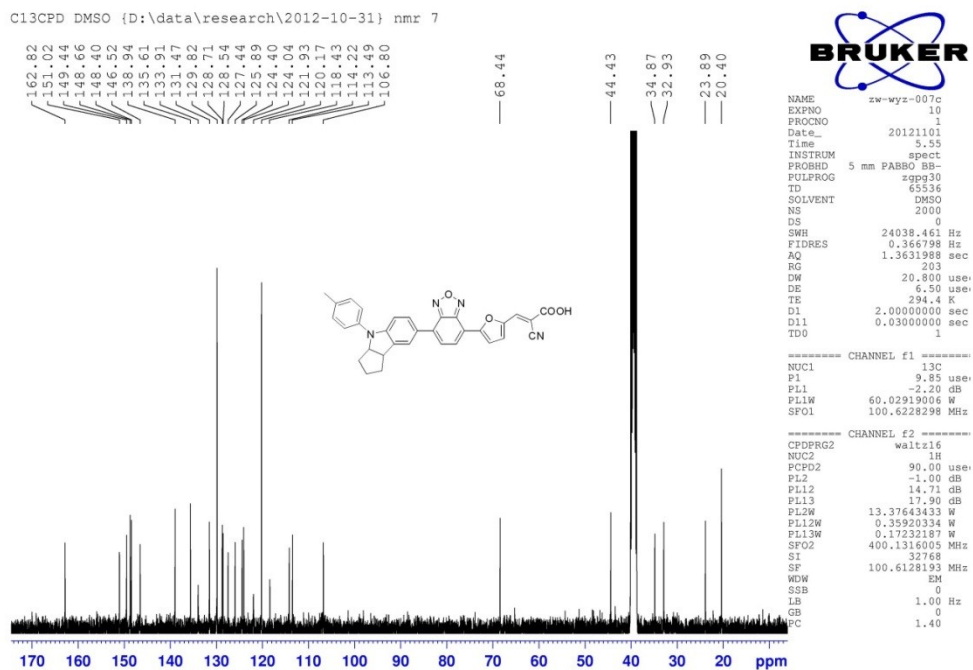


Fig. S8 ^{13}C NMR of WS-24 in $\text{DMSO-}d_6$

Single Mass Analysis

Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

33 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-32 H: 0-70 N: 0-4 O: 0-4

WH-ZHU

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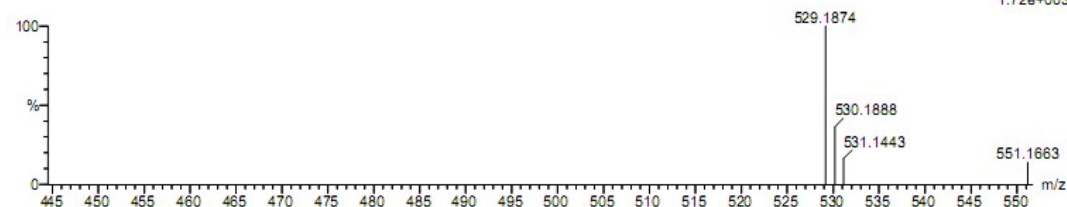
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1: TOF MS ES+

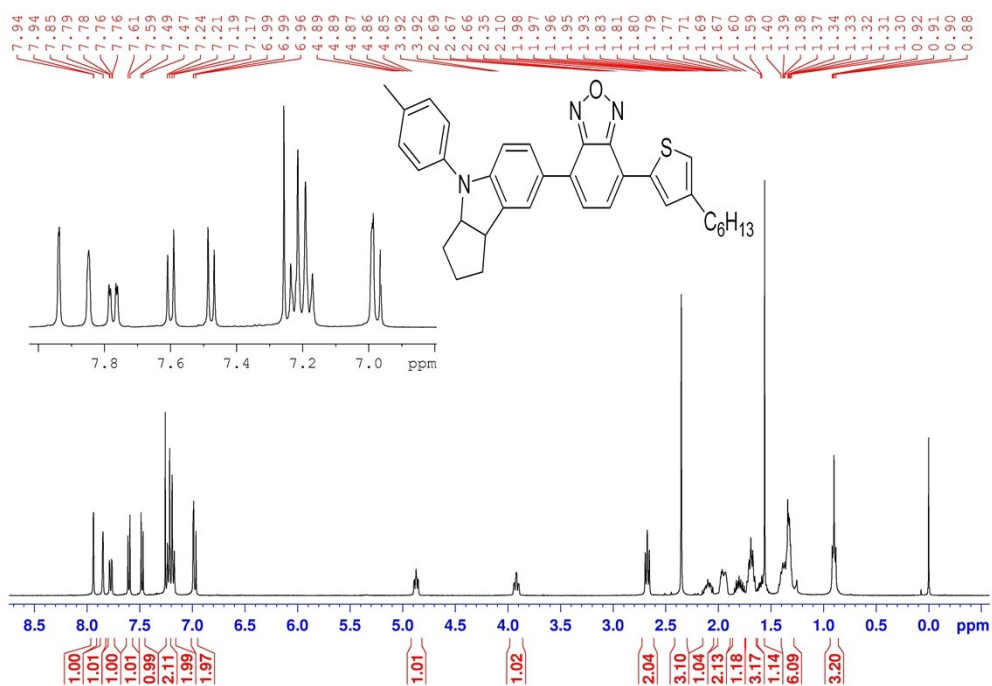
1.72e+003

ZW-WYZ-6 6 (0.274) Cm (5:8)



Mass	Calc. Mass	mDa	PFM	DBE	i-FIT	i-FIT (Norm)	Formula
529.1874	529.1876	-0.2	-0.4	22.5	8.0	0.0	C32 H25 N4 O4

Fig. S9 HRMS of compound WS-24

Fig. S10 ^1H NMR of compound **3** in CDCl_3

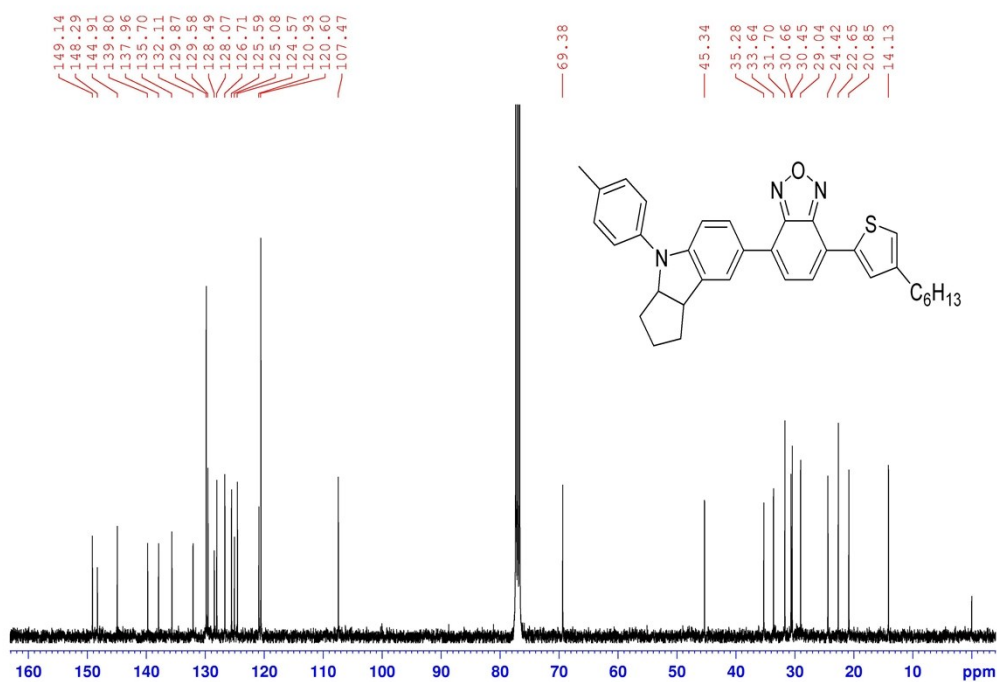


Fig. S11 ¹³C NMR of compound 3 in CDCl₃

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

260 formula(e) evaluated with 16 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-45 H: 0-40 N: 0-4 O: 0-4 S: 0-2

WH-ZHU

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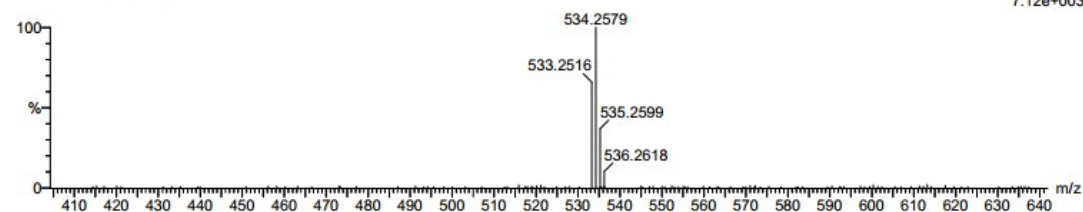
09-Oct-2013

15:03:32

1: TOF MS ES+

7.12e+003

ZWH-ZHB-3 35 (0.314) Cm (28:36)



Minimum: -1.5
Maximum: 30.0 50.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
534.2579	534.2579	0.0	0.0	18.5	73.2	0.0	C34 H36 N3 O S

Fig. S12 HRMS of compound 3

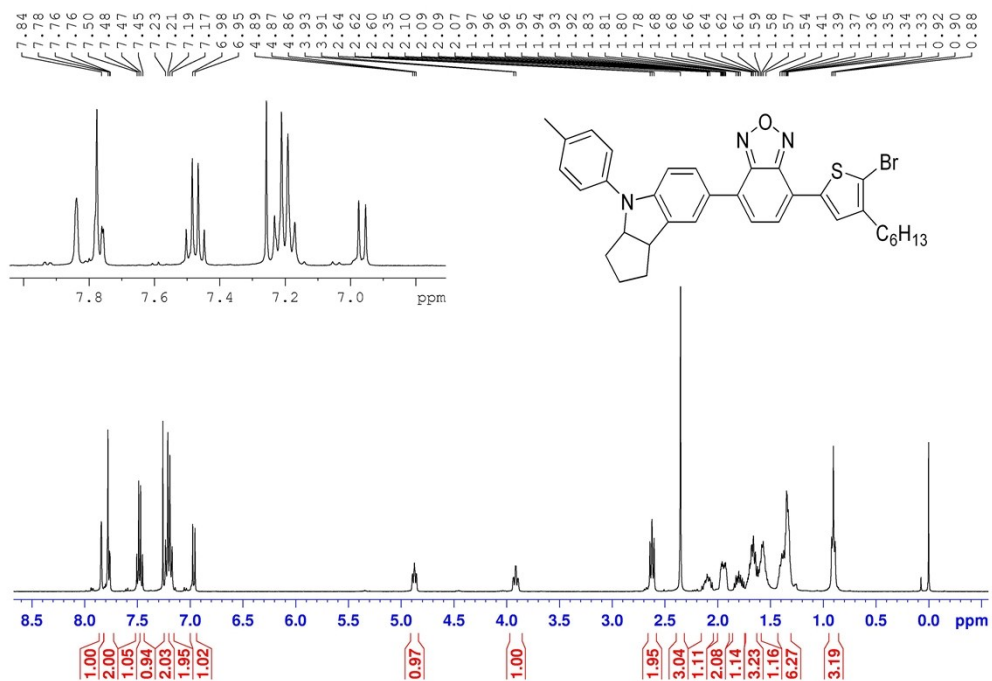


Fig. S13 ¹H NMR of compound 4 in CDCl₃

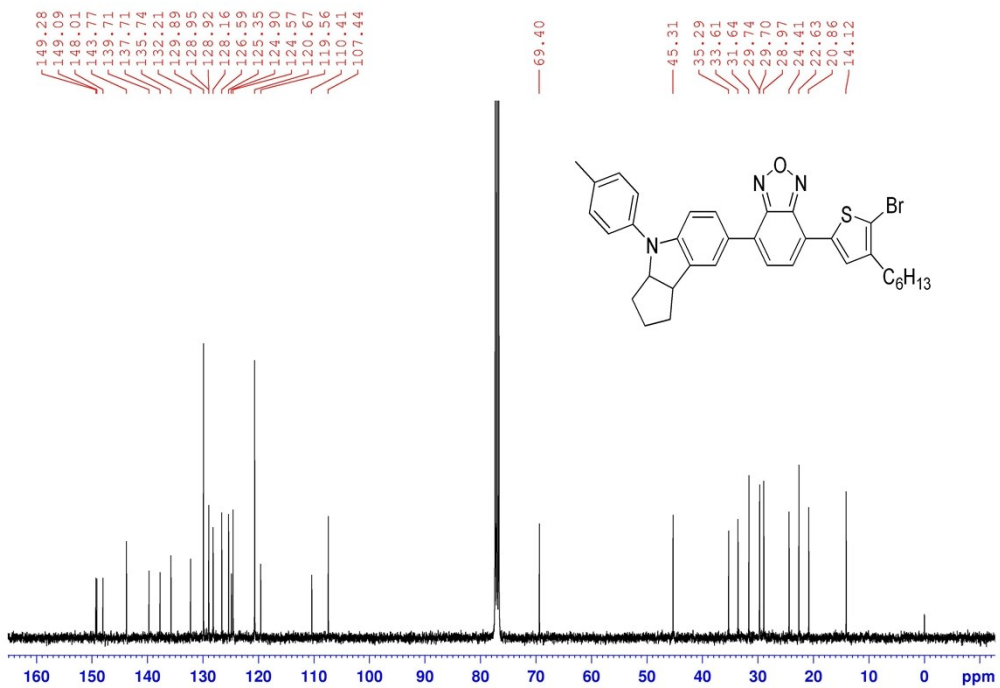


Fig. S14 ¹³C NMR of compound 4 in CDCl₃

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

27 formula(e) evaluated with 2 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 0-36 H: 0-40 N: 0-3 O: 0-1 S: 0-1 Br: 0-1

WH-ZHU

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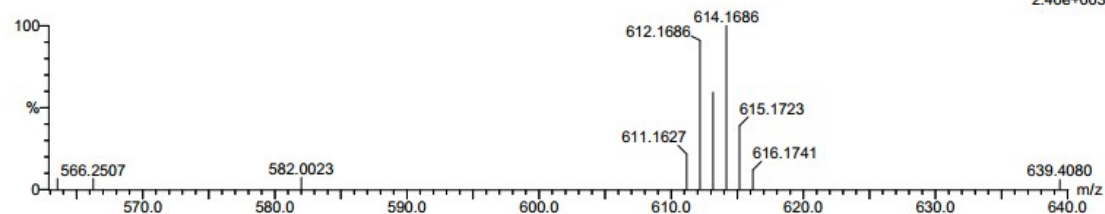
09-Oct-2013

ZWH-ZHB-4 83 (0.608) Cm (80:84)

15:08:32

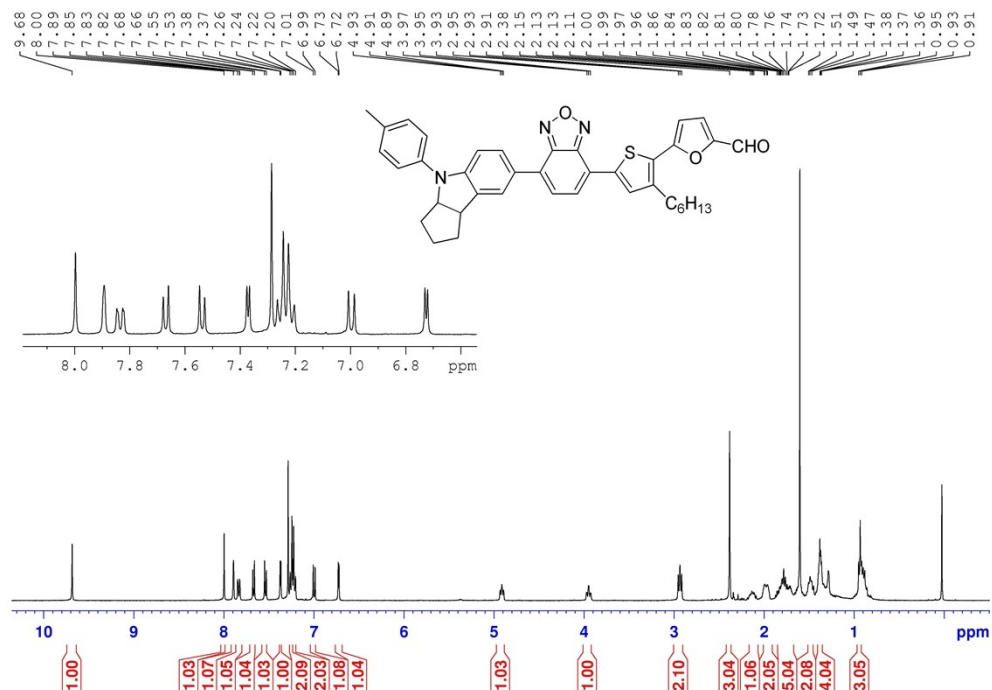
1: TOF MS ES+

2.40e+003



Minimum:	Maximum:							
		300.0	50.0	-1.5				
				100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
612.1686	612.1684	0.2	0.3	18.5	15.0	0.0	C34 H35 N3 O S Br	

Fig. S15 HRMS of compound 4

Fig. S16 ¹H NMR of compound 5 in CDCl₃

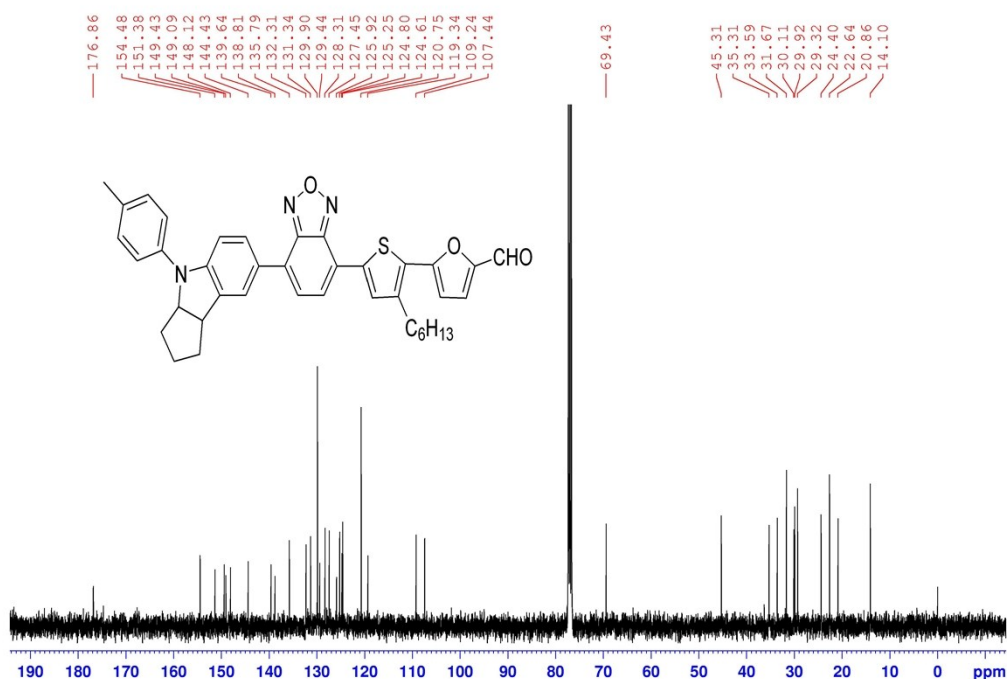


Fig. S17 ^{13}C NMR of compound 5 in CDCl_3

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

199 formula(e) evaluated with 11 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-45 H: 0-40 N: 0-4 O: 0-4 S: 0-2

WH-ZHU

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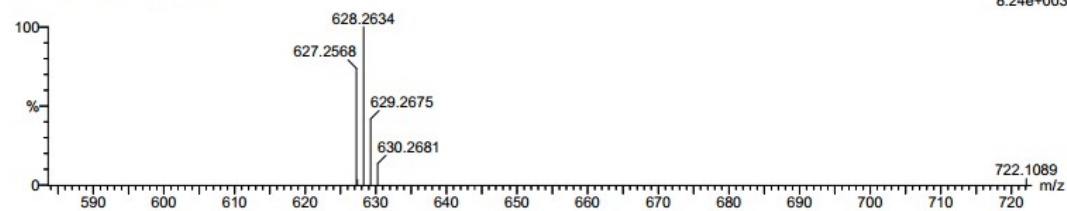
09-Oct-2013

15:16:31

1: TOF MS ES+

8.24e+003

ZWH-ZHB-5 65 (0.494) Cm (65.69)



Minimum: -1.5
Maximum: 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
628.2634	628.2634	0.0	0.0	22.5	11.6	0.0	$\text{C}_{39}\text{H}_{38}\text{N}_3\text{O}_3\text{S}$

Fig. S18 HRMS of compound 5

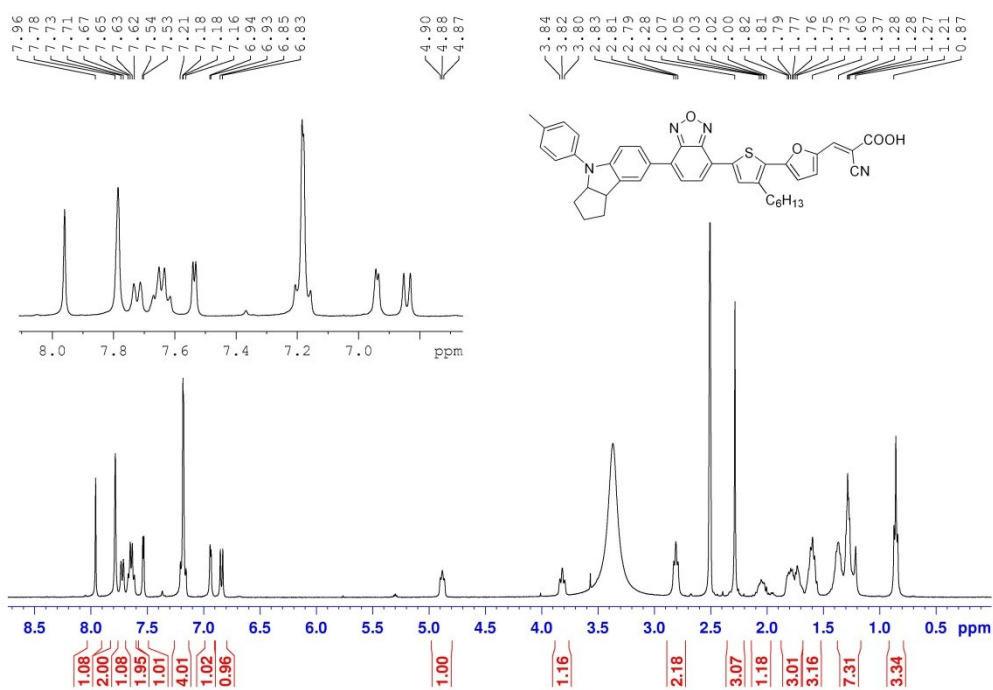


Fig. S19 ¹H NMR of WS-26 in DMSO-*d*₆

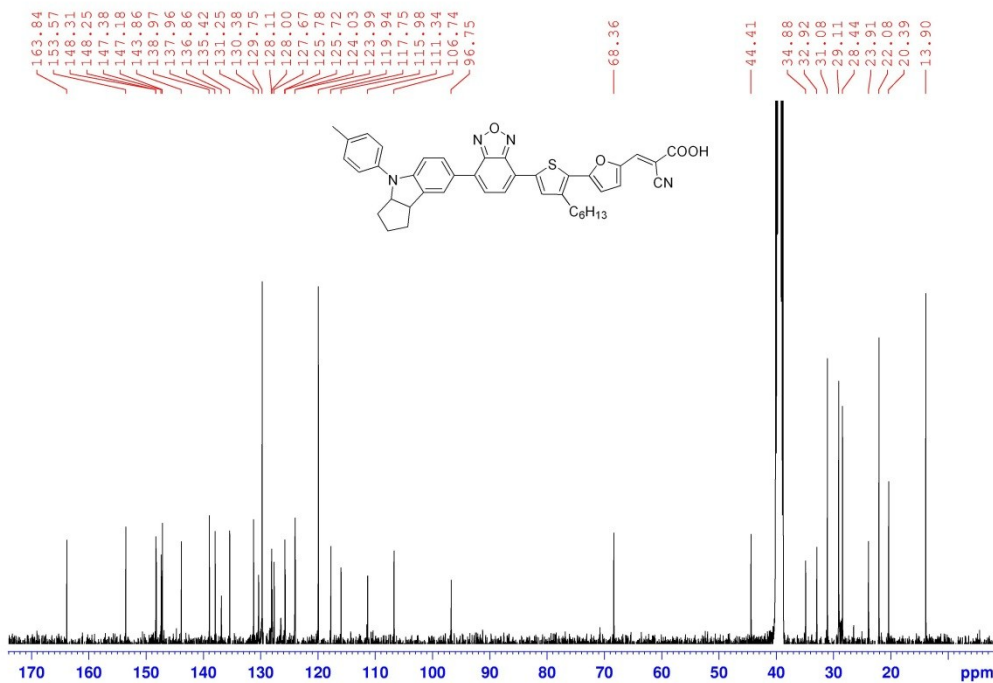


Fig. S20 ¹³C NMR of dye WS-26 in DMSO-*d*₆

Single Mass Analysis

Tolerance = 1000.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Odd and Even Electron Ions

34 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 0-42 H: 0-40 N: 0-4 O: 0-4 S: 0-1

WH-ZHU

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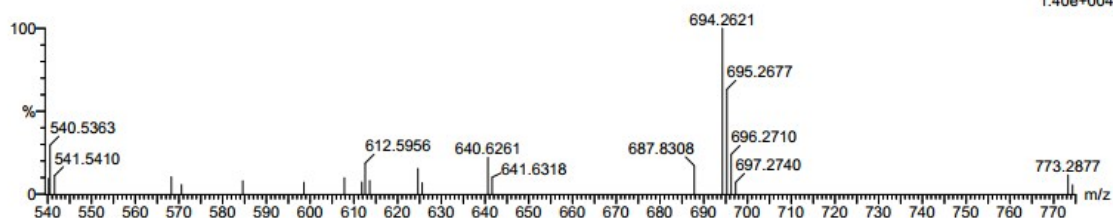
23-Mar-2015

08:35:59

1: TOF MS ES+

1.40e+004

ZWH-ZHB-2 199 (1.309) Cm (196:200)



Minimum: -1.5
 Maximum: 1000.0 50.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
694.2621	694.2614	0.7	1.0	26.0	17.6	0.0	C42 H38 N4 O4 S

Fig. S21 HRMS of WS-26