

Electronic Supplementary Information (ESI)

A red fluorescent turn-on chemosensor for Al³⁺ based on dimethoxy triarylamine-benzothiadiazole derivative with aggregation-induced emission

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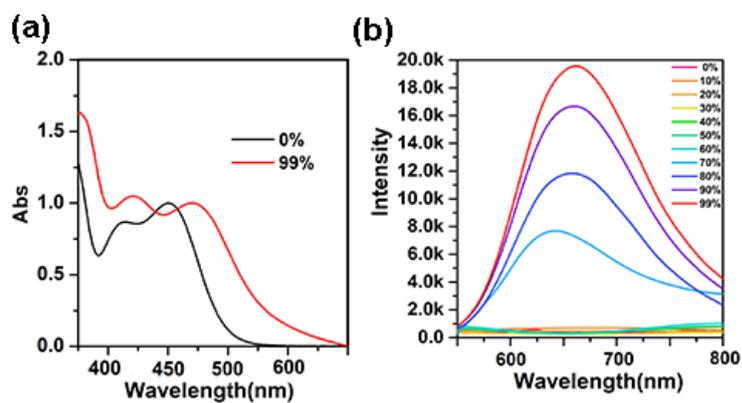


Fig. S1. (a) Normal absorption of **TB-COOH** in DMSO and DMSO/HEPES mixtures ($f_w = 99$ vol %). (b) Fluorescence emission spectra of **TB-COOH** in DMSO and DMSO/HEPES mixtures with different HEPES fractions (f_w). Solution concentration: 1×10^{-4} M.

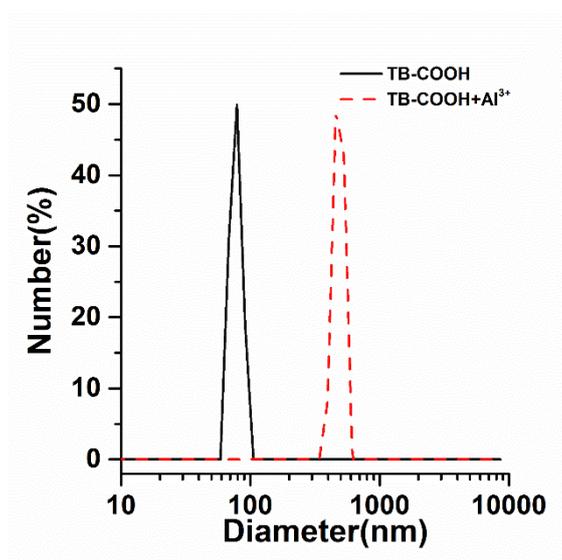


Fig. S2. Dynamic light scattering data for **TB-COOH** (20 μ M) with and without Al^{3+} (10 μ M) the DMSO/HEPES mixtures containing 50 vol% DMSO)

Characterization Data

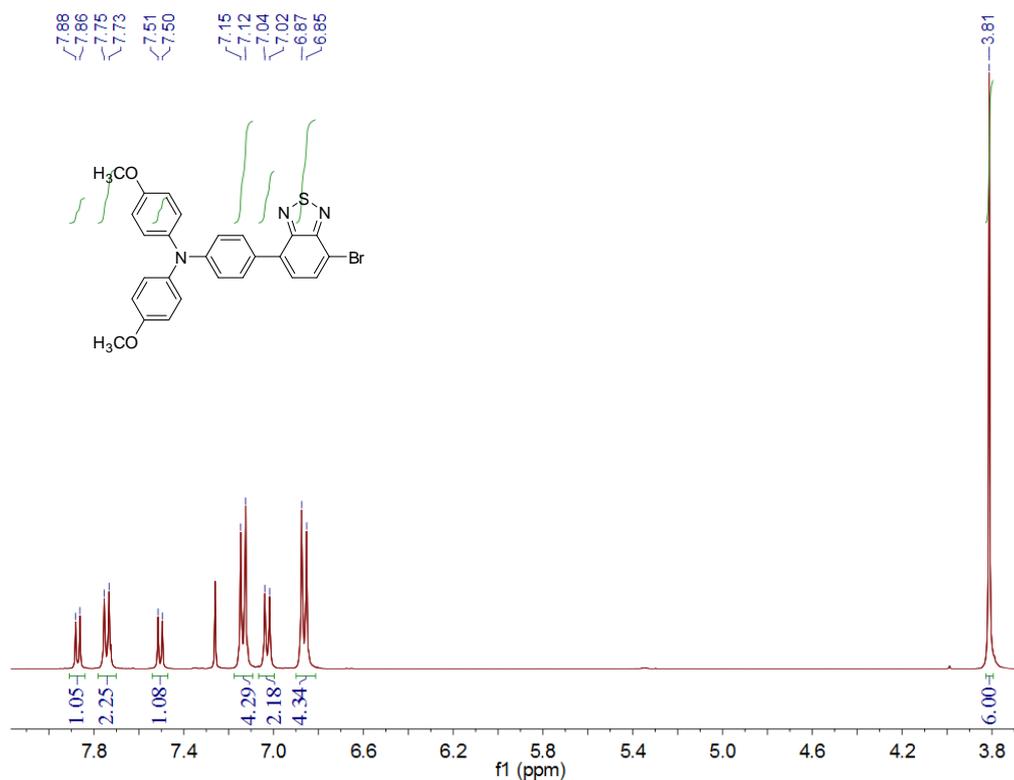


Fig. S3. ¹H NMR spectrum of **2** in CDCl₃

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 100.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

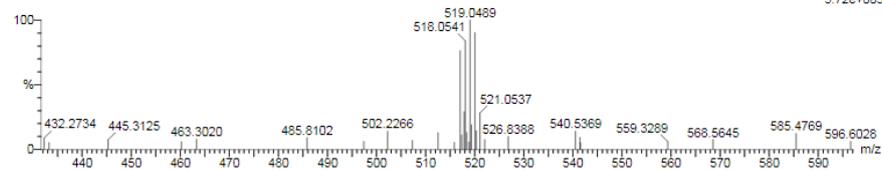
Monoisotopic Mass, Even Electron Ions
 41 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
 Elements Used:
 C: 0-26 H: 0-21 N: 0-3 O: 0-2 S: 0-1 Br: 0-1

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06-Nov-2016
 19:17:09
 1: TOF MS ES+
 3.72e+003

HL-LN-018 44 (0.629) Cm (44.46)



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
518.0541	518.0538	0.3	0.6	17.5	76.6	0.0	C ₂₆ H ₂₁ N ₃ O ₂ S Br

Fig. S4. High-Resolution mass spectrum of **2**

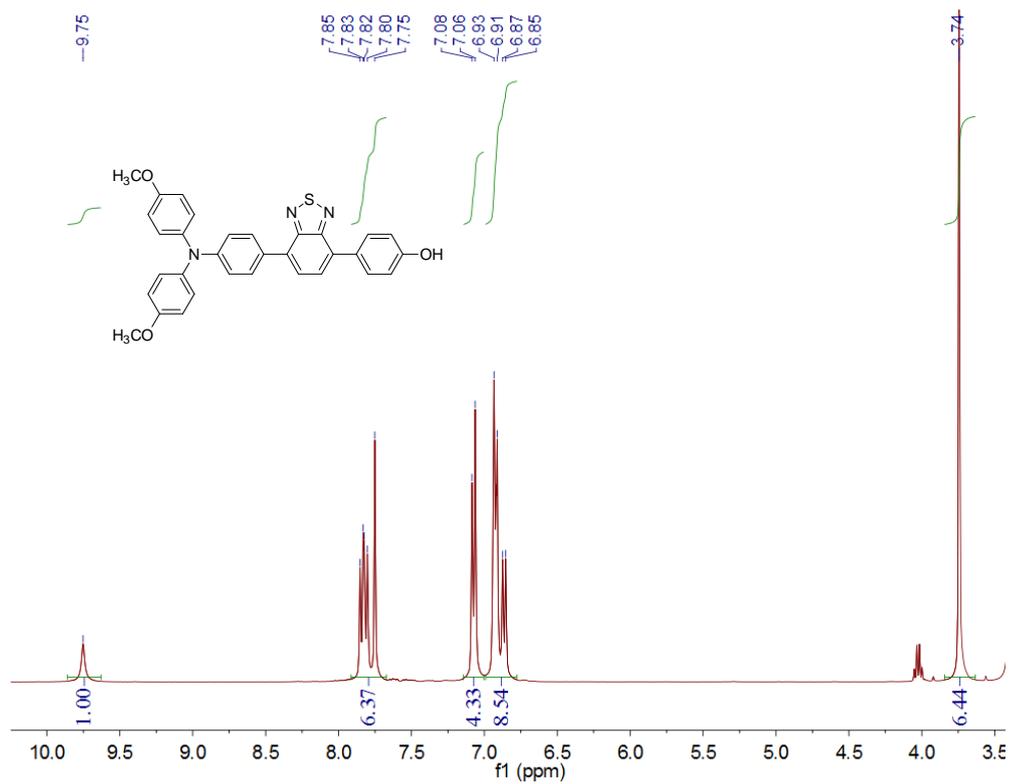


Fig. S5. ¹H NMR spectrum of 3 in DMSO-d₆

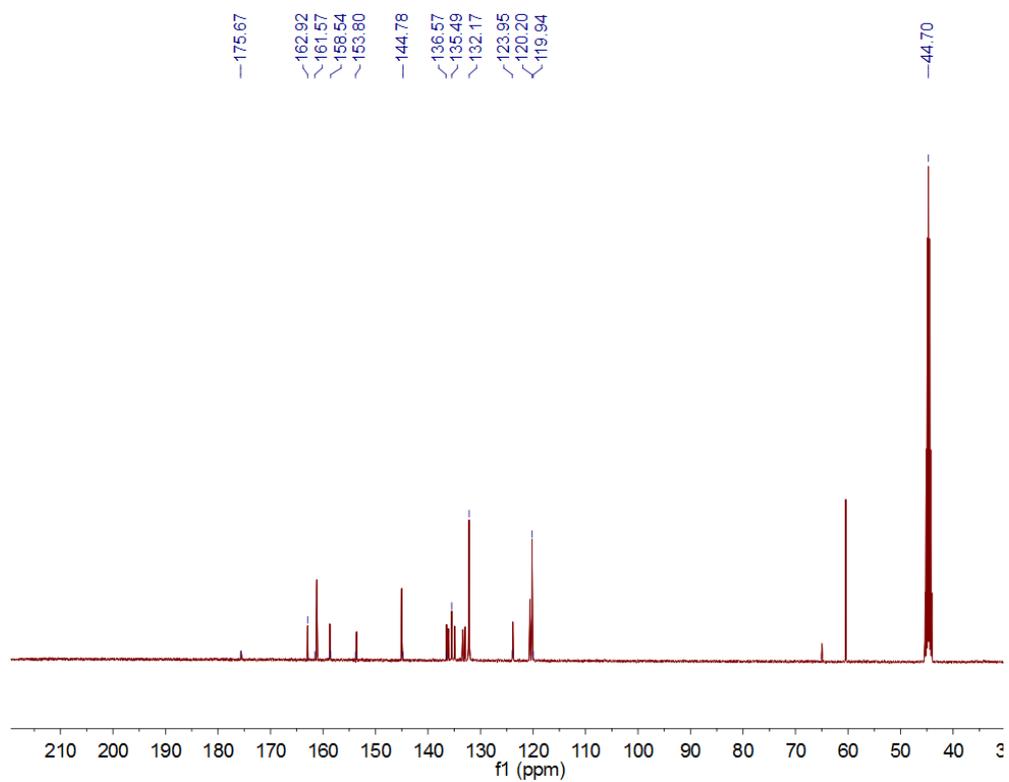


Fig. S6. ¹³C NMR spectrum of 3 in DMSO-d₆

Elemental Composition Report

Page 1

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 = 3

Monoisotopic Mass, Even Electron Ions

112 formula(e) evaluated with 12 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-35 H: 0-33 N: 0-3 O: 0-5 S: 0-2

JL-HUA

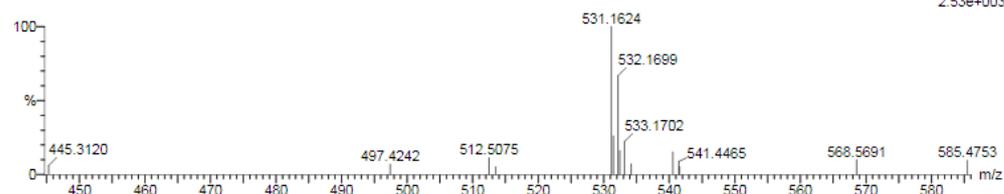
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17-Oct-2016

20:32:17

1: TOF MS ES+
2.53e+003

HL-LN-0019 (0.202) Cm (8:9)



Minimum: -1.5
Maximum: 300.0 50.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
532.1699	532.1695	0.4	0.8	21.5	21.8	0.0	C32 H26 N3 O3 S

Fig. S7. High-Resolution mass spectrum of 3

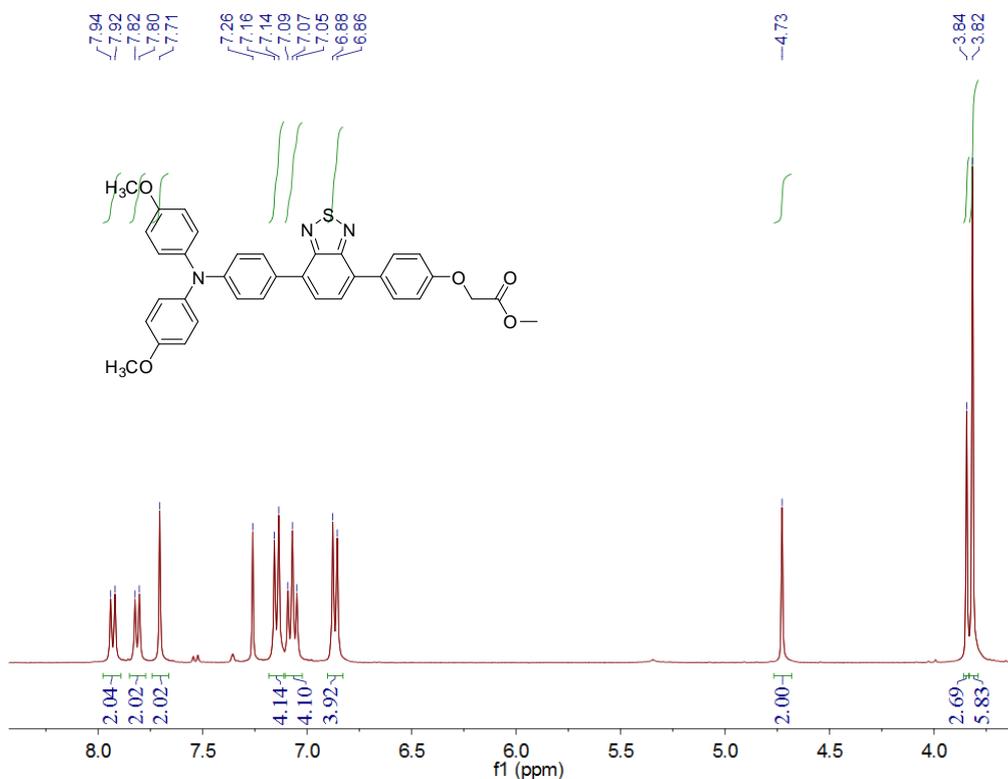


Fig. S8. ¹H NMR spectrum of 4 in CDCl₃

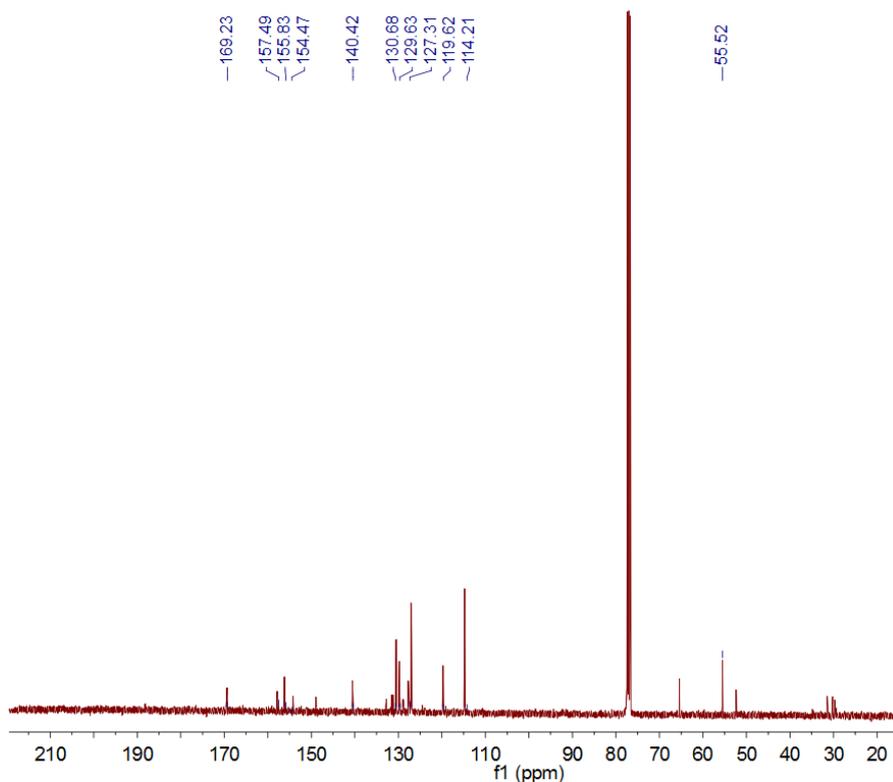


Fig. S9. ¹³C NMR spectrum of **4** in CDCl₃

Elemental Composition Report

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 = 3

Monoisotopic Mass, Even Electron Ions

51 formula(e) evaluated with 2 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-35 H: 0-33 N: 0-3 O: 0-5 S: 0-2

JL-HUA

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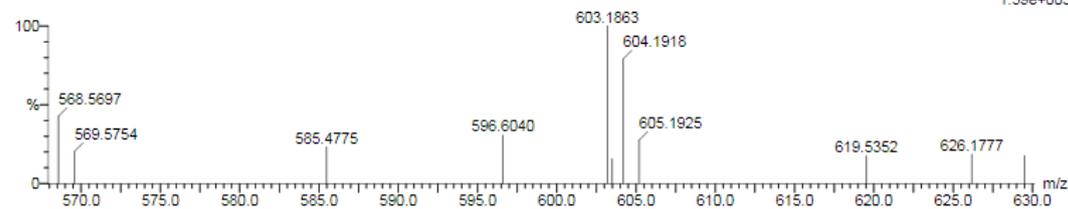
17-Oct-2016

20:27:02

1: TOF MS ES+

1.39e+003

HL-LN-002 117 (1.515) Cm (112:117)



Minimum:

Maximum: 300.0 50.0 -1.5

100.0

Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

604.1918 604.1906 1.2 2.0 22.5 22.8 0.0 C35 H30 N3 O5 S

Fig. S10. High-Resolution mass spectrum of **4**

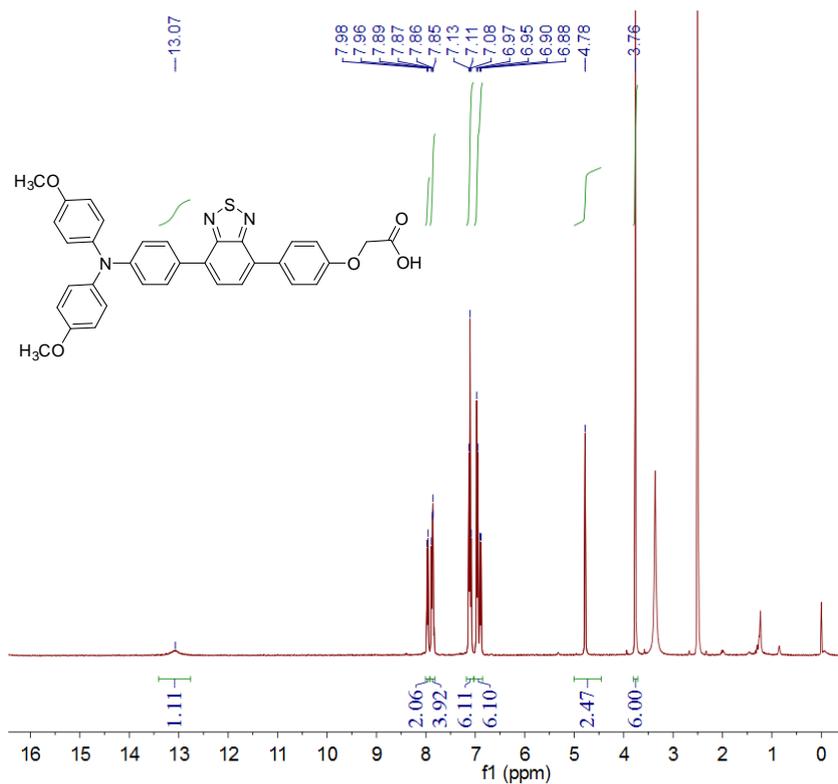


Fig. S11. ¹H NMR spectrum of TB-COOH in DMSO-d₆

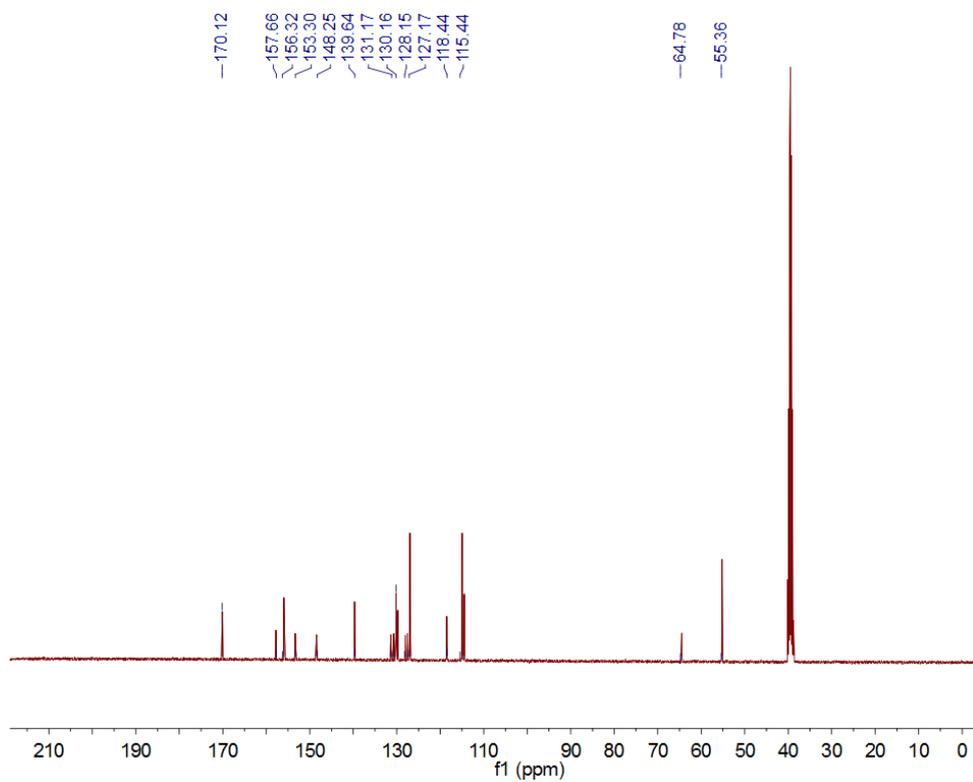


Fig. S12. ¹³C NMR spectrum of TB-COOH in DMSO-d₆

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 = 3

Monoisotopic Mass, Even Electron Ions

204 formula(e) evaluated with 24 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-94 H: 0-33 N: 0-3 O: 0-5 S: 0-2

JL-HUA

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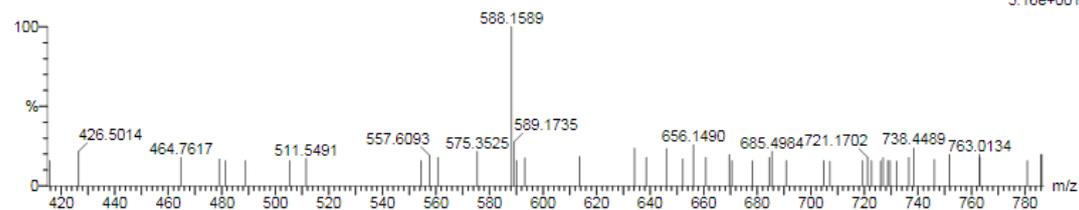
17-Oct-2016

20:21:03

1: TOF MS ES-

5.16e+001

HL-LN-003 74 (1.705) Cm (74.75)



Minimum:

Maximum: 300.0 50.0 -1.5

100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
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588.1589	588.1593	-0.4	-0.7	23.5	7.7	0.0	C34 H26 N3 O5 S
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Fig. S13. High-Resolution mass spectrum of TB-COOH