Electronic Supplementary Information (ESI)

Reversible mechanofluorochromism and acidochromism using a cyanostyrylbenzimidazole derivative with aggregation-induced emission

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Table S1. Photophysical data of **TBM** in different solvents.

Solvent	λ_{abs} (nm)	ε^{max} (M^{-1} cm^{-1})	λ_{em} (nm)	$\Delta\nu_{st}$[a] (cm^{-1})	Φ_f[b]
Hexane	296, 397	28900	490	4781	0.010
Cyclohexane	296, 400	28600	491	4633	0.016
Toluene	295, 409	26800	510	4842	0.019
THF	295, 404	29100	524	5669	0.004
DCM	295, 412	29100	542	5822	0.005
DMF	295, 415	26900	551	5948	0.011
DMSO	296, 416	27000	560	6181	0.012

[a]$\Delta\nu_{st} = \nu_{abs}-\nu_{em}$; [b]The fluorescence quantum yield (Φ_f) was measured using 9,10-diphenylanthracene (Φ_F = 0.85 in benzene, λ_{ex} = 390 nm) as the standard.

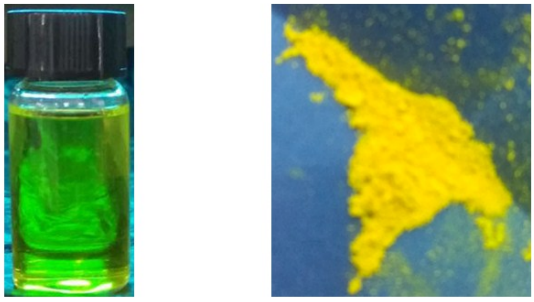


Fig. S1 Images of **TBM** in THF solution (10^{-5} M, left) and solid state (right) under 365 nm illumination.

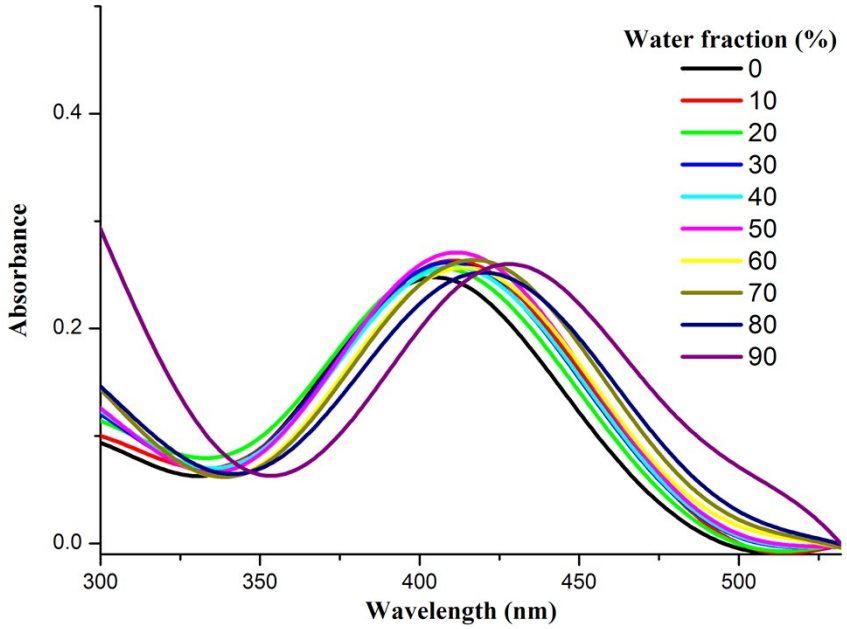


Fig. S2 UV-Vis spectra of **TBM** in the mixtures of THF and water, and concentration is 10^{-5} M.

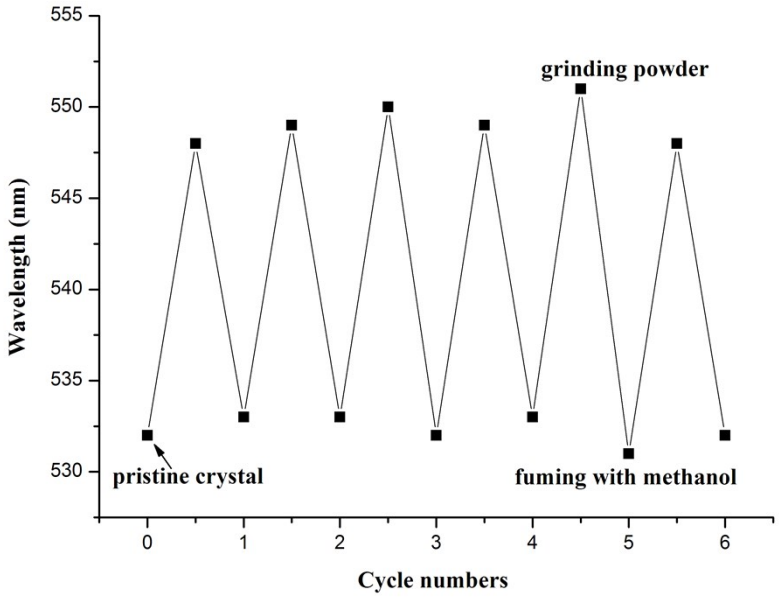


Fig. S3 Maximum fluorescent emission of compound **TBM** upon repeating treatment by grinding and fuming with methanol vapor.

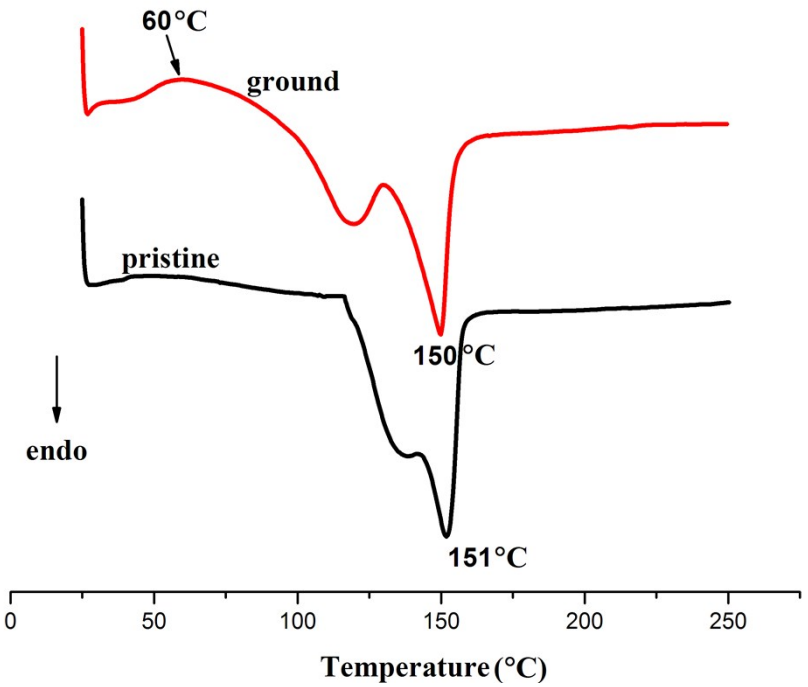


Fig. S4 DSC curves of compound **TBM** in the pristine crystal and ground powder under nitrogen atmosphere at a heating rate at 10 °C/min.

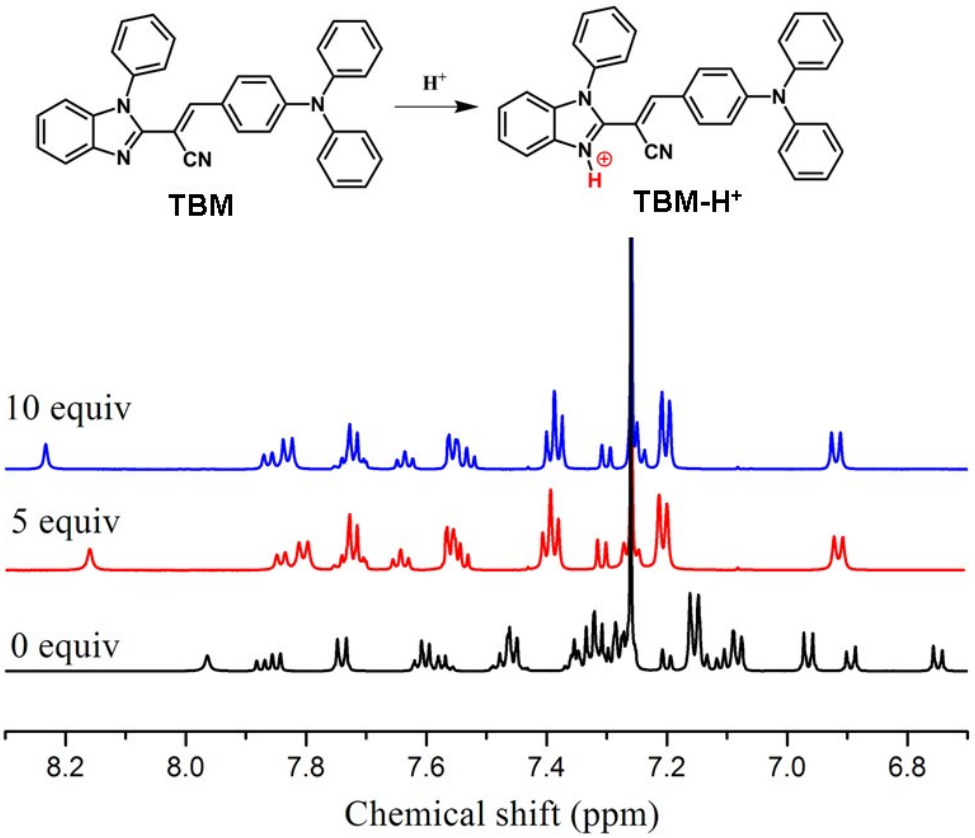


Fig. S5 ^{1}H NMR spectra of **TBM** in $CDCl_3$ in the: absence (0 equiv) and presence of 5 equiv and 10 equiv of TFA.

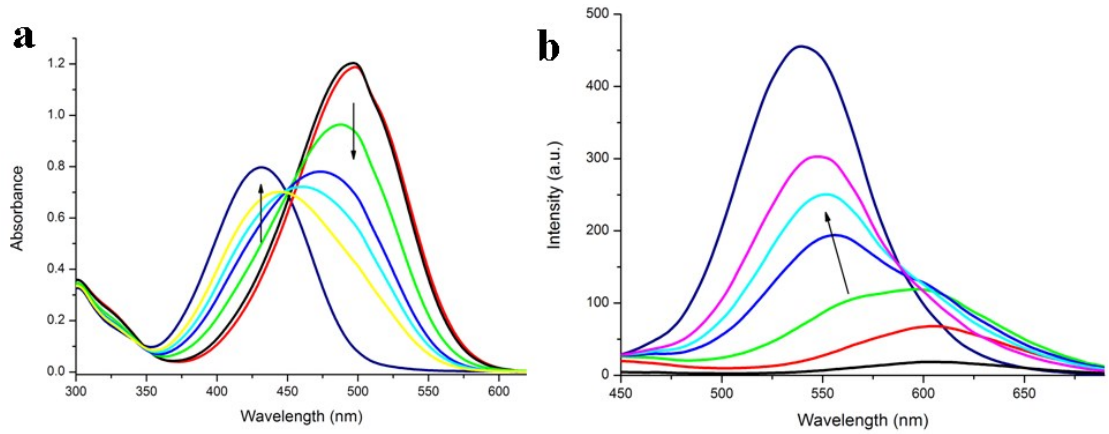


Fig. S6 UV-vis absorption (a) and emission (b) spectral changes of **TBM** chloroform solution containing 500 equiv. TFA from 0 equiv. to 500 equiv. with additional TEA at room temperature. The concentration of **TBM** was maintained at 2.5 × 10^{-5} M; Excitation wavelength is 410 nm.

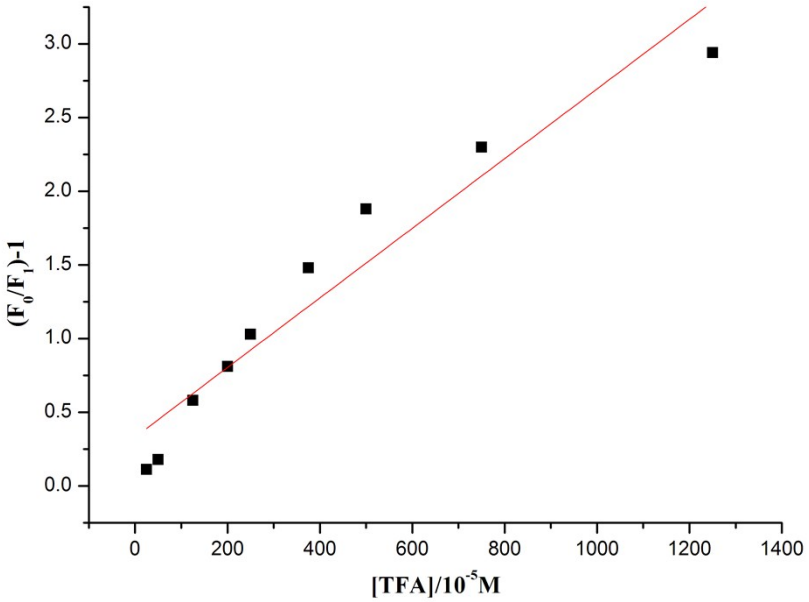


Fig. S7 Stern-Volmer plot for **TBM** towards TFA in $CHCl_3$, the concentration of **TBM** was maintained at 2.5 × 10^{-5} M.

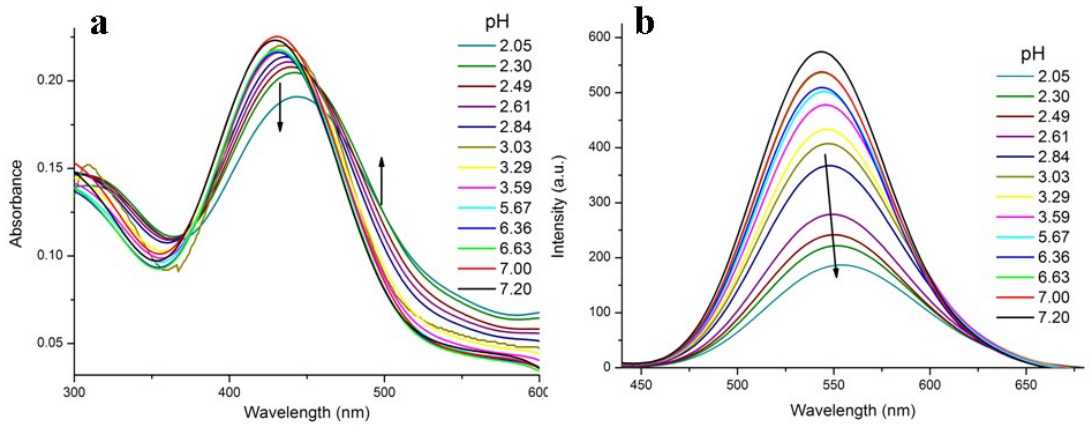


Fig. S8 The changes of absorption (a) and emission (b) spectra in the THF/H_2O (1:9, v/v) solution upon addition of H^+.

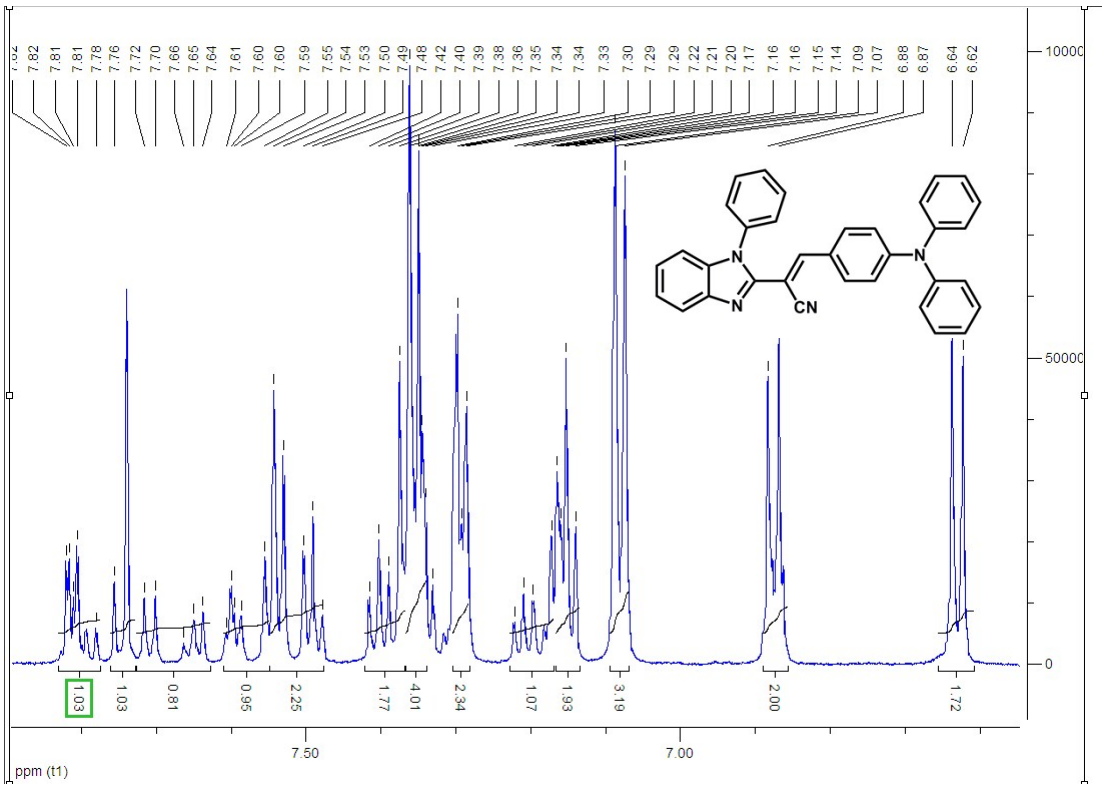


Fig. S9 ^{1}H-NMR (600 MHz, DMSO-d_6) spectra of compound **TBM**.

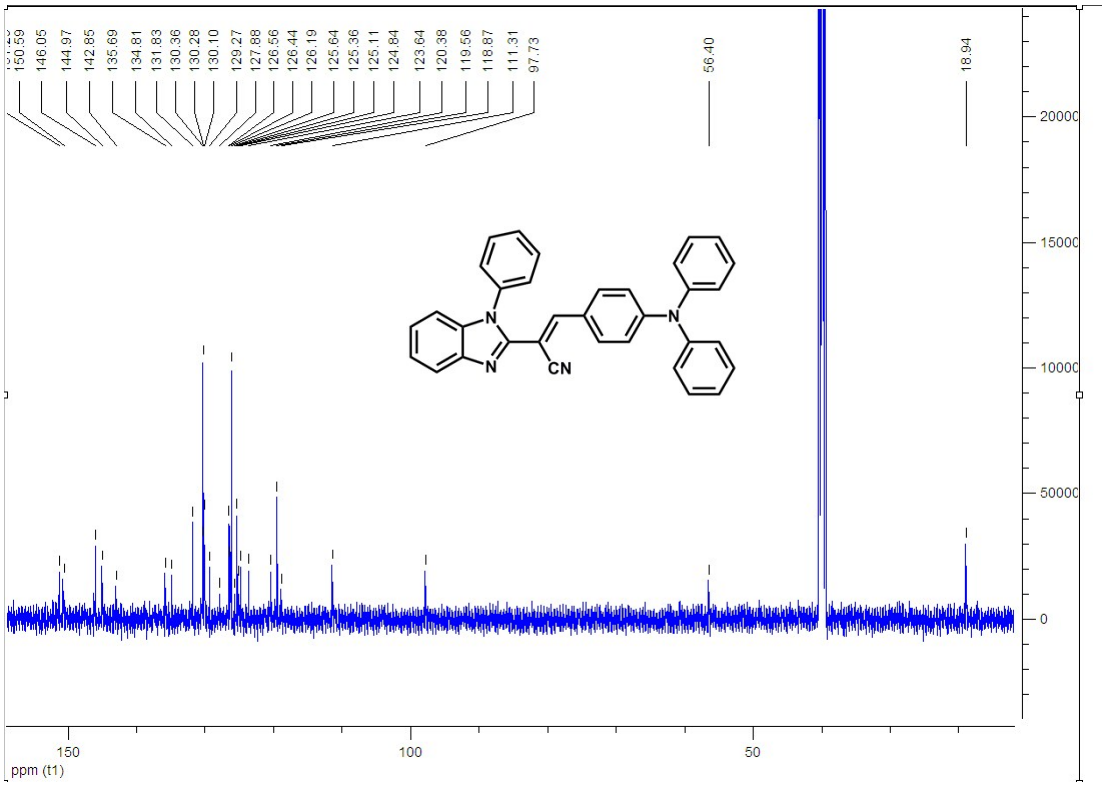


Fig. S10 ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **TBM**.

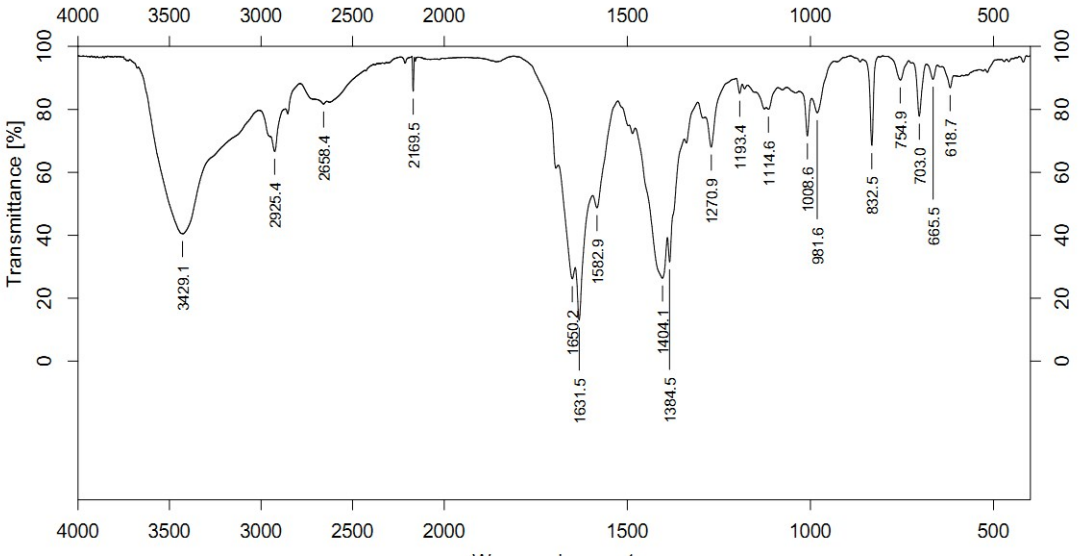
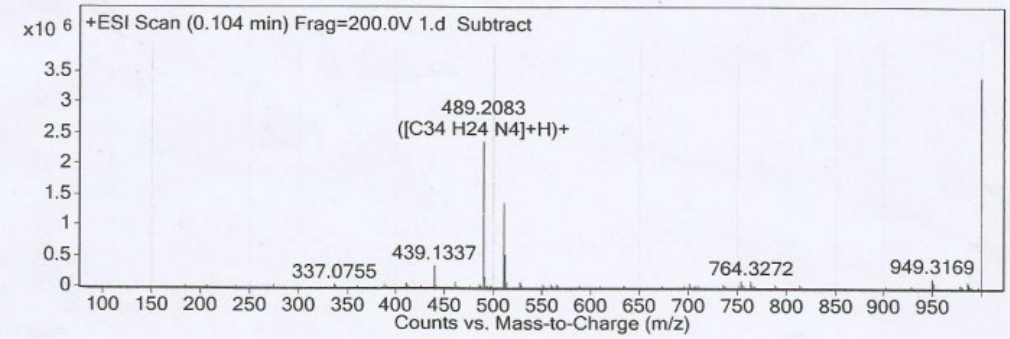


Fig. S11 FT-IR spectrum of compound **TBM**.

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
439.1337	1	344047.47		
489.2083	1	2371546.75	C34 H24 N4	(M+H)+
490.2125	1	870282.75	C34 H24 N4	(M+H)+
491.2147	1	162961.77	C34 H24 N4	(M+H)+
511.1911	1	1364347.75	C34 H24 N4	(M+Na)+
512.1944	1	527584.88	C34 H24 N4	(M+Na)+
754.2522	1	99309.31		
764.3272	1	104296.09		
949.3169	1	148879.36		
999.392		3417776.75		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C34 H24 N4	TRUE	488.2013	488.2001	-2.54	C34 H25 N4	95.53
C34 H24 N4	TRUE	488.2019	488.2001	-3.61	C34 H24 N4 Na	93.97

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Fig. S12 The HRMS spectrum of compound **TBM**.