

Electronic Supplementary Material

New Journal of Chemistry

A highly sensitive colorimetric chemodosimeter for cyanide anion by Michael addition based on coumarin derivative

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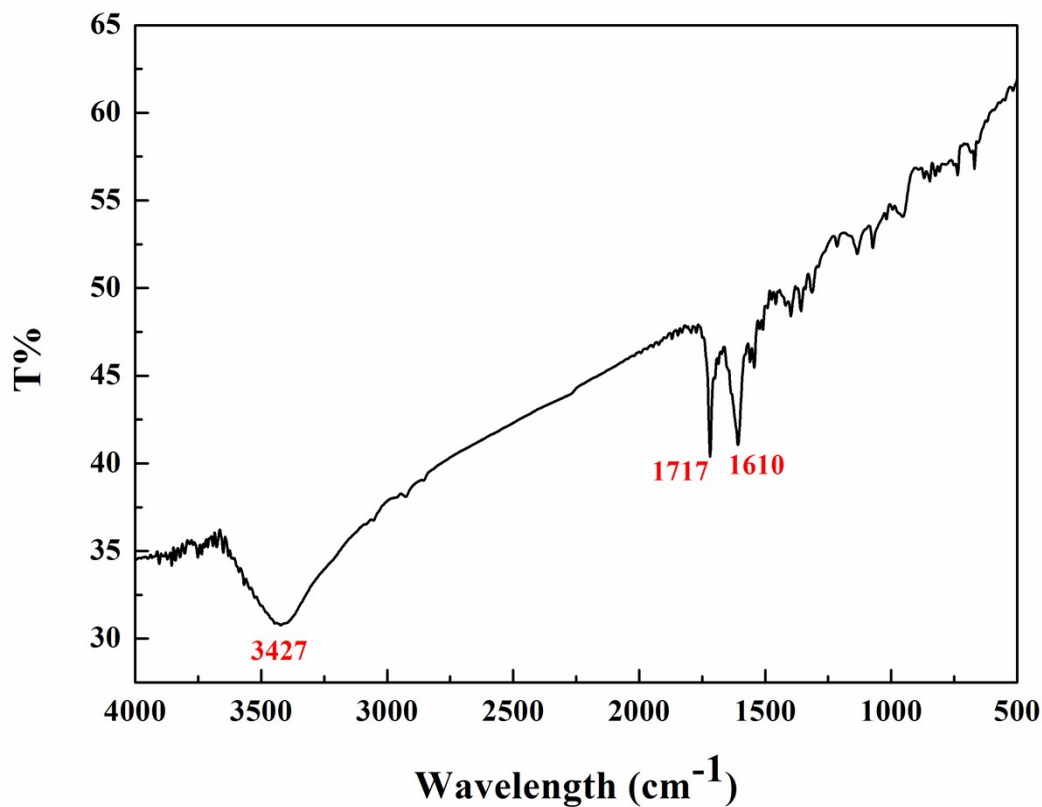


Fig. S1 FT-IR spectra of powdered L1.

LENGYANLI-XDS1-1H-0625
STANDARD 1H OBSERVE

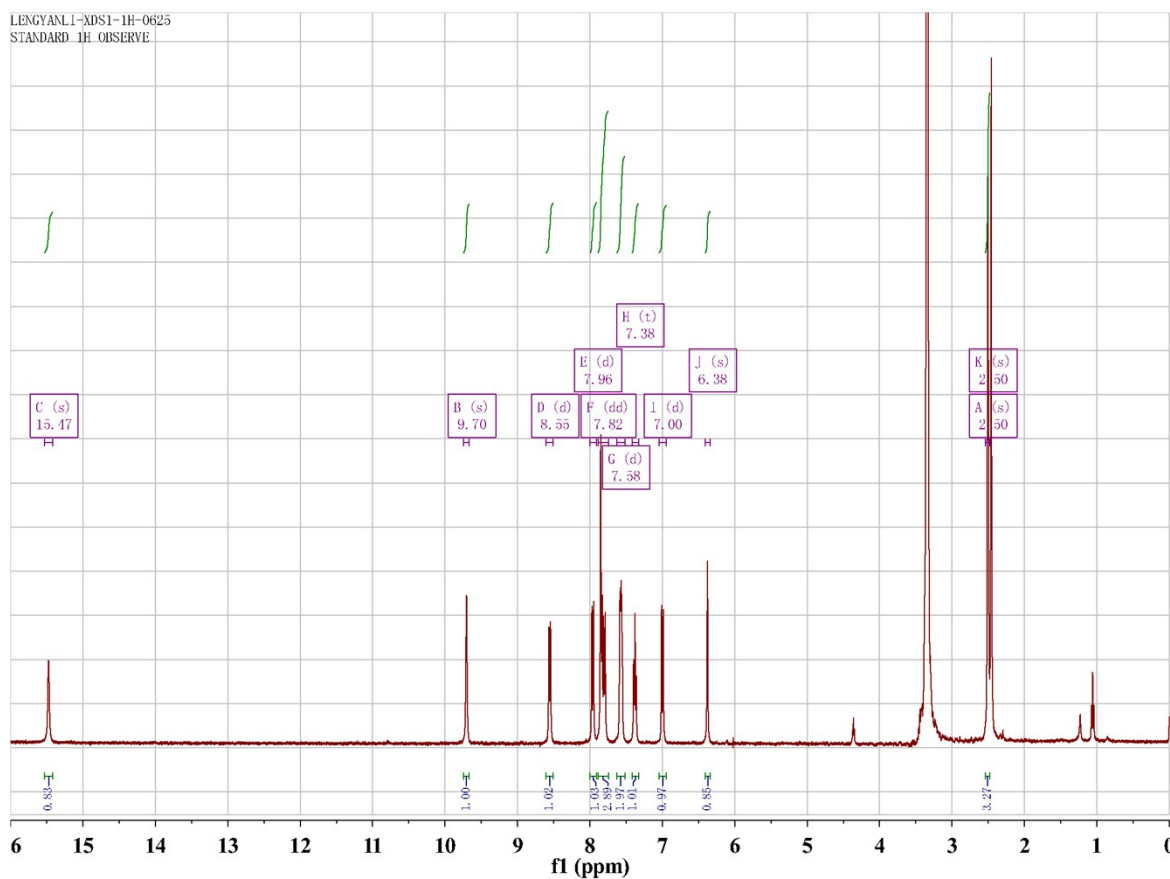


Fig. S2 Partial ^1H NMR spectra of L1 (0.05 M, $\text{DMSO-}d_6$).

Generic Display Report

Analysis Info

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Sample Name
Comment

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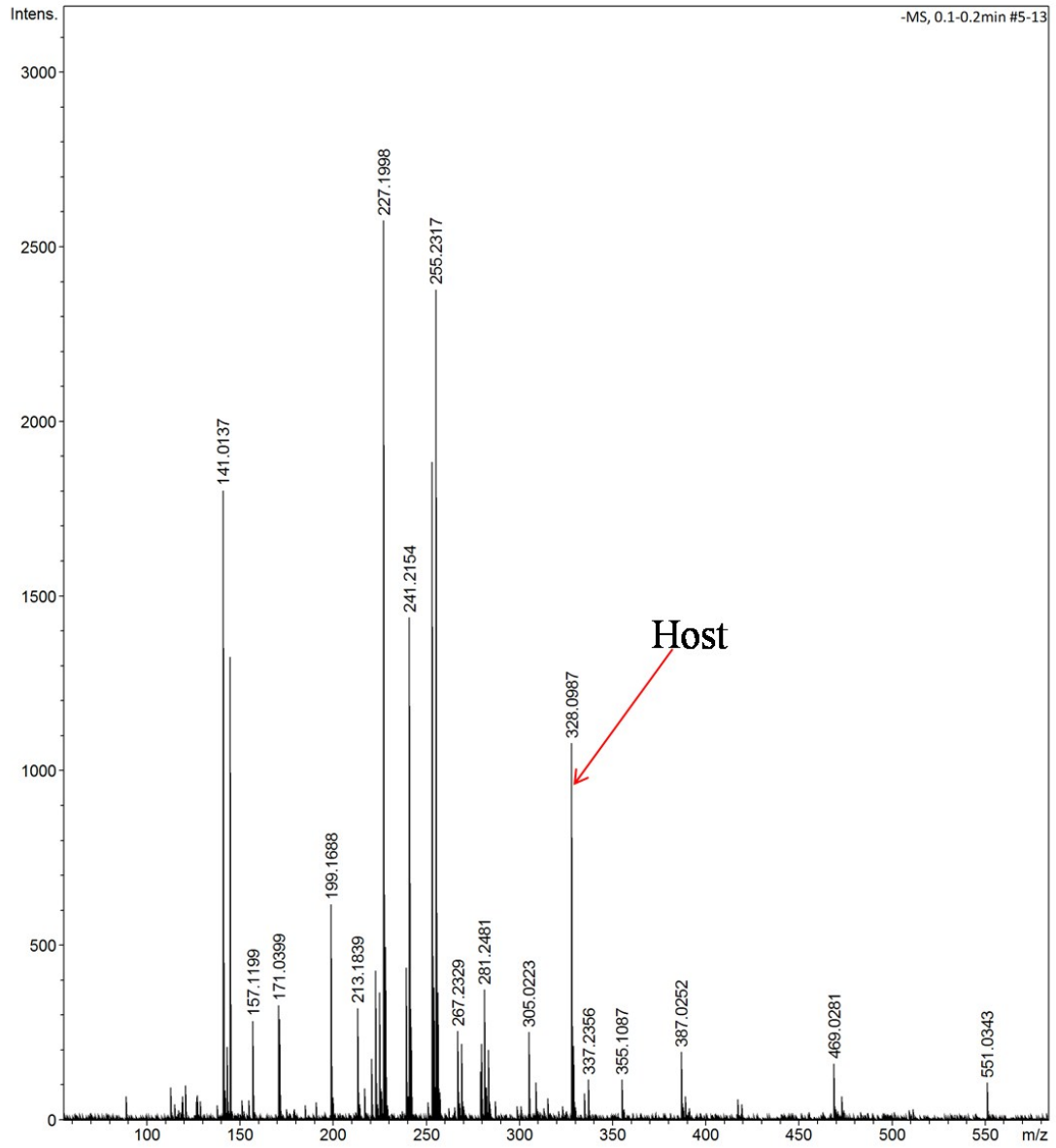


Fig. S3 ESI-MS spectrum of L1 in DMSO.

Generic Display Report

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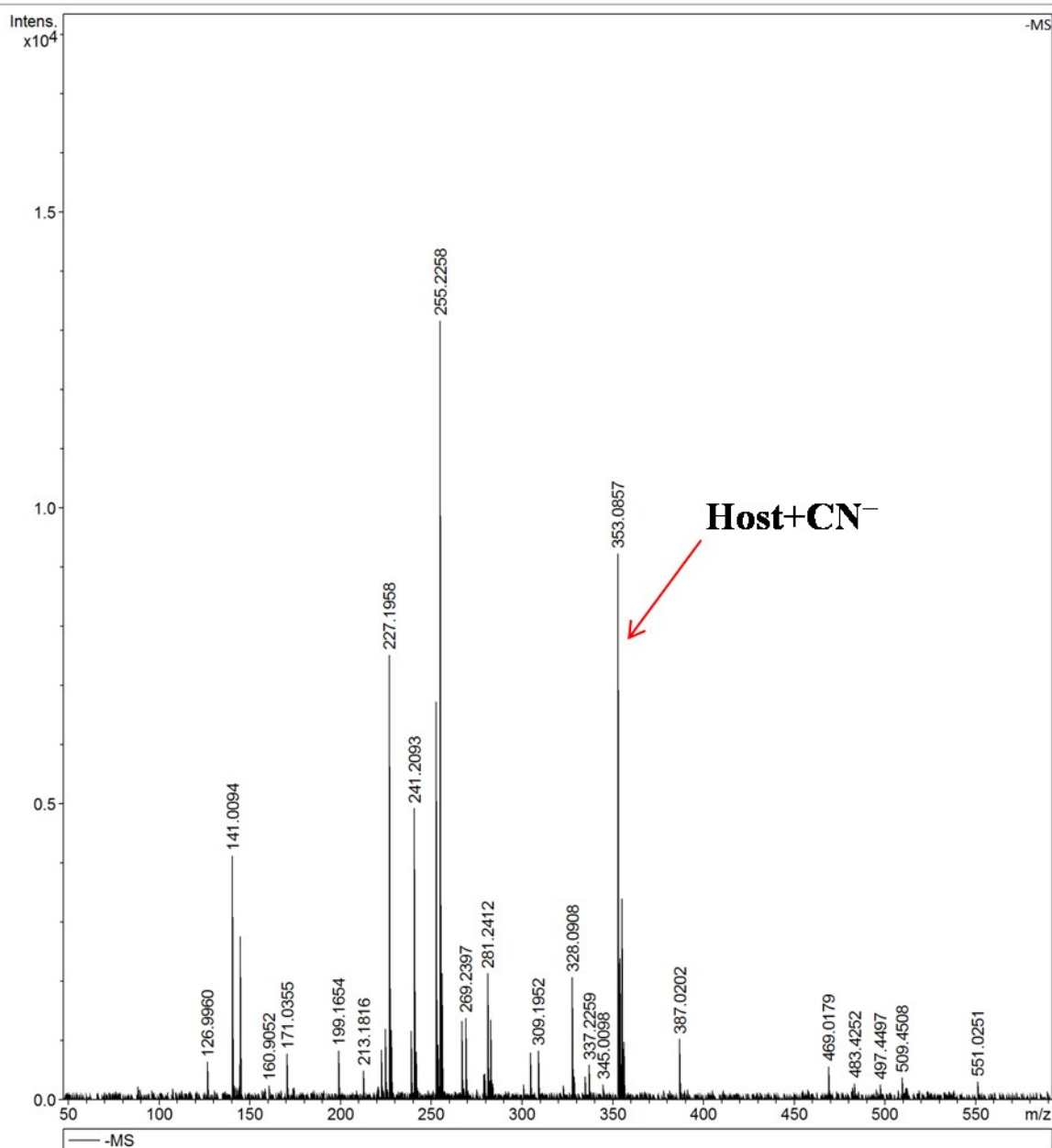


Fig. S4 ESI-MS spectrum of **L1+CN⁻** in DMSO.

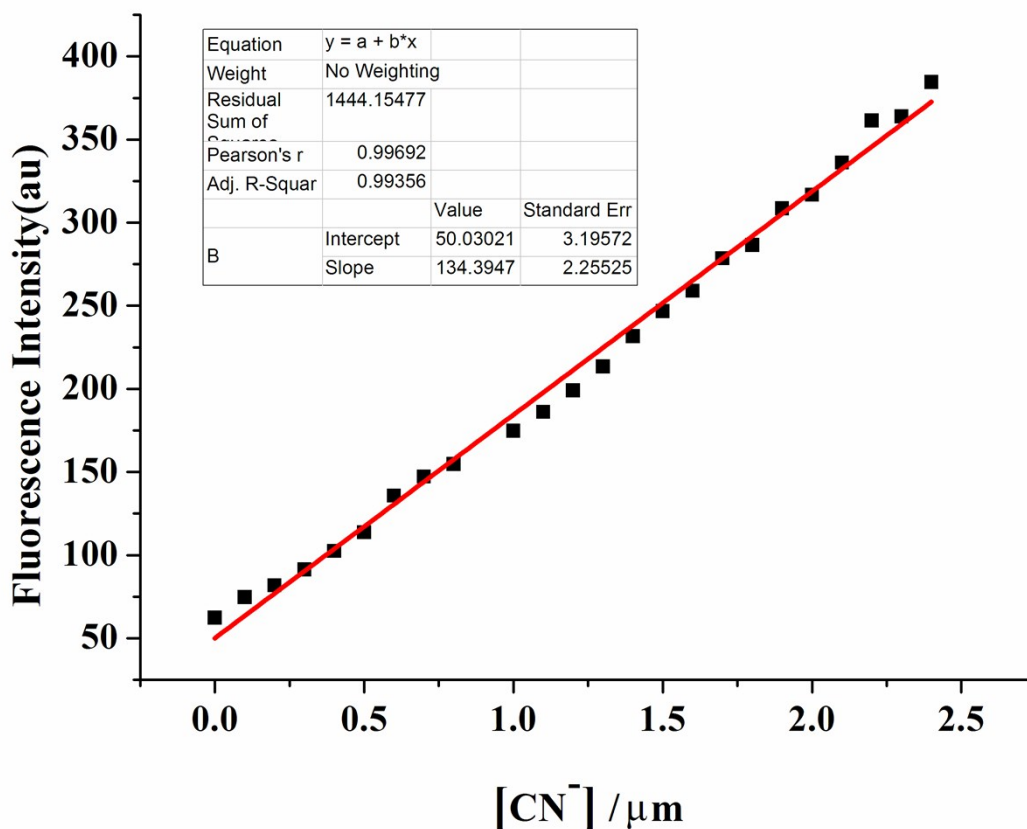


Figure S5 Plot of the intensity at 426 nm for a mixture of probe **L1** (25.0 μM) and CN^- in DMSO/ H_2O (8:2, v/v) solution in the range 0–2.6 μM ($\lambda_{\text{ex}} = 370 \text{ nm}$).

The result of the analysis as follows:

Linear Equation: $Y = 134.3947 \times X + 50.03021$ $R = 0.9936$

$$S = 134.3947 \times 10^6 \quad \delta = \sqrt{\frac{\sum (F_0 - F_0)^2}{N - 1}} = 3.4600 \text{ (N=10)} \quad K = 3$$

$$\text{LOD} = K \times \delta / S = 7.72 \times 10^{-8} \text{ M}$$

F_0 is the fluorescence intensity of **L1**.



Fig. S6 Optimized structure of sensor CN^- .

Charge = -1 Multiplicity = 1

C	0.00000000	0.00000000	-0.63086800
N	0.00000000	0.00000000	0.54074400

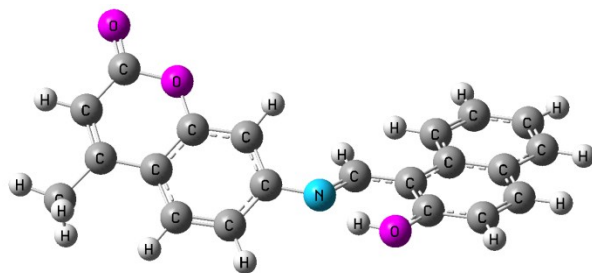


Fig. S7 Optimized structure of sensor **L1**.

Charge = 0 Multiplicity = 1

C	-3.09860600	-1.80069200	-0.46602200
C	-2.63674100	-0.53454000	-0.05884800
C	-3.59591800	0.52214700	0.17043400
C	-4.98232000	0.25448400	-0.03531200
C	-5.38356000	-1.04350400	-0.45300300
C	-4.47903600	-2.04078800	-0.66068500
H	-2.20839500	2.08565600	0.76892600
C	-3.24316100	1.82659900	0.59270600
C	-5.93903700	1.27197400	0.17831000
H	-6.44041000	-1.23325500	-0.60531600
H	-4.78084600	-3.03117800	-0.97648200
C	-5.56001900	2.52664200	0.58577100
C	-4.19665200	2.79829000	0.79366000
H	-6.98568600	1.04079500	0.01375700
H	-6.30002100	3.30066100	0.74711800
H	-3.88906000	3.78577000	1.11688800
O	-2.27458100	-2.82568300	-0.68600700
H	-1.34294900	-2.50465800	-0.49881800
C	-1.22425300	-0.31816900	0.11634900
H	-0.89422700	0.67452000	0.42267300

N	-0.34502900	-1.25179800	-0.05824400
C	3.21079600	-1.80084900	0.68662000
C	3.81168200	-0.59461400	0.28629800
C	1.85255100	-2.00241900	0.56443700
C	5.23130800	-0.31809900	0.36845600
C	2.97279000	0.39817000	-0.24475100
C	1.02570300	-0.98761700	0.05104100
H	1.40093000	-2.93658900	0.87222200
C	5.68451400	0.88048900	-0.06566000
C	1.60193800	0.21210300	-0.36749800
C	4.81799600	1.90565400	-0.61410000
H	6.73371800	1.14100300	-0.02809300
H	1.01306900	0.99657600	-0.82393100
O	3.46156100	1.59309500	-0.67880900
O	5.16105600	2.98786700	-1.01287100
C	6.17282900	-1.34718900	0.92437600
H	5.90978100	-1.60462600	1.95395000
H	6.13319000	-2.27071200	0.34043900
H	7.19845300	-0.98067000	0.91493800
H	3.82655300	-2.59139200	1.09545500

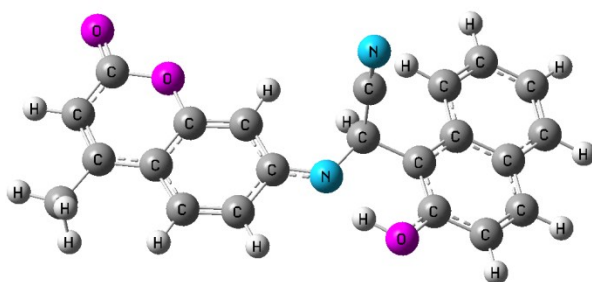


Fig. S8 Optimized structure of IM.

Charge = -1 Multiplicity = 1

C	2.92308000	-1.87727400	0.01914900
C	2.57871400	-0.52728100	0.11533400
C	3.55681900	0.46851300	-0.17665700
C	4.87778700	0.07914000	-0.57360000
C	5.18457100	-1.30249900	-0.65359000
C	4.24263400	-2.24443900	-0.36824500
H	2.32188900	2.21145300	0.23226000

C	3.29458500	1.86448100	-0.08850500
C	5.84374500	1.06619200	-0.87266600
H	6.18564100	-1.60008600	-0.94933800
H	4.46129000	-3.30403500	-0.42889300
C	5.54891400	2.40462000	-0.78549700
C	4.25718900	2.79912400	-0.38483300
H	6.83490700	0.74184600	-1.17447400
H	6.29997400	3.15114000	-1.01676600
H	4.01806200	3.85360500	-0.30338200
O	2.07020300	-2.87259500	0.26855000
H	1.13007200	-2.39485900	0.35554400
C	1.15722700	-0.11261800	0.52205900
H	0.86329200	0.73665200	-0.11214500
N	0.22887200	-1.21216300	0.37864000
C	-3.27832700	-1.95370600	-0.20957700
C	-3.90231300	-0.67959400	-0.22482900
C	-1.93831900	-2.10001600	0.00291600
C	-5.28877900	-0.44216900	-0.44304100
C	-3.05770100	0.42880600	0.00386800
C	-1.07406200	-0.97065000	0.21900300
H	-1.48472000	-3.08394000	0.00458300
C	-5.76543300	0.83983500	-0.43015100
C	-1.70127400	0.30748600	0.22937300
C	-4.91552600	1.97437300	-0.19964400
H	-6.81137000	1.06124200	-0.59394400
H	-1.14569500	1.21276200	0.43062100
O	-3.56840400	1.70196600	0.01651900
O	-5.25438300	3.14066700	-0.17556400
C	-6.23059400	-1.59167700	-0.68764900
H	-5.93444700	-2.16364000	-1.57158700
H	-6.23267100	-2.28588800	0.15745800
H	-7.24941200	-1.23326700	-0.83787000
H	-3.88268100	-2.83841900	-0.37417700
C	1.16797500	0.41462200	1.92077200
N	1.16556600	0.79837800	3.00737900

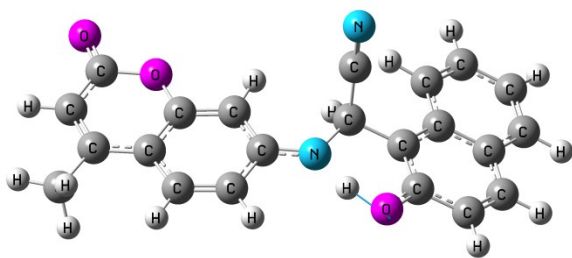


Fig. S9 Optimized structure of TS.

Charge = -1 Multiplicity = 1

C	2.86783100	-1.87745300	0.04058200
C	2.57928100	-0.50654800	0.12159400
C	3.58617900	0.45352600	-0.17748400
C	4.89610500	0.01715500	-0.56492600
C	5.15549300	-1.37613200	-0.62973000
C	4.18309600	-2.28463900	-0.34088700
H	2.40626300	2.24181400	0.20095100
C	3.36905500	1.85886900	-0.10981800
C	5.89398800	0.96813800	-0.87069100
H	6.14796000	-1.70886300	-0.91830500
H	4.36897500	-3.35119700	-0.39189200
C	5.64329500	2.31761300	-0.80208700
C	4.36293100	2.75821900	-0.41383200
H	6.87546600	0.60789000	-1.16384800
H	6.41950500	3.03617200	-1.03881200
H	4.15718700	3.82096400	-0.34794300
O	1.97705400	-2.81977500	0.29103000
H	0.99061400	-2.22356400	0.37143800
C	1.16976400	-0.04694100	0.51610200
H	0.88339100	0.78630600	-0.14175700
N	0.23187200	-1.14159100	0.39728700
C	-3.26430500	-1.94757300	-0.17714400
C	-3.90323300	-0.68279300	-0.21161900
C	-1.92112200	-2.07388500	0.03431500
C	-5.29540900	-0.46756900	-0.43004900
C	-3.07389300	0.44022100	-0.00544400
C	-1.07728100	-0.92906800	0.22971900
H	-1.45553800	-3.05187500	0.05111900
C	-5.78687900	0.80718300	-0.43849500

C	-1.71451700	0.33977200	0.21800700
C	-4.95025900	1.95755500	-0.23141000
H	-6.83589000	1.01322100	-0.60263600
H	-1.16596200	1.25345700	0.39924200
O	-3.59945600	1.70647000	-0.01437500
O	-5.30514700	3.11840900	-0.22802500
C	-6.22203400	-1.63360400	-0.65080800
H	-5.92153500	-2.21635500	-1.52613500
H	-6.21088600	-2.31316700	0.20602200
H	-7.24625600	-1.29192200	-0.80269900
H	-3.85741000	-2.84249800	-0.32539300
C	1.17649300	0.51623500	1.90074600
N	1.17056200	0.93432000	2.97439300

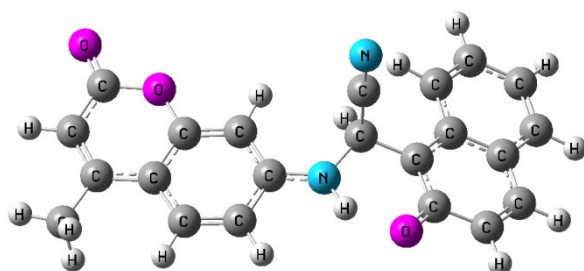


Fig. S10 Optimized structure of **L1**+**CN⁻**.

Charge = -1 Multiplicity = 1

C	2.94067200	-1.89716200	0.13785200
C	2.61815400	-0.50940900	0.16568600
C	3.57516700	0.48315700	-0.17423300
C	4.88860500	0.09066300	-0.60414800
C	5.19462800	-1.29765400	-0.65454600
C	4.27768300	-2.23602000	-0.30395900
H	2.37002200	2.24943800	0.25187200
C	3.32485500	1.88540500	-0.10560900
C	5.83895000	1.06691900	-0.95969000
H	6.18808700	-1.59574100	-0.97938100
H	4.51109600	-3.29466500	-0.33659900
C	5.55247100	2.41301000	-0.89747600
C	4.27749500	2.81377900	-0.45816100
H	6.81956000	0.73249900	-1.28621600

H	6.29630900	3.15183600	-1.17245500
H	4.04044100	3.87010600	-0.38659600
O	2.13130800	-2.83755400	0.46078300
H	0.68770400	-2.04485700	0.32493500
C	1.21433700	-0.07572900	0.57962400
H	0.95243100	0.83153200	0.02697400
N	0.24105000	-1.10250500	0.27021200
C	-3.24627000	-1.92867200	-0.35821300
C	-3.89656200	-0.67549300	-0.29174300
C	-1.89811500	-2.05492500	-0.16004800
C	-5.29856100	-0.46268200	-0.48974000
C	-3.08483800	0.43828900	-0.00197900
C	-1.08596600	-0.91722100	0.12292400
H	-1.42051800	-3.02516700	-0.22143400
C	-5.80122900	0.79949400	-0.39583900
C	-1.72117200	0.33690700	0.21095100
C	-4.97596300	1.94380800	-0.10242500
H	-6.85296500	1.00745800	-0.53874800
H	-1.17564900	1.23672400	0.45716900
O	-3.62129200	1.69365900	0.08829200
O	-5.34780700	3.09262800	-0.00807900
C	-6.20712400	-1.62123000	-0.79960100
H	-5.90204400	-2.12397400	-1.72158400
H	-6.17771400	-2.36818500	-0.00154500
H	-7.23770200	-1.28612000	-0.91720200
H	-3.82808000	-2.81666400	-0.57381100
C	1.16215500	0.30083100	2.02480400
N	1.12111000	0.60386400	3.13551200