Electronic Supplementary Information

Polymorphism and mechanochromic luminescence of a highly solid-emissive Quinoline-*β*-Ketone Boron-Difluoride

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Contents

1. Photophysical data of $QKBF_2$

Table S1. Photophysical data of **$QKBF_2$**

Solvent	**λ_{abs} (nm)**	**λ_{em} (nm)**	**Φ_F**
THF	468	543	0.44
Methanol	464	574	0.03
Chloroform	476	541	0.67
Acetonitrile	463	598	0.03
Hexane	446, 474	489, 518	0.67
Solid	454, 495	566	0.56

2. DFT calculation

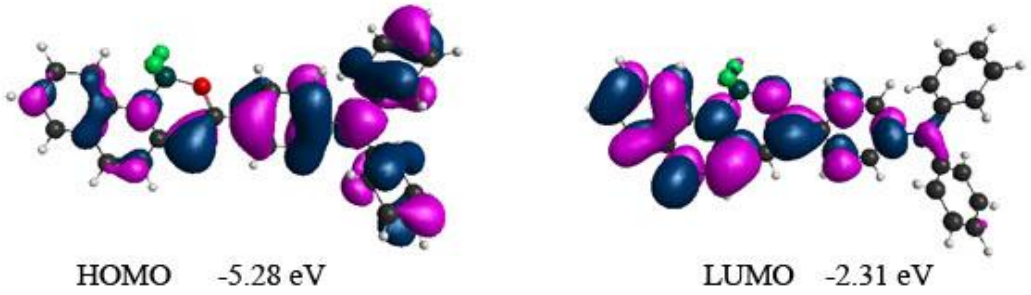
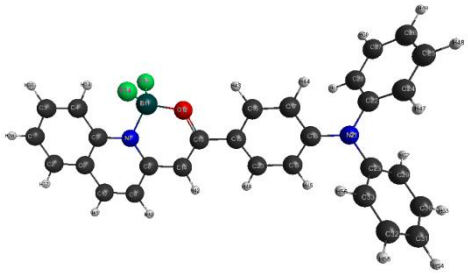


Figure S1. HOMO and LUMO levels of **$QKBF_2$**

Table S1. Atomic cartesian coordinates for DFT optimized ground state structure



C	6.0	-5.34942150	1.70290768	0.17344031
C	6.0	-4.75021839	0.53544939	-0.24090099
C	6.0	-4.54498720	2.78452301	0.57631075
C	6.0	-3.16792893	2.70413351	0.56024194
C	6.0	-2.53307343	1.51706910	0.13107547
C	6.0	-3.34324908	0.41828933	-0.26780581
N	7.0	-1.14583170	1.41295898	0.09454708
C	6.0	-0.54458702	0.26713181	-0.30519992
C	6.0	-1.34094739	-0.85498929	-0.69739276
C	6.0	-2.69557762	-0.77927577	-0.68498862

B	5.0	-0.25376526	2.68719220	0.50442082
O	8.0	1.18084788	2.36917543	0.36894542
C	6.0	1.68589628	1.22074449	-0.01294783
C	6.0	0.86836141	0.16399768	-0.34466940
C	6.0	3.15463090	1.16770720	-0.04014849
C	6.0	3.89846087	2.21945906	0.51918310
C	6.0	5.28335333	2.19990373	0.52347350
C	6.0	5.98796749	1.12665629	-0.04900621
C	6.0	5.24744034	0.07741163	-0.62497646
C	6.0	3.86417699	0.09948040	-0.61421424
N	7.0	7.39596653	1.09590316	-0.05170747
C	6.0	8.14865589	2.30516696	-0.12561332
C	6.0	8.08821011	-0.14373548	0.08466040
C	6.0	9.22918415	2.51725078	0.73967671
C	6.0	9.96830940	3.69384217	0.66298467
C	6.0	9.63425064	4.67944813	-0.26408064
C	6.0	8.55750370	4.47140265	-1.12511039
C	6.0	7.82349014	3.29046988	-1.06671417
C	6.0	9.18308163	-0.44045669	-0.73635870
C	6.0	9.86136341	-1.64696002	-0.58852011
C	6.0	9.45164490	-2.57801270	0.36477315
C	6.0	8.36022949	-2.28542447	1.18120205
C	6.0	7.68776274	-1.07464814	1.05211461
F	9.0	-0.52041095	3.00603008	1.82606101
F	9.0	-0.57501841	3.72289419	-0.35631916
H	1.0	-6.42937326	1.79110467	0.19174048
H	1.0	-5.34702539	-0.31484008	-0.55373645
H	1.0	-5.01238585	3.70464087	0.90865129
H	1.0	-2.57322526	3.54635763	0.87532133
H	1.0	-0.82791519	-1.75522864	-1.01073456
H	1.0	-3.30091596	-1.62632573	-0.99104667
H	1.0	1.28963923	-0.78447419	-0.63762283
H	1.0	3.37008333	3.04847813	0.97141057
H	1.0	5.82835865	3.01609898	0.98040777
H	1.0	5.76736355	-0.74981904	-1.09126556
H	1.0	3.33534765	-0.71685773	-1.09116459
H	1.0	9.48428154	1.75808430	1.46917892
H	1.0	10.80038166	3.84435606	1.34203112
H	1.0	10.20651531	5.59861279	-0.31535244
H	1.0	8.29218674	5.22693110	-1.85657346
H	1.0	6.99486160	3.12922835	-1.74630916
H	1.0	9.49864578	0.27632582	-1.48520935
H	1.0	10.70796967	-1.86460459	-1.23053348
H	1.0	9.97827625	-3.51931953	0.47219121
H	1.0	8.03754902	-2.99583721	1.93448091
H	1.0	6.84938812	-0.84267819	1.69772863

3. Concentration-dependent fluorescent spectra

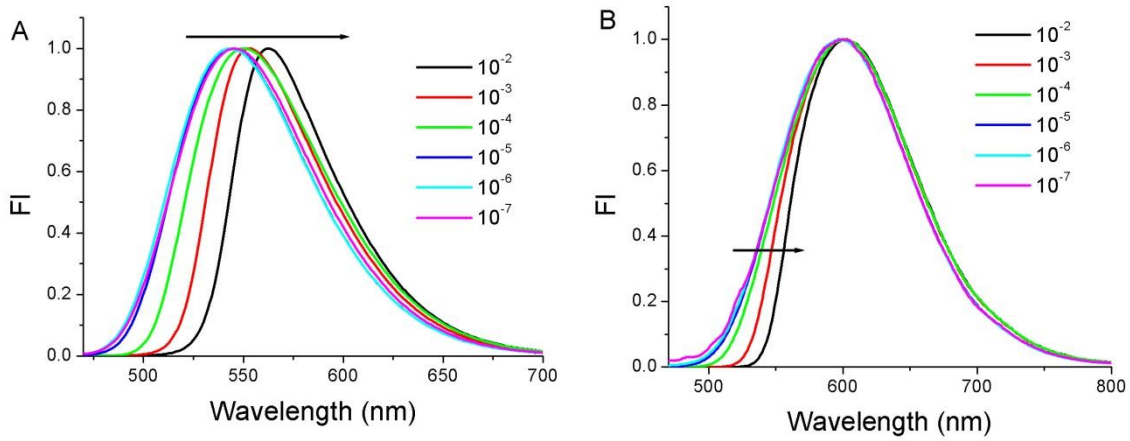


Figure S2. Concentration-dependent fluorescent spectra in THF (A) and in acetonitrile (B)

4. Non-covalent interactions in C1

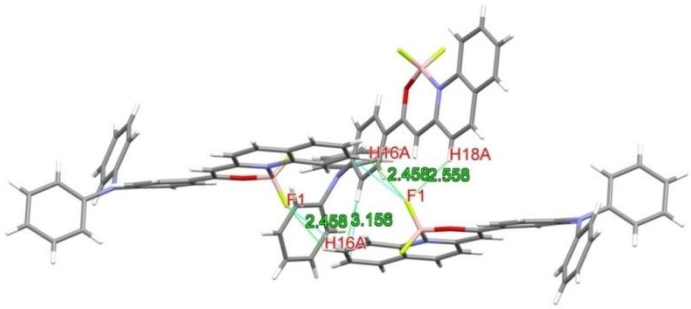


Figure S3. Non-covalent interactions of **QKBF$_2$** with neighbouring molecules in **C1**

5. Mechanochromism of crystal C2

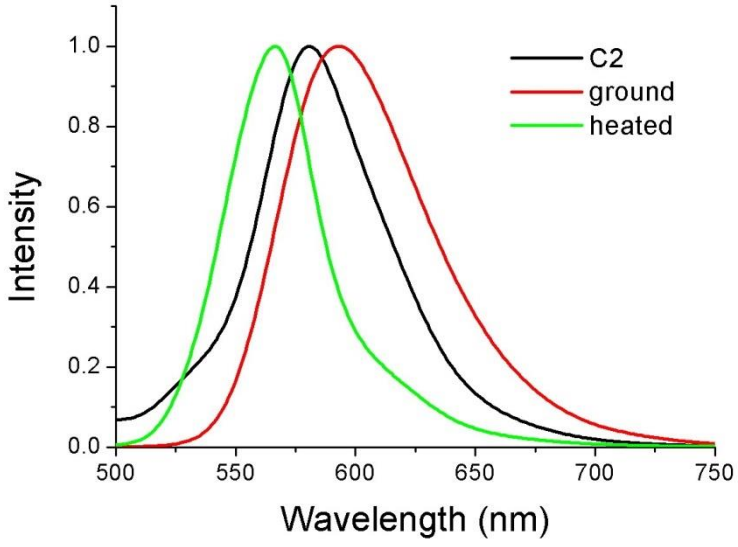


Figure S4. Fluorescence changes of **C2** upon grinding and heating

6. Reversibility of mechanochromism

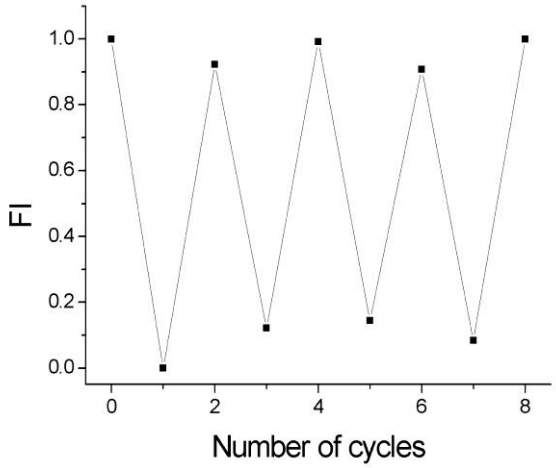


Figure S5. Reversibility of **$QKBF_2$** emissions by cycles of grinding and annealing.

7. XRD

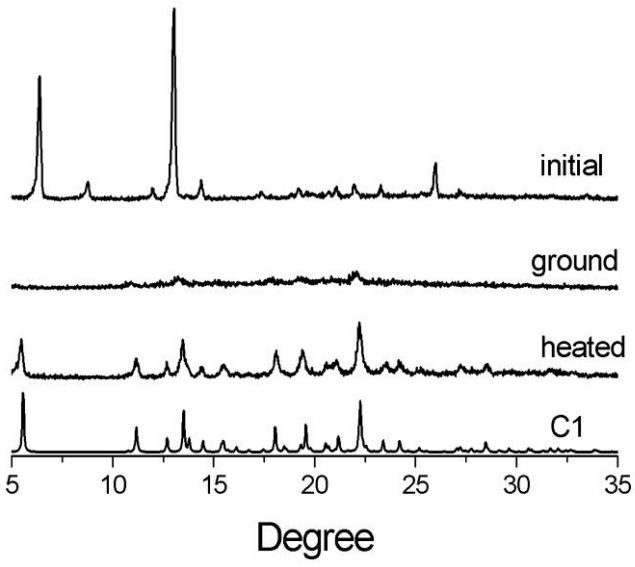


Figure S6. XRD patterns of **$QKBF_2$** powder during mechanochromism.

8. DSC curves

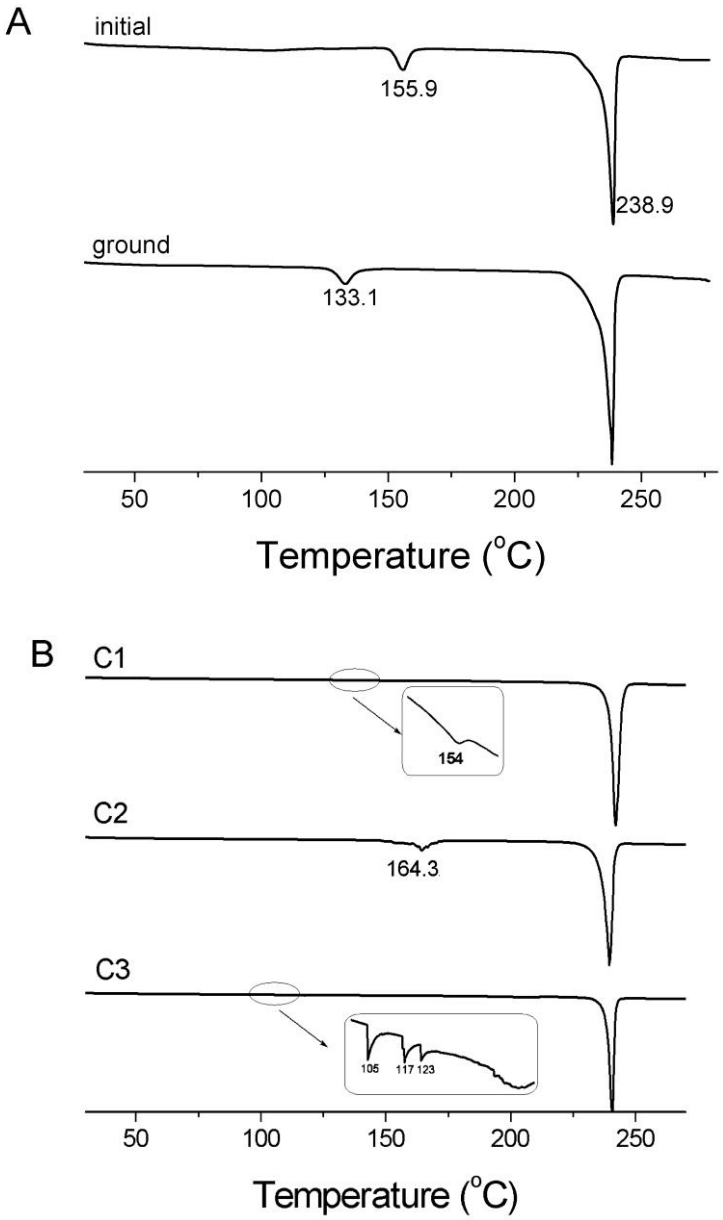


Figure S7. (A) DSC curves of the initial and grinded sample; (B) DSC curves of the three crystals

9. NMR spectra

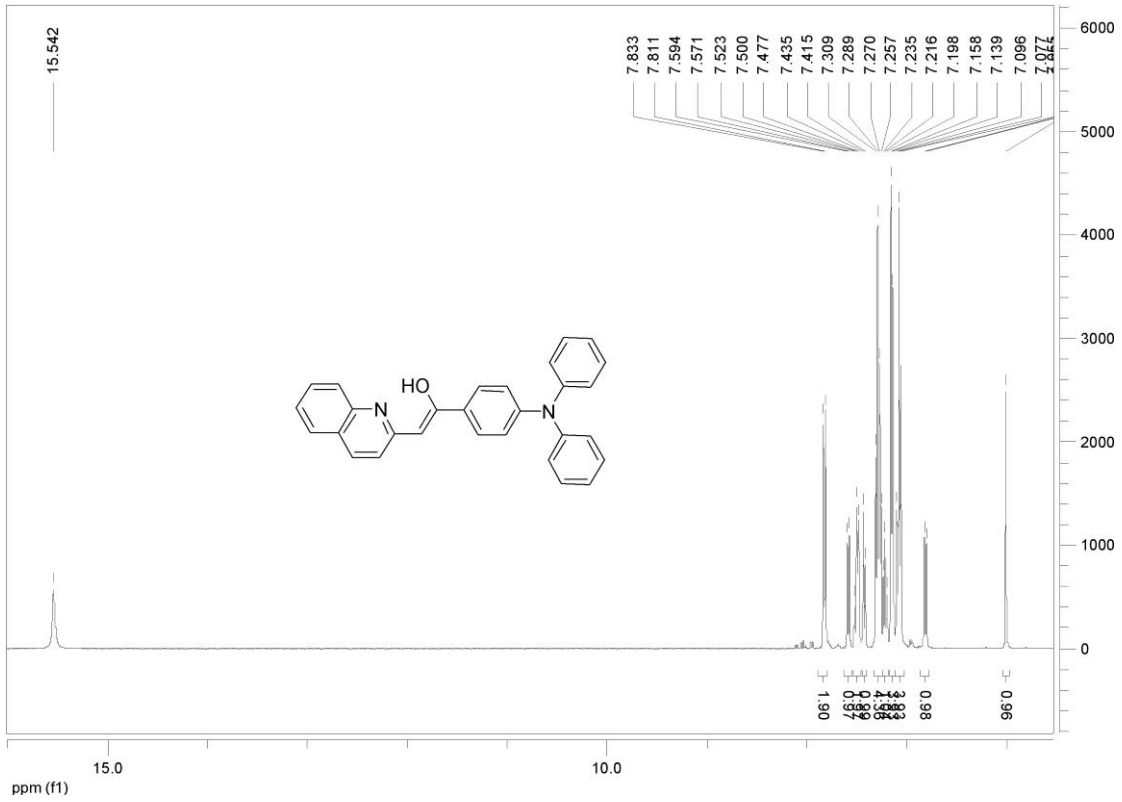


Figure S8. ^{1}H NMR of the ligand **QK-L** (400 MHz, $CDCl_3$)

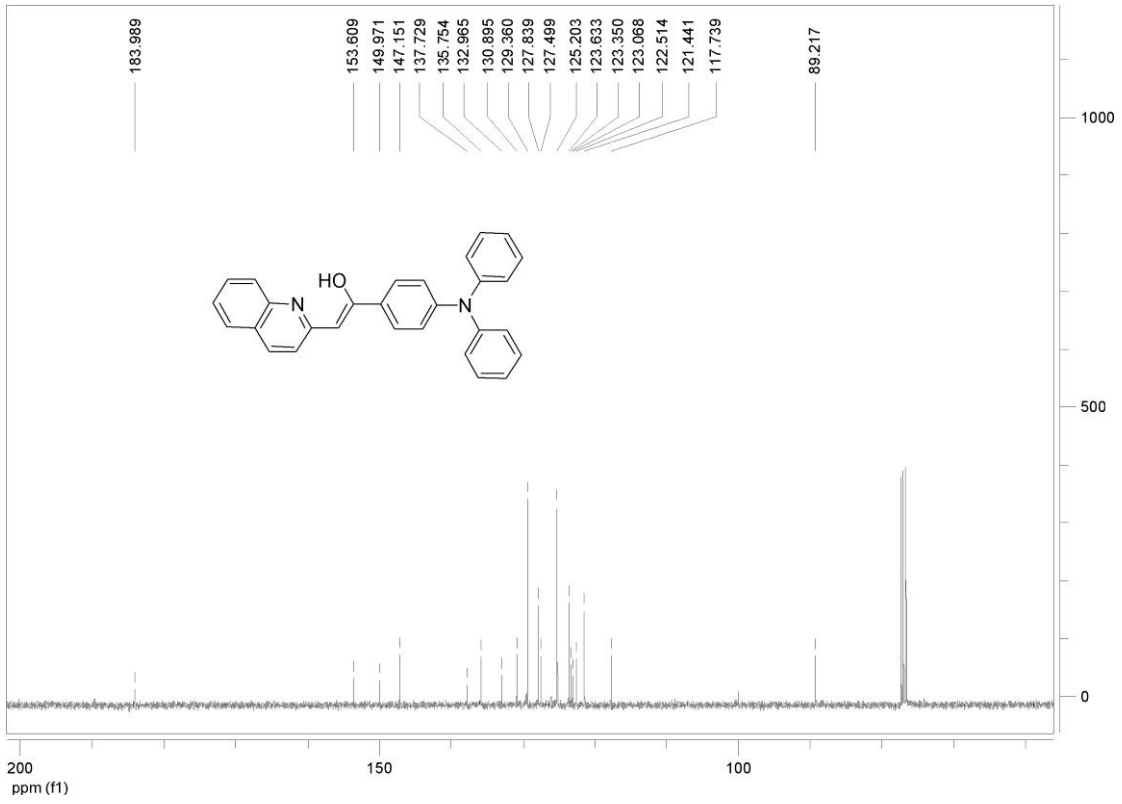


Figure S9. ^{13}C NMR of the ligand **QK-L** (100 MHz, $CDCl_3$)

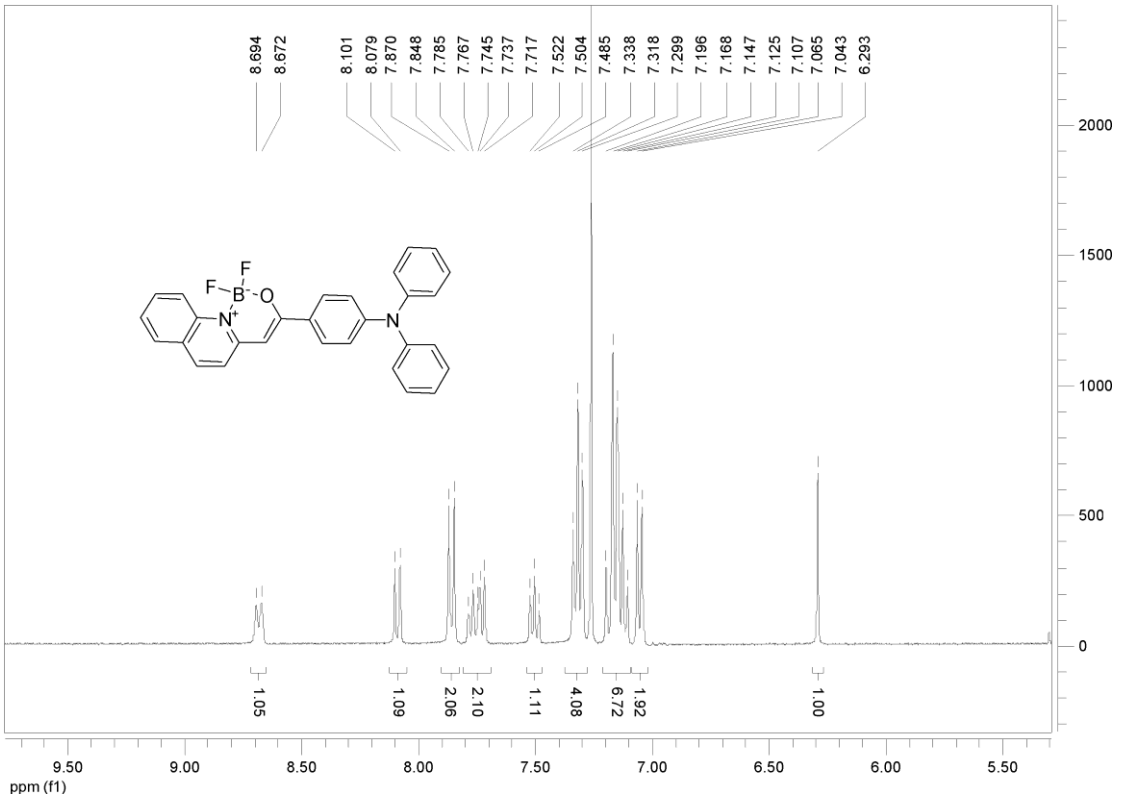


Figure S10. ^{1}H NMR of **QKBF$_2$** (400 MHz, $CDCl_3$)

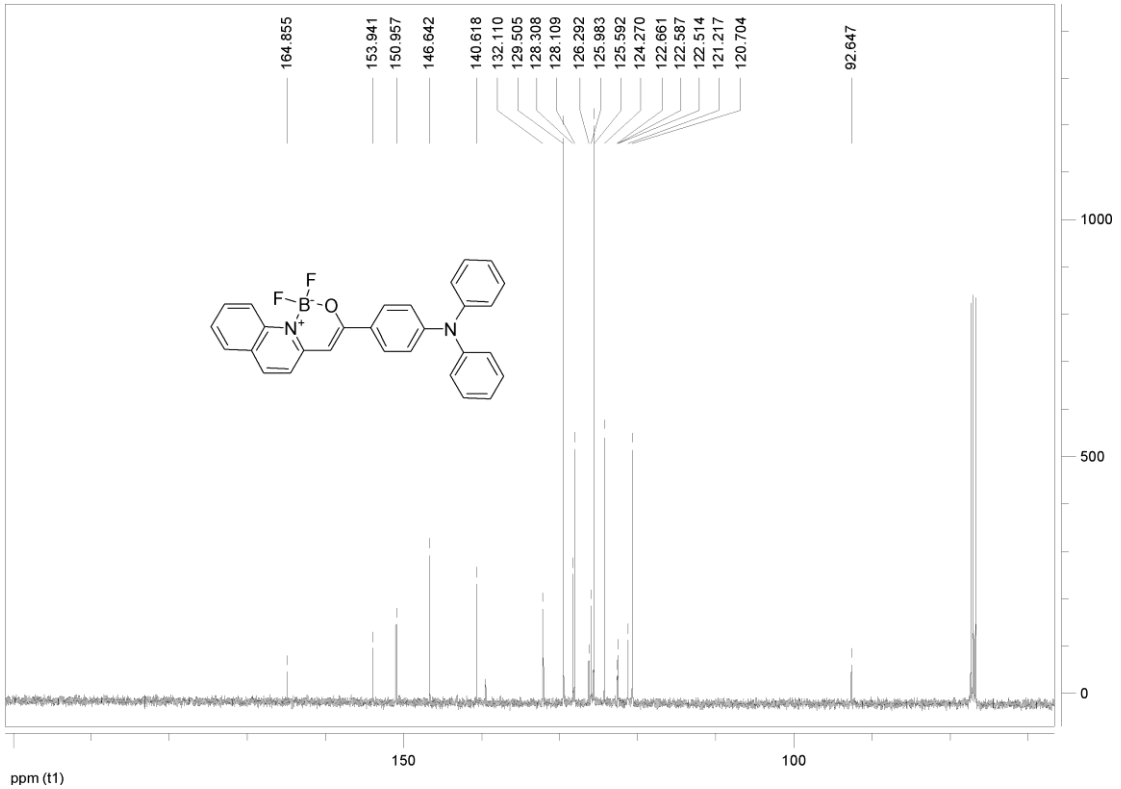


Figure S11. ^{13}C NMR of **QKBF$_2$** (100 MHz, $CDCl_3$)

10. Ms spectra

Display Report

Analysis Info

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Method	tune_200-800_hcoona-pos-10min.m	Operator	gftang
Sample Name	TRH-5A	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

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Focus	Not active			Set Dry Heater	200 ℃
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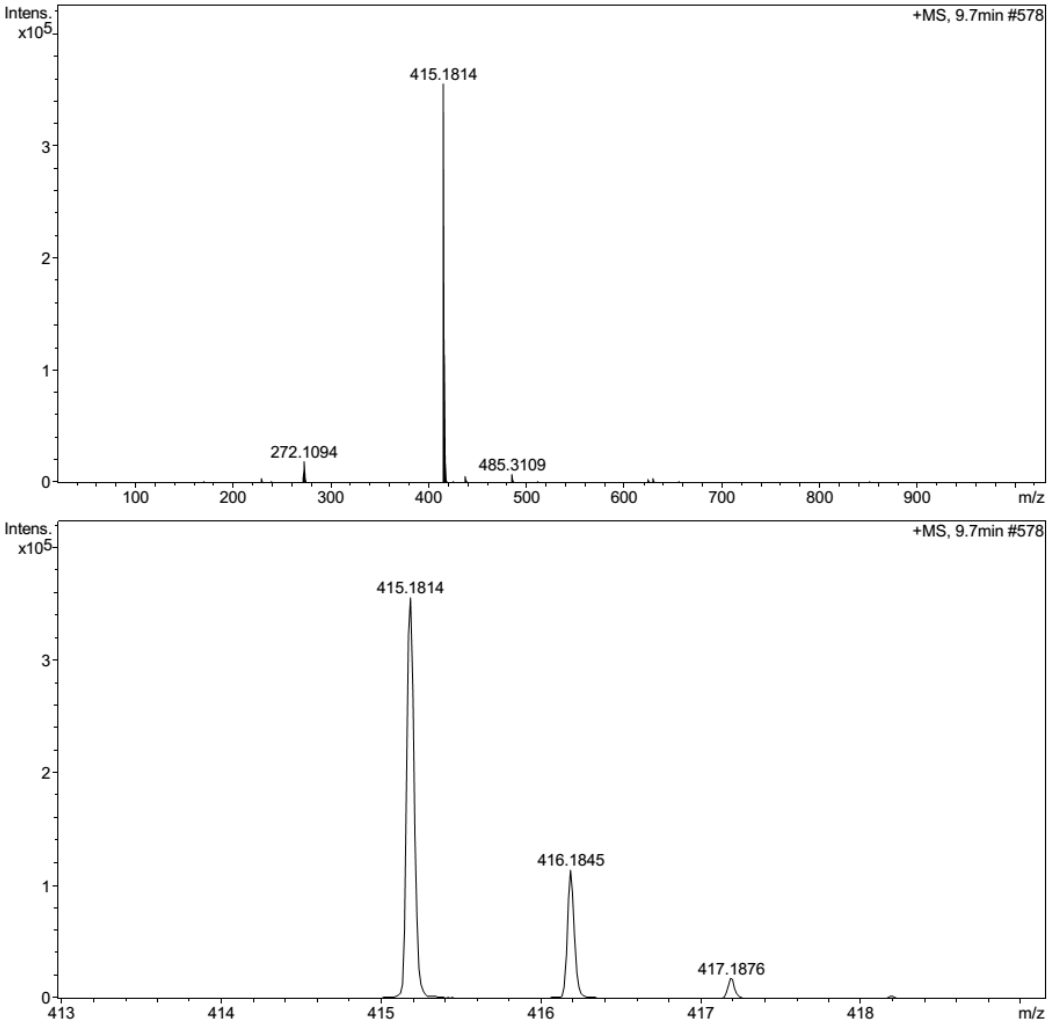
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Bruker Compass DataAnalysis 4.0 printed: 1/23/2015 10:08:34 AM Page 1 of 1

Figure S12. HRMs of **QK-L**

Display Report

Analysis Info

Analysis Name	D:\Data\MS\YT\0122\TRH-3A_RA6_01_768.d	Acquisition Date	1/22/2015 4:29:59 PM
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Sample Name	TRH-3A	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

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Focus	Not active			Set Dry Heater	200 ℃
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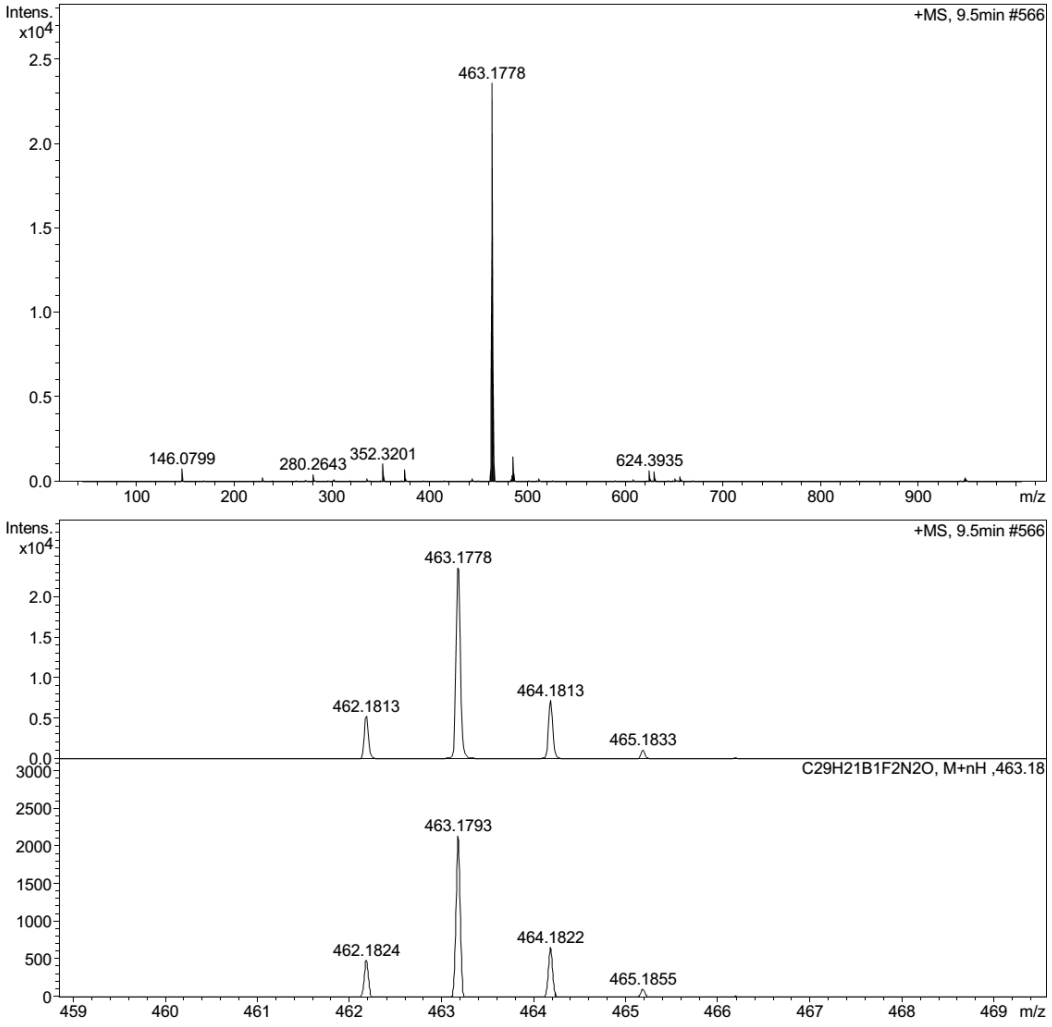

Figure S13. HRMs of **QKBF$_2$**

11. Crystal data and structure refinements of the $QKBF_2$ crystals

CCDC number	1039804	1052996	1044705
Empirical formula	C29 H21 B F2 N2 O	C29 H21 B F2 N2 O	C29 H21 B F2 N2 O
Formula weight	462.29	462.29	462.29
Temperature, K	293(2)	293(2)	293(2)
Wavelength, Å	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
space group	P 21/a	P 21/c	P2(1)/c
a, Å	15.823(17)	17.149(14)	17.097(15)
b, Å	9.588(10)	8.780(7)	8.764(7)
c, Å	17.462(19)	17.692(14)	17.682(16)
alpha, deg	90	90	90
beta, deg	114.623(13)	117.636(8)	117.686(9)
gamma,deg	90	90	90
volume, $Å^3$	2408(4)	2360(3)	2346(4)
Z	4	4	4
Mg/m^3	1.275	1.301	1.309
Reflections collected	24860	24403	24315
Unique Reflections	5519	5418	5395
R(int)	0.2212	0.1188	0.1079
GOF	1.125	1.082	1.088
R1[I>2sigma(I)]	0.1377	0.0880	0.0848
wR2[I>2sigma(I)]	0.1868	0.1776	0.1616
R1 (all data)	0.2985	0.1784	0.1630
wR2(all data)	0.2393	0.2169	0.1950