

## Supporting Information

### Design and synthesis of new boron-based benzo[c][1,2,5]oxadiazoles and benzo[c][1,2,5]thiadiazoles as Hypoxia inhibitors

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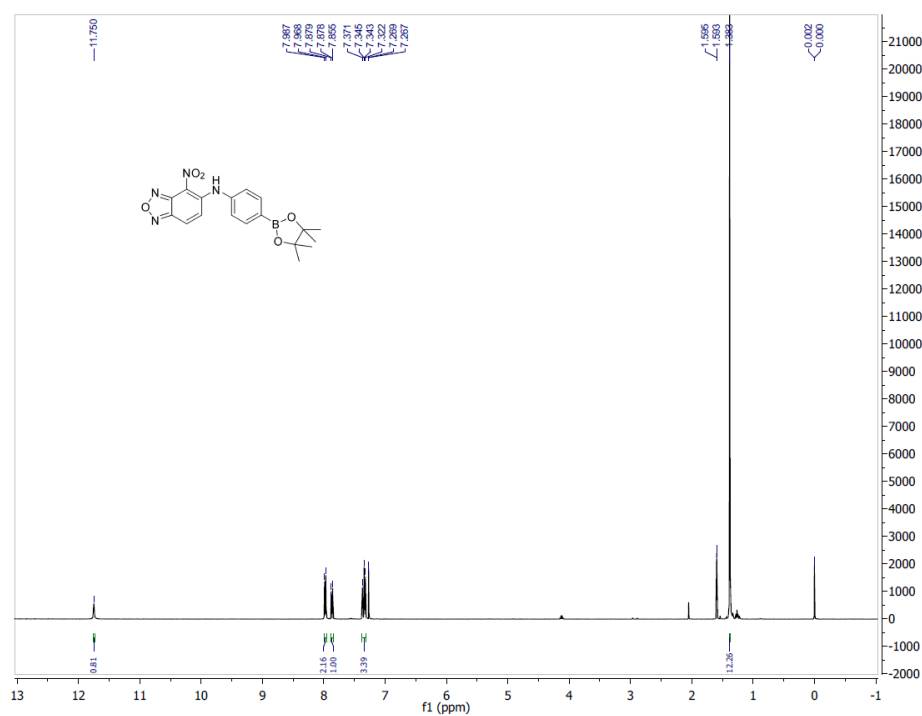
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\* Correspondence: sasmita.das@liu.edu (S.D.); bhaskar.das@liu.edu (B.C.D.)

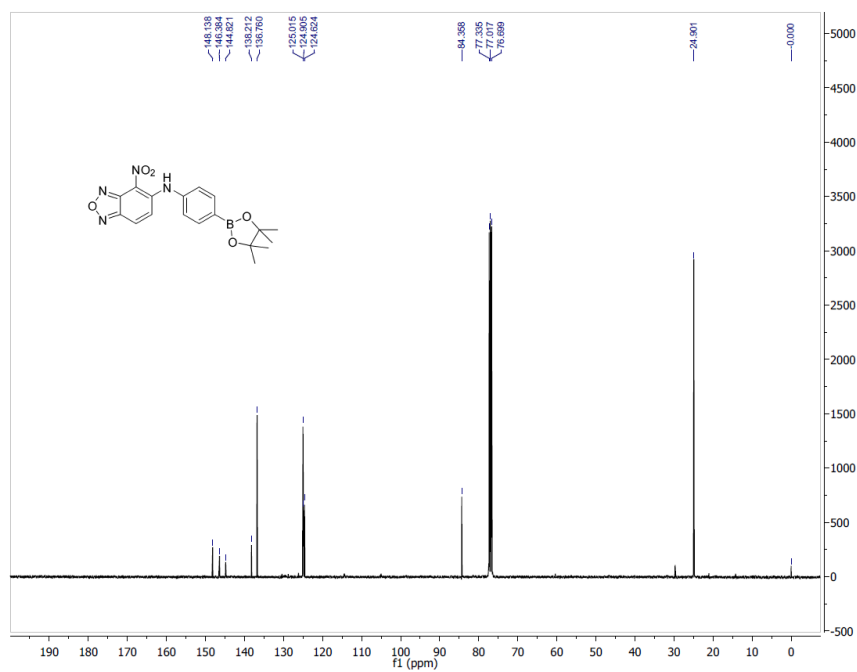
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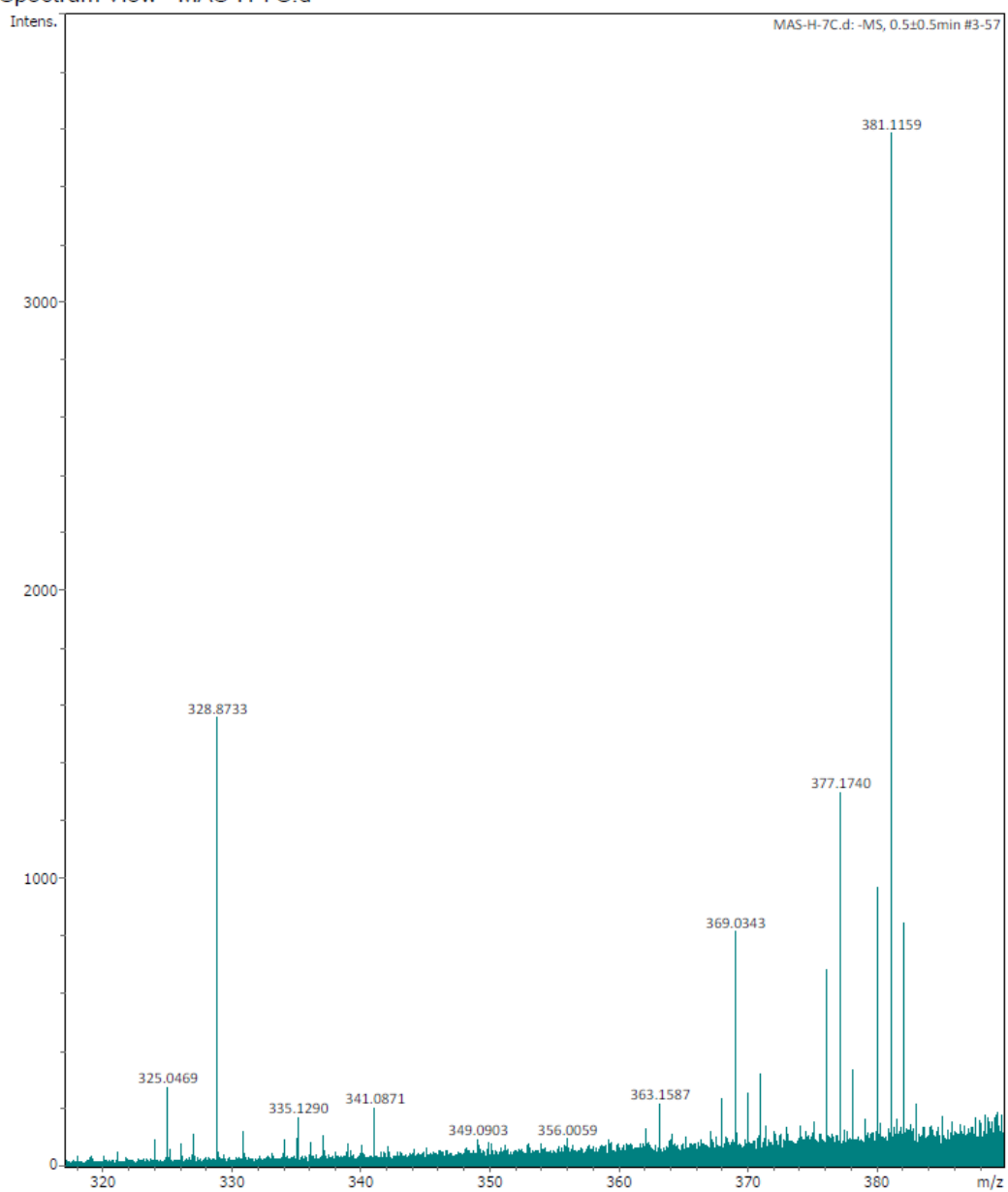


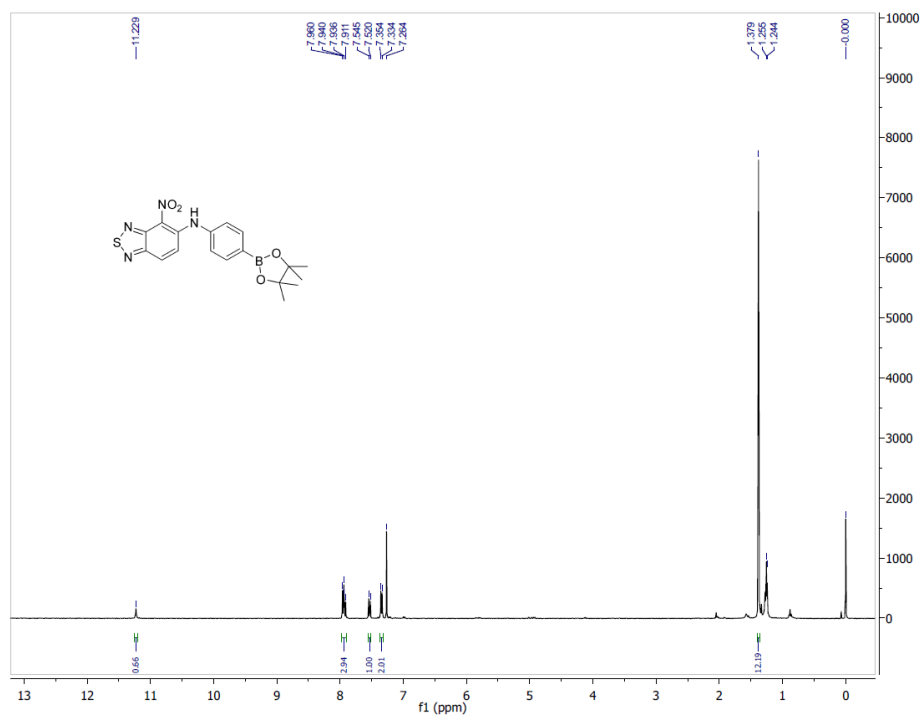
**<sup>1</sup>H NMR of compound (7)**



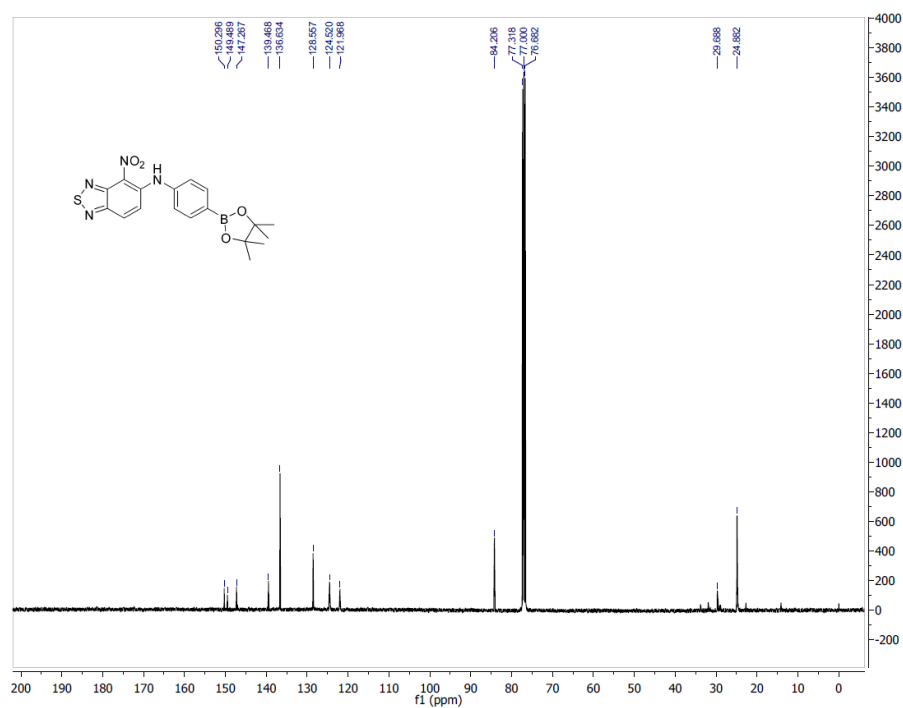
**<sup>13</sup>C NMR of compound (7)**

Spectrum View - MAS-H-7C.d

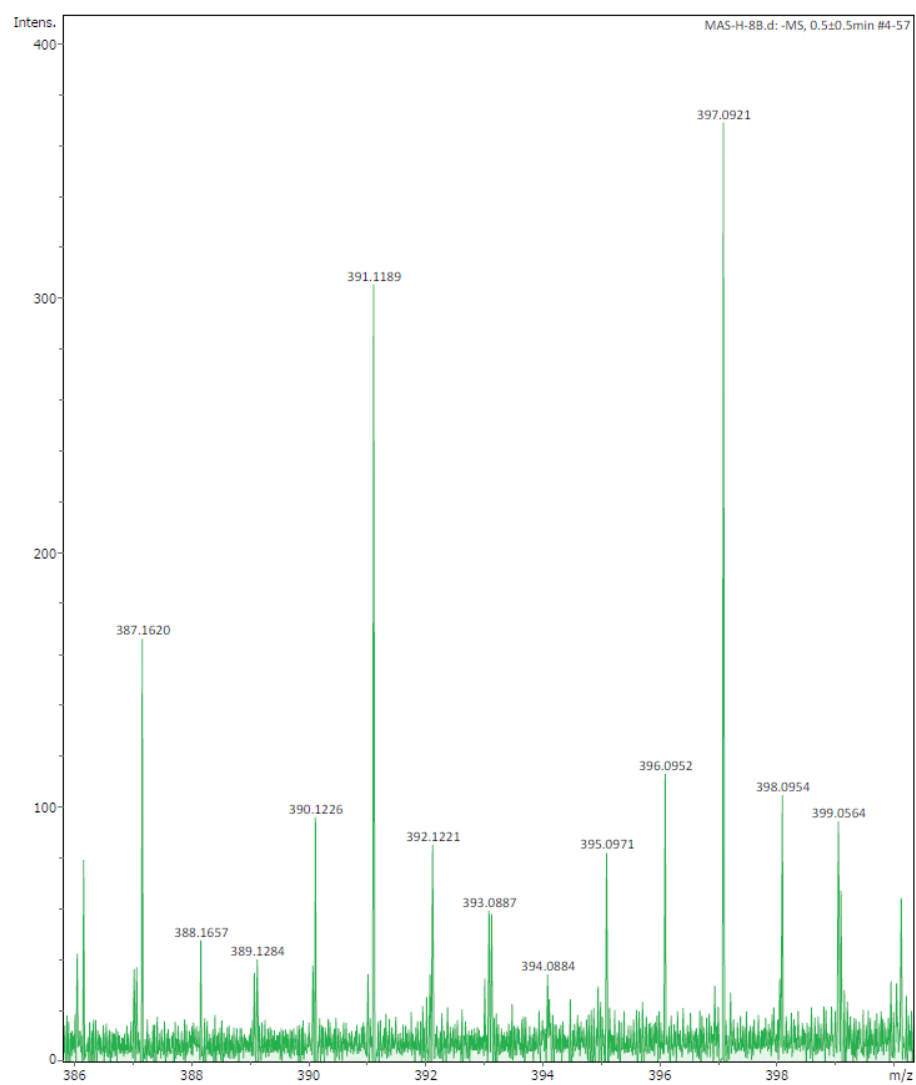


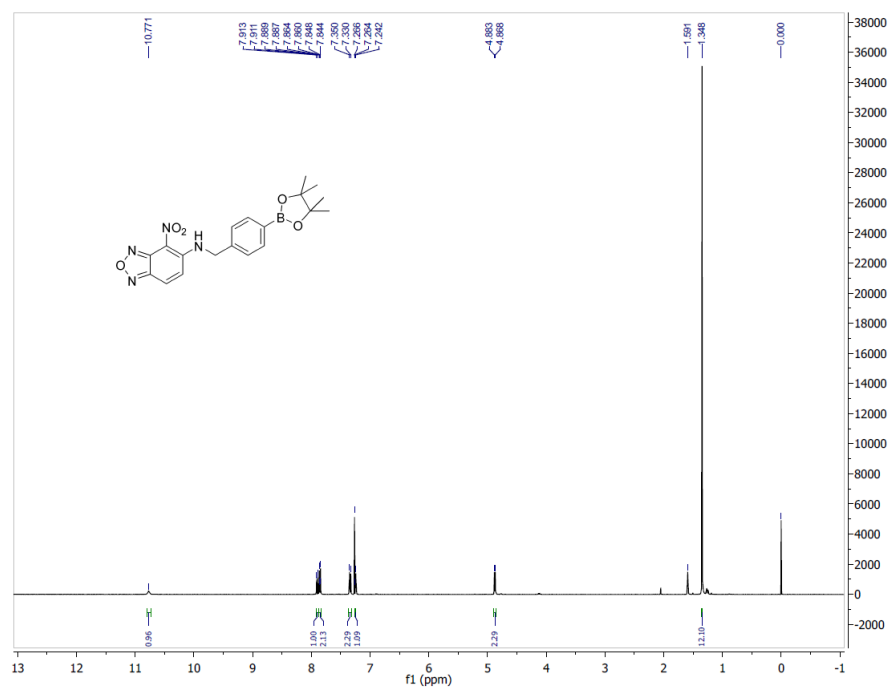


**<sup>1</sup>H NMR of compound (8)**

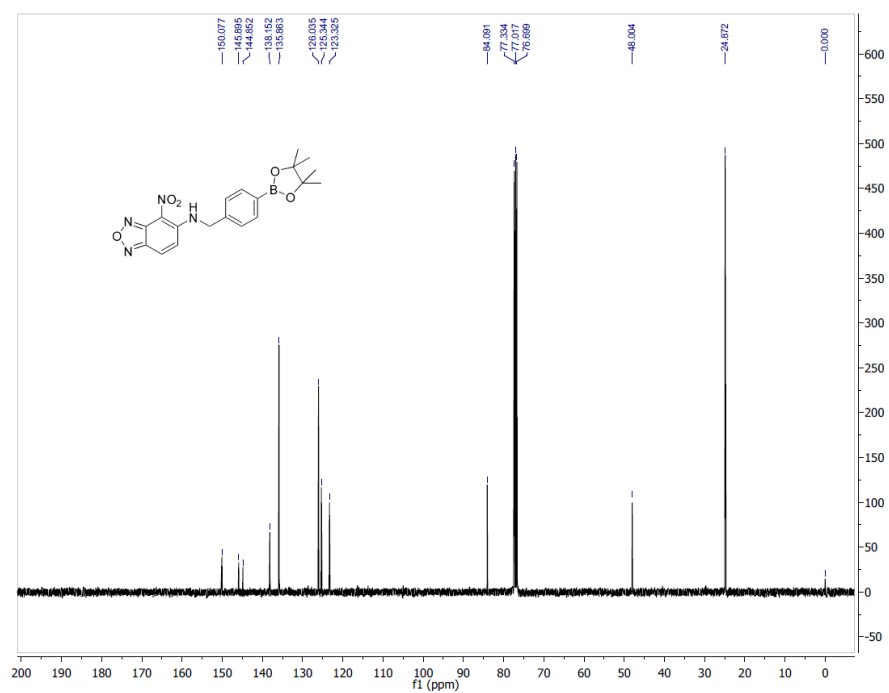


**<sup>13</sup>C NMR of compound (8)**



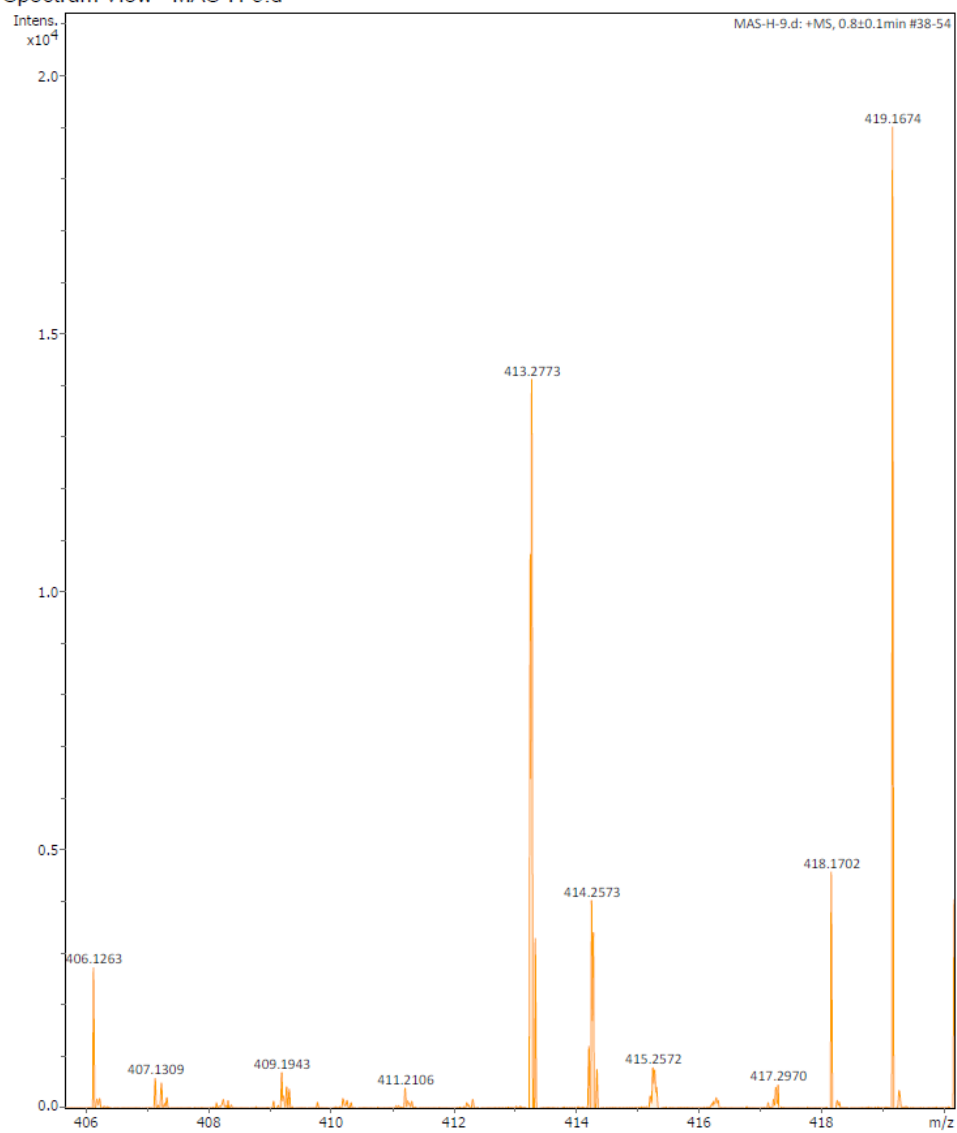


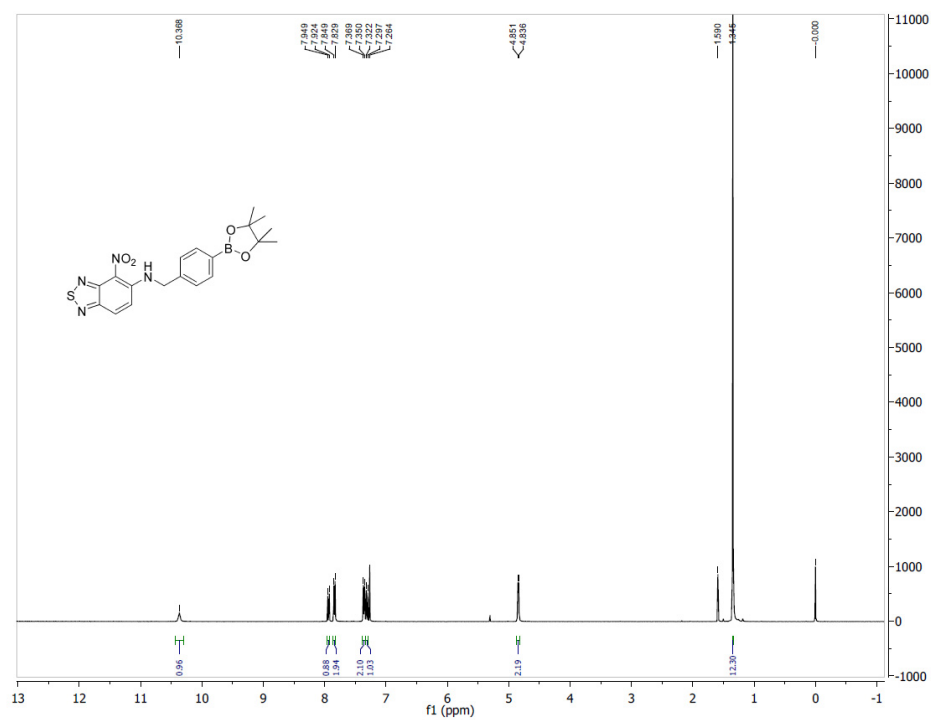
**<sup>1</sup>H NMR of compound (9)**



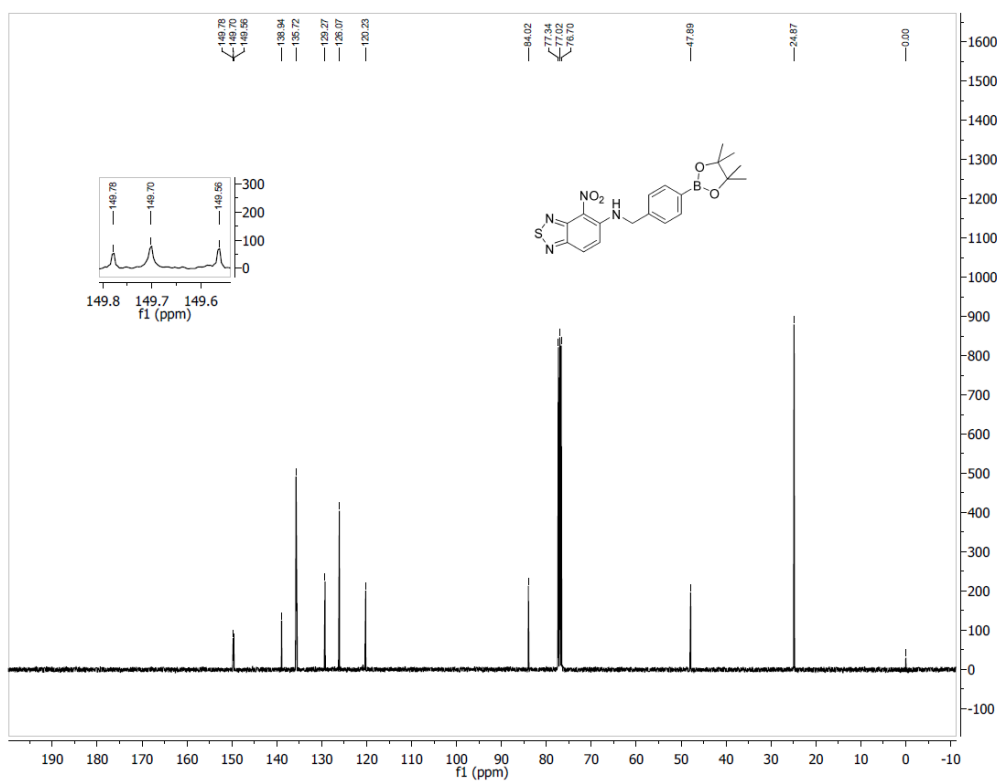
**<sup>13</sup>C NMR of compound (9)**

Spectrum View - MAS-H-9.d





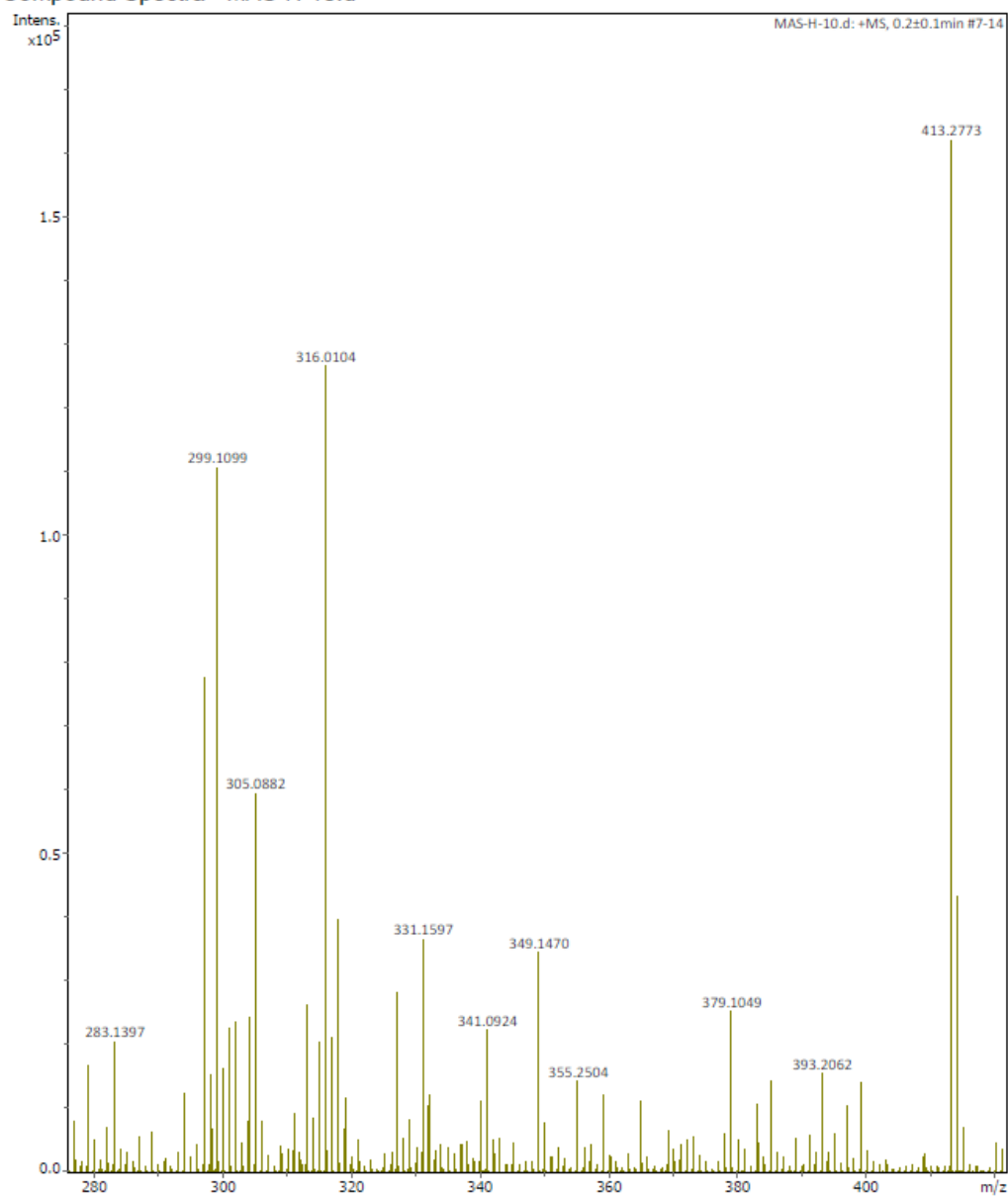
**<sup>1</sup>H NMR of compound (10)**

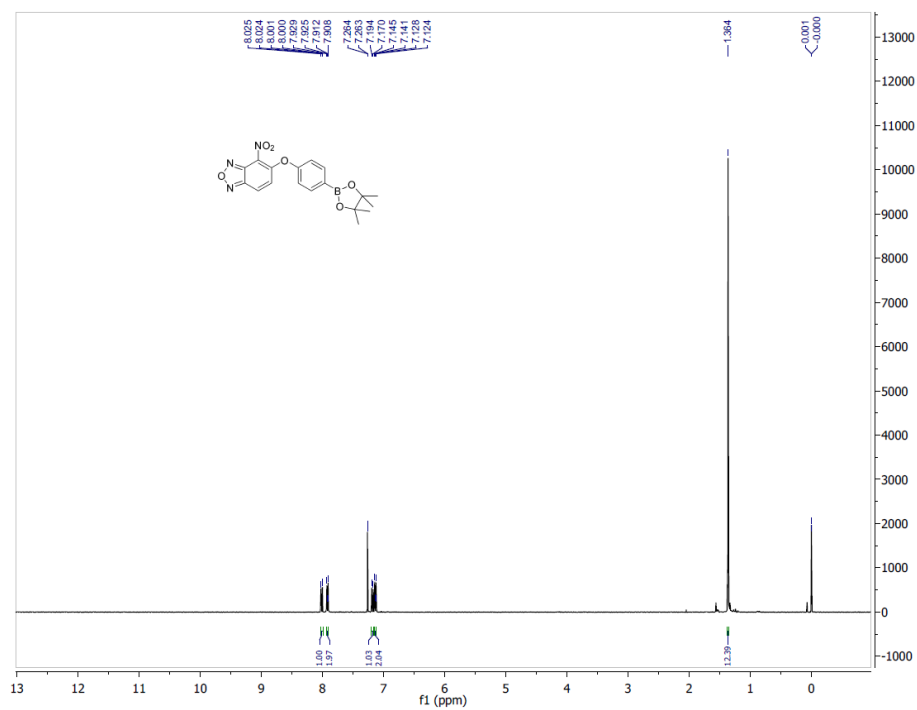




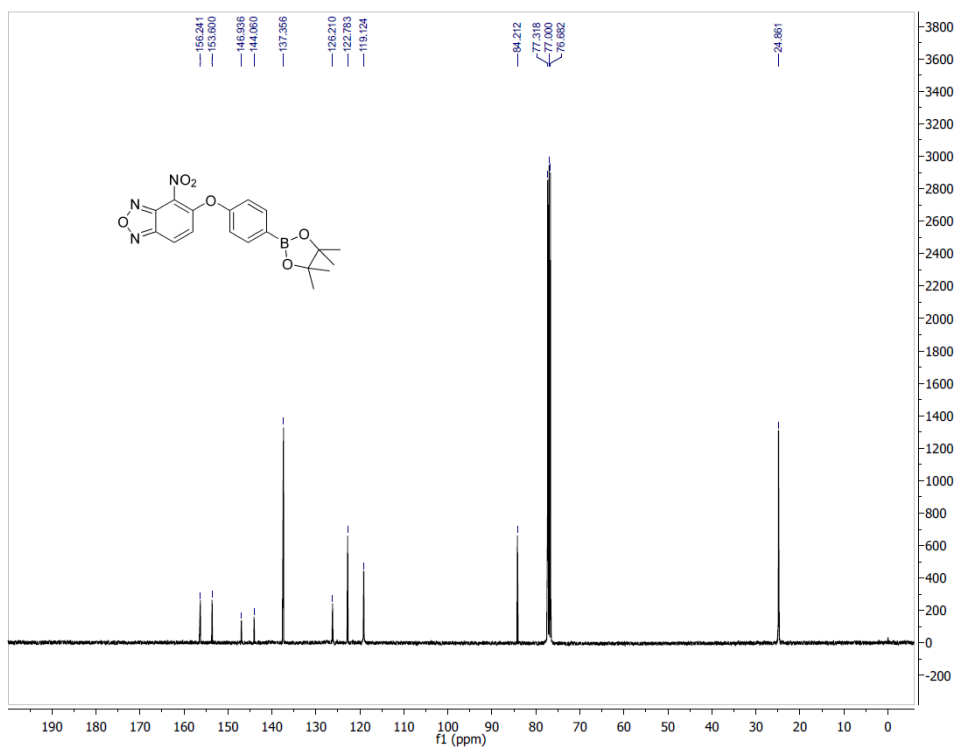
# <sup>13</sup>C NMR of compound (10)

Compound Spectra - MAS-H-10.d



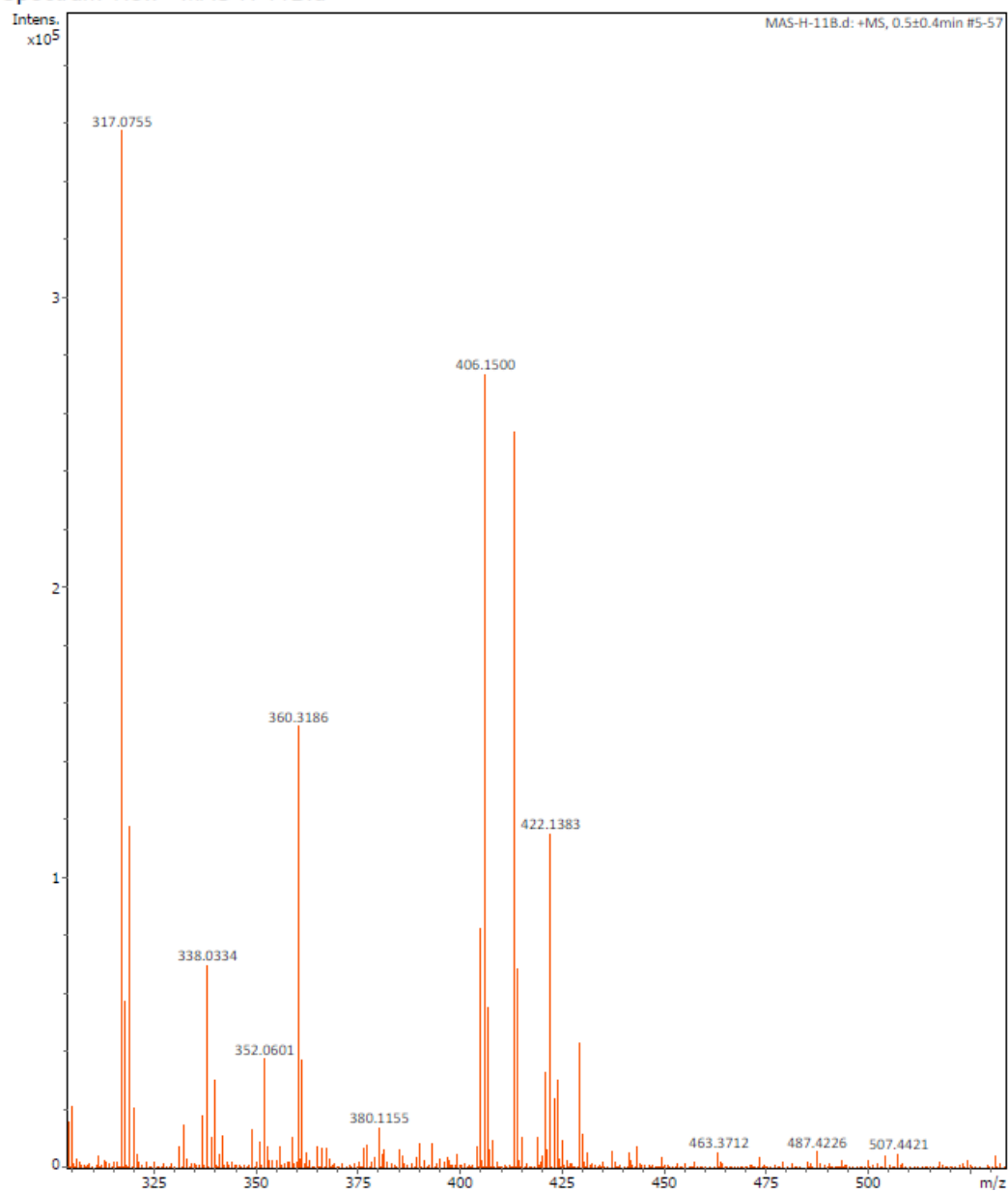


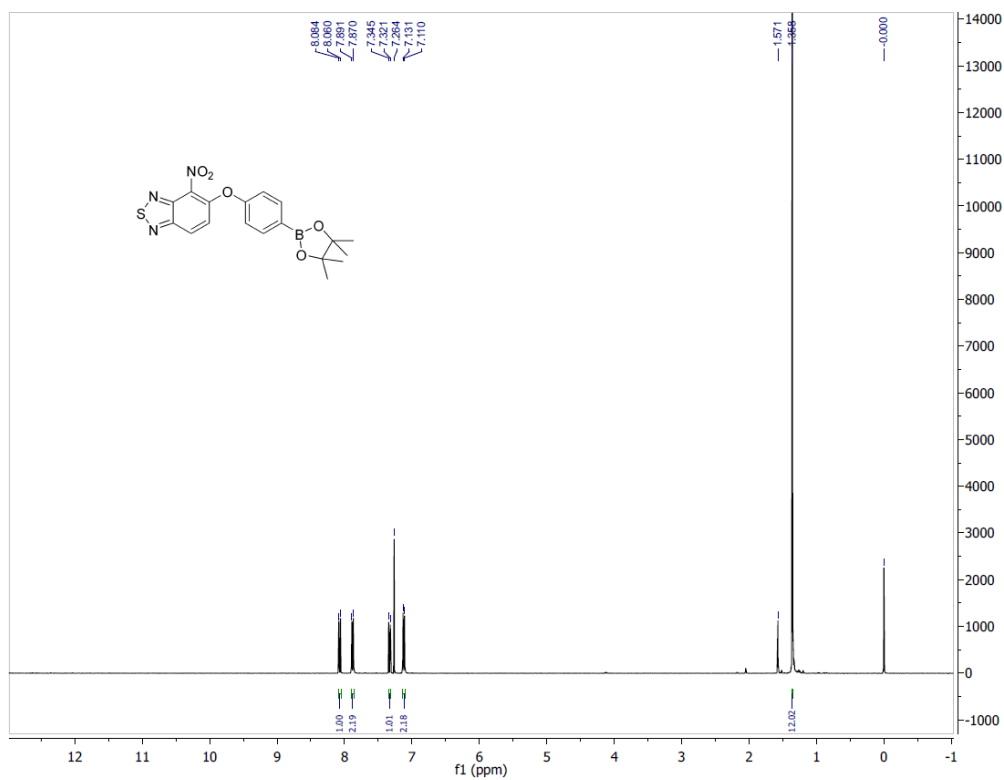
**<sup>1</sup>H NMR of compound (11)**



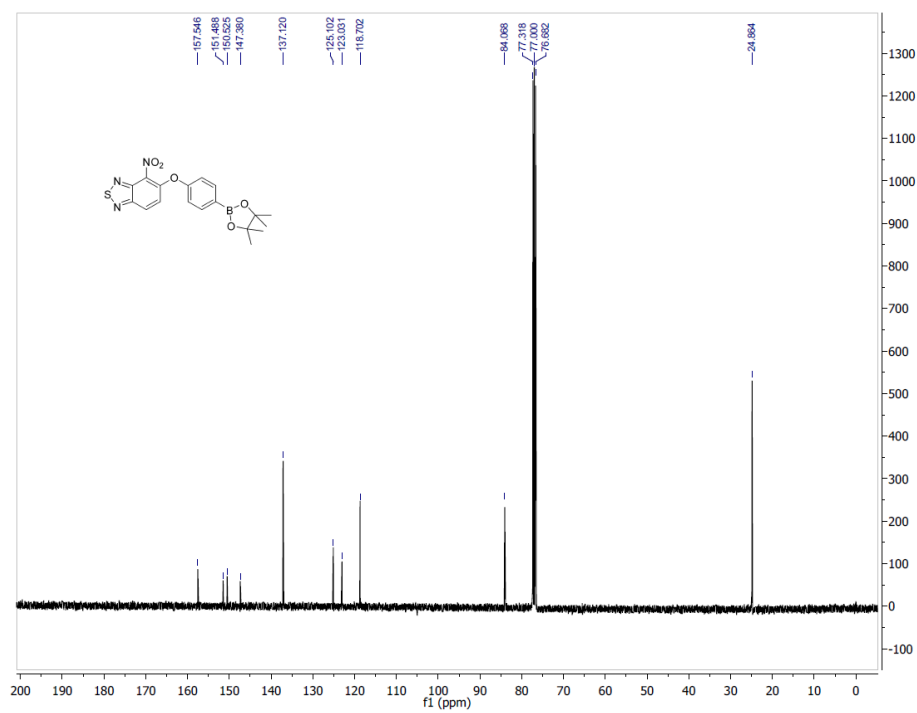
# <sup>13</sup>C NMR of compound (11)

Spectrum View - MAS-H-11B.d



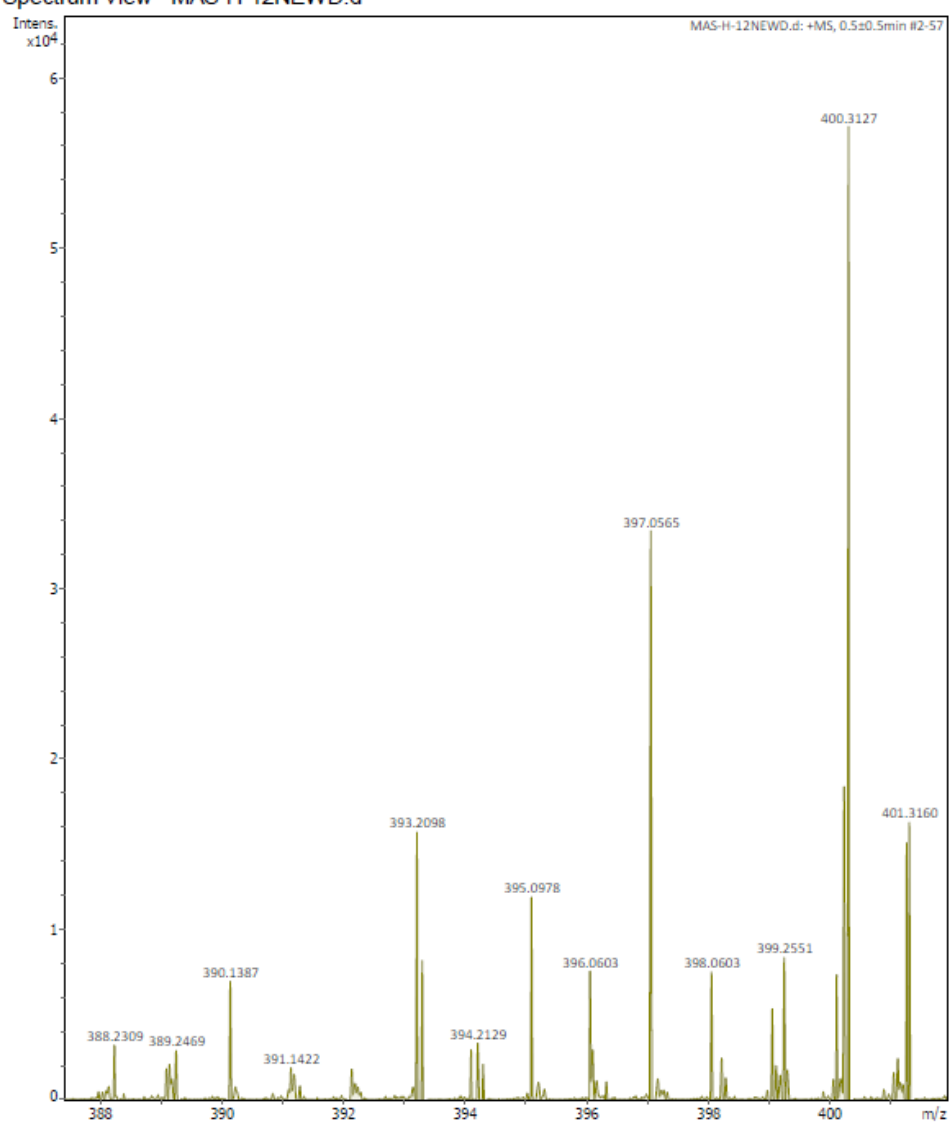


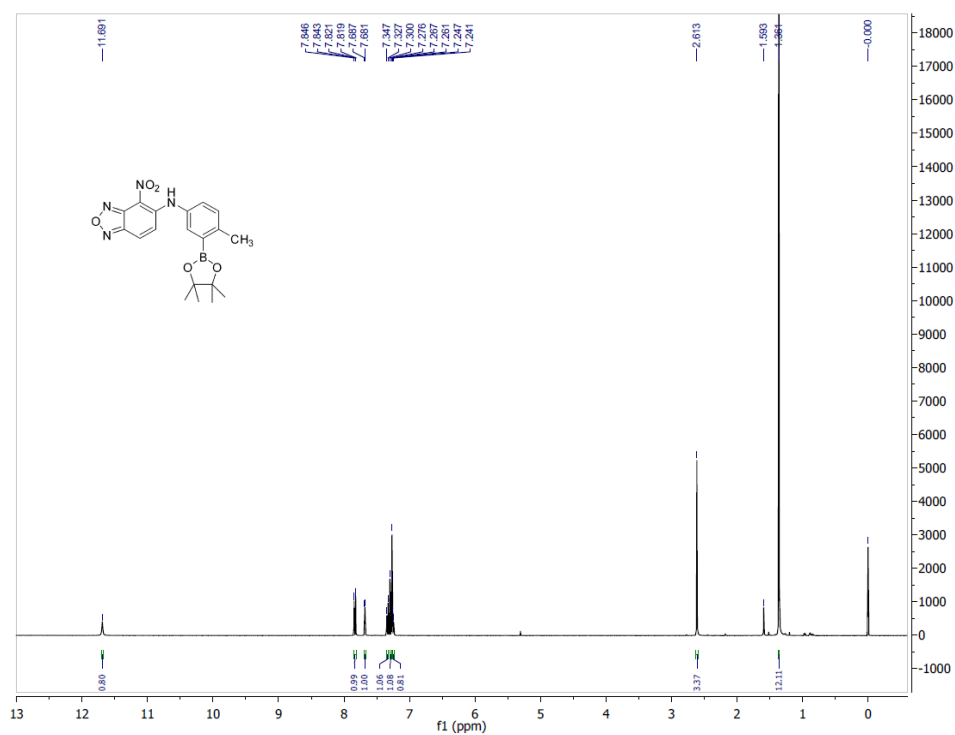
**<sup>1</sup>H NMR of compound (12)**



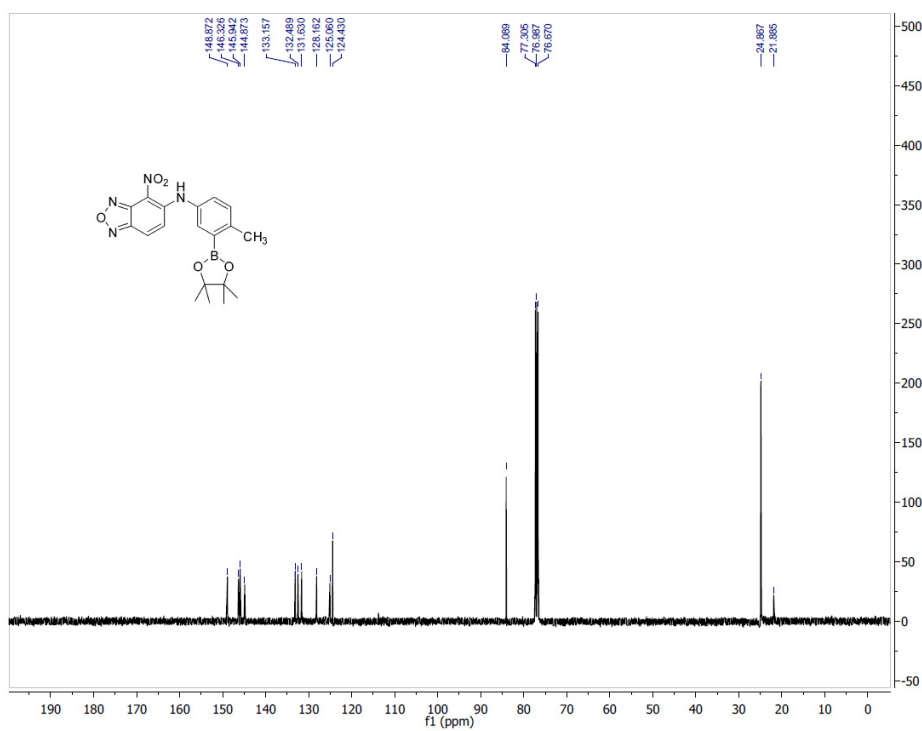
**<sup>13</sup>C NMR of compound (12)**

Spectrum View - MAS-H-12NEWD.d



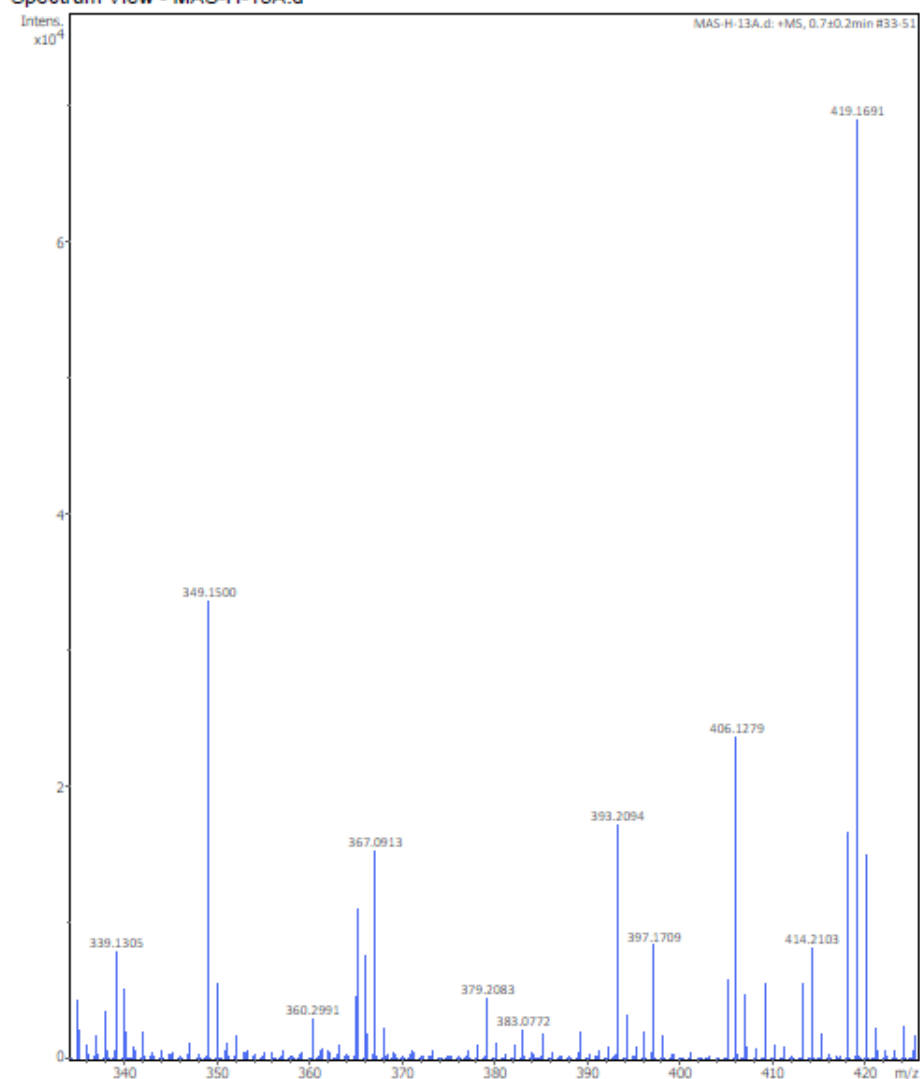


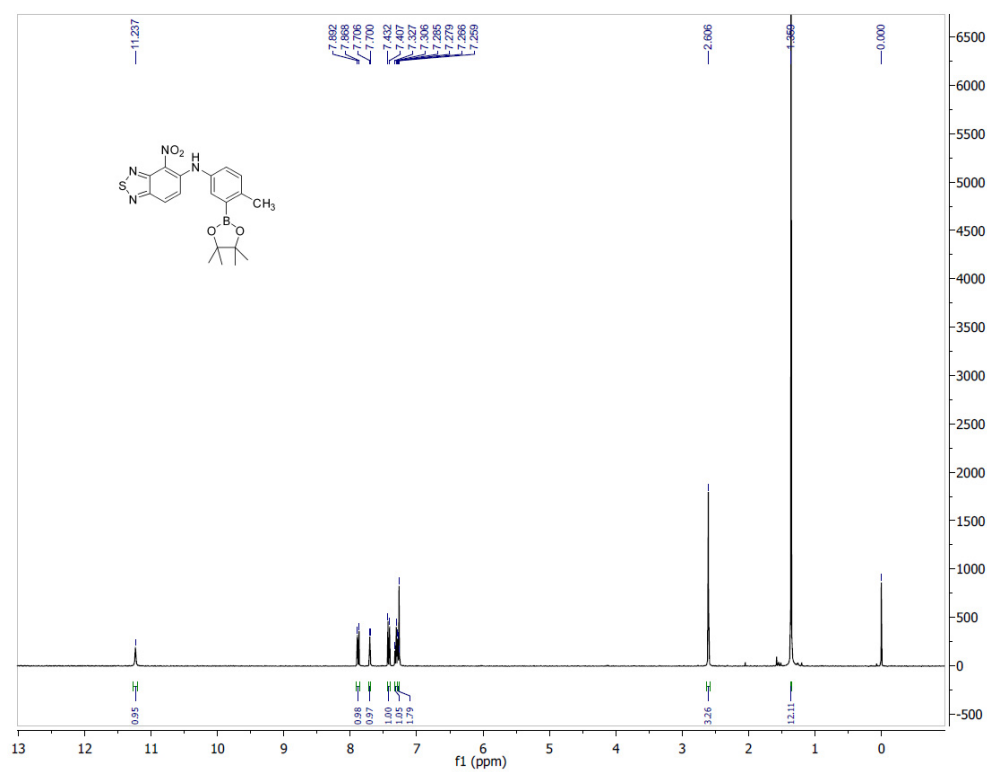
<sup>1</sup>H NMR of compound (13)



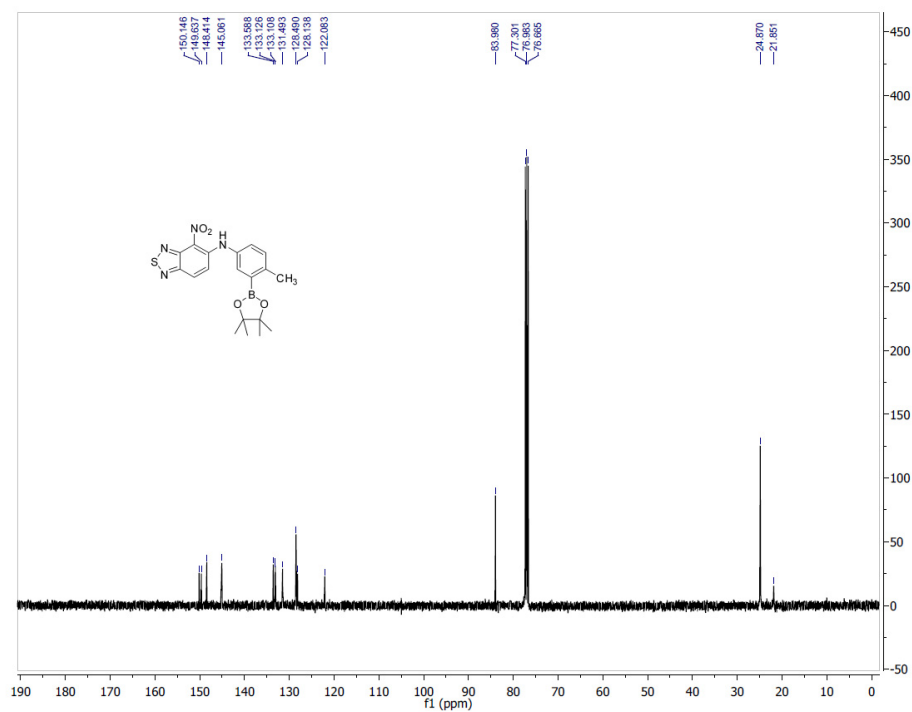
<sup>13</sup>C NMR of compound (13)

Spectrum View - MAS-H-13A.d



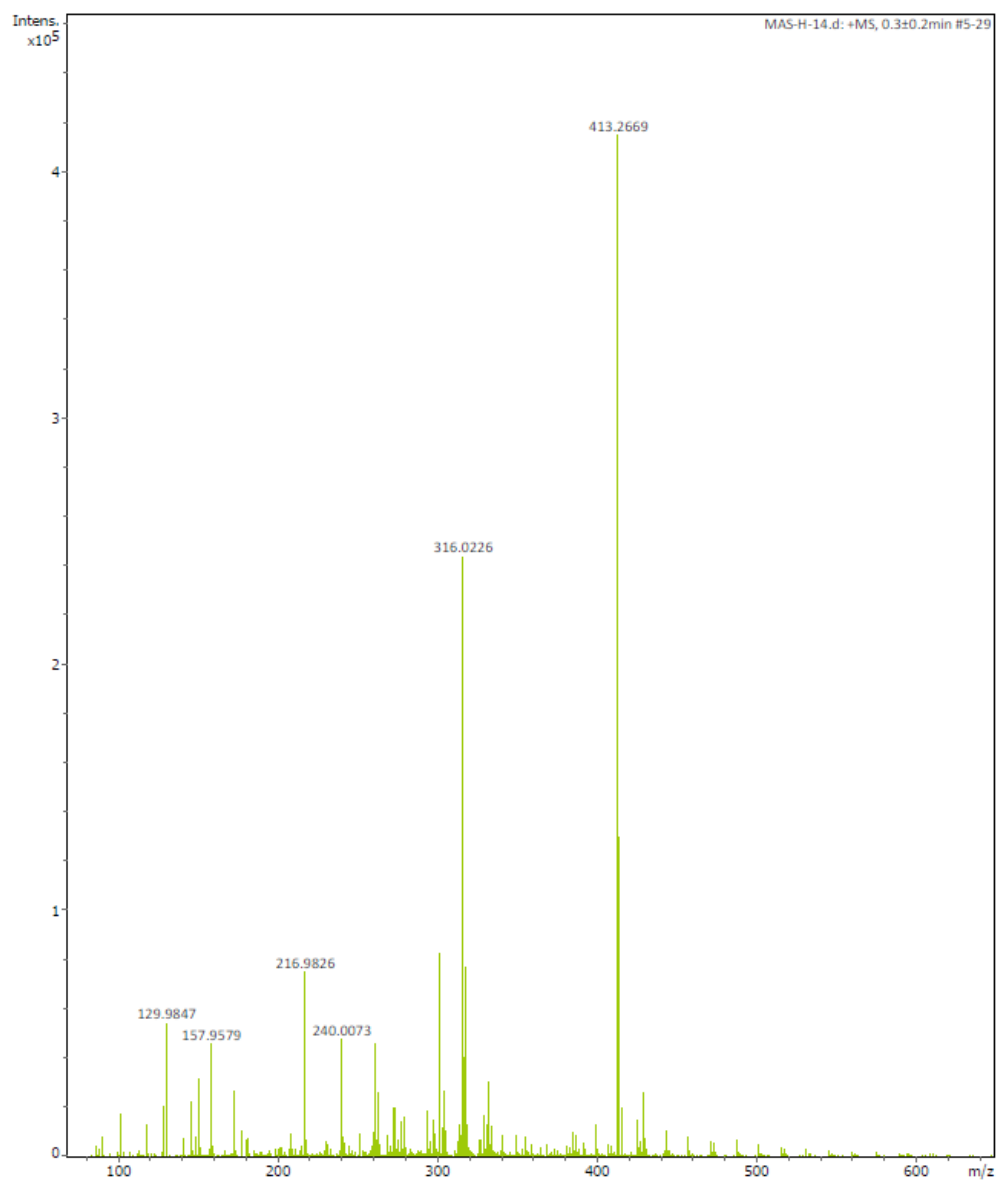


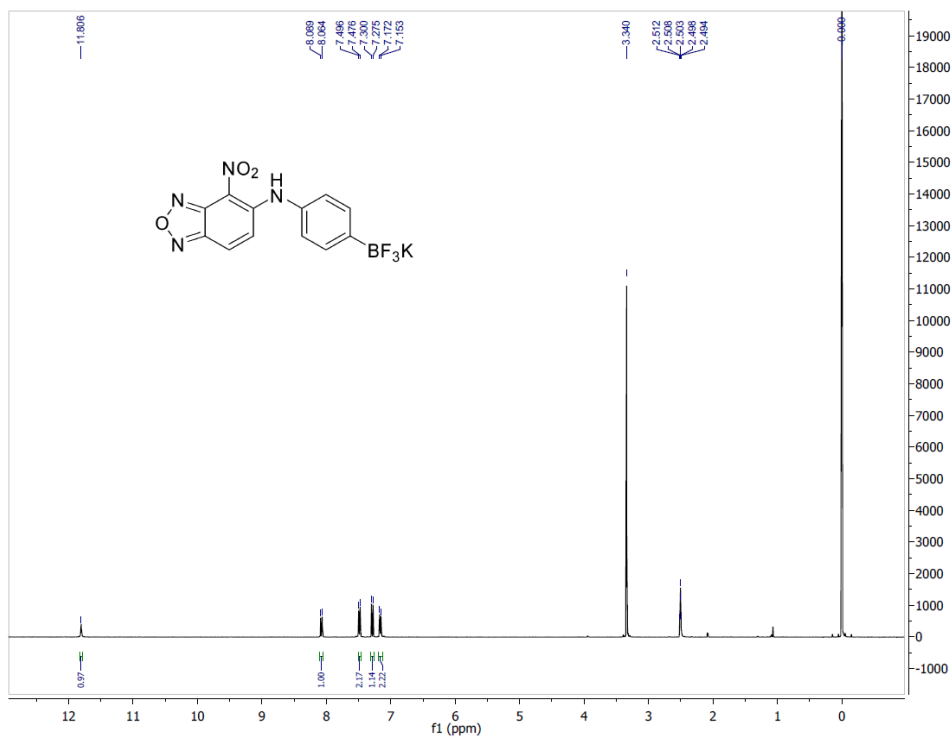
**<sup>1</sup>H NMR of compound (14)**



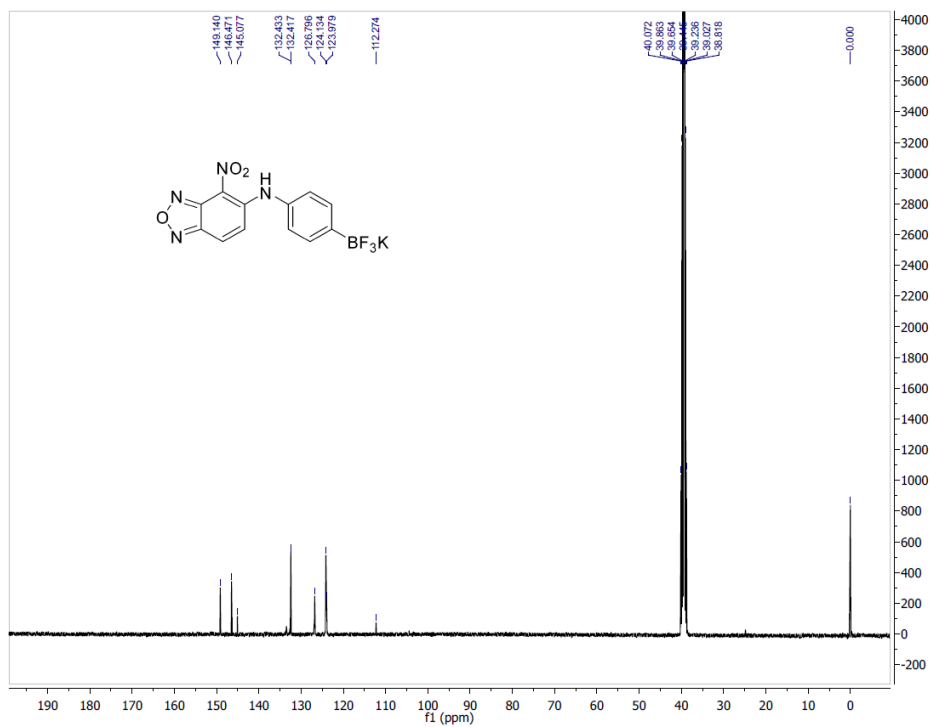


# <sup>13</sup>C NMR of compound (14)





**<sup>1</sup>H NMR of compound (15)**



**<sup>13</sup>C NMR of compound (15)**

COMP-15

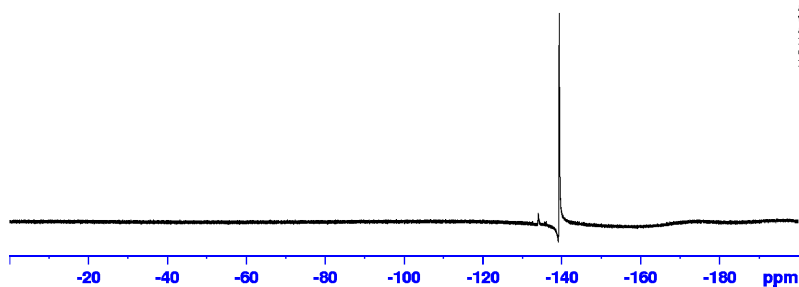
—139.41



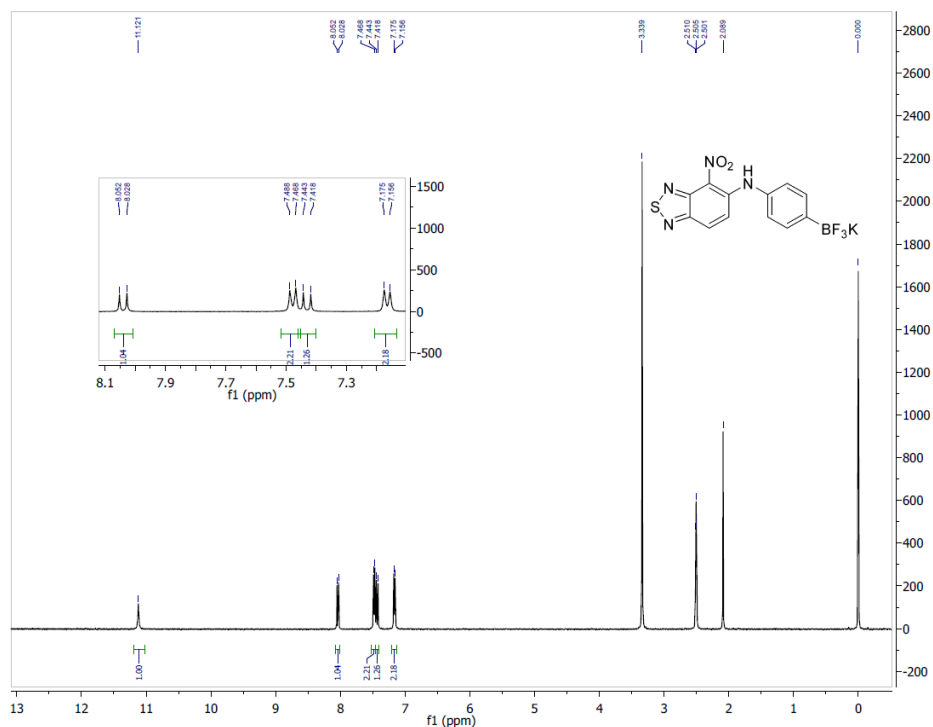
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 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
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 INSTRUM Avance Neo 400 Nanobay  
 PROBHD Z163739\_0311 ( )  
 PULPROG zg  
 TD 131072  
 SOLVENT DMSO  
 NS 64  
 DS 4  
 SWH 90909.094 Hz  
 FIDRES 1.387163 Hz  
 AQ 0.7208960 sec  
 RG 101  
 DW 5.500 usec  
 DE 6.50 usec  
 TE 295.8 K  
 D1 1.00000000 sec  
 TD0 1  
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 NUC1 19F  
 P1 12.00 usec  
 PLW1 30.18459947 W

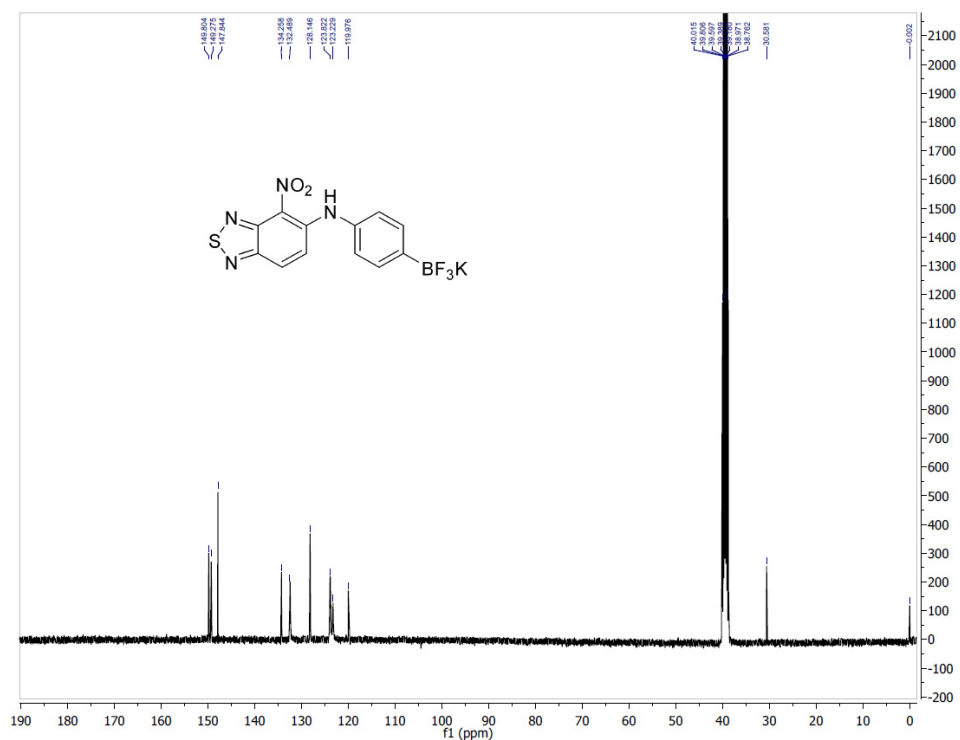
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 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



<sup>19</sup>F NMR of compound (15)



<sup>1</sup>H NMR of compound (16)



<sup>13</sup>C NMR of compound (16)

COMP-16

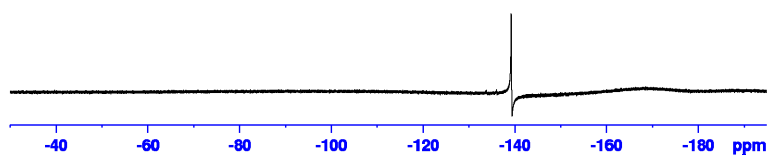
— -139.22



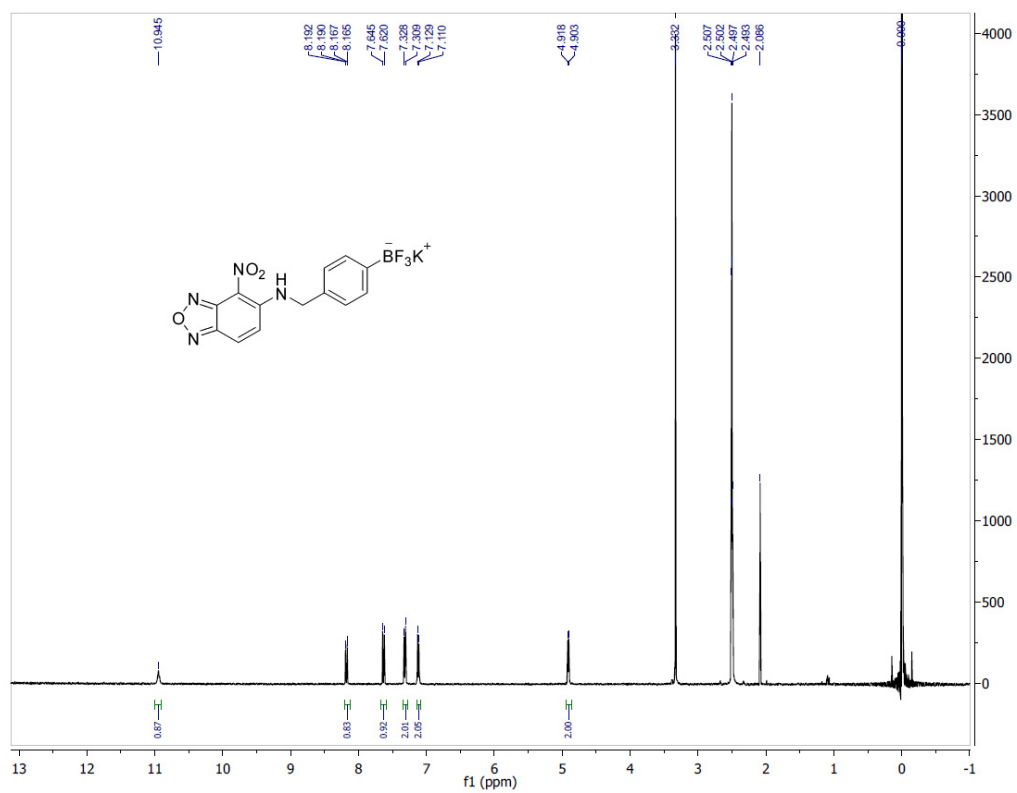
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EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
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Time 17.16 h  
INSTRUM Avance Neo 400 Nanobay  
PROBHD 2163739\_0311 (   
PULPROG zgpg30  
TD 131072  
SOLVENT DMSO  
NS 64  
DS 4  
SWH 90909.094 Hz  
FIDRES 1.387163 Hz  
AQ 0.7208960 sec  
RG 101  
DW 5.500 usec  
DE 6.50 usec  
TE 295.2 K  
D1 1.00000000 sec  
TD0 1  
SFO1 376.4748291 MHz  
NUC1 19F  
P1 12.00 usec  
PLW1 30.18499947 W

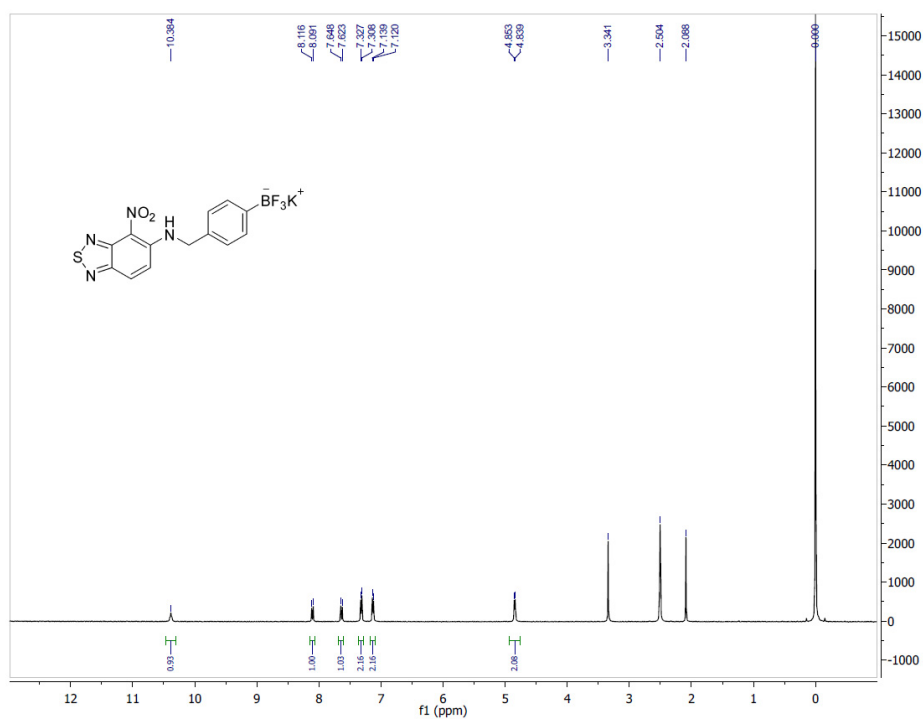
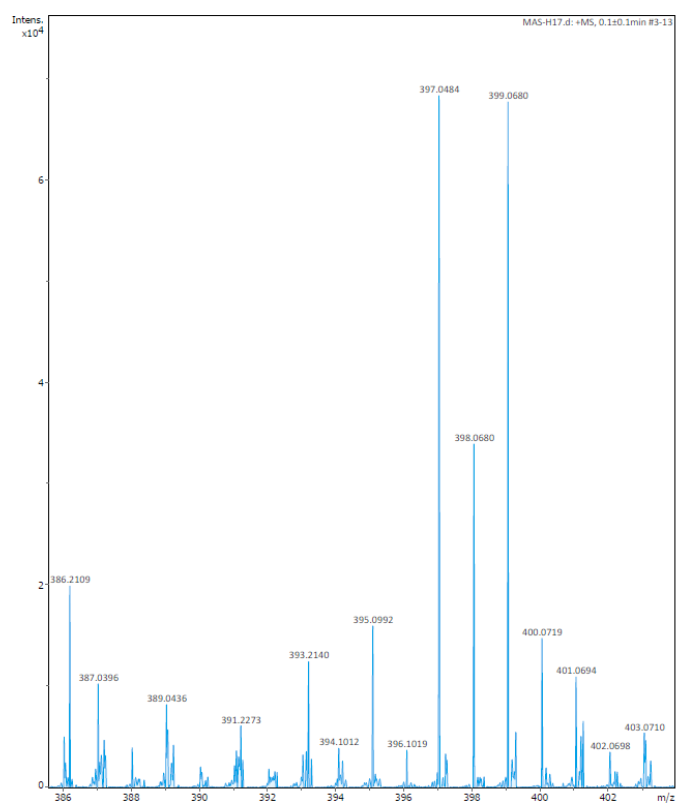
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WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



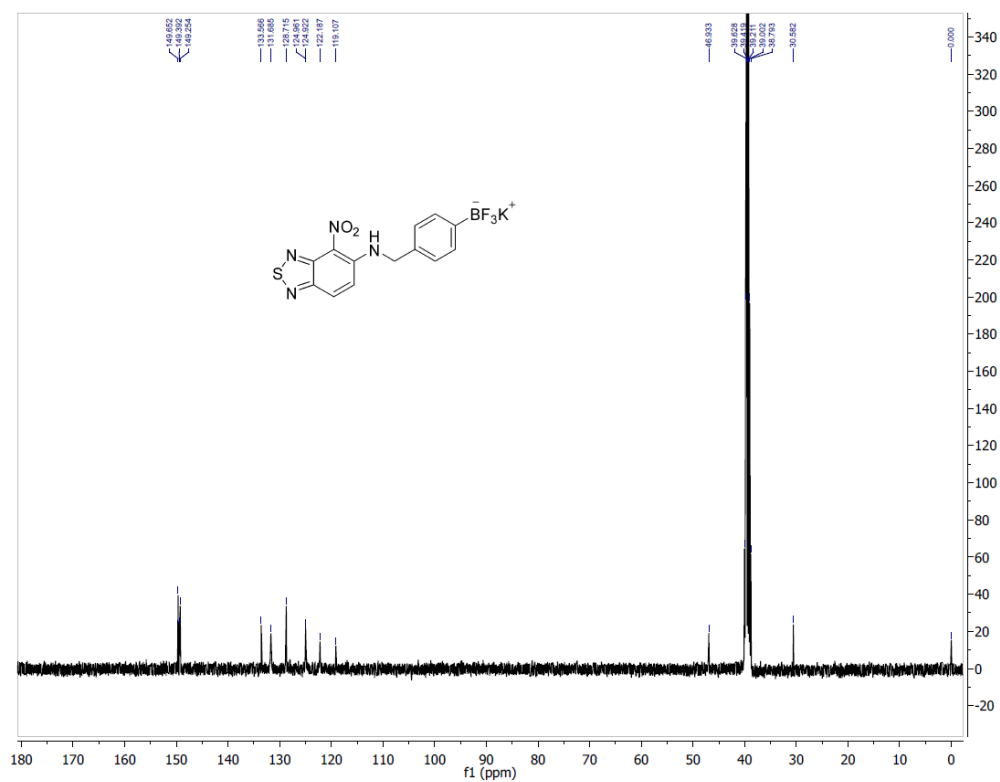
<sup>19</sup>F NMR of compound (16)



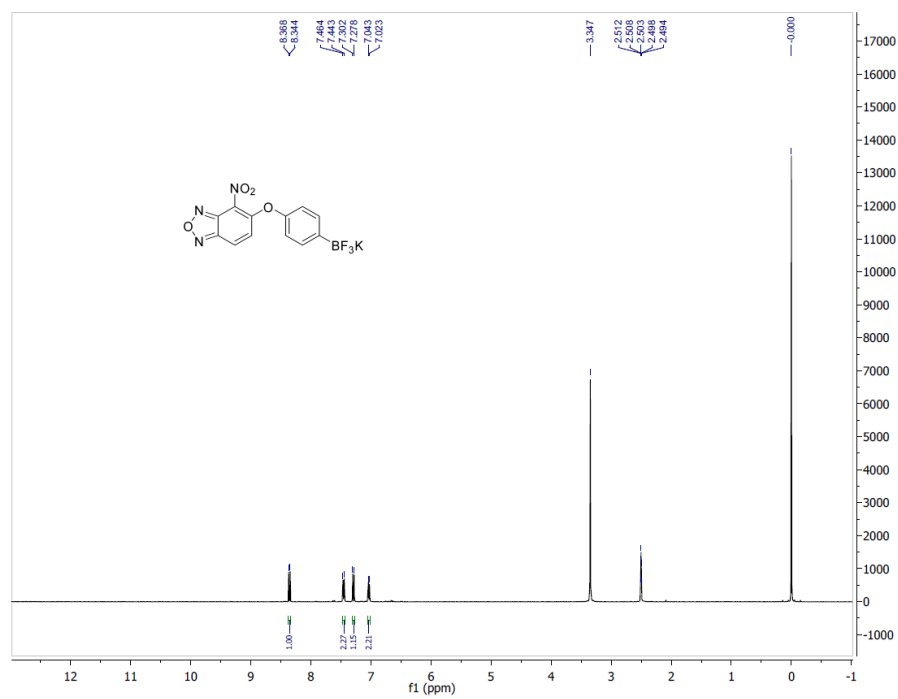
**<sup>1</sup>H NMR of compound (17)**



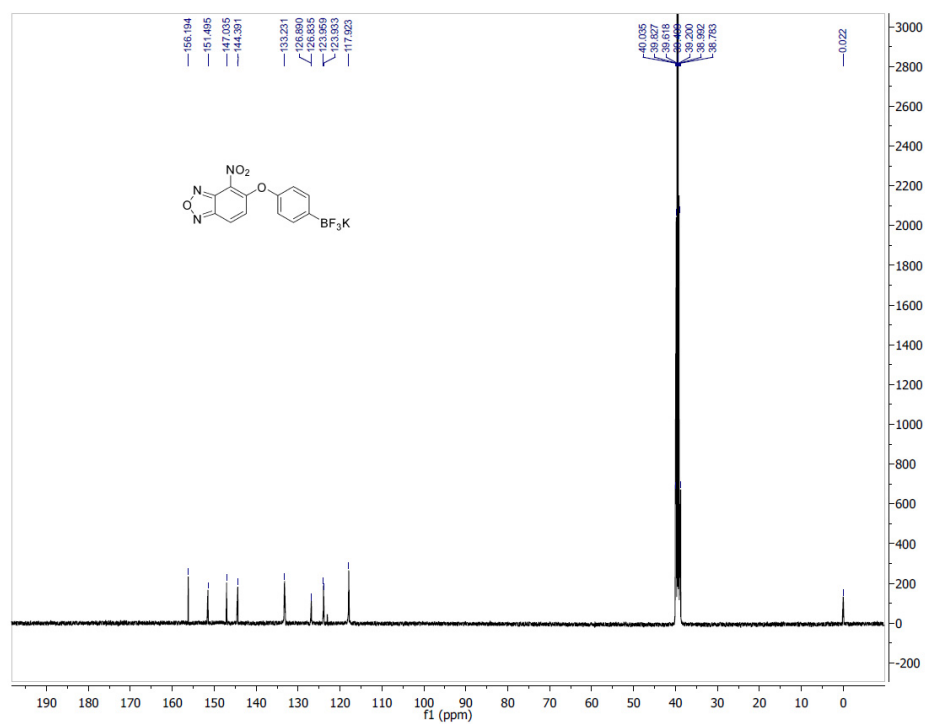
$^1\text{H}$  NMR of compound (18)



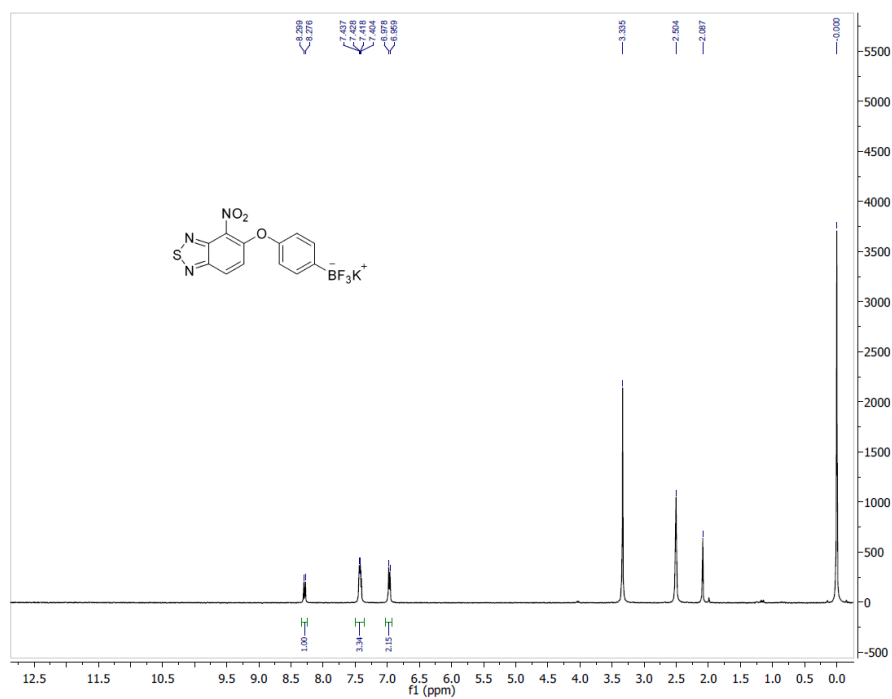
<sup>13</sup>C NMR of compound (18)



<sup>1</sup>H NMR of compound (19)

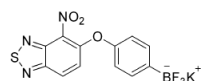


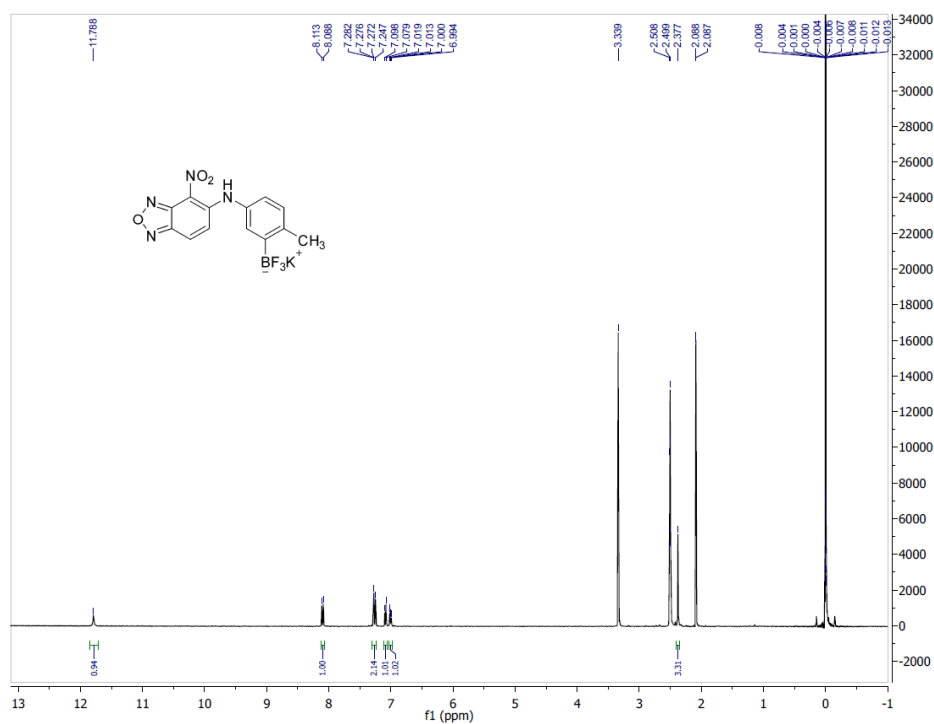
**<sup>13</sup>C NMR of compound (19)**



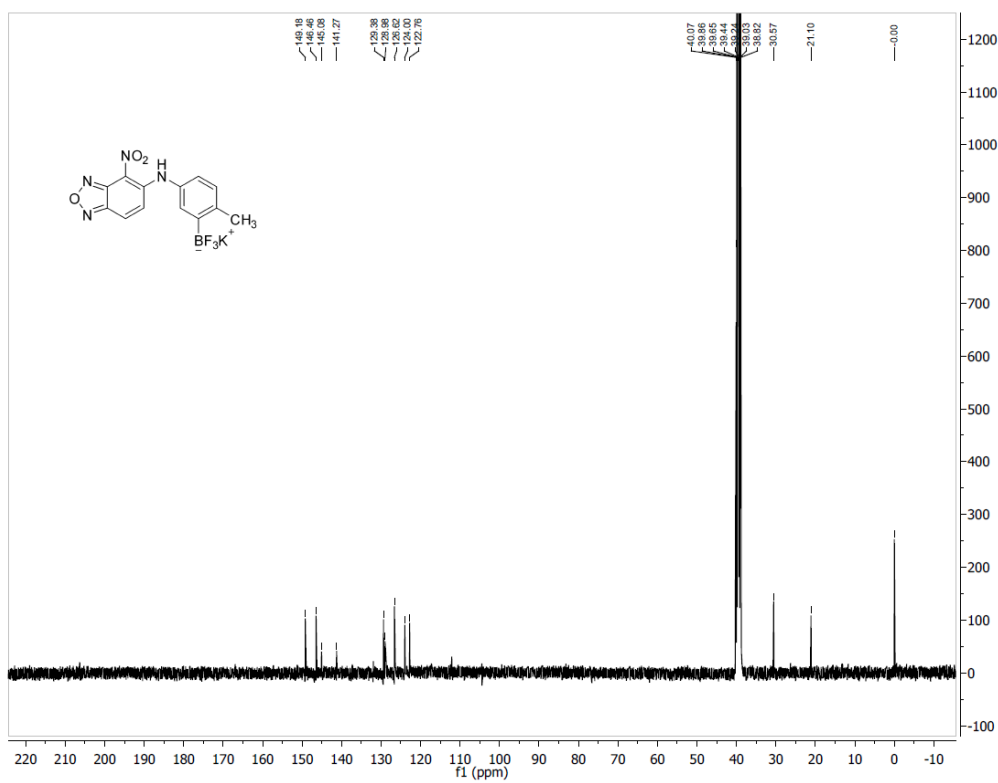
**<sup>1</sup>H NMR of compound (20)**







**<sup>1</sup>H NMR of compound (21)**



# <sup>13</sup>C NMR of compound (21)

COMPOUND 21

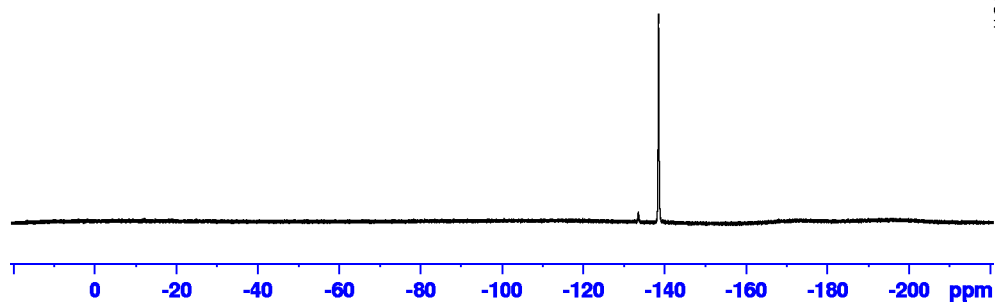
— -138.29



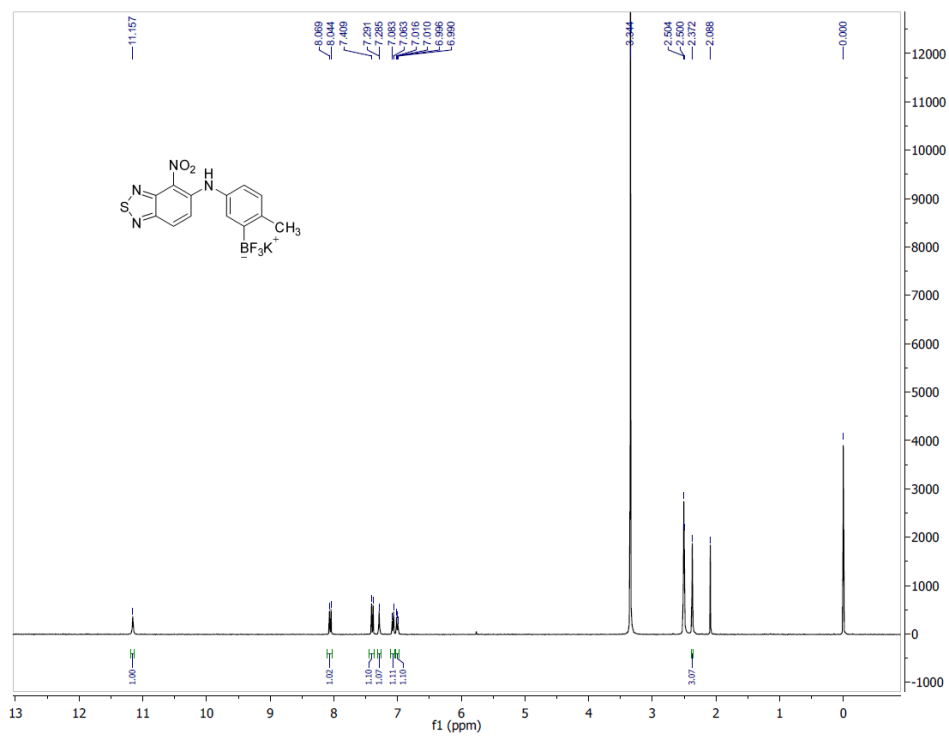
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NAME Oct13-2022  
EXPNO 2  
PROCNO 1

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PULPROG zg  
TD 131072  
SOLVENT DMSO  
NS 16  
DS 4  
SWH 90909.094 Hz  
FIDRES 1.387163 Hz  
AQ 0.7208960 sec  
RG 101  
DW 5.500 usec  
DE 6.50 usec  
TE 295.9 K  
D1 1.00000000 sec  
TD0 1  
SFO1 376.4748291 MHz  
NUC1 19F  
P1 12.00 usec  
PLW1 30.18499947 W

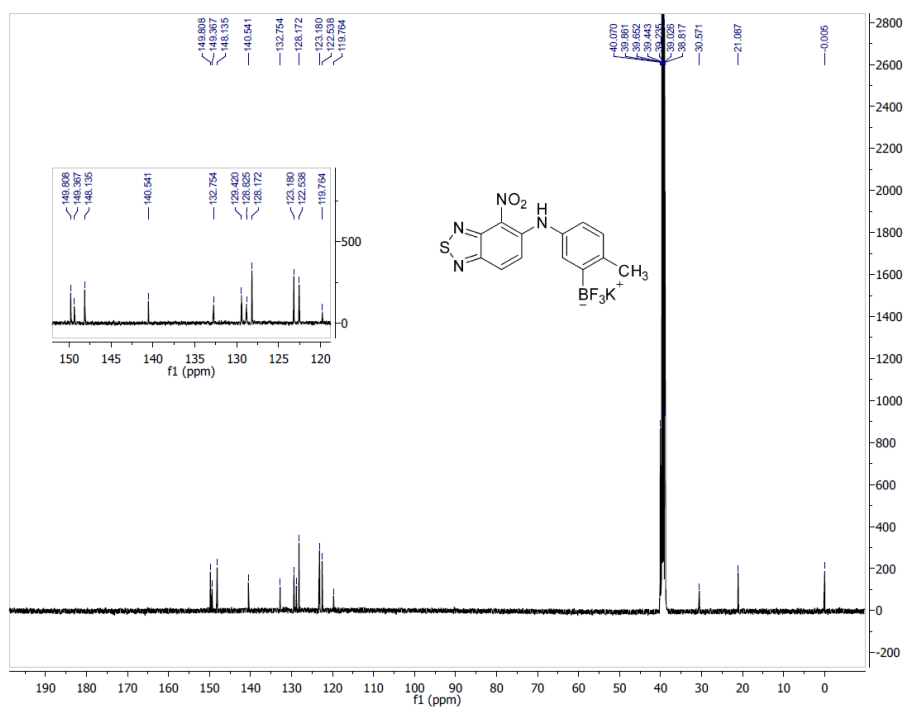
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SF 376.5124803 MHz  
WDW EM  
SSR 0  
LB 0.30 Hz  
GB 0  
PC 1.00



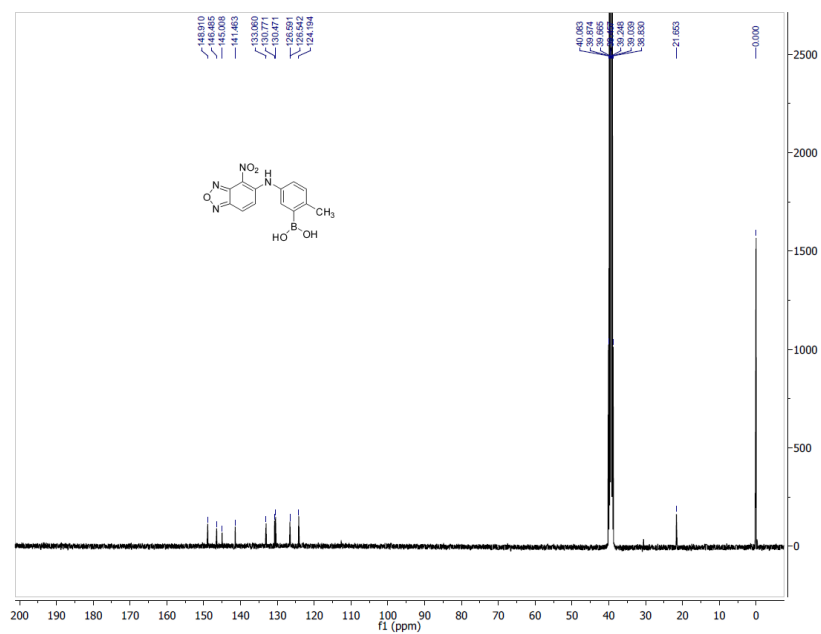
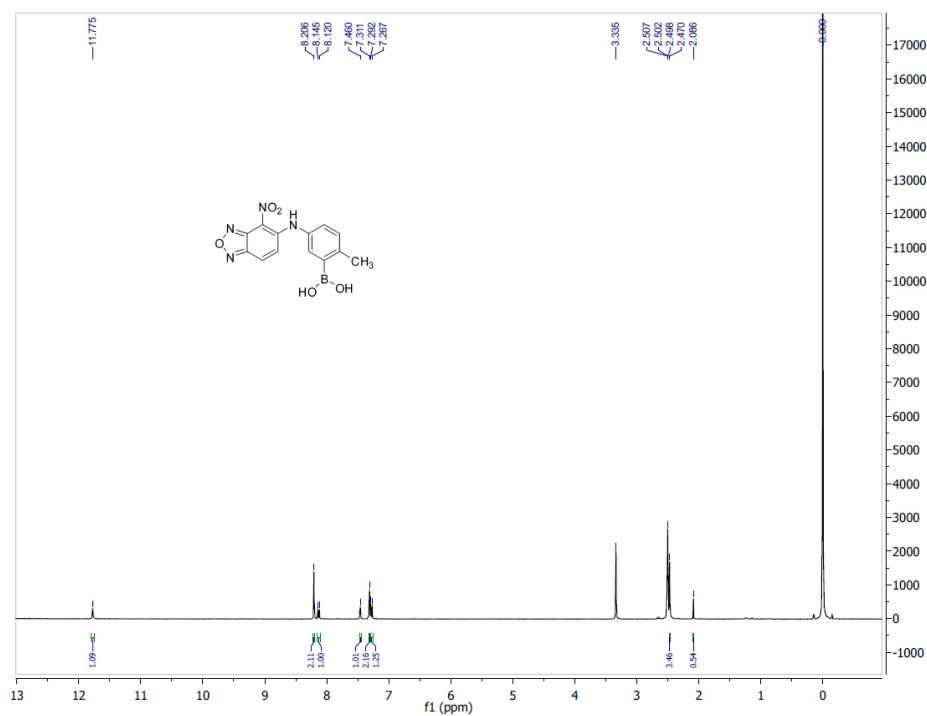
# <sup>19</sup>F NMR of compound (21)



**<sup>1</sup>H NMR of compound (22)**



**<sup>13</sup>C NMR of compound (22)**



**Figure S1.** Spectra of the products (7–23).