Replacement of nitro function by free boronic acid in the group of non-steroidal anti-androgens.

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Supporting information

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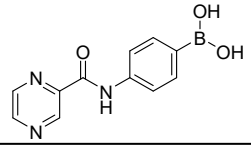
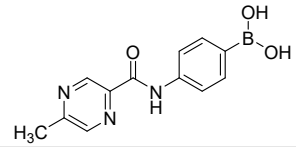
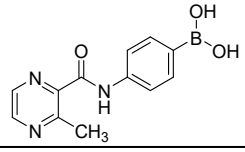
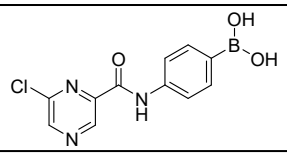
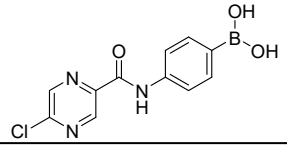
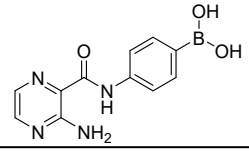
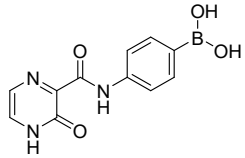
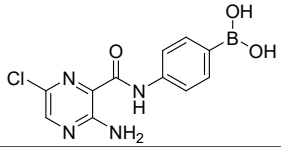
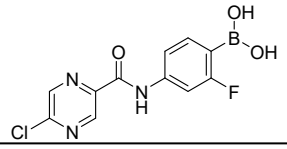
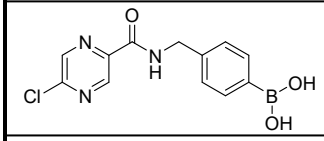
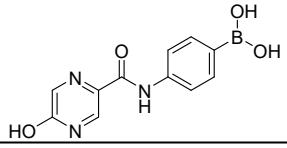
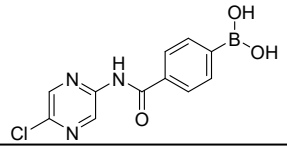
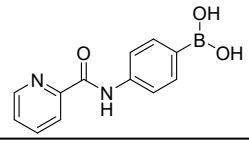
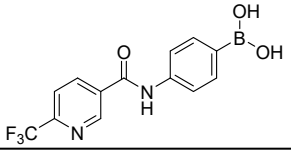
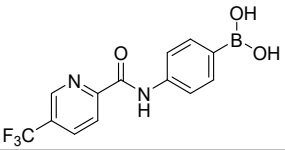
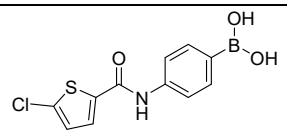
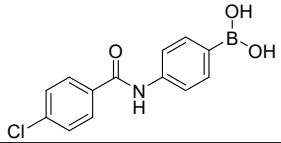
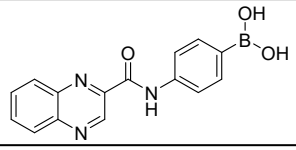
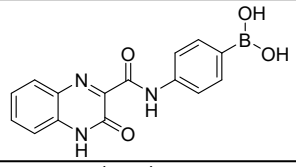
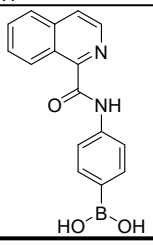
Results of *in vitro* cytotoxicity screening

Table S1: Complete results of in vitro cytotoxicity screening for aromatic amides against the tested cell lines with indicated incubation time and calculated selectivity index (SI).

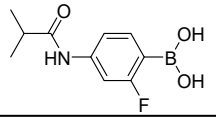
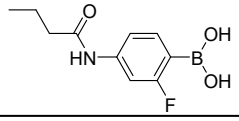
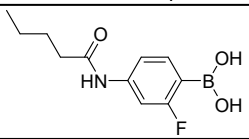
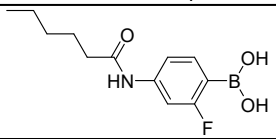
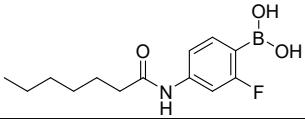
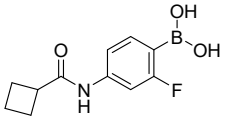
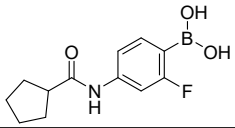
Structure	Code	IC_{50} (μM)					
		HepG2 (24 h)	PC3 (24 h)	PC3 (72 h)	HK-2 (72 h)	LAPC4 (72 h)	SI (HK-2/LAPC4)
	**1a**	>250	>100	na	na	>100	na
	**2a**	>100	>100	na	na	>100	na
	**3a**	>500	>1000	na	na	>100	na

	**4a**	>500	>250	na	na	>100	na
	**5a**	139.3	133.4	121.6	194.5	27.8	7.0
	**6a**	>250	>250	na	na	>100	na
	**7a**	>500	>500	na	na	>100	na
	**8a**	126.4	193.3	375.2	422.4	78.3	5.4
	**9a**	71.26	118.4	78.1	137.7	19.2	7.2
	**10a**	187	>1000	227.9	183.7	48.0	3.8
	**11a**	>1000	296	779.6	1000	>100	na
	**12a**	>1000	na	na	na	>100	na
	**13a**	>250	>250	na	na	>100	na
	**14a**	>100	>100	na	na	>100	na
	**15a**	>25	>50	na	na	>100	na

	**16a**	>50	>50	na	na	>100	na
	**17a**	>25	>100	na	na	>100	na
	**18a**	>50	>50	na	na	>100	na
	**19a**	>50	>50	na	na	>100	na
	**20a**	322.2	>250	na	na	>100	na

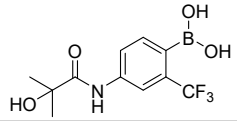
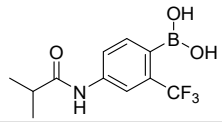
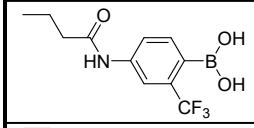
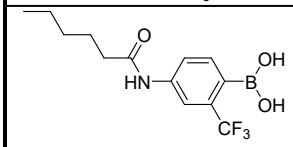
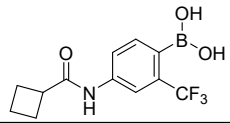
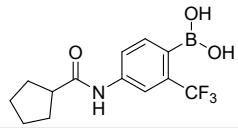
NOTE: na= not available.

Table S2: Complete results of in vitro cytotoxicity screening for aliphatic and alicyclic amides against the tested cell lines with indicated incubation time and calculated selectivity index (SI).

Structure	Code	IC_{50} (μM)					
		HepG2 (24 h)	PC3 (24 h)	PC3 (72 h)	HK-2 (72 h)	LAPC4 (72 h)	SI (HK-2/LAPC4)
	**1b**	>1000	>1000	na	na	>100	na
	**2b**	>1000	>1000	na	na	>100	na
	**3b**	>1000	877.7	na	na	>100	na
	**4b**	>250	>250	na	na	>100	na
	**5b**	>250	>250	na	na	>100	na
	**6b**	>1000	>1000	na	na	>100	na
	**7b**	>500	>1000	na	na	>100	na

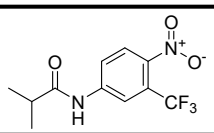
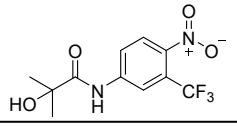
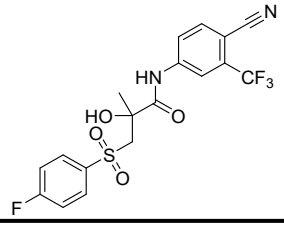
NOTE: na= not available.

Table S3: Complete results of in vitro cytotoxicity screening for aliphatic and alicyclic amides substituted with trifluoromethyl group against the tested cell lines with indicated incubation time and calculated selectivity index (SI).

Structure	Code	IC_{50} (μM)					
		HepG2 (24h)	PC3 (24h)	PC3 (72h)	HK-2 (72h)	LAPC4 (72h)	SI (HK-2/LAPC4)
	**HFB**	>1000	>1000	>1000	>1000	403.8	na
	**1c**	>1000	>1000	697.1	>1000	>100	na
	**2c**	>1000	>1000	na	na	>100	na
	**3c**	>1000	>500	na	na	>100	na
	**4c**	>1000	>1000	na	na	>100	na
	**5c**	>1000	>1000	185.6	>1000	>100	na

NOTE: na= not available.

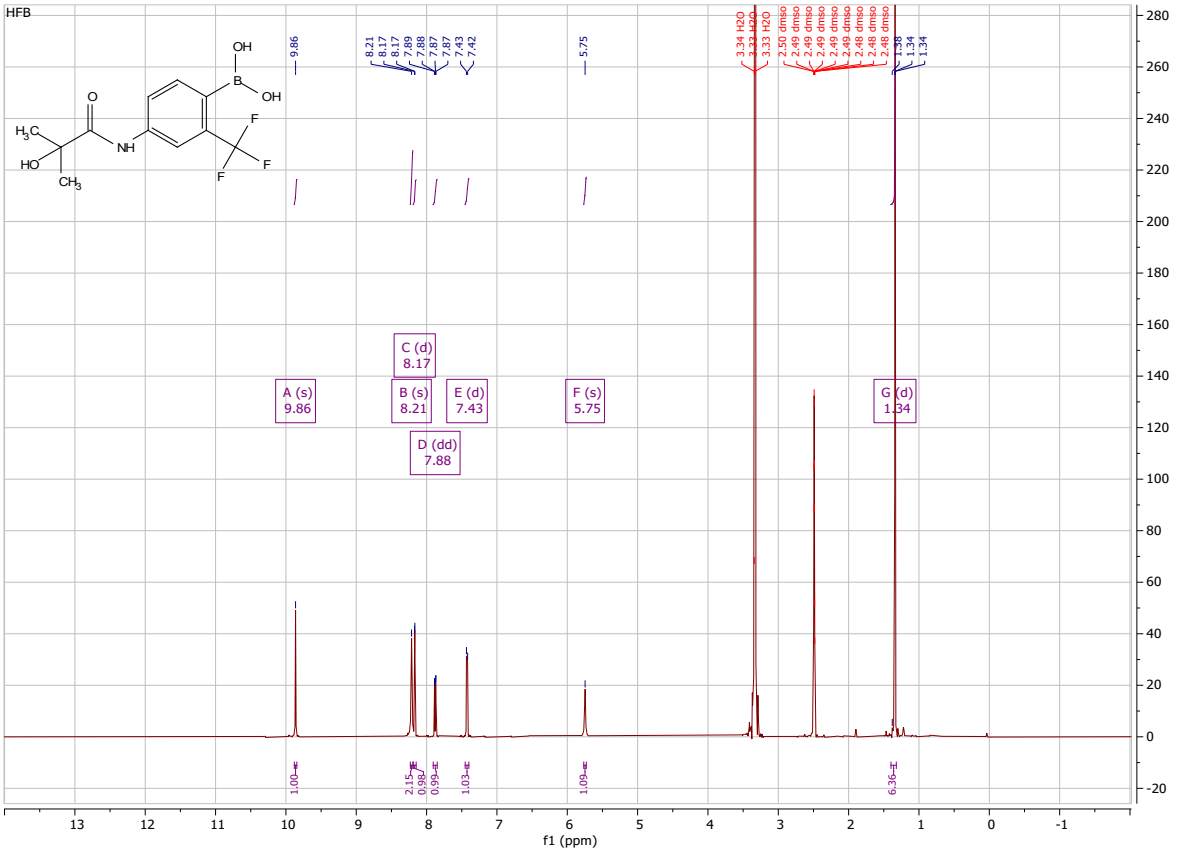
Table S4: Results of in vitro cytotoxicity screening for standards against the tested cell lines with indicated incubation time and calculated selectivity index (SI).

Structure	Code	IC_{50} (μM)					
		HepG2 (24 h)	PC3 (24 h)	PC3 (72 h)	HK-2 (72 h)	LAPC4 (72 h)	SI (HK-2/LAPC4)
	**flutamide**	137.2	34.7	50.8	76.2	60.5	1.3
	**HF**	103.2	229.2	41.8	231.0	136.1	1.7
	**bicalutamide (racemic mixture)**	na	na	na	na	37.2	na

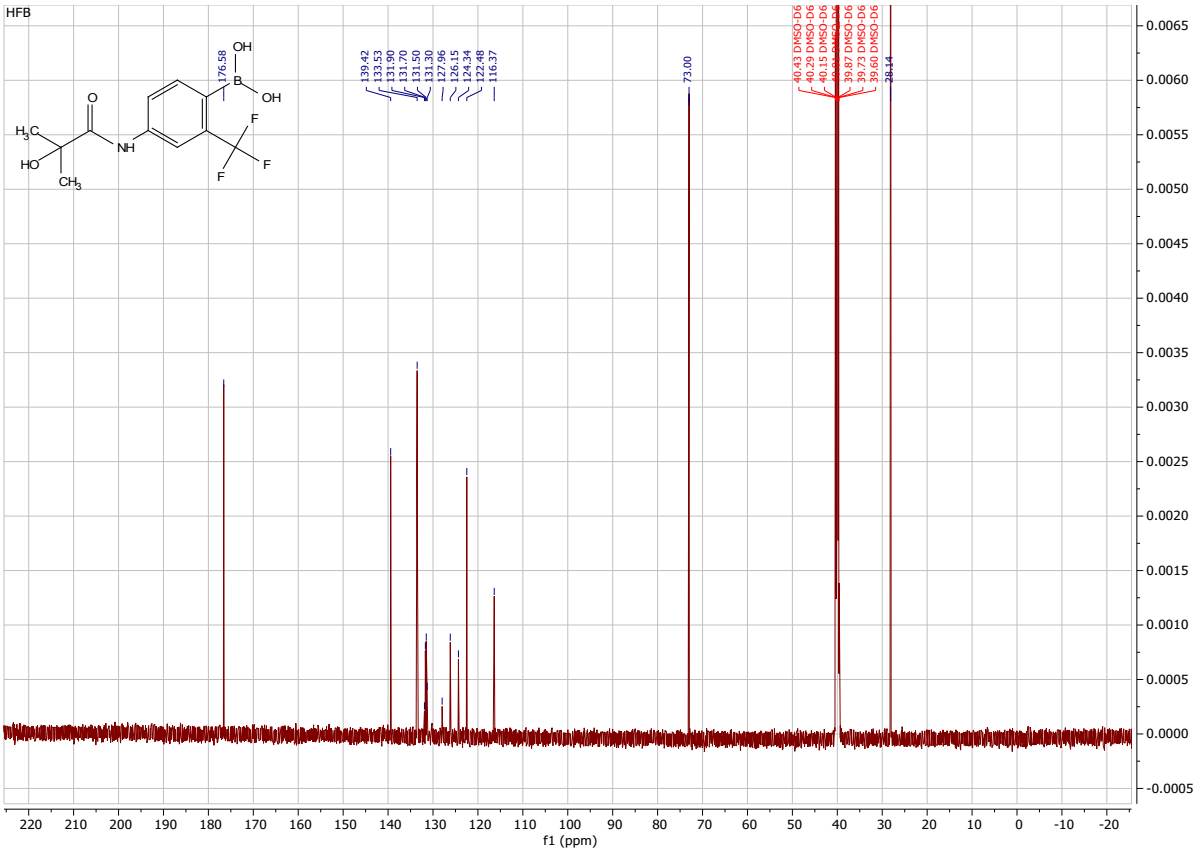
NOTE: na= not available.

NMR spectra of final compounds

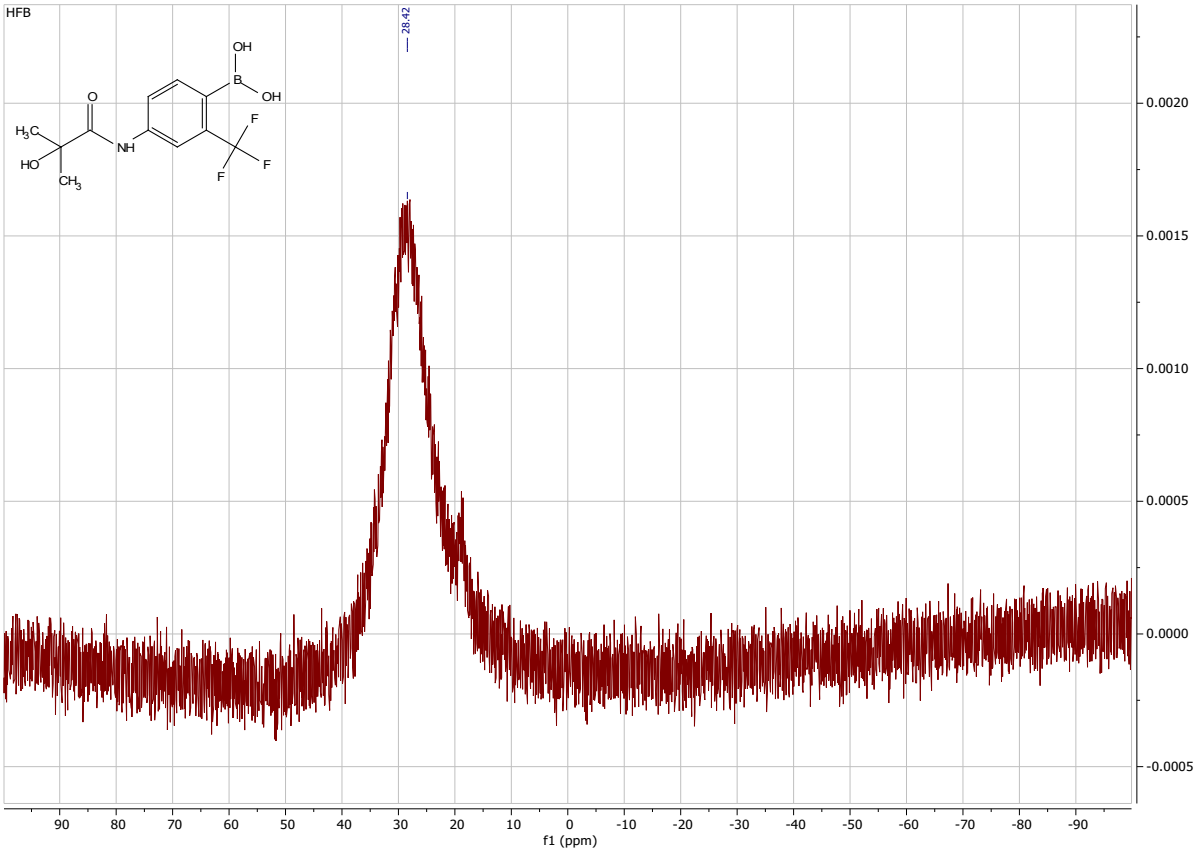
HFB ^{1}H NMR spectrum



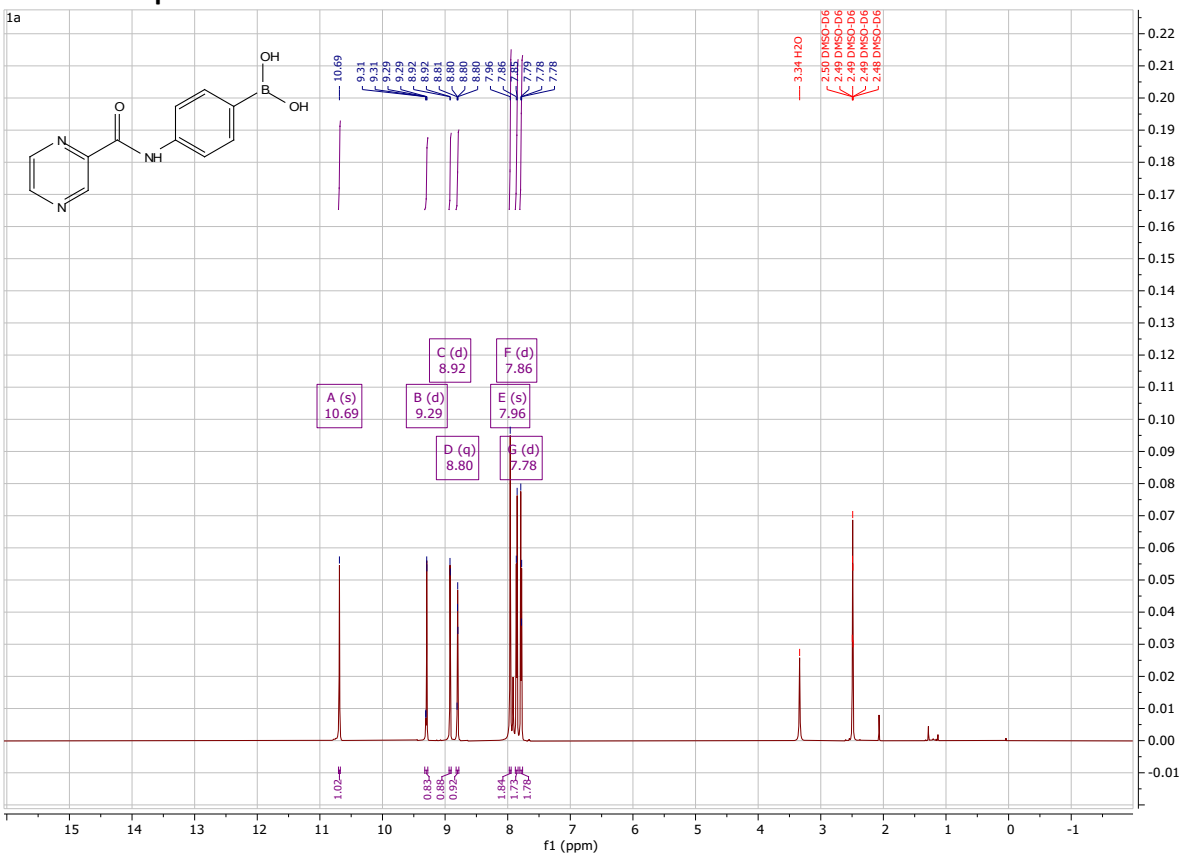
HFB ^{13}C NMR spectrum



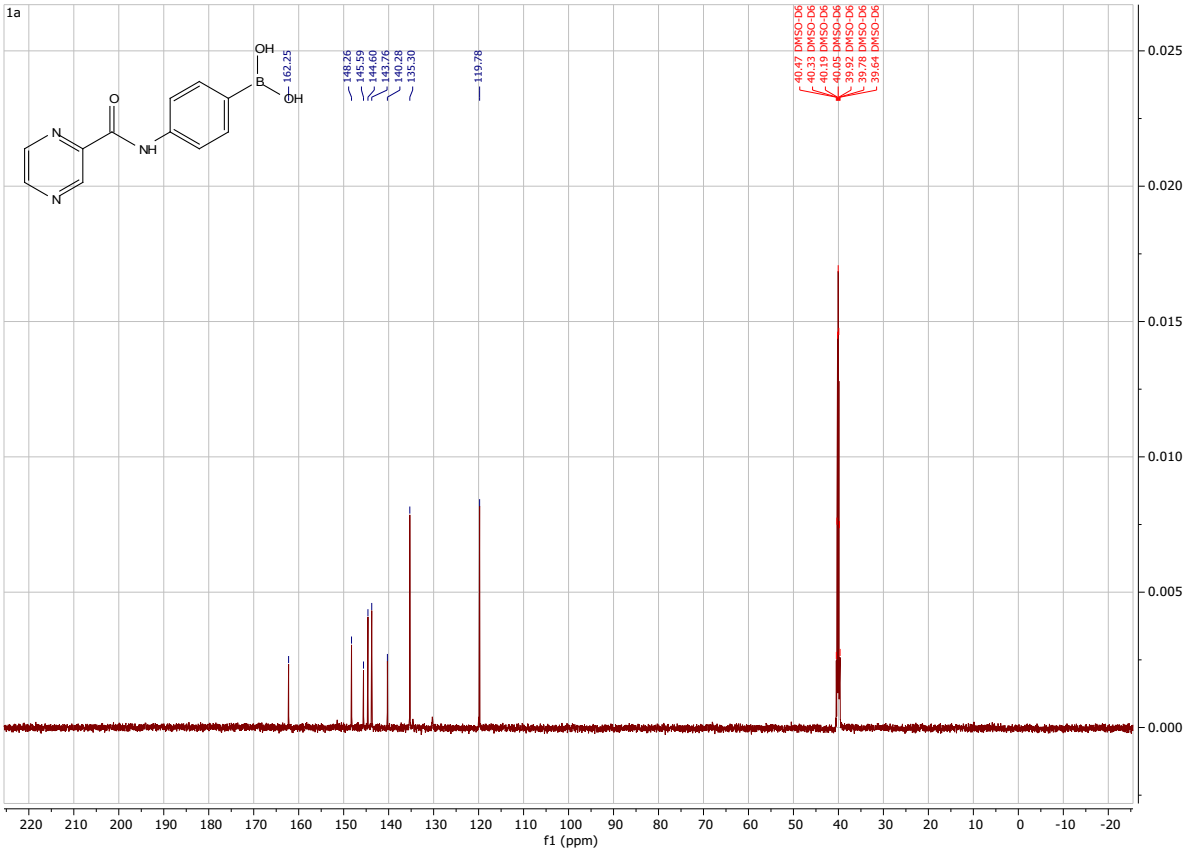
HFB ^{11}B NMR spectrum



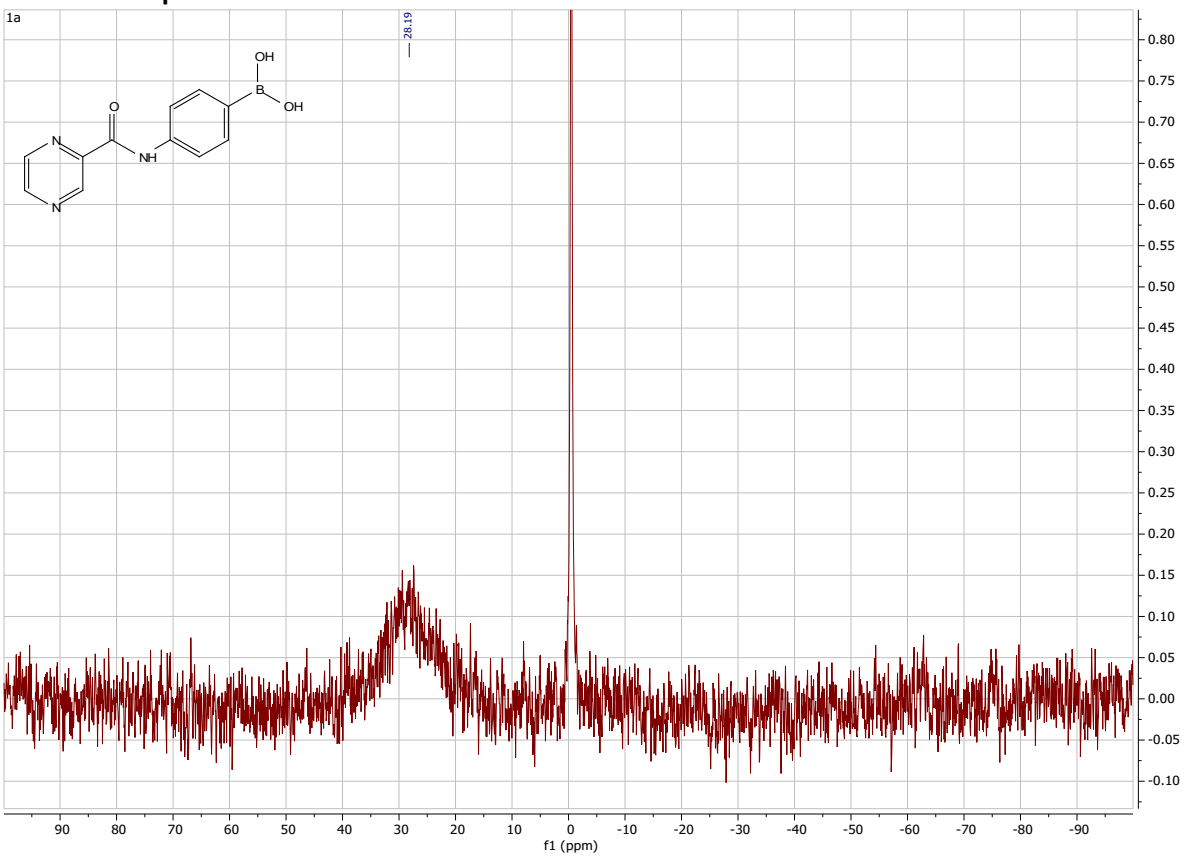
1a ^{1}H NMR spectrum



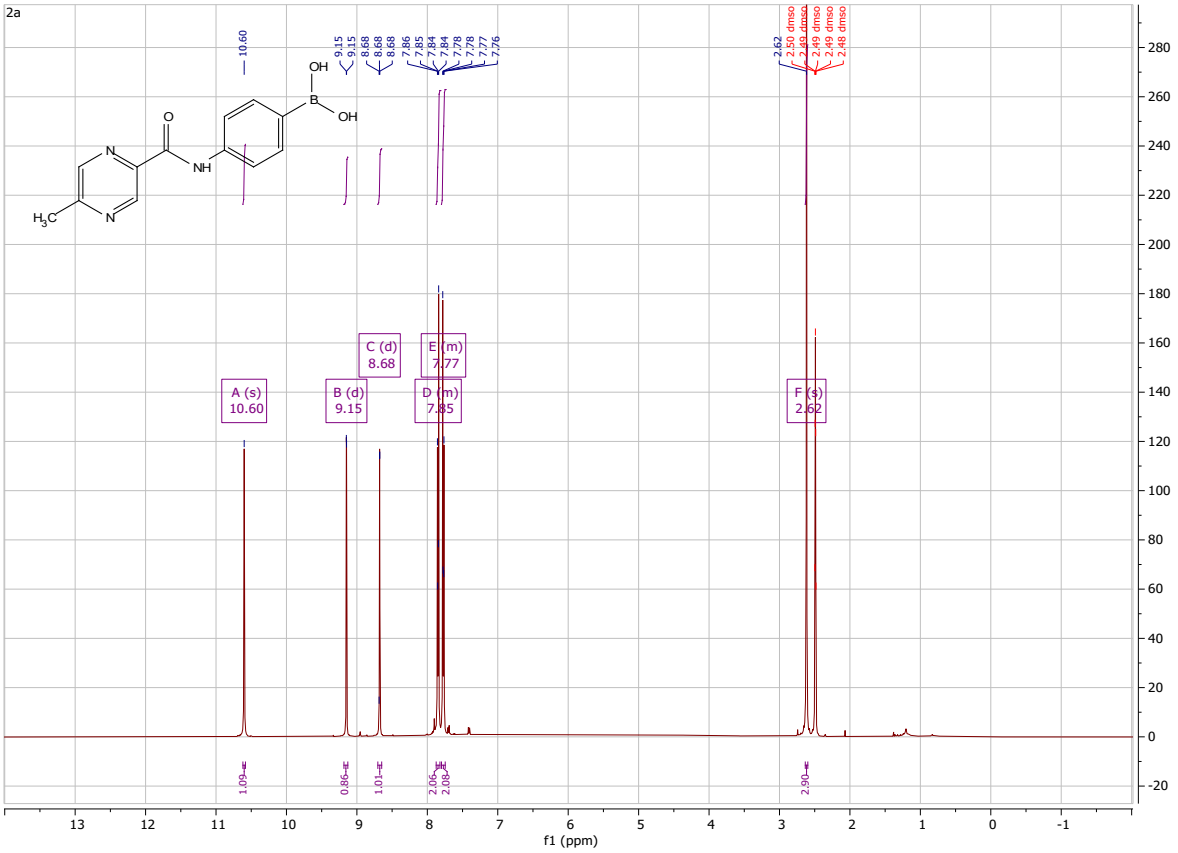
1a ^{13}C NMR spectrum



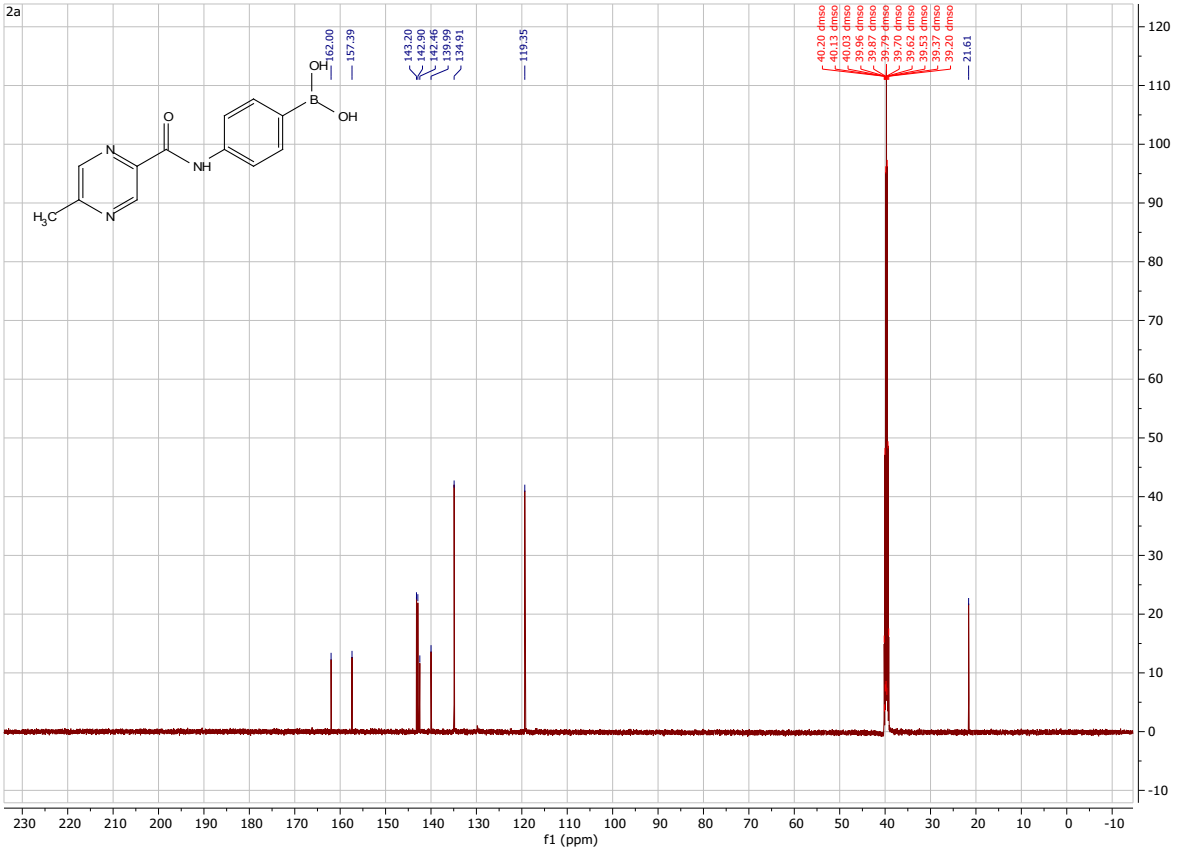
1a ^{11}B NMR spectrum



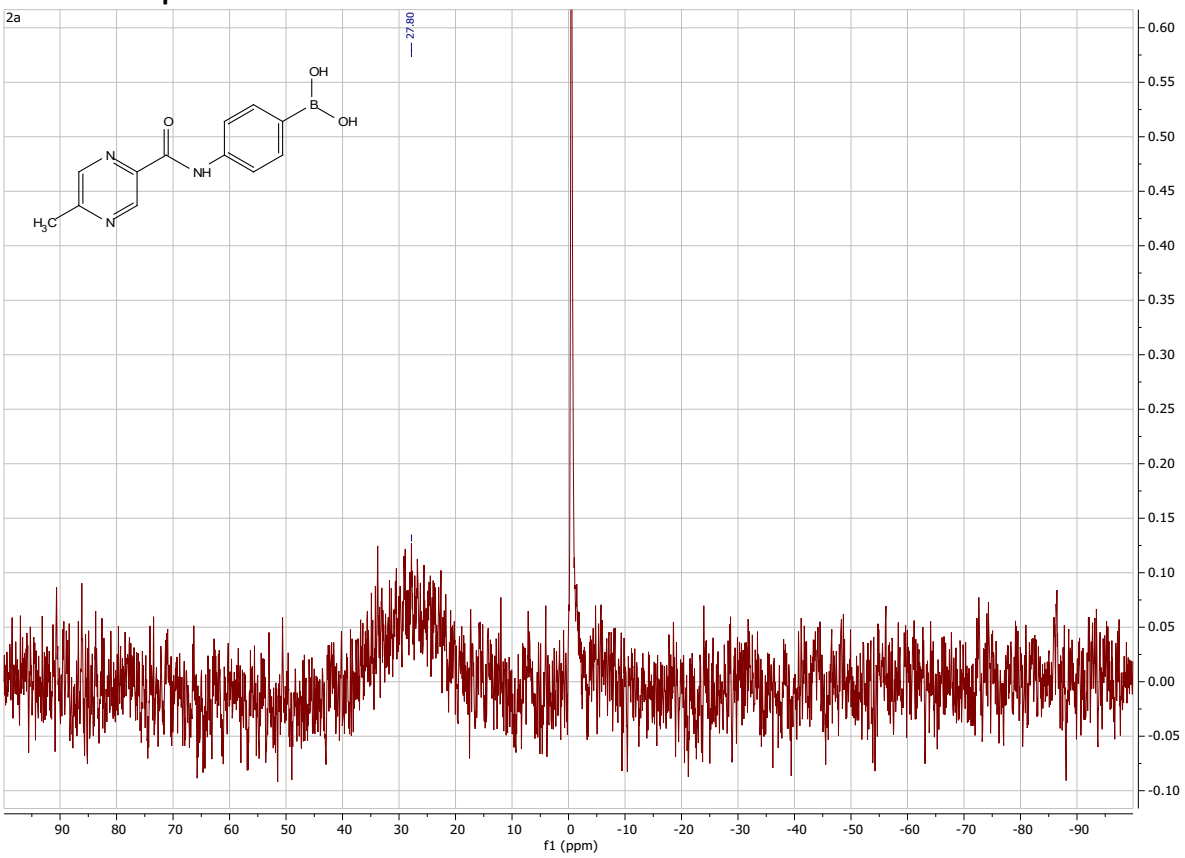
2a ^{1}H NMR spectrum



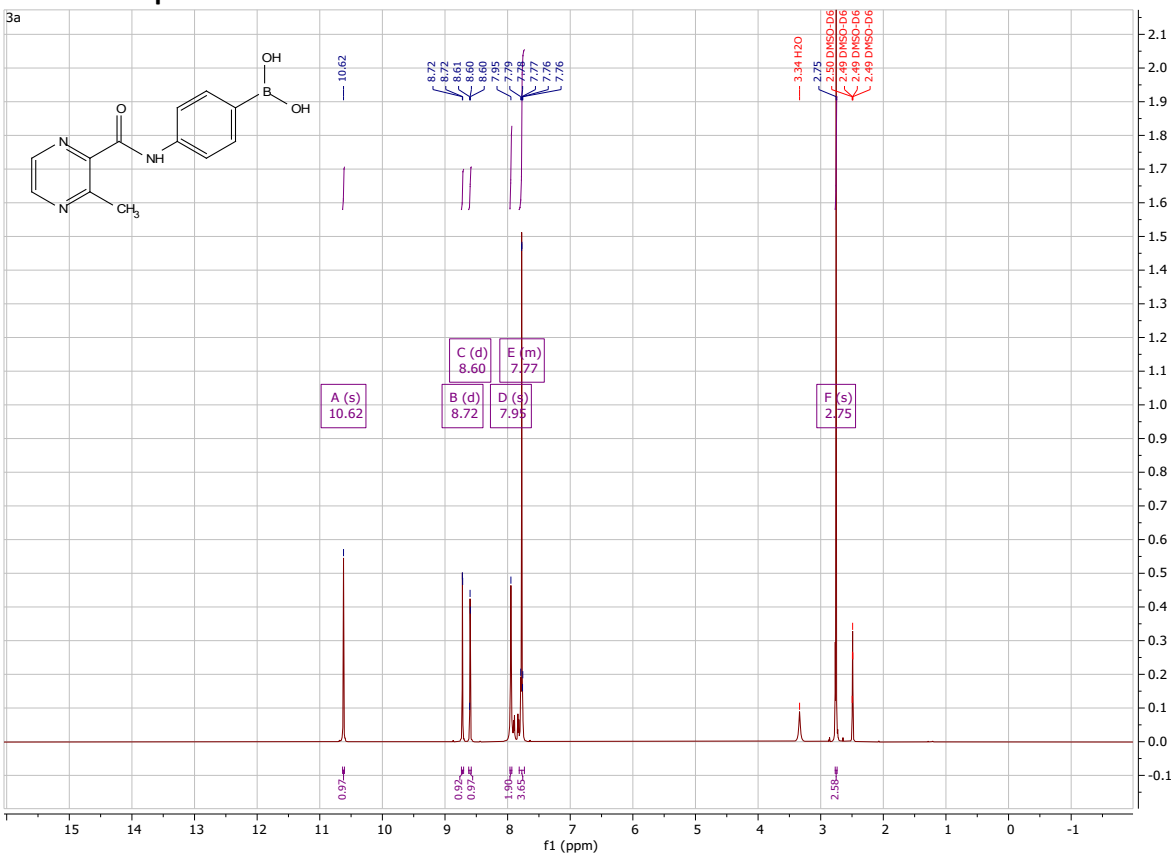
2a ^{13}C NMR spectrum



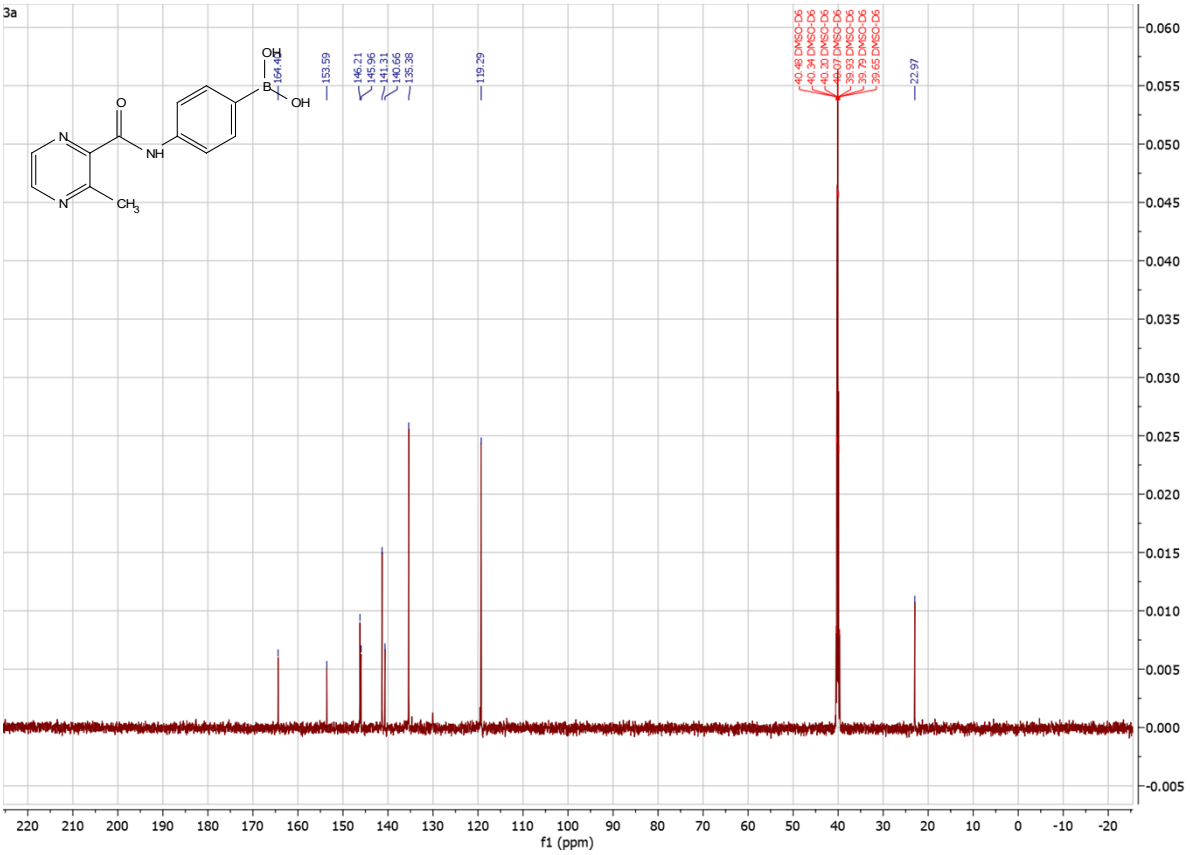
2a ^{11}B NMR spectrum



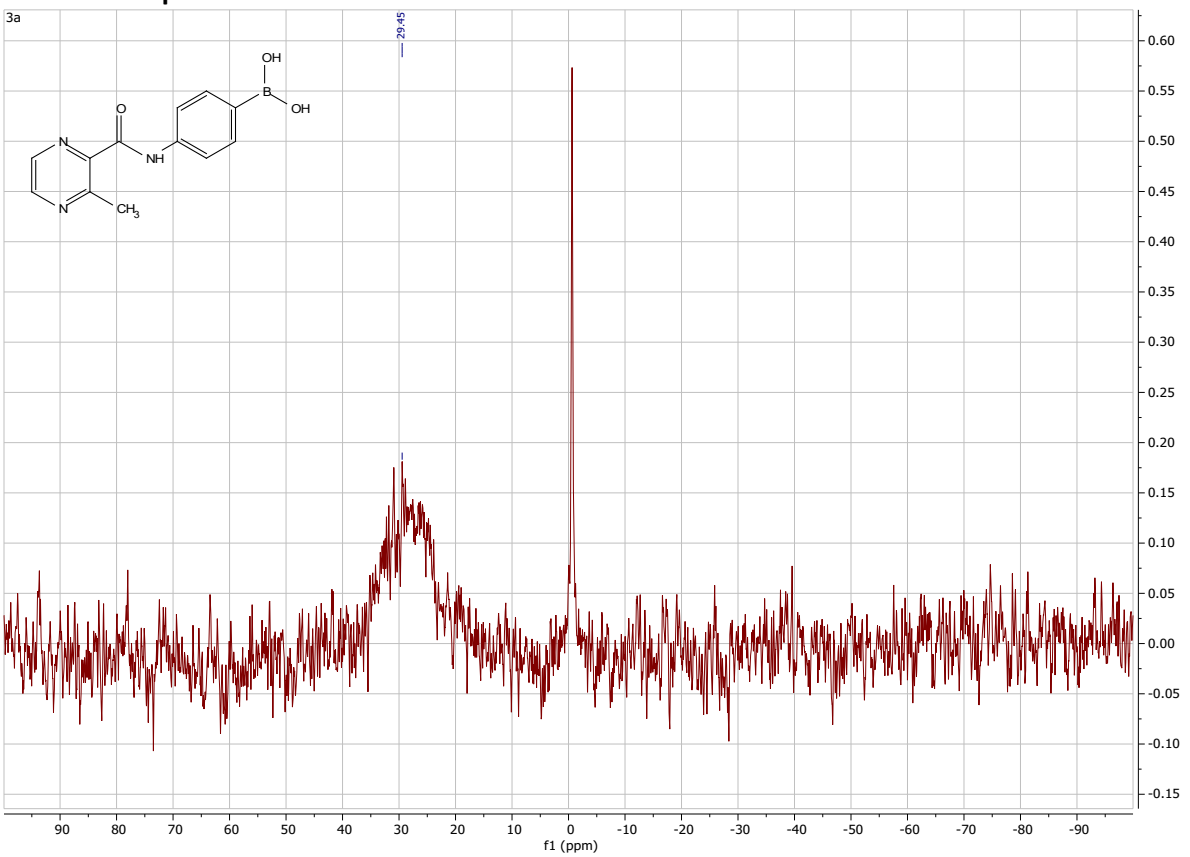
3a ^{1}H NMR spectrum



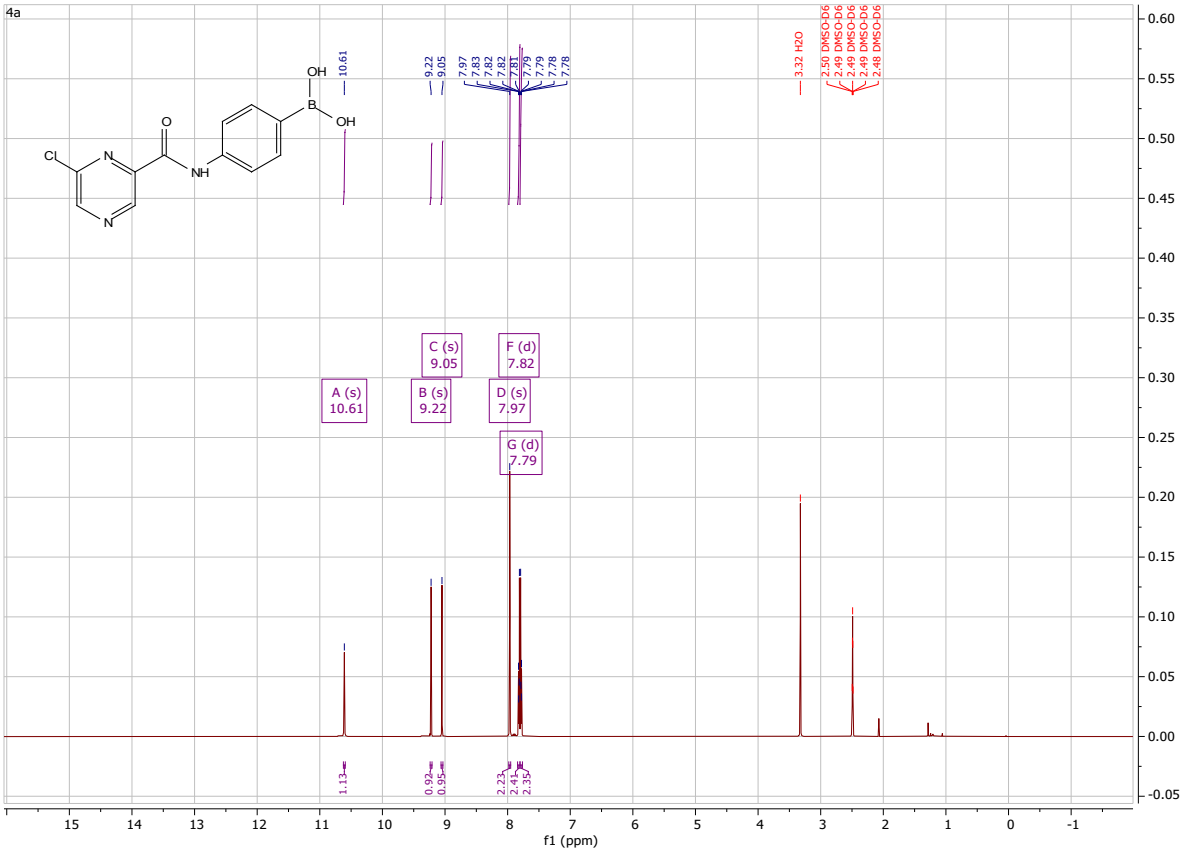
3a ^{13}C NMR spectrum



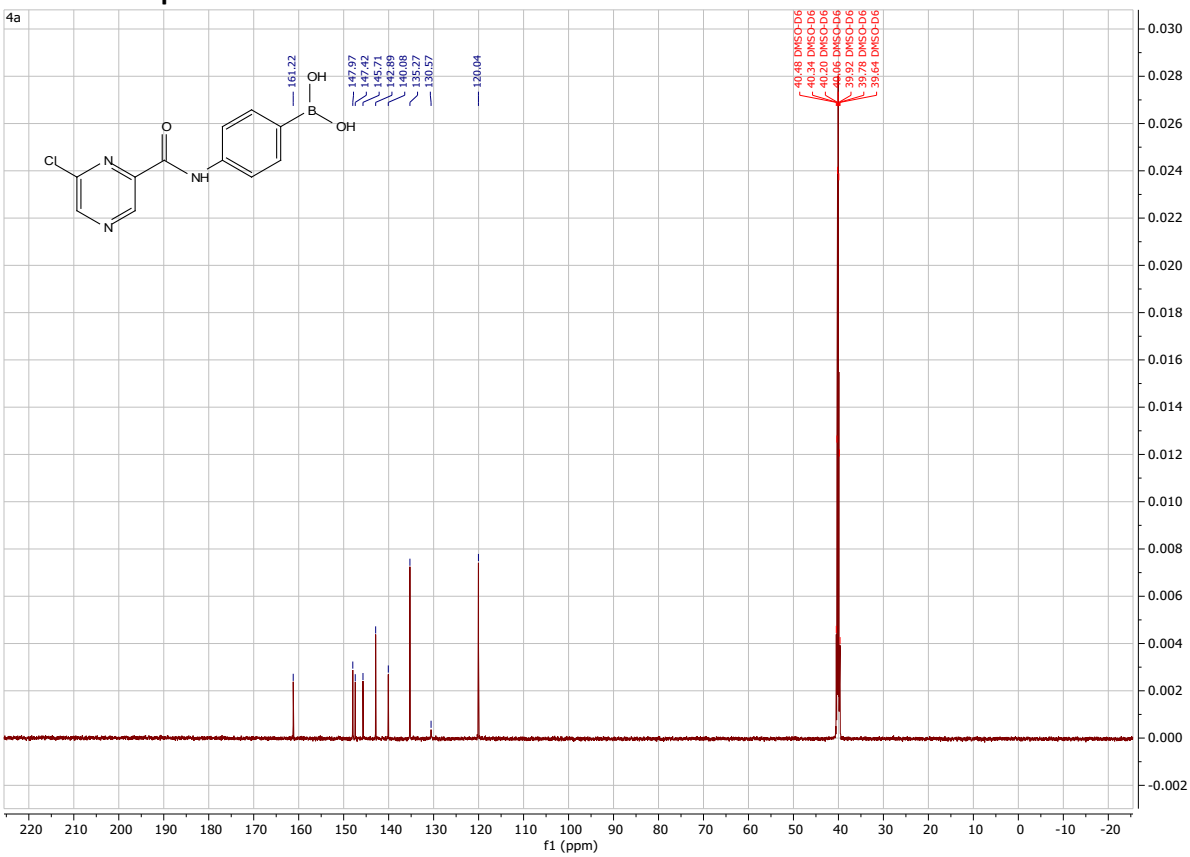
3a ^{11}B NMR spectrum



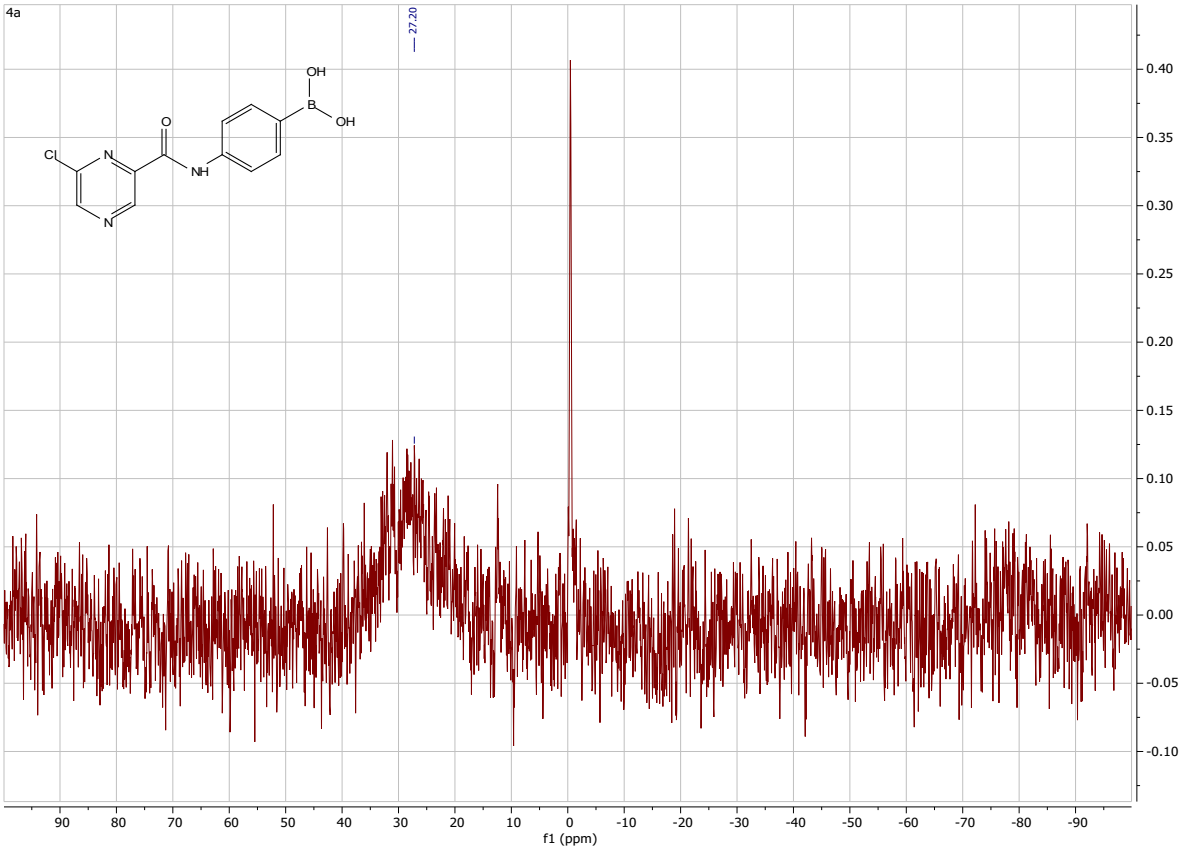
4a ^{1}H NMR spectrum



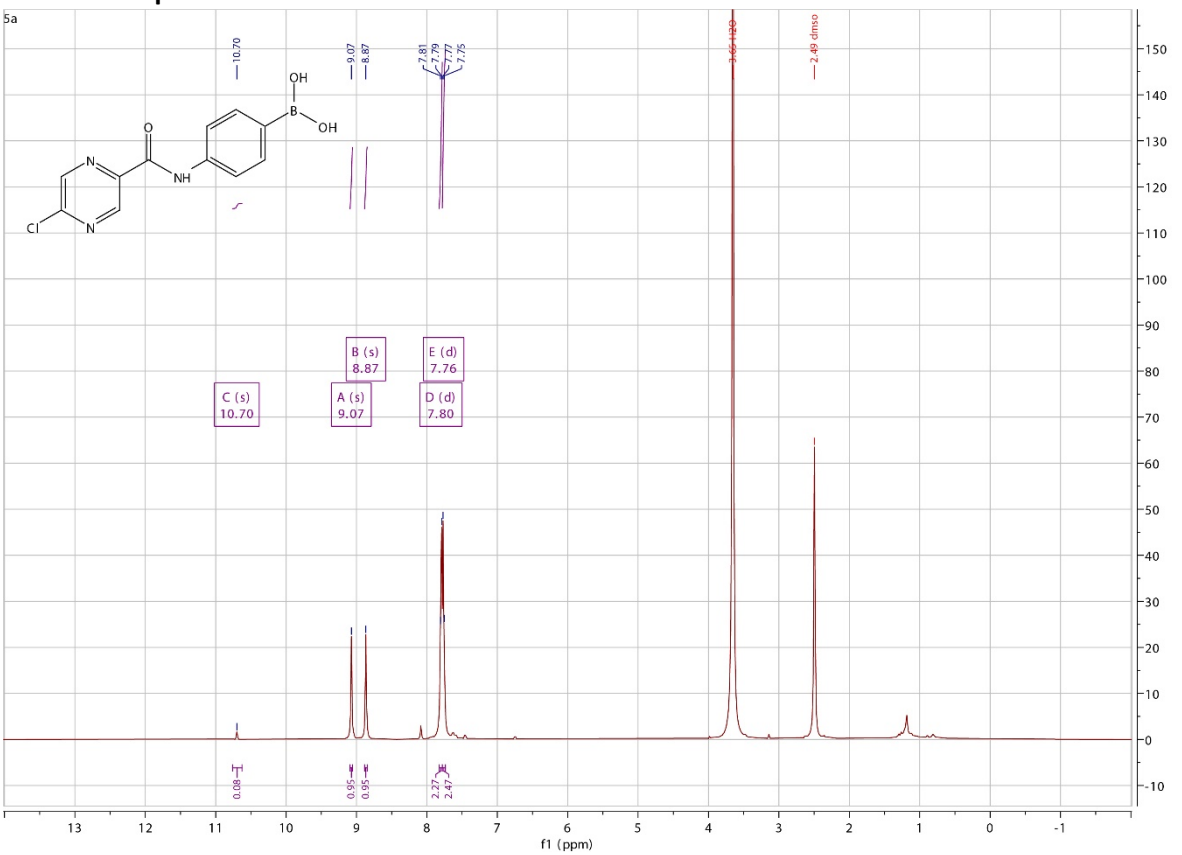
4a ^{13}C NMR spectrum



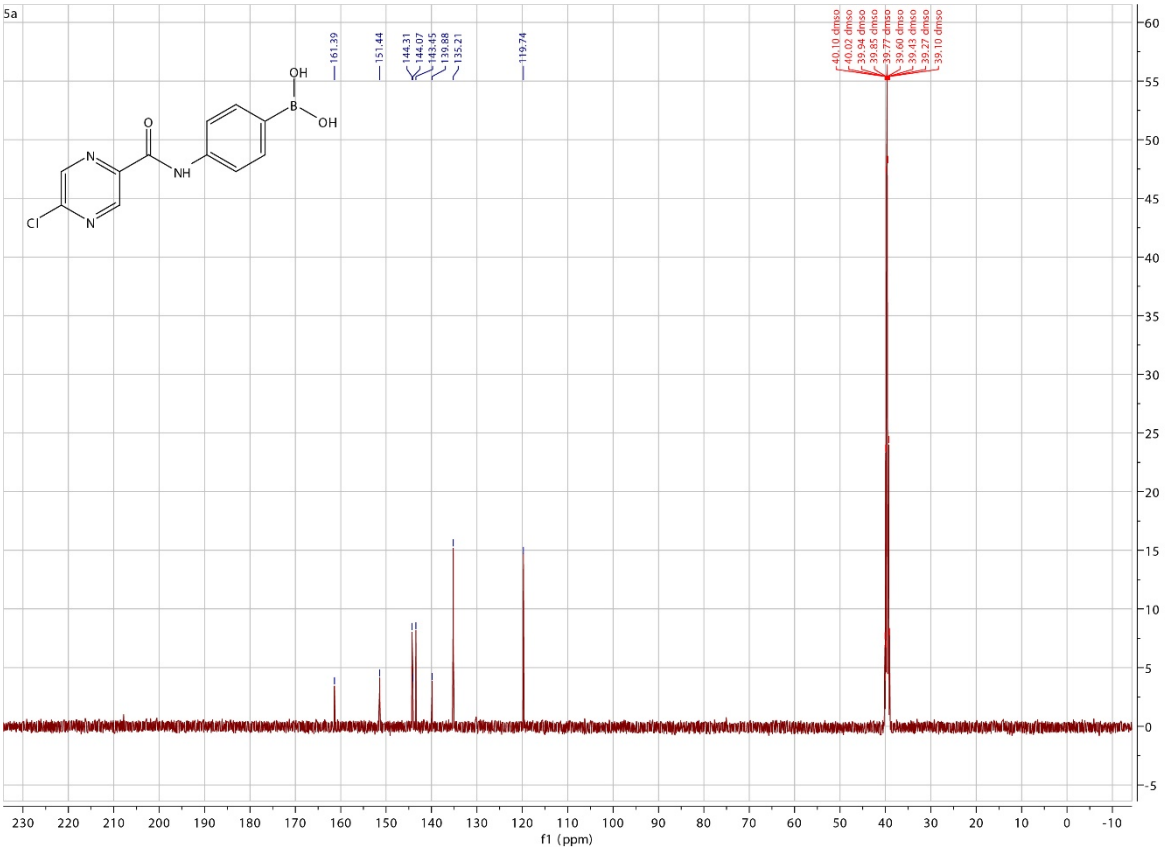
4a ^{11}B NMR spectrum



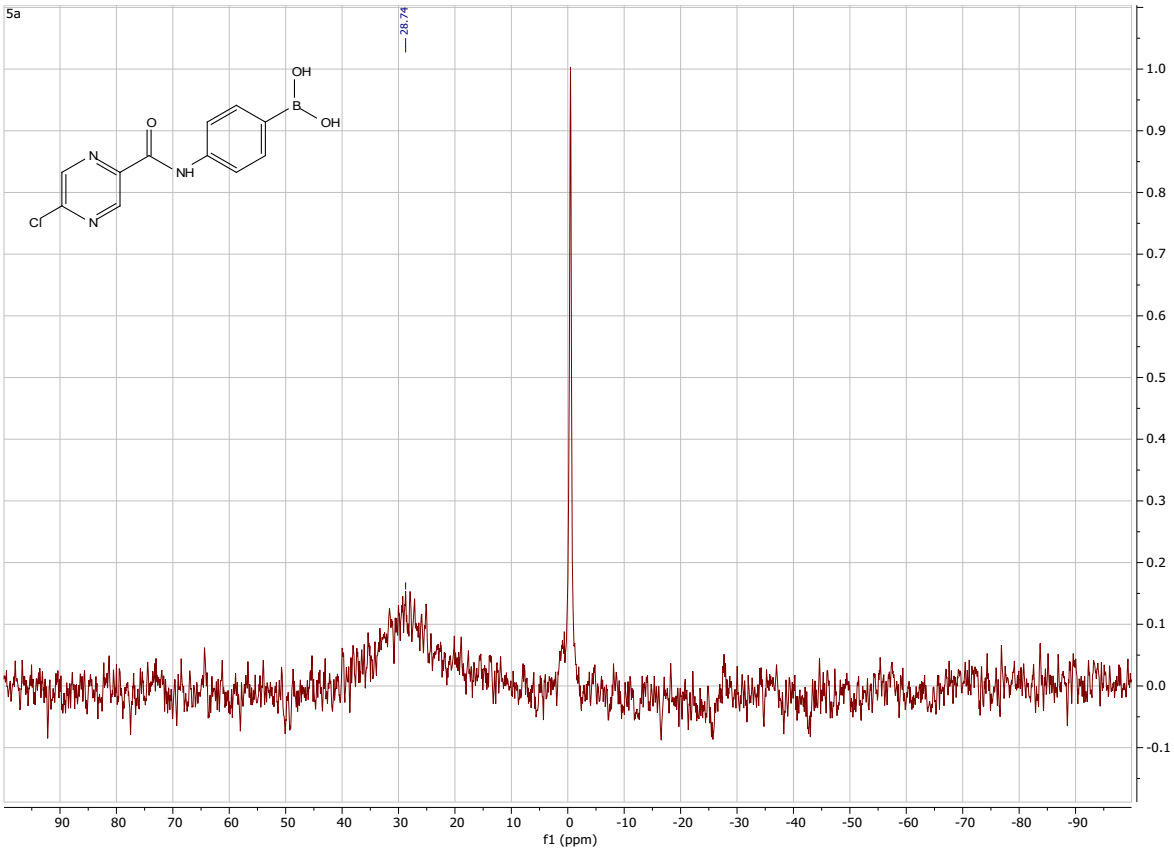
5a ^{1}H NMR spectrum



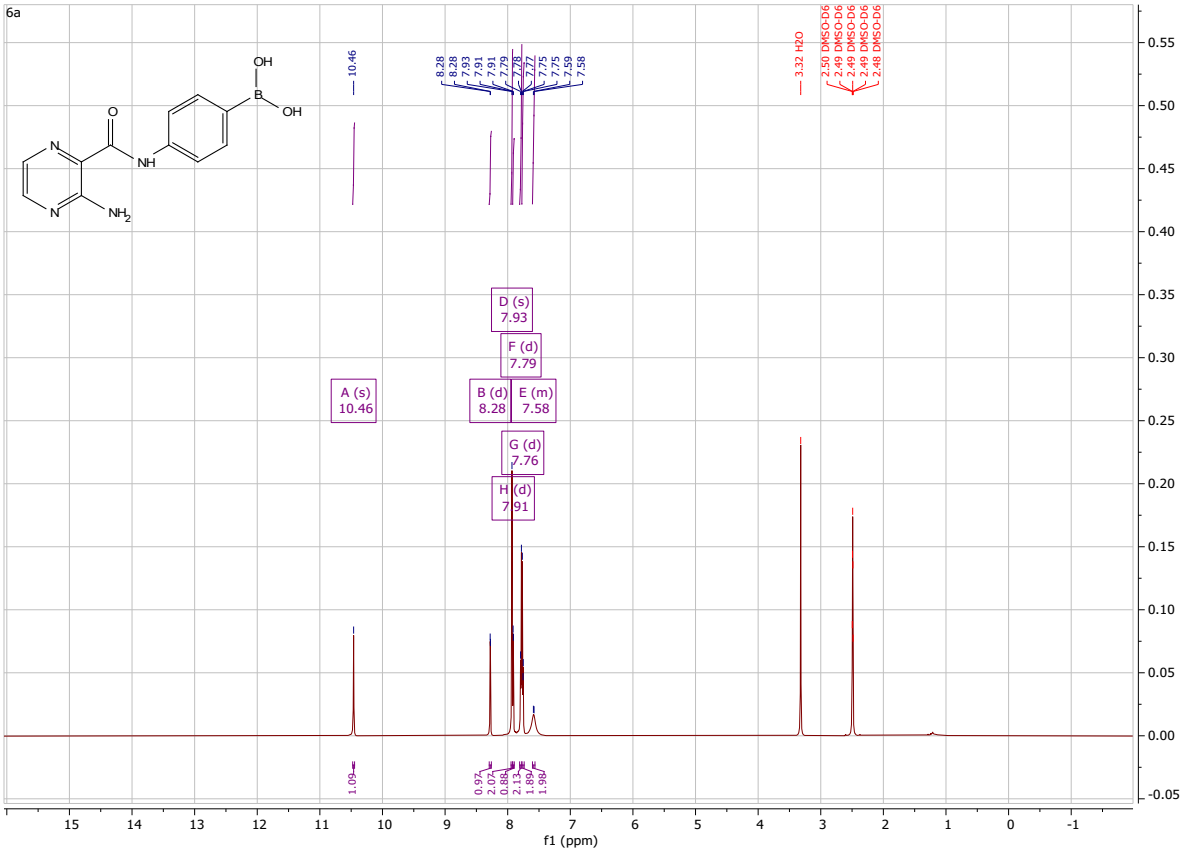
5a ^{13}C NMR spectrum



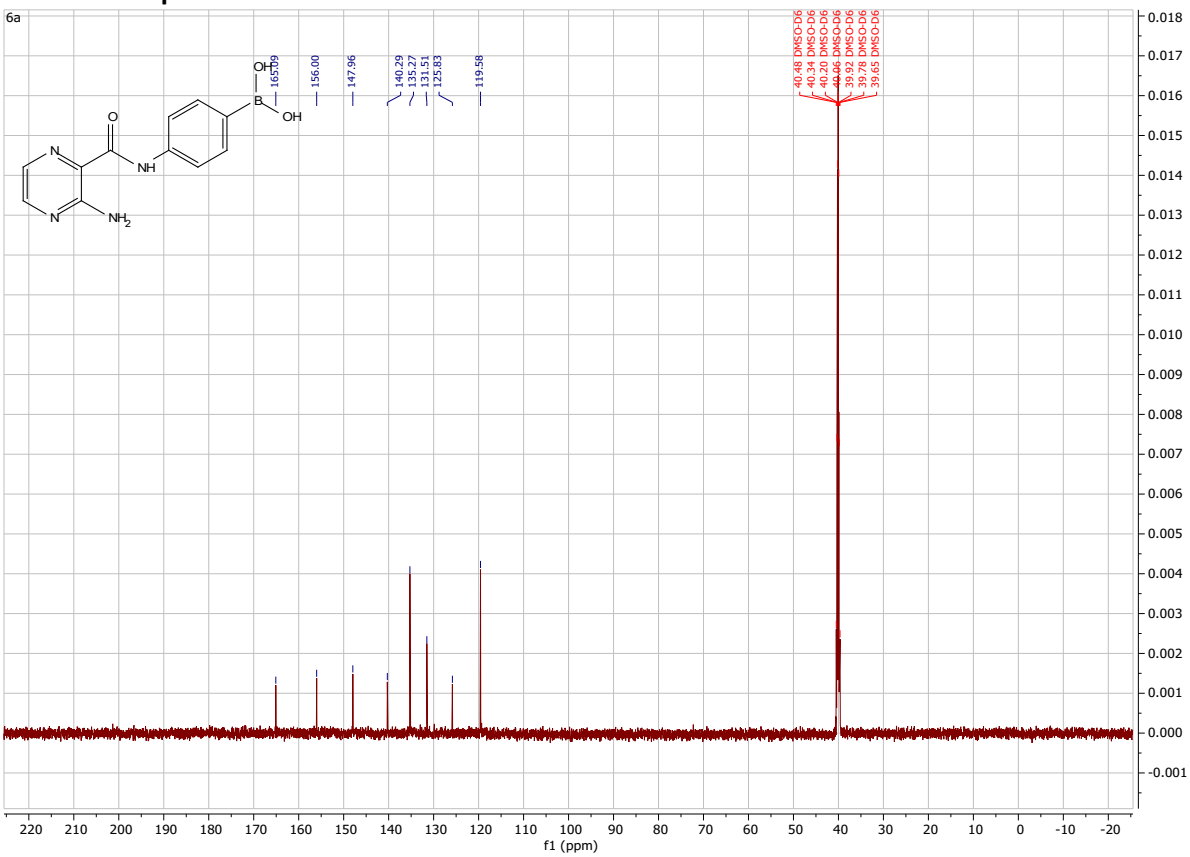
5a ^{11}B NMR spectrum



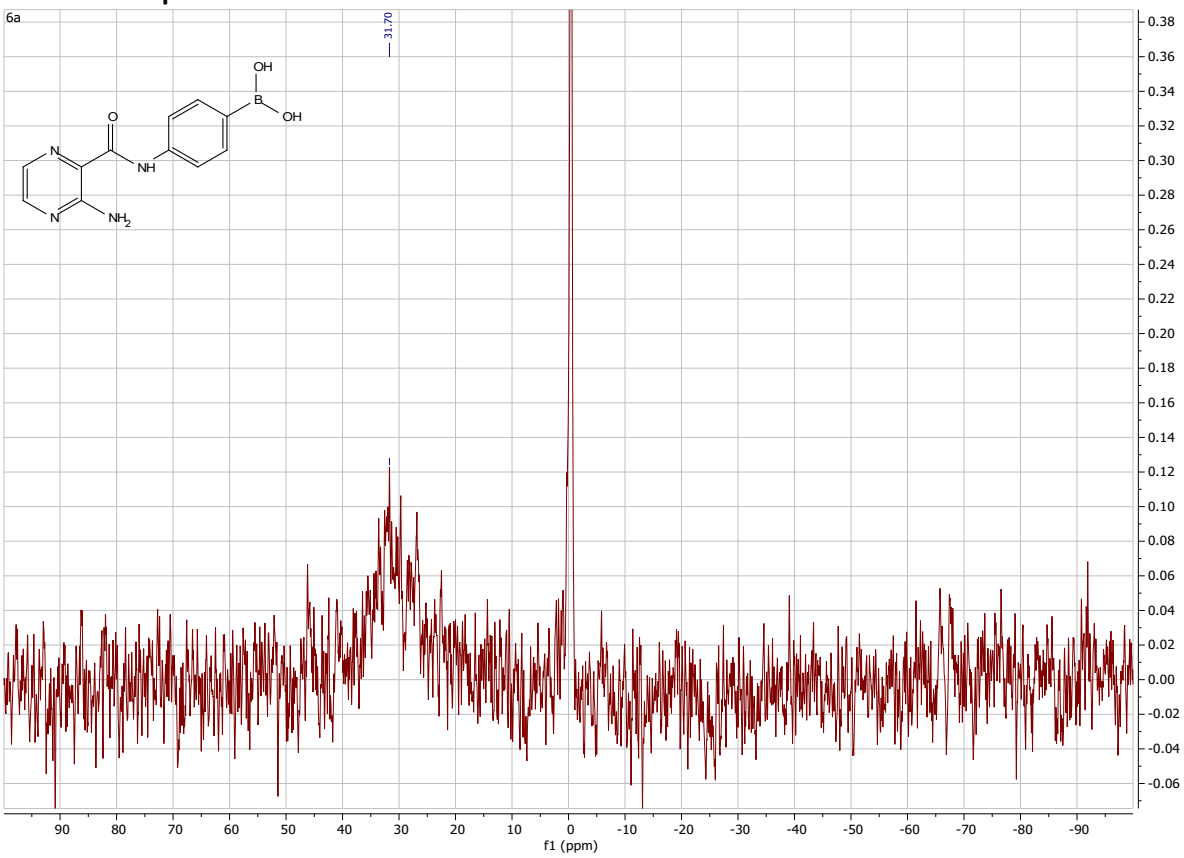
6a ^{1}H NMR spectrum



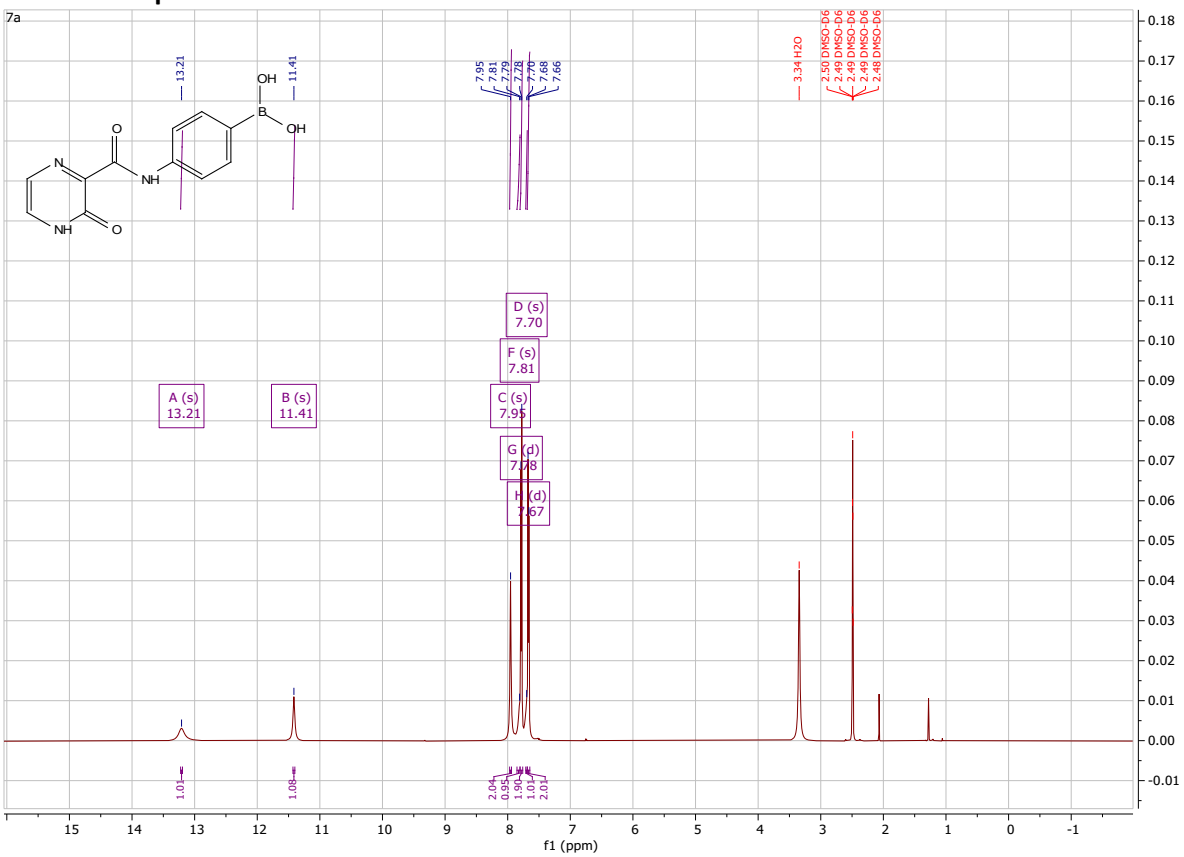
6a ^{13}C NMR spectrum



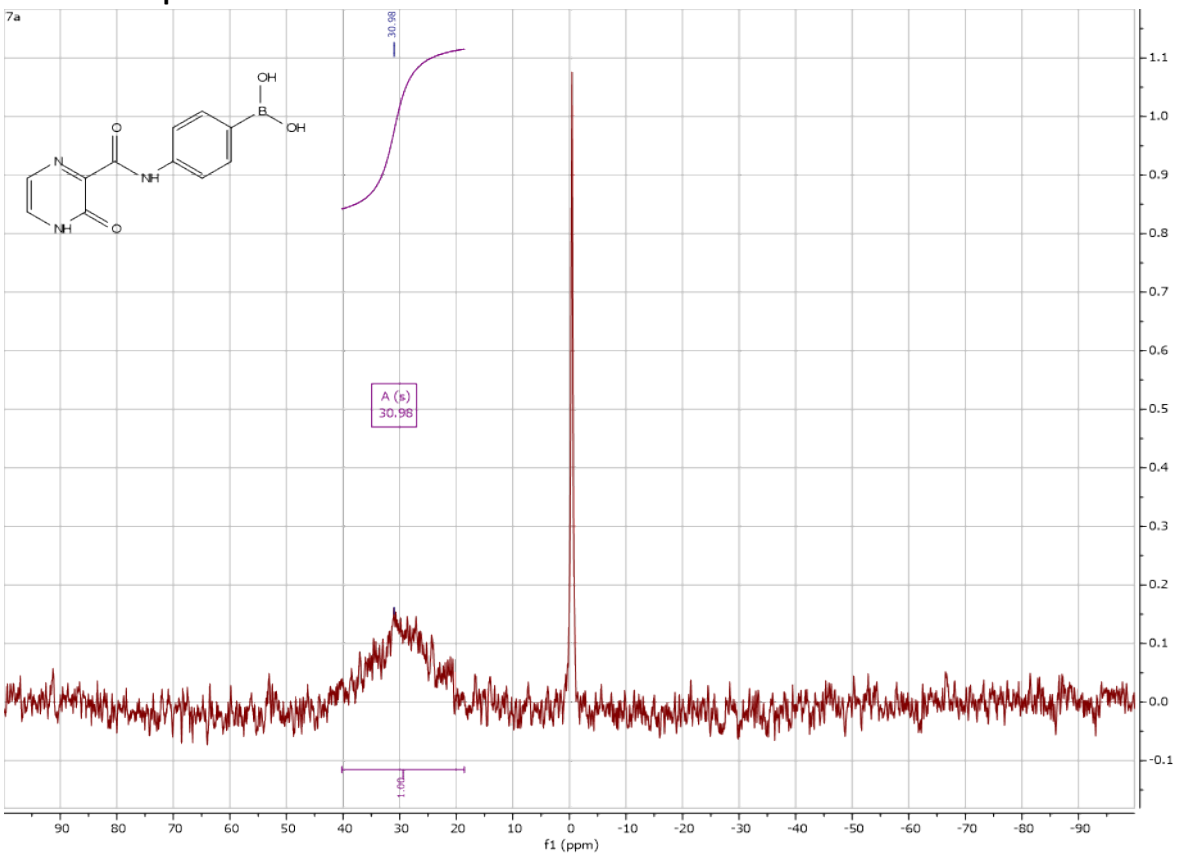
6a ^{11}B NMR spectrum



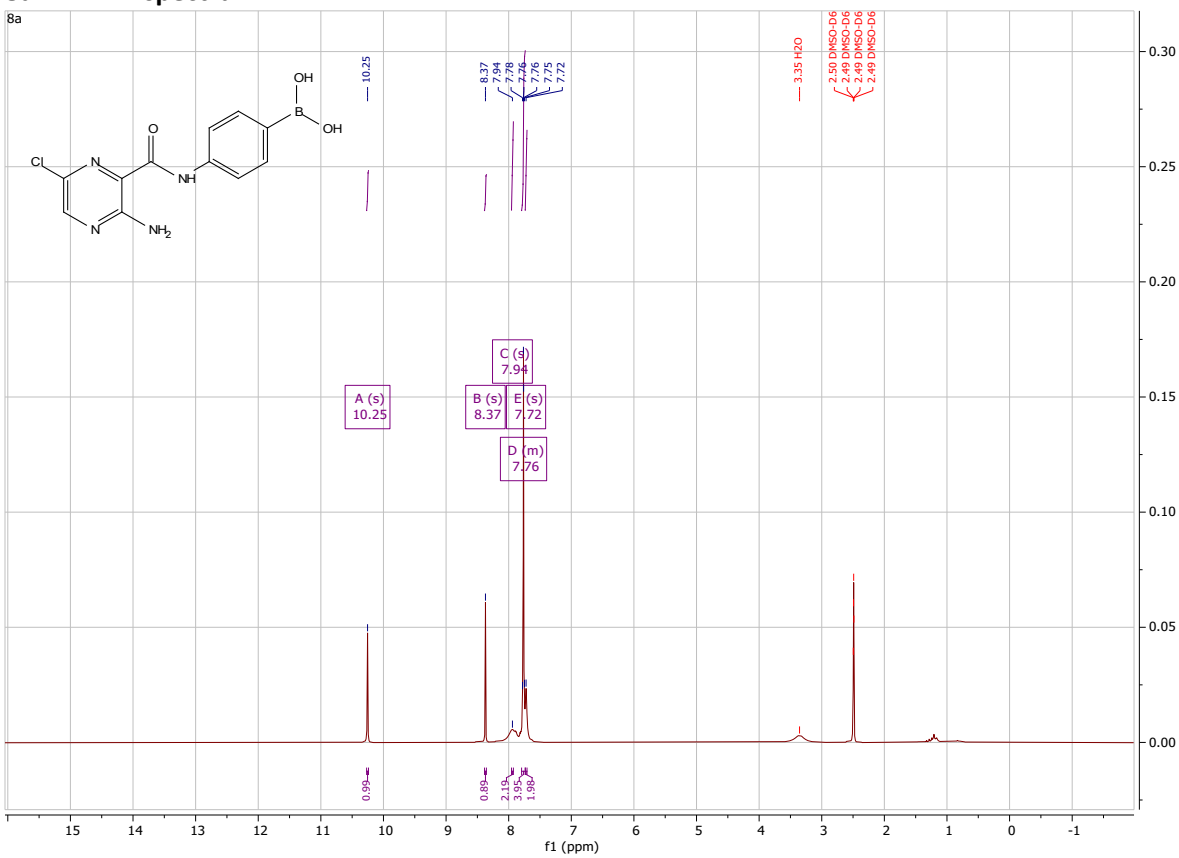
7a ^{1}H NMR spectrum



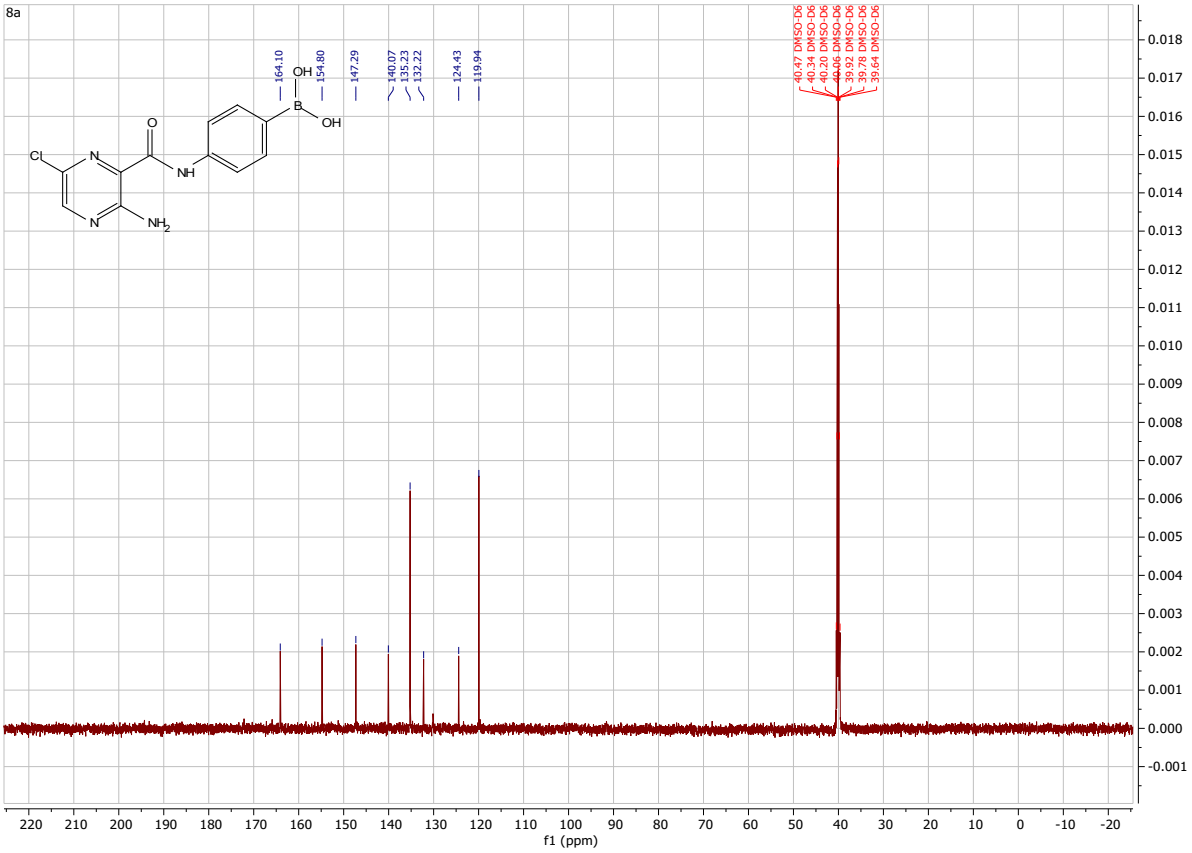
7a ^{11}B NMR spectrum



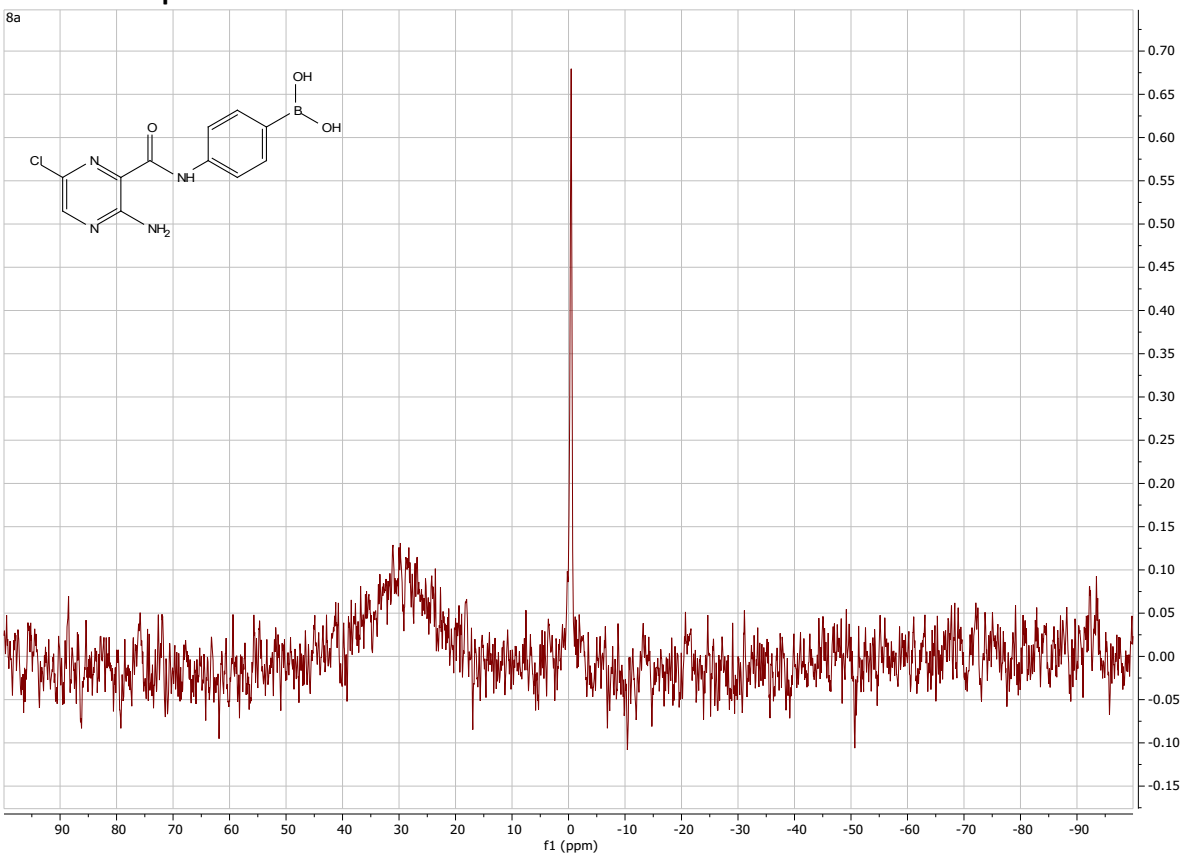
8a ^{1}H NMR spectrum



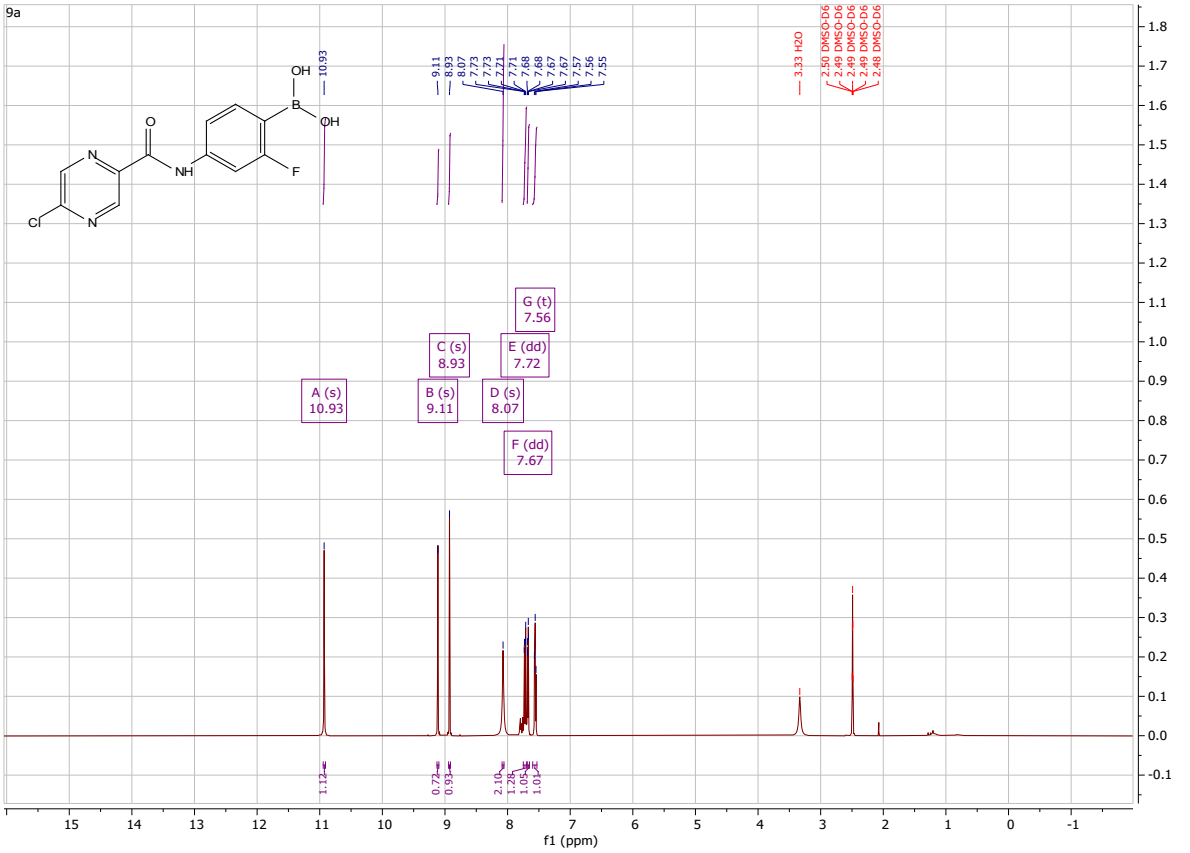
8a ^{13}C NMR spectrum



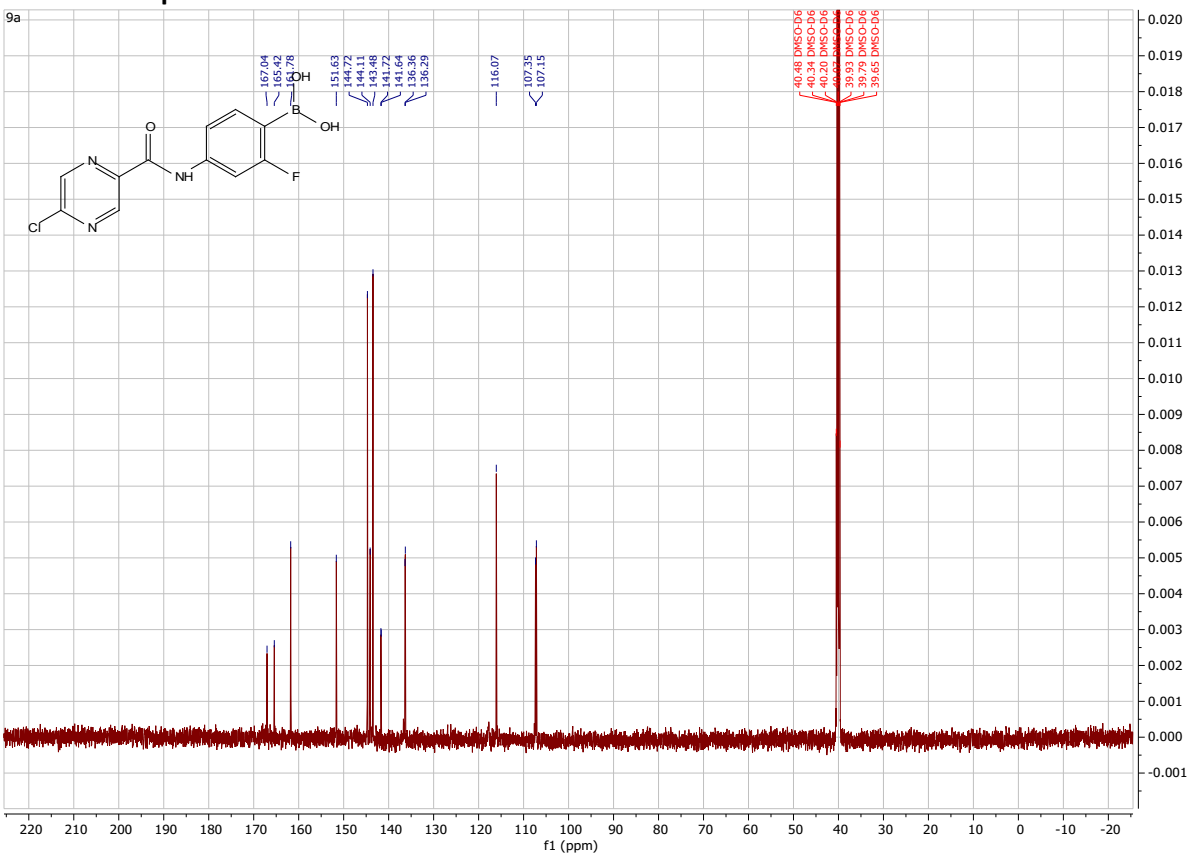
8a ^{11}B NMR spectrum



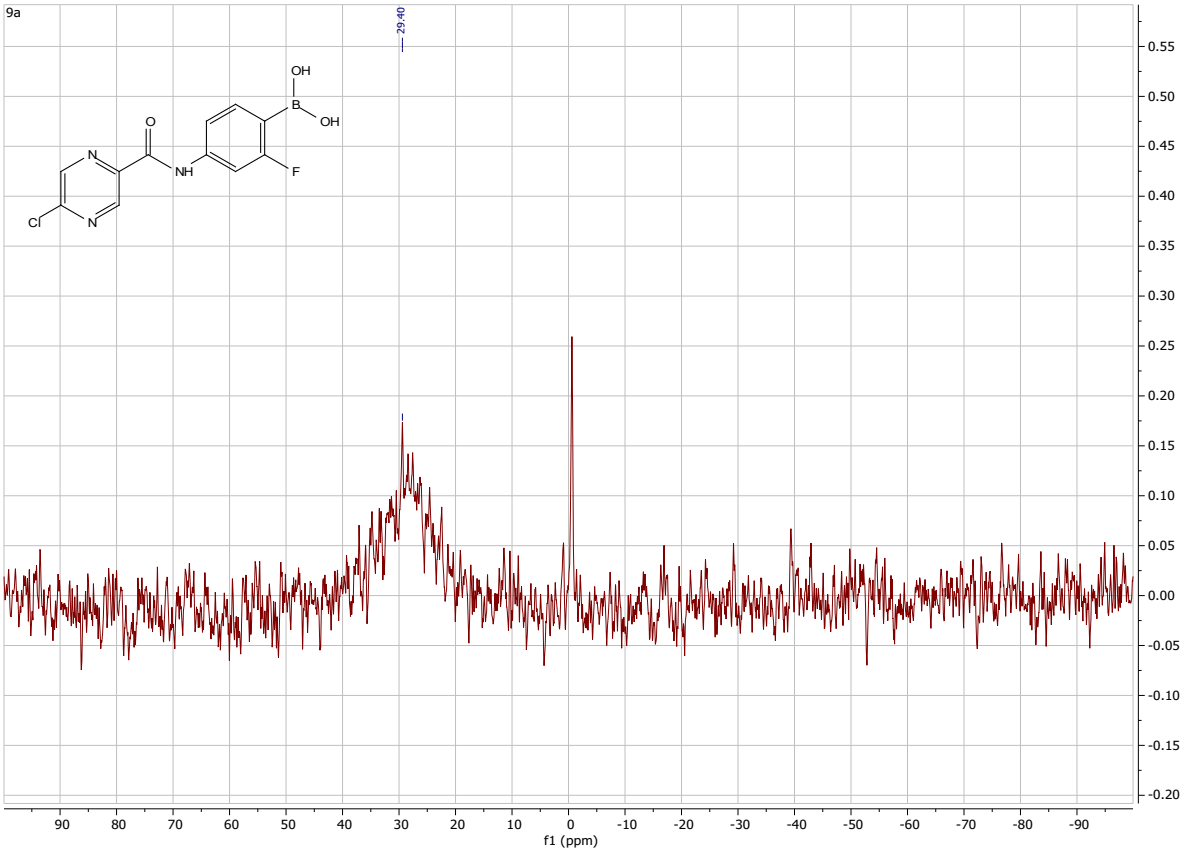
9a ^{1}H NMR spectrum



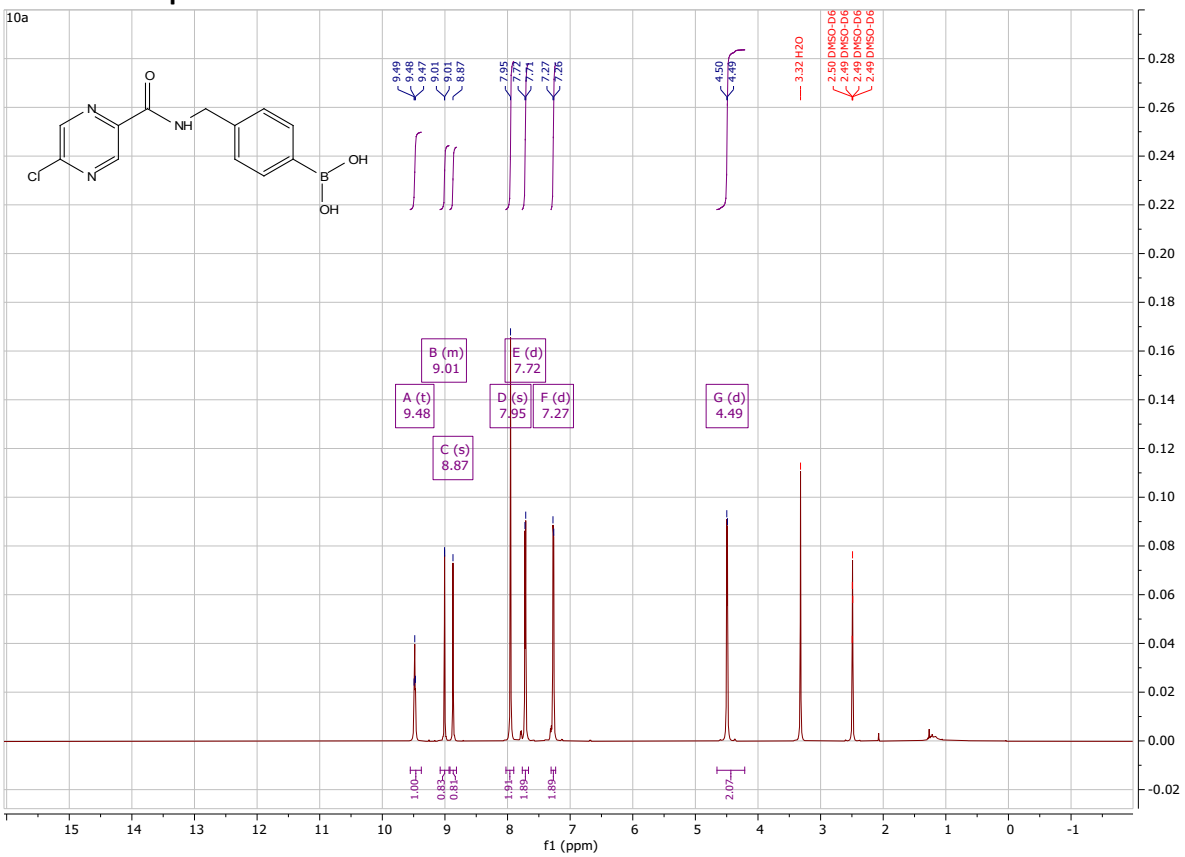
9a ^{13}C NMR spectrum



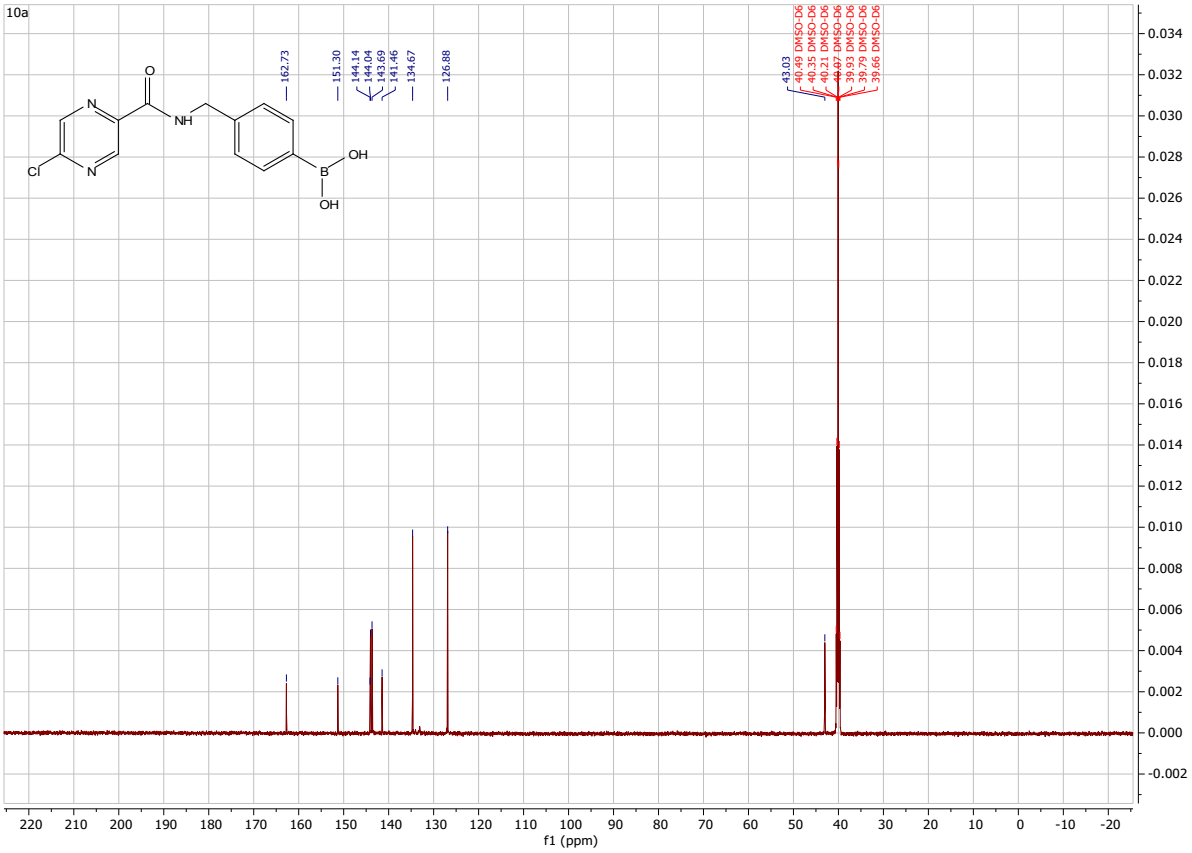
9a ^{11}B NMR spectrum



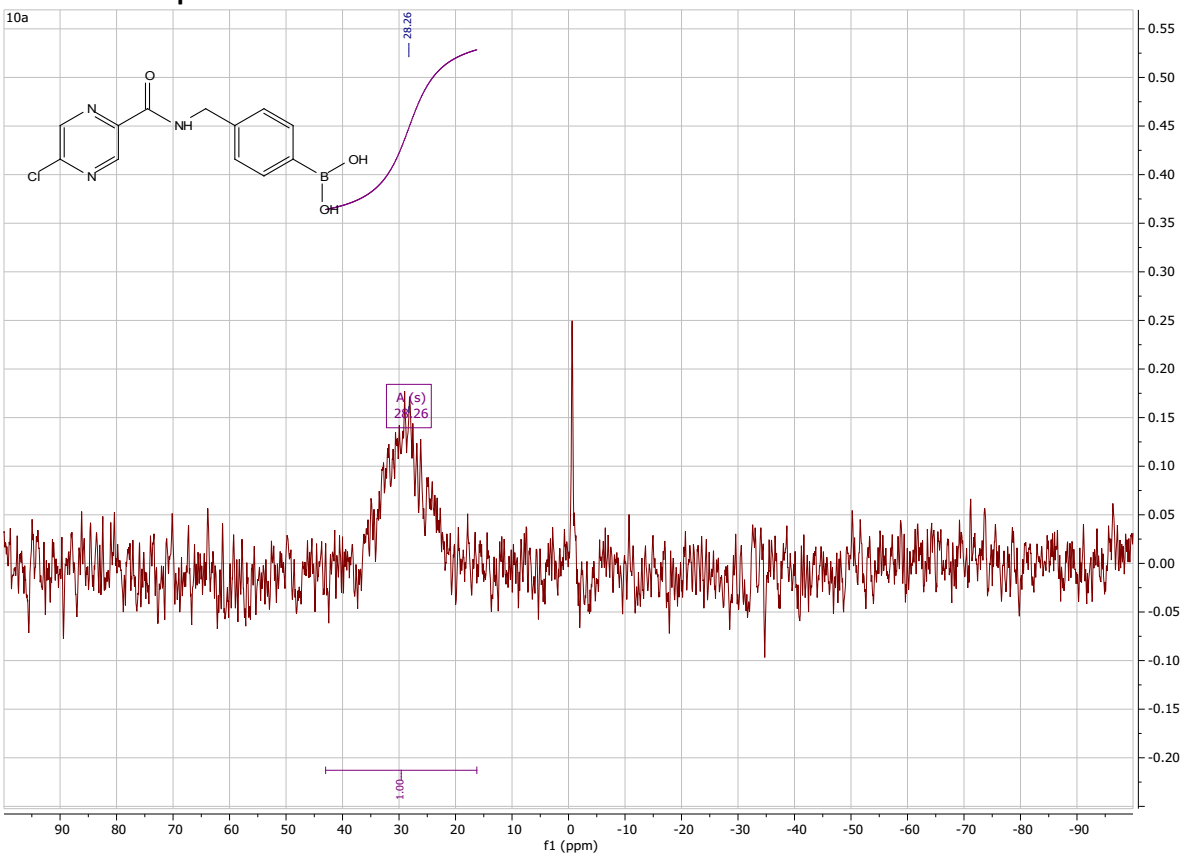
10a ^{1}H NMR spectrum



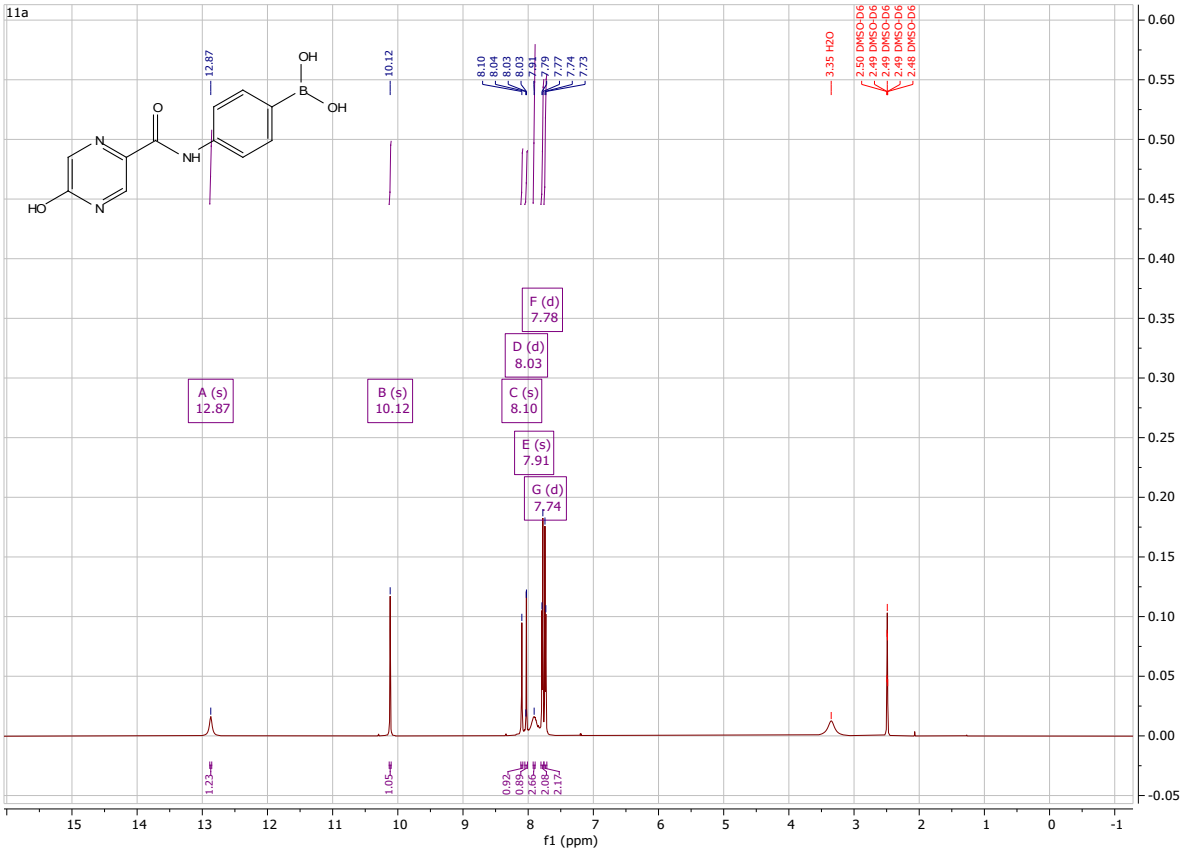
10a ^{13}C NMR spectru



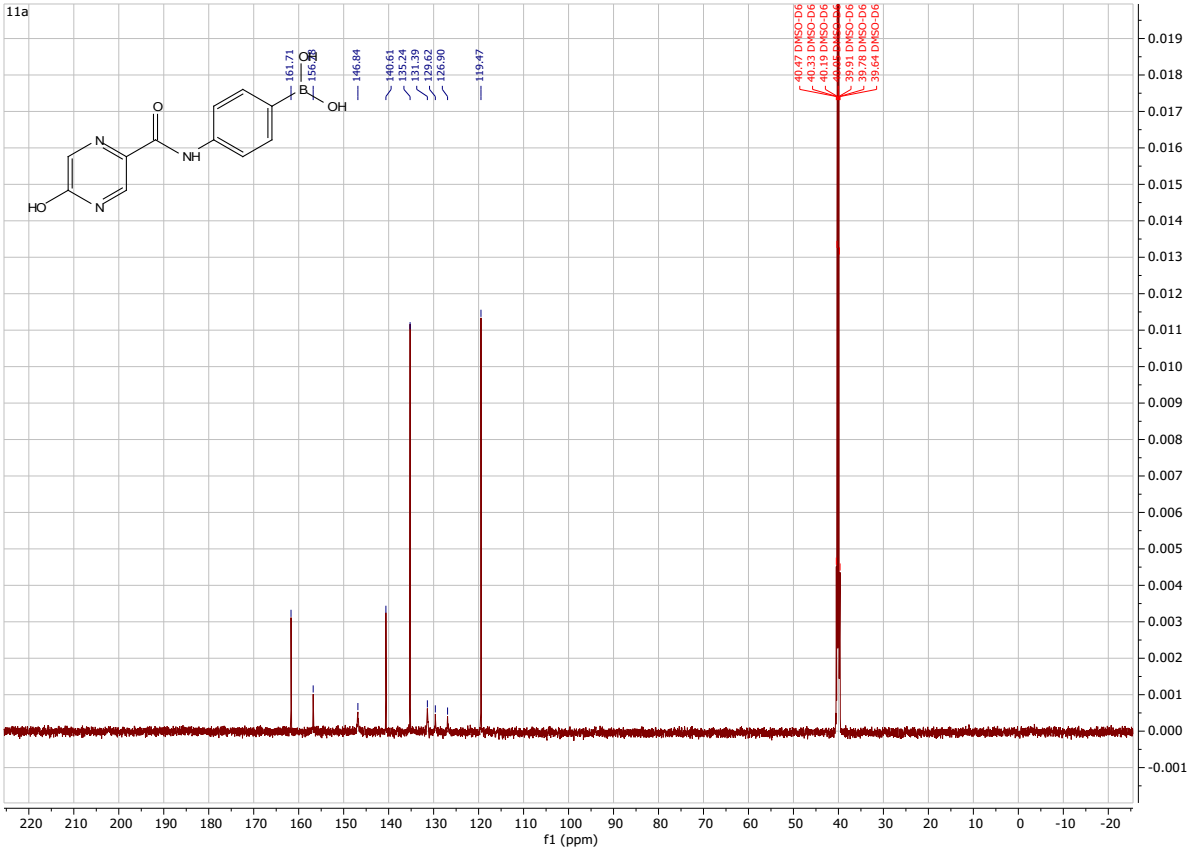
10a ^{11}B NMR spectrum



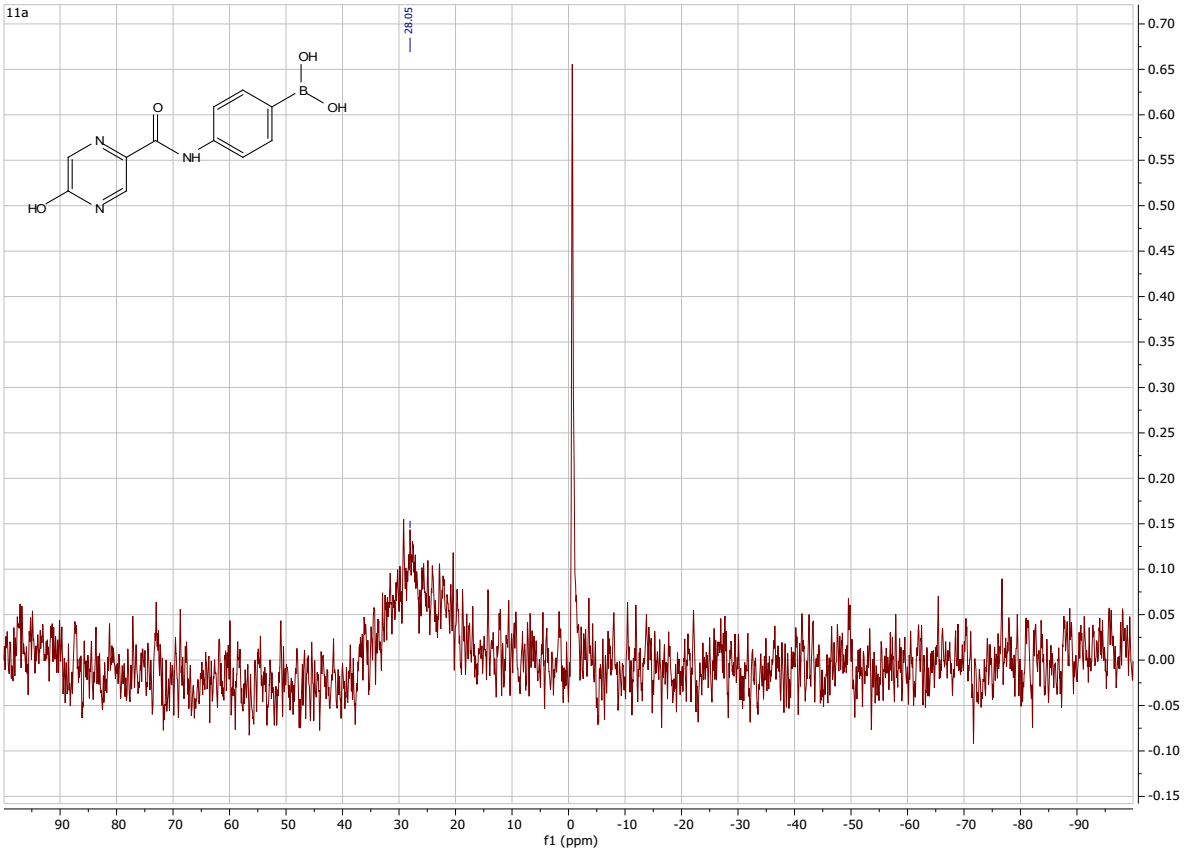
11a ^{1}H NMR spectrum



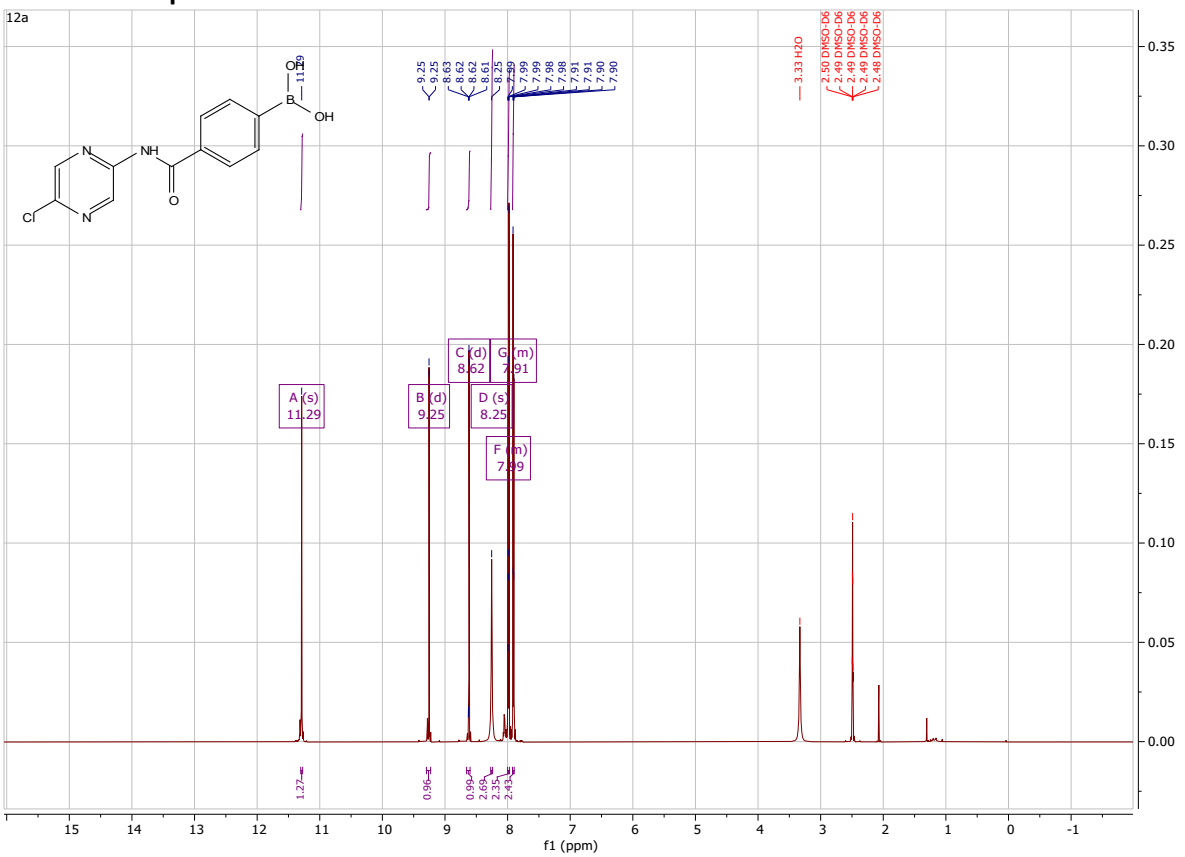
11a ^{13}C NMR spectrum



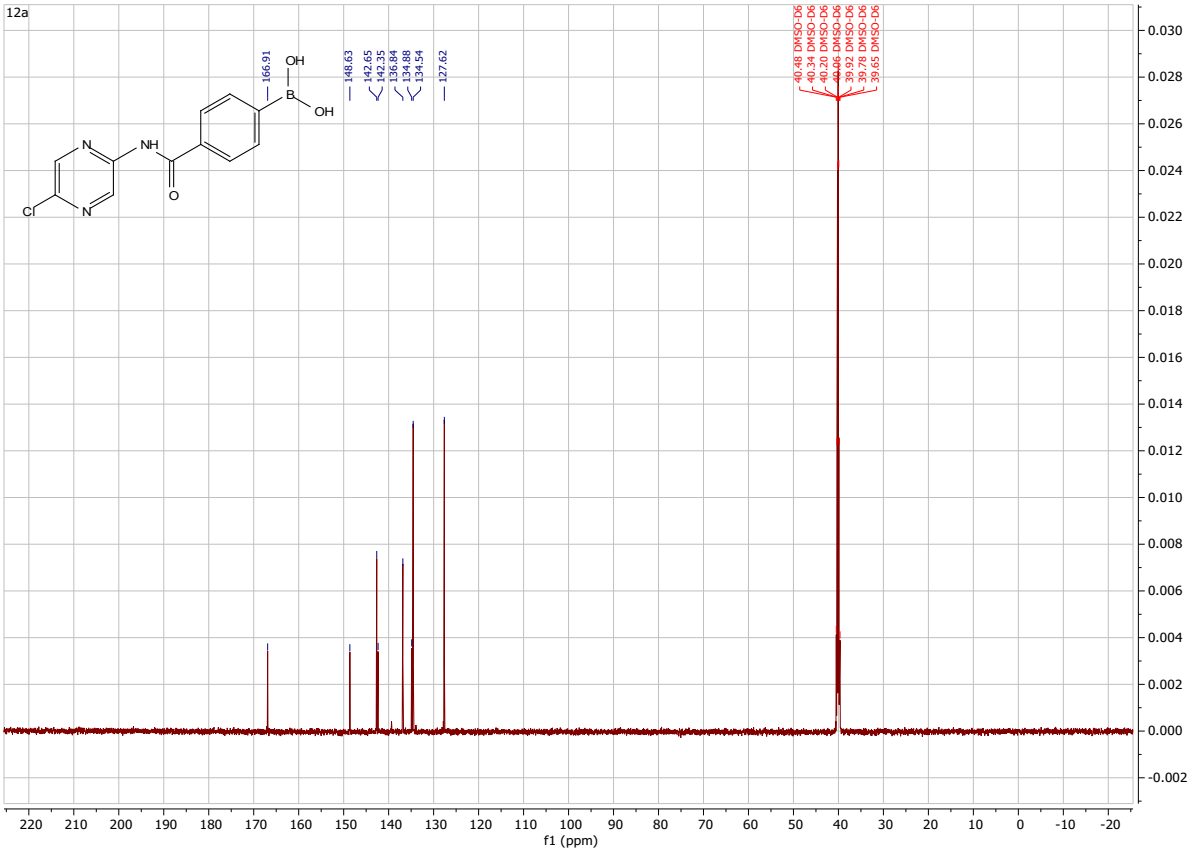
11a ^{11}B NMR spectrum



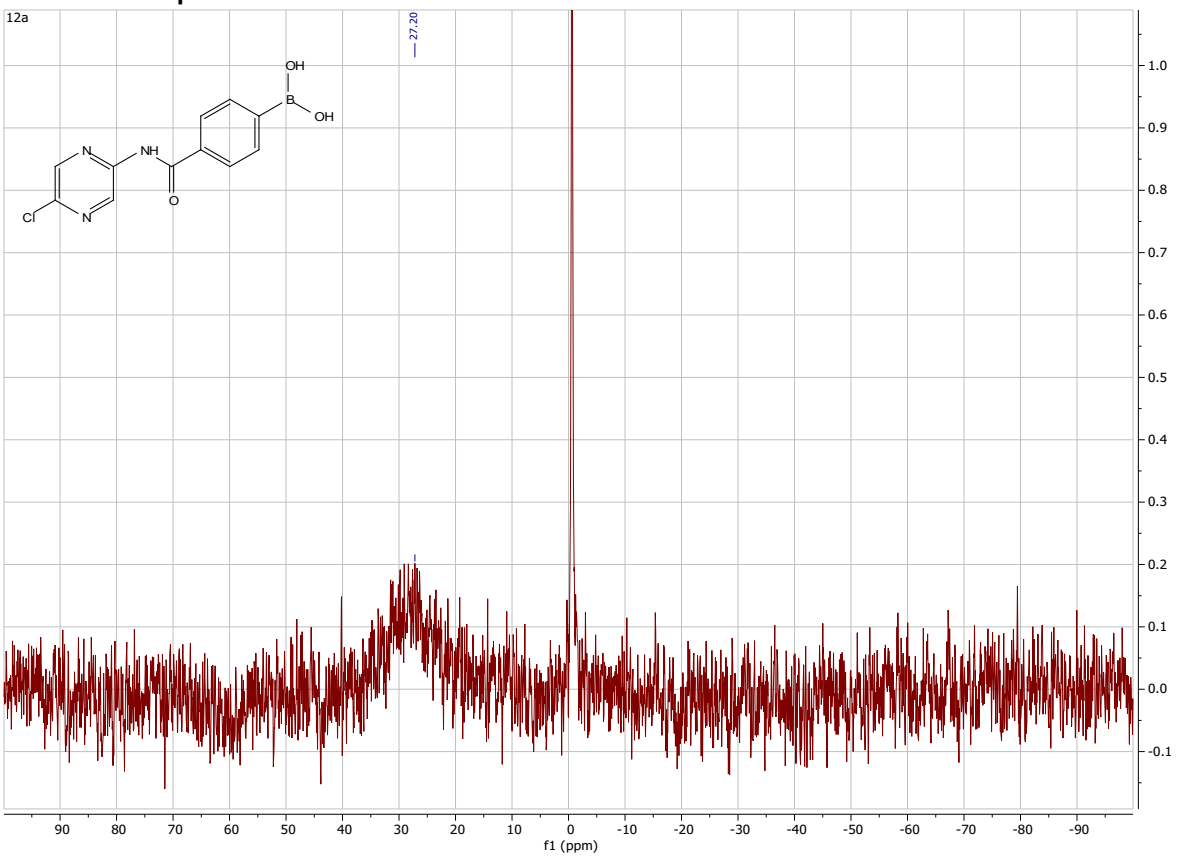
12a ^{1}H NMR spectrum



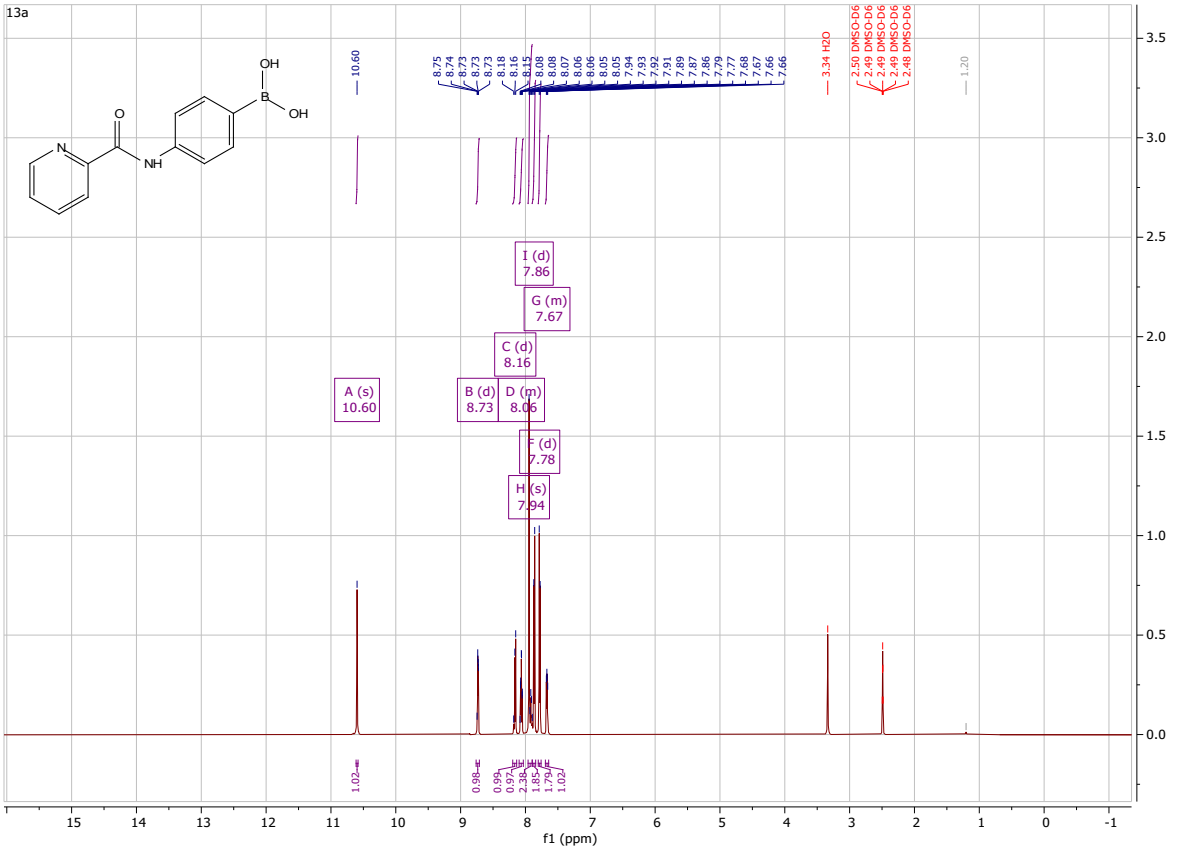
12a ^{13}C NMR spectrum



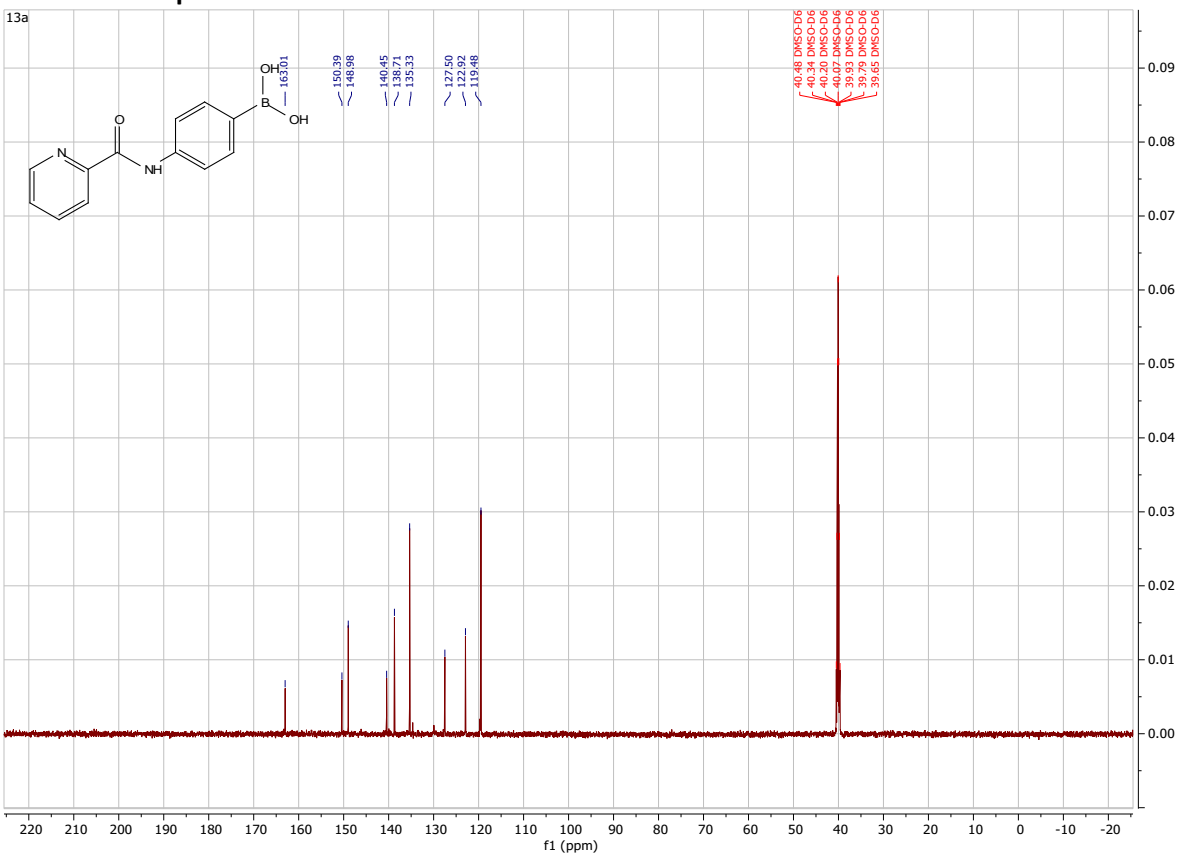
12a ^{11}B NMR spectrum

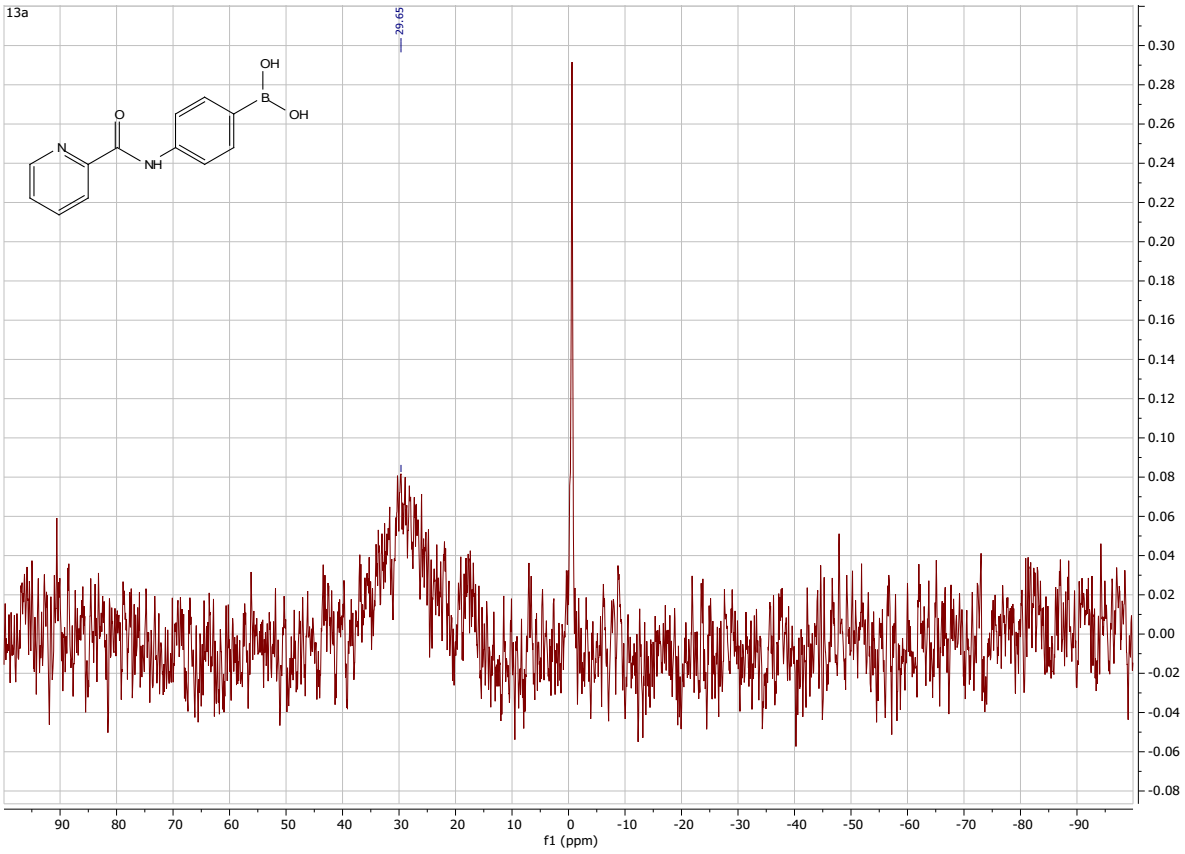


13a ^{1}H NMR spectrum

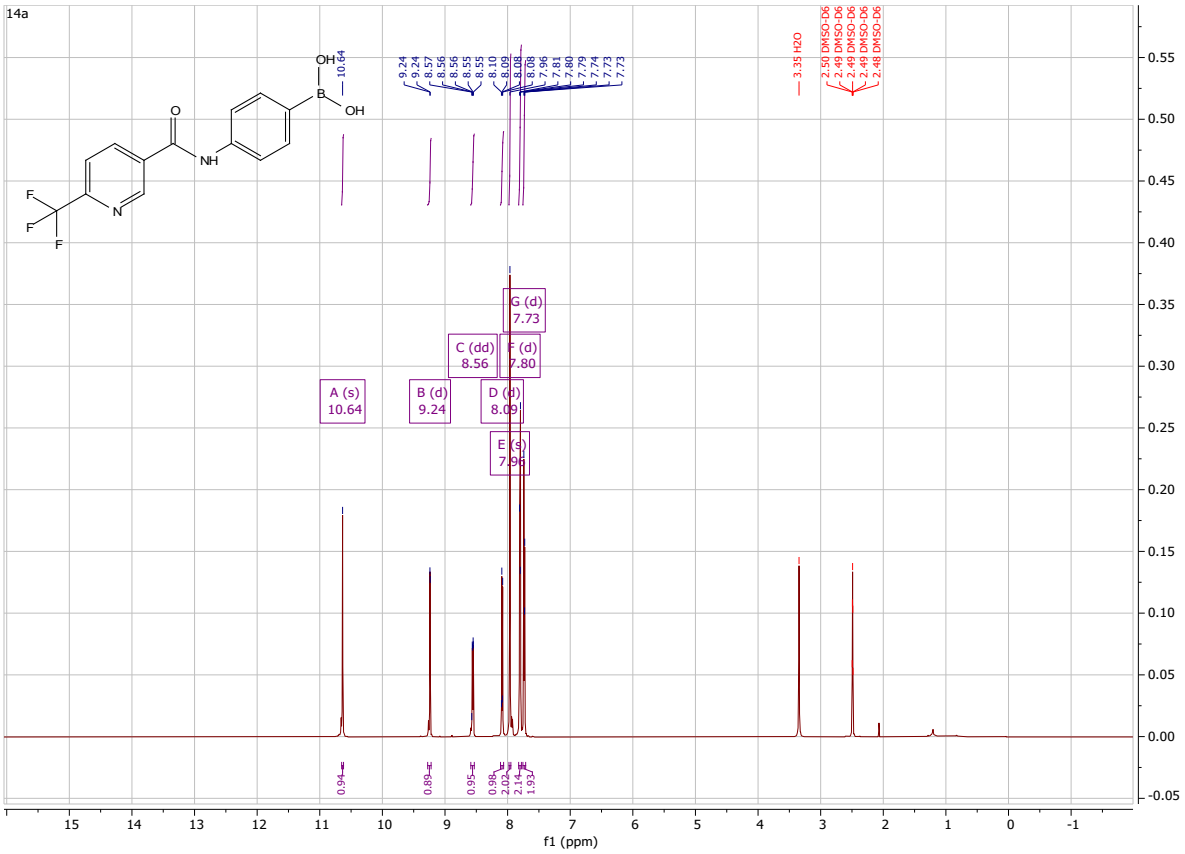


13a ^{13}C NMR spectrum



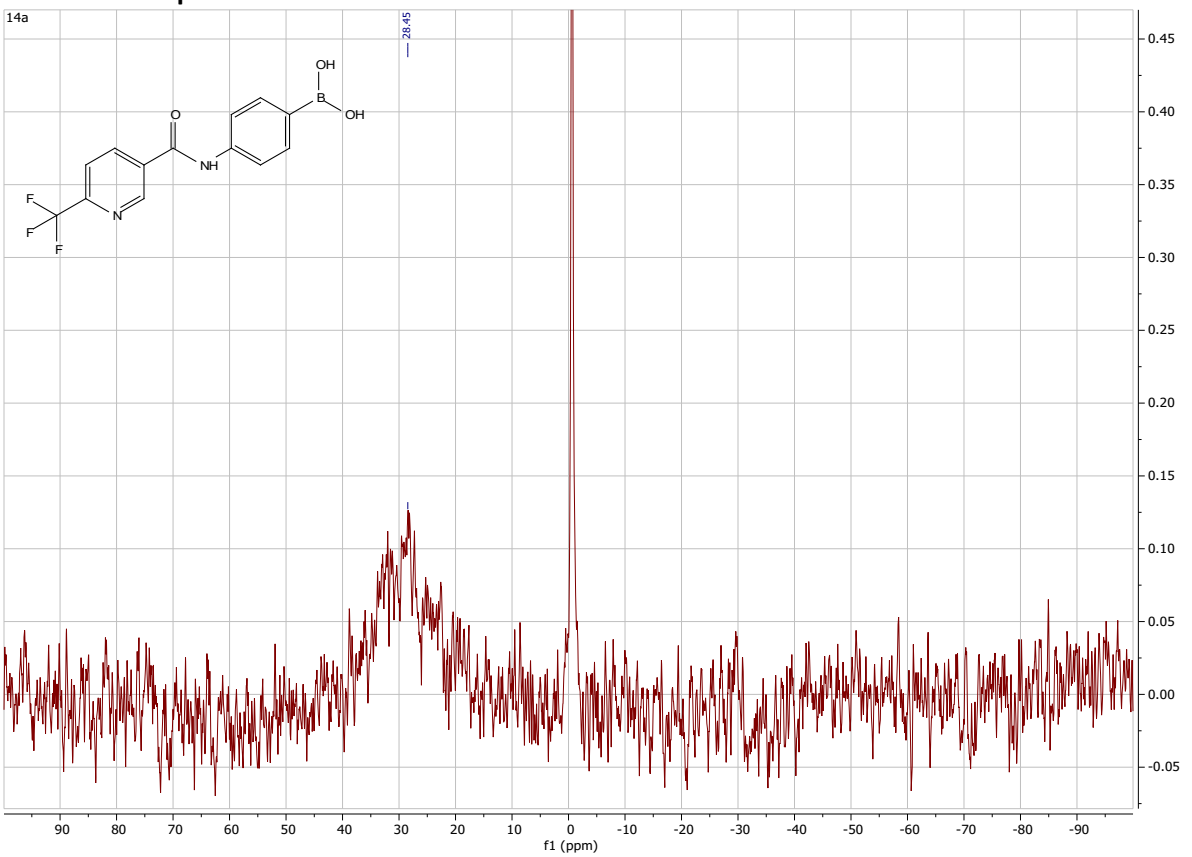


14a ^{1}H NMR spectrum

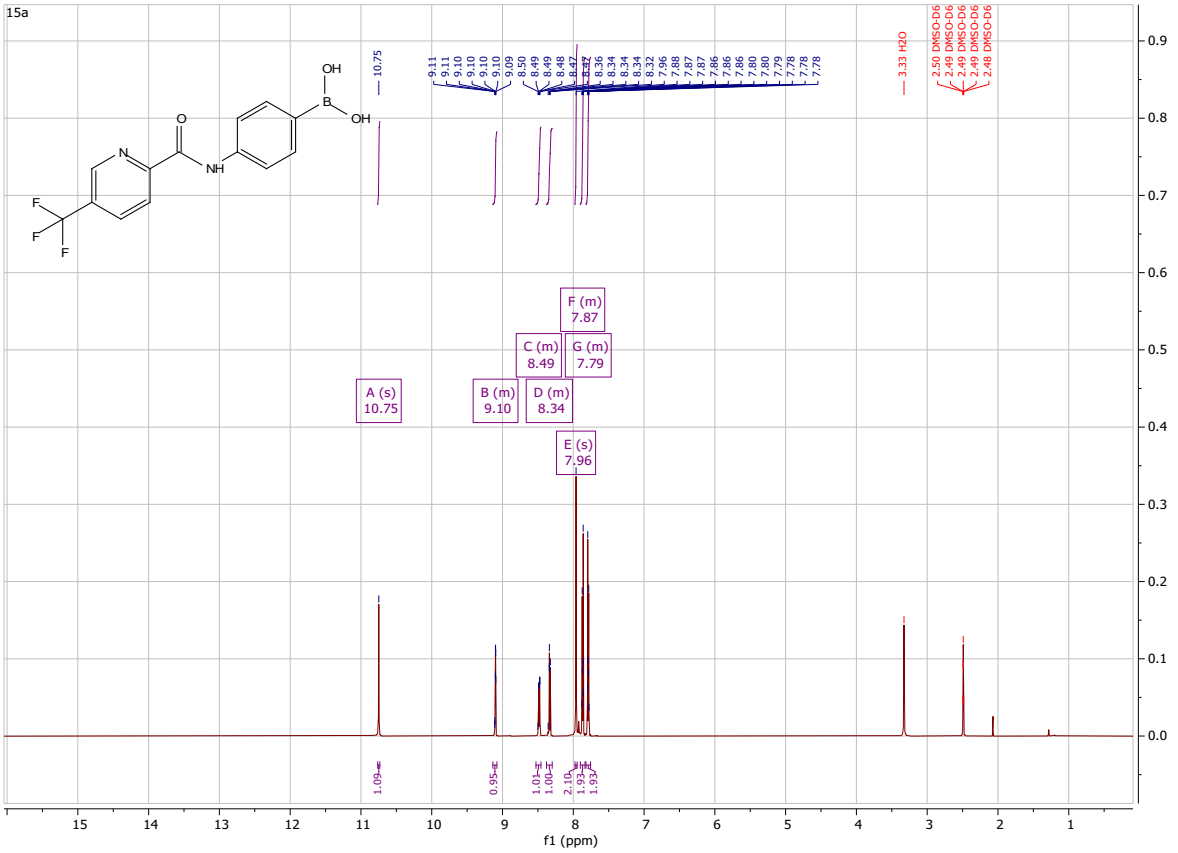


14a ^{13}C NMR spectrum

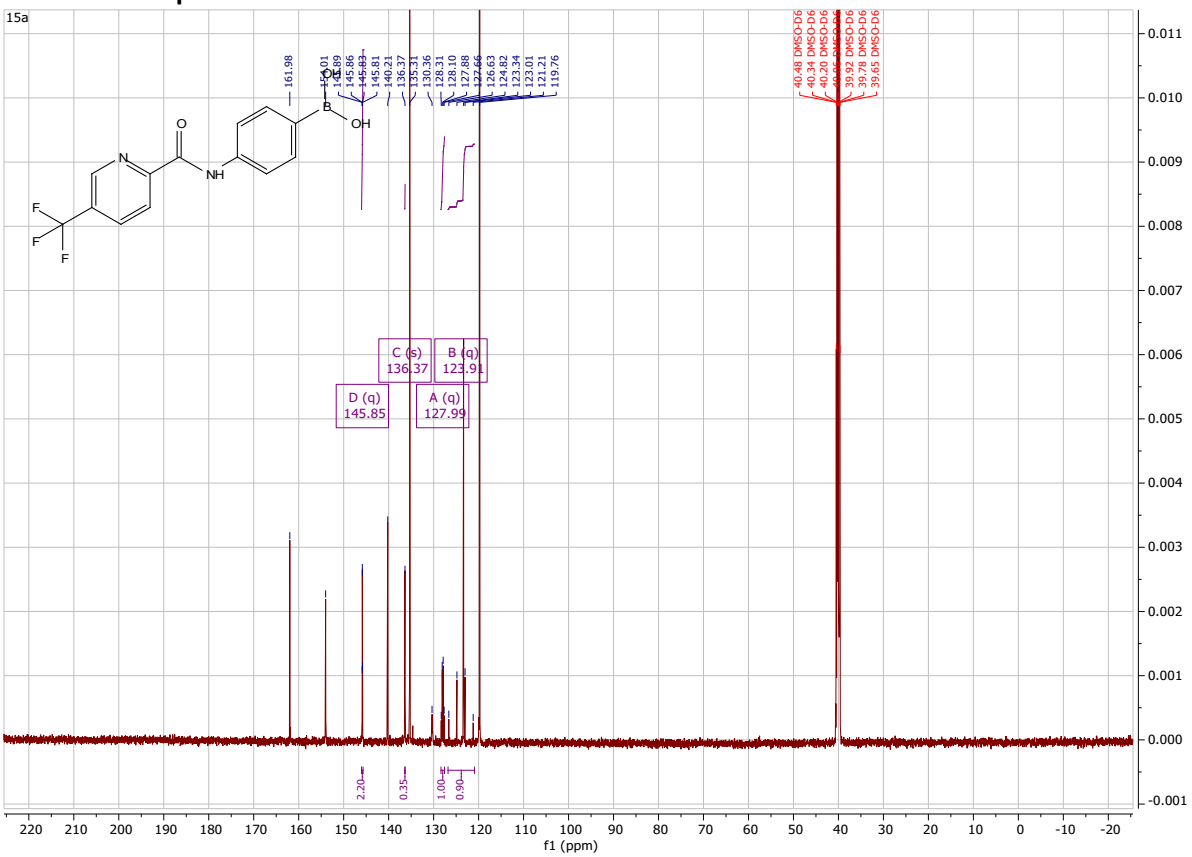
14a ^{11}B NMR spectrum



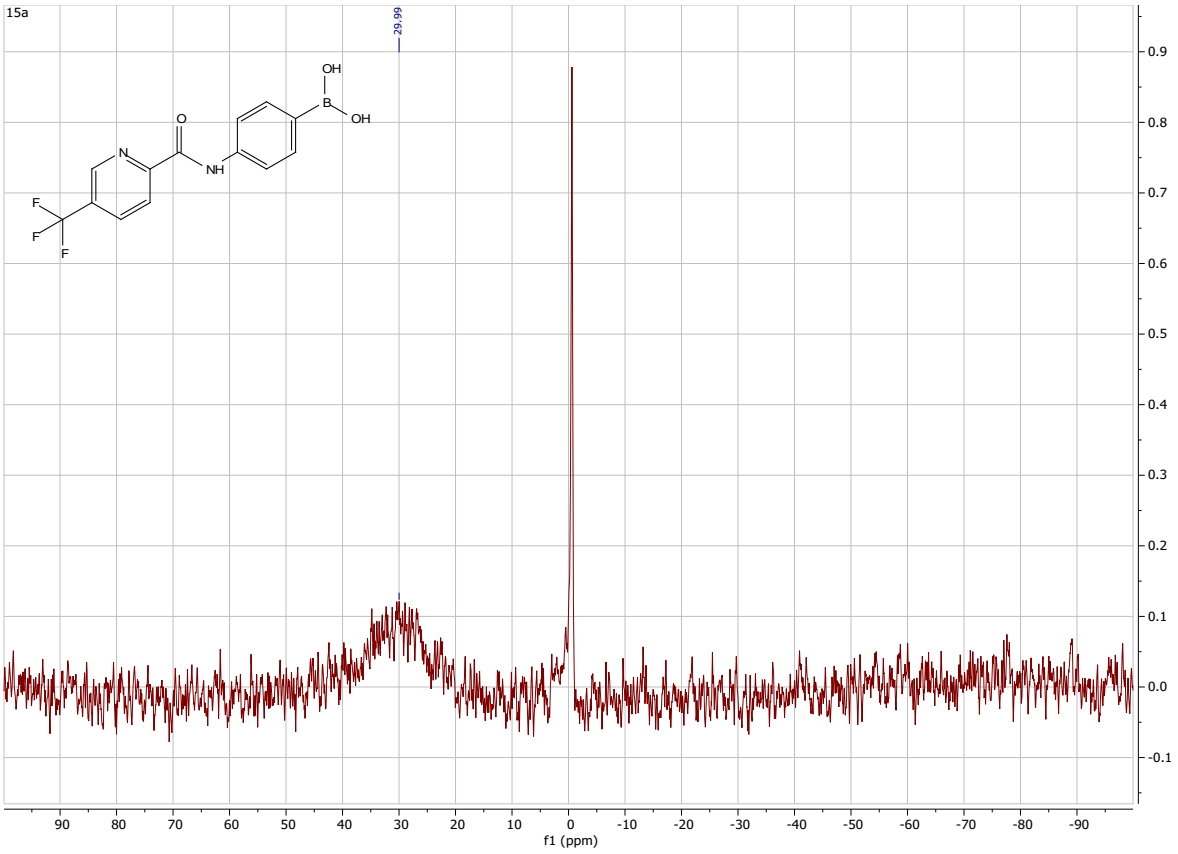
15a ^{1}H NMR spectrum



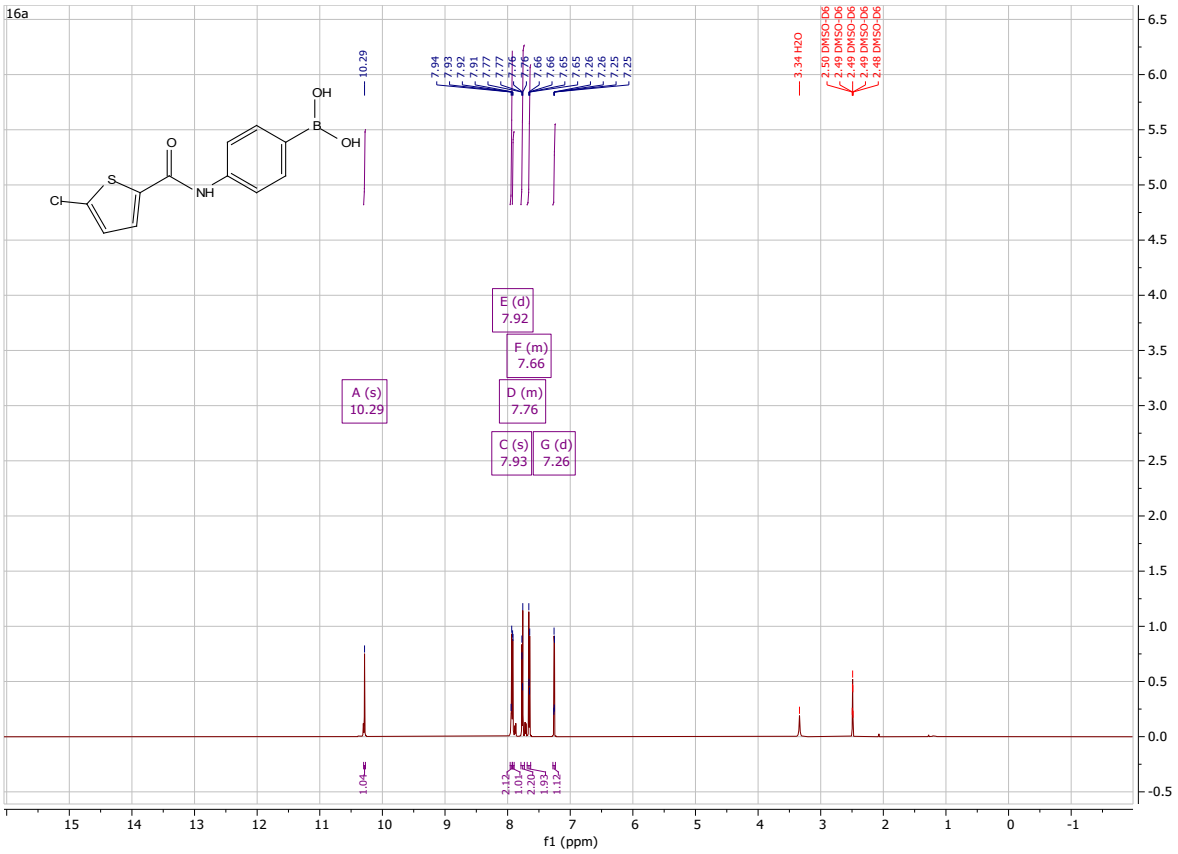
15a ^{13}C NMR spectrum



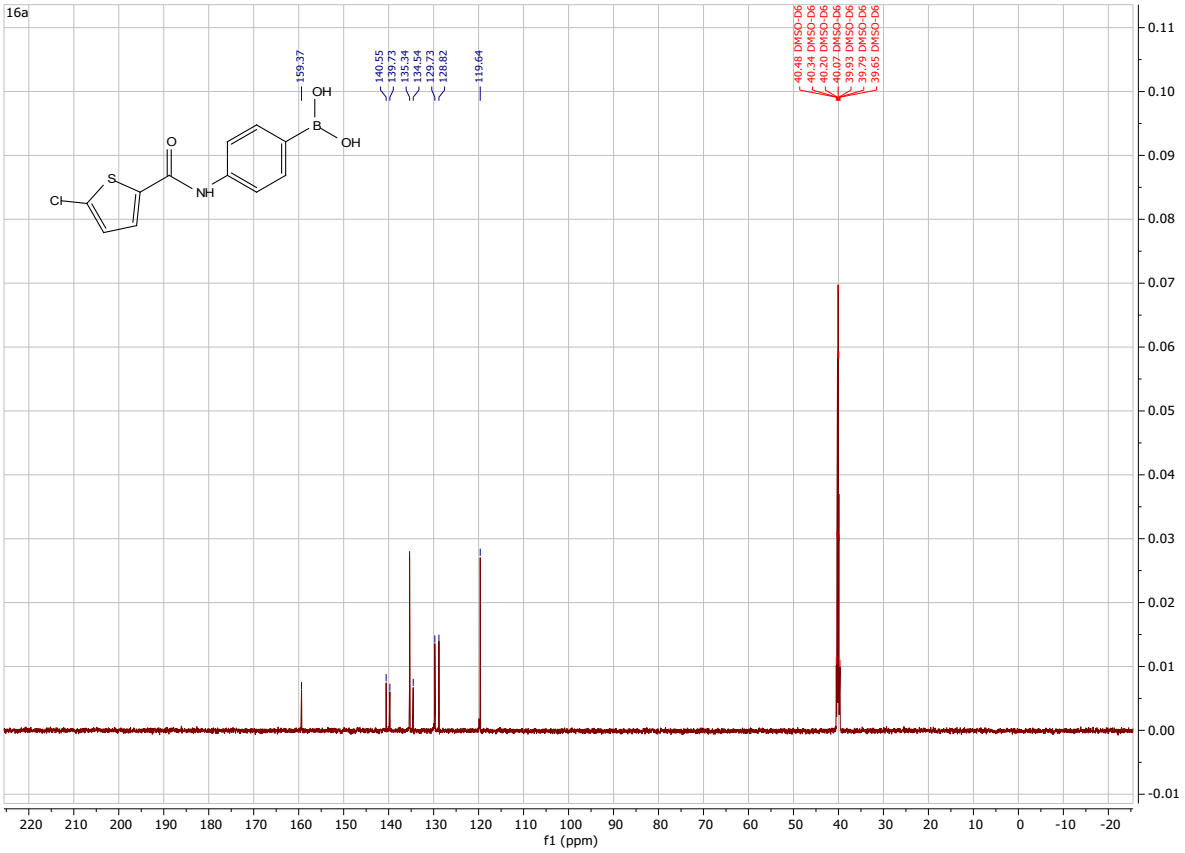
15a ^{11}B NMR spectrum



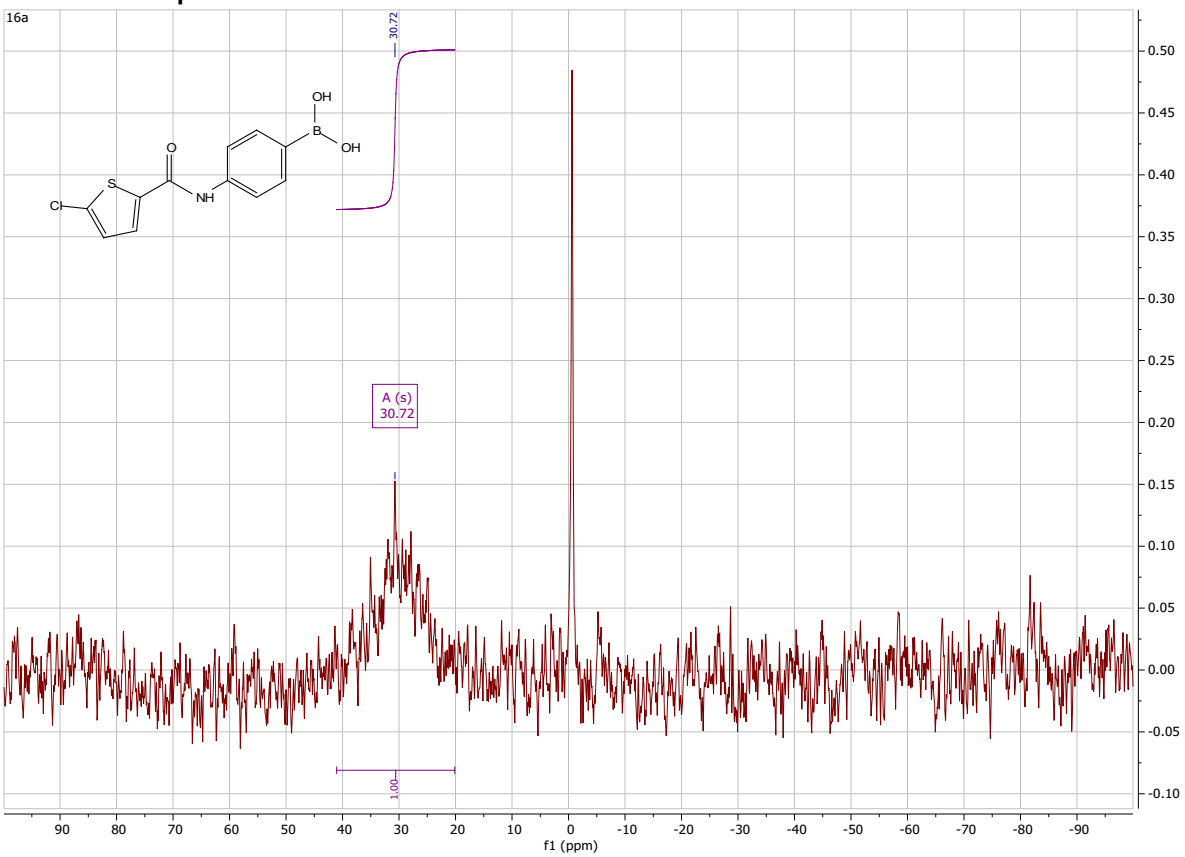
16a ^{1}H NMR spectrum



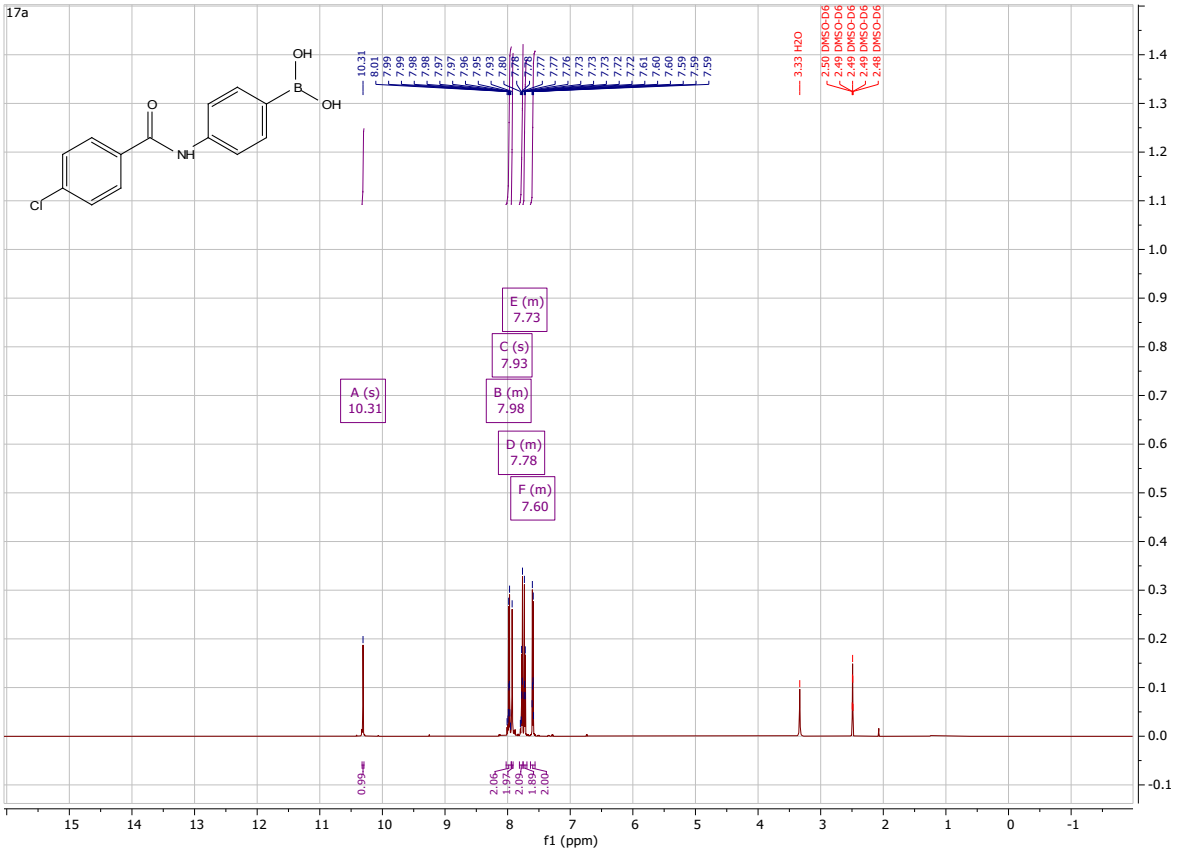
16a ^{13}C NMR spectrum



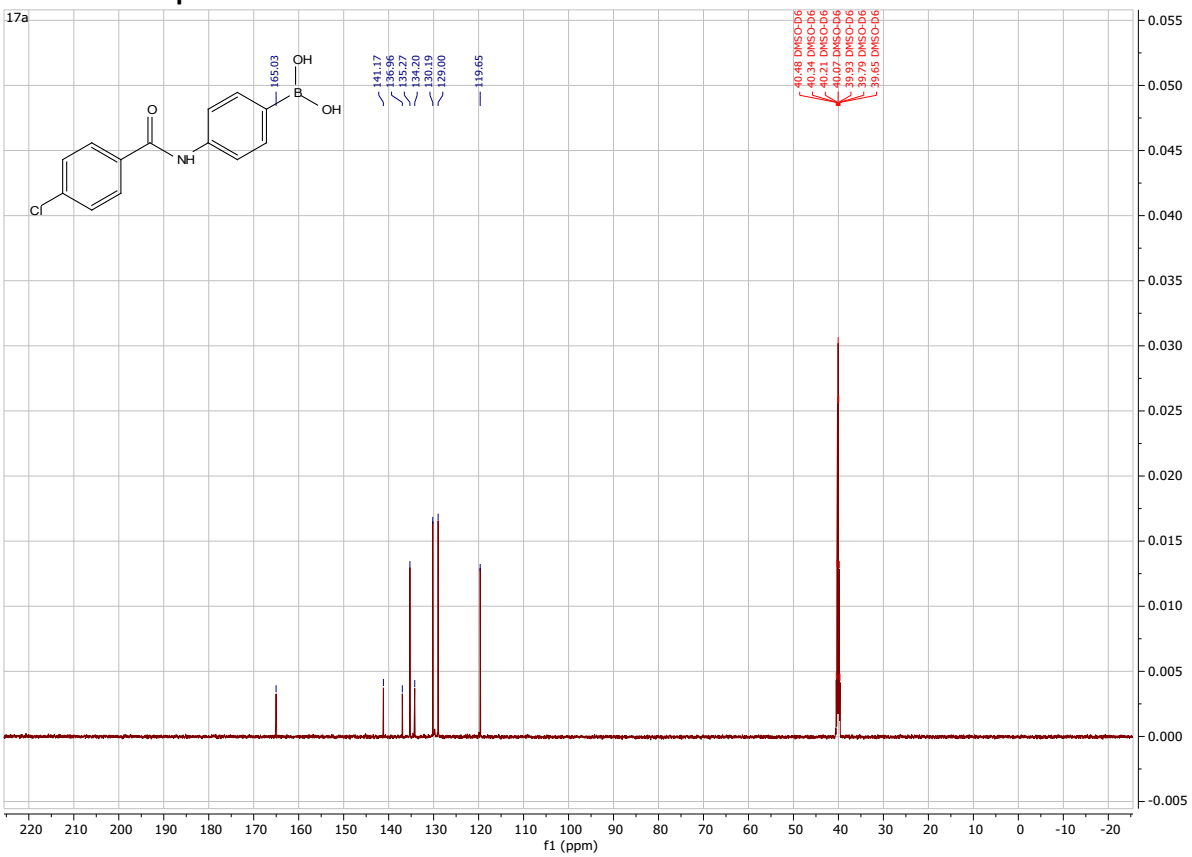
16a ^{11}B NMR spectrum



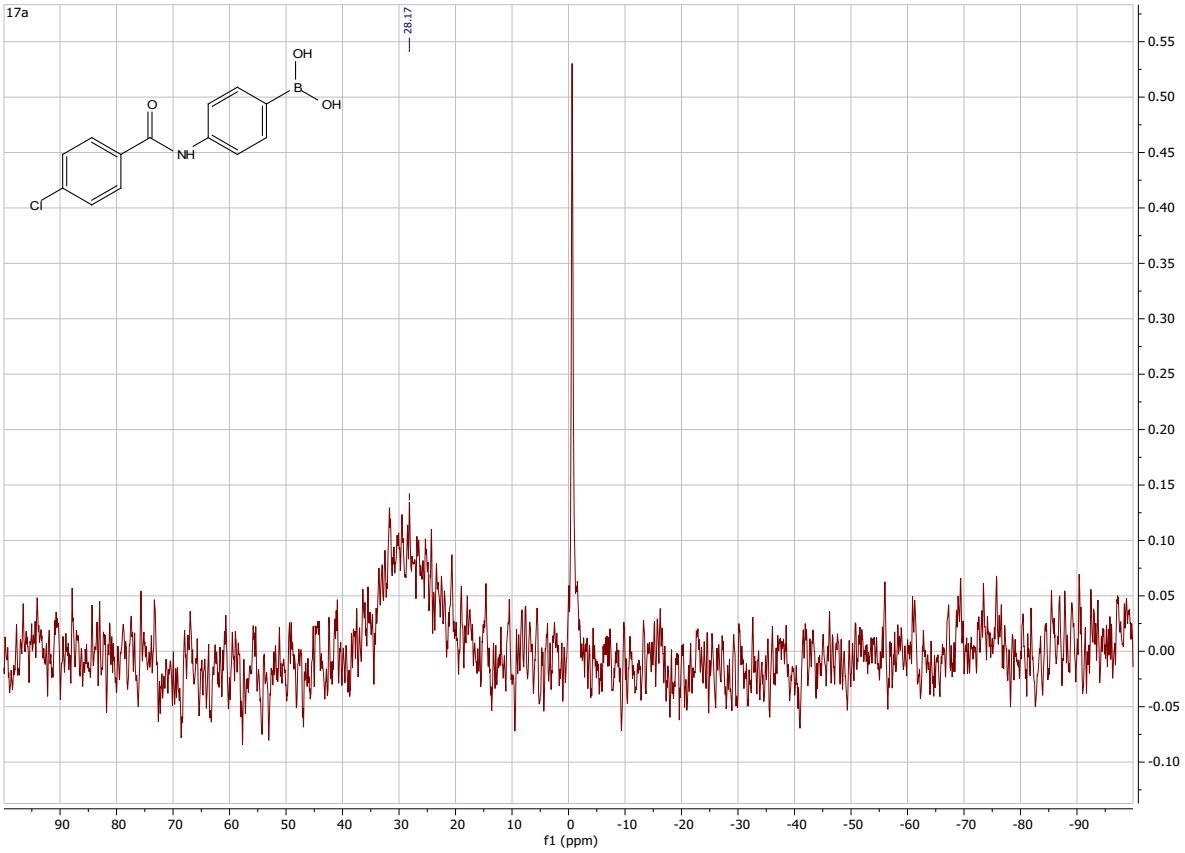
17a ^{1}H NMR spectrum



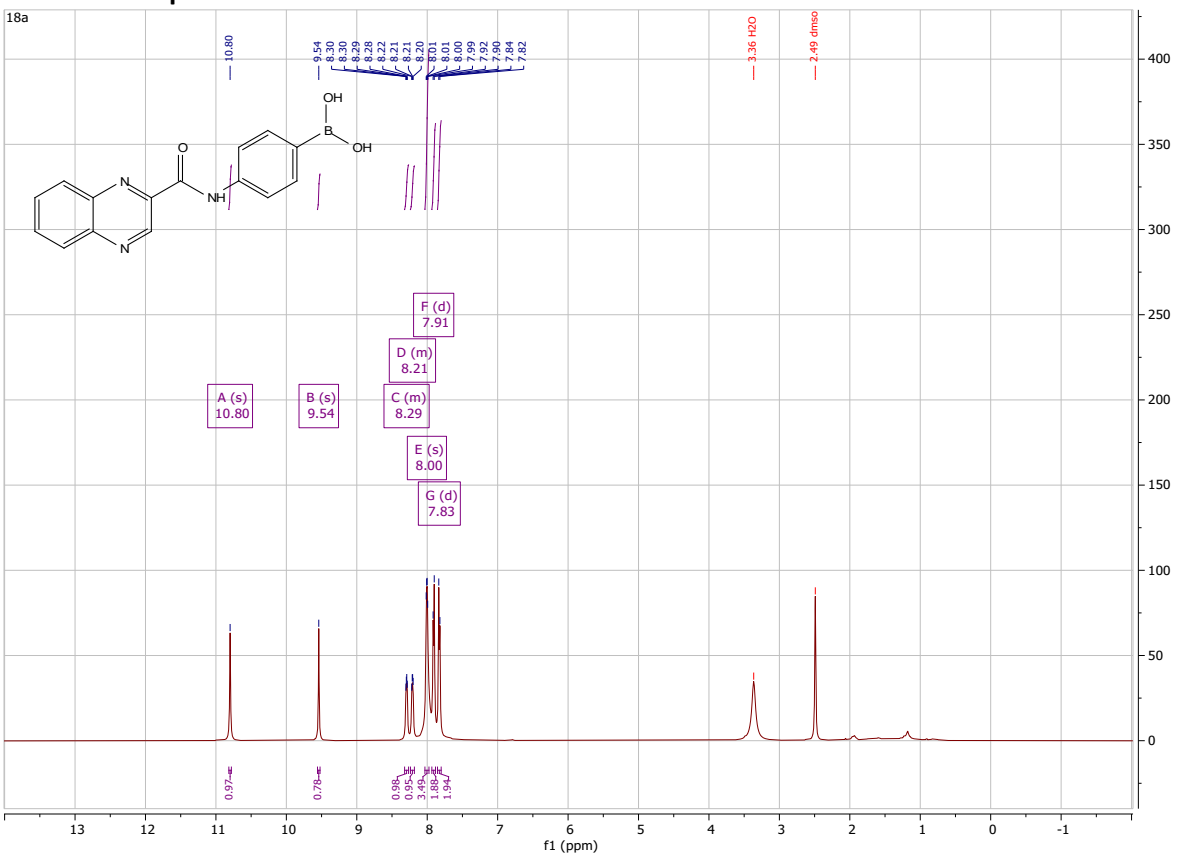
17a ^{13}C NMR spectrum



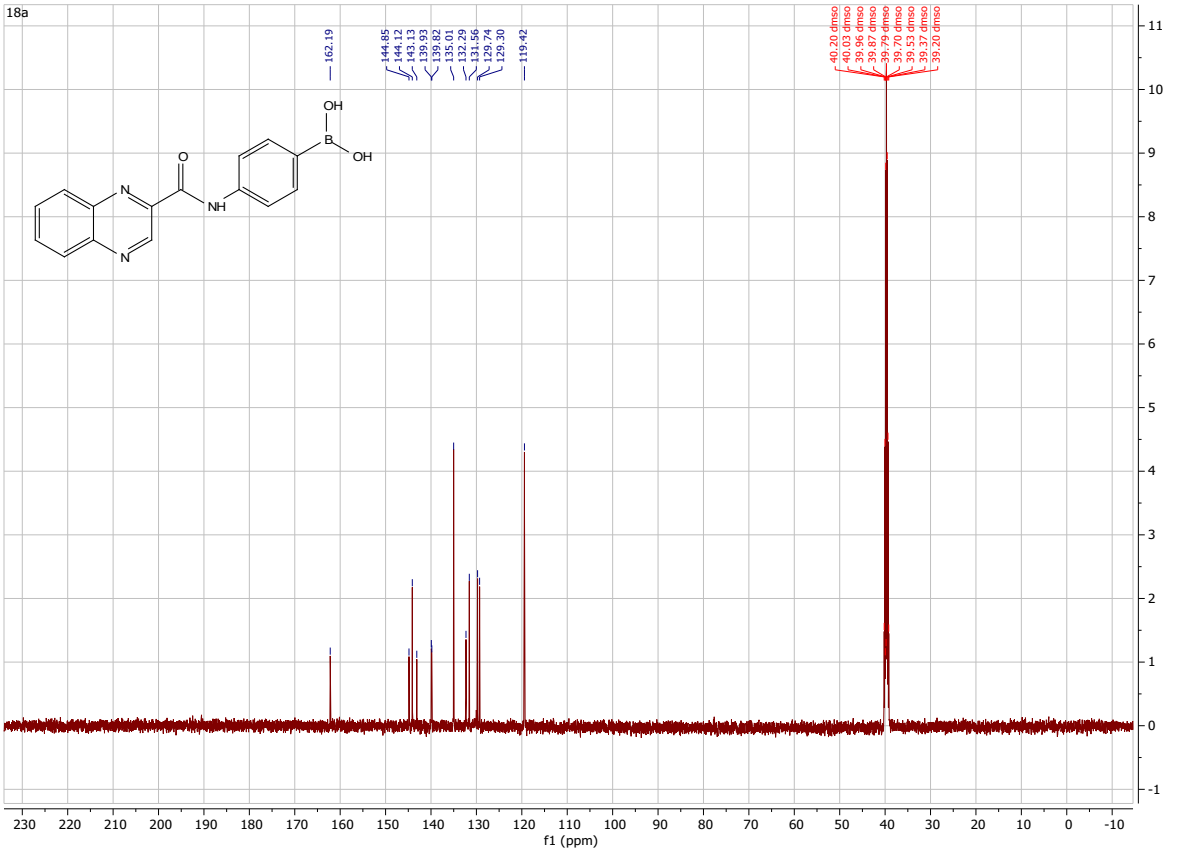
17a ^{11}B NMR spectrum



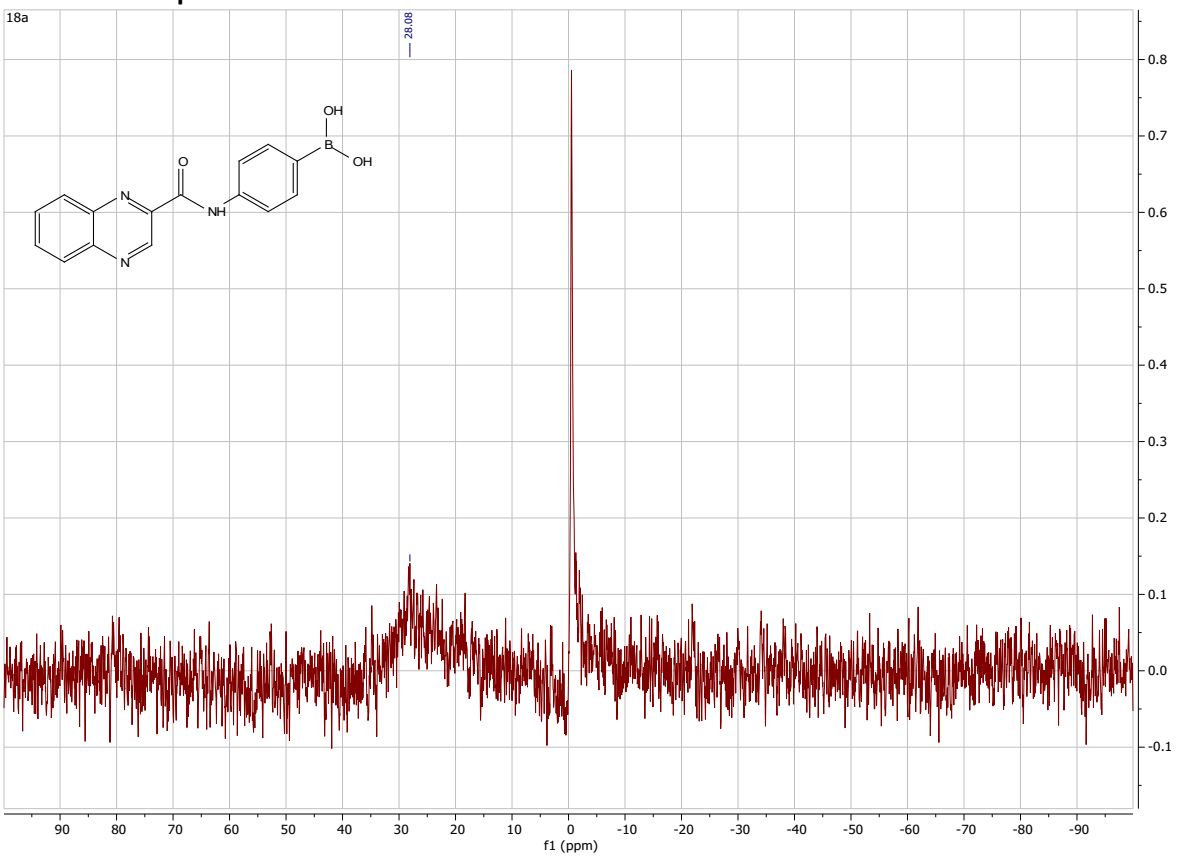
18a ^{1}H NMR spectrum



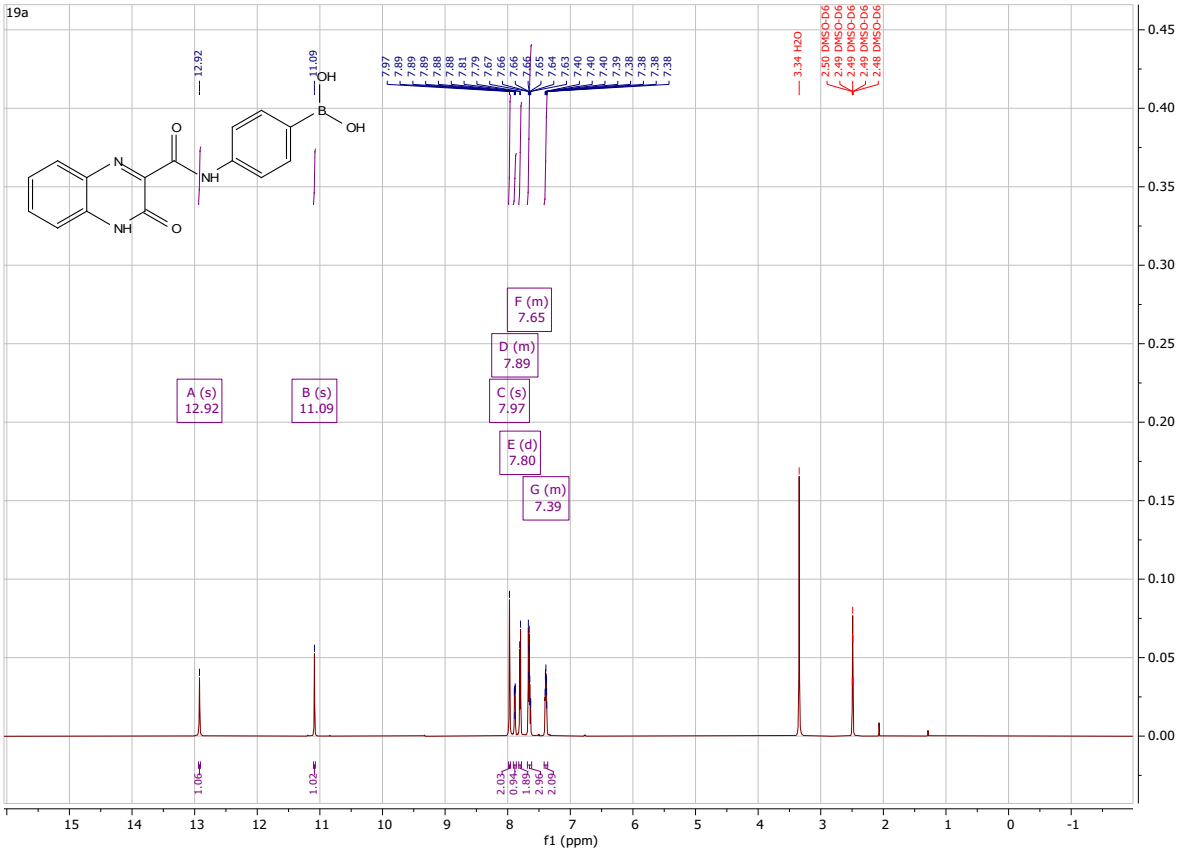
18a ^{13}C NMR spectrum



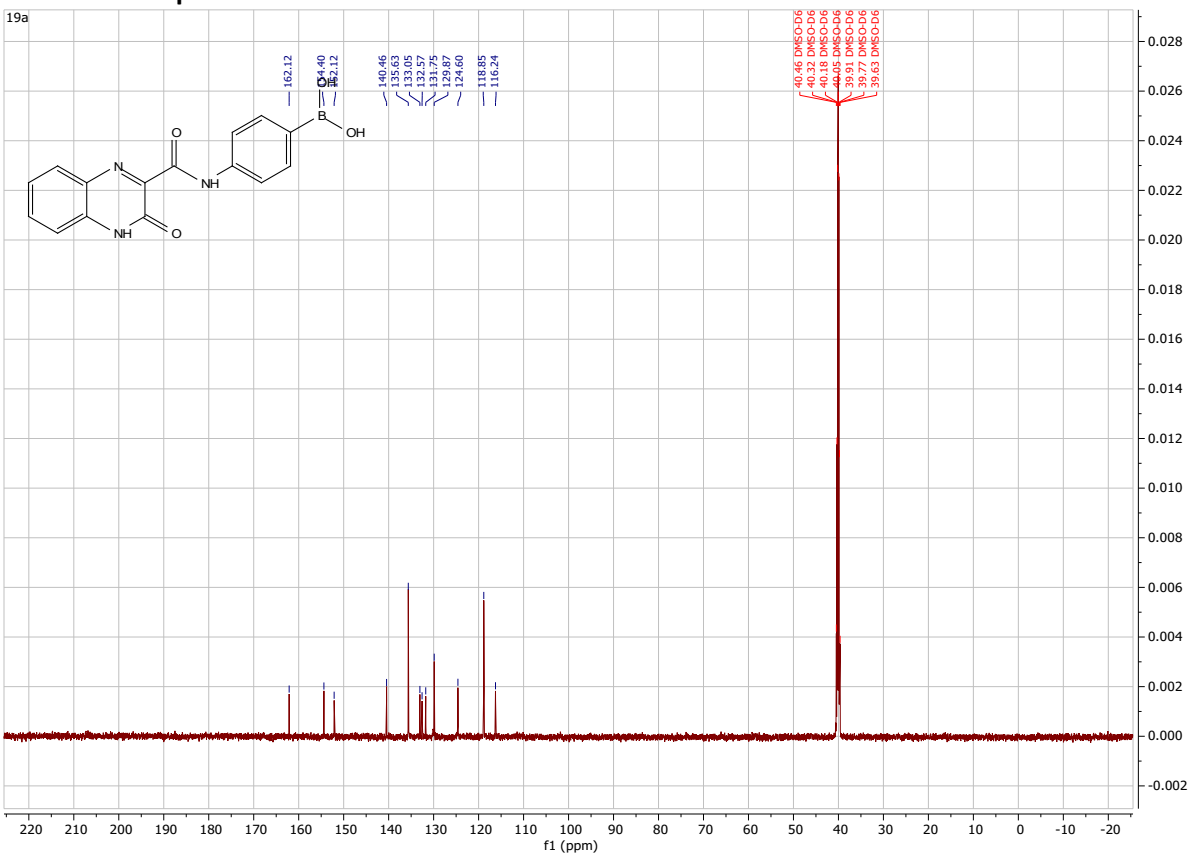
18a ^{11}B NMR spectrum



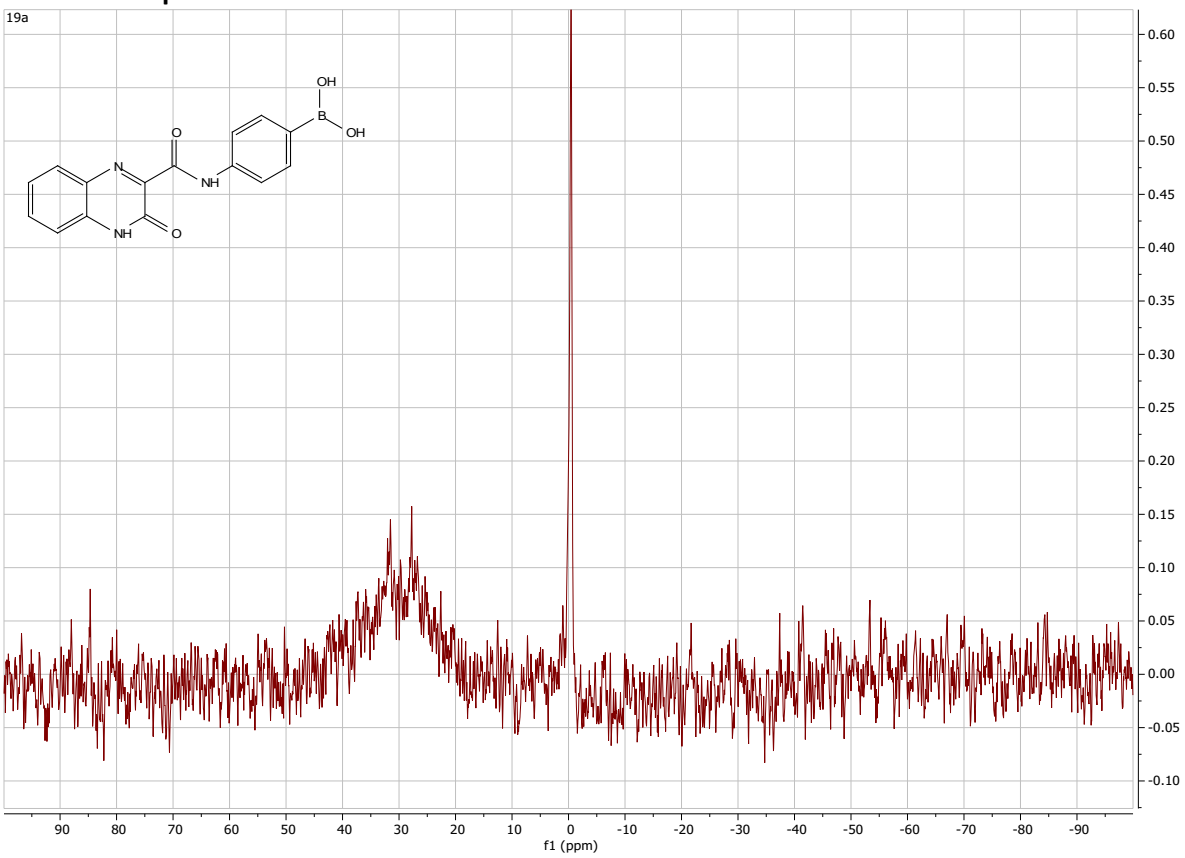
19a ^{1}H NMR spectrum



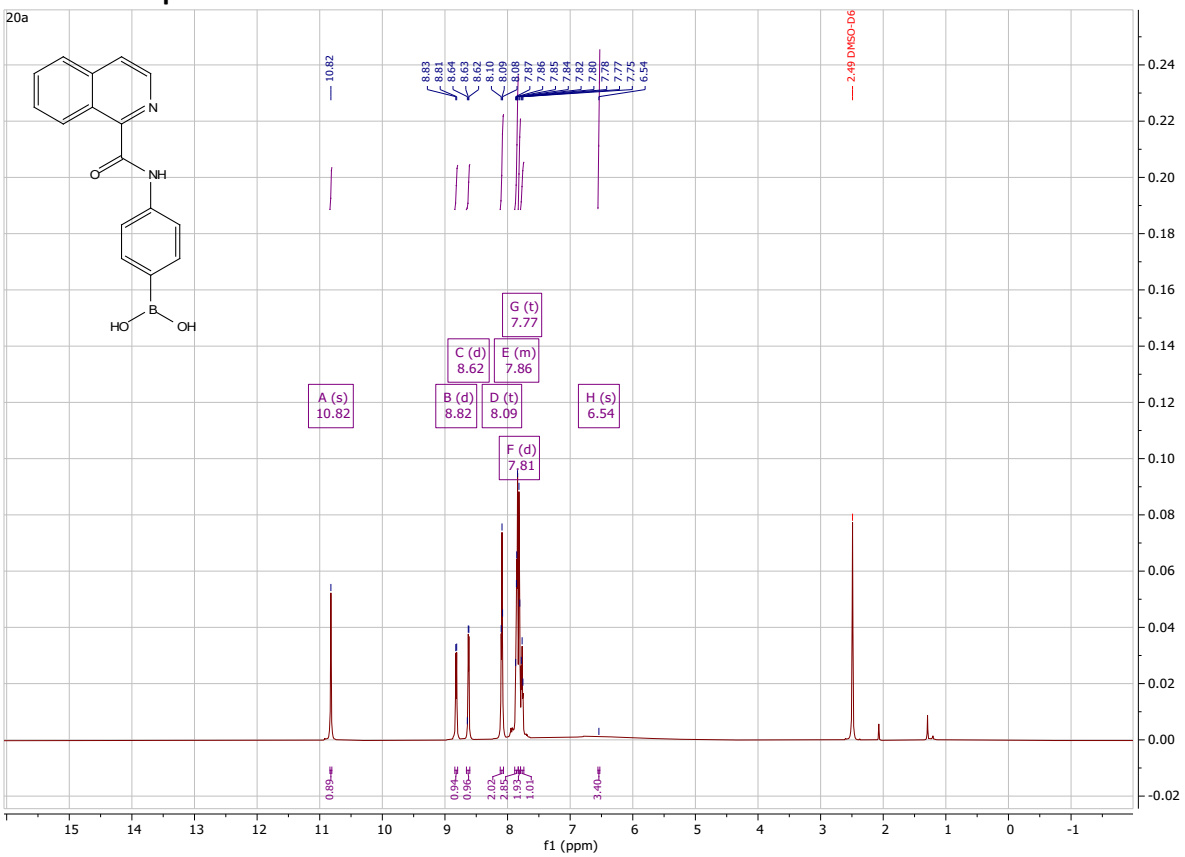
19a ^{13}C NMR spectrum



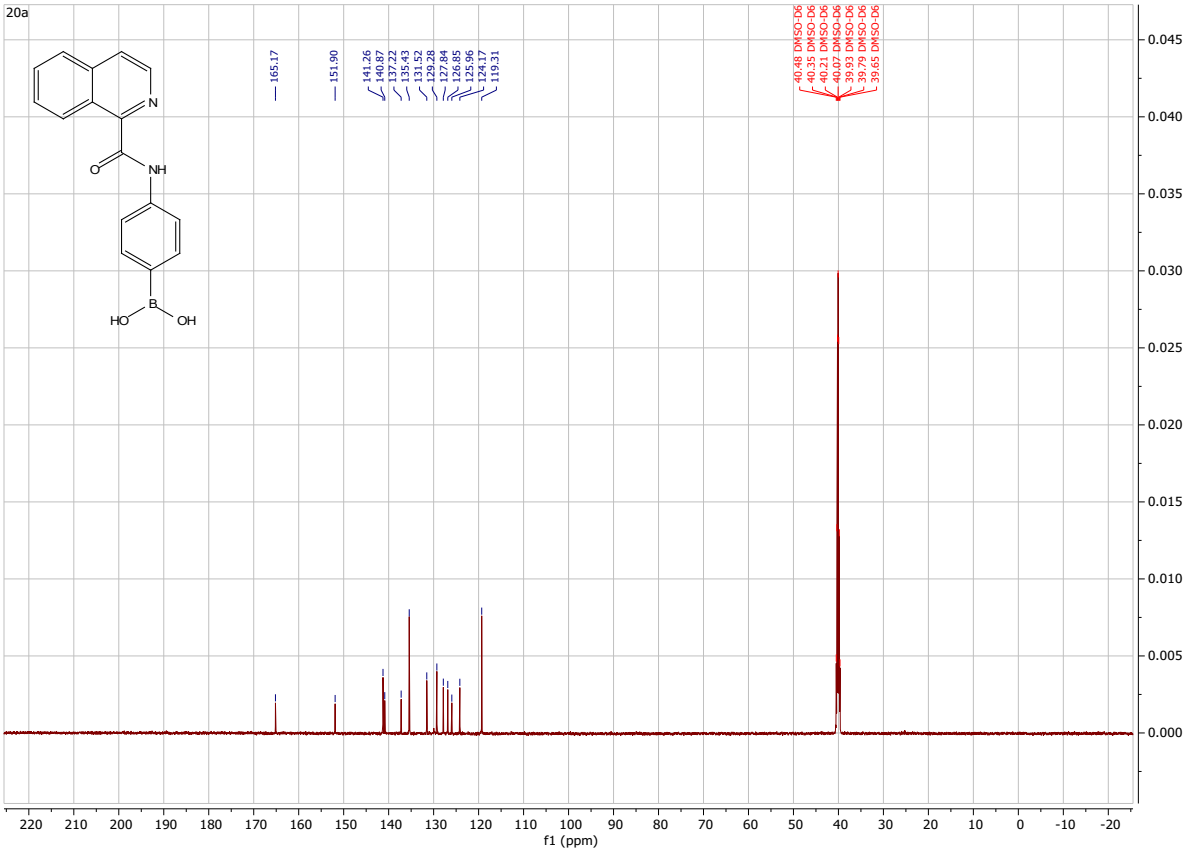
19 ^{11}B NMR spectrum



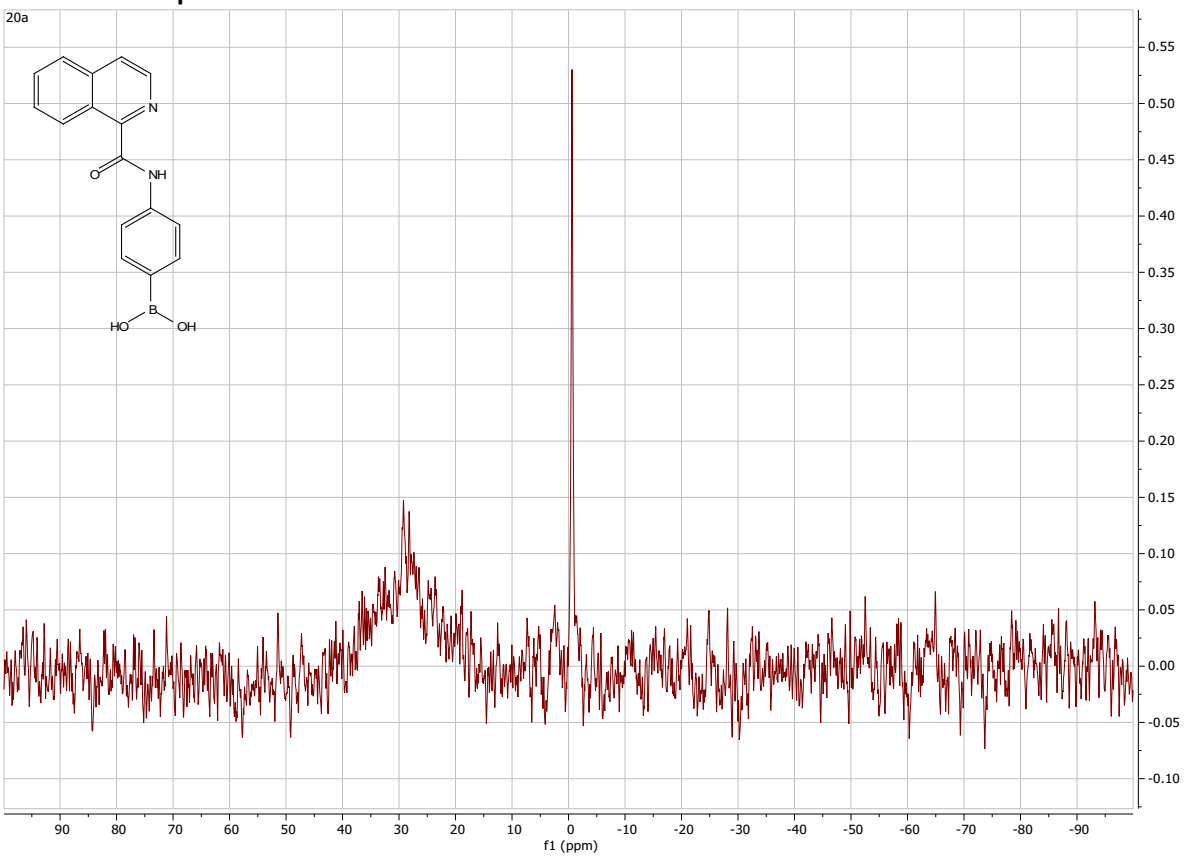
20a ^{1}H NMR spectrum



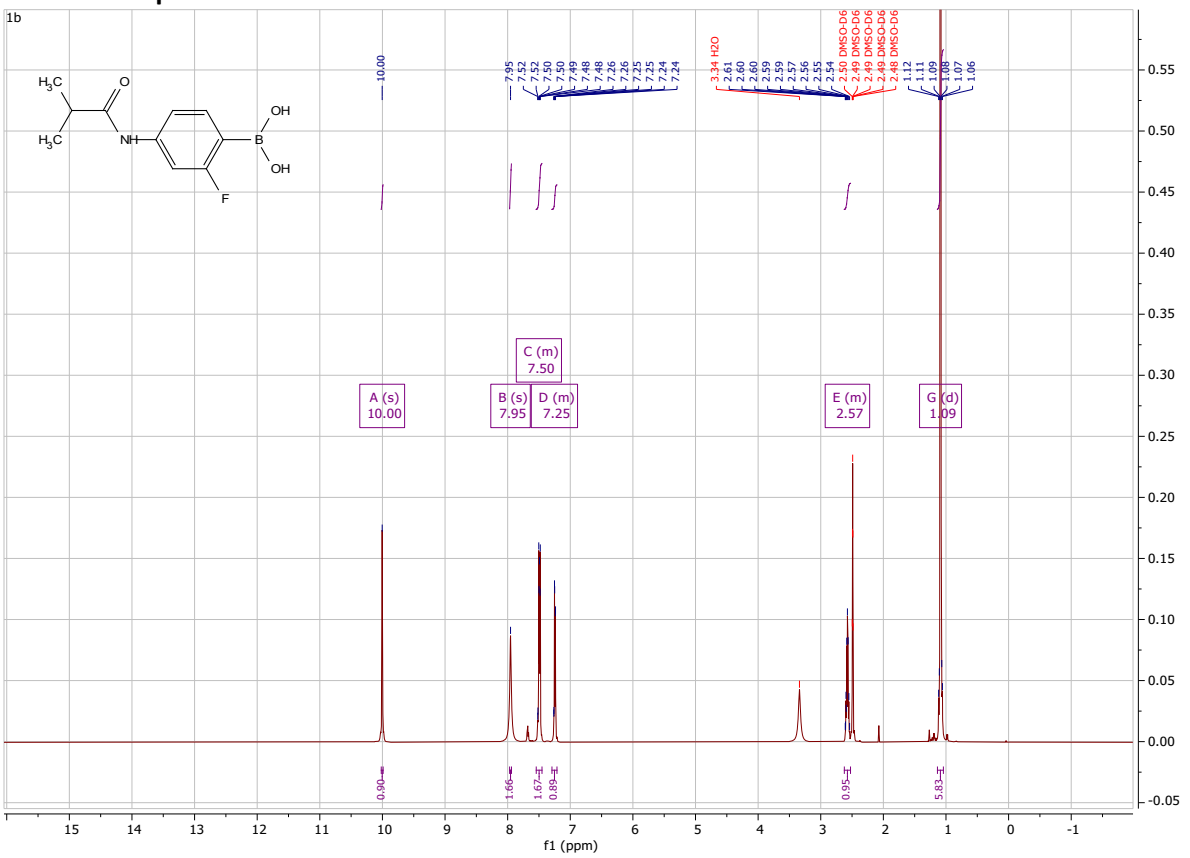
20a ^{13}C NMR spectrum



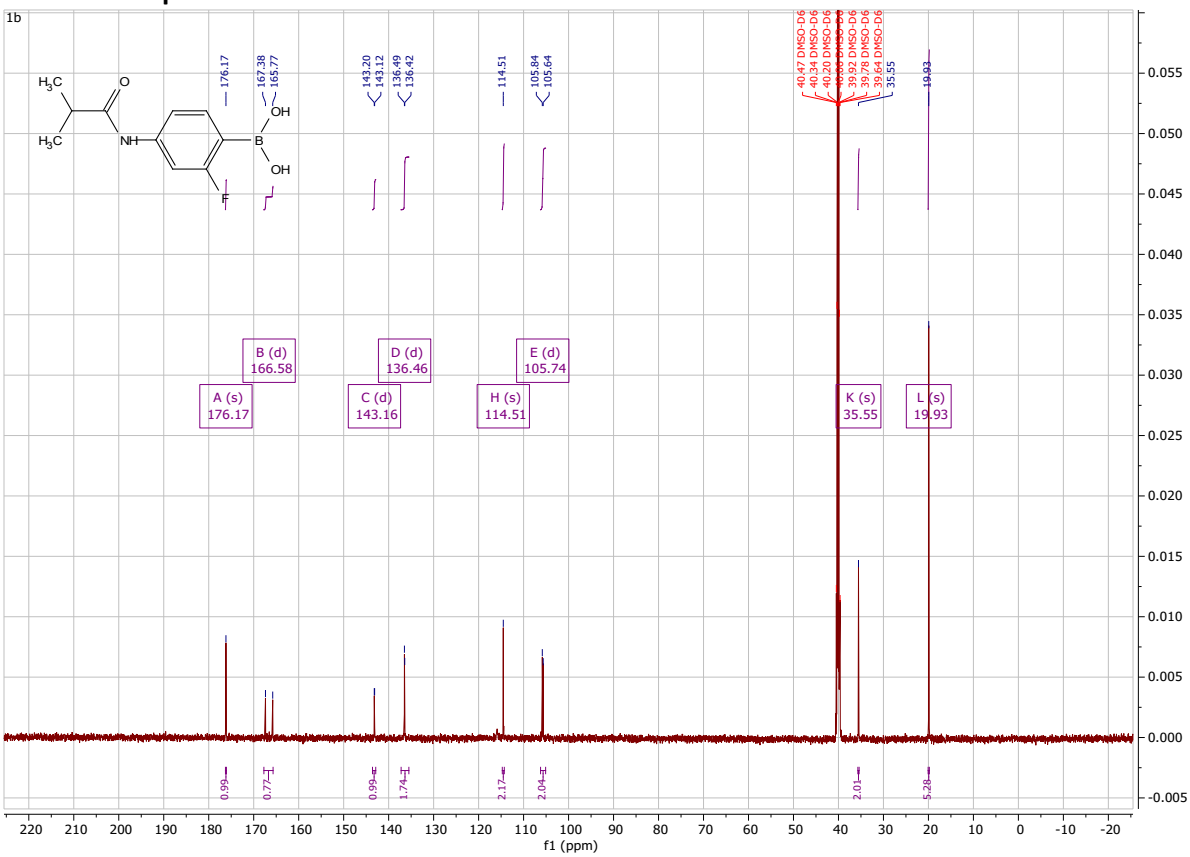
20a ^{11}B NMR spectrum



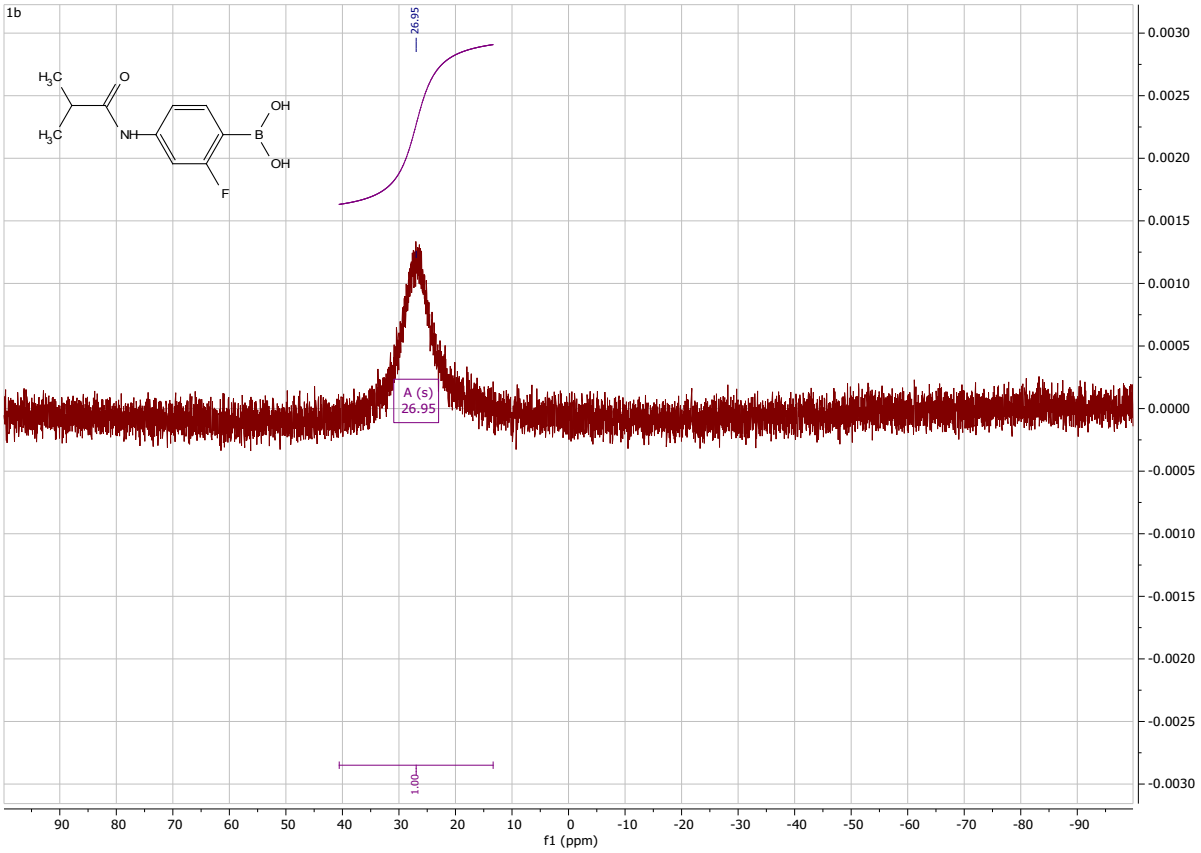
1b ^{1}H NMR spectrum



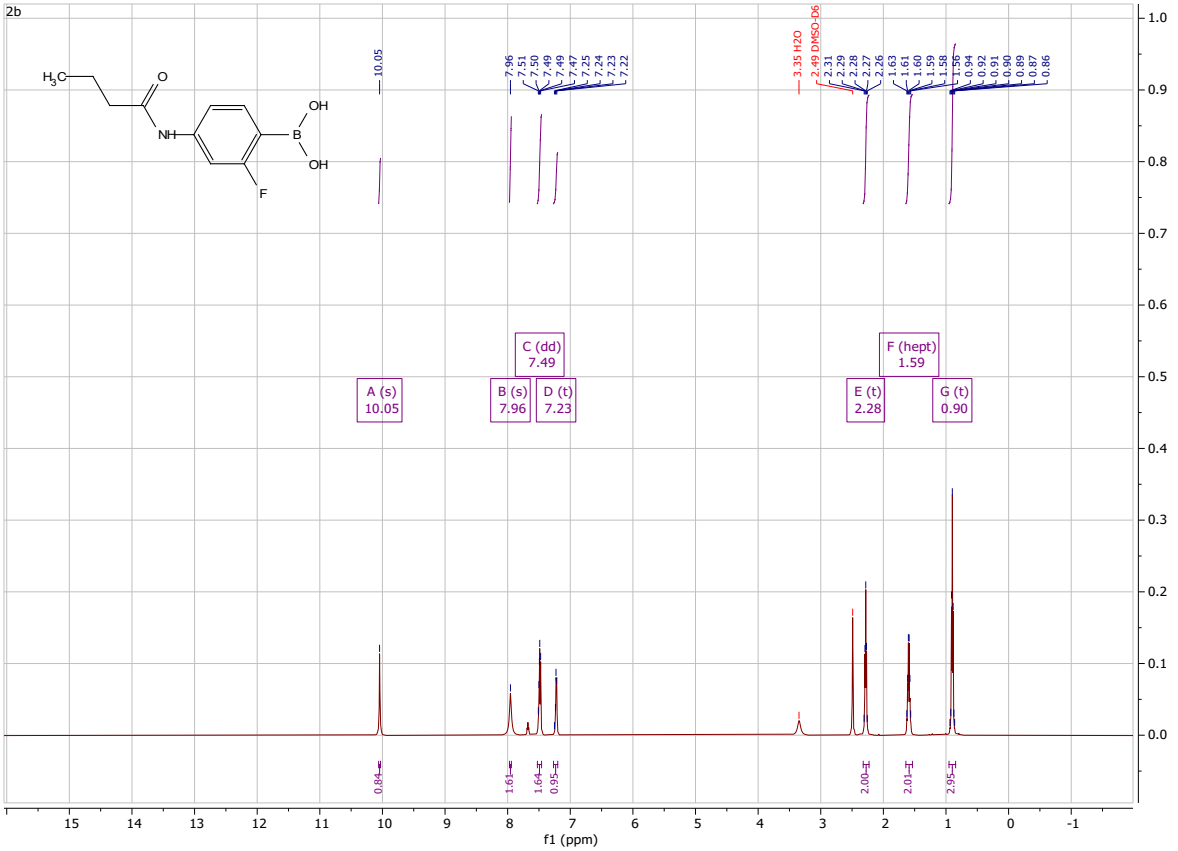
1b ^{13}C NMR spectrum



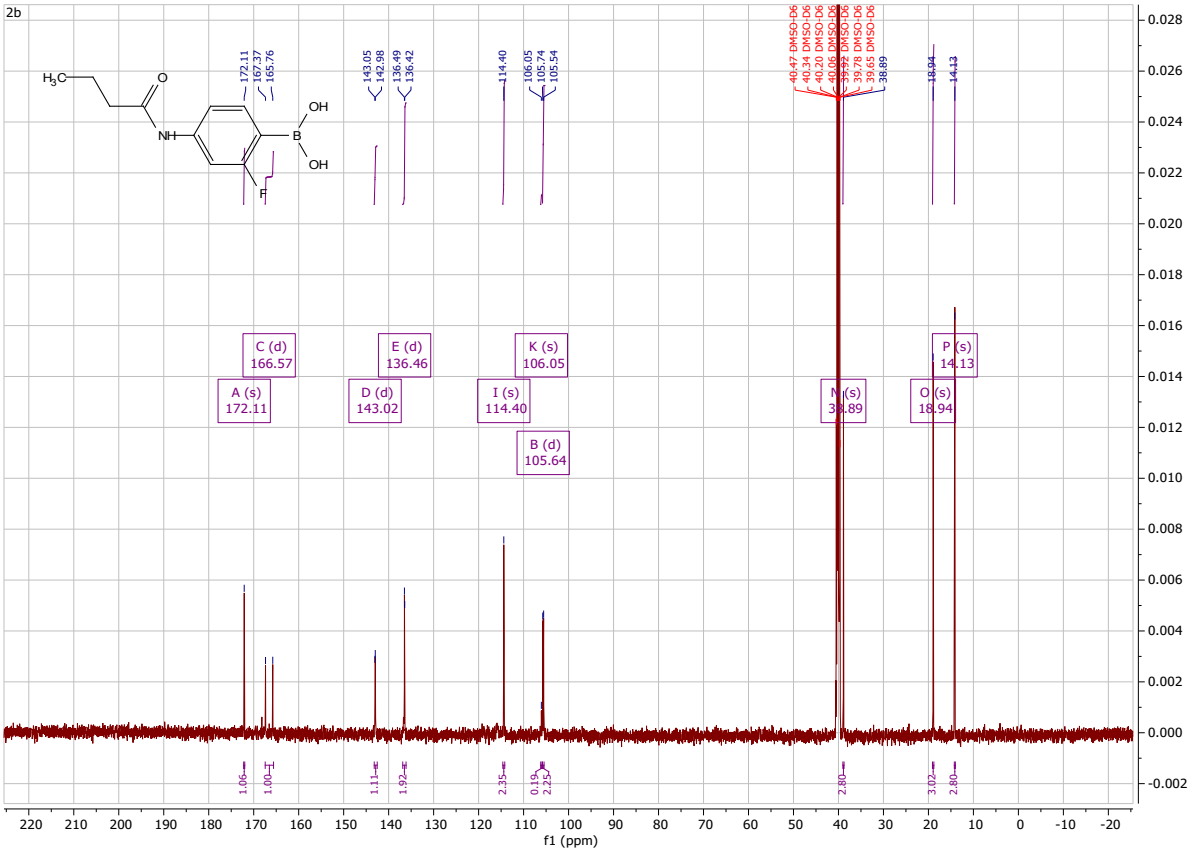
1b ^{11}B NMR spectrum



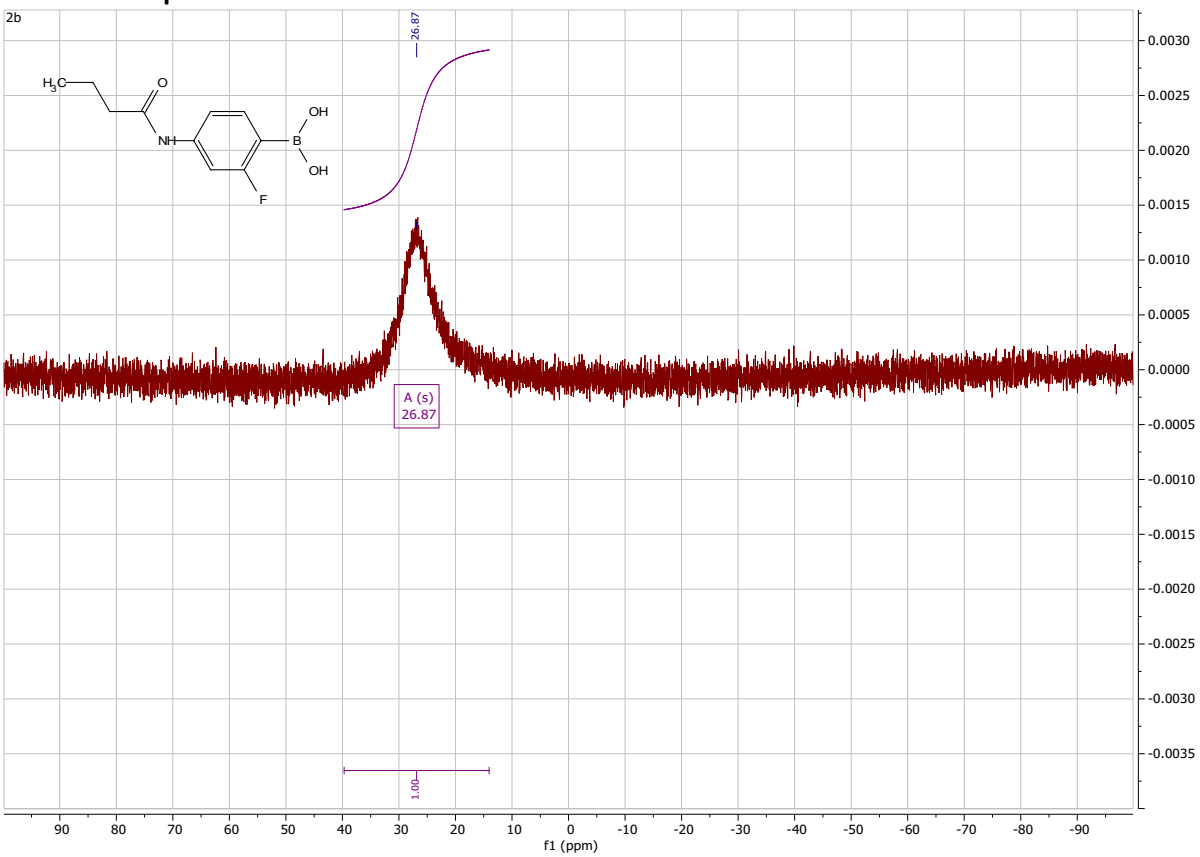
2b ^{1}H NMR spectrum



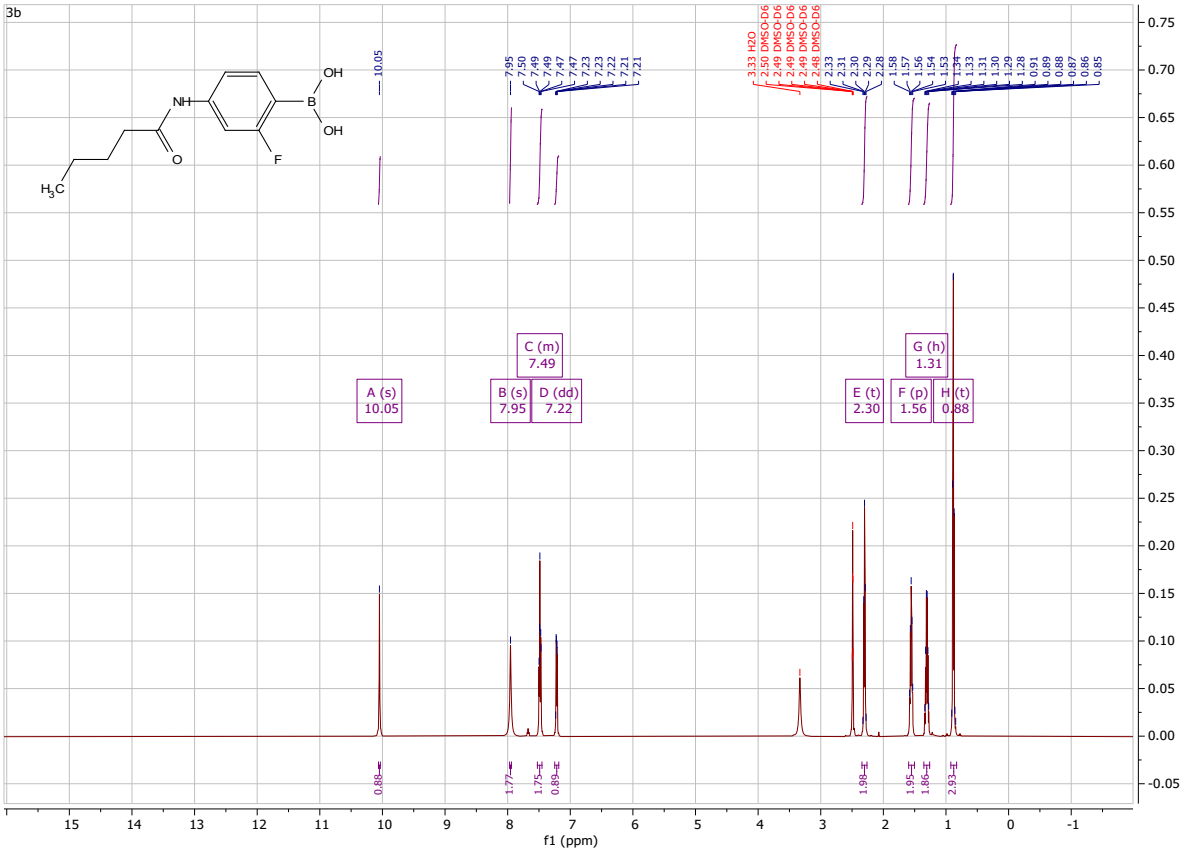
2b ^{13}C NMR spectrum



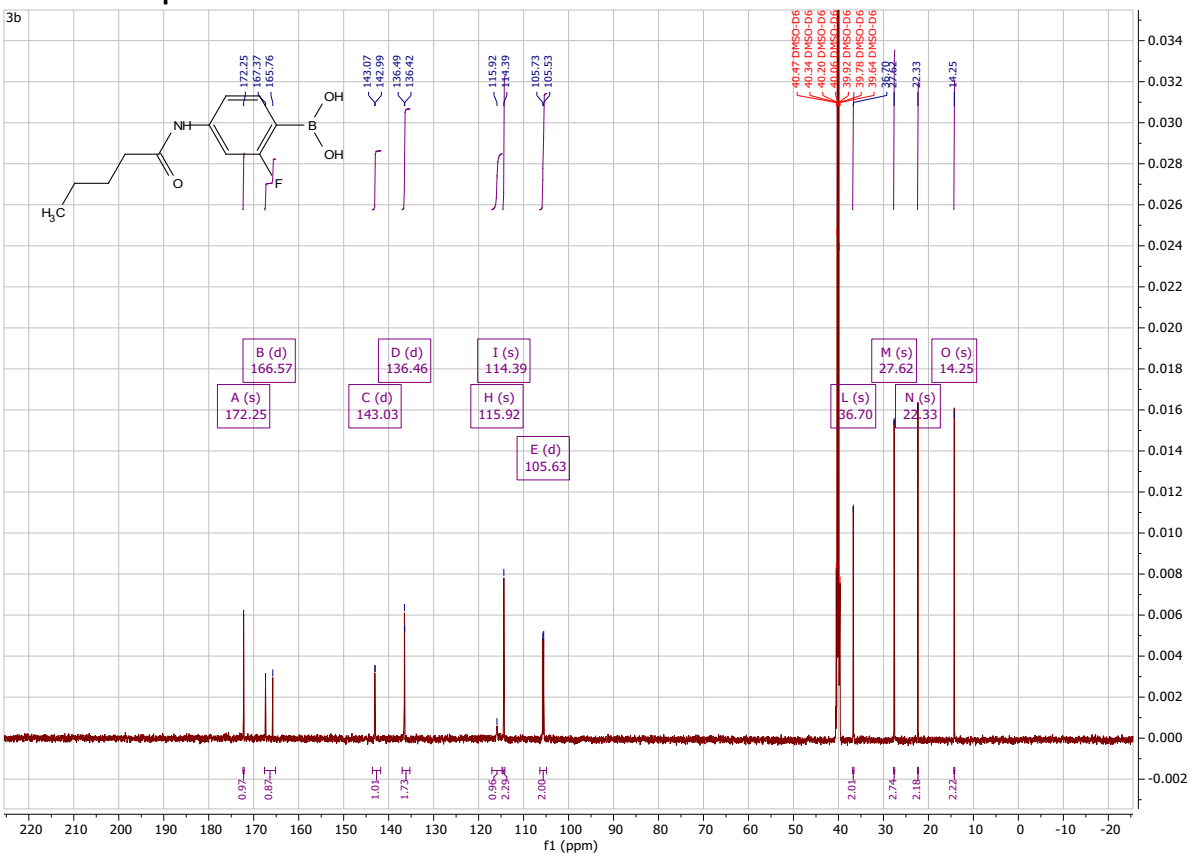
2b ^{11}B NMR spectrum



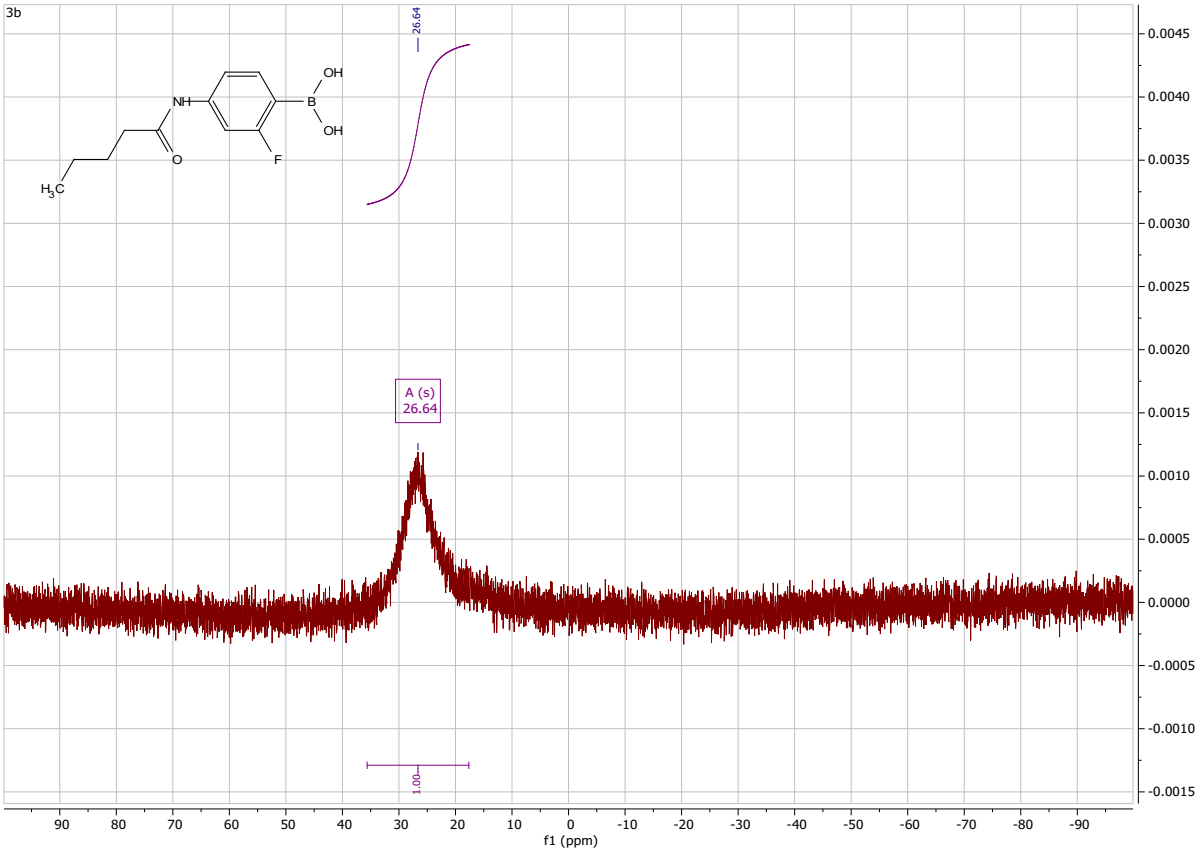
3b ^{1}H NMR spectrum



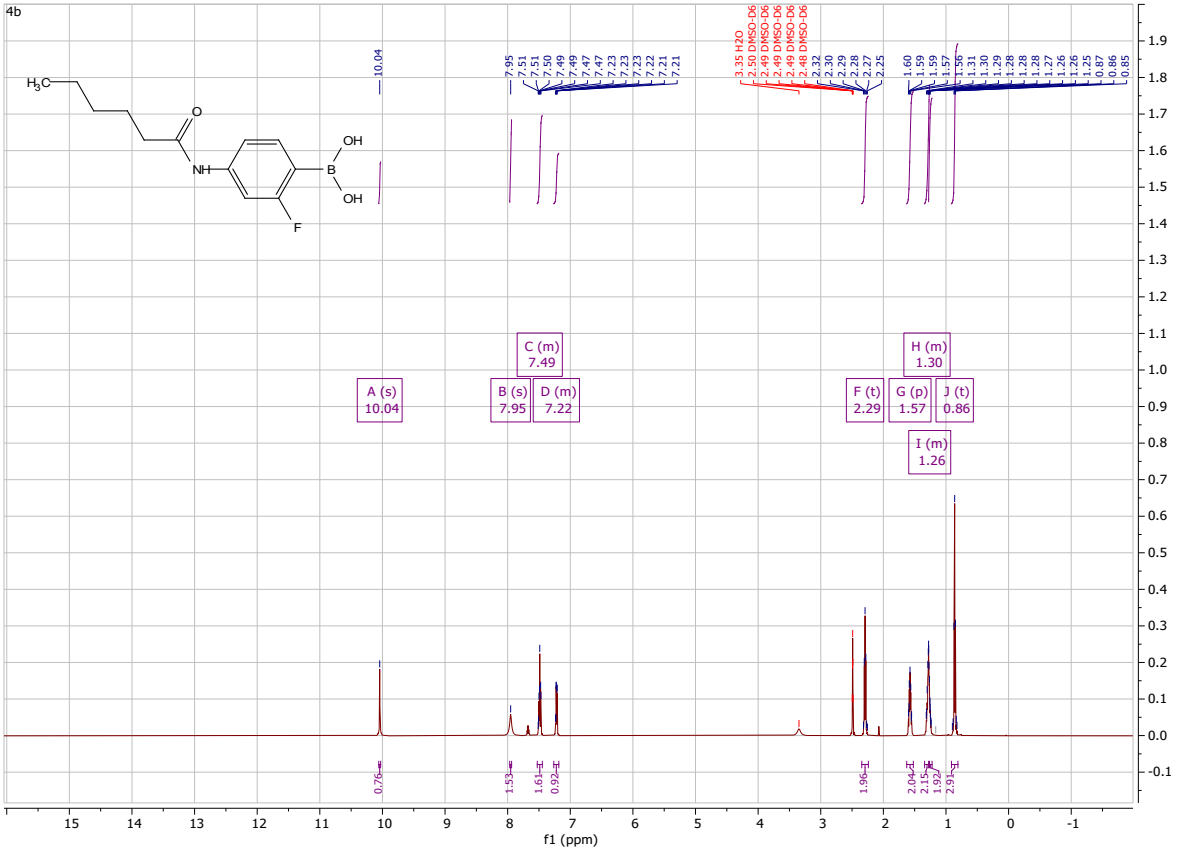
3b ^{13}C NMR spectrum



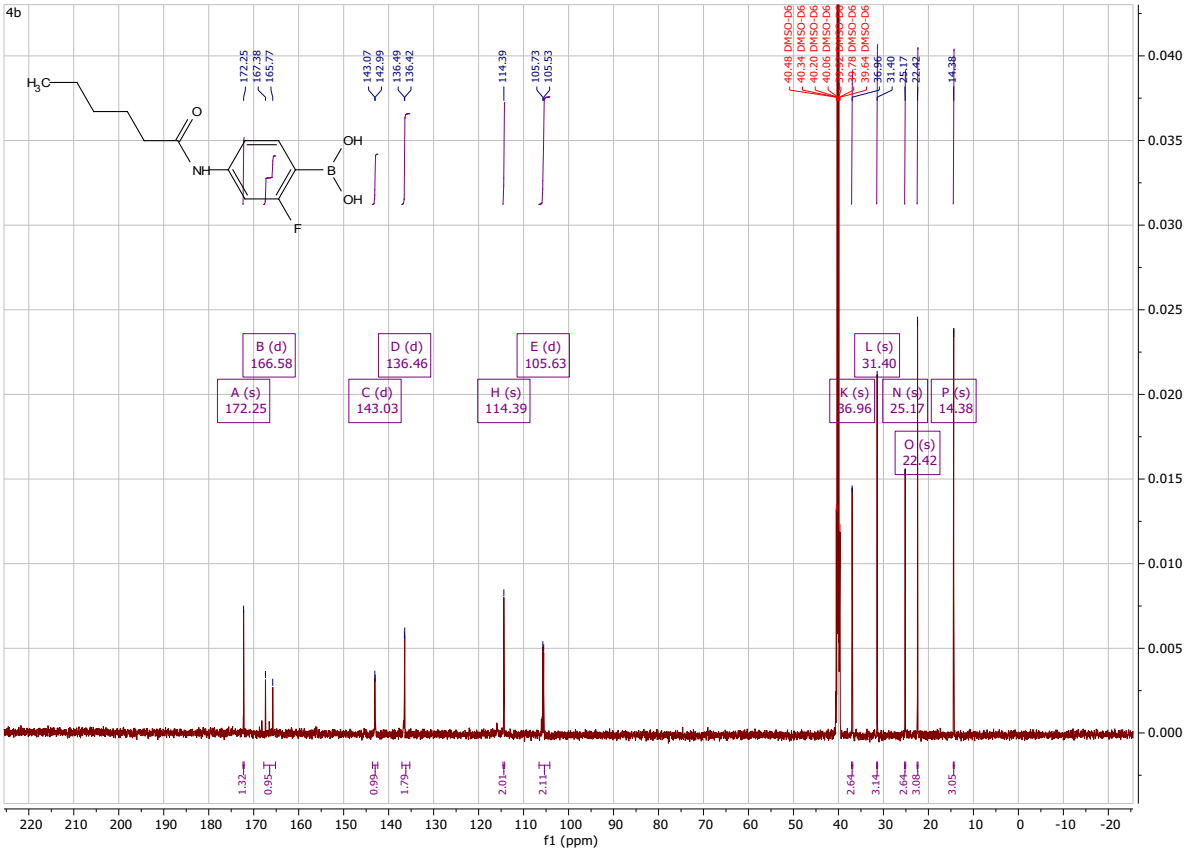
3b ^{11}B NMR spectrum



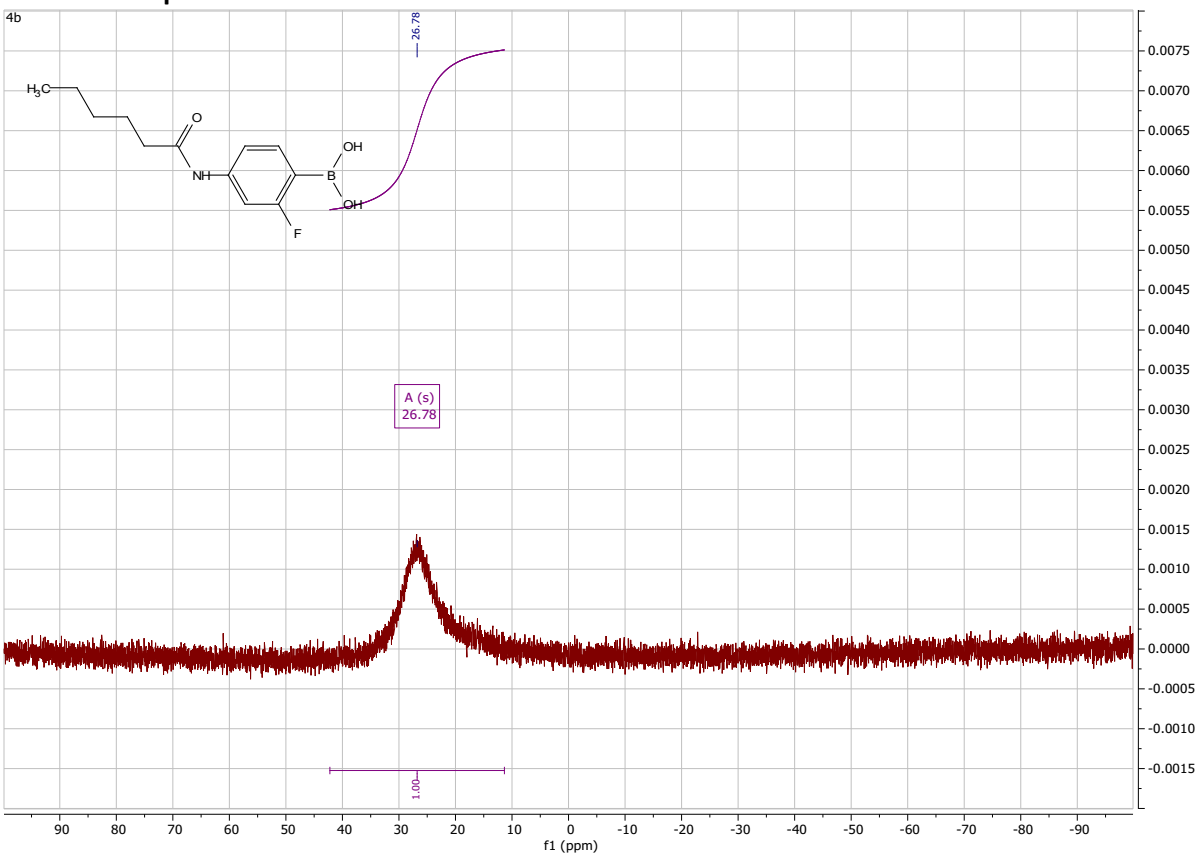
4b ^{1}H NMR spectrum



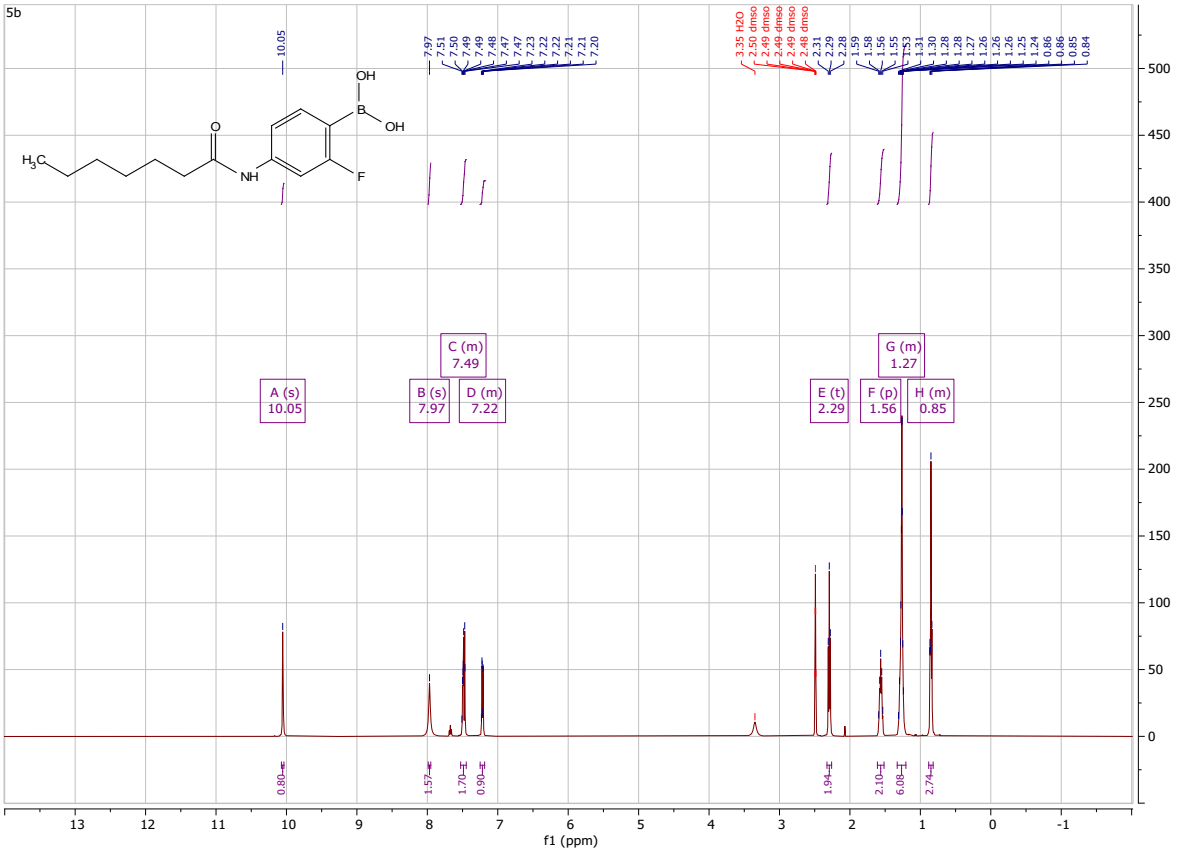
4b ^{13}C NMR spectrum



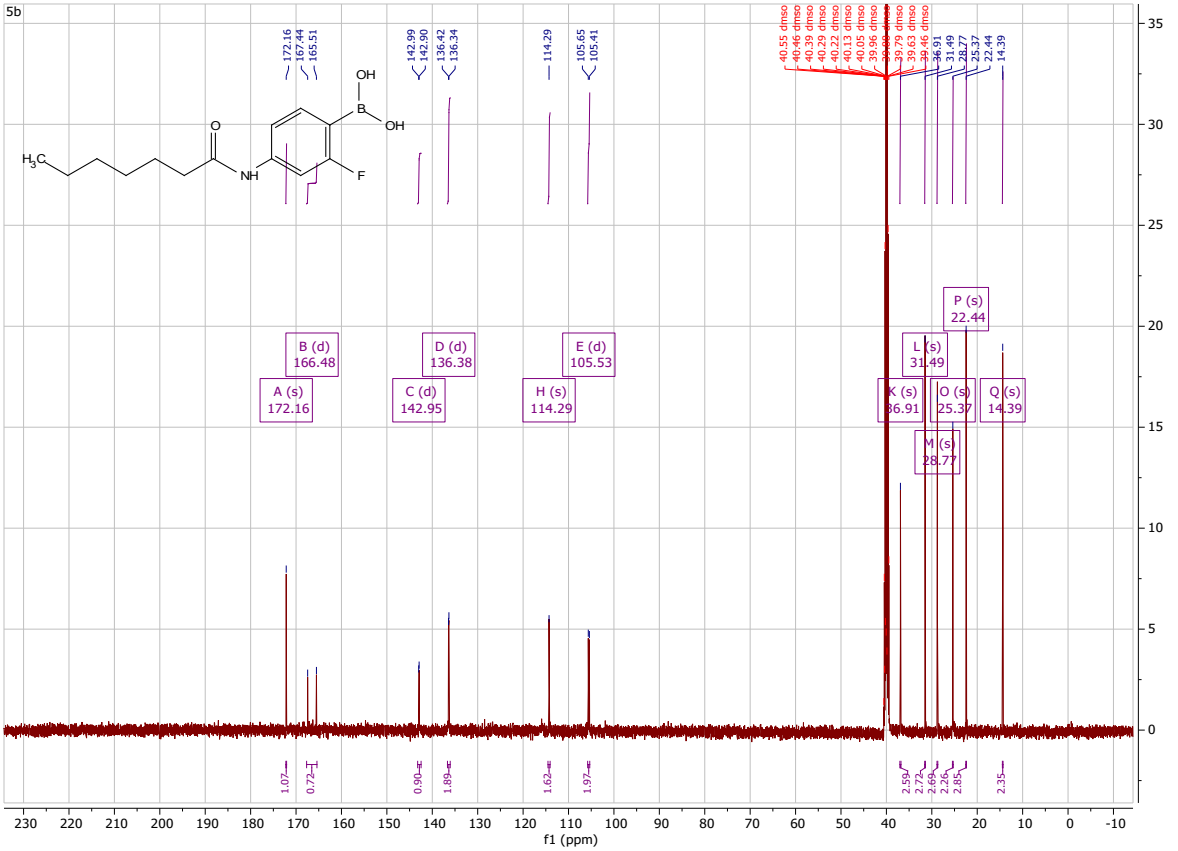
4b ^{11}B NMR spectrum



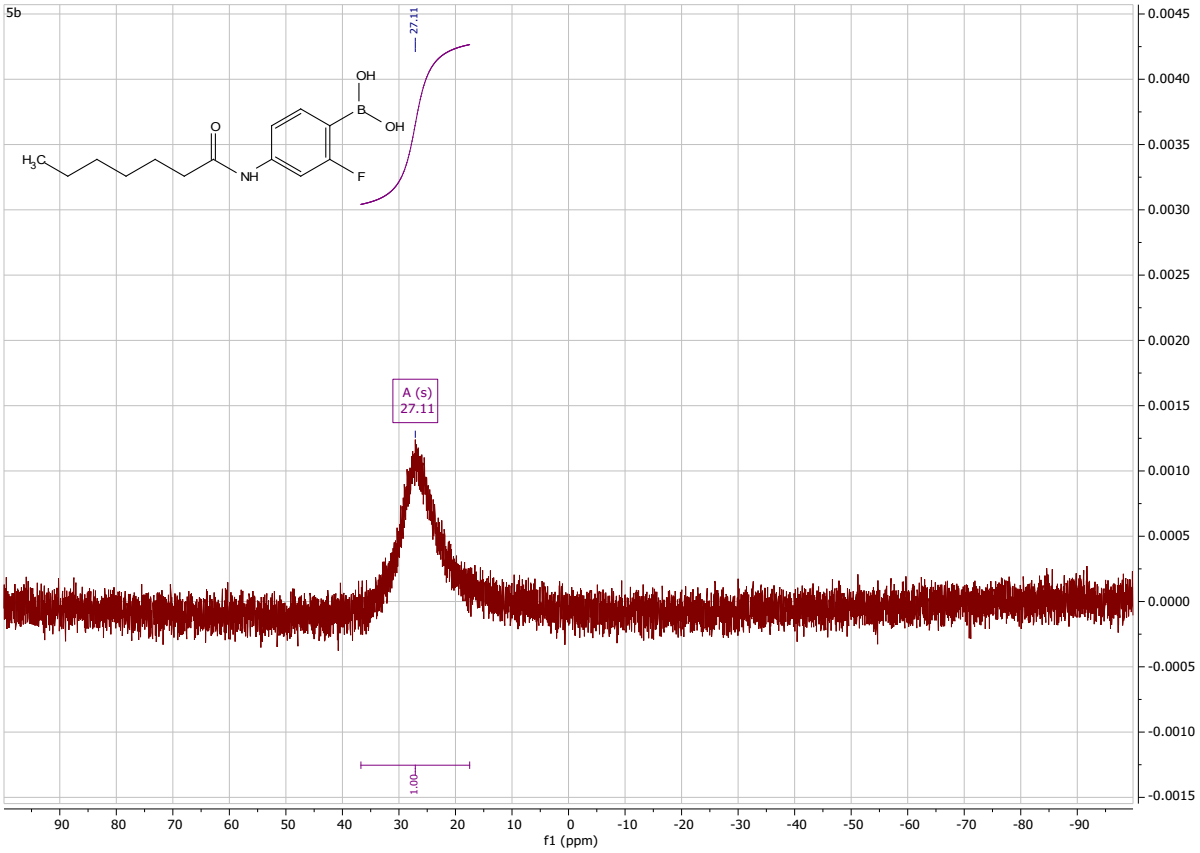
5b ^{1}H NMR spectrum



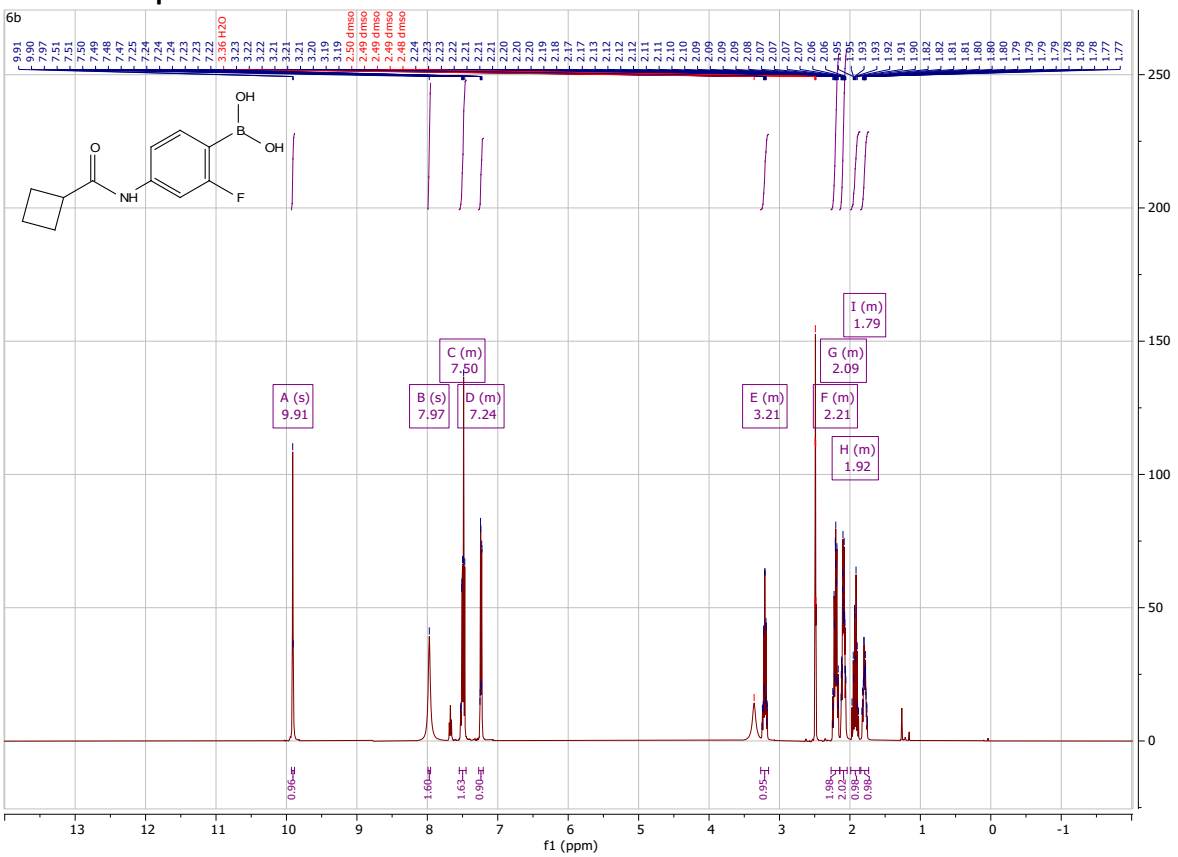
5b ^{13}C NMR spectrum



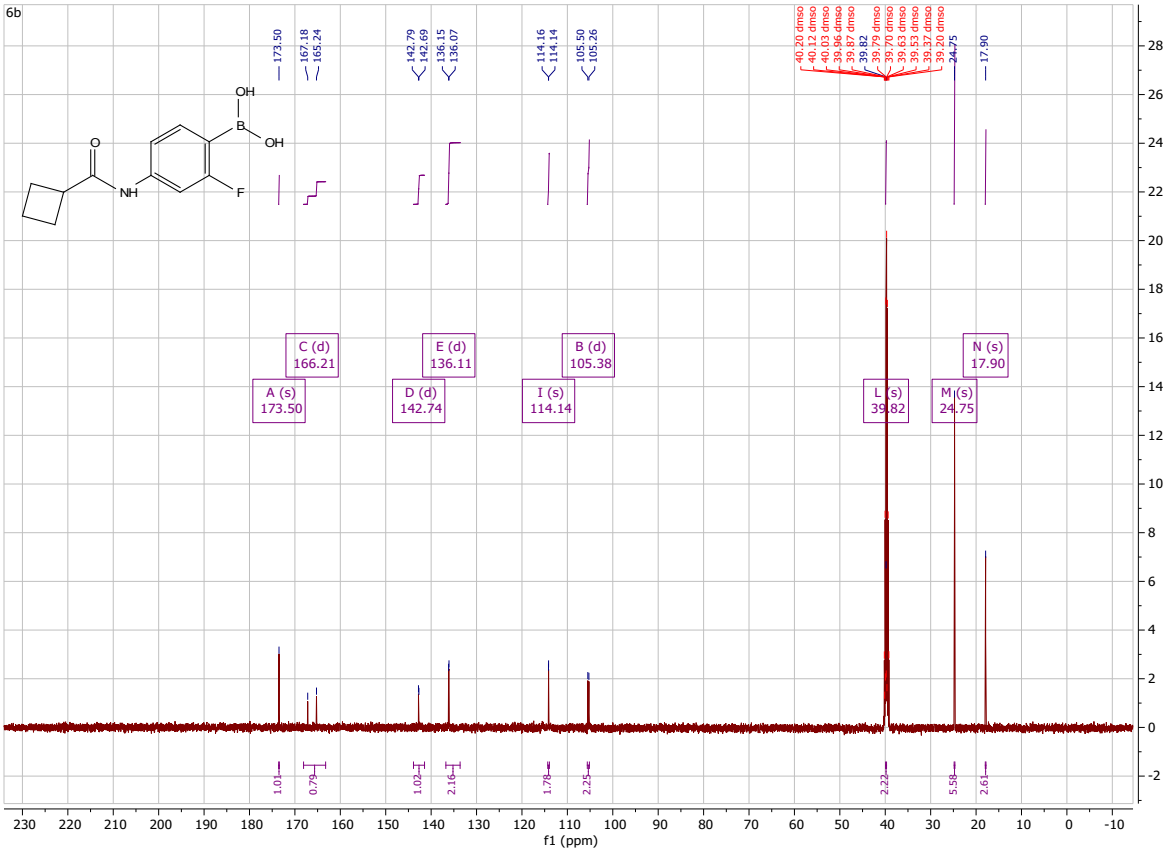
5b ^{11}B NMR spectrum



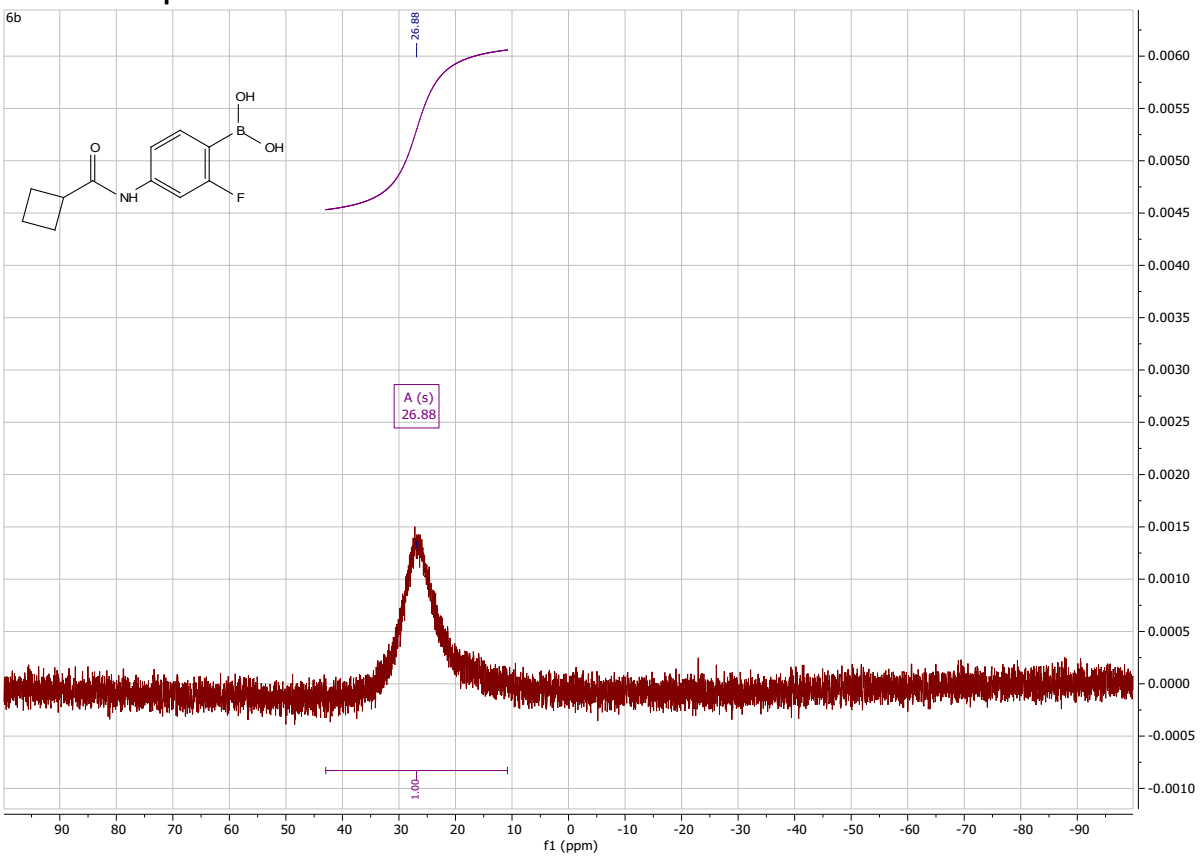
6b ^{1}H NMR spectrum



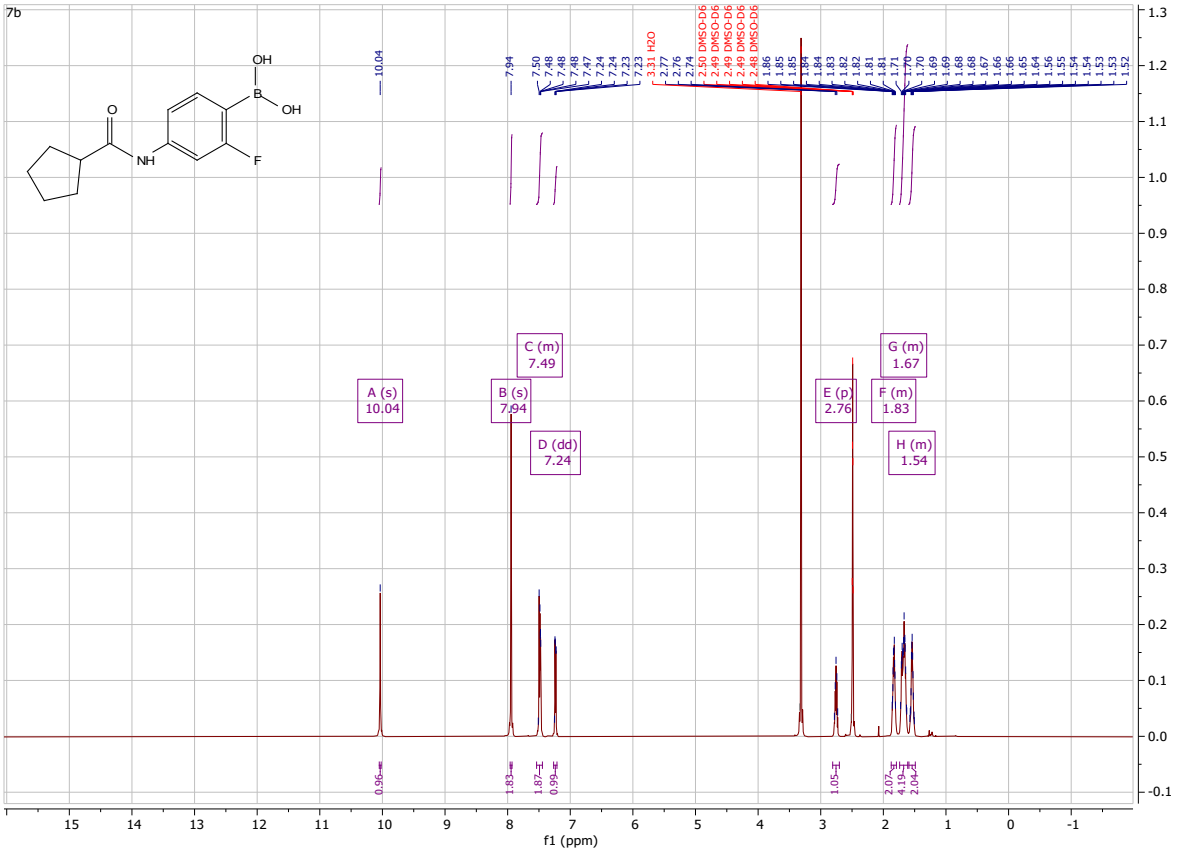
6b ^{13}C NMR spectrum



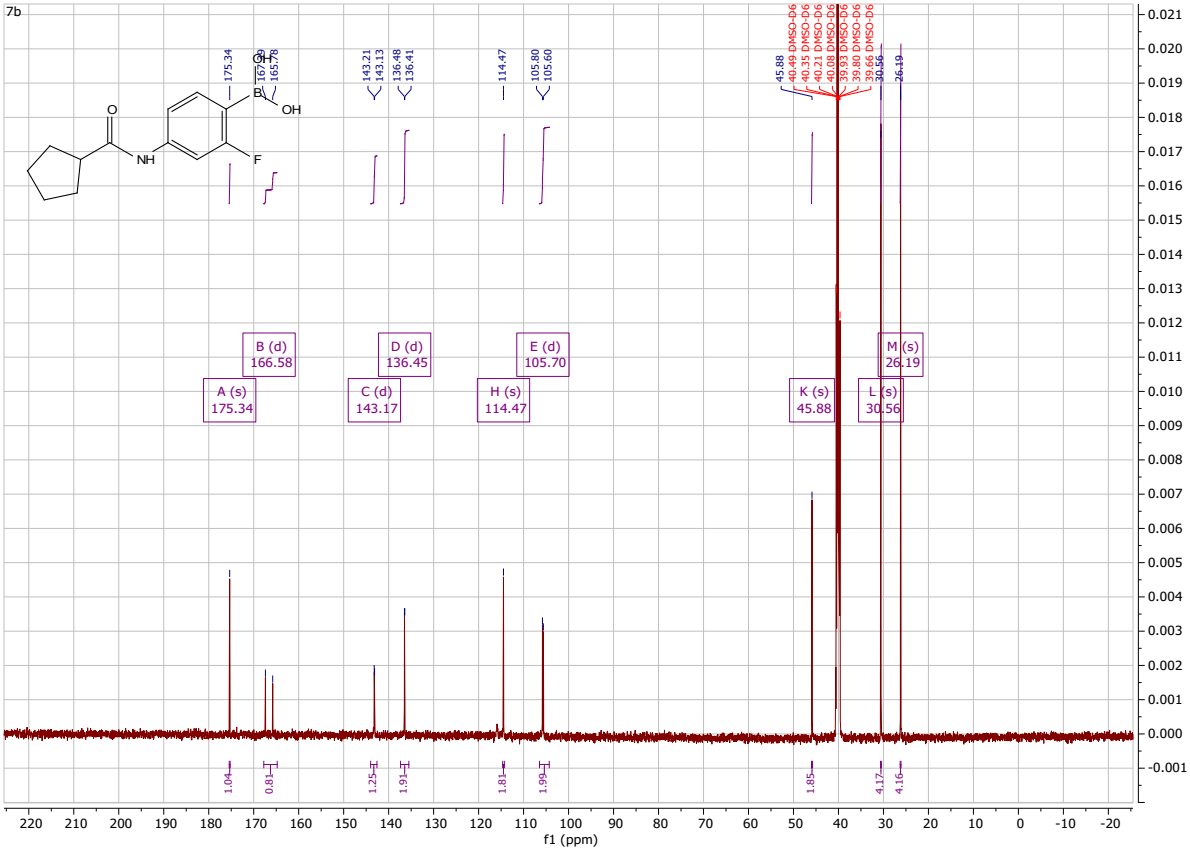
6b ^{11}B NMR spectrum



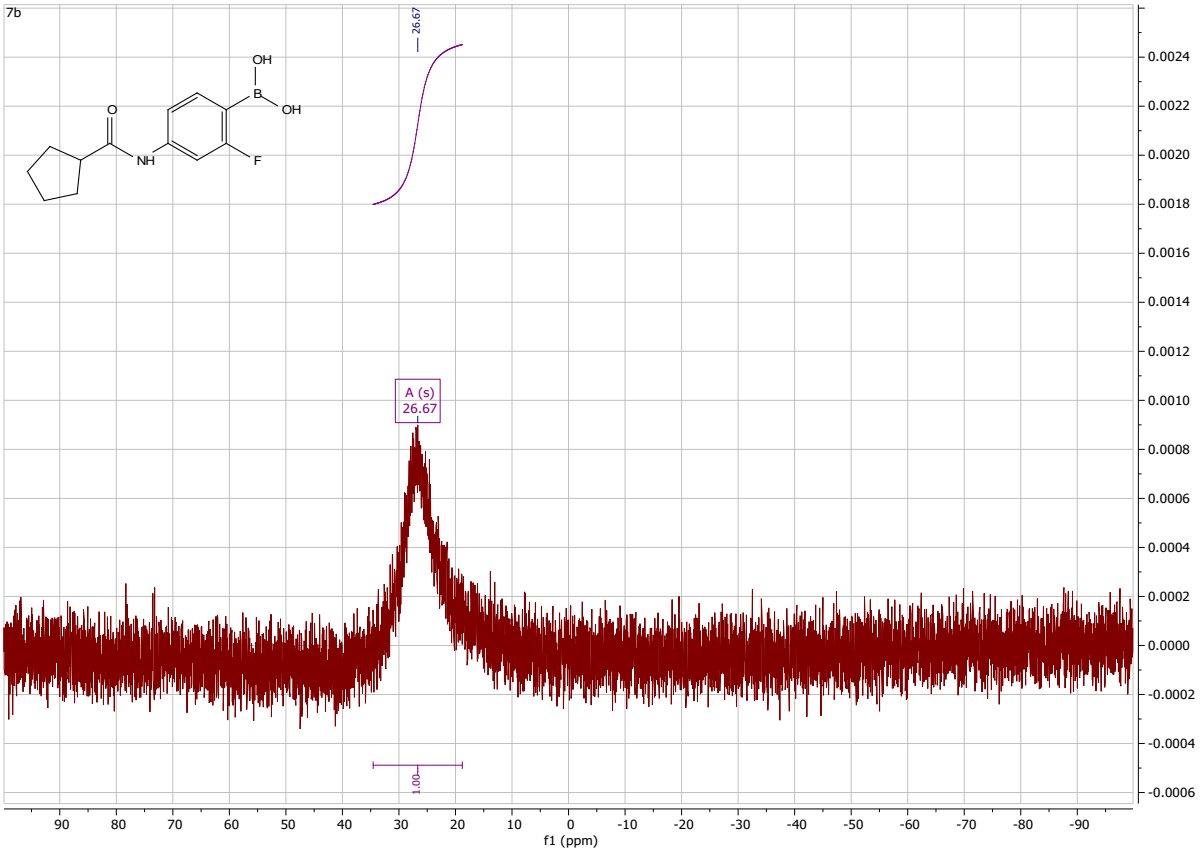
7b ^{1}H NMR spectrum



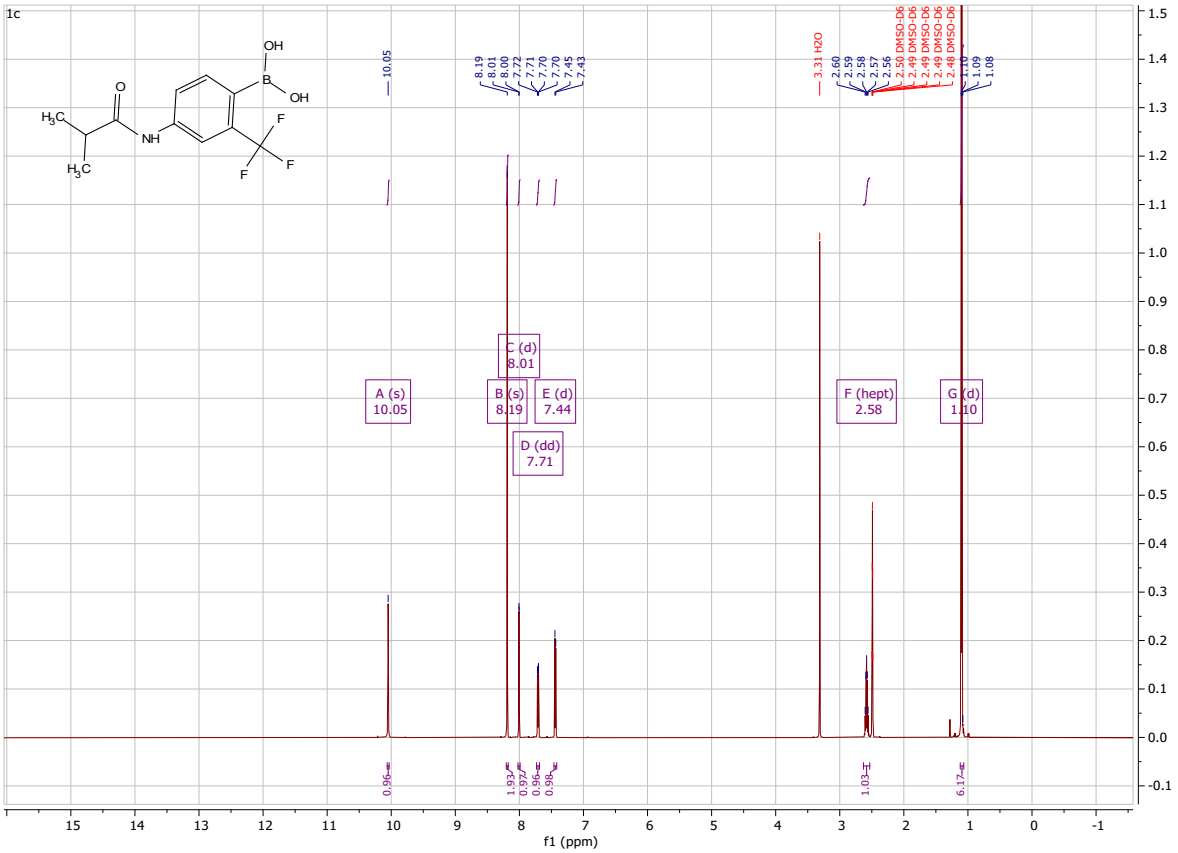
7b ^{13}C NMR spectrum



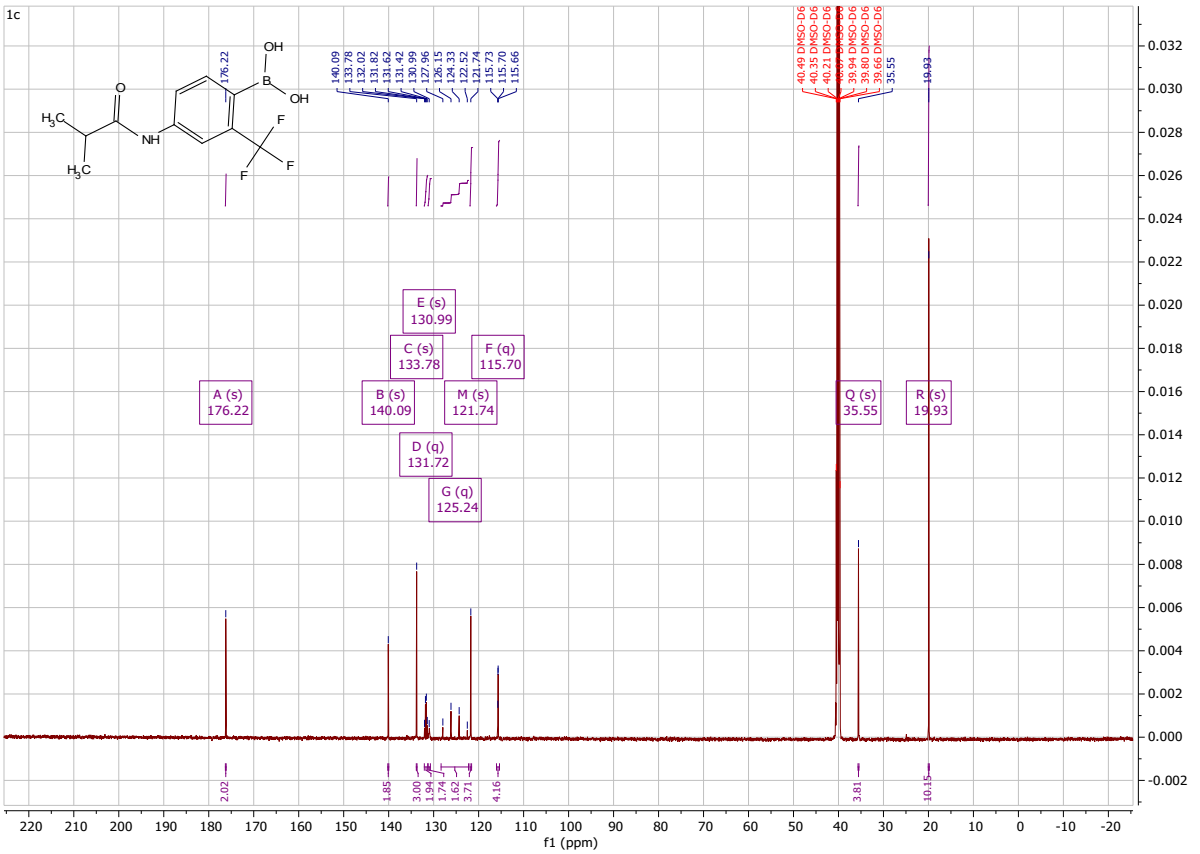
7b ^{11}B NMR spectrum



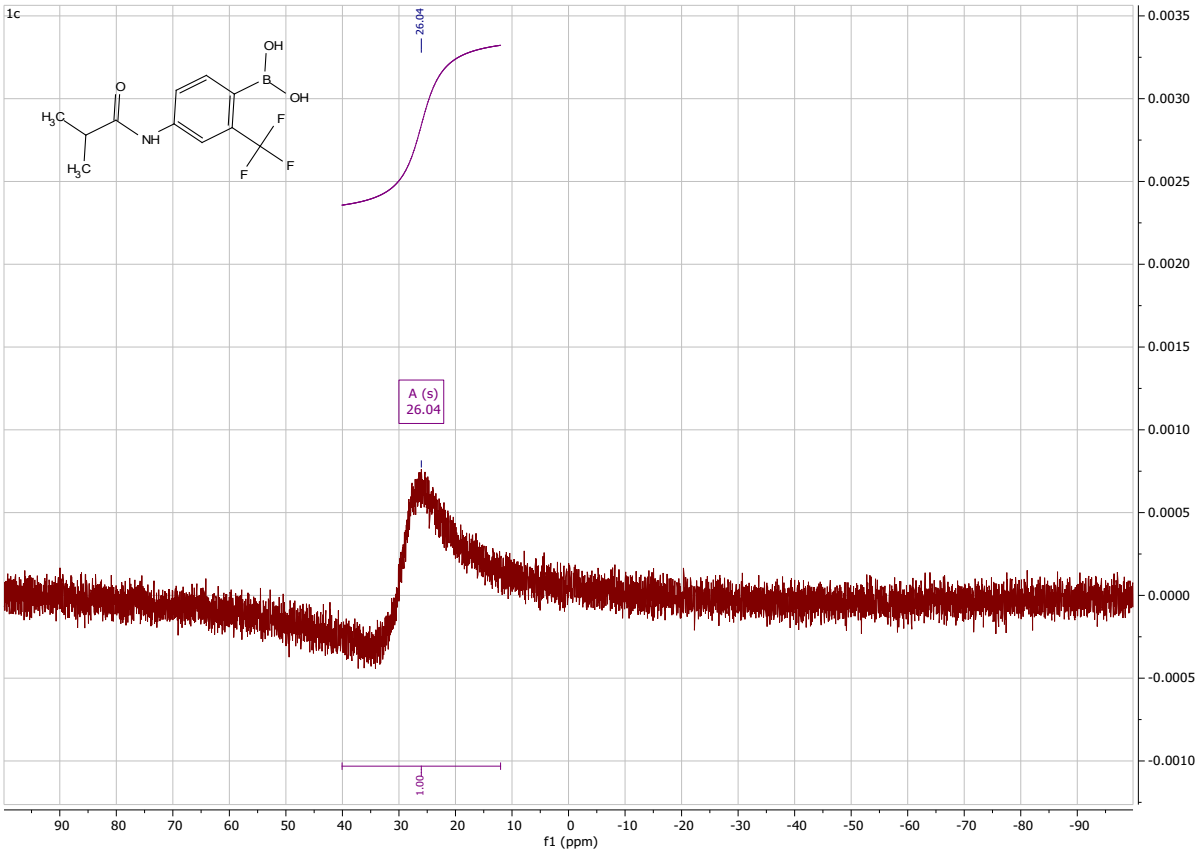
1c ^{1}H NMR spectrum



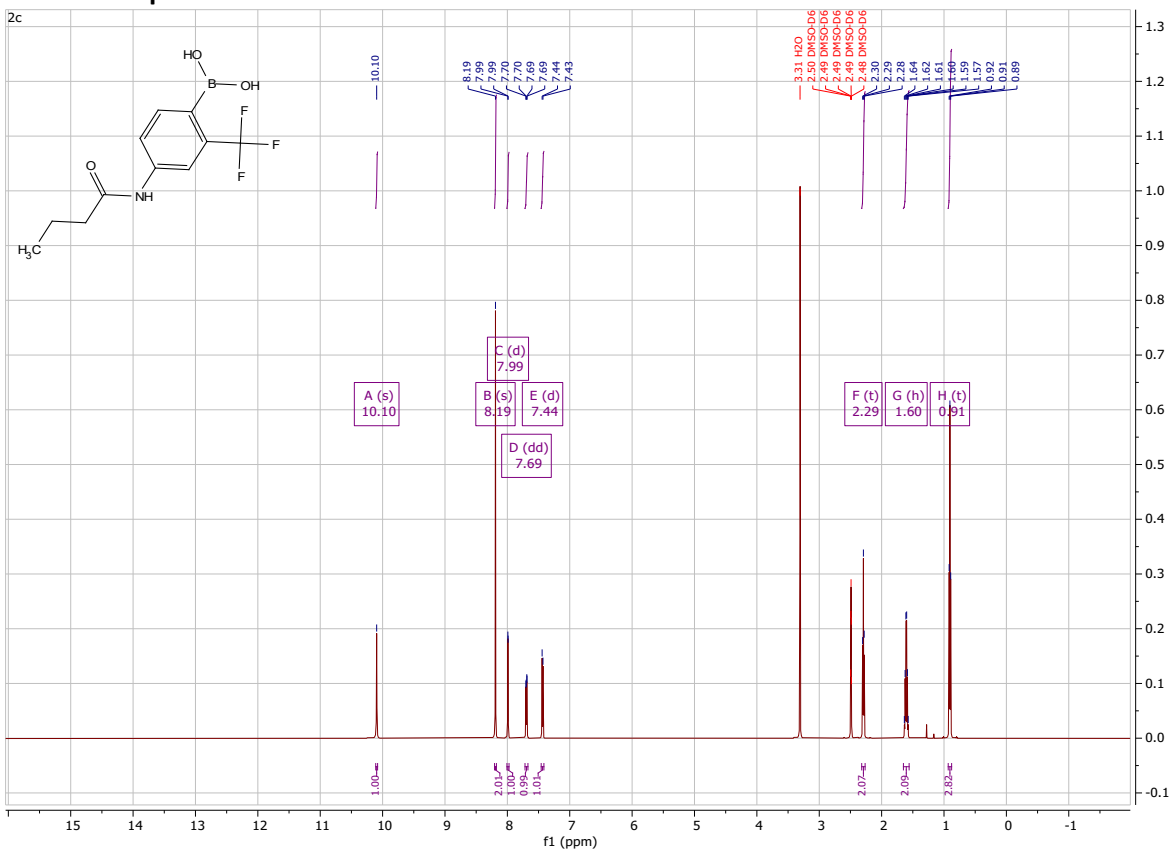
1c ^{13}C NMR spectrum



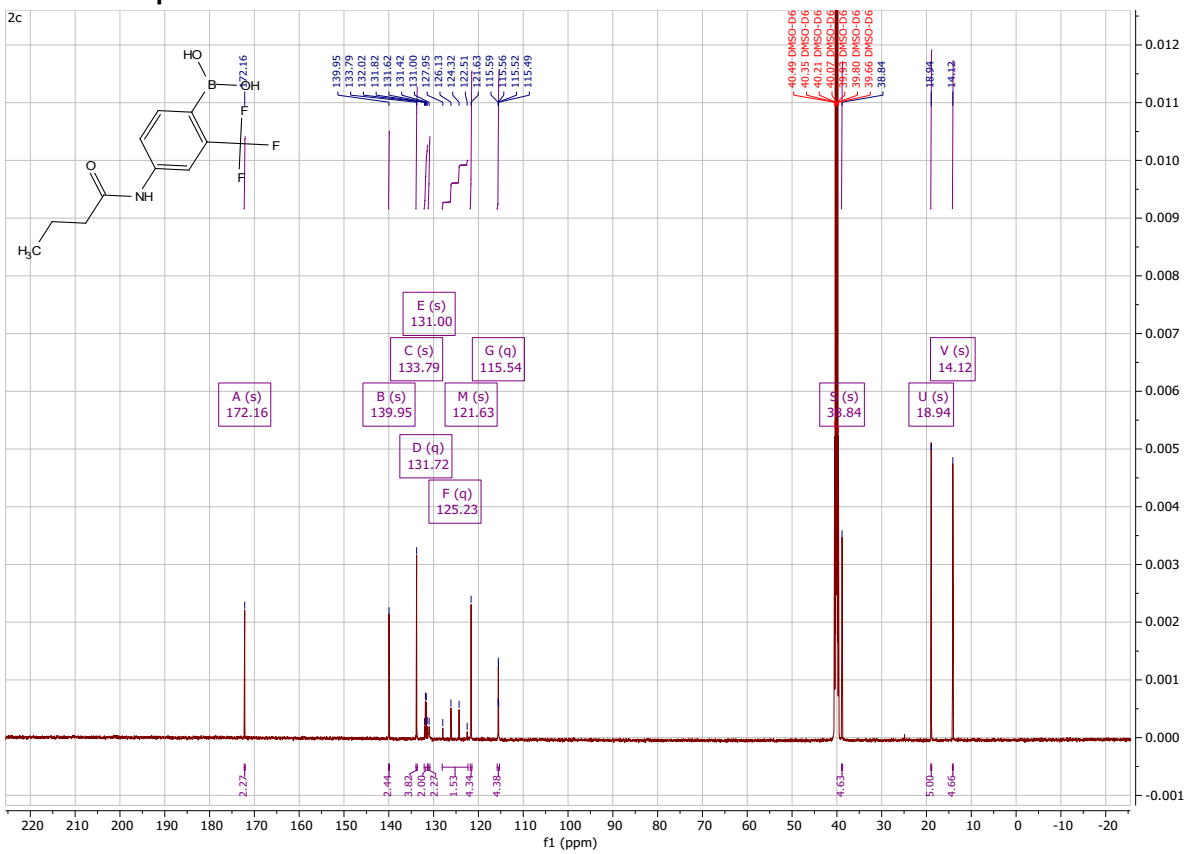
1c ^{11}B NMR spectrum



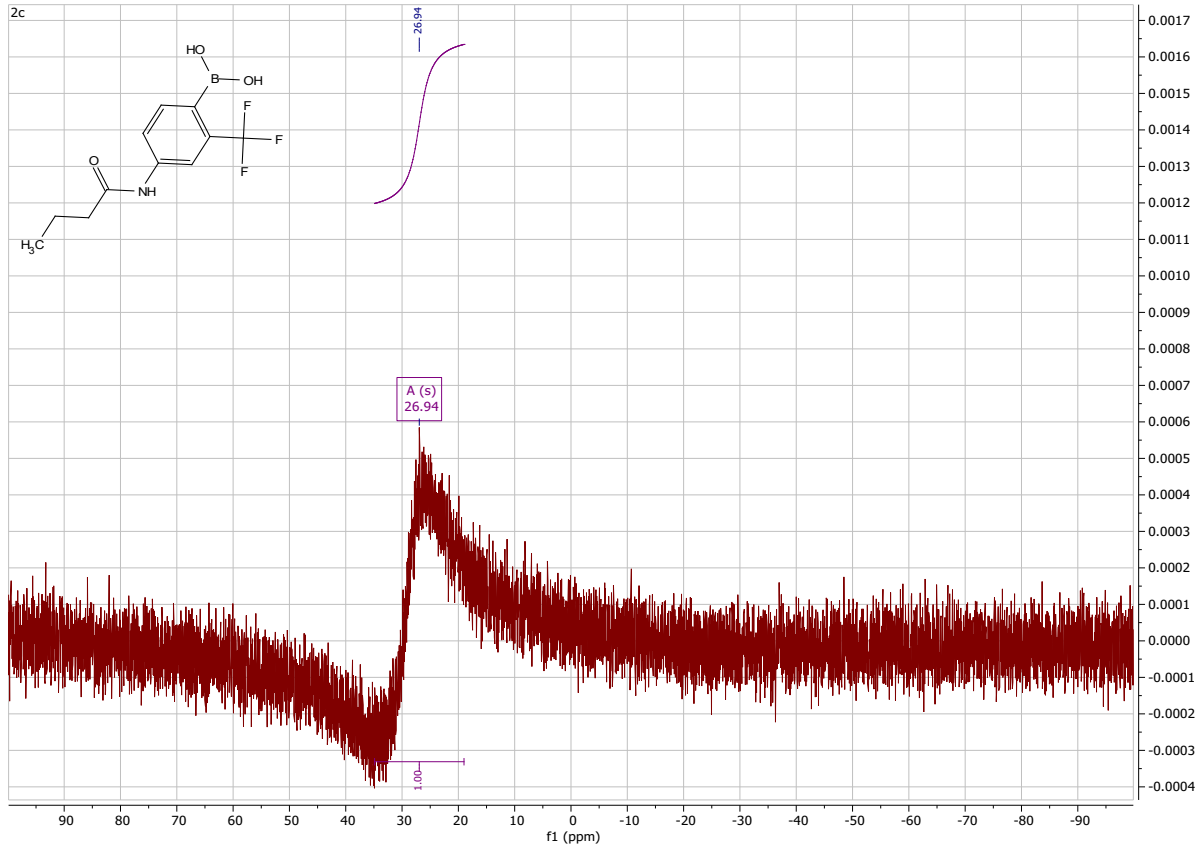
2c ^{1}H NMR spectrum



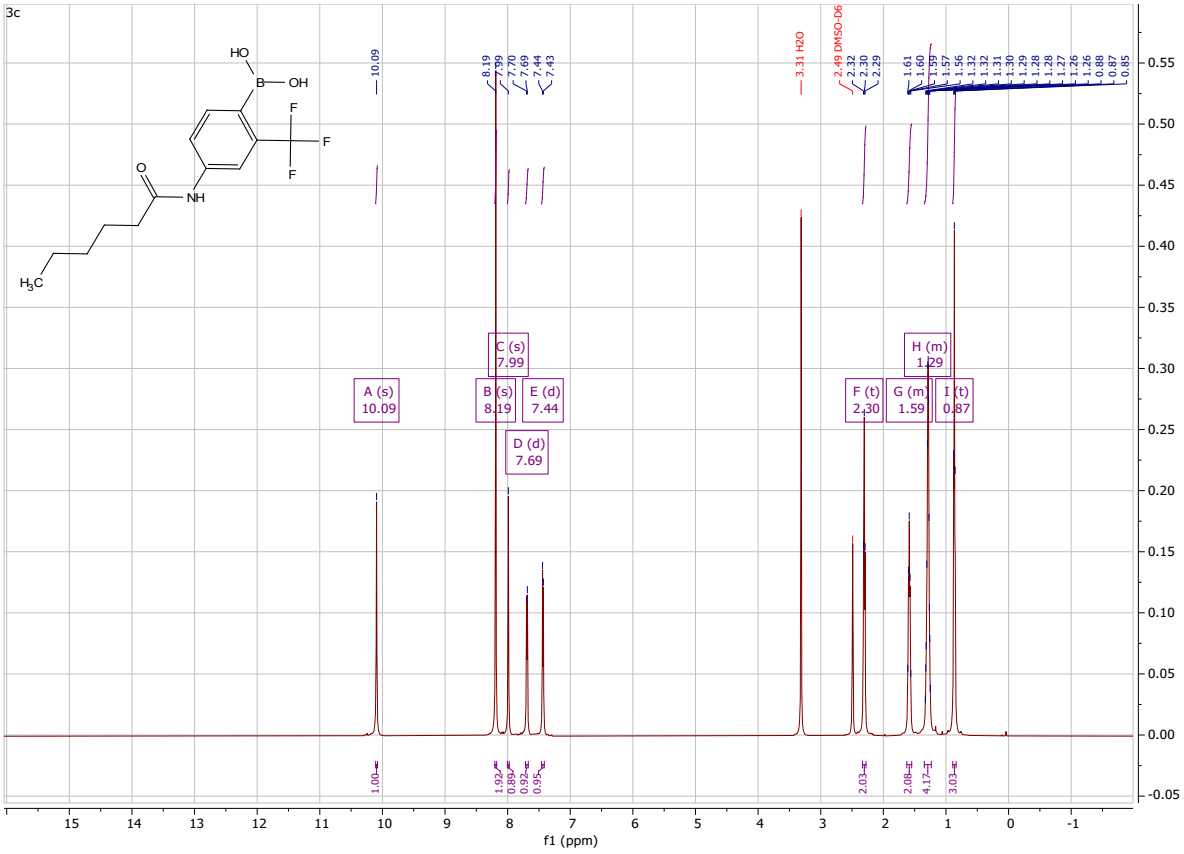
2c ^{13}C NMR spectrum



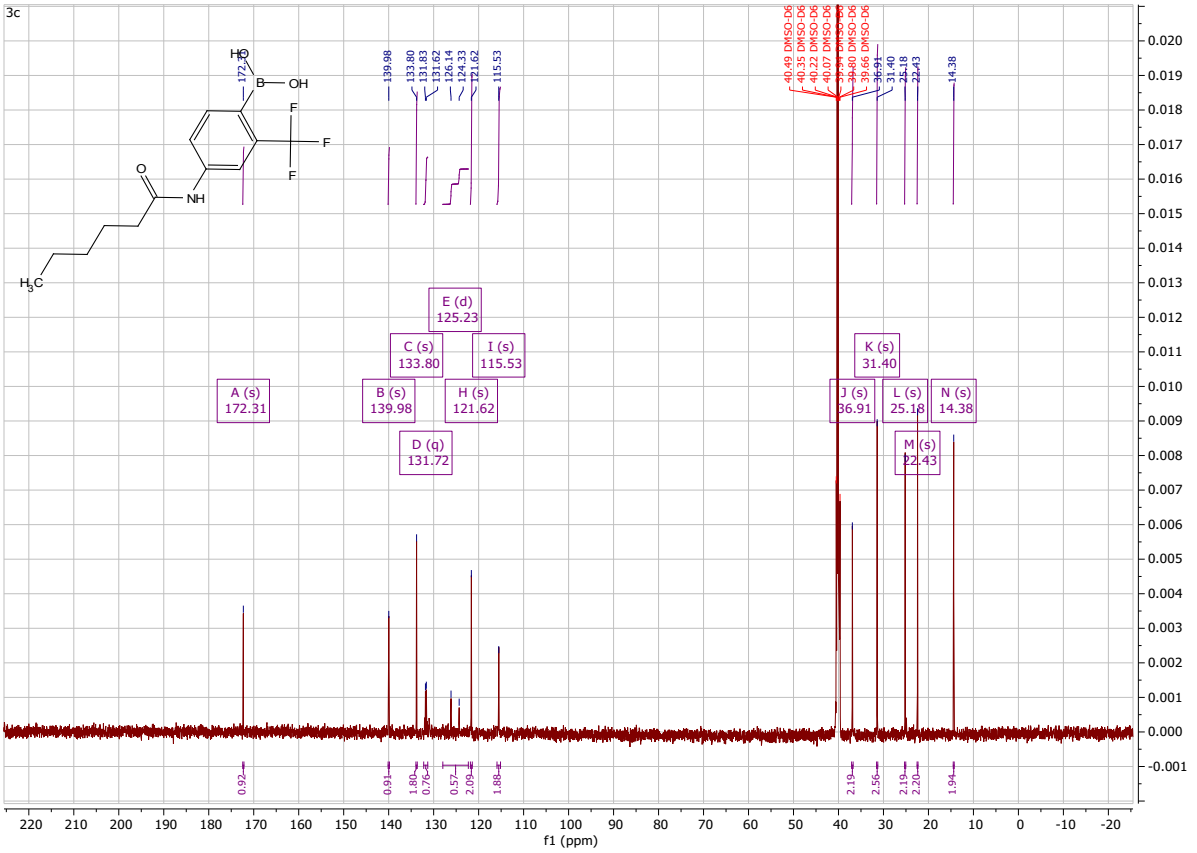
2c ^{11}B NMR spectrum



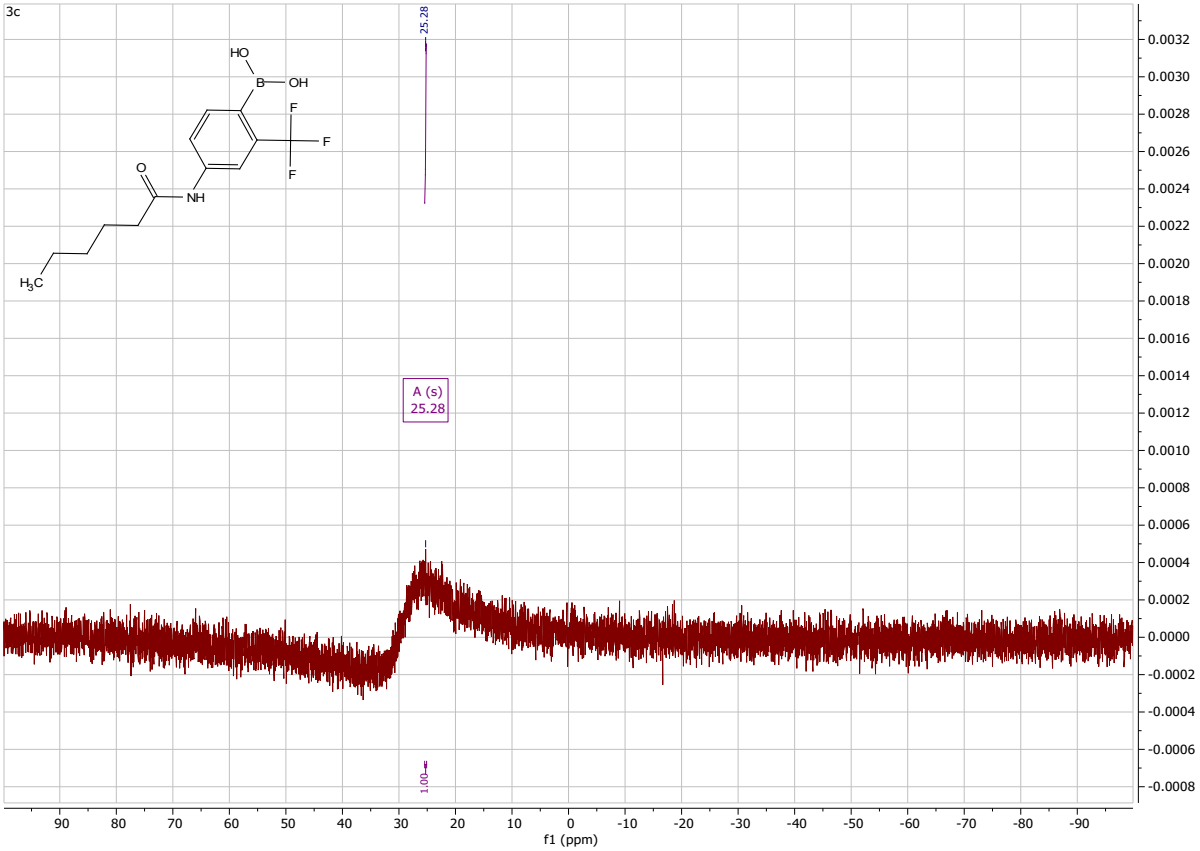
3c ^{1}H NMR spectrum



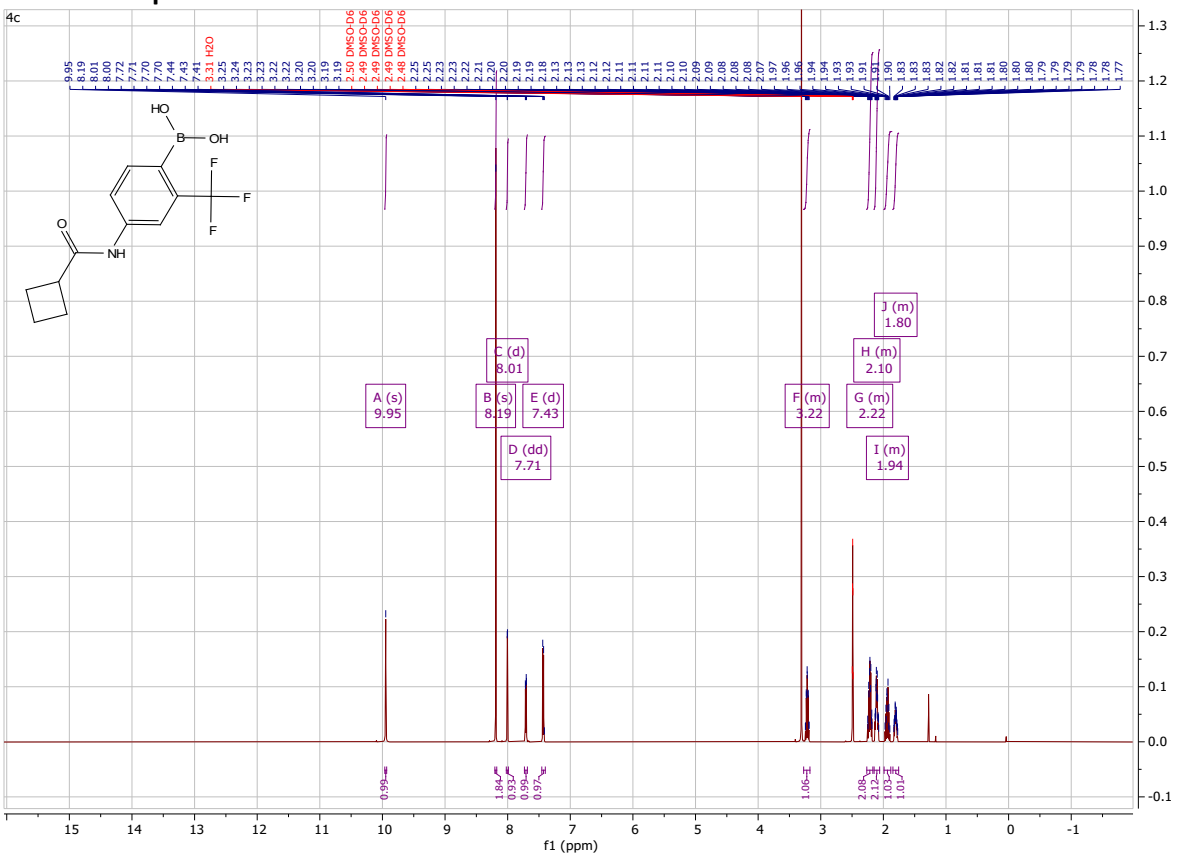
3c ^{13}C NMR spectrum



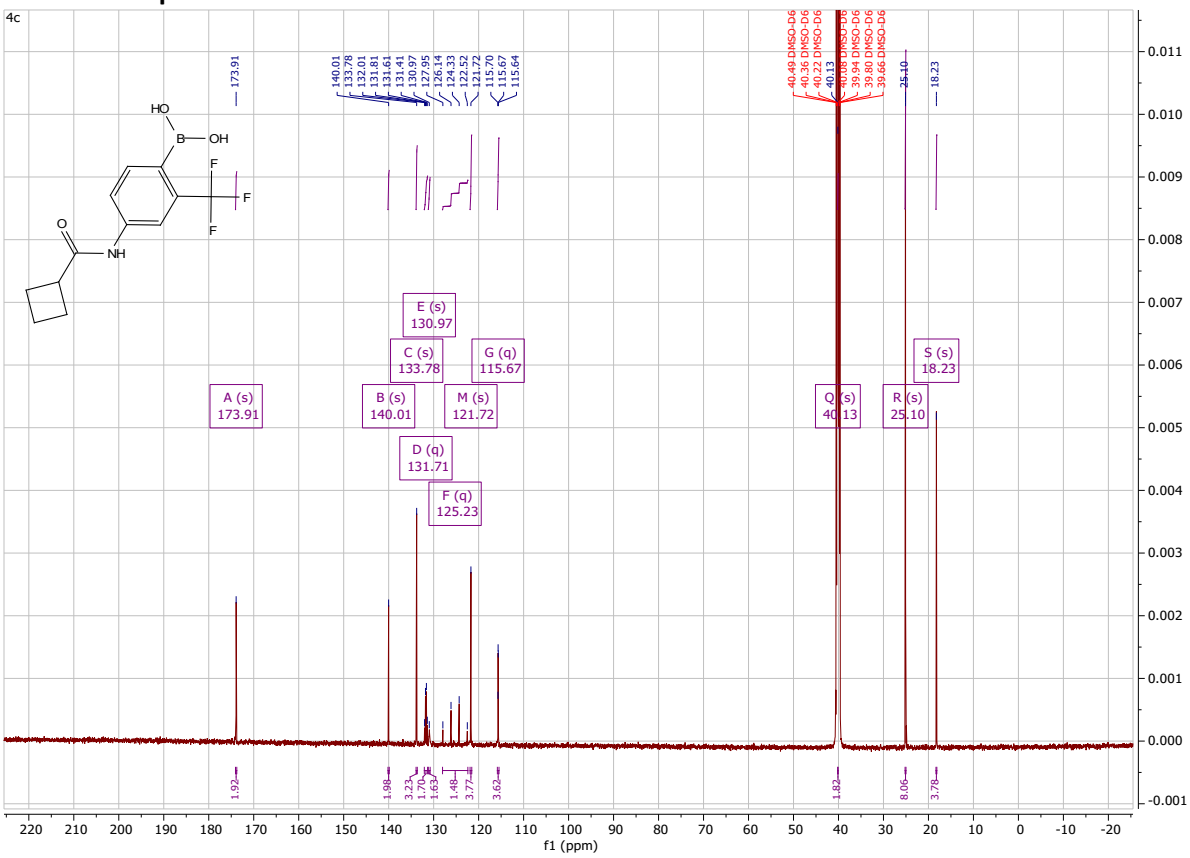
3c ^{11}B NMR spectrum



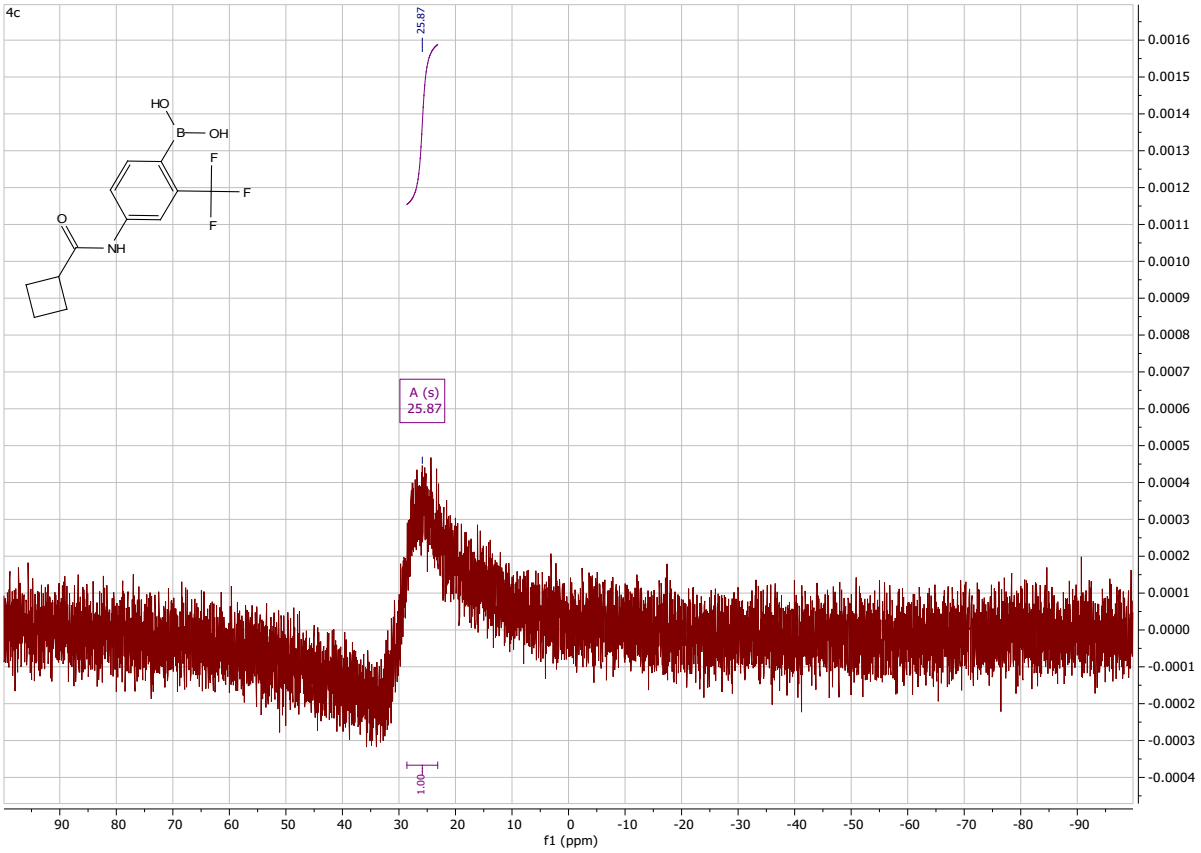
4c ^{1}H NMR spectrum



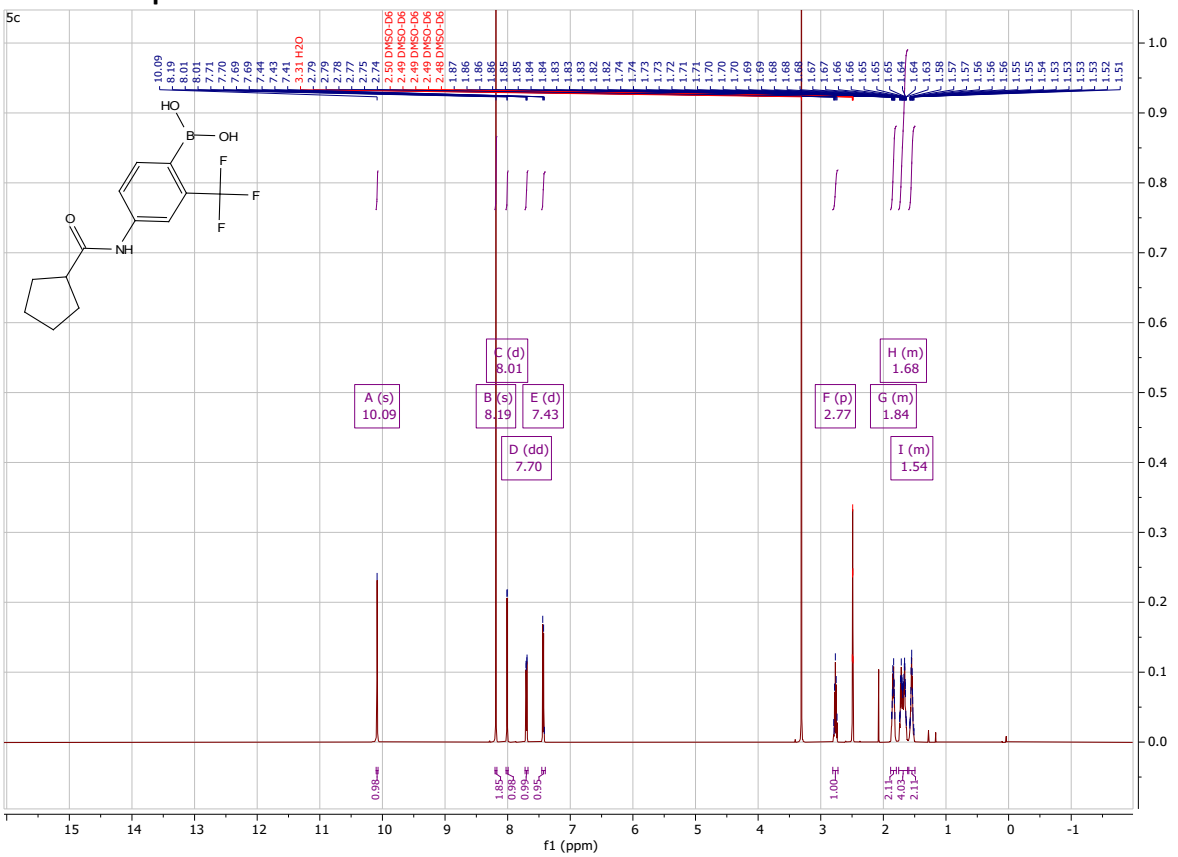
4c ^{13}C NMR spectrum



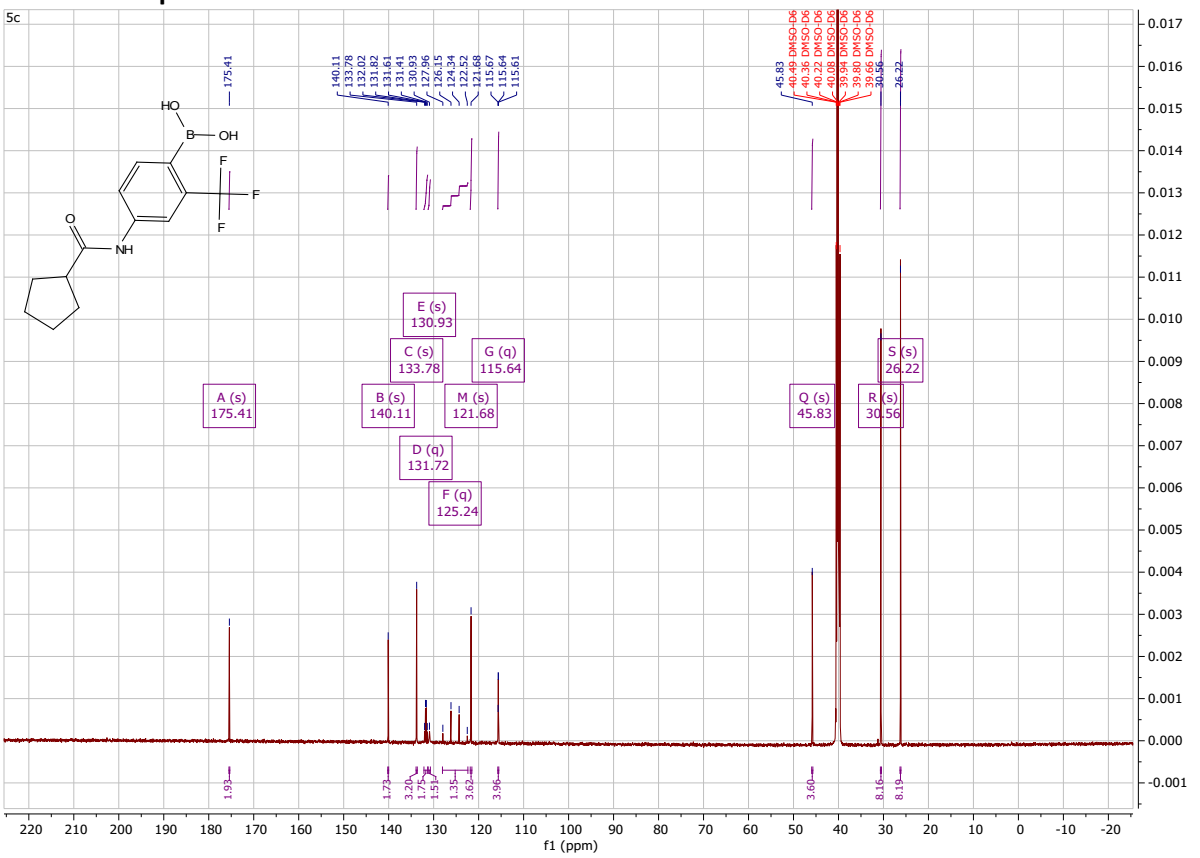
4c ^{11}B NMR spectrum



5c ^{1}H NMR spectrum



5c ^{13}C NMR spectrum



5c ^{11}B NMR spectrum