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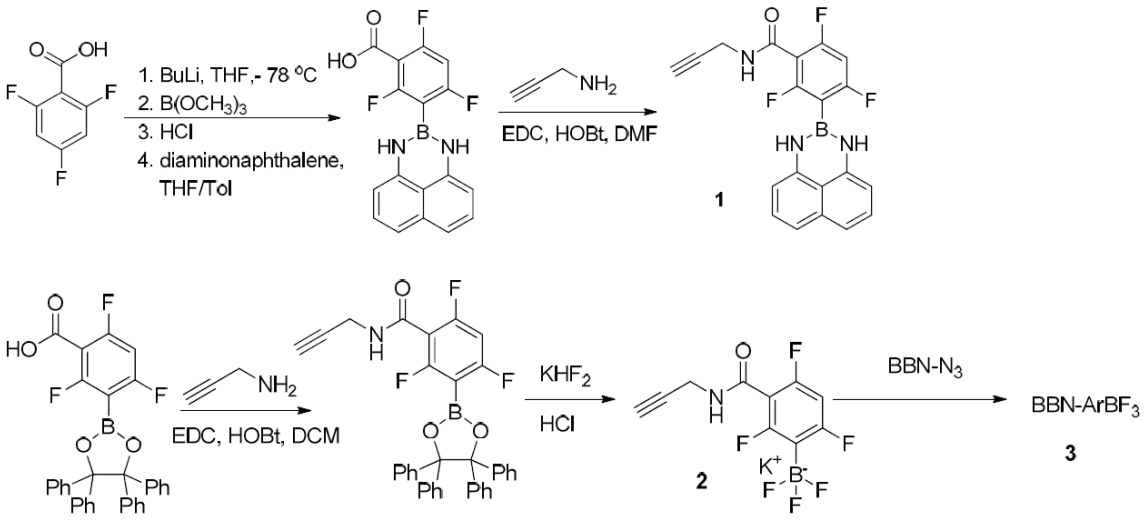
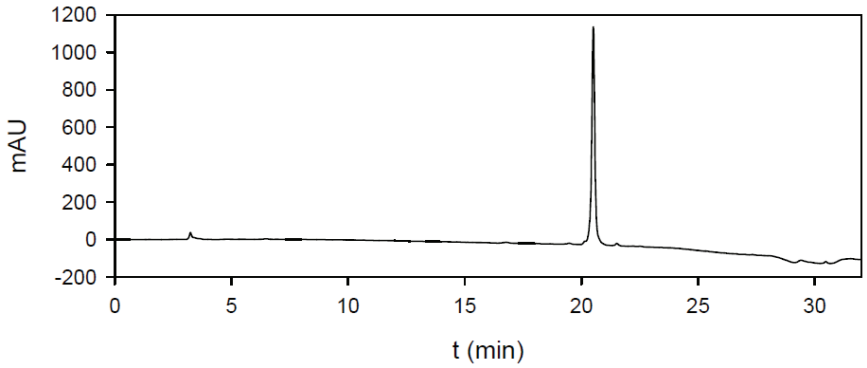
Synthetic Schemes: Below production of the arylborimidine which is used to give the aryltrifluoroborate and the tetraphenylpinacolate arylboronate which is also converted to the aryltrifluoroborate.



HPLC reinjection of the purified 3 (BBN-ArBF$_3$ after lyophilization) at 229 nm.



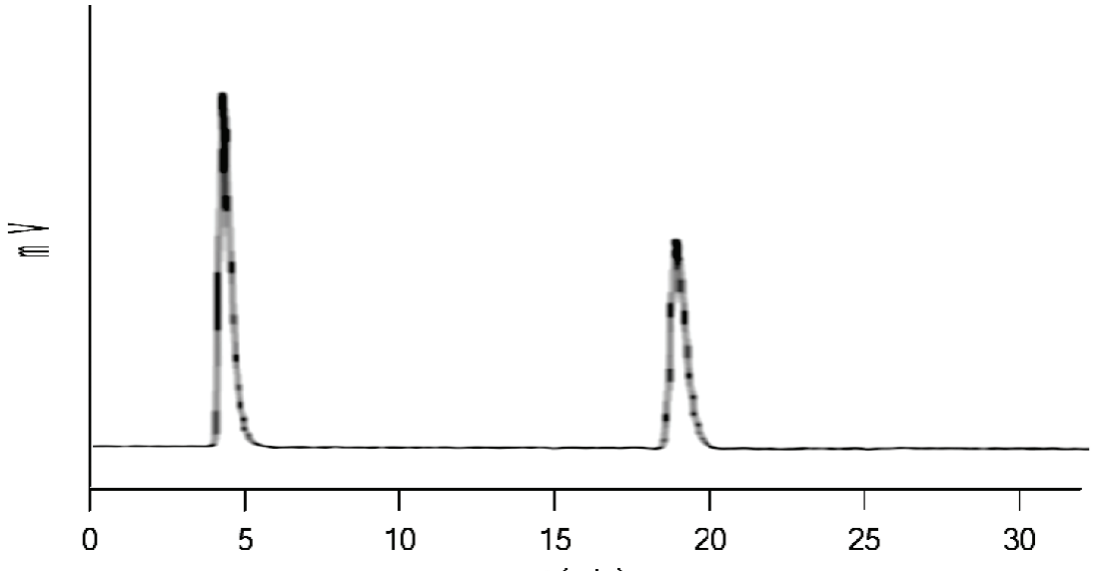
Concentration determination of BBN-ArBF3. An extinction coefficient was calculated to be: 7550 $M^{-1}cm^{-1}$at 280 nm based on values of individual functional groups. Using this value, the concentration of a solution of purified BBN-ArBF$_3$ was determined. This solution was diluted for receptor binding assays by competition with a ^{125}I-labeled variant of bombesin to measure the K_d for the GRP-receptor.

IC50 Assay for BBN-ArBF3.BBN-ArBF$_3$ was stored dry or in 35% aqueous DMSOand was diluted serially for a receptor binding assay using whole cells. The inhibition constant (K_i) of BBN-ArBF$_3$ was determined by performing competitive binding assay using ^{125}I-Tyr-BBN (PerkinElmer) as the radioligand. Briefly, PC-3 human prostate adenocarcinoma cells were cultured in Ham's F-12 and 10% fetal bovine serum and seeded in 6-well plates (1 x 10^5 cells/well). For the binding assay the medium was replaced with RPMI 1640 containing 4.8 mg/mL HEPES, 2 mg/mL BSA and 0.1μM penicillin/streptavidin. The cells were incubated with increasing concentration of BBN-ArBF$_3$peptide ranging from 10 pM to 0.1 μM, in the presence of a constant concentration of 4.2 pmol/L of radioligand in triplicates for 45 min at 37˚C. The cells were rinsed with ice-cold PBS three times and then detached by trypsin and counted in a gamma counter (Cobra-II Auto Gamma, Canberra Packard Canada) to determine the amount of bound radioactivity. Results are shown as counts per minute (CPM) of radioactivity bound to cells vs. log of molar concentration of BBN-ArBF3. Data are presented as mean ± SEM of experiment with each point being performed in triplicate.

The data were analyzed using the GraphPad Prism software.The K_i was calculated to be 3.06 nM.

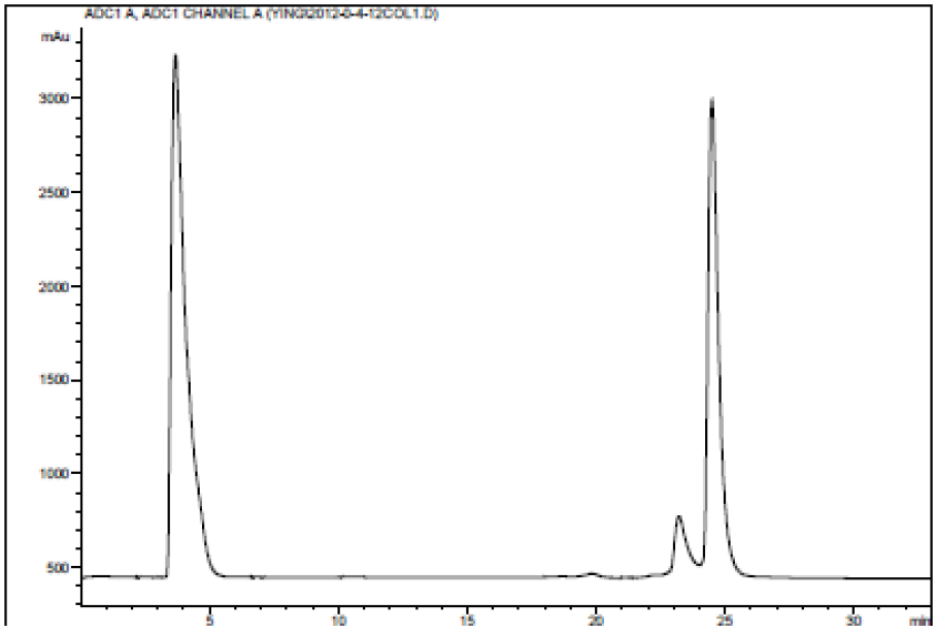
Radiosynthesis of the alkynyl-^{18}F-ArBF$_3$ and click labeling of N_3-BBN

Following labeling, the reaction was quenched and loaded directly onto the HPLC column. The crude HPLC radiotrace is shown below.

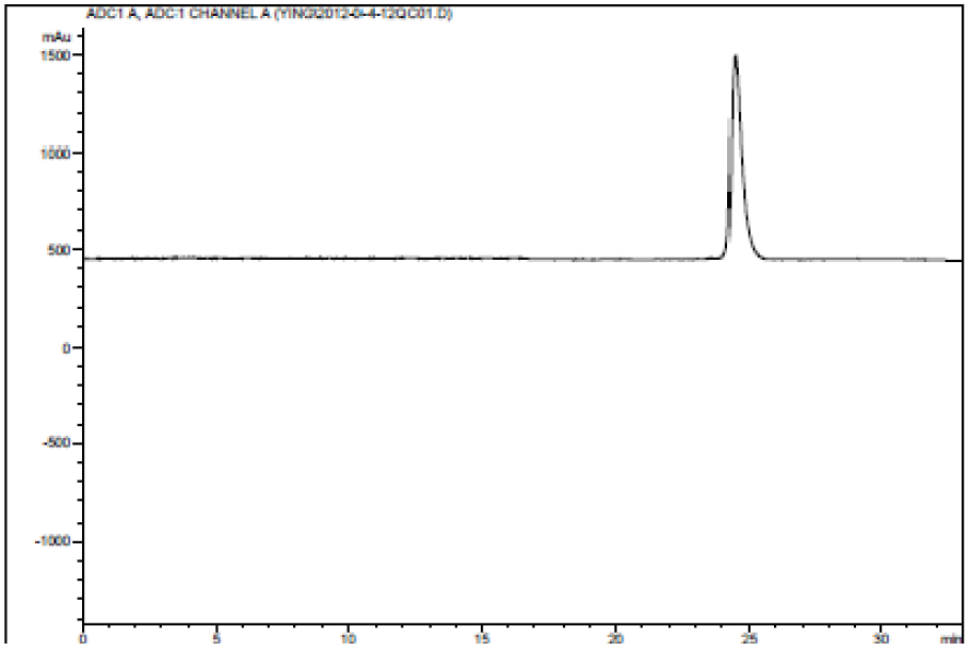


Crude HPLC Radiotrace of the labeled **2**, which eluted at 19 minutes.

Radiolabeling for biodistribution study: The desalted product (2.17 mCi at t= 118 min) was diluted with saline buffer (2 mL) and expedited for biodistribution studies (specific activity calculated to be ~ 0.077 Ci/mmol)

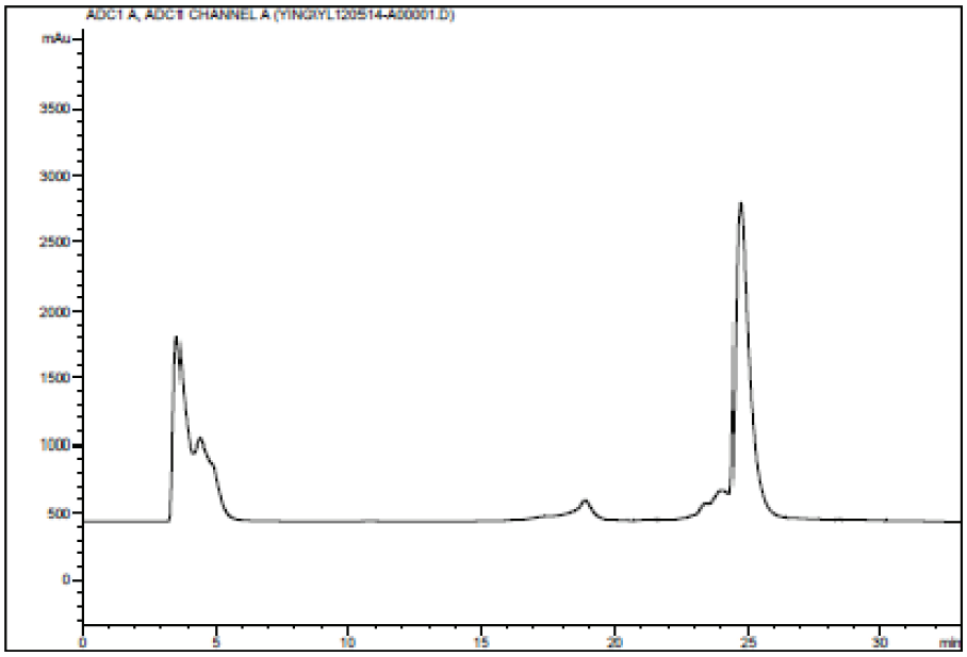


Crude radiotrace of one-pot-two-step radiolabeling: desired conjugate **3** eluted at 25 minutes. A small peak which was less prominent in subsequent labeling reactions was not collected or identified.

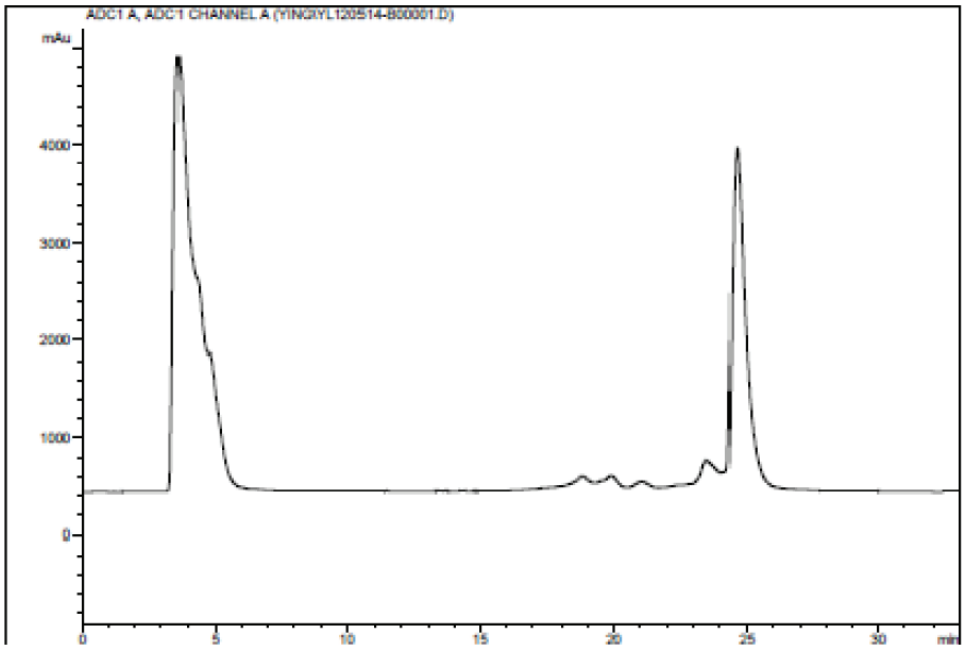


Reinjection to verify the radiochemical purity.

Radiolabeling for animal imaging



Crude radiotrace of the labeling reaction for animal imaging



Crude radiotrace of the reaction used for plasma stability assays.

Plasma stability test

BBN-^{18}F-ArBF$_3$ (4.27 mCi at t= 150 min post EOB) in EtOH (100 mL) was diluted in saline buffer (2 mL). For each assay, the saline solution (200 mL) was mixed with plasma (200 mL), incubated at 30 ^{o}C for 0, 15, 30, 60 and 120, and quenched by the addition of 75% aqueous CH_3CN (400 mL). The resulting mixture was then vortexed and centrifuged at 13k rpm for 20 min. The supernatant was isolated, filtered, and analyzed by HPLC for further analysis shown below the percent converted to other products was plotted on the graph below and is similar to serum stabilities seen for bombesin.

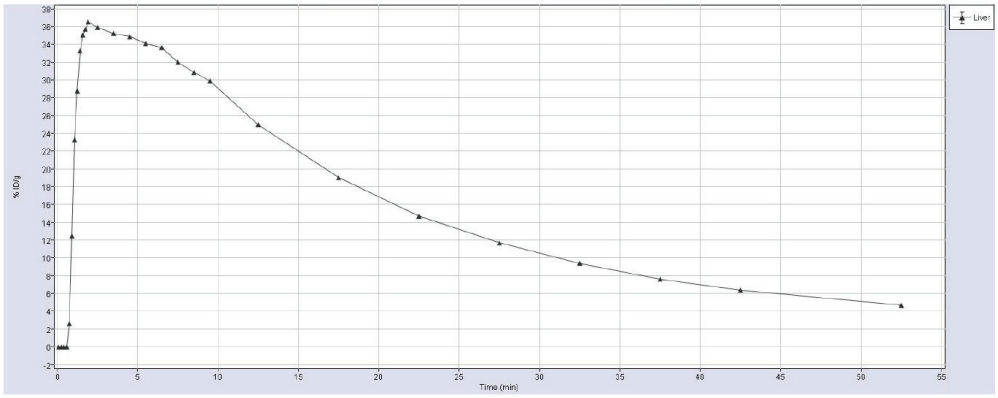
Imaging data from healthy mice (5, 30 and 60 min dynamic scans)

Dynamic scan of mice 1&2 from 0-5 min.

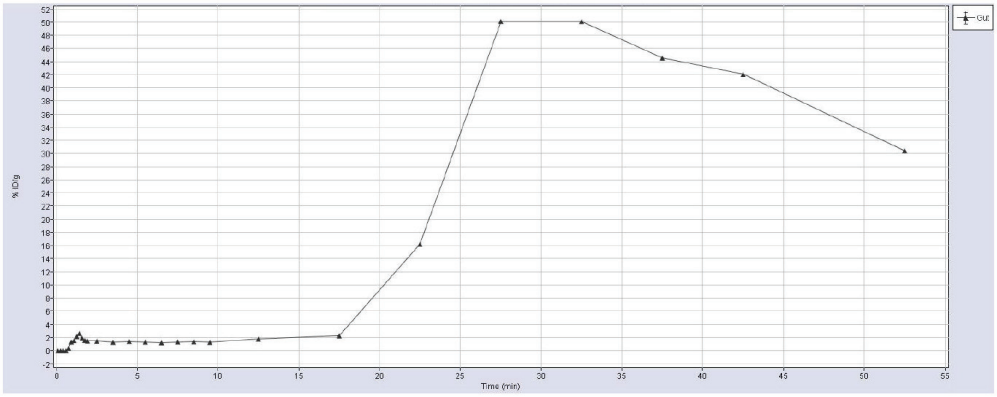
Dynamic scan of mice 1&2 from 6-30 min.

Dynamic scan of mice 1&2 from 31-60 min.

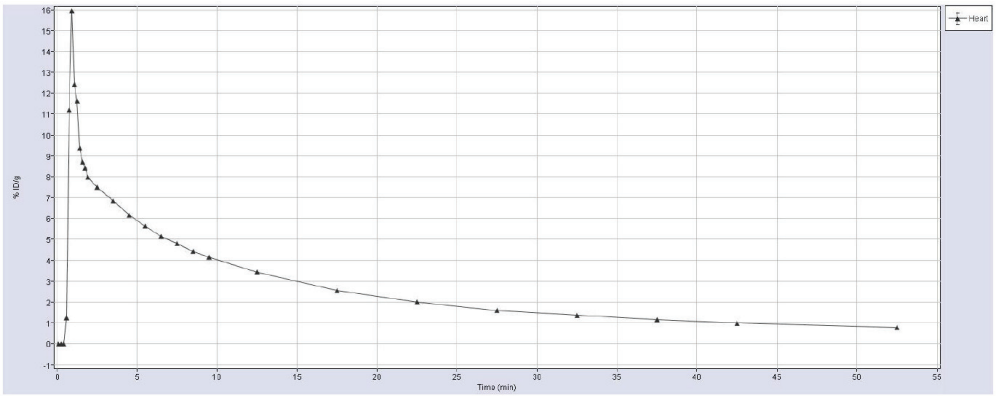
Time activity curves for various organs (Liver, Intestine, Heart, Lung, Bone, Kidney, Muscle, Brain, Bladder) :



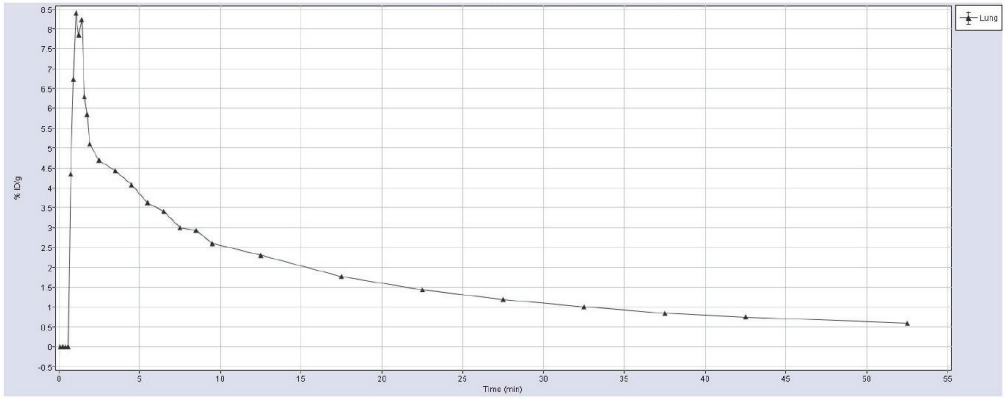
Liver



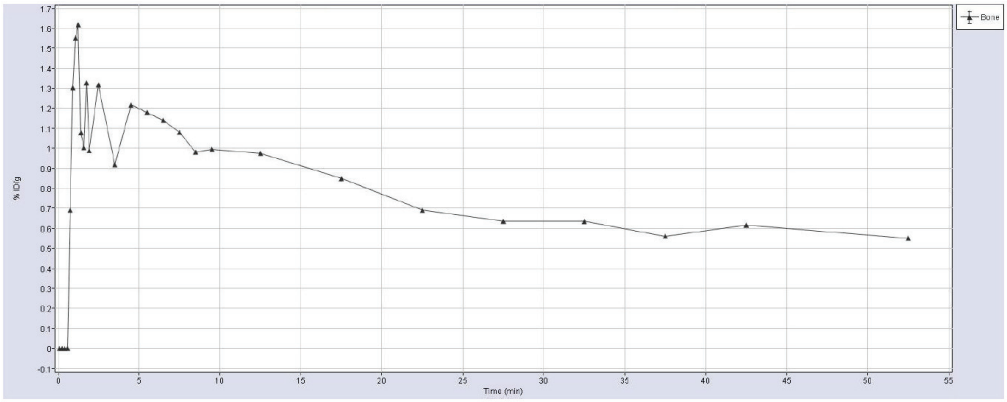
Gut



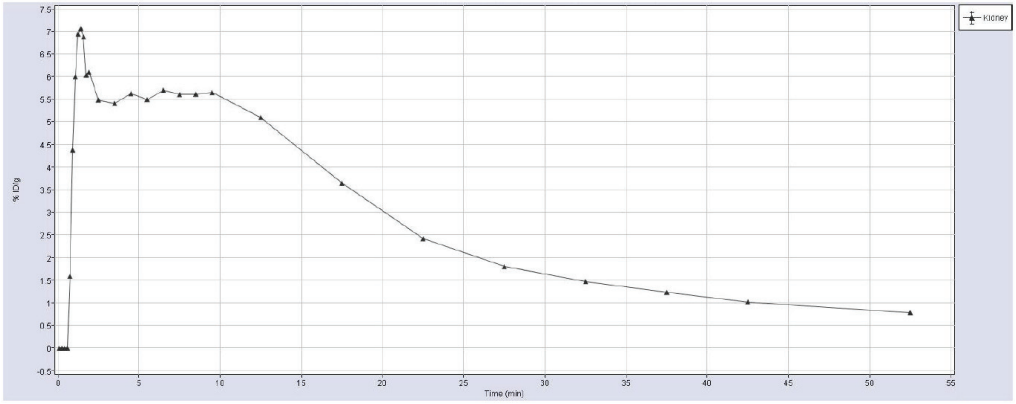
Heart



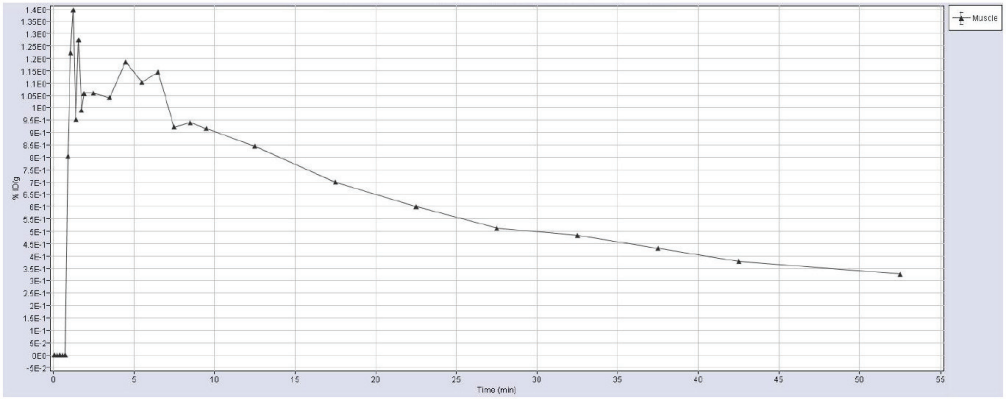
Lung



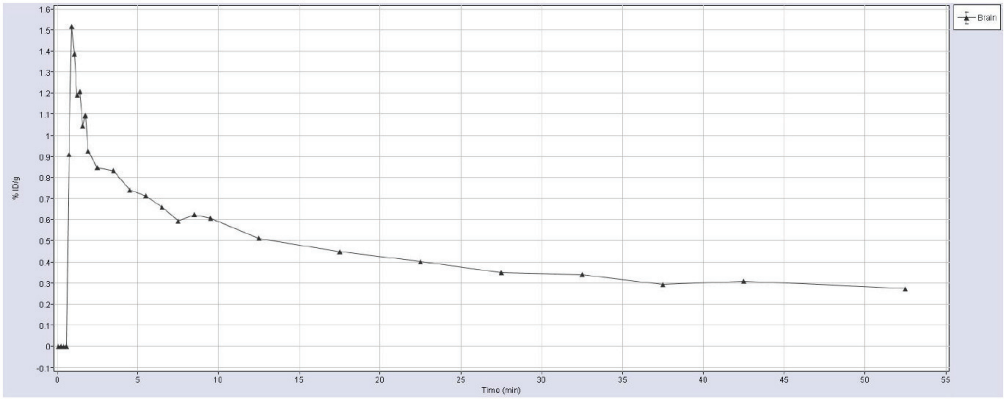
Bone



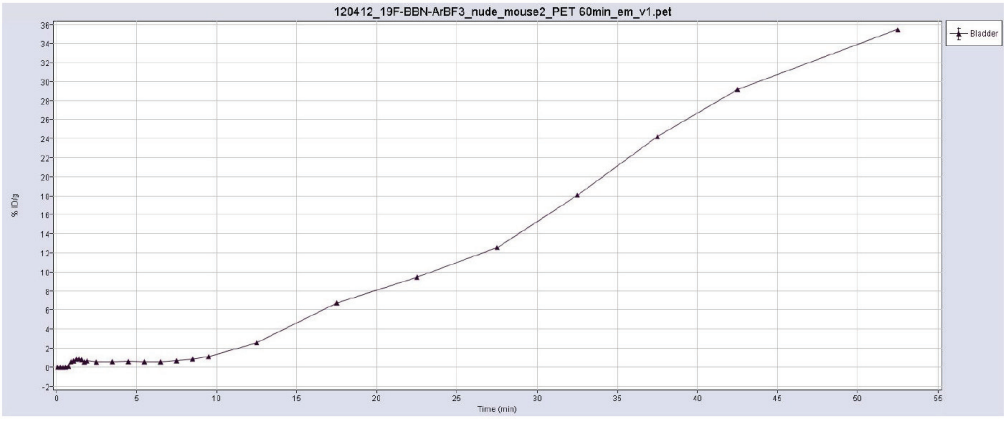
Kidney



Muscle



Brain

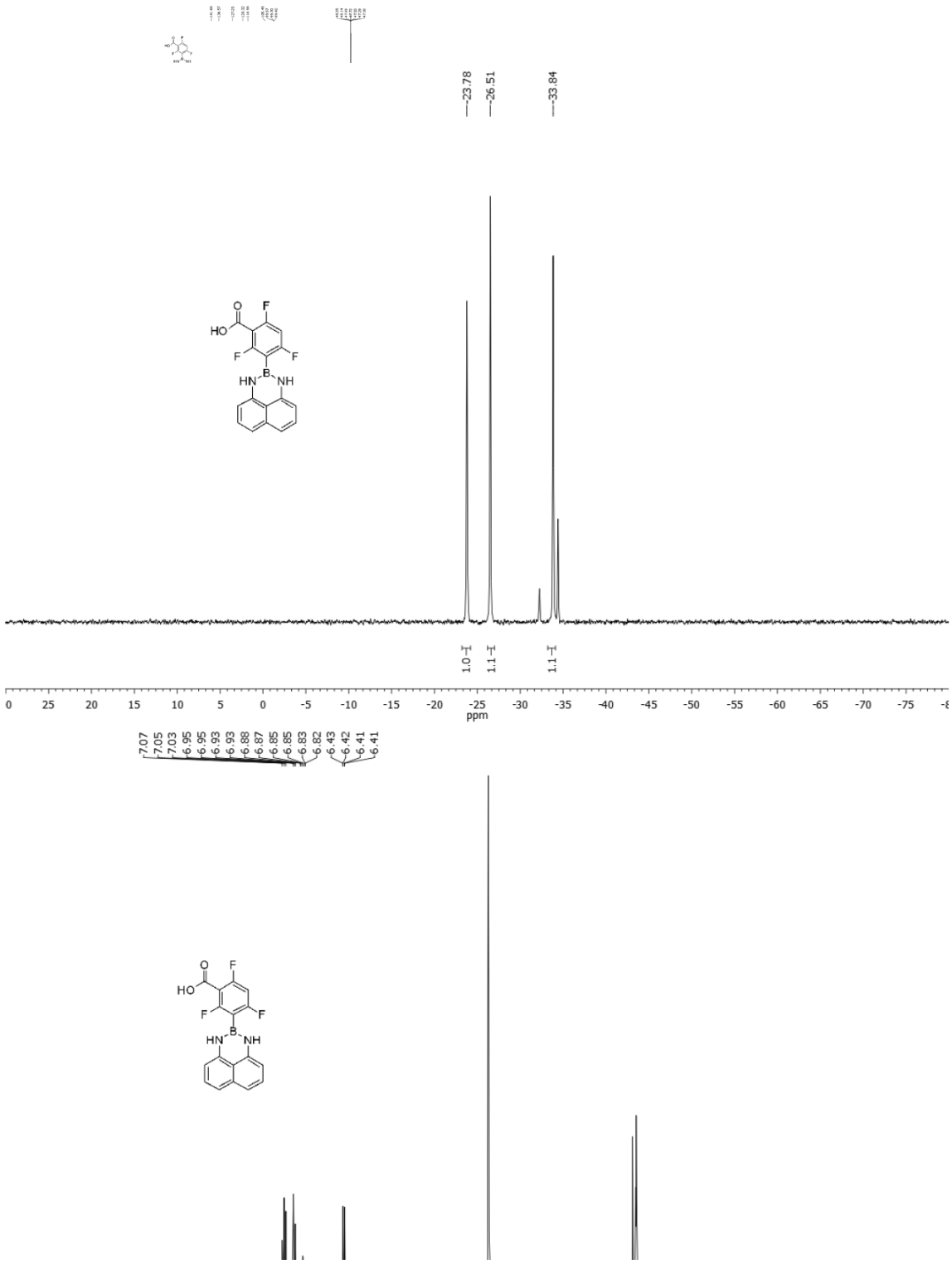


Bladder

Biodistribution of ^{18}F-ArBF$_3$-BBN 60 min post-injection using ROI analysis in healthy mice

Tissue	%ID/g
Heart	0.85 ± 0.09
Lung	0.65 ± 0.07
Liver	4.55 ± 0.21
Intestine*	41.95 ± 10.54
Kidney	0.85 ± 0.08
Bone	0.67 ± 0.19
Muscle	0.30 ± 0.02
Brain	0.33 ± 0.03

* Value for intestine is shown as percentage injected dose (%ID)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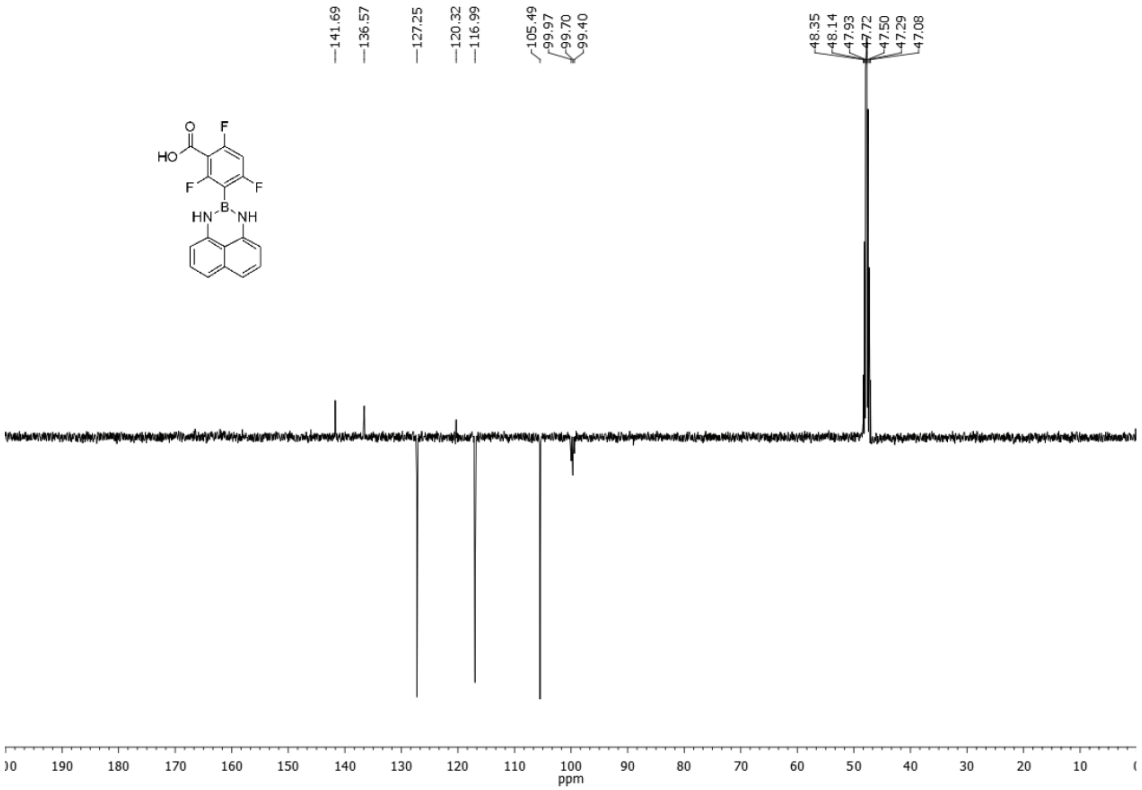
-33.84
1.0
1.1
1.1
ppm
7.07
7.05
7.03
6.95
6.95
6.93
6.93
6.88
6.87
6.85
6.85
6.83
6.82
6.43
6.42
6.41
6.41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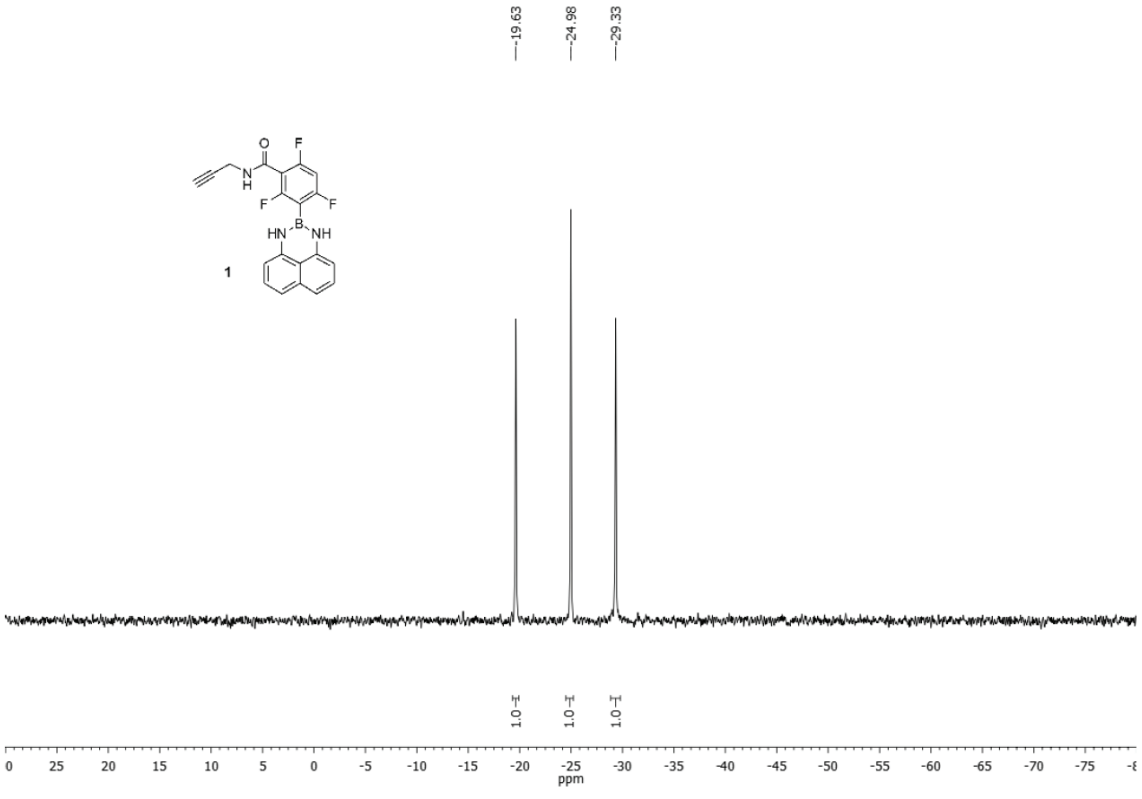
136.57
127.25
120.32
116.99
105.49
99.97
99.70
99.40
48.35
48.14
47.93
47.72
47.50
47.29
47.08
ppm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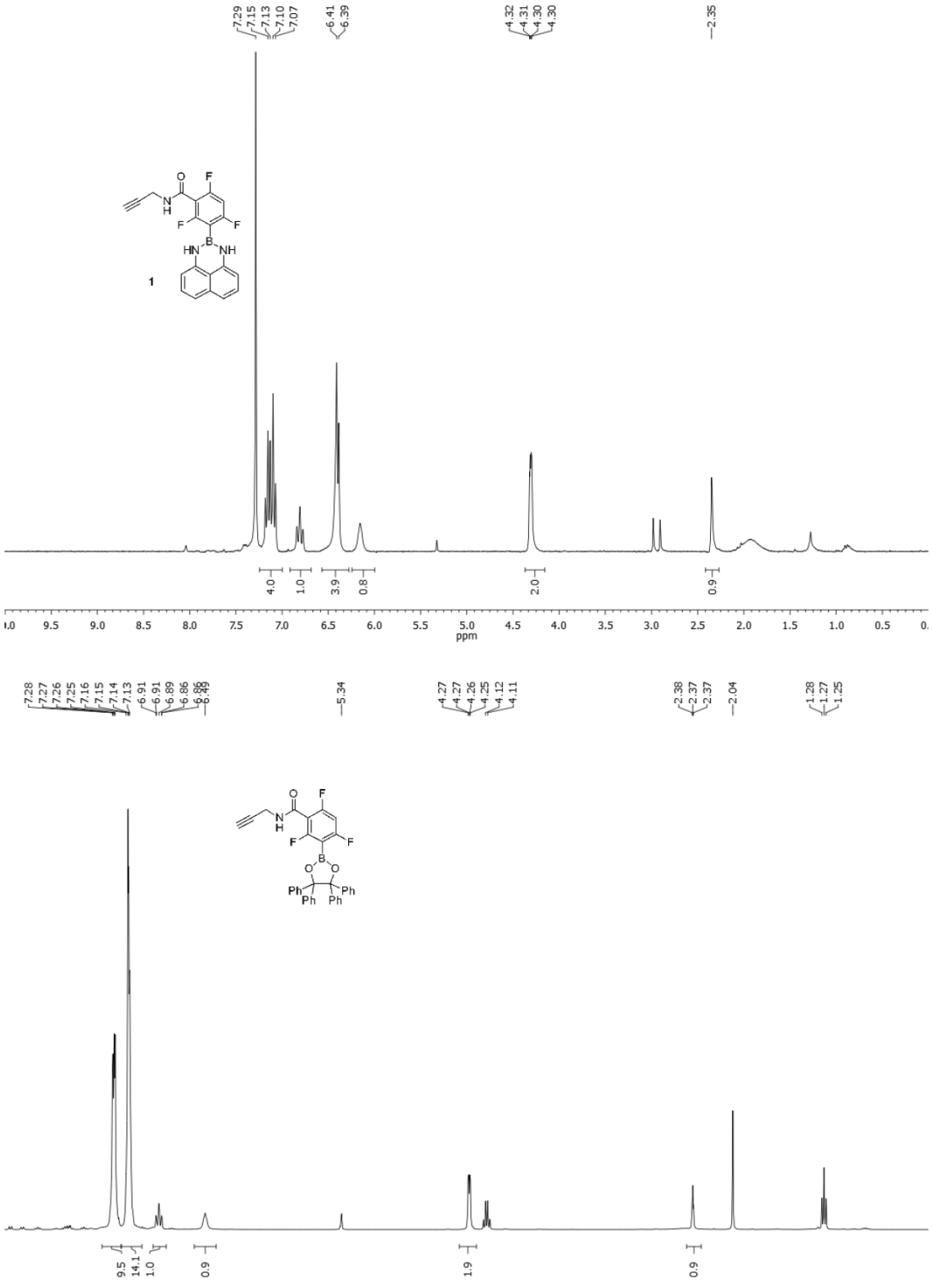
1.0
1.0
ppm

1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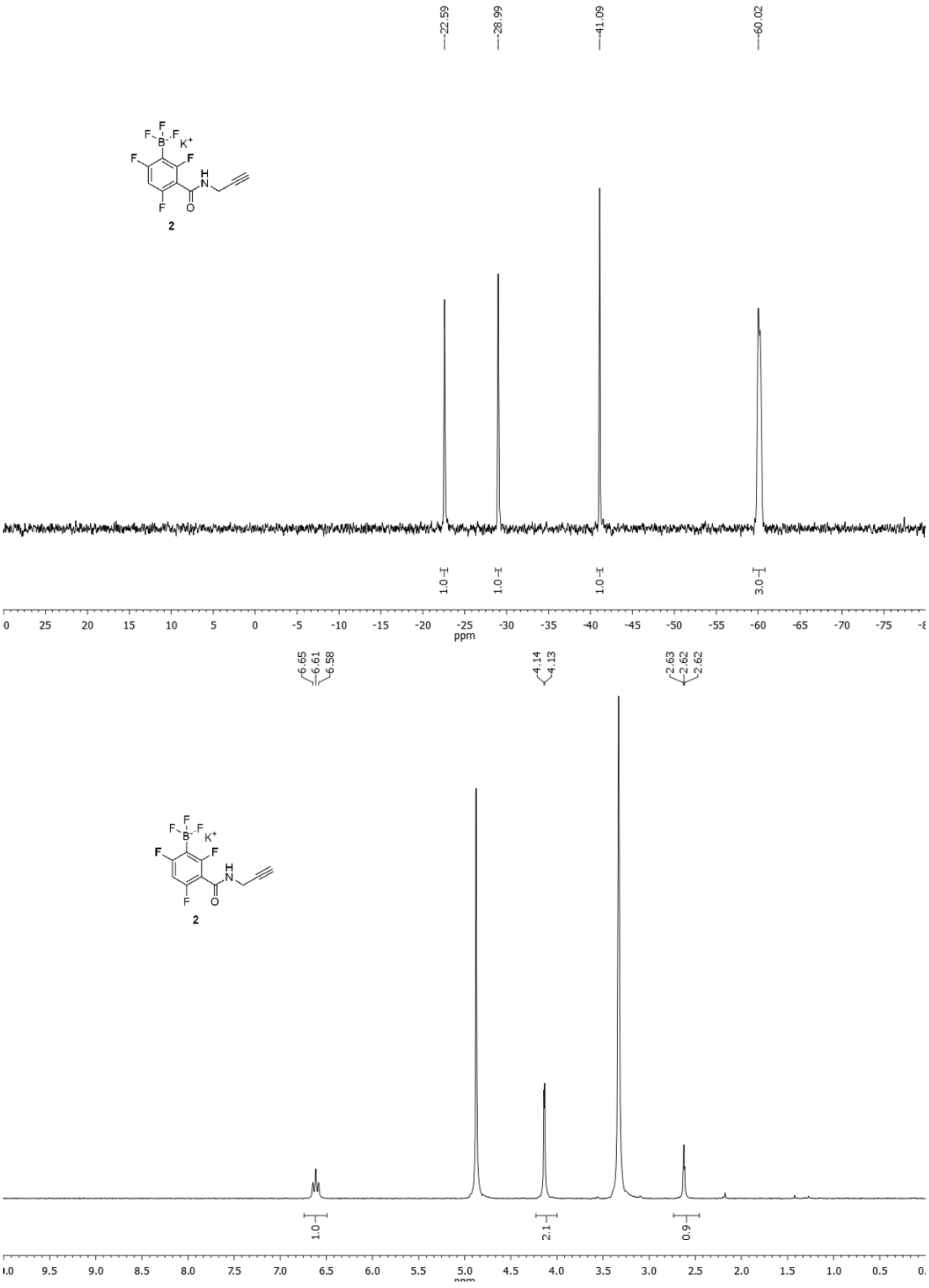
7.13
7.10
7.07
6.41
6.39
4.32
4.31
4.30
4.30
2.35
1
4.0
1.0
3.9
0.8
2.0
0.9
ppm
7.28
7.27
7.26
7.25
7.16
7.15
7.14
7.13
6.91
6.91
6.89
6.86
5.34
4.27
4.27
4.26
4.25
4.12
4.11
2.38
2.37
2.37
2.04
1.28
1.27
1.25
Ph
Ph
Ph
Ph
9.5
14.1
1.0
0.9
1.9
0.9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-41.09
-60.02
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1.0
1.0
1.0
3.0
ppm
6.65
6.61
6.58
4.14
4.13
2.63
2.62
2.62
2
1.0
2.1
0.9