Supporting Information

Preparation of a First ^{18}F-Labeled Agonist for M_1 Muscarinic Acetylcholine Receptors

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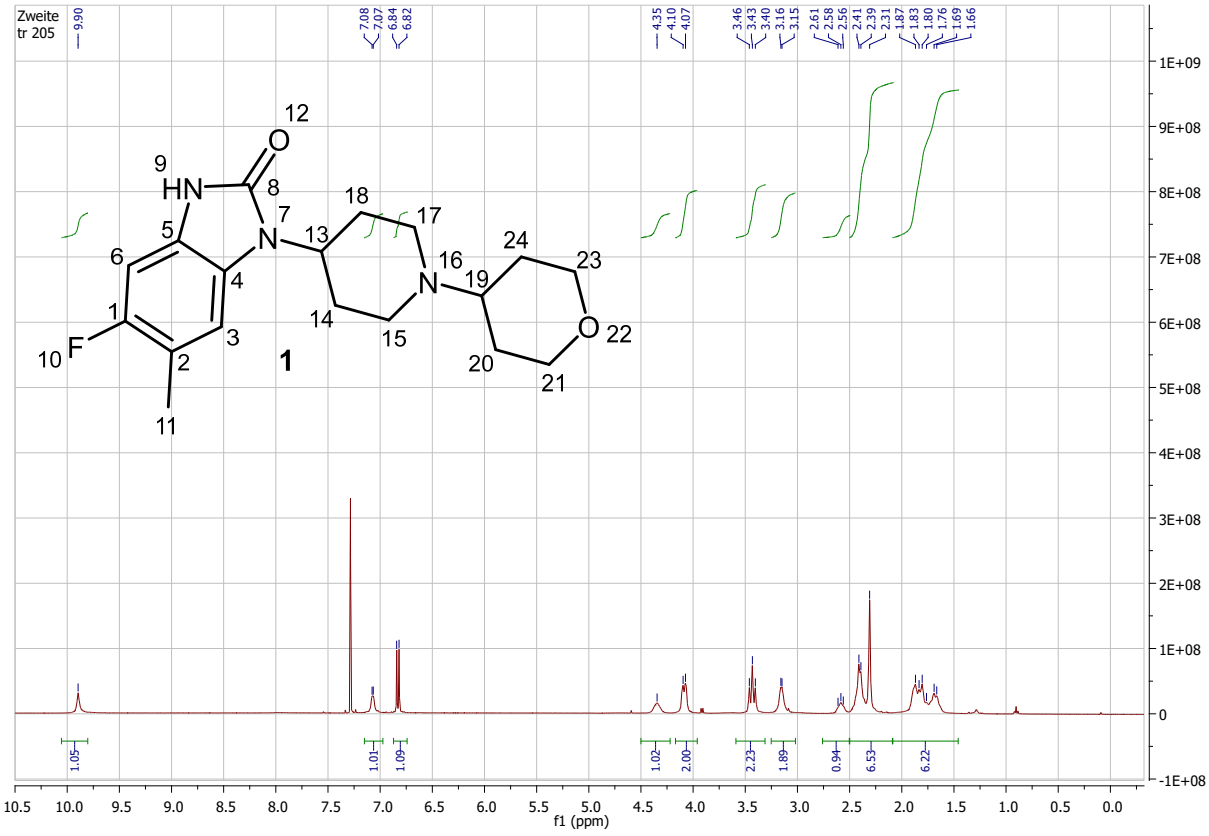
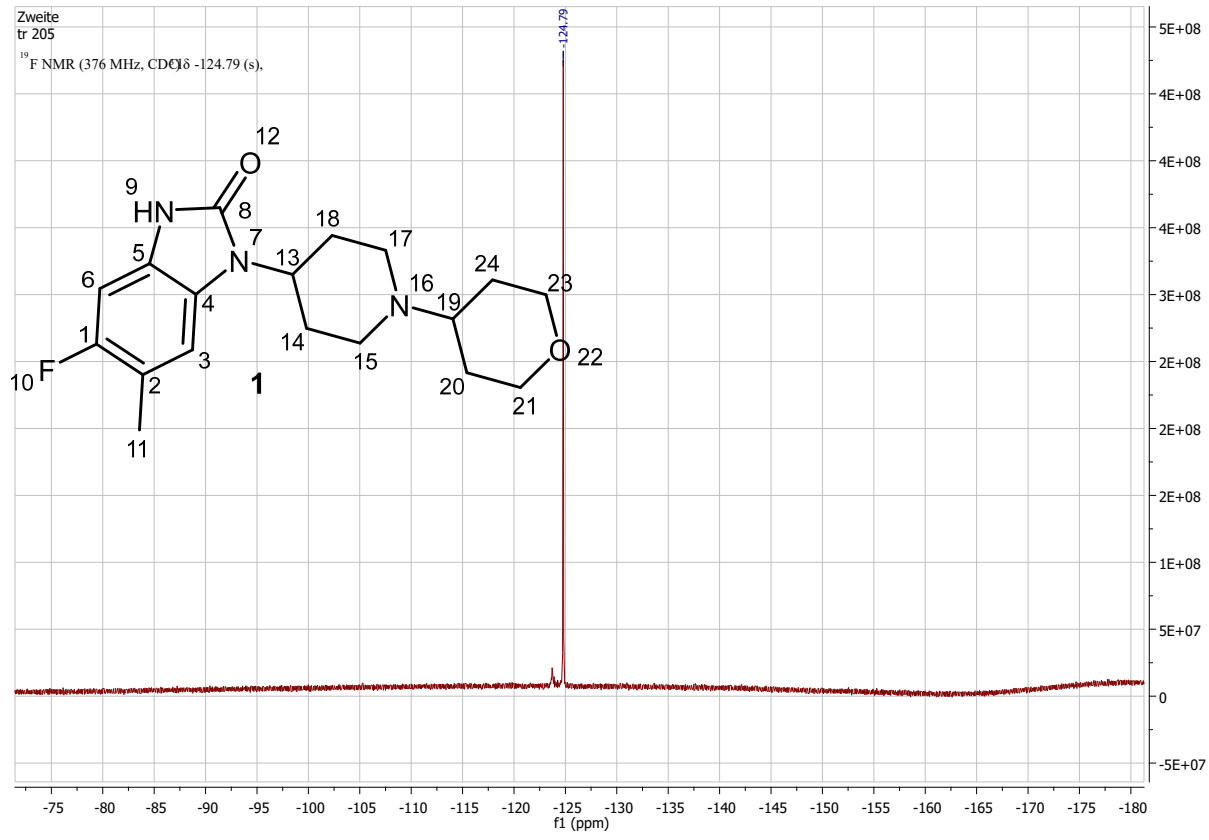
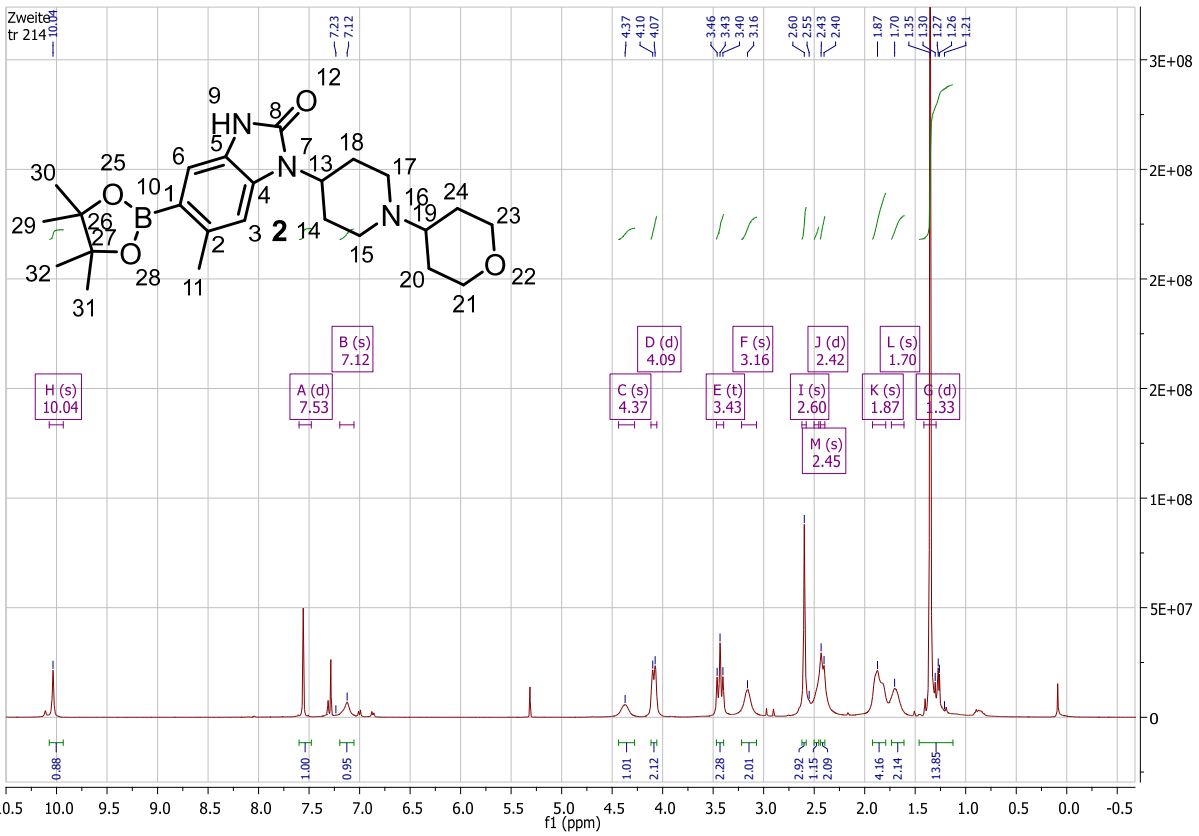
NMR-Spectra

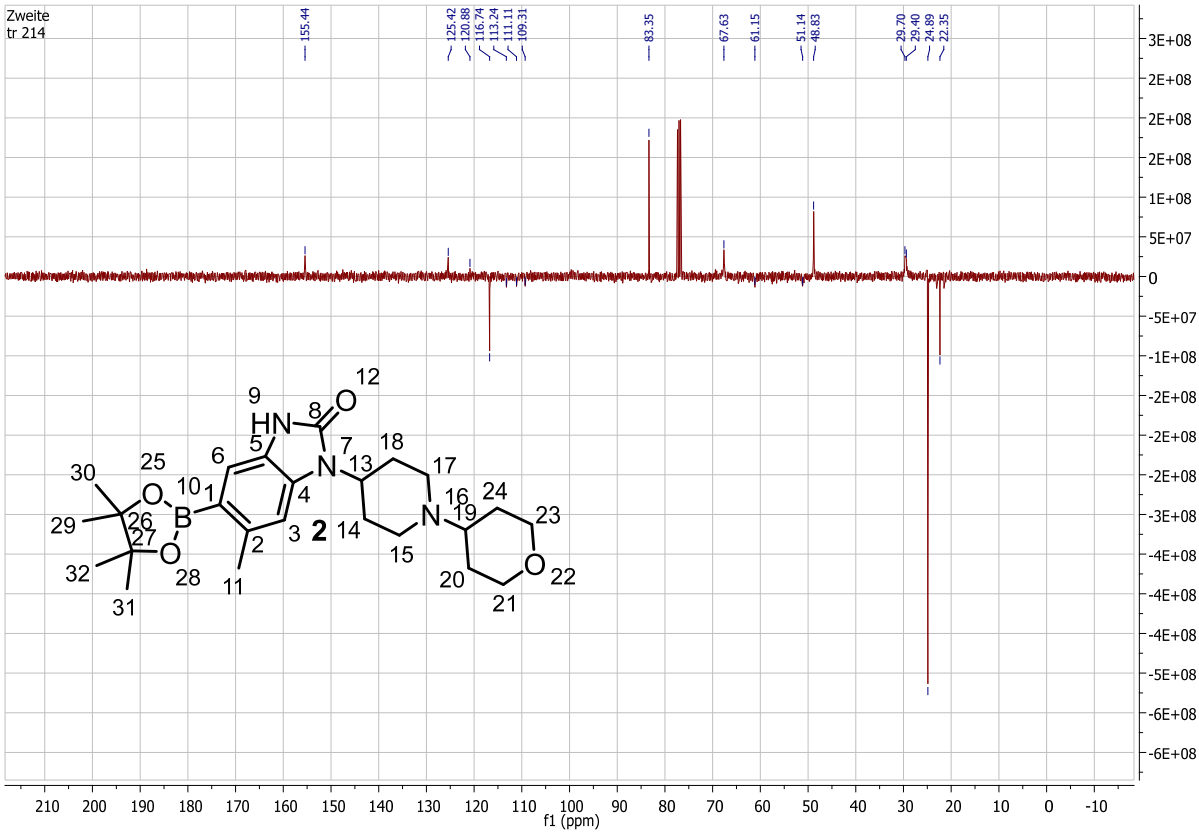
5-Fluoro-6-methyl-1-[1-(tetrahydro-2*H*-pyran-4-yl)piperidin-4-yl]-1,3-dihydro-2H-benz[d]-imidazole-2-one (**1**)



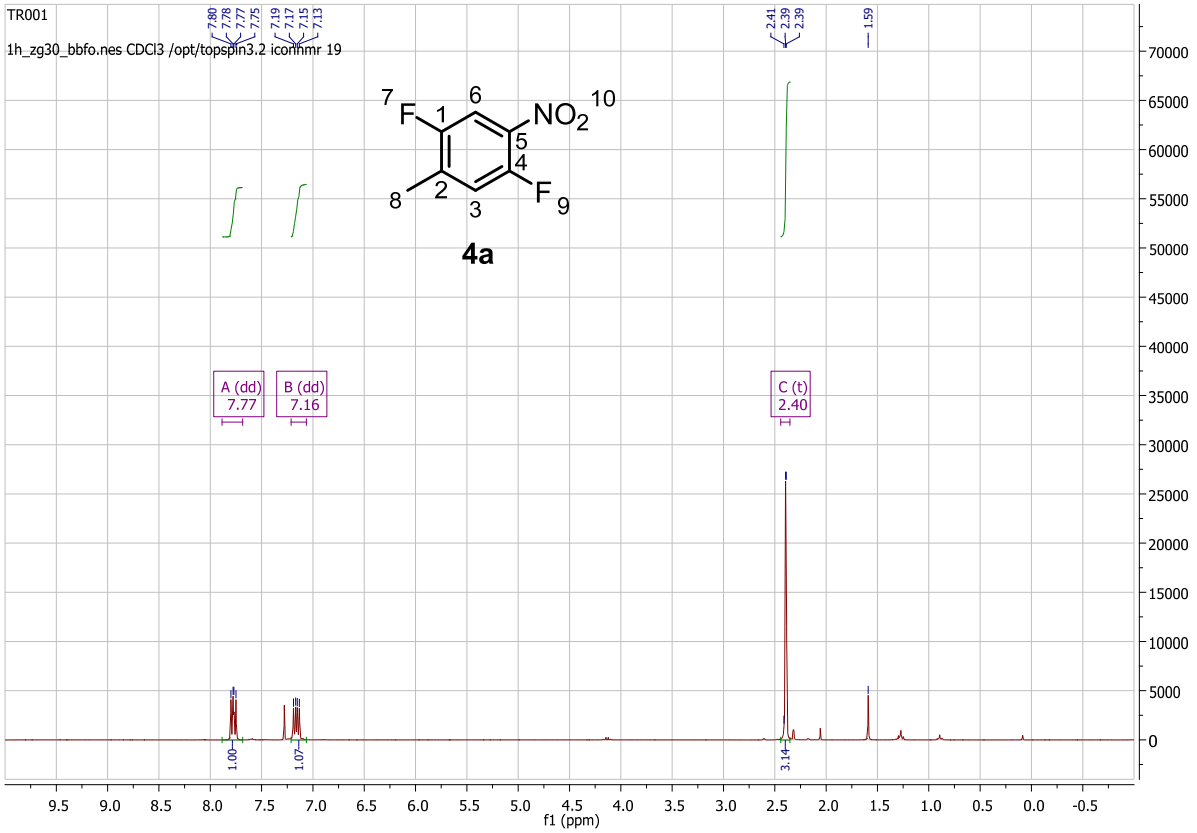


6-Methyl-1-[1-(tetrahydro-2*H*-pyran-4-yl)piperidin-4-yl]-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3-dihydro-2H-benz[d]imidazol-2-one (**2**)



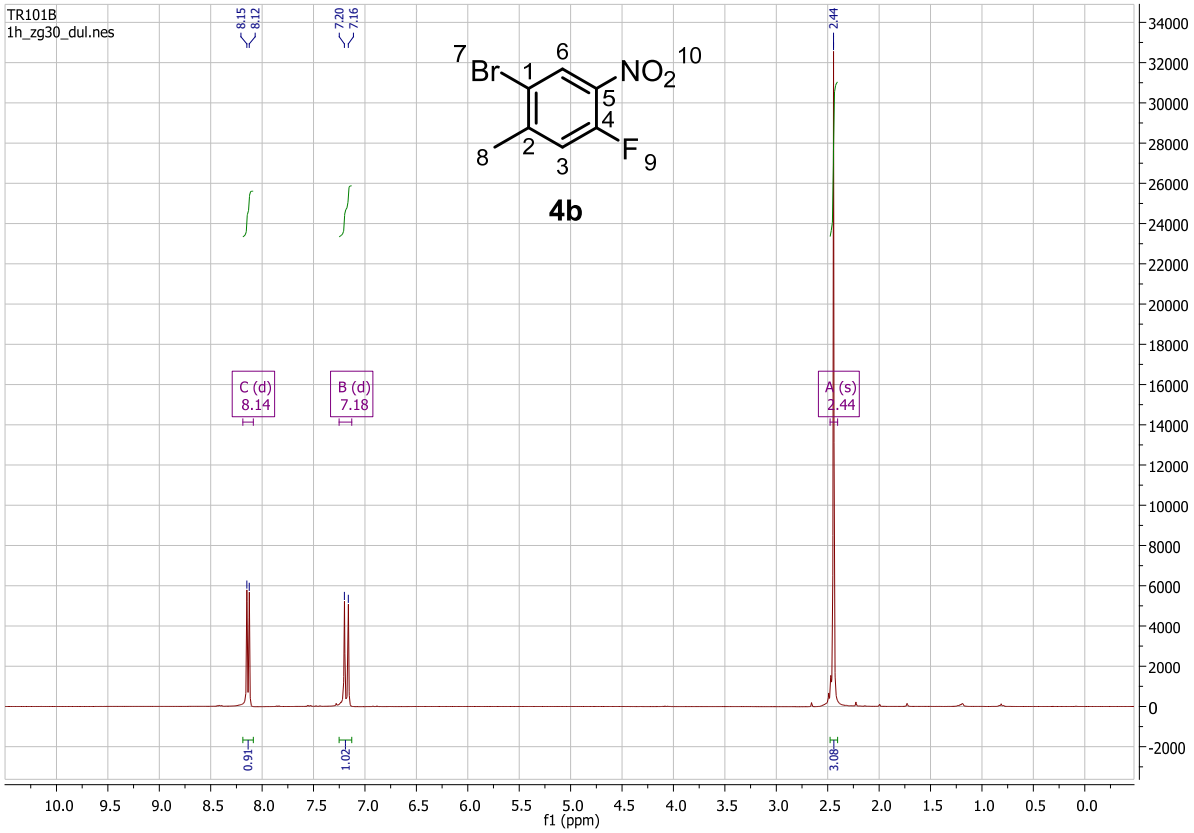


2,5-Difluoro-4-nitrotoluene (**4a**)

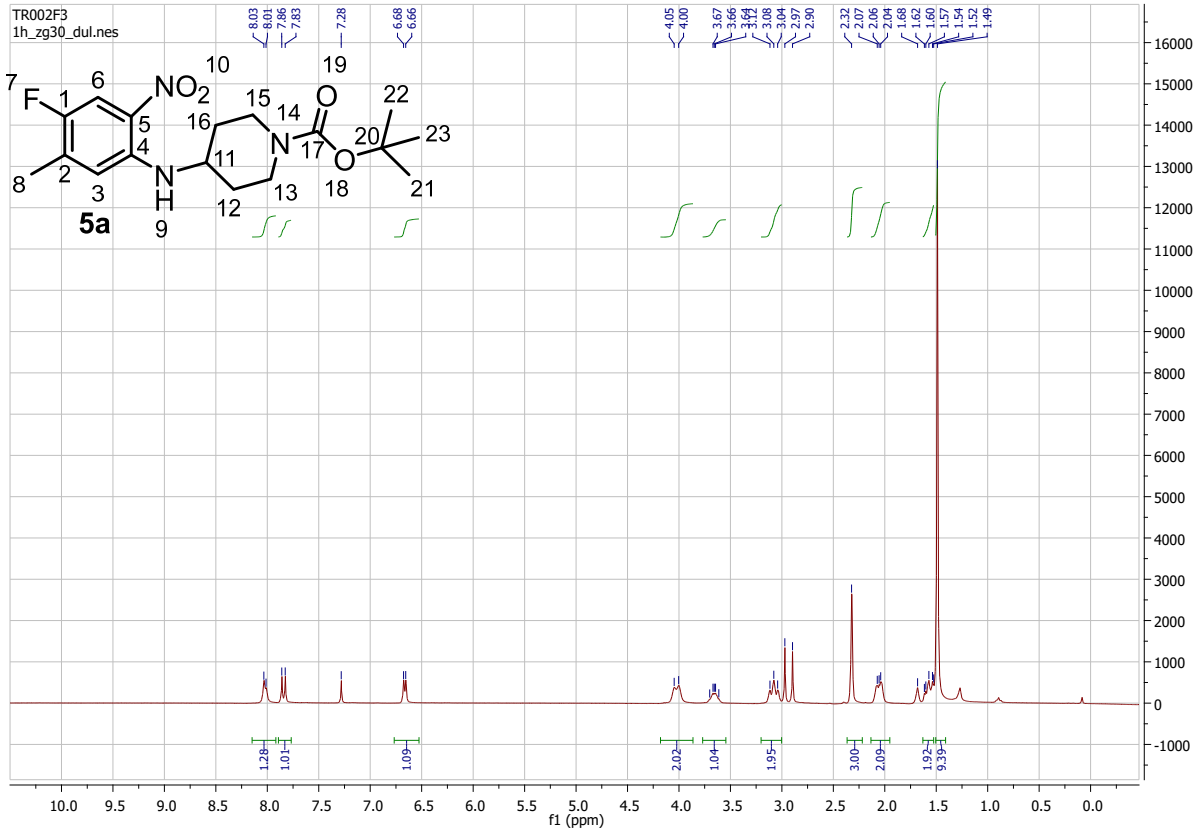


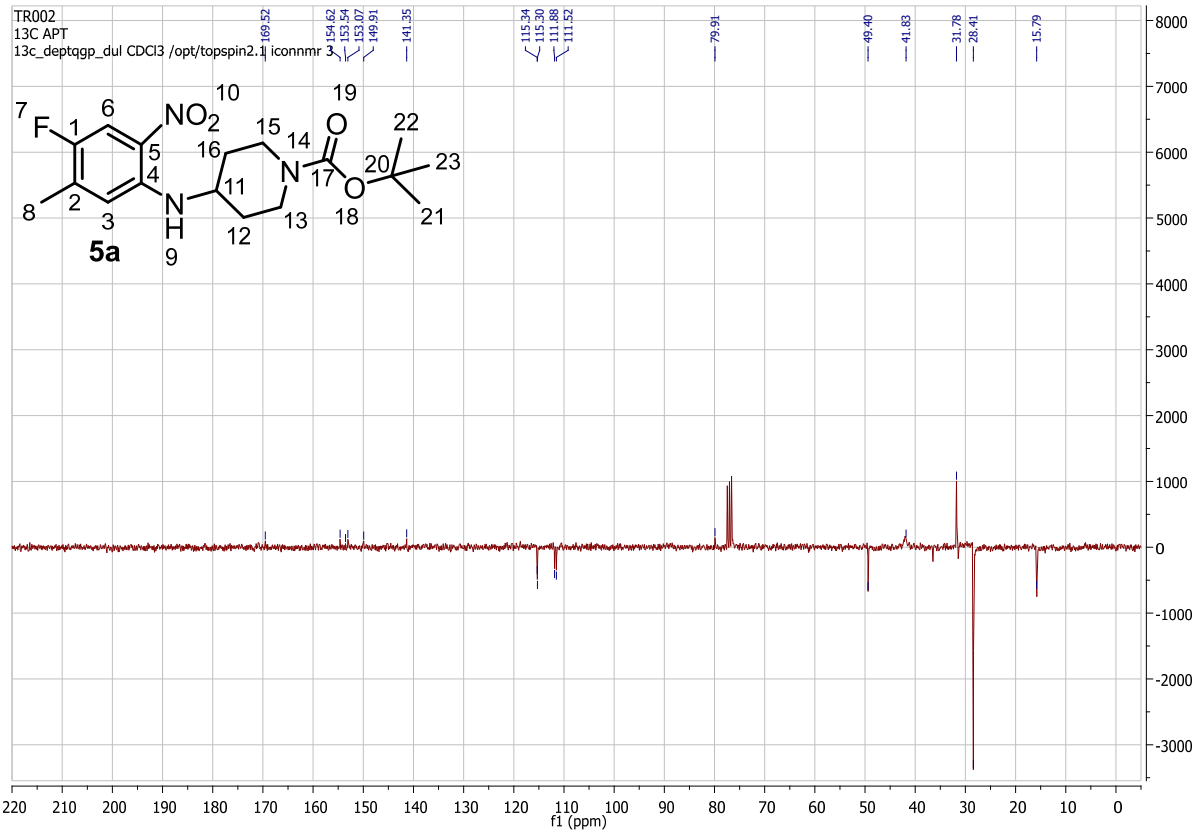
4a

2-Bromo-5-fluoro-4-nitrotoluene (**4b**)

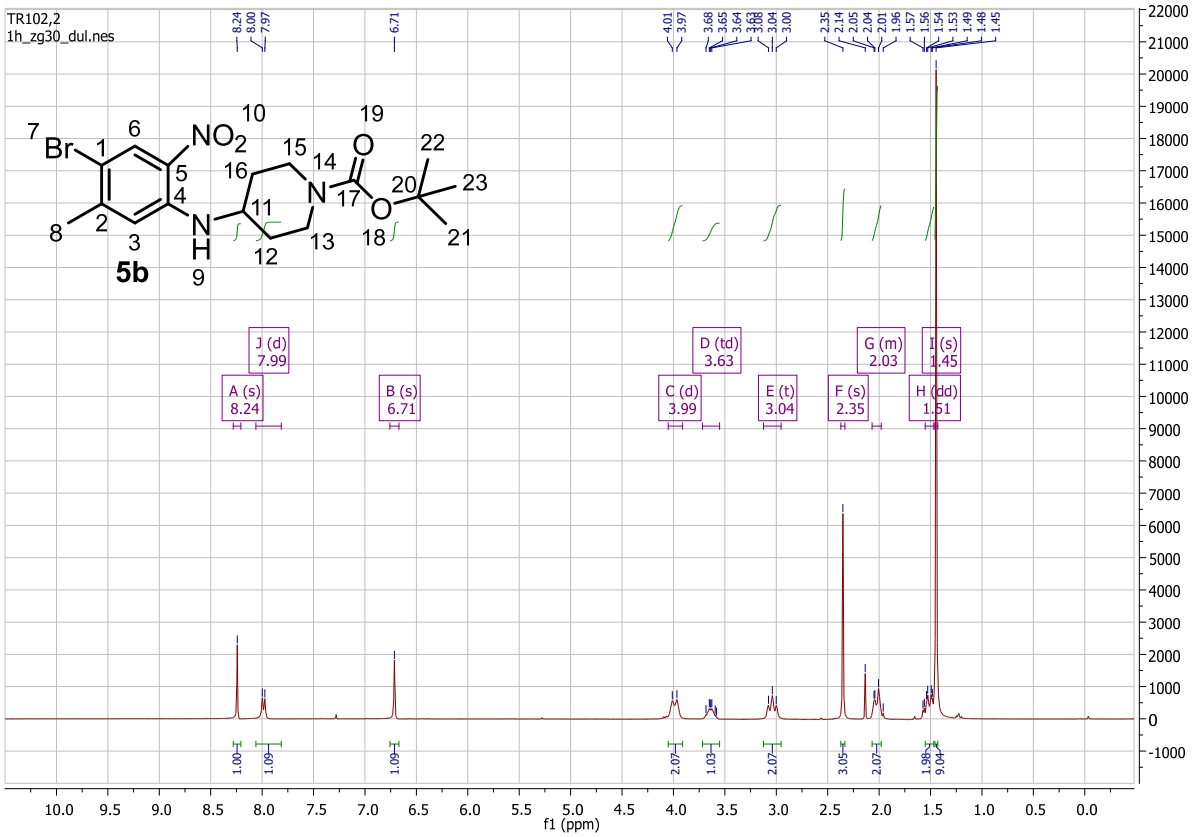


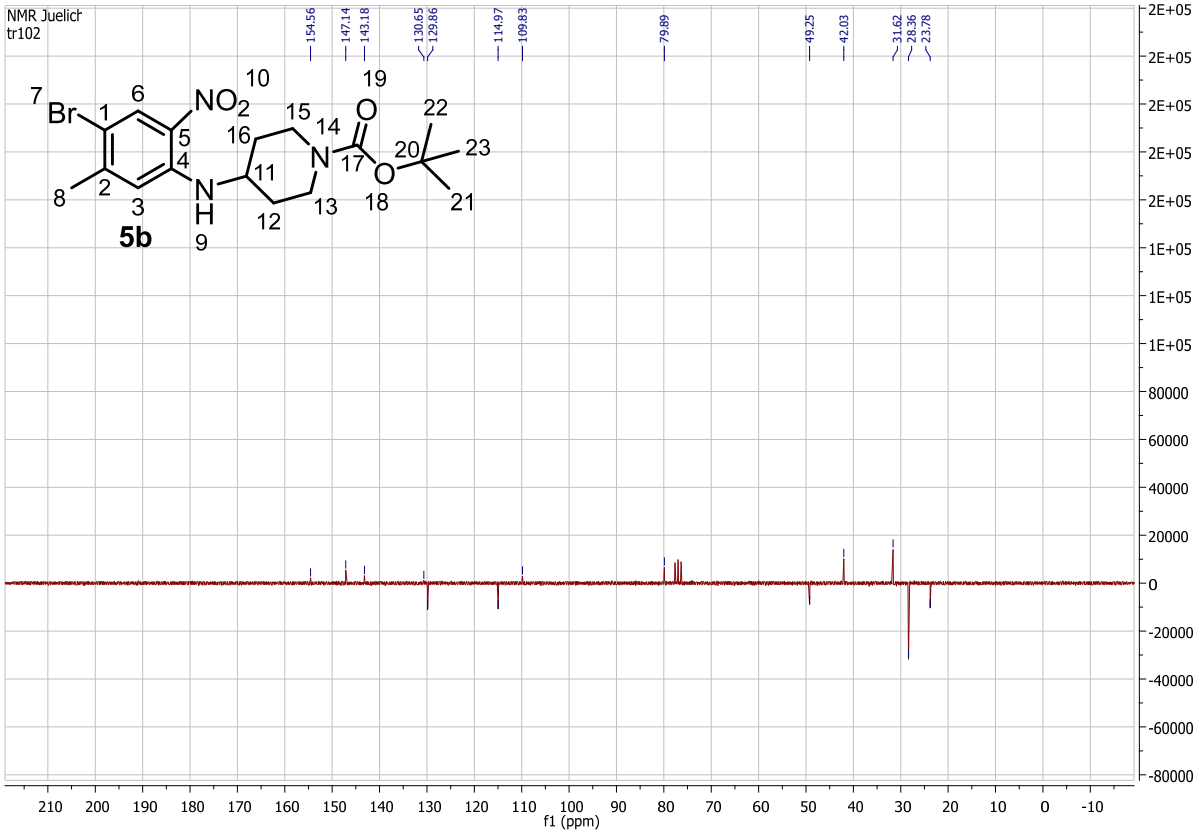
tert-Butyl 4-[(4-fluoro-5-methyl-2-nitrophenyl)amine]piperidine-1-carboxylate (**5a**)



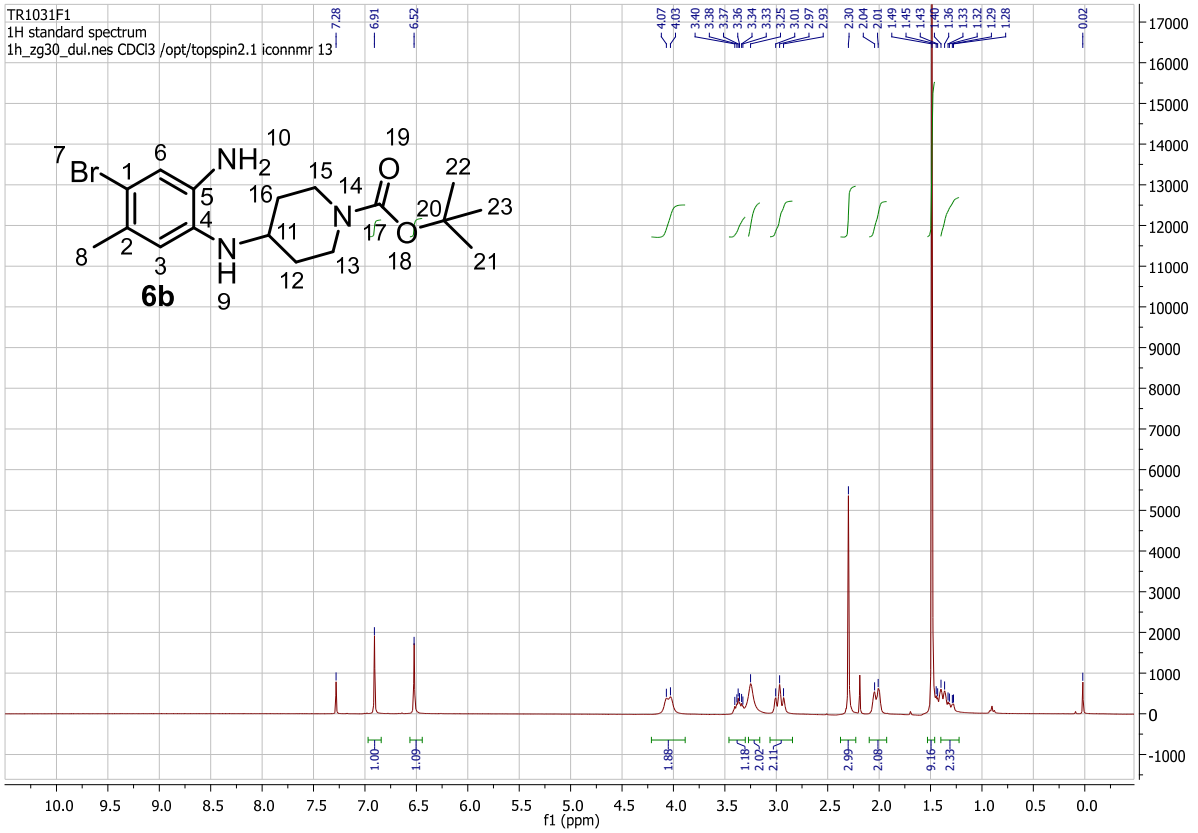


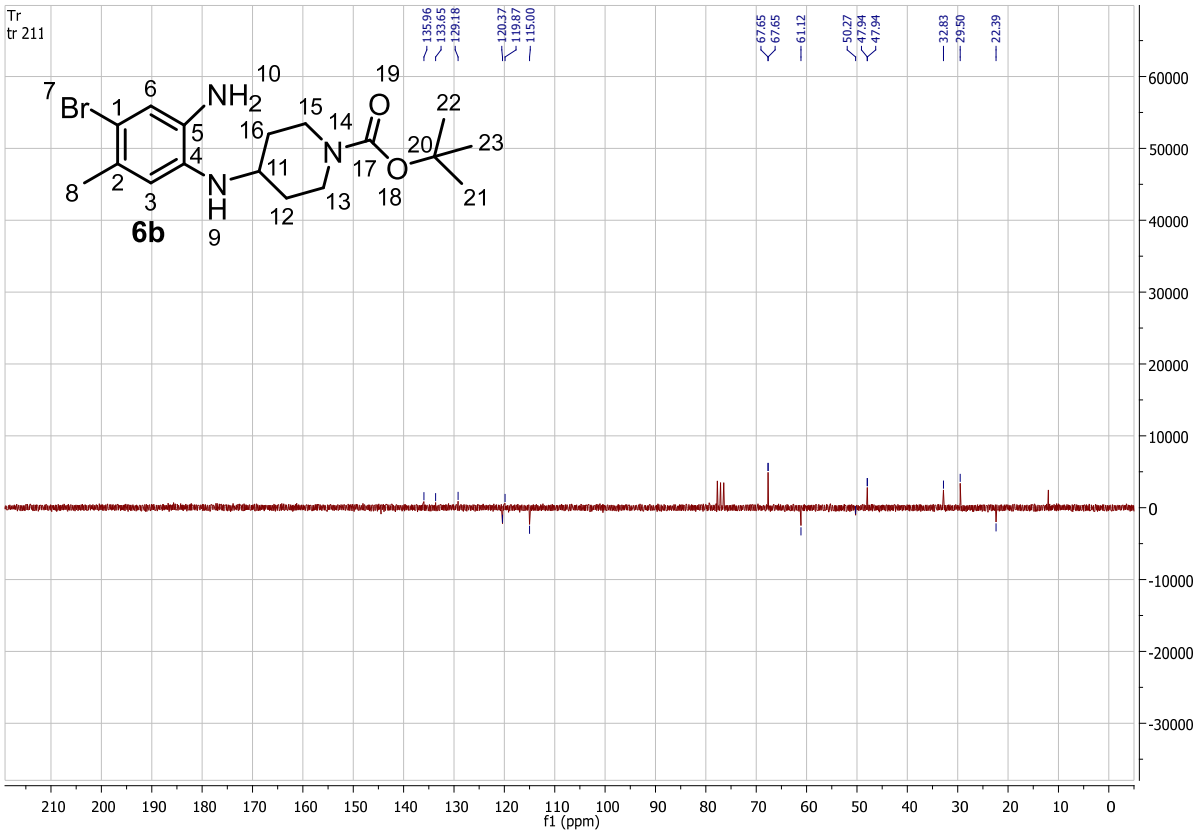
tert-Butyl 4-[(4-bromo-5-methyl-2-nitrophenyl)amine]piperidine-1-carboxylate (**5b**)



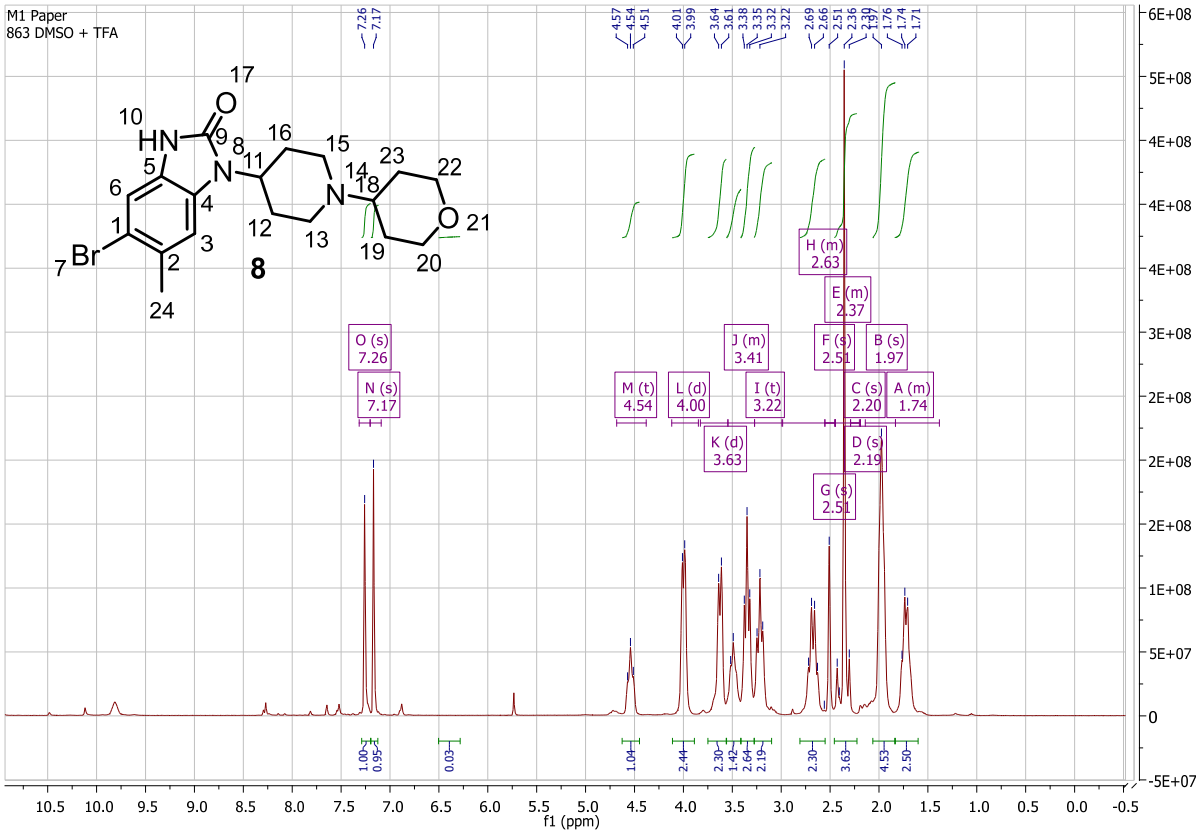


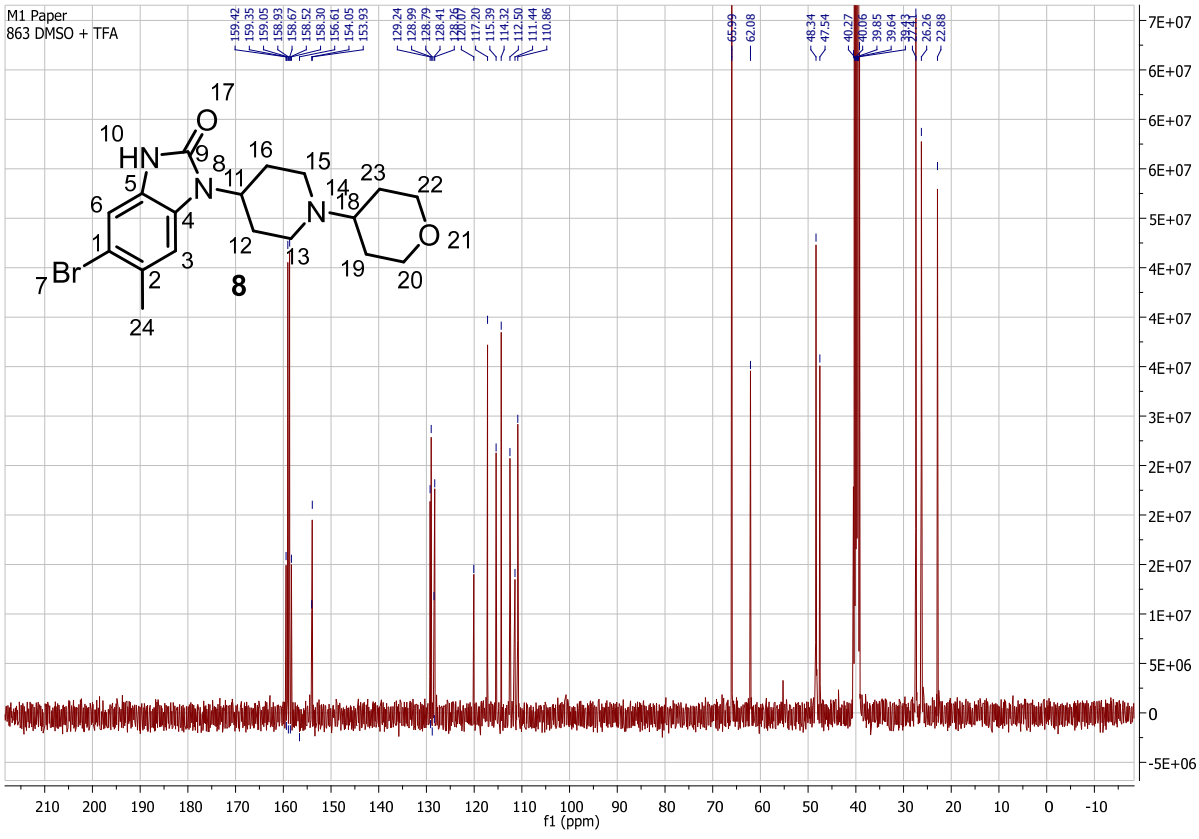
tert-Butyl 4-[(2-amine-4-bromo-5-methylpheny)]amine]piperidine-1-carboxylate (**6b**)

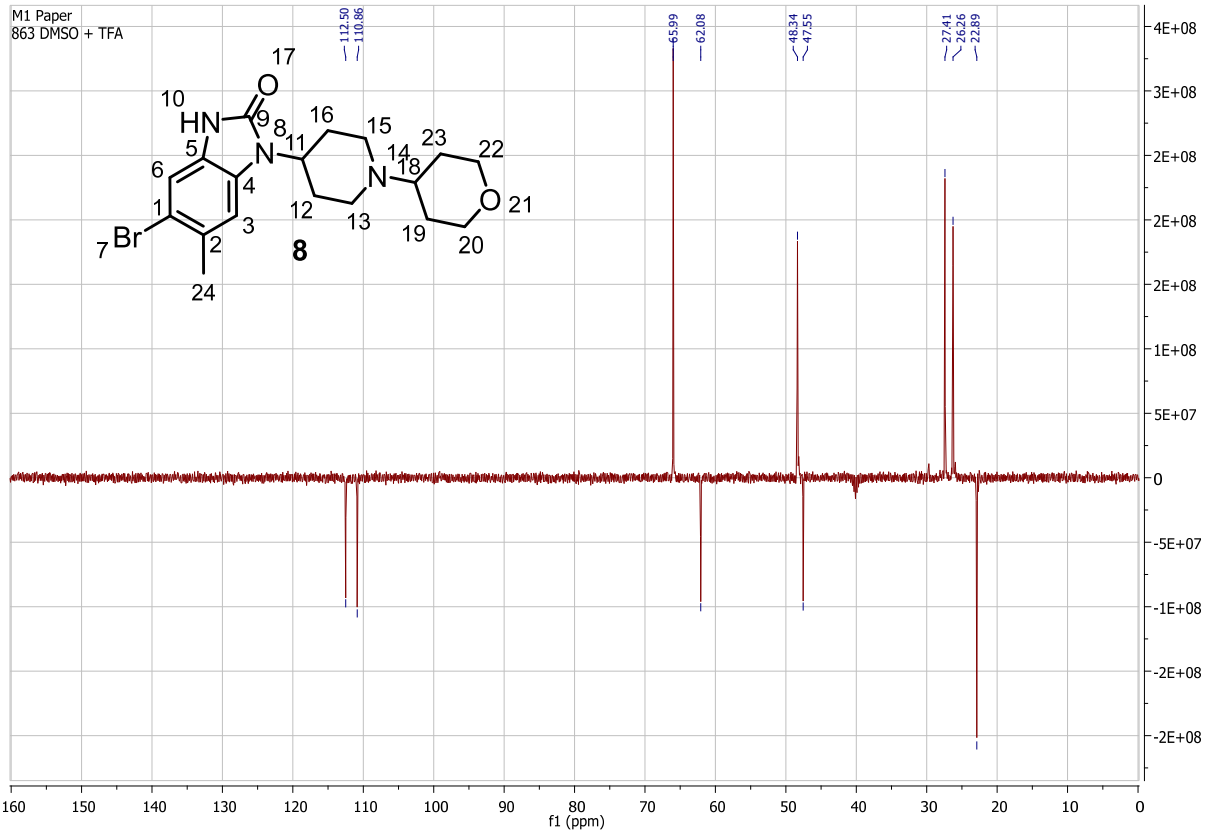




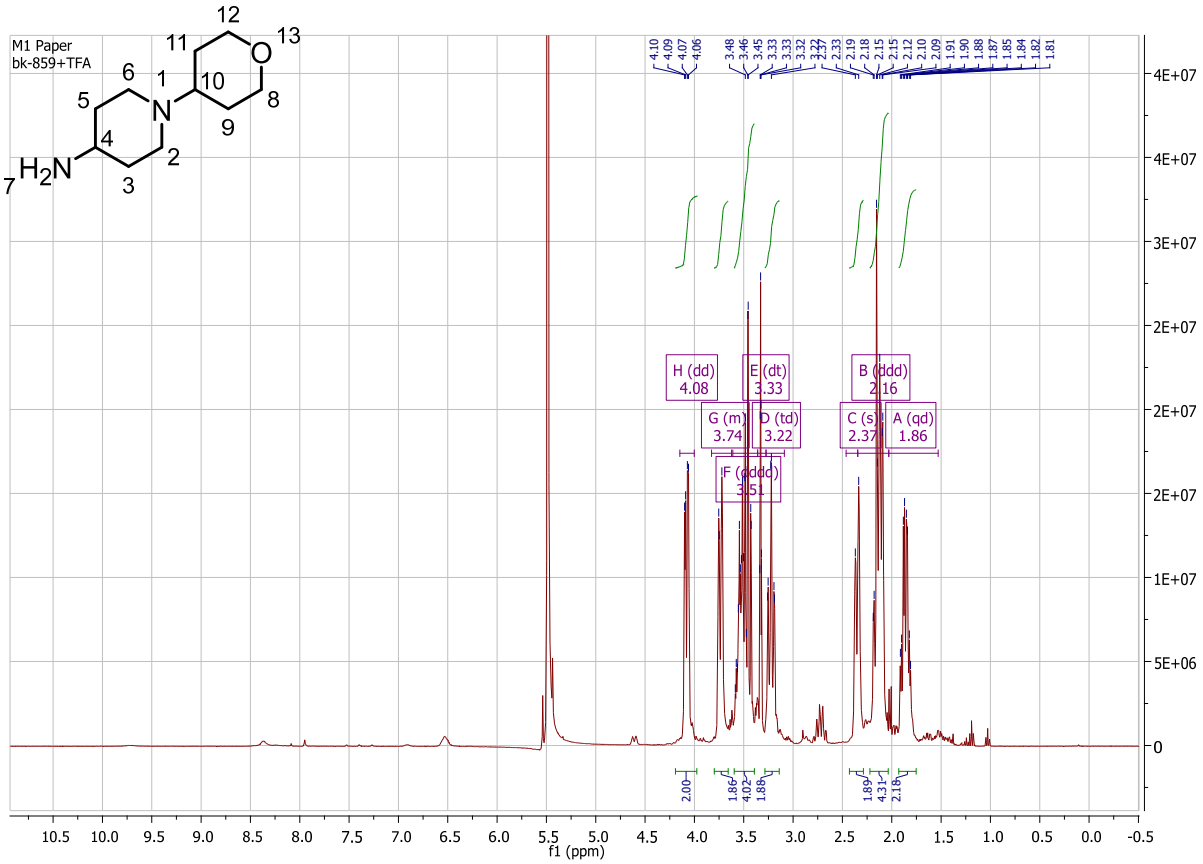
5-Bromo-6-methyl-1-[1-(tetrahydro-2*H*-pyran-4-yl)piperidin-4-yl]-1,3-dihydro-2*H*-benz[d]imidazol-2-one (mixture of **8** and **8**·TFA)



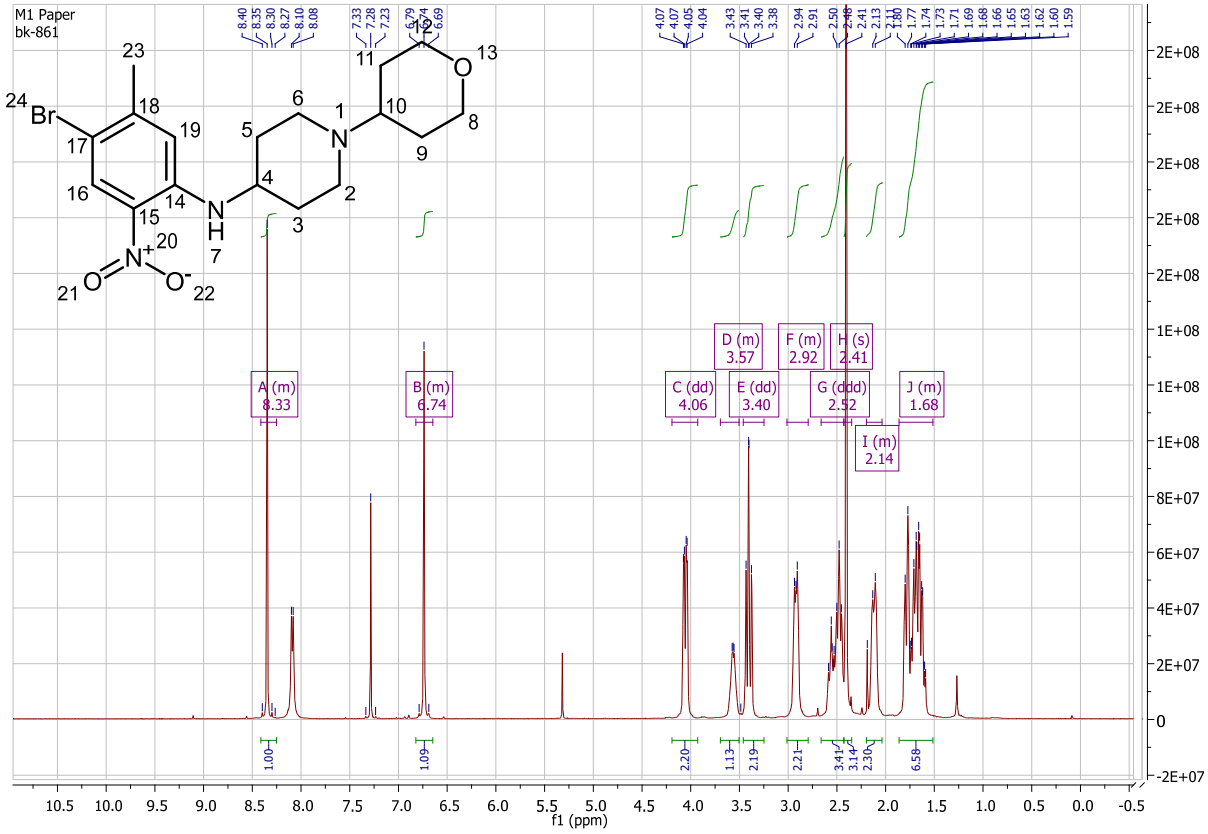


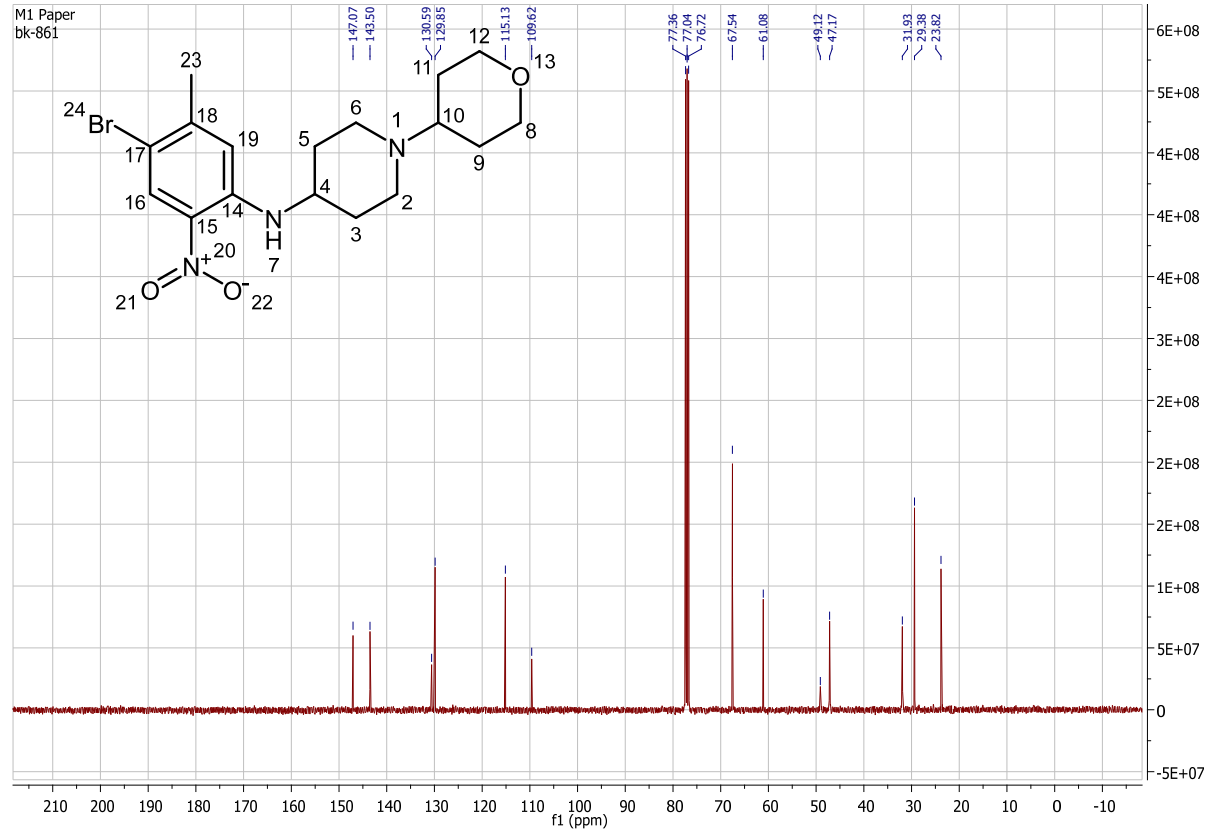

M1 Paper
863 DMSO + TFA
112.50
110.86
65.99
62.08
48.34
47.55
27.41
26.26
22.89
8
f1 (ppm)

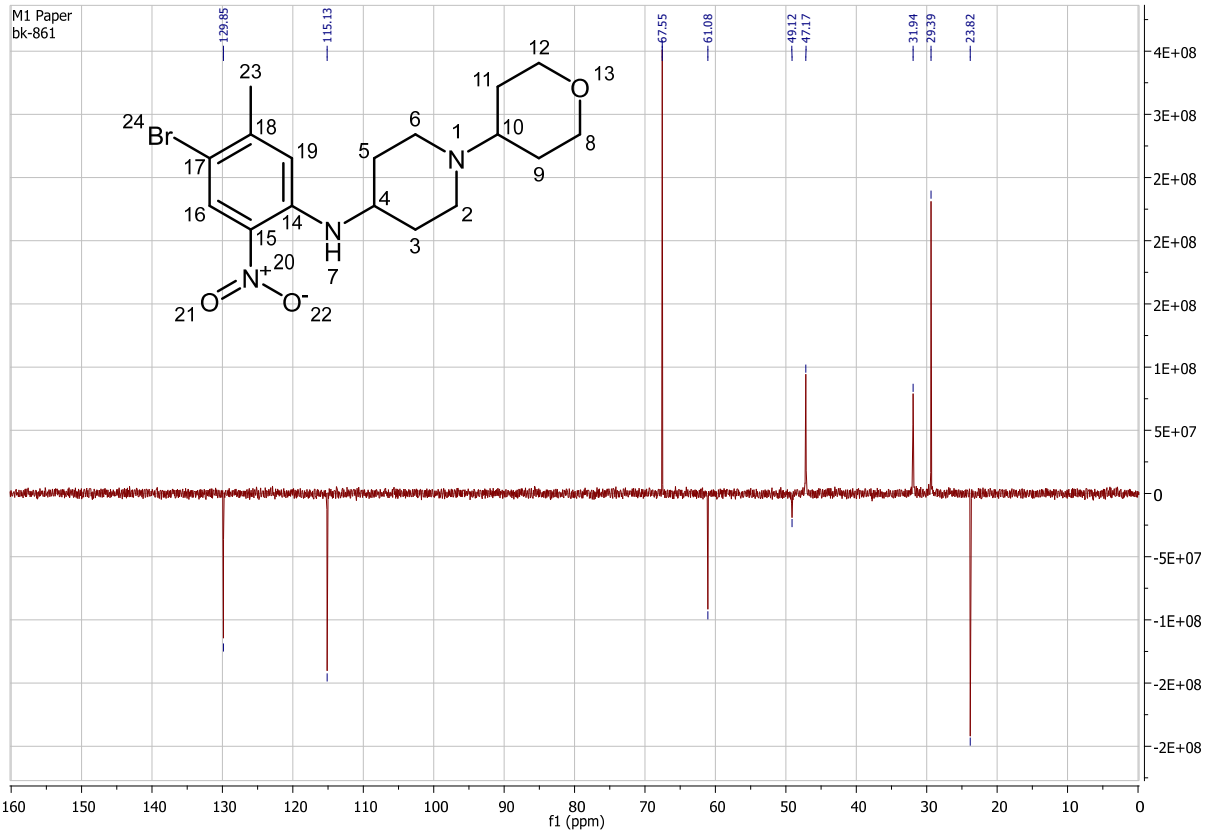
1-(Tetrahydro-2*H*-pyran-4-yl)piperidine-4-amine (mixture of **10**·TFA and **10**·2 TFA)



N-(4-Bromo-5-methyl-2-nitrophenyl)-1-(tetrahydro-2*H*-pyran-4-yl)piperidine-4-amine (**11b**)






M1 Paper
bk-861
129.85
115.13
67.55
61.08
49.12
47.17
31.94
29.39
23.82
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
-2E+08
-2E+08
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
Br
N
H
O
O
N+
O-
1
2
3
4
5
6
7
8
9
10
11
12
13
14
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Determination of carrier amount and molar activity

The batch of [^{18}F]**1** obtained after HPLC purification (770 MBq) was left to stay for 24 h and thereafter concentrated under reduced pressure. The residue was redissolved in 20% MeCN (0.1% TFA) (1.5 mL) and an aliquot of the solution (0.5 mL) was injected into the HPLC system. The peak area was determined and the carrier amount as well as the molar activity were calculated according to the calibration curve (λ=210 nm) (Figure S1).

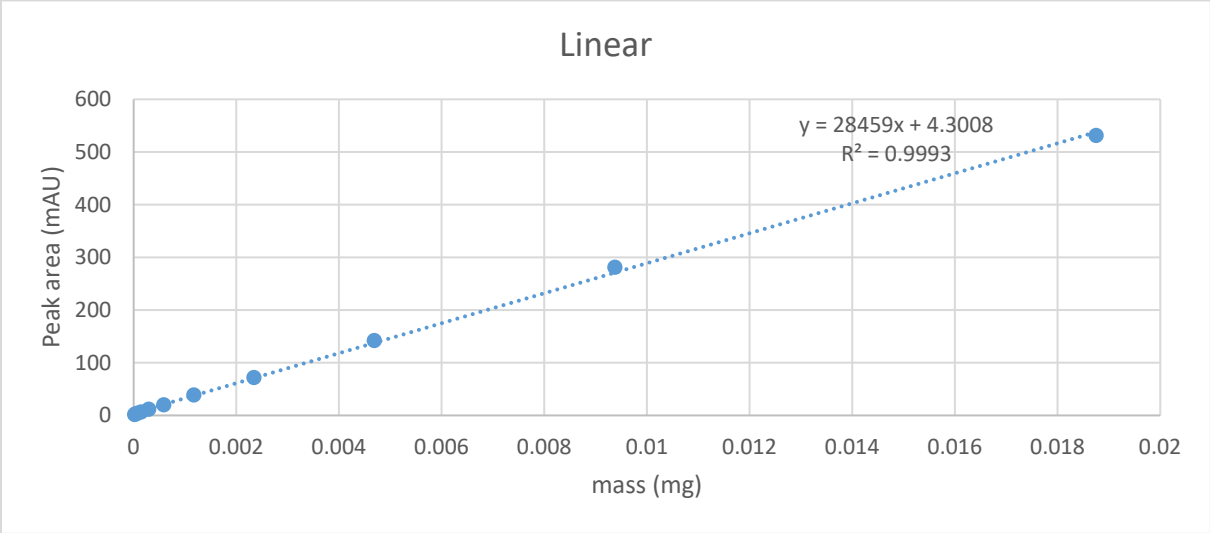

Figure S1. Calibration curve.

1/3 Batch; peak area: 83.92 mAU (corresponds to 2.8 µg). Batch; peak area: 230.21 mAU (corresponds to 8.4 µg).

Mr(**1**) = 333.4 g/mol.

Carrier amount = 25.2 nmol/batch.

Molar activity = 30.6 GBq/µmol.