

Supporting information

Synthesis and evaluation of novel ^{18}F labeled 2-pyridinyl benzoxazole and benzothiazole derivatives as ligands for Positron Emission Tomography (PET) Imaging of β -amyloid plaques

Mengchao Cui,^{†, §, *} Xuedan Wang,^{†, §} Pingrong Yu,[†] Jinming Zhang,[‡] Zijing Li,[†] Xiaojun Zhang,[‡] Yanping Yang,[†] Masahiro Ono,[£] Hongmei Jia,[†] Hideo Saji,[£] Boli Liu,^{†, *}

[†]Key Laboratory of Radiopharmaceuticals, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing 100875, PR China.

[‡]Department of Nuclear Medicine, Chinese PLA General Hospital, Beijing 100853, PR China.

[£]Department of Patho-Functional Bioanalysis, Graduate School of Pharmaceutical Sciences, Kyoto University, 46-29 Yoshida Shimoadachi-cho, Sakyo-ku, Kyoto 606-8501, Japan.

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1. Purity of key target compounds.

UV-wavelength: 254 nm

Compd	Flow rate (mL/min)	Mobile phase (AcCN%)	Column (Venusil MP C18, 5 μ m)	Retention time (RT, min)	Purity (%)
28	1	60	4.6 $\times$ 250 mm	6.41	97.62
29	1	60	4.6 $\times$ 250 mm	6.07	99.63
30	1	60	4.6 $\times$ 250 mm	11.00	98.40
31	1	60	4.6 $\times$ 250 mm	10.32	98.00
32	1	60	4.6 $\times$ 250 mm	6.01	98.34
33	1	60	4.6 $\times$ 250 mm	11.73	96.92
40	1	60	4.6 $\times$ 250 mm	7.36	97.02
41	1	60	4.6 $\times$ 250 mm	7.04	97.23
42	1	60	4.6 $\times$ 250 mm	13.92	97.53
43	1	60	4.6 $\times$ 250 mm	12.97	98.79
44	1	60	4.6 $\times$ 250 mm	7.76	96.63
45	1	60	4.6 $\times$ 250 mm	15.00	97.21

2. HPLC chromatograms of key target compounds.

Compd	Flow rate (mL/min)	Mobile phase (AcCN%)	Column (Venusil MP C18, 10 μ m)	Retention time (RT, min)
29	4	60	10 $\times$ 250 mm	7.72
[¹⁸ F] 29	4	60	10 $\times$ 250 mm	7.78
31	4	70	10 $\times$ 250 mm	8.95
[¹⁸ F] 31	4	70	10 $\times$ 250 mm	9.09
32	4	60	10 $\times$ 250 mm	6.22
[¹⁸ F] 32	4	60	10 $\times$ 250 mm	6.36
33	4	70	10 $\times$ 250 mm	5.80
[¹⁸ F] 33	4	70	10 $\times$ 250 mm	5.93
41	4	60	10 $\times$ 250 mm	5.14
[¹⁸ F] 41	4	60	10 $\times$ 250 mm	5.28
43	4	70	10 $\times$ 250 mm	8.07
[¹⁸ F] 43	4	70	10 $\times$ 250 mm	8.23
44	4	60	10 $\times$ 250 mm	7.68
[¹⁸ F] 44	4	60	10 $\times$ 250 mm	7.81

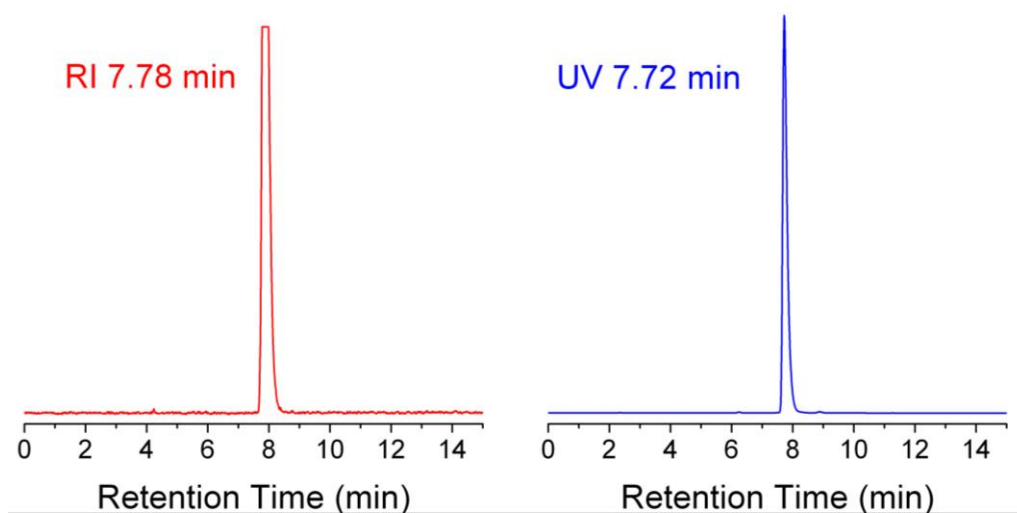


Figure S1. HPLC profiles of [^{18}F]29 and 29

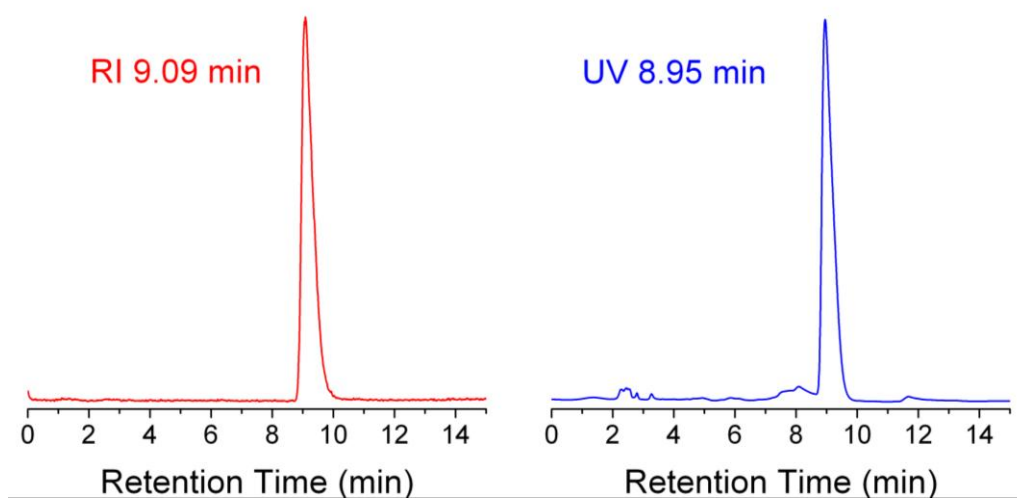


Figure S2. HPLC profiles of [^{18}F]31 and 31

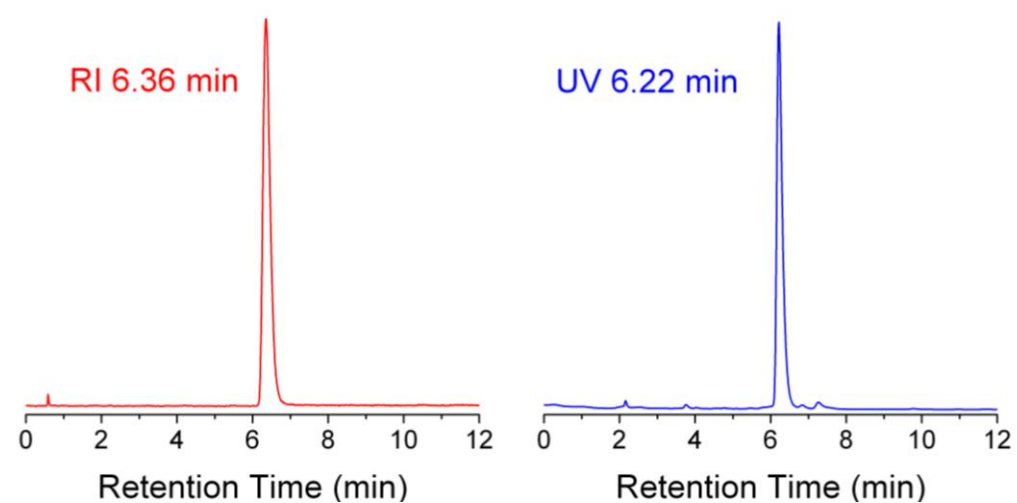


Figure S3. HPLC profiles of [^{18}F]32 and 32

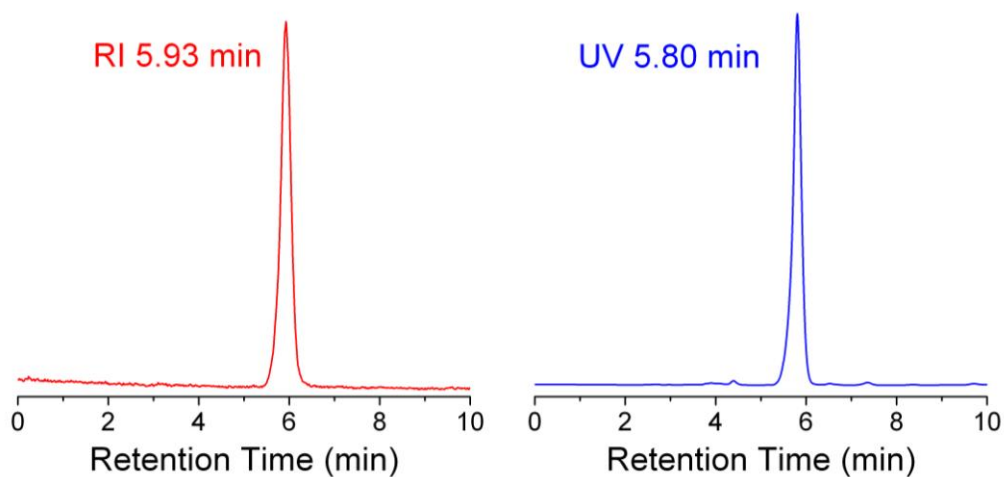


Figure S4. HPLC profiles of [^{18}F]**33** and **33**

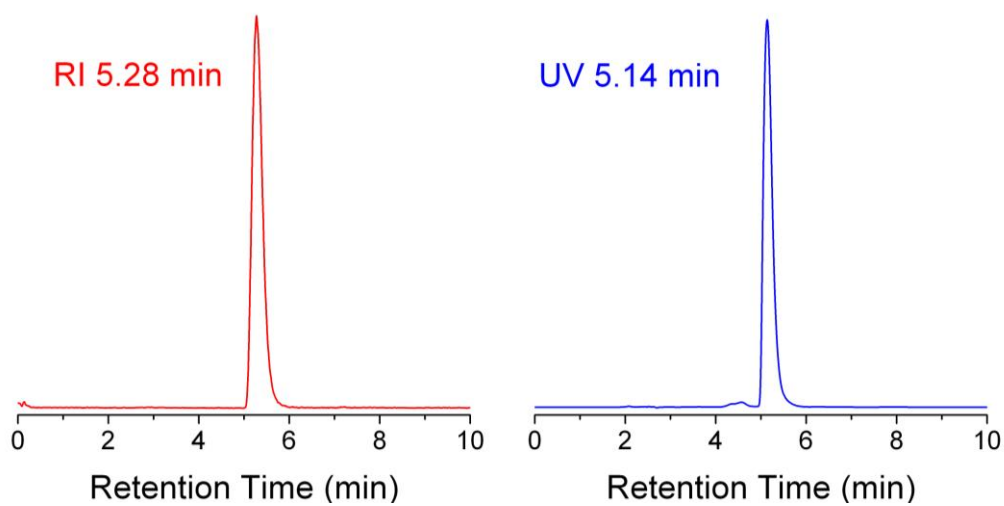


Figure S5. HPLC profiles of [^{18}F]**41** and **41**

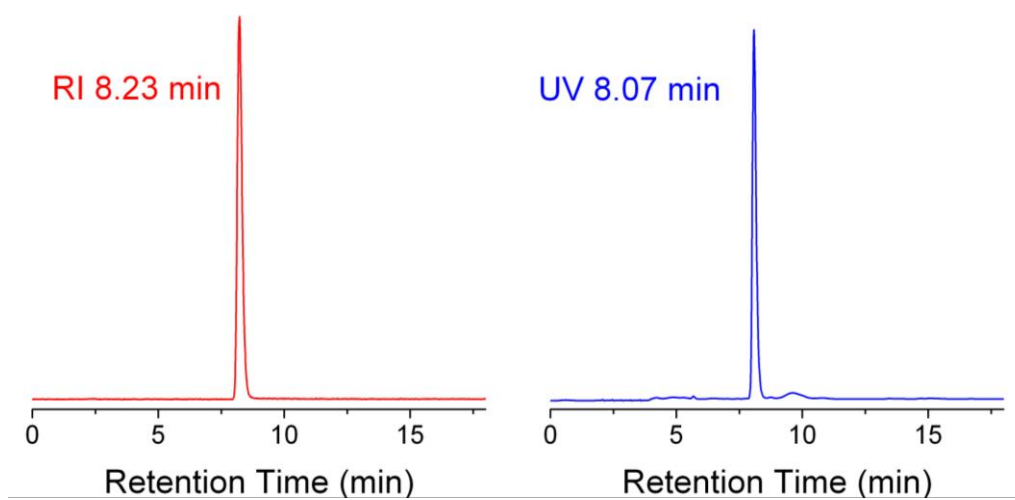


Figure S6. HPLC profiles of [^{18}F]**43** and **43**

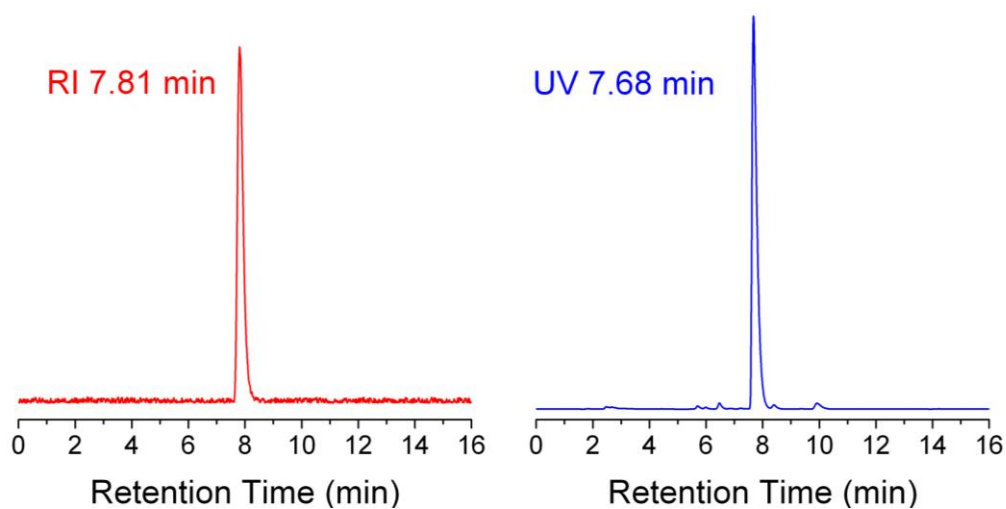
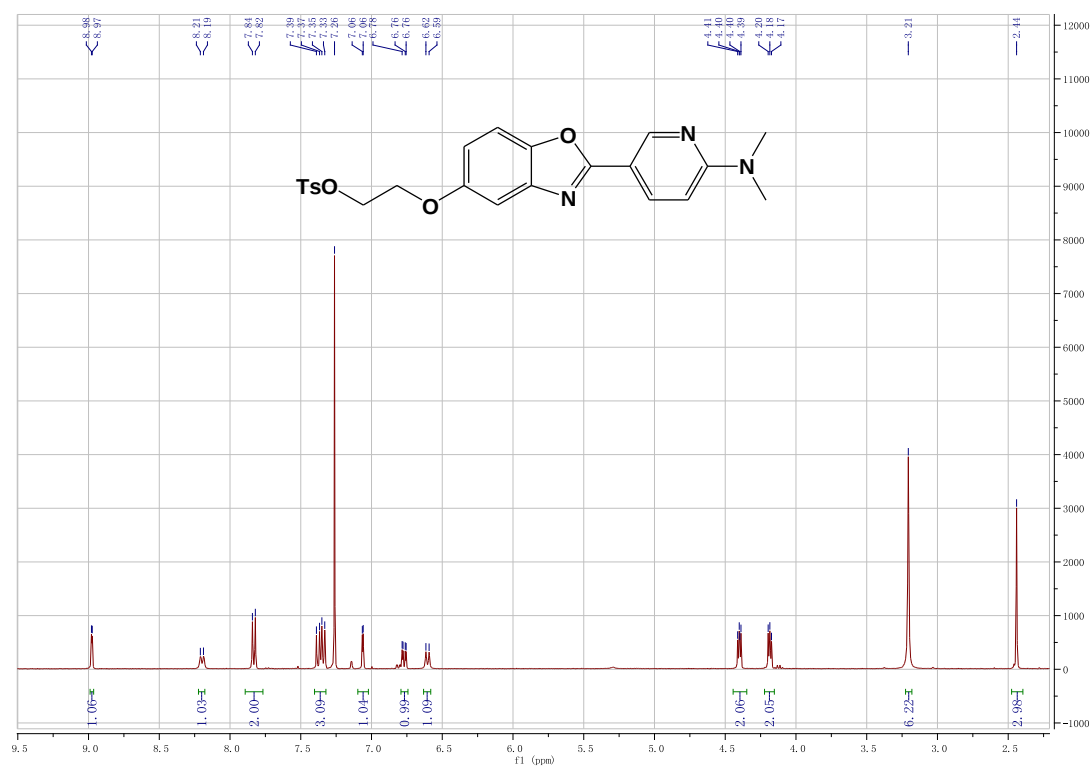


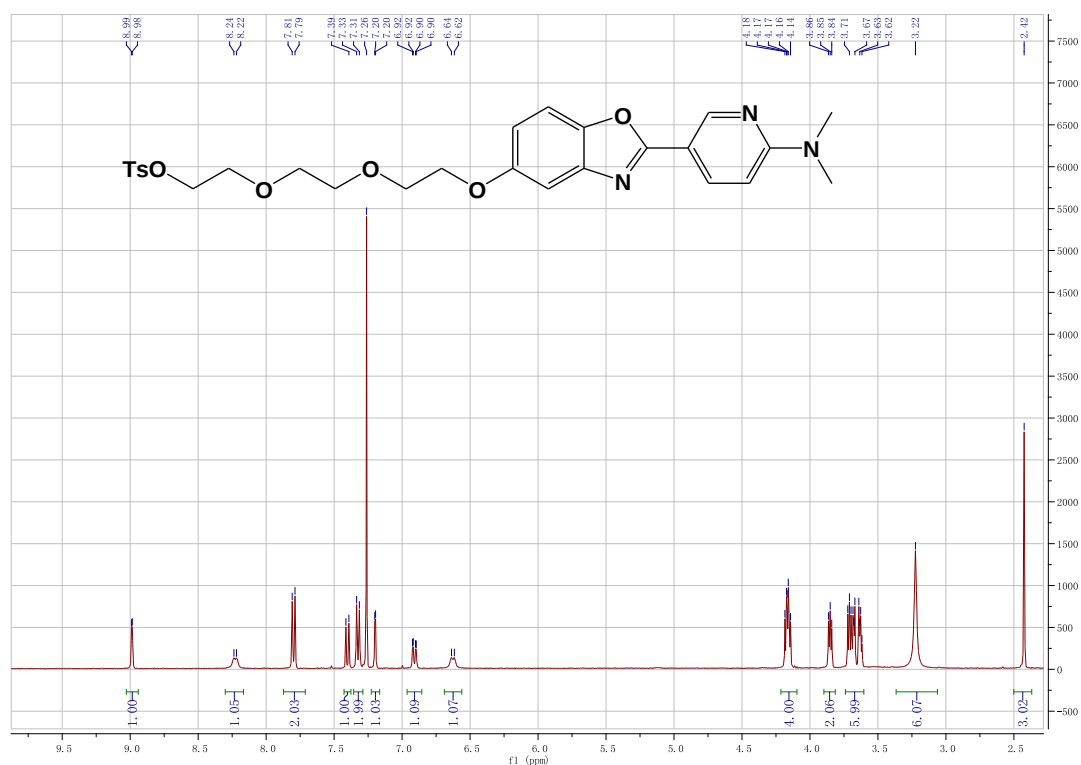
Figure S7. HPLC profiles of [^{18}F]44 and 44

3. ^1H -NMR for precursors

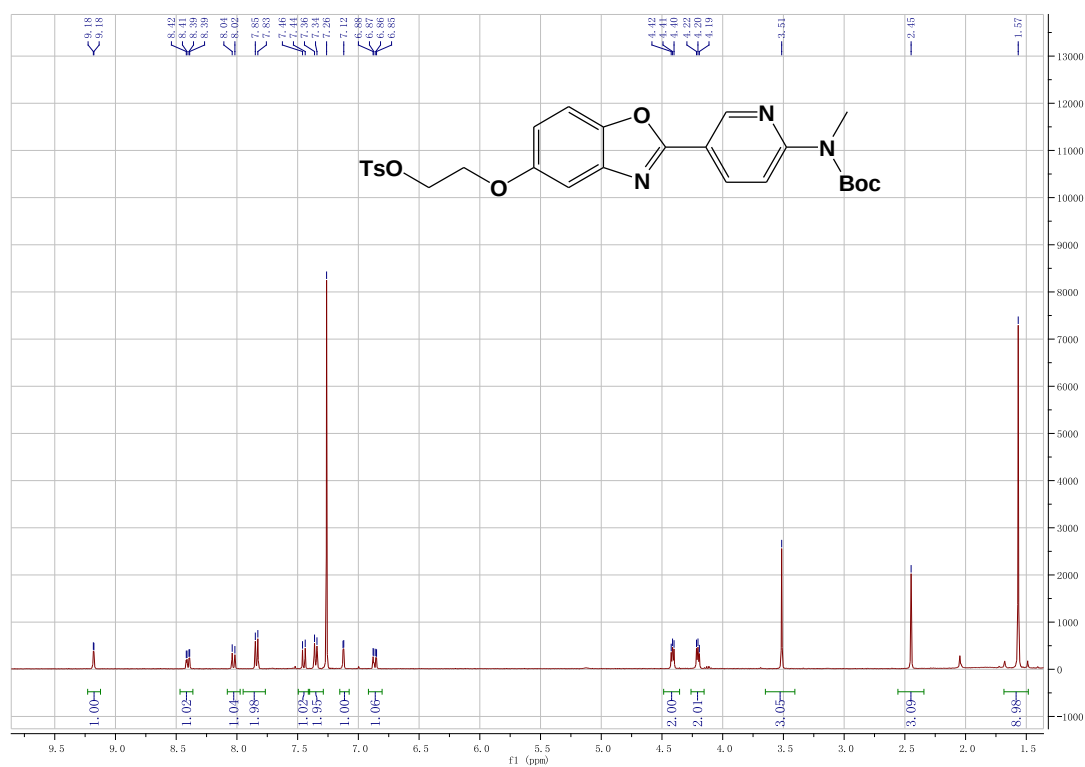
^1H -NMR for compound 46

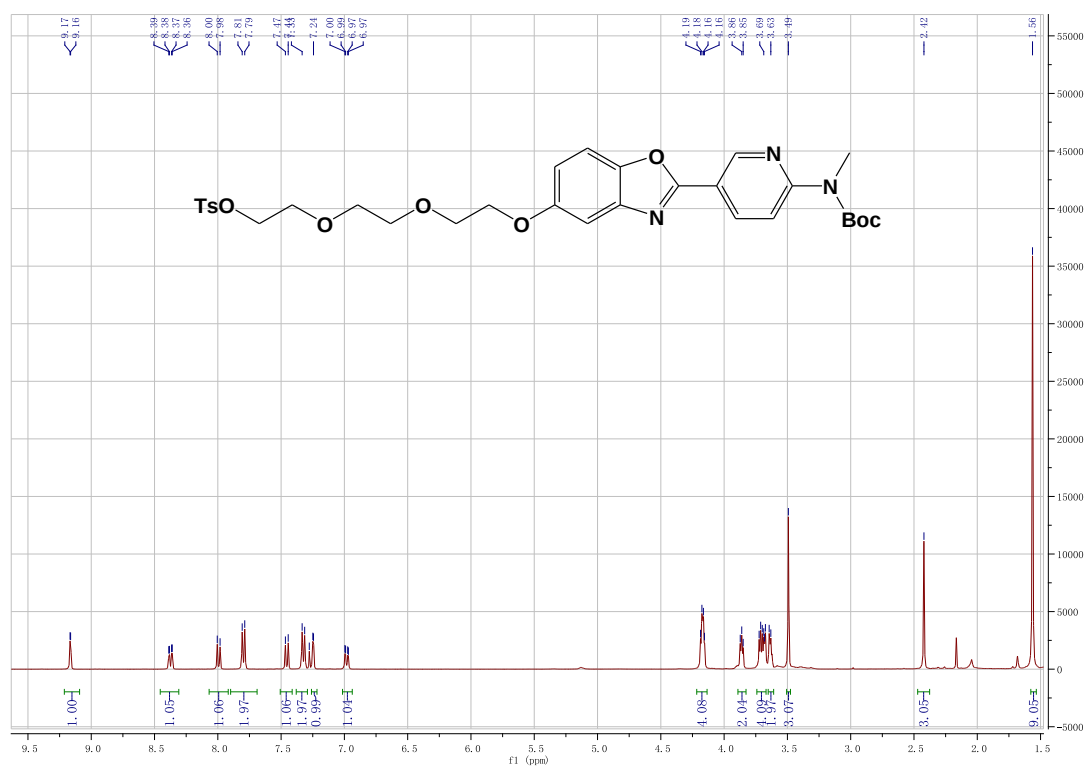
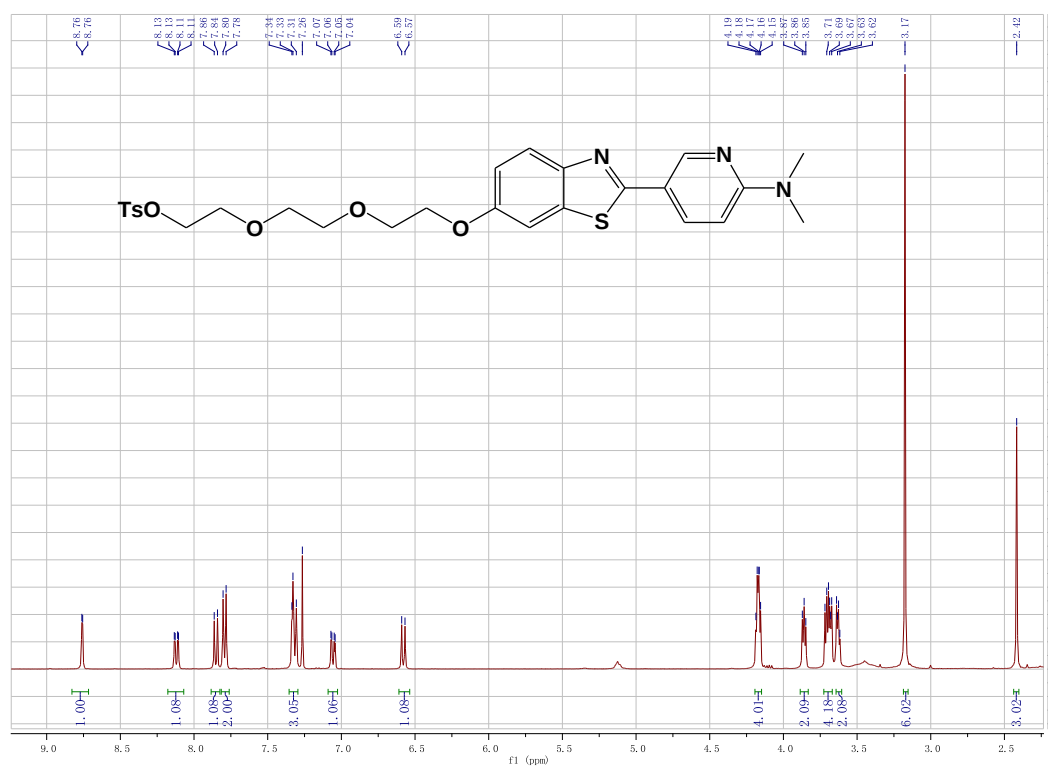


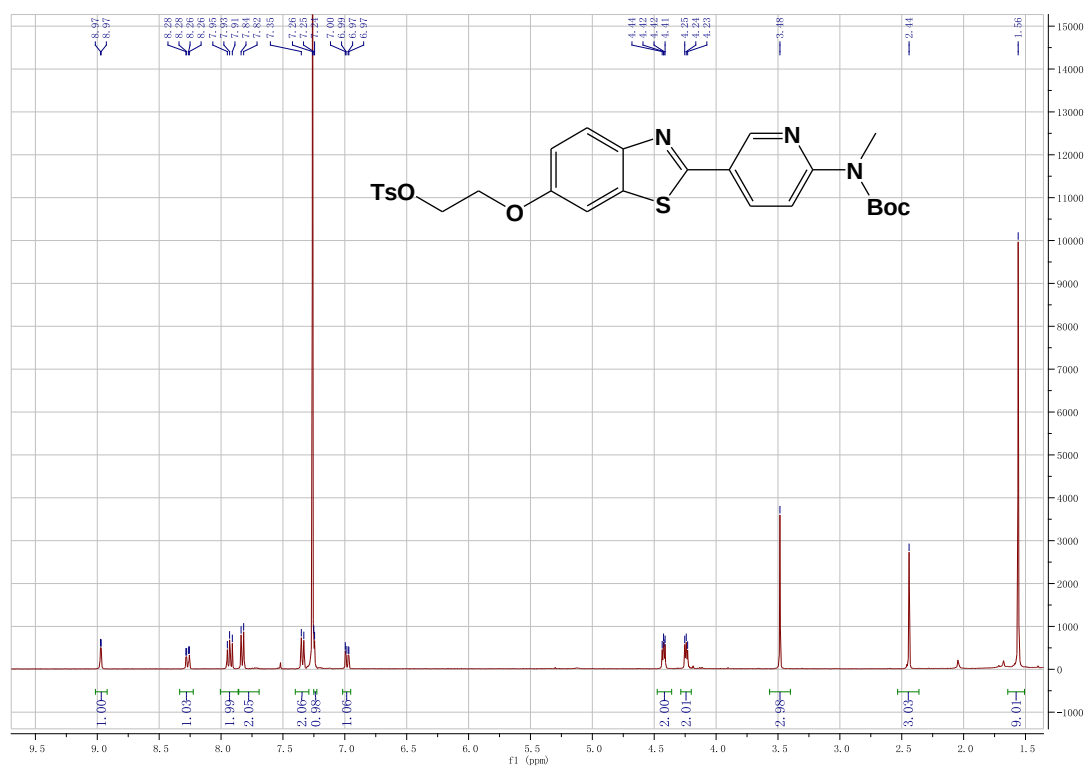
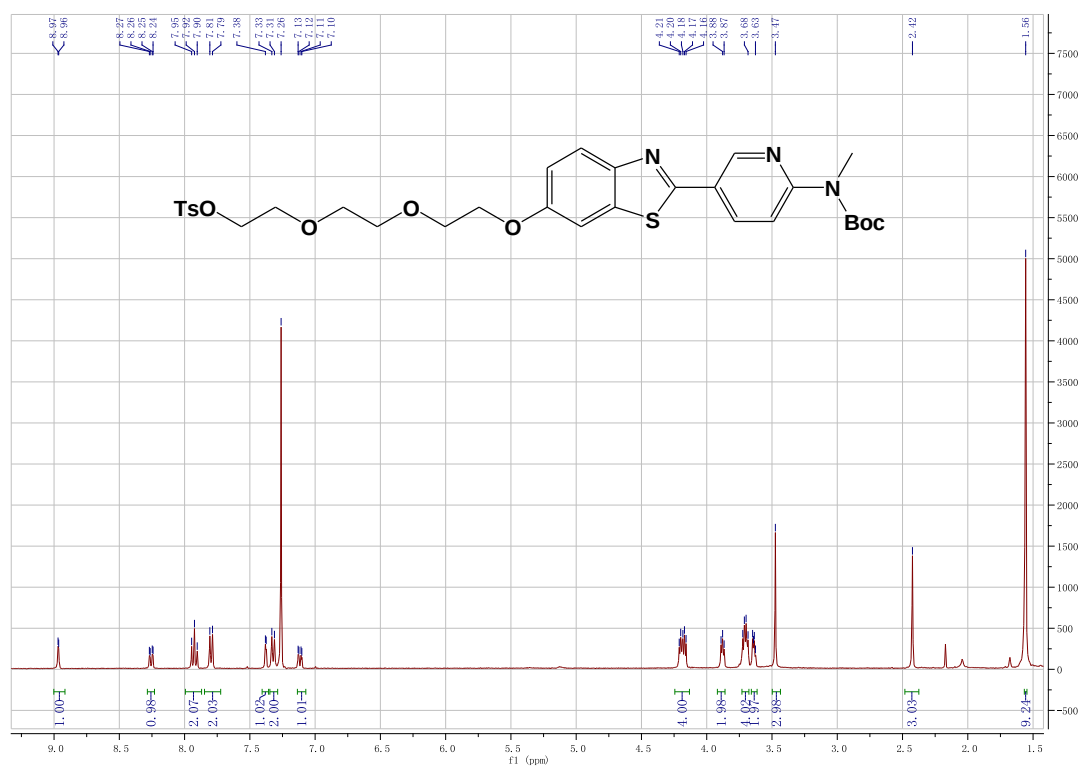
¹H-NMR for compound 47



¹H-NMR for compound 50

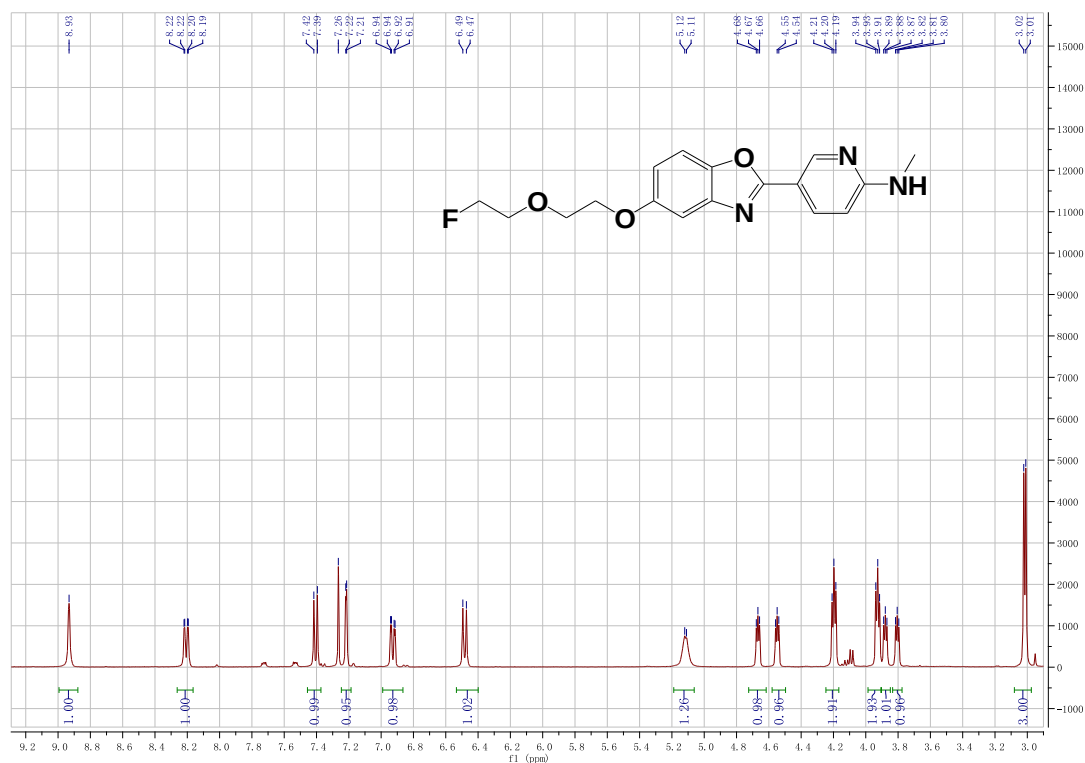


¹H-NMR for compound **51**¹H-NMR for compound **52**

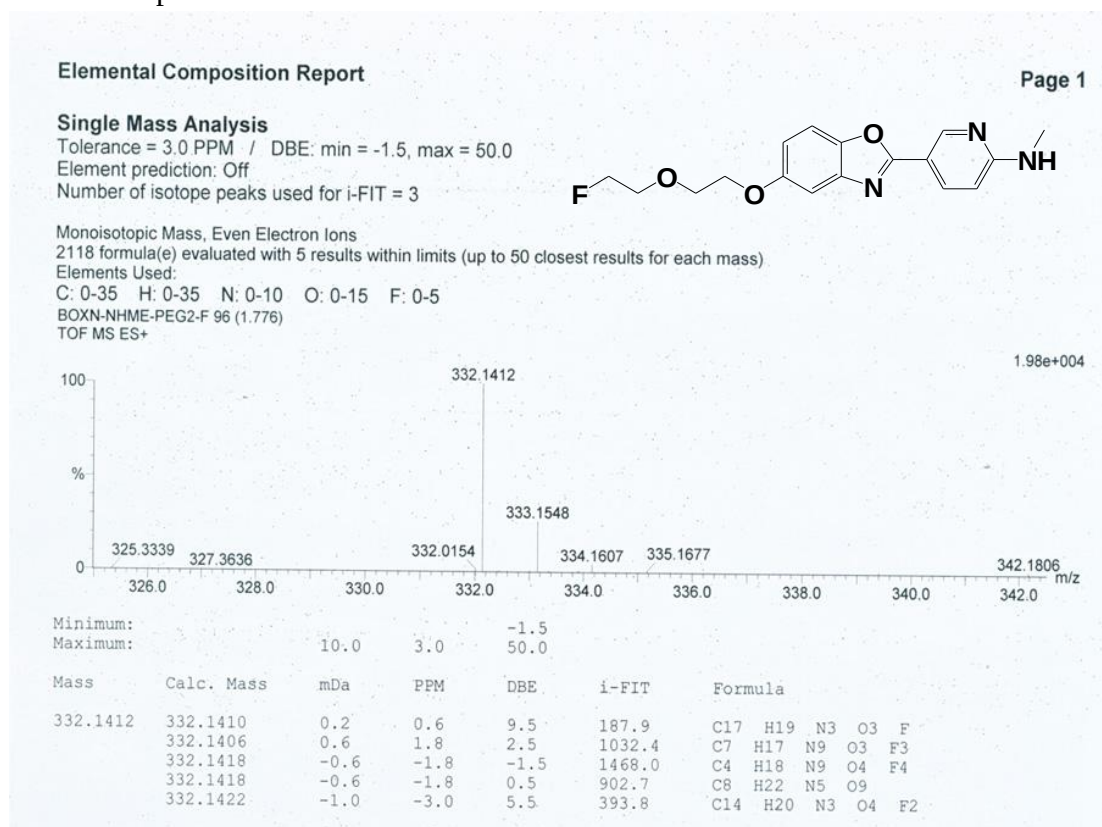
¹H-NMR for compound 55¹H-NMR for compound **56**

4. ¹H-NMR and HRMS of key target compounds.

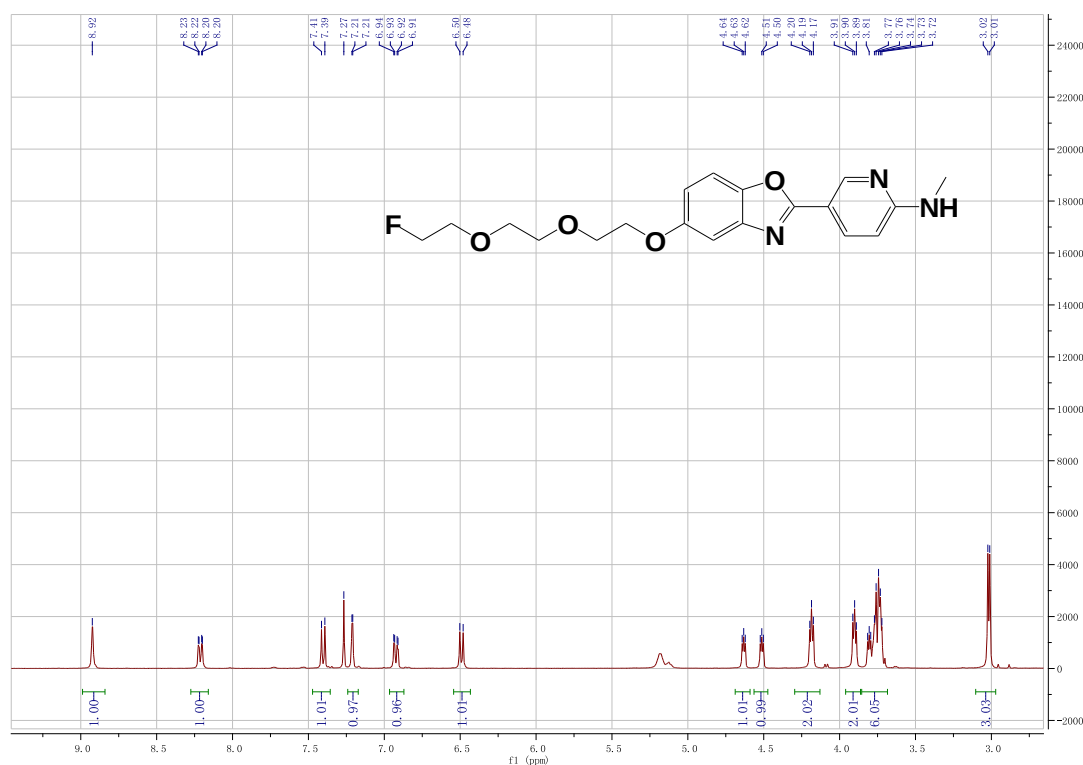
¹H-NMR for compound 28



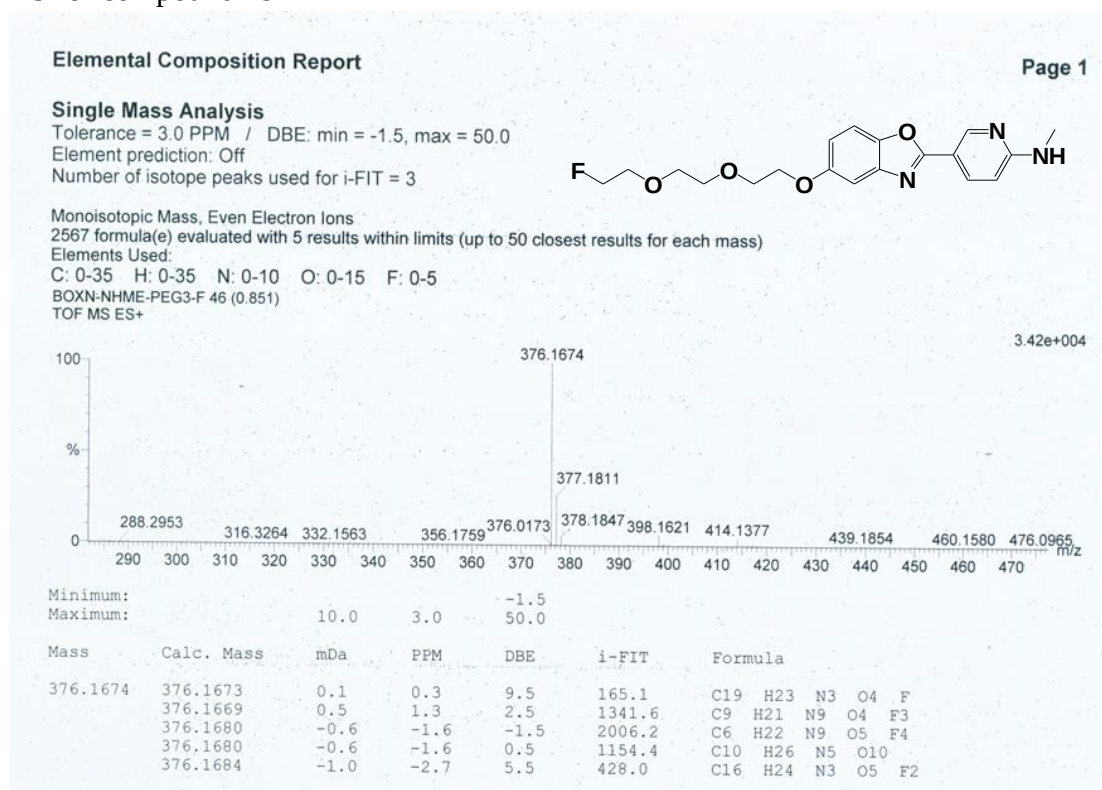
HRMS for compound 28



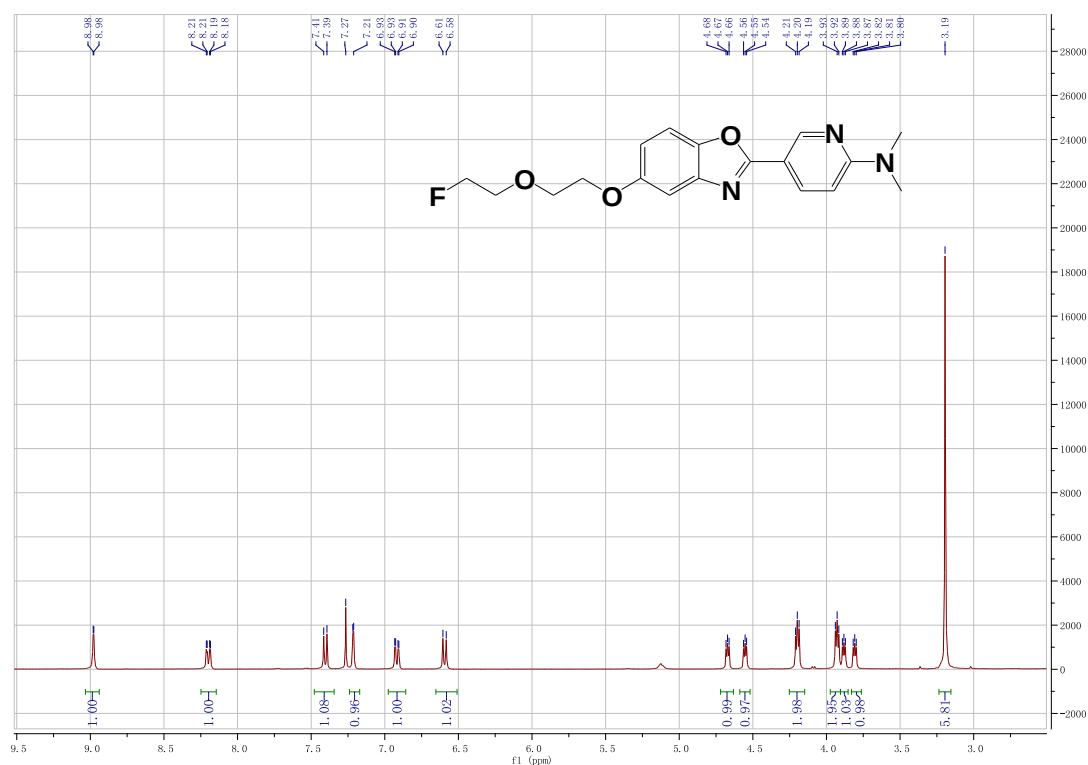
¹H-NMR for compound 29



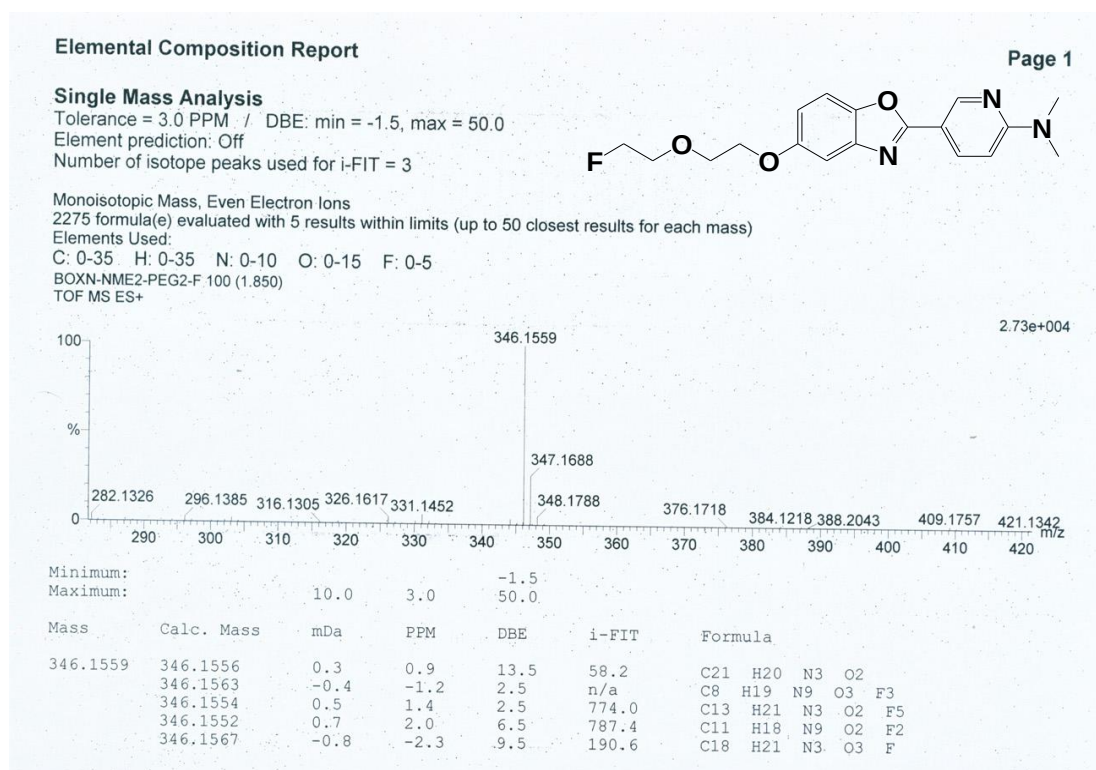
HRMS for compound 29



¹H-NMR for compound 30



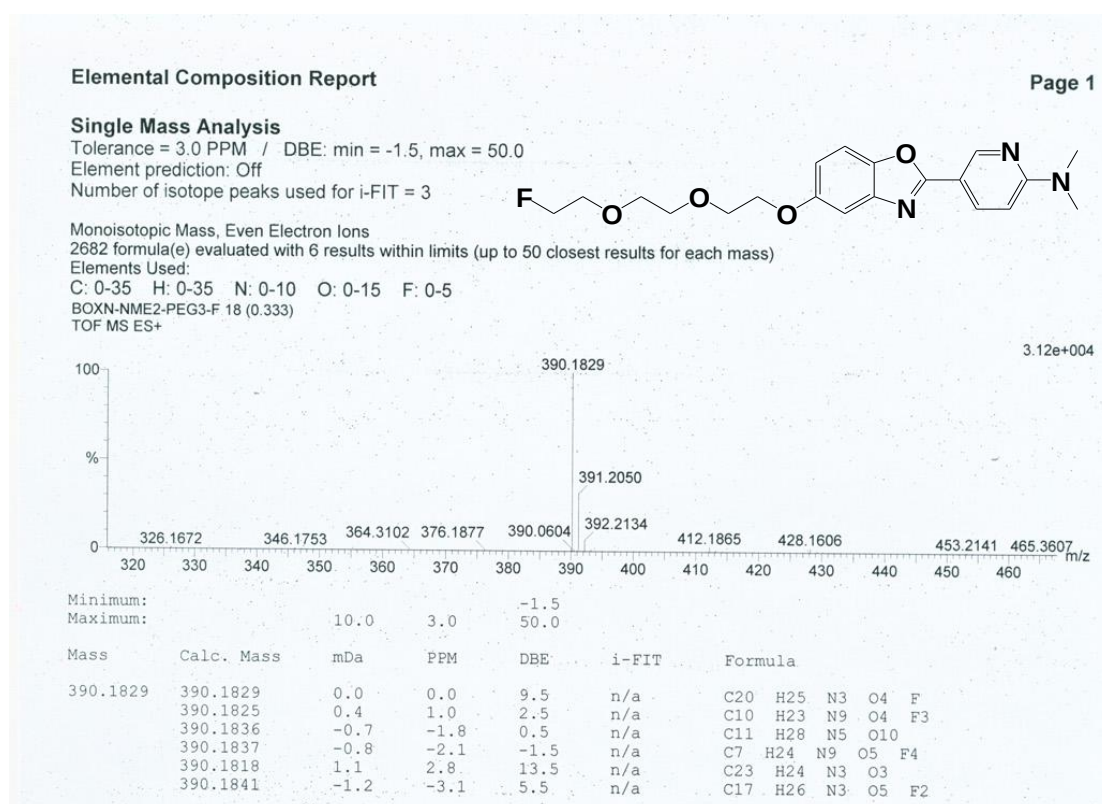
HRMS for compound 30



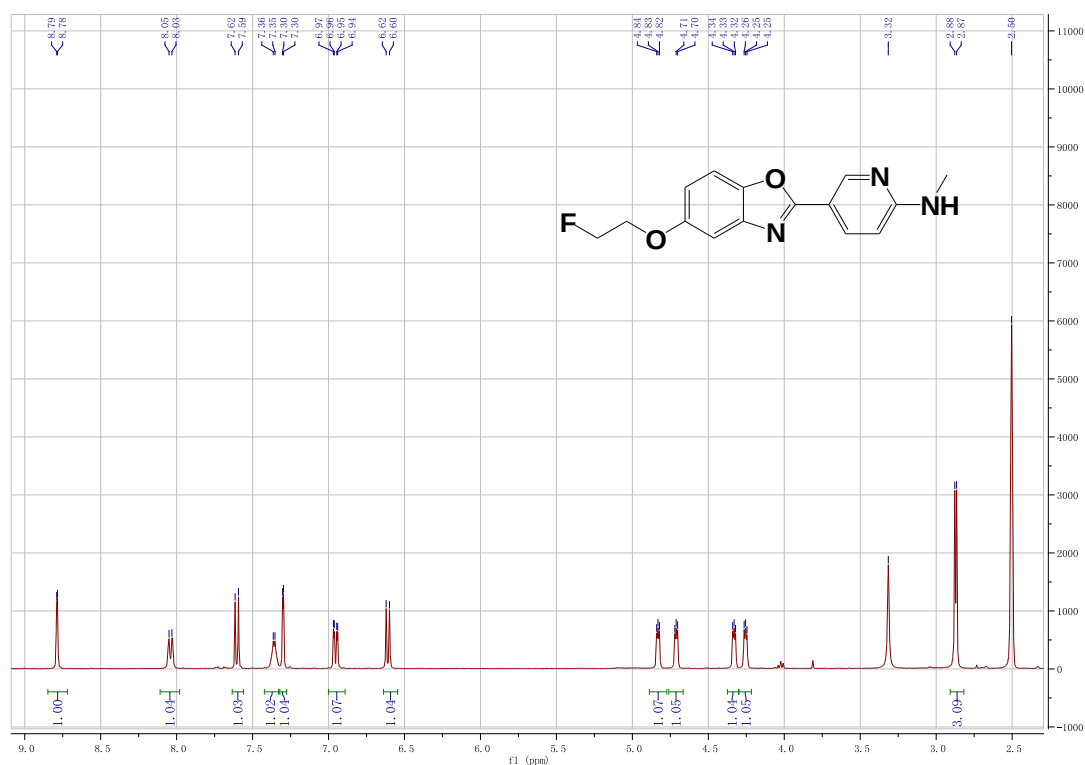
¹H-NMR for compound **31**



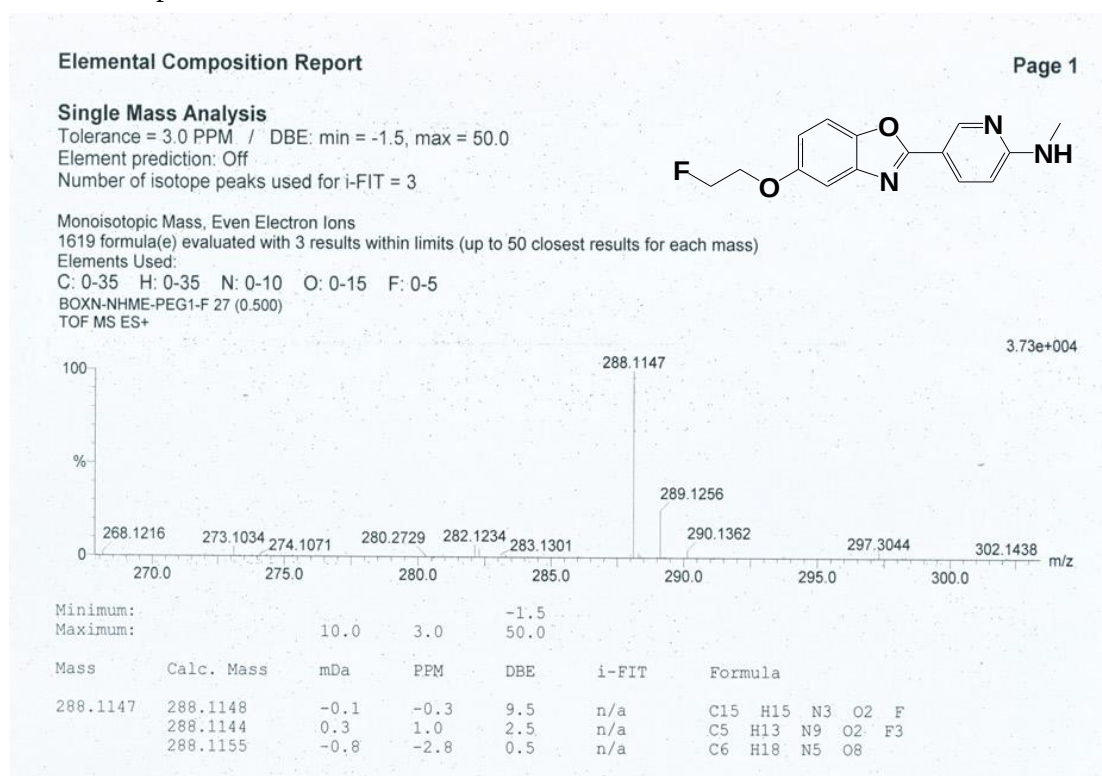
HRMS for compound **31**



¹H-NMR for compound 32



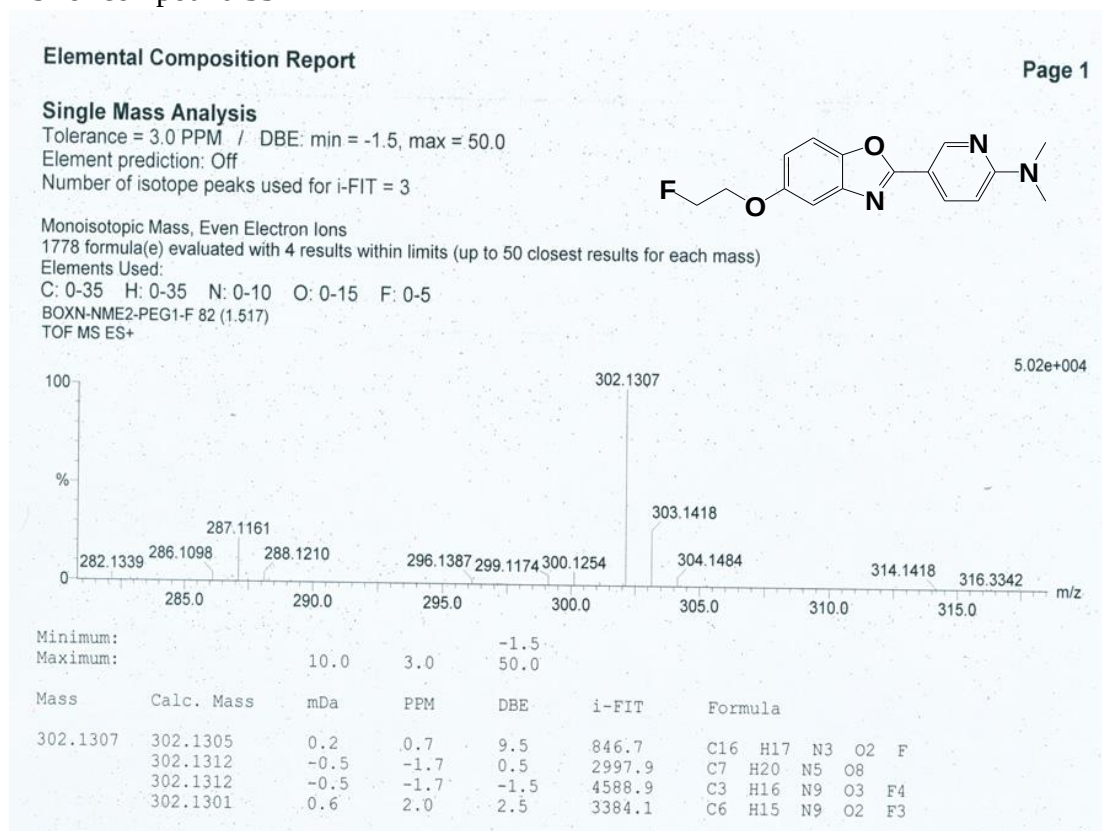
HRMS for compound 32



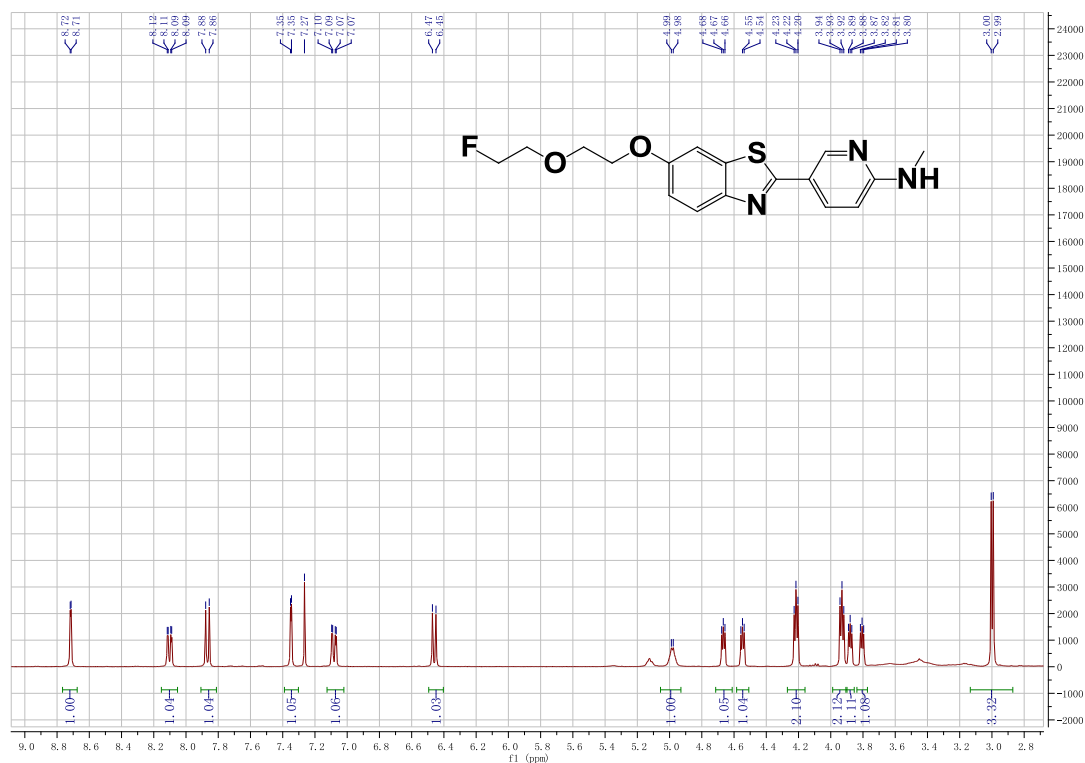
¹H-NMR for compound **33**



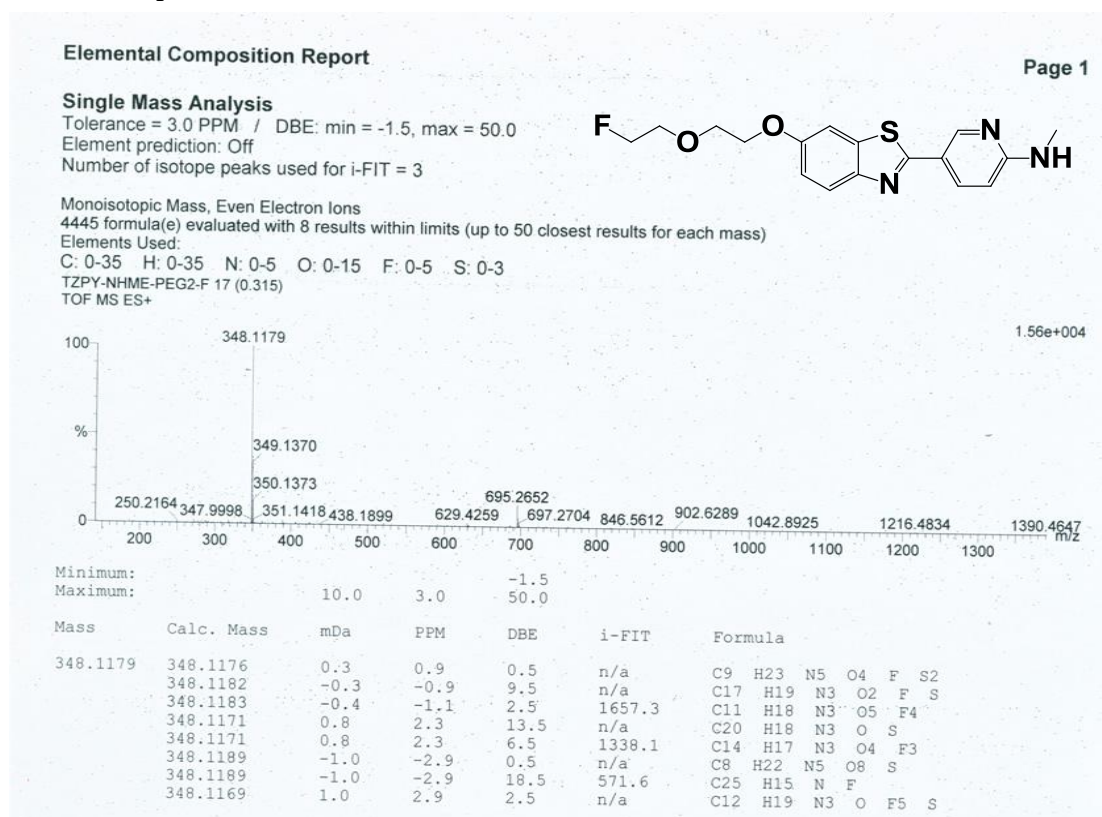
HRMS for compound **33**



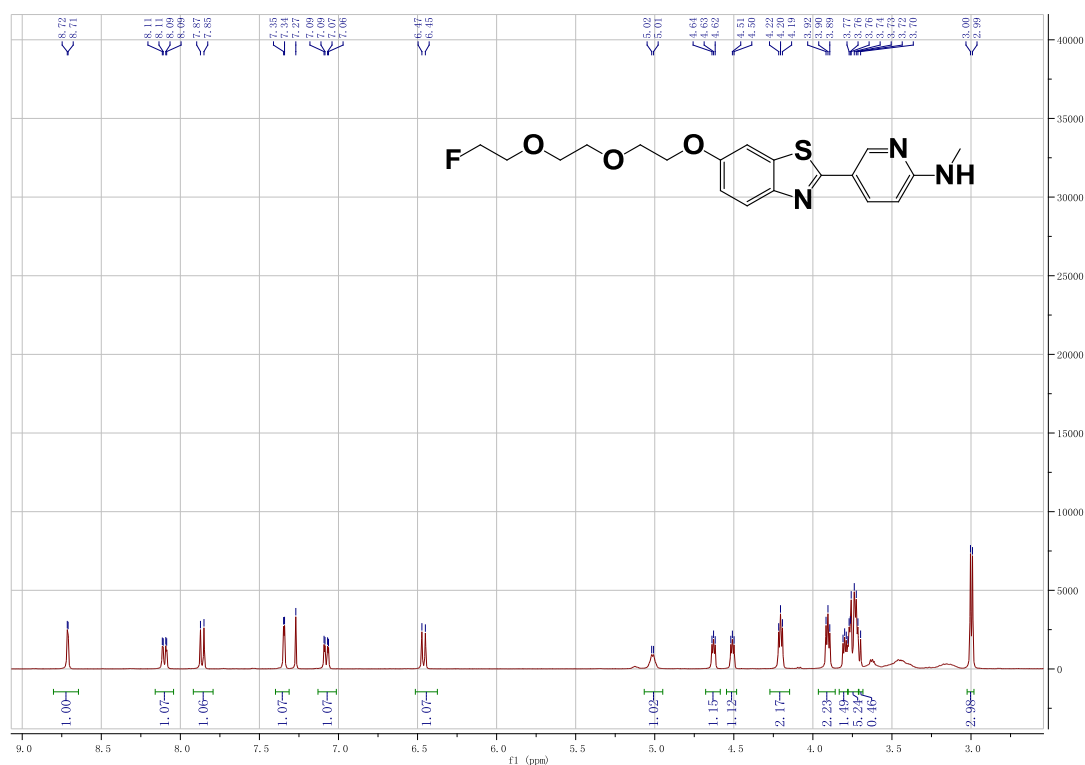
¹H-NMR for compound 40



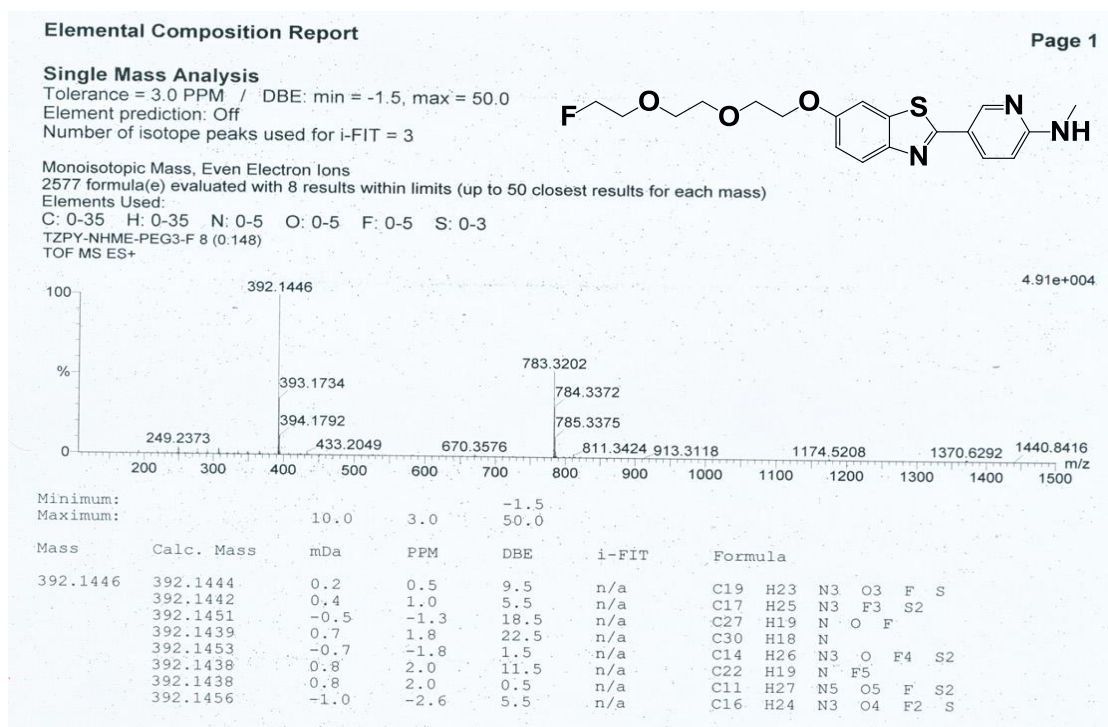
HRMS for compound 40



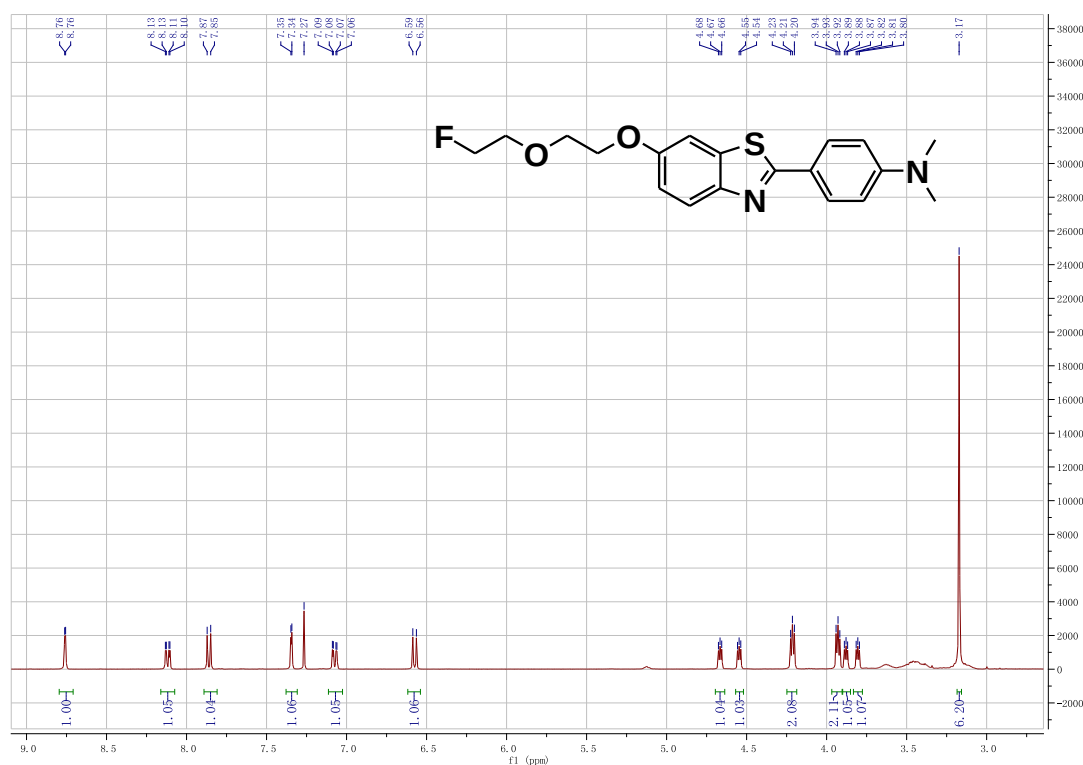
¹H-NMR for compound **41**



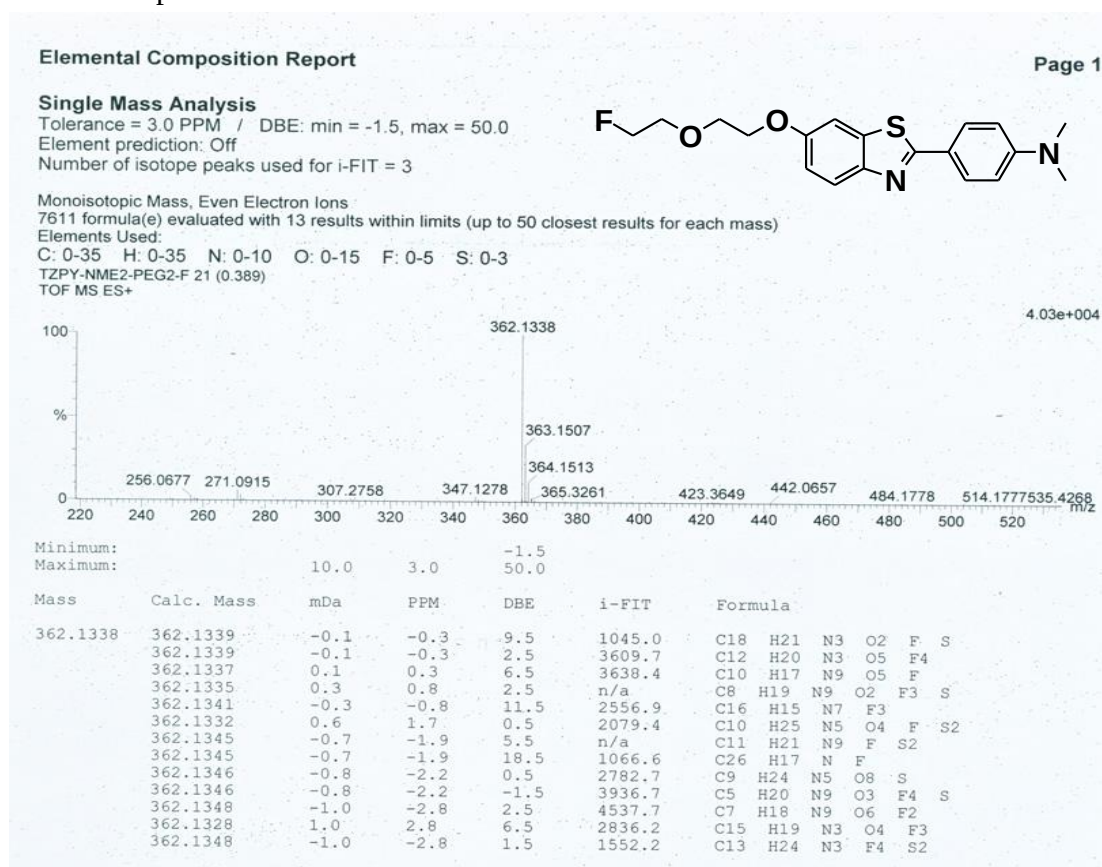
HRMS for compound **41**



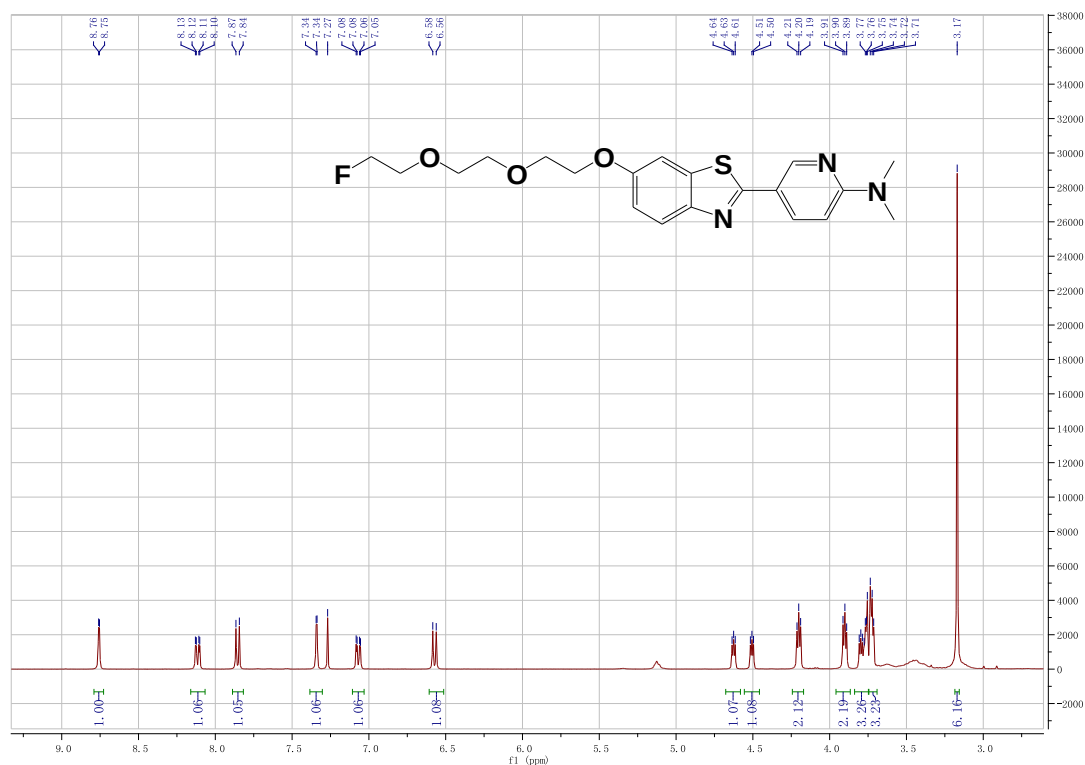
¹H-NMR for compound 42



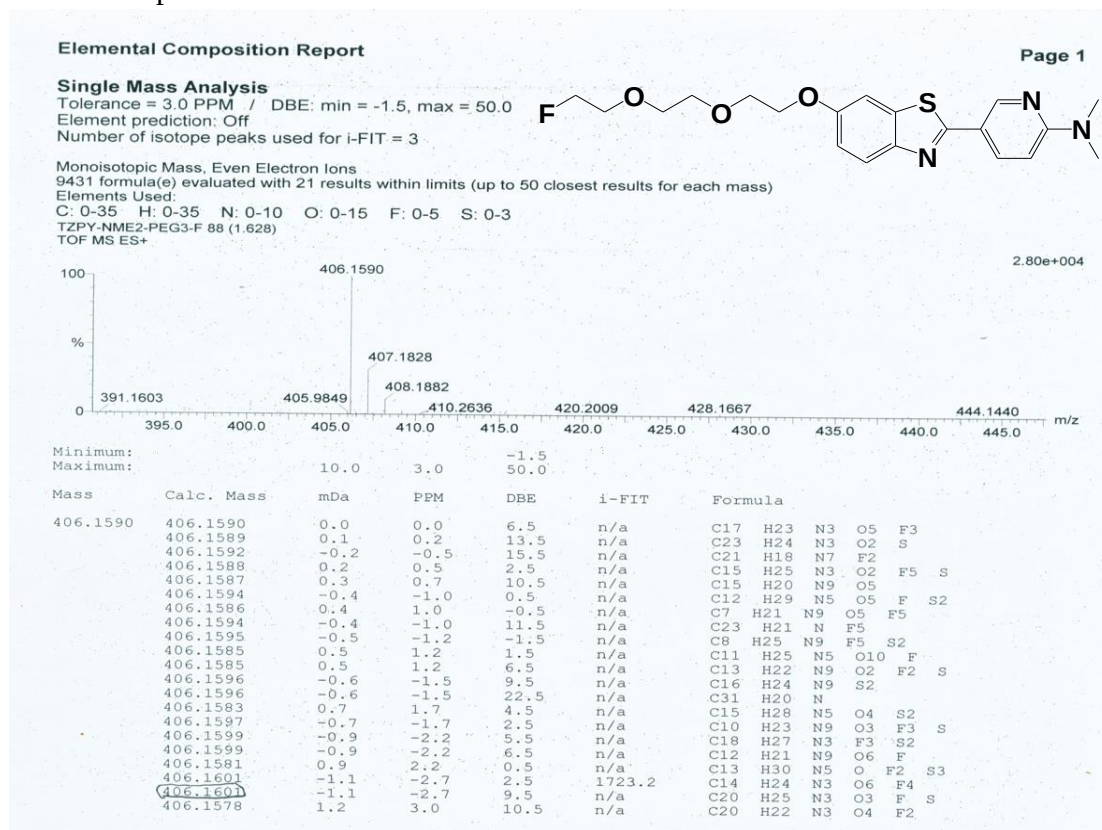
HRMS for compound 42



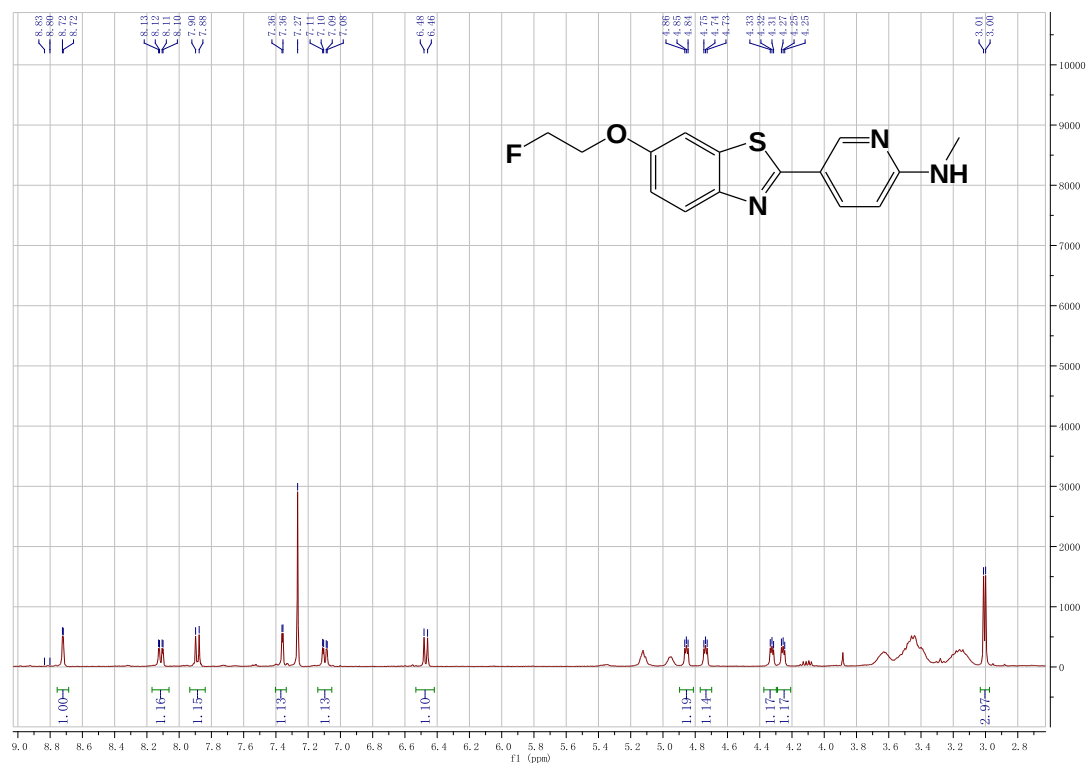
¹H-NMR for compound 43



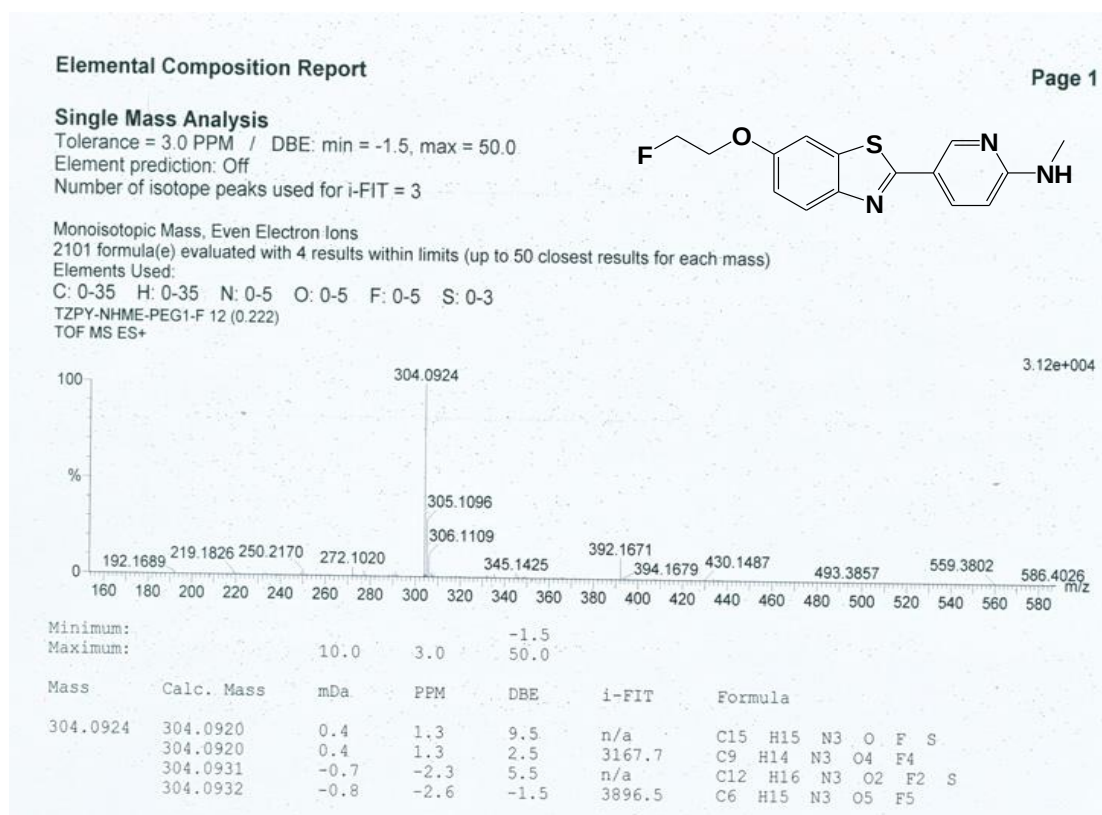
HRMS for compound 43



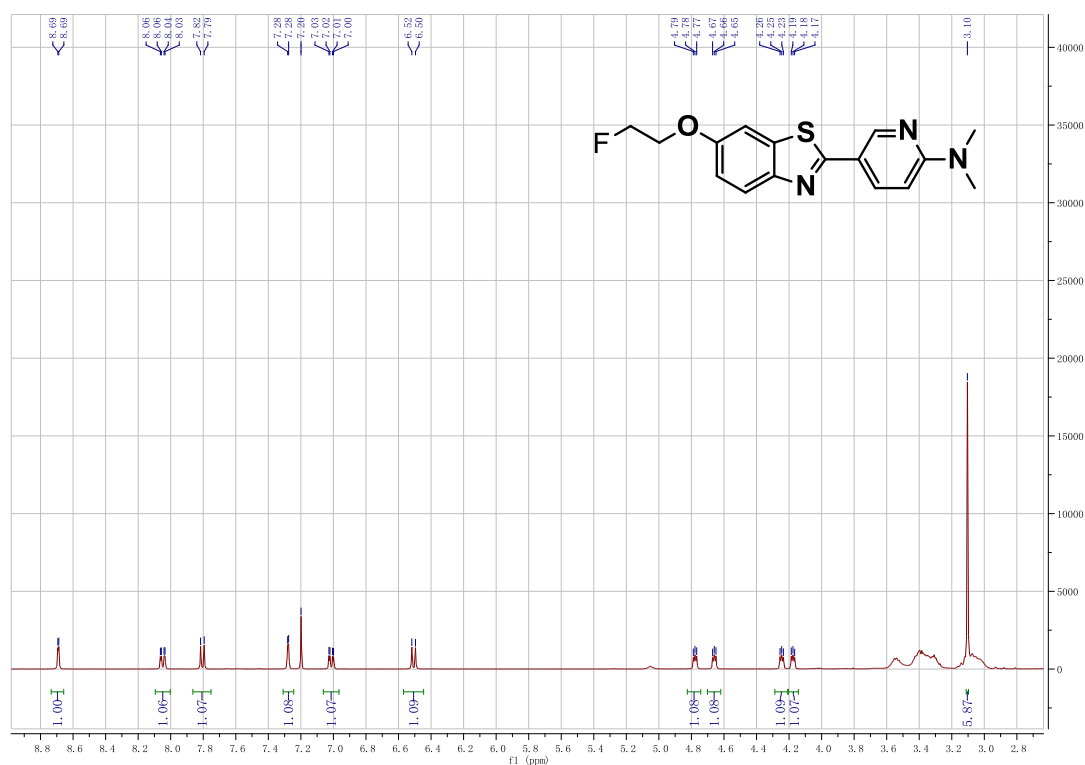
¹H-NMR for compound 44



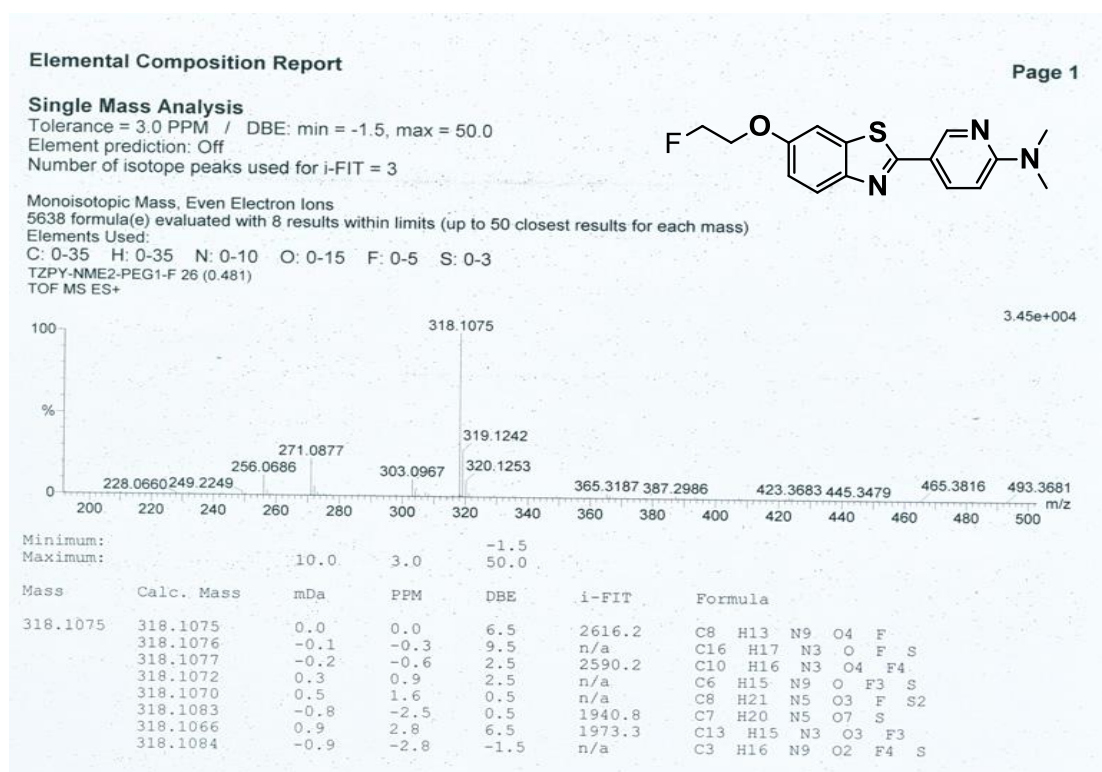
HRMS for compound 44



¹H-NMR for compound 45

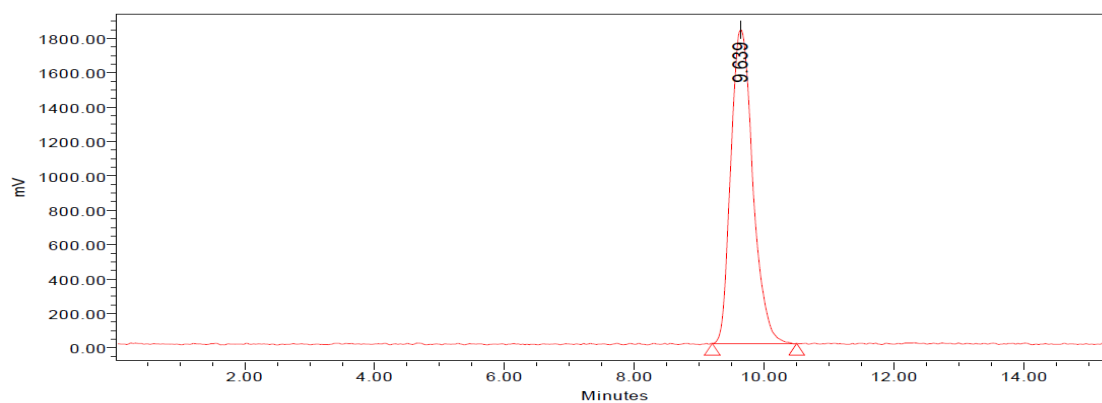


HRMS for compound 45



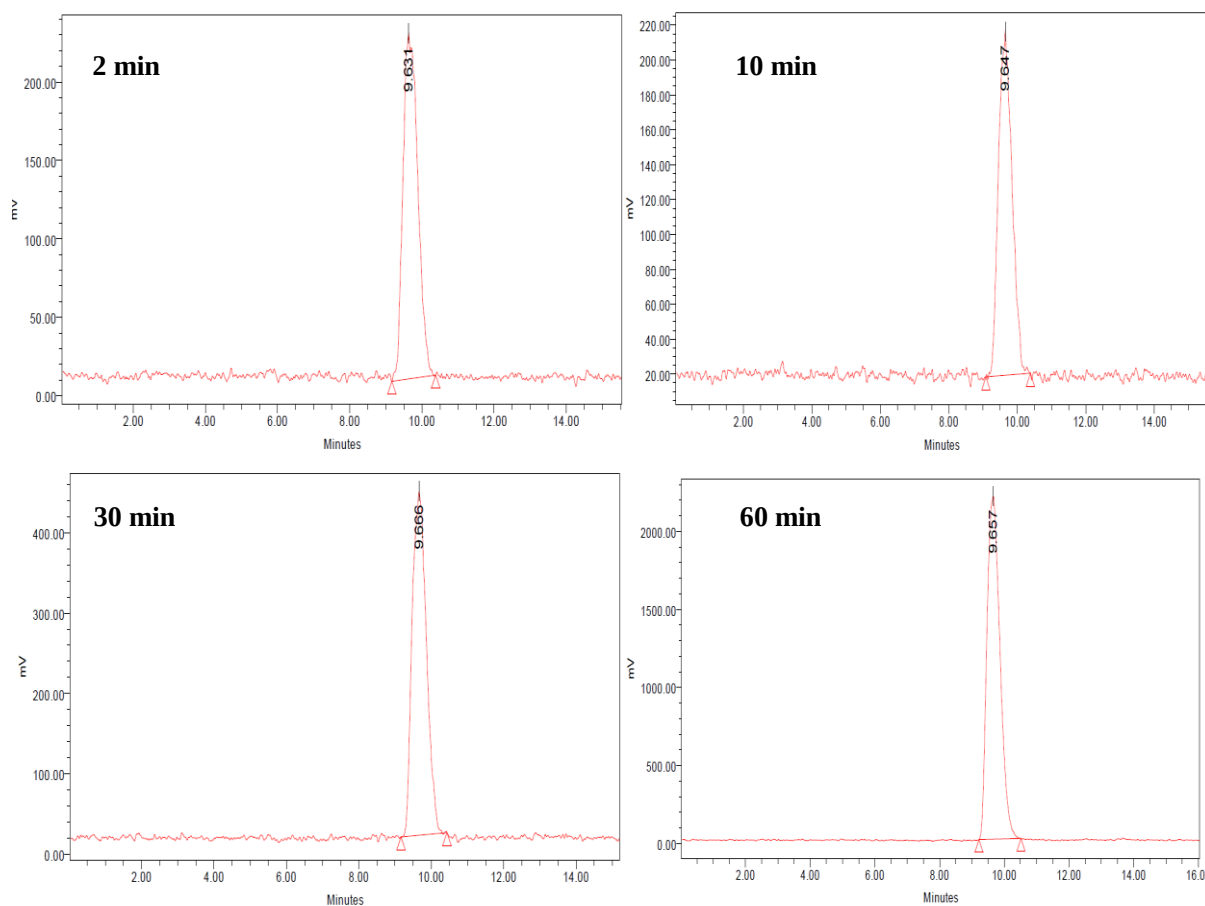
5. In vitro stability studies of [^{18}F]32

In vitro stability studies of [^{18}F]32 in saline solutions



6 h Saline Stability			
RT	Area	Height	% Area
9.639	43022077	1826031	100

In vitro stability studies of [^{18}F]32 in mice plasma



Plasma Stability									
Time	RT	Area	Height	% Area	Time	RT	Area	Height	% Area
2 min	9.631	6311912	219808	100	10 min	9.647	5441379	196177	100
30 min	9.666	11730286	428164	100	60 min	9.657	61454369	2201124	100