Supporting Information

Novel Aryltriazole Acyclic *C*-Azanucleosides as Anticancer Candidates

Yanhua Zhang[a#], Yun Lin[a#], Qianqian Hou[a], Xi Liu[a], Sabrina Pricl[b,c], Ling Peng[d], Yi Xia[a]*

[a] Chongqing Key Laboratory of Natural Product Synthesis and Drug Research, School of Pharmaceutical Sciences, Chongqing University, Chongqing, 401331, China.

[b] Molecular Biology and Nanotechnology Laboratory (MolBNL@UniTS), DEA, University of Trieste, Trieste, Italy

[c] Department of General Biophysics, Faculty of Biology and Environmental Protection, University of Lodz, 90-236 Lodz, Poland

[d] Aix-Marseille Université, CNRS, Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), UMR 7325, Equipe Labellisé par La Ligue, 13288 Marseille, France.

*Corresponding Author

Dr. Yi XIA, Email: yixia@cqu.edu.cn

[#] These authors contribute equally to this work

Table of Contents

Figure S1. The UV-Visible spectrum of **Ia**, **If**, **Ig**, **Ii**, **Ij**, **Ik**, **Il** and **II** in MeOH (50 μM) was recorded on Agilent Cary 60 UV-Vis Spectrophotometer within the spectral region of 200-400 nm.

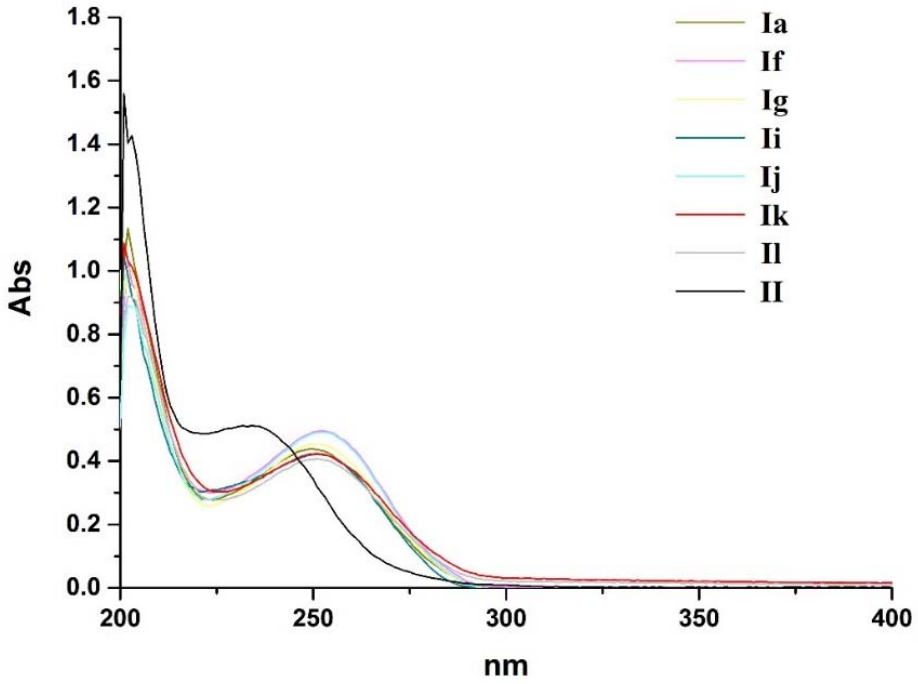


Figure S2. 1D NOESY spectra of **Ia**, **If**, **Ig**, **Ij** and **Ik** dissolved in $CDCl_3$ (20mg/mL) using a 800 ms NOESY mixing time was recorded on Agilent DD2 600-MR. The proton (H*) in triazole ring was selectively irradiated and the strong NOE at 7.6 ppm (H_A) and 4.0 ppm (H_B) was observed.

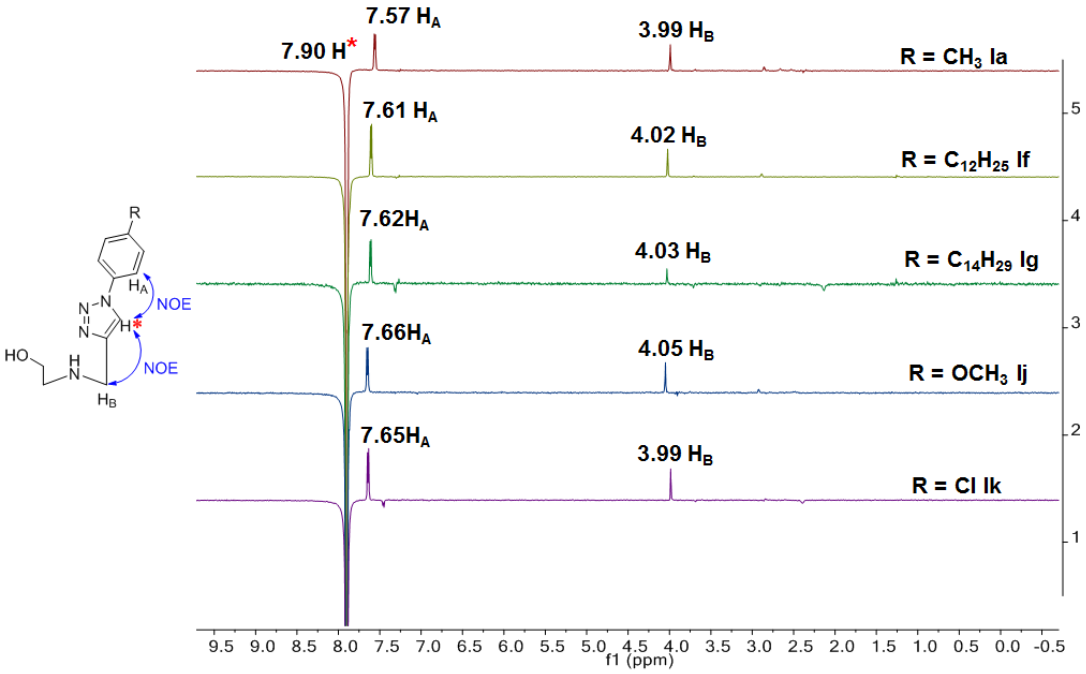


Figure S3. Compound **Ig** predominantly induced apoptosis in cancer cells with negligible necrosis. (A) Panc-1 cells were treated with different doses of **Ig** for 48 h and the percentage of cells undergoing apoptosis (Annexin V-positive cells) and necrosis (PI-positive cells) was determined with flow cytometry. Untreated cells were used as the reference control. (B) Compound **Ig** efficiently induced the cleavage of PARP and downregulation of BCL-2 in Panc-1 cells. BCL-2 and PARP protein levels after treatment with different concentrations of compound **Ig** were analyzed by use of western blotting, with β-actin as the reference. (C) Necrosis induced by different concentrations of **Ig** in Panc-1 cells was assessed by LDH assays.

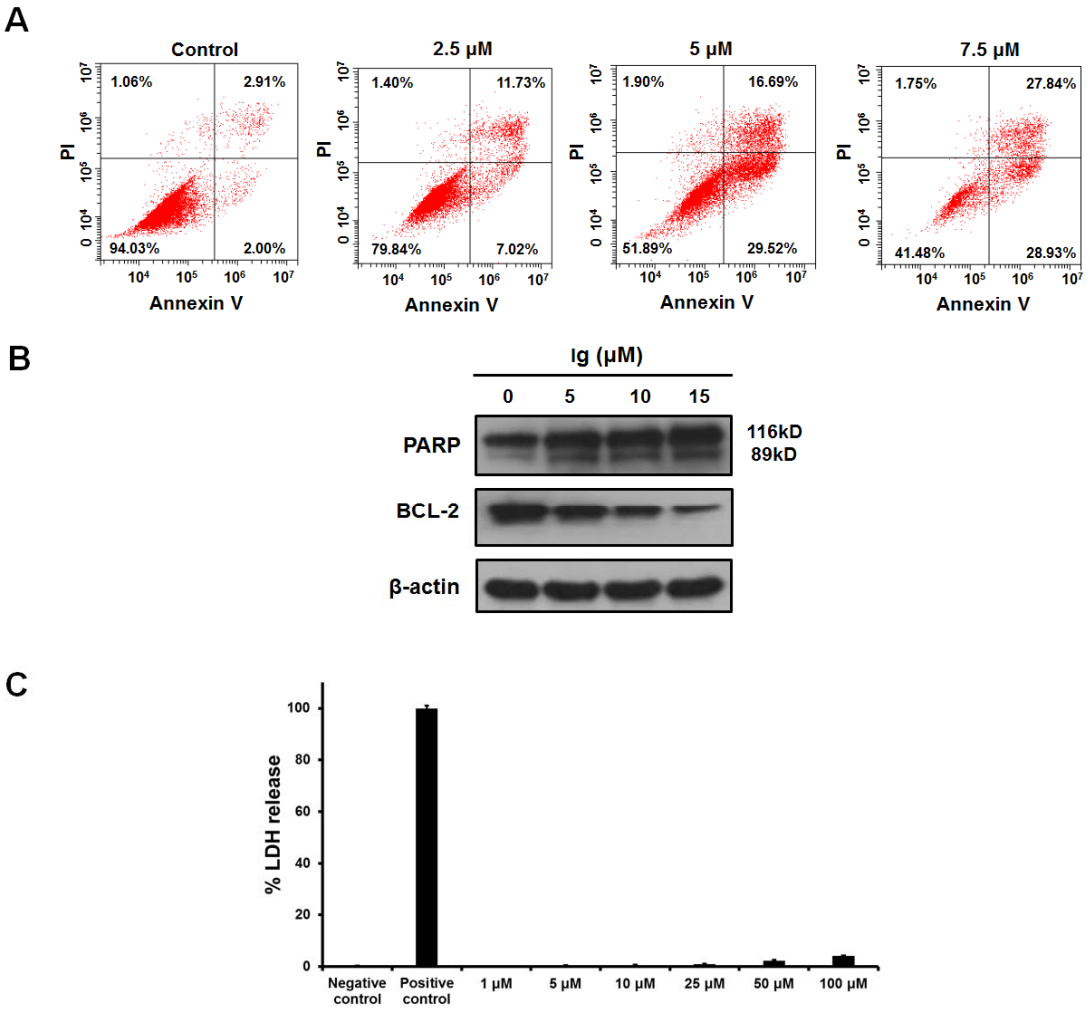


Figure S4. Compound **Ic** and **Ik** could not induce apoptosis or inhibit the expression of HSF1, HSP27, HSP70, HSP90α and eIF4E in Panc-1 cells. (A) Panc-1 cells were treated with **Ic** and **Ik** (15μM) for 48 h and the percentage of cells undergoing apoptosis (Annexin V-positive cells) and necrosis (PI-positive cells) was determined with flow cytometry. Untreated cells were used as the reference control. (B) Panc-1 cells were treated with **Ic** and **Ik**. Then the BCL-2 and PARP protein levels after treatment were analyzed by western blotting, with β-actin as the reference. (C) Necrosis induced by different concentrations of **Ic** and **Ik** in Panc-1 cells was assessed by LDH assays. (D) Panc-1 cells were treated with **Ic** and **Ik**. Then the **p**rotein levels of HSF1, HSP27, HSP70, HSP90α and eIF4E were analyzed by western blotting, with β-actin as the reference.

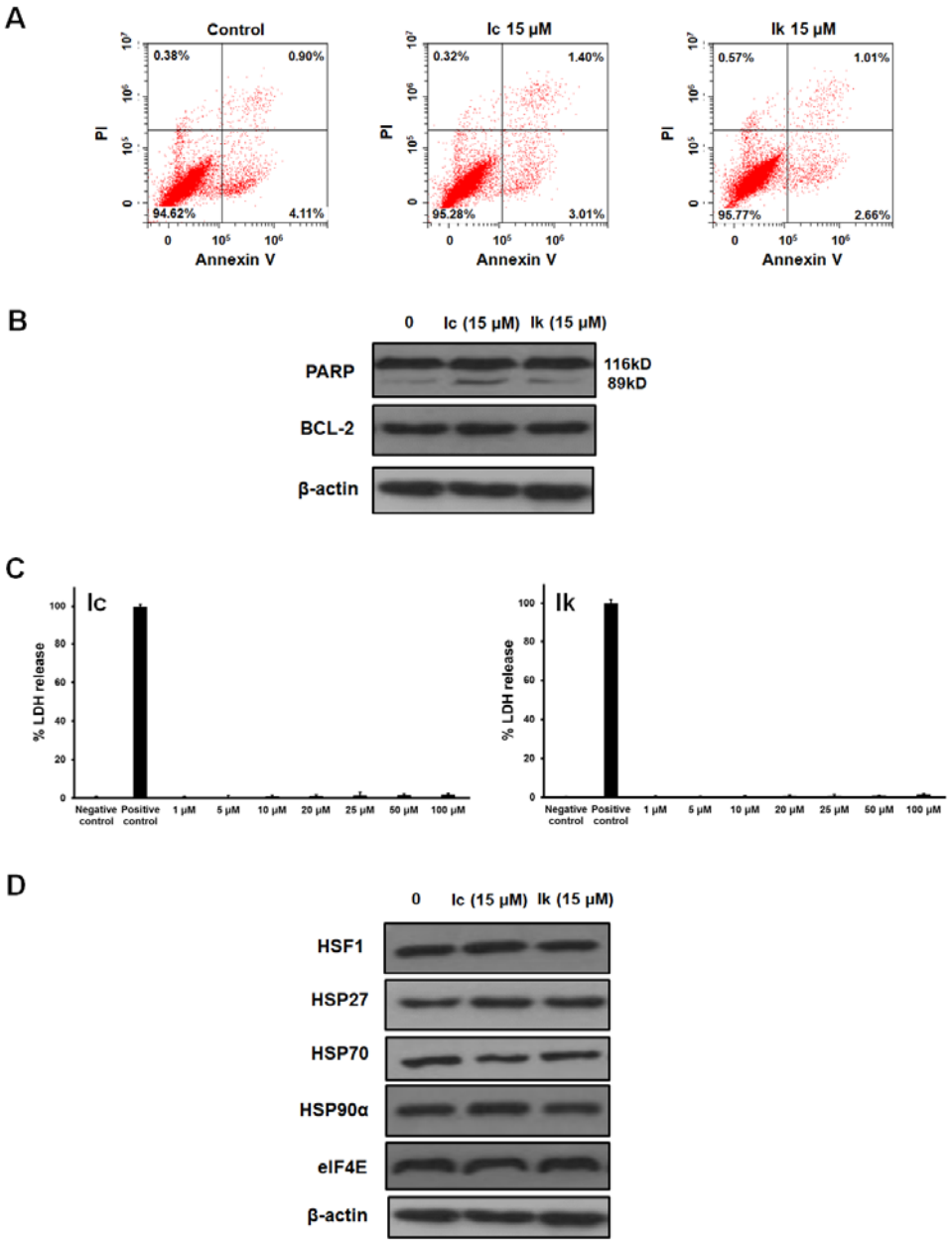


Figure S5. Compound **Ig** efficiently inhibited the expression of HSF1, HSP27, HSP70, HSP90α and eIF4E in Panc-1 cells (B). Panc-1 cells were treated with **If** at indicated concentrations. Protein levels of HSF1, HSP27, HSP70, HSP90α and eIF4E were then analyzed by western blotting, with β-actin as the reference.

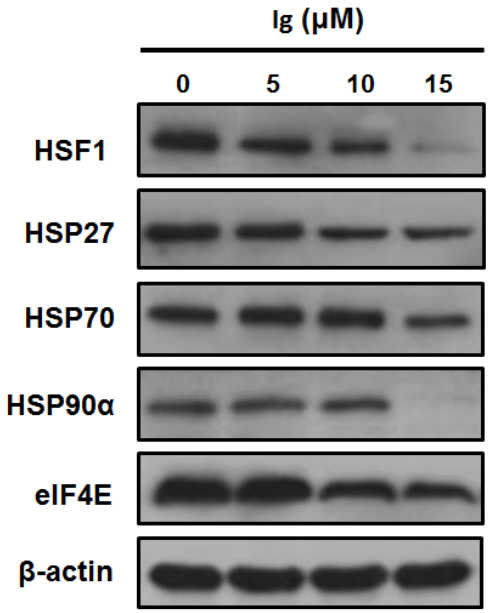
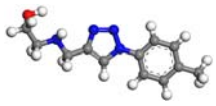
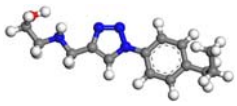
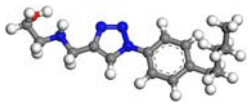
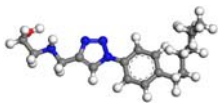
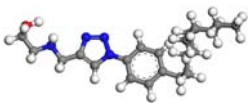
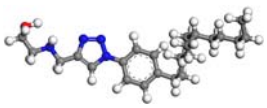
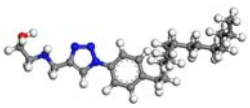
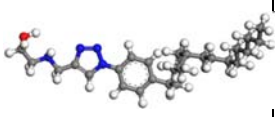
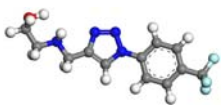
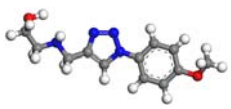
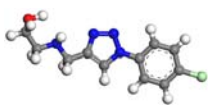


Table S1. Optimized structures and the corresponding values of the geometrical parameters for compounds **Ia-Il** as obtained from Density Functional (DFT) calculations performed at the B3LYP/6-311++G(d,p) level. Molecular structures are shown as atom-colored sticks-and-balls (C, gray; O, red; N, blue; H, white; F, light cyan; Cl, light green; Br, dark red).

Compound	**Structure**	**Dihedral angle 1 (º)**[a]	**Dihedral angle 2 (º)**[b]	**H-H distance (Å)**[c]
Ia		178.1	-178.2	2.21
Ib		178.7	-178.9	2.22
Ic		177.8	-177.6	2.21
Id		178.3	-178.1	2.21
Ie		177.4	-177.9	2.23
If		177.4	-177.2	2.23
Ig		177.3	-177.1	2.23
Ih		177.2	-177.3	2.23
Ii		178.4	-178.9	2.27
Ij		179.0	-178.6	2.24
Ik		178.6	-178.6	2.33

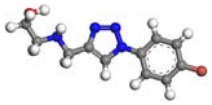
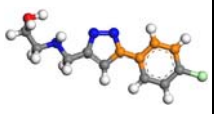
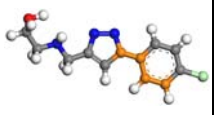
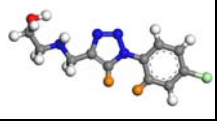
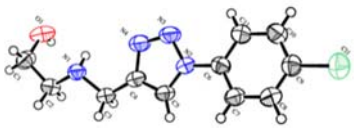
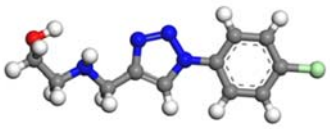
Il		178.9	-178.4	2.27
[a]Atoms involved in dihedral angle 1 (N2-C6-C7-C8) are shown in orange for **Ik** as an example				
[b]Atoms involved in dihedral angle 2 (N2-C6-C11-C10) are shown in orange for **Ik** as an example				
[c]Atoms involved in H-H distance are shown in orange for **Ik** as an example				

Table S2. Comparison between experimental (X-ray) and calculated (B3LYP/6-311++G(d,p)) values of the main structural parameters for compound **Ik**. The first row shows the X-ray derived (left) and DFT-optimized (right) molecular structure of **I**k (atom color code: C, gray; O, red; N, blue; Cl, light green; H, white).

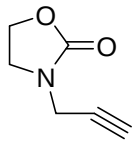
					
Atoms	**Experimental**	**Calculated**	**Atoms**	**Experimental**	**Calculated**
Bond length (Å)			***Bond length*** (Å)		
Cl1-C9	1.742(5)	1.76(0)	C6-C7	1.378(6)	1.39(0)
N2-N3	1.347(5)	1.35(1)	N4-C4	1.363(6)	1.36(1)
N2-C6	1.426(5)	1.44(2)	C5-C4	1.356(6)	1.36(0)
N2-N5	1.352(6)	1.35(8)	C3-C4	1.483(6)	1.49(0)
O1-C1	1.408(6)	1.41(0)	C10-C9	1.377(6)	1.37(3)
N1-C3	1.465(5)	1.48(4)	C10-C11	1.386(7)	1.38(2)
N1-C2	1.460(5)	1.48(3)	C9-C8	1.362(7)	1.37(3)
N3-N4	1.315(6)	1.33(0)	C2-C1	1.512(6)	1.52(3)
C6-C11	1.385(6)	1.39(2)	C7-C8	1.372(7)	1.38(1)
Bond angle (º)			***Bond angle*** (º)		
N3-N2-C6	120.6(4)	120.5(1)	C5-C4-N4	107.5(4)	108.8(2)
N3-N2-C5	109.7(4)	108.5(7)	C5-C4-C3	130.3(4)	129.6(9)
C5-N2-C6	129.7(4)	130.8(9)	C9-C10-Cl1	118.7(5)	119.9(7)
C2-N1-C3	111.5(4)	111.8(6)	C10-C9-Cl21	118.7(4)	119.9(6)
N4-N3-N2	107.3(4)	107.9(3)	C8-C9-C11	120.3(4)	120.0(3)
C11-C6-N2	119.4(4)	119.8(1)	C8-C9-C10	121.1(4)	120.0(1)
C7-C6-N2	120.3(4)	120.1(4)	N1-C2-C1	110.1(4)	112.3(4)
C7-C6-C11	120.3(4)	120.0(4)	C6-C11-C10	120.0(4)	119.9(8)
N3-N4-C4	109.4(4)	107.4(4)	C8-C7-C6	119.2(5)	119.9(9)
N2-C5-C4	106.2(4)	107.2(0)	C9-C8-C7	120.6(4)	120.0(0)
N1-C3-C4	111.5(4)	111.7(3)	O1-C1-C2	111.6(4)	112.3(2)
N4-C4-C3	122.1(4)	121.3(1)			
Torsion angle (º)			***Torsion angle*** (º)		
Cl1-C9-C8-C7	-177.5(4)	-179.3(9)	C6-N2-N3-N4	178.2(3)	178.8(1)
N2-N3-N4-C4	-0.5(6)	-0.4(8)	C6-N2-C5-C4	-177.9(4)	-178.0(9)
N2-C6-C11-C10	-178.3(4)	-178.6(1)	C6-C7-C8-C9	0.5(7)	0.08(9)
N2-C6-C7-C8	177.4(4)	178.6(7)	C5-N2-N3-N4	1.0(6)	0.5(1)
N2-C5-C4-N4	0.7(5)	0.8(4)	C5-N2-C6-C11	164.2(5)	165.1(0)
N2-C5-C4-C3	177.7(4)	176.3(2)	C5-N2-C6-C7	-15.1(6)	-15.6(8)
N1-C3-C4-N4	-21.6(6)	-23.2(5)	C3-N1-C2-C1	-167.2(4)	-168.1(3)
N1-C3-C4-C5	161.8(4)	161.5(3)	C10-C9-C8-C7	1.7(7)	0.6(4)
N1-C2-C1-O1	58.5(5)	58.7(5)	C9-C10-C11-C6	1.2(7)	0.7(4)

N3-N2-C6-C11	-12.4(6)	-13.2(0)	C2-N1-C3-C4	172.4(3)	171.4(4)
N3-N2-C6-C7	168.4(5)	166.0(2)	C11-C6-C7- C8	-1.8(7)	-0.5(5)
N3-N2-C5-C4	-1.1(5)	-0.9(8)	C11-C10-C9-Cl1	176.7(4)	179.4(6)
N3-N4-C4-C5	-0.1(6)	-0.094(4)	C11-C10-C 9-C8	-2.5(7)	-0.5(8)
N3-N4-C4-C3	-177.4(4)	-176.7(0)	C7-C6-C11-C10	1.0(7)	0.6(1)

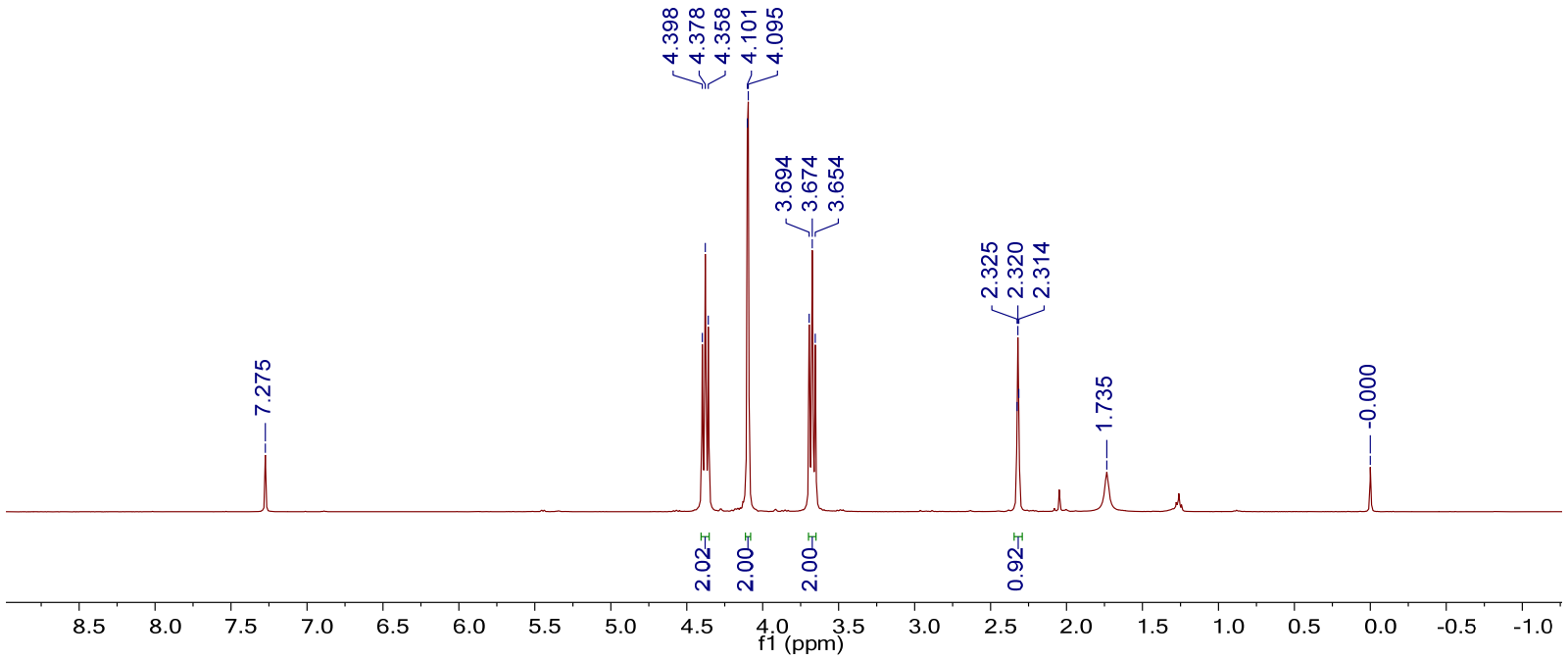
Table S3. *In silico* predicted main pharmacokinetic parameters of compounds **Ia-Il**.

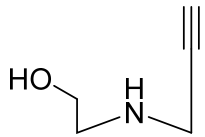
Cpd.	MW[a]	HBA[b]	HBD[c]	logP[d]	logS[e]	PSA[f]	BBB score[g]	Rule of 5 violation	Drug likeness
Rule of 5	<500	≤10	≤5	≤5	≤5	-	-	≤1	-
Ia	232.13	4	2	0.83	-0.94	55.63	4.44	0	-0.53
Ib	260.16	4	2	1.81	-1.41	55.63	4.59	0	-0.47
Ic	288.20	4	2	2.86	-2.99	55.63	4.69	0	-0.37
Id	316.23	4	2	3.87	-3.85	55.63	4.76	0	-0.37
Ie	358.27	4	2	5.39	-5.32	55.63	4.79	**1**	-0.37
If	386.30	4	2	6.40	-6.04	55.63	4.78	**1**	-0.37
Ig	414.34	4	2	7.41	-6.12	55.63	4.74	**1**	-0.37
Ih	442.37	4	2	8.43	-6.23	55.63	4.70	**1**	-0.37
Ii	286.10	4	2	1.33	-1.13	55.63	4.69	0	-0.82
Ij	284.13	5	2	0.35	-1.44	63.18	4.06	0	-0.42
Ik	252.08	4	2	0.98	-1.60	55.63	4.54	0	-0.20
Il	286.03	4	2	1.23	-0.91	55.63	4.71	0	-0.62

[a]Molecular weight; [b]number of hydrogen bond acceptors; [c]number of hydrogen bond donors; [d]logarithm of n-octanol/water partition coefficient; [e]logarithm of water solubility (in log(mol/L)); [f]polar surface area; [g]Blood-brain barrier score: 6 = High; 0 = low.

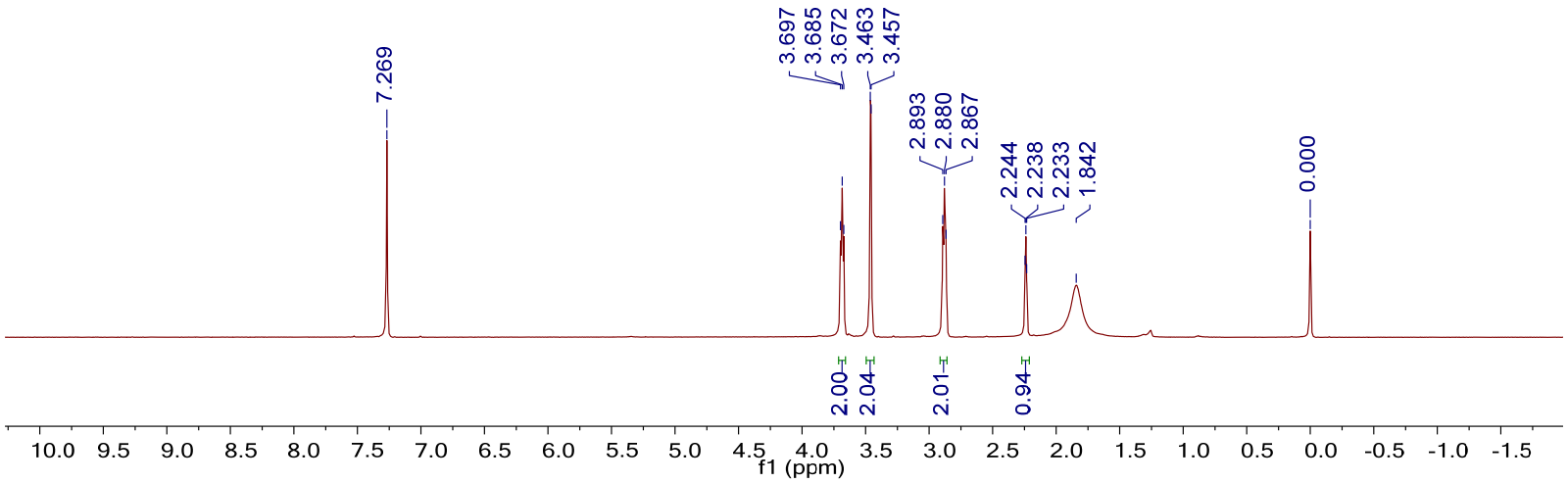


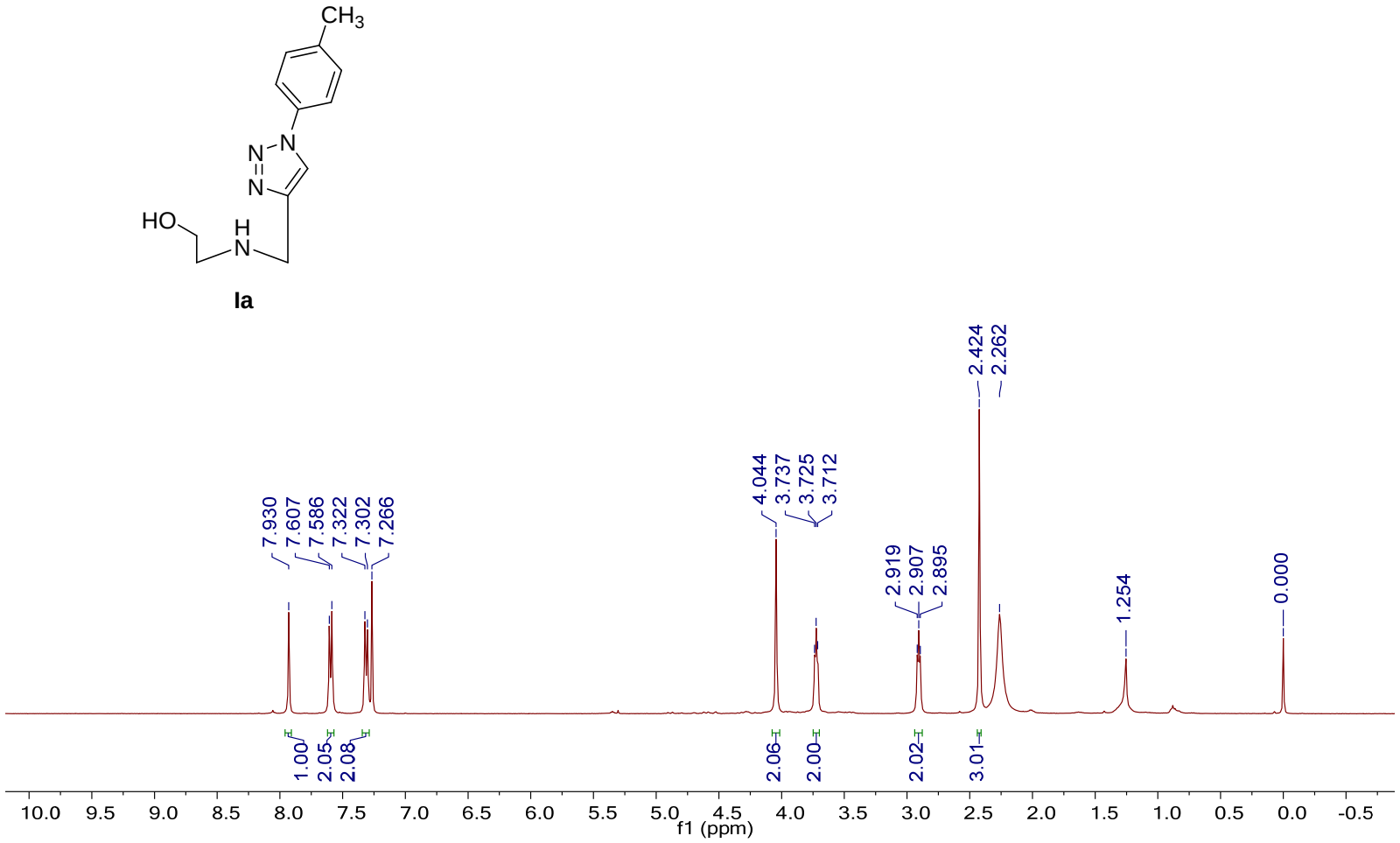
I-2

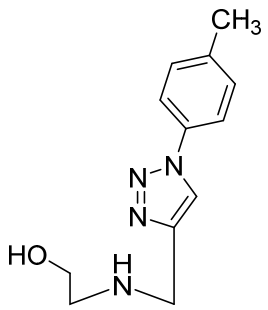

4.398
4.378
4.358
4.101
4.095
3.694
3.674
3.654
2.325
2.320
2.314
7.275
1.735
-0.000
2.02
2.00
2.00
0.92
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


HO
H
N

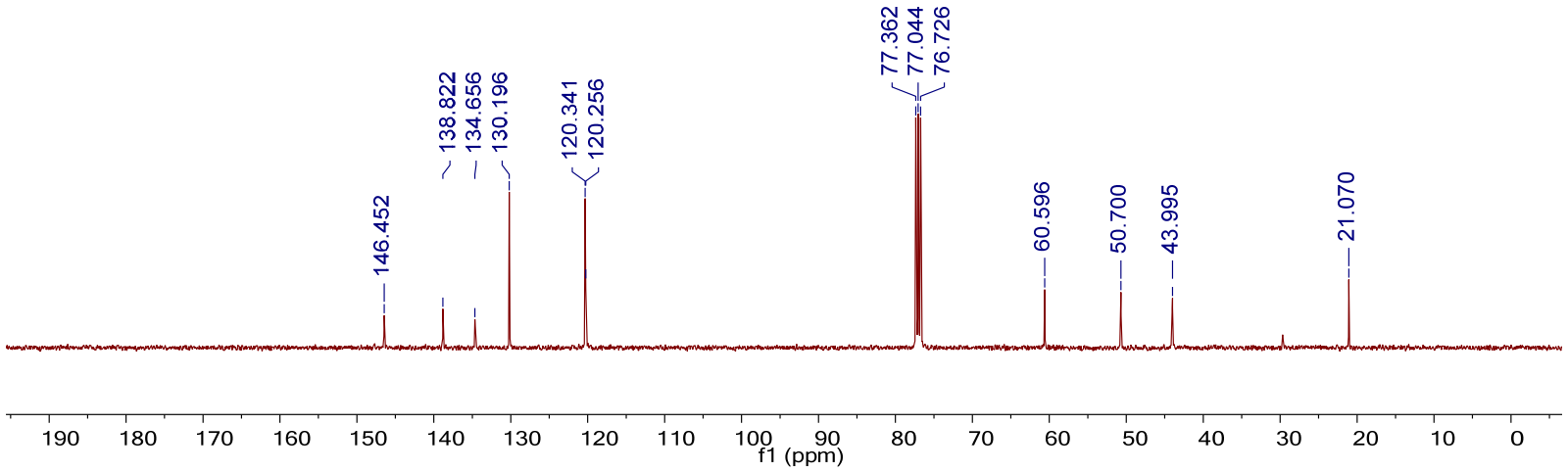
I-3

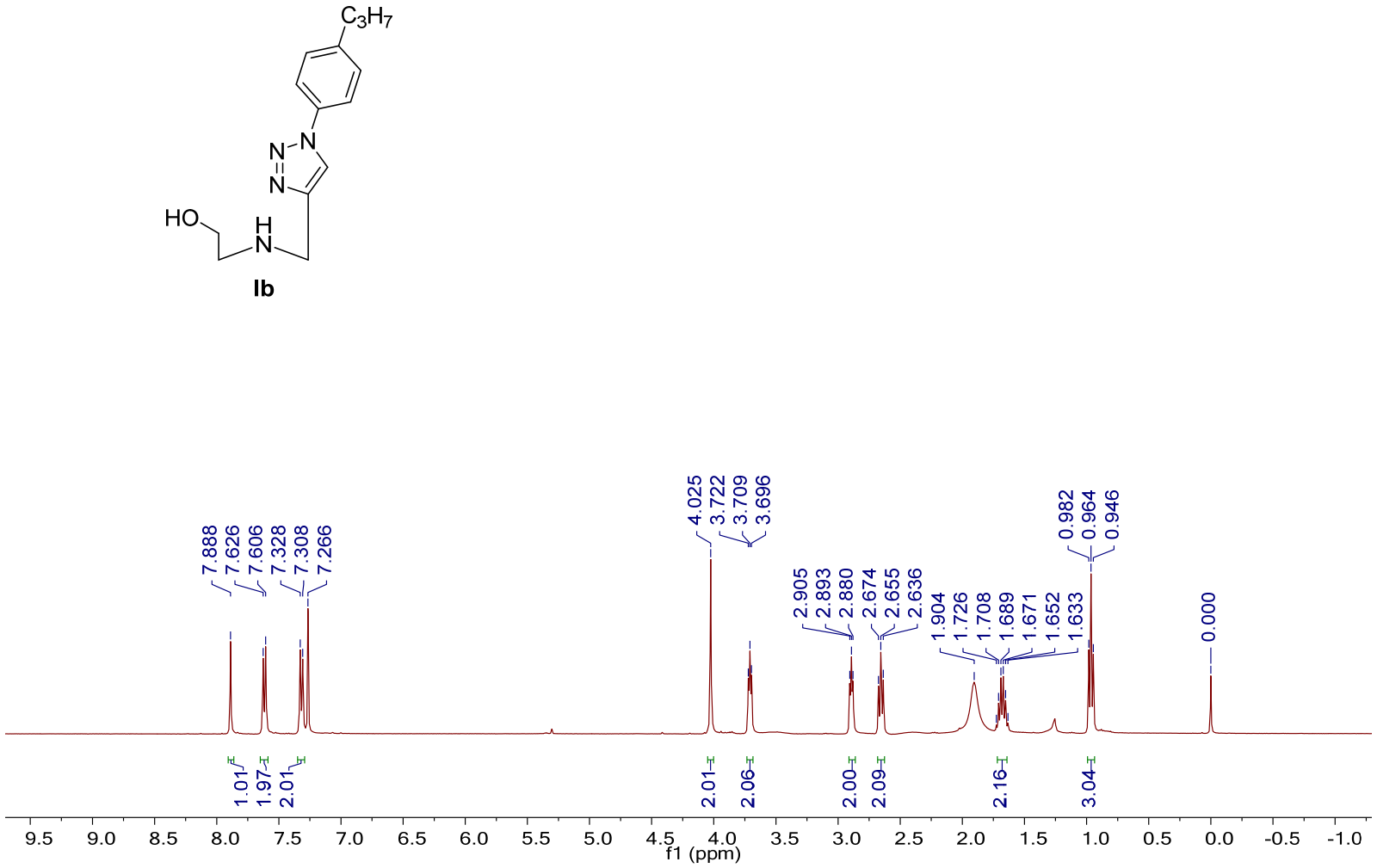

7.269
3.697
3.685
3.672
3.463
3.457
2.893
2.880
2.867
2.244
2.238
2.233
1.842
0.000
2.00
2.04
2.01
0.94
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

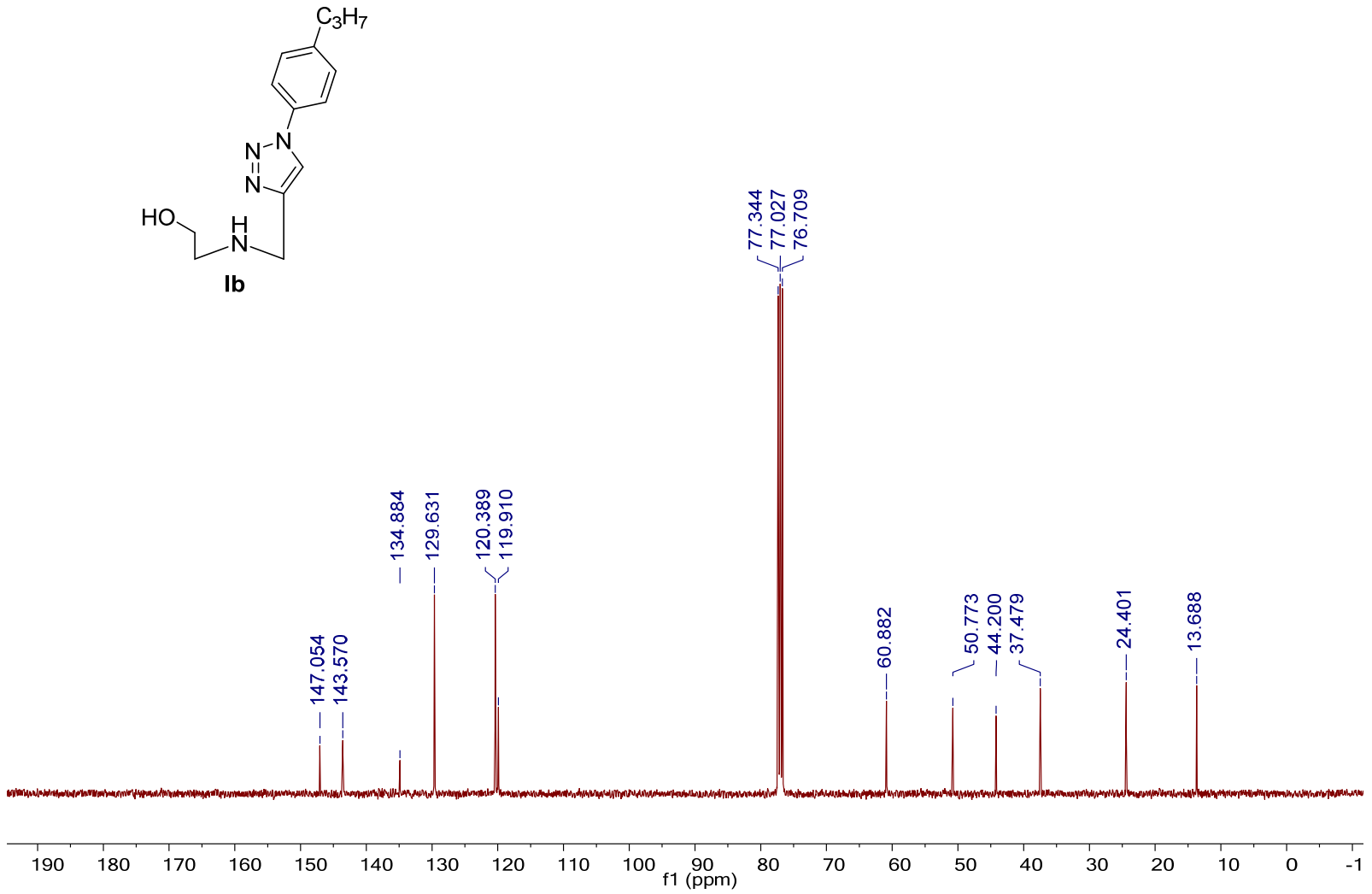

CH3
N
N
N
HO
H
N
Ia
7.930
7.607
7.586
7.322
7.302
7.266
4.044
3.737
3.725
3.712
2.919
2.907
2.895
2.424
2.262
1.254
0.000
1.00
2.05
2.08
2.06
2.00
2.02
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

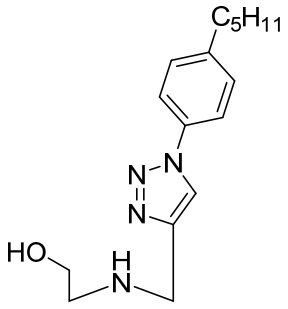

CH3
N
N
N
HO
H
N

Ia

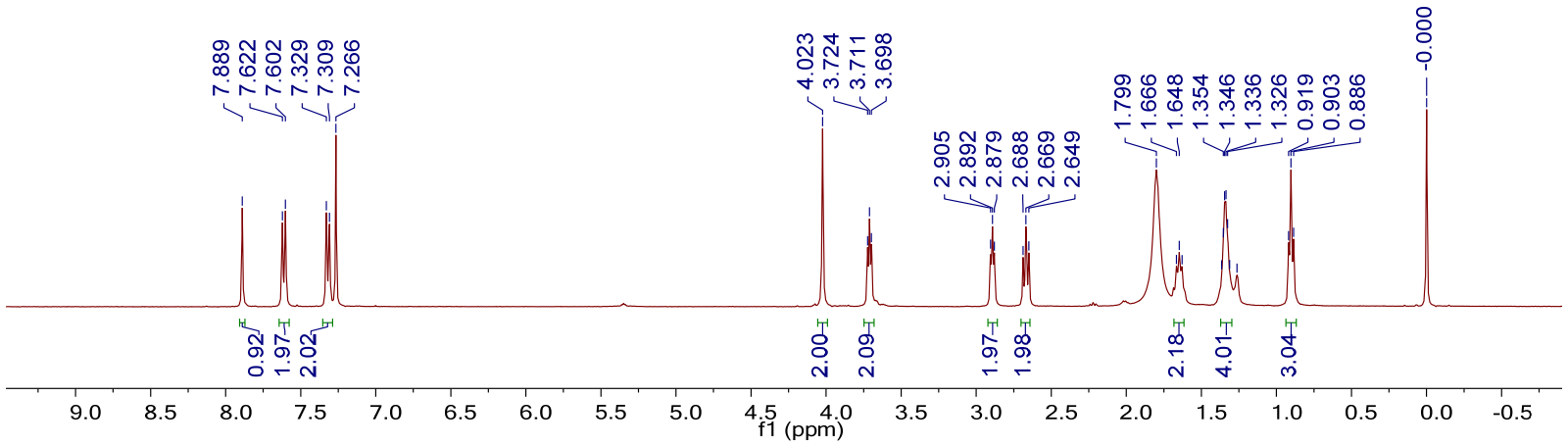

146.452
138.822
134.656
130.196
120.341
120.256
77.362
77.044
76.726
60.596
50.700
43.995
21.070
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

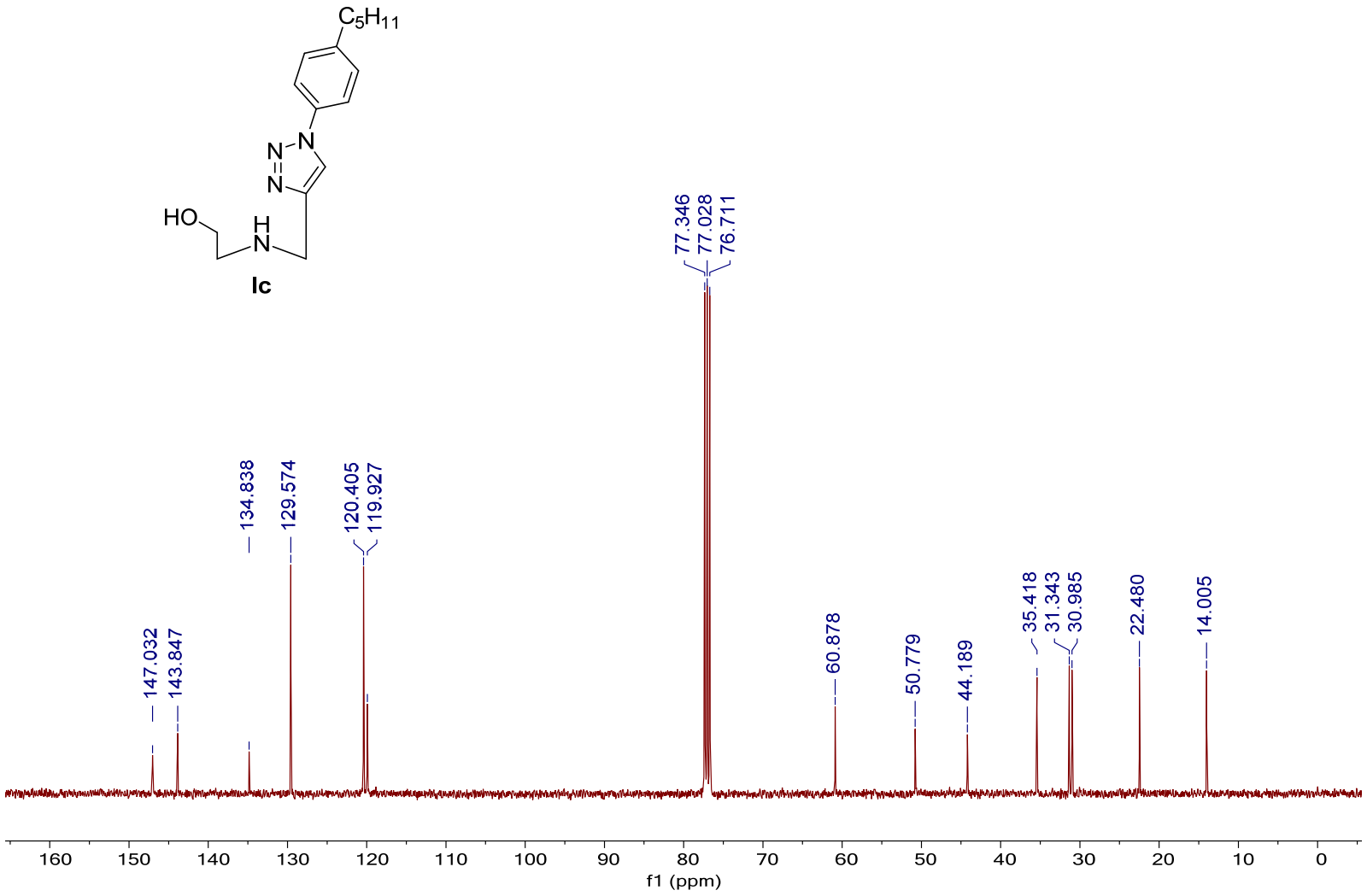

C3H7
HO
H
N
N
N
N
Ib
7.888
7.626
7.606
7.328
7.308
7.266
4.025
3.722
3.709
3.696
2.905
2.893
2.880
2.674
2.655
2.636
1.904
1.726
1.708
1.689
1.671
1.652
1.633
0.982
0.964
0.946
0.000
1.01
1.97
2.01
2.01
2.06
2.00
2.09
2.16
3.04
f1 (ppm)

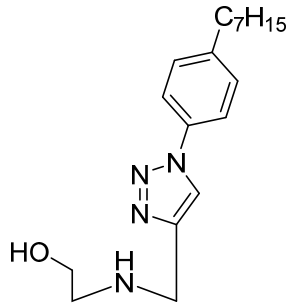

C3H7
HO
H
N
N
N
N
Ib
147.054
143.570
134.884
129.631
120.389
119.910
77.344
77.027
76.709
60.882
50.773
44.200
37.479
24.401
13.688
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


C5H11
N
N
N
HO
H
N

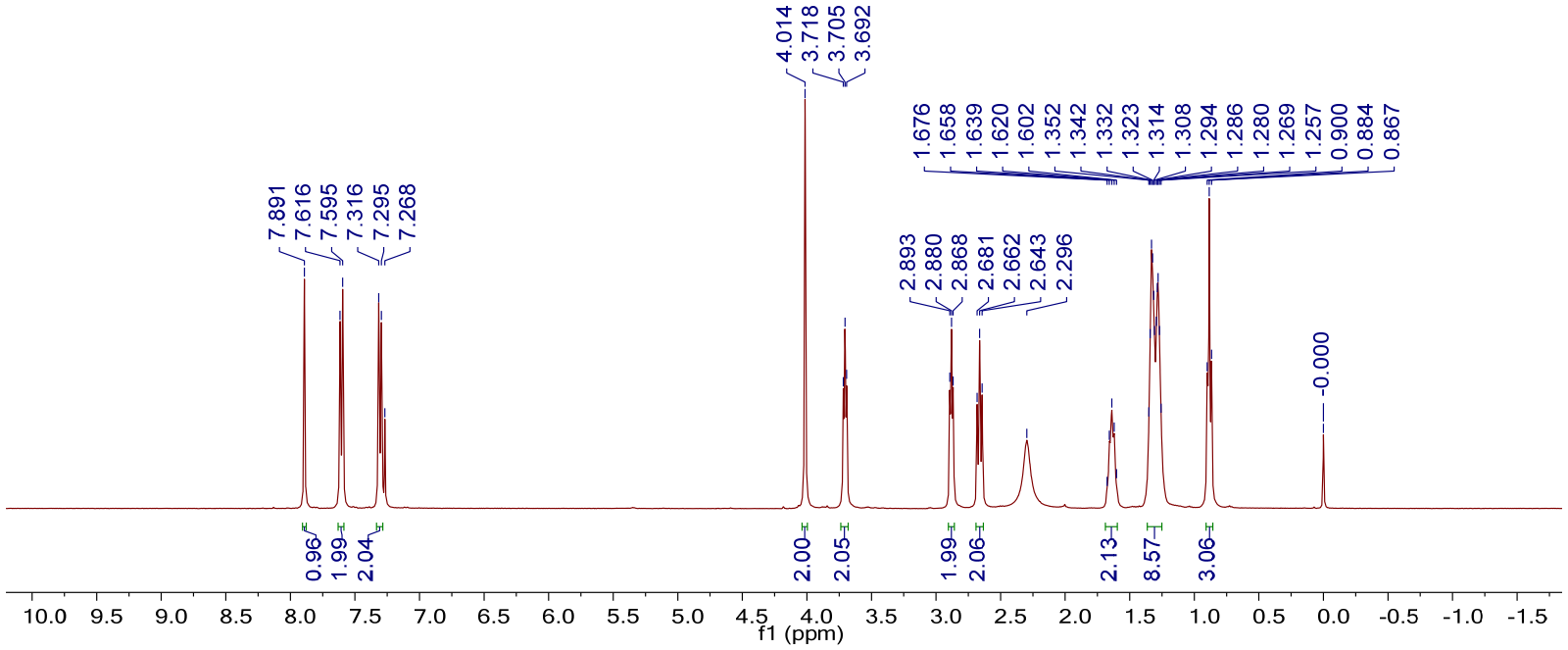
Ic

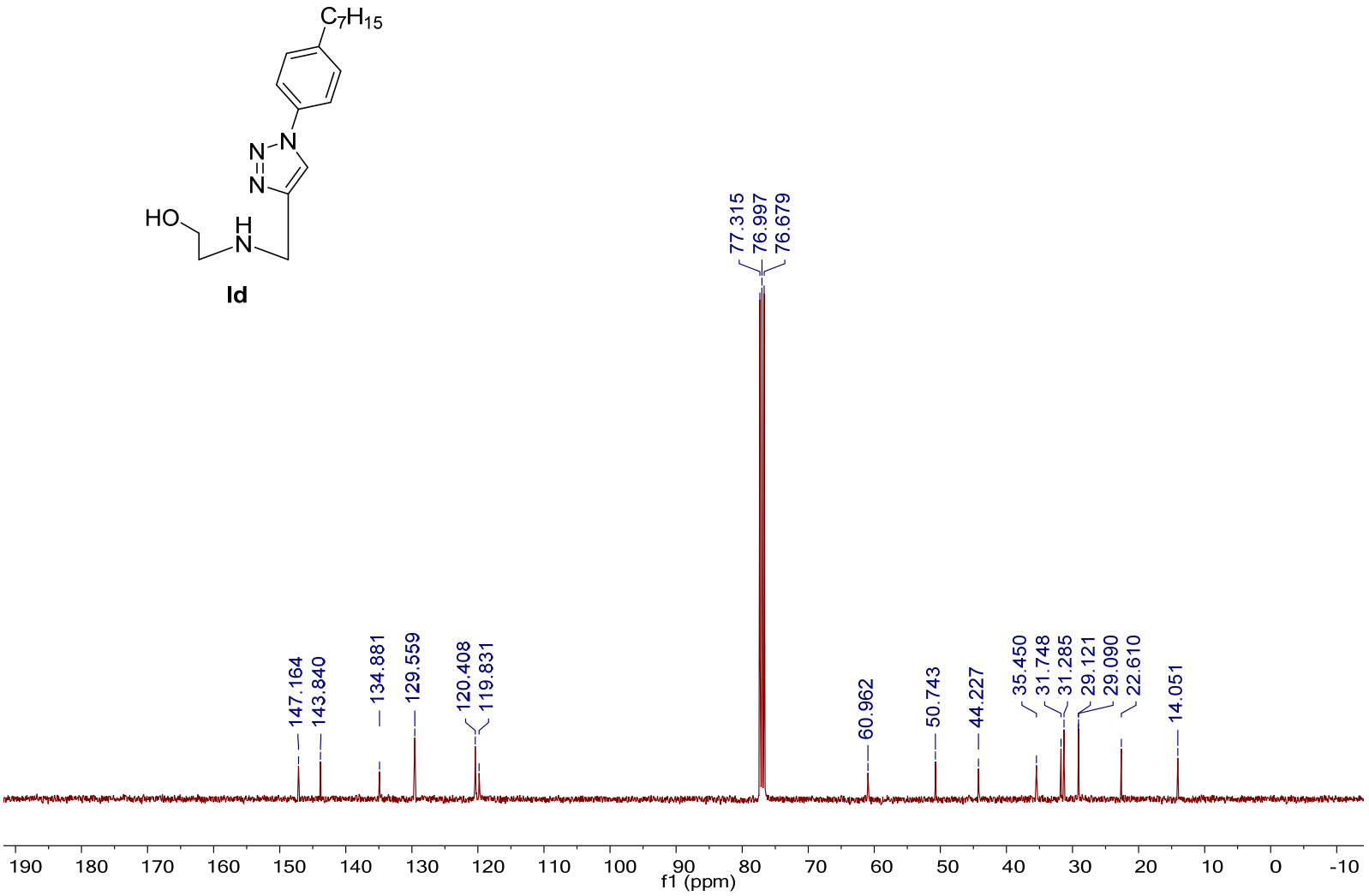

7.889
7.622
7.602
7.329
7.309
7.266
4.023
3.724
3.711
3.698
2.905
2.892
2.879
2.688
2.669
2.649
1.799
1.666
1.648
1.354
1.346
1.336
1.326
0.919
0.903
0.886
-0.000
0.92
1.97
2.02
2.00
2.09
1.97
1.98
2.18
4.01
3.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

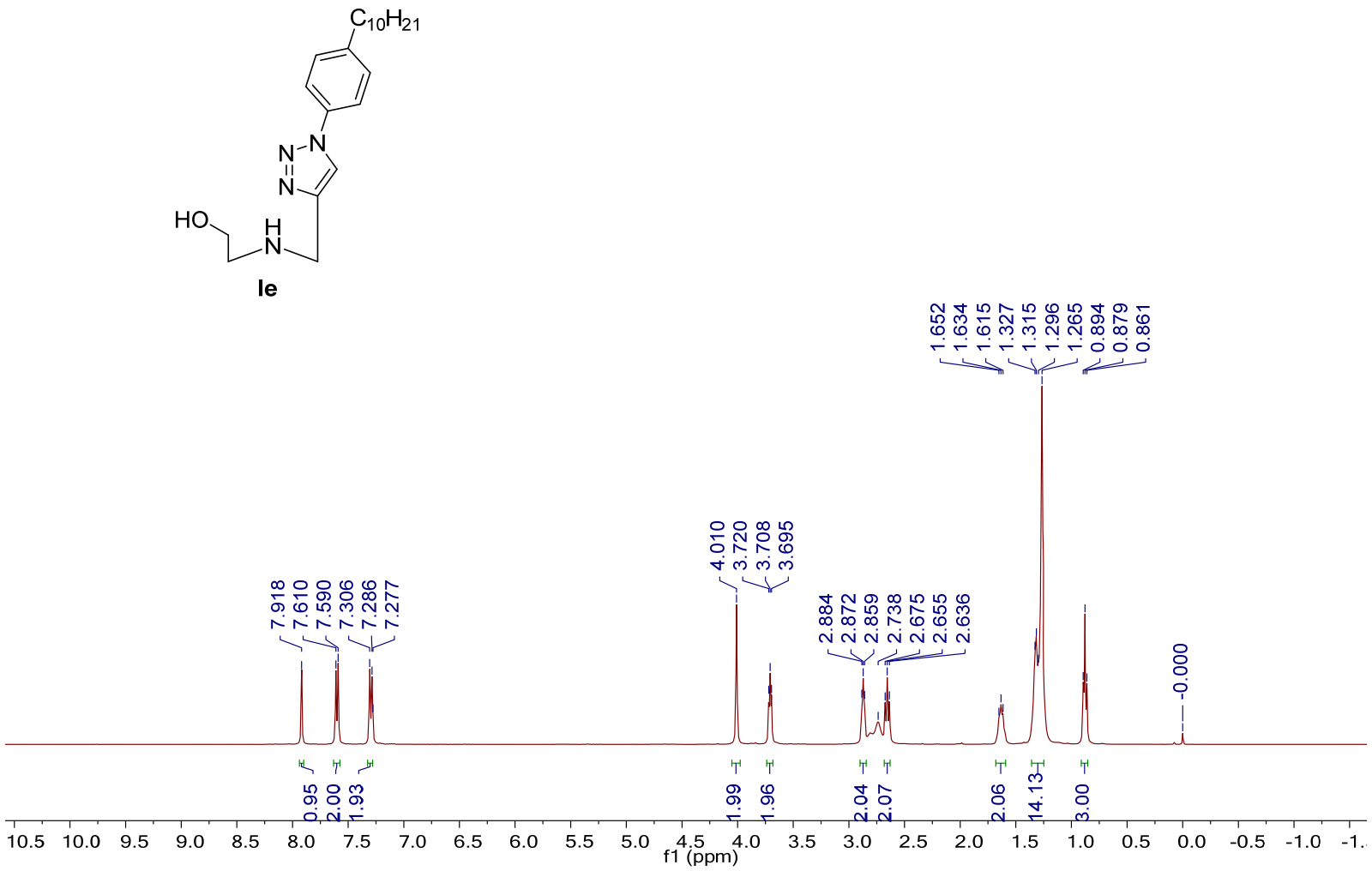

C5H11
N
N
N
HO
H
N
Ic
77.346
77.028
76.711
147.032
143.847
134.838
129.574
120.405
119.927
60.878
50.779
44.189
35.418
31.343
30.985
22.480
14.005
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

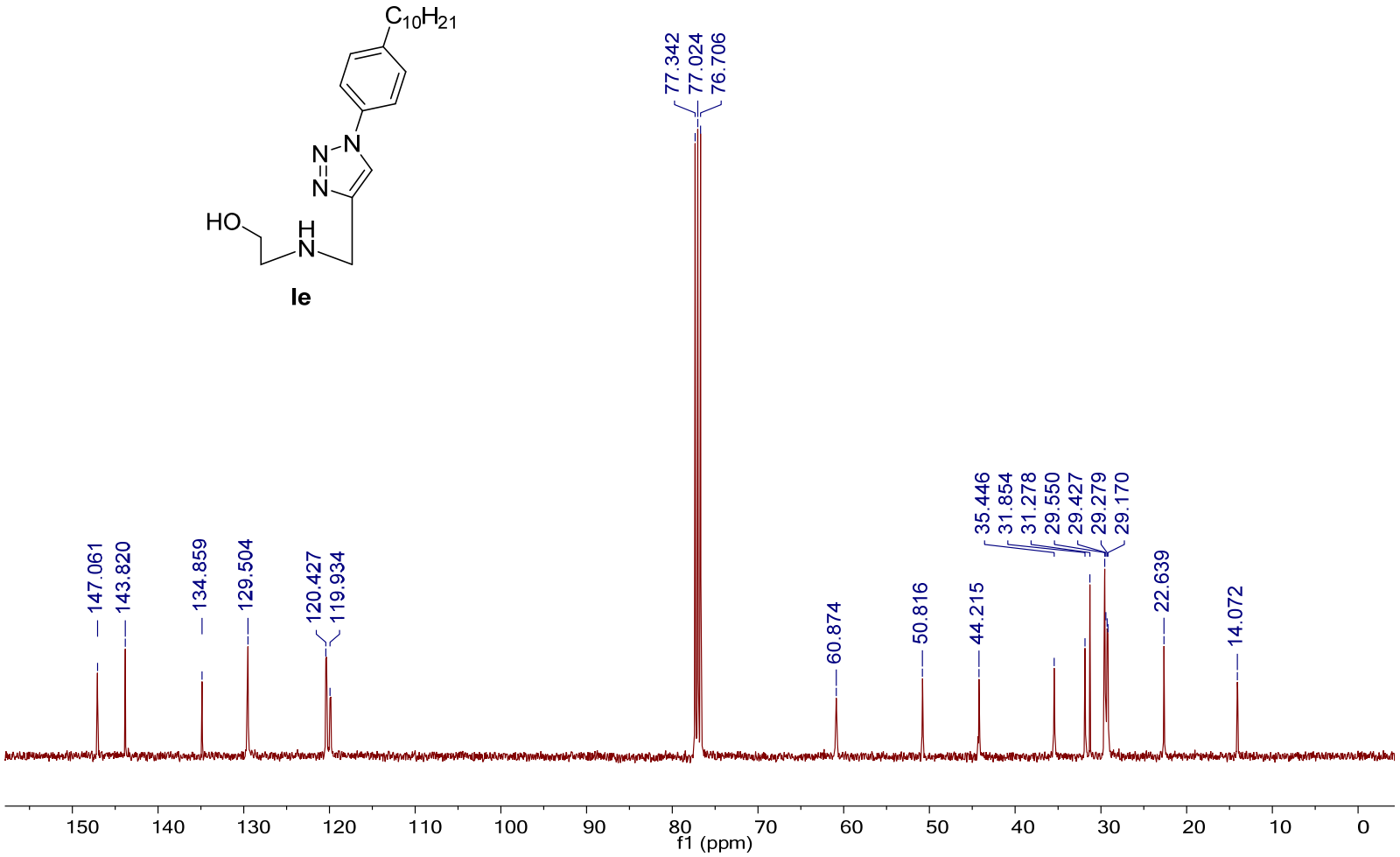

C7H15
N
N
N
HO
H
N

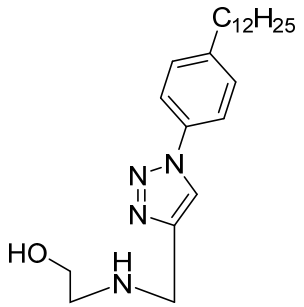
Id


4.014
3.718
3.705
3.692
1.676
1.658
1.639
1.620
1.602
1.352
1.342
1.332
1.323
1.314
1.308
1.294
1.286
1.280
1.269
1.257
0.900
0.884
0.867
7.891
7.616
7.595
7.316
7.295
7.268
2.893
2.880
2.868
2.681
2.662
2.643
2.296
-0.000
0.96
1.99
2.04
2.00
2.05
1.99
2.06
2.13
8.57
3.06
f1 (ppm)

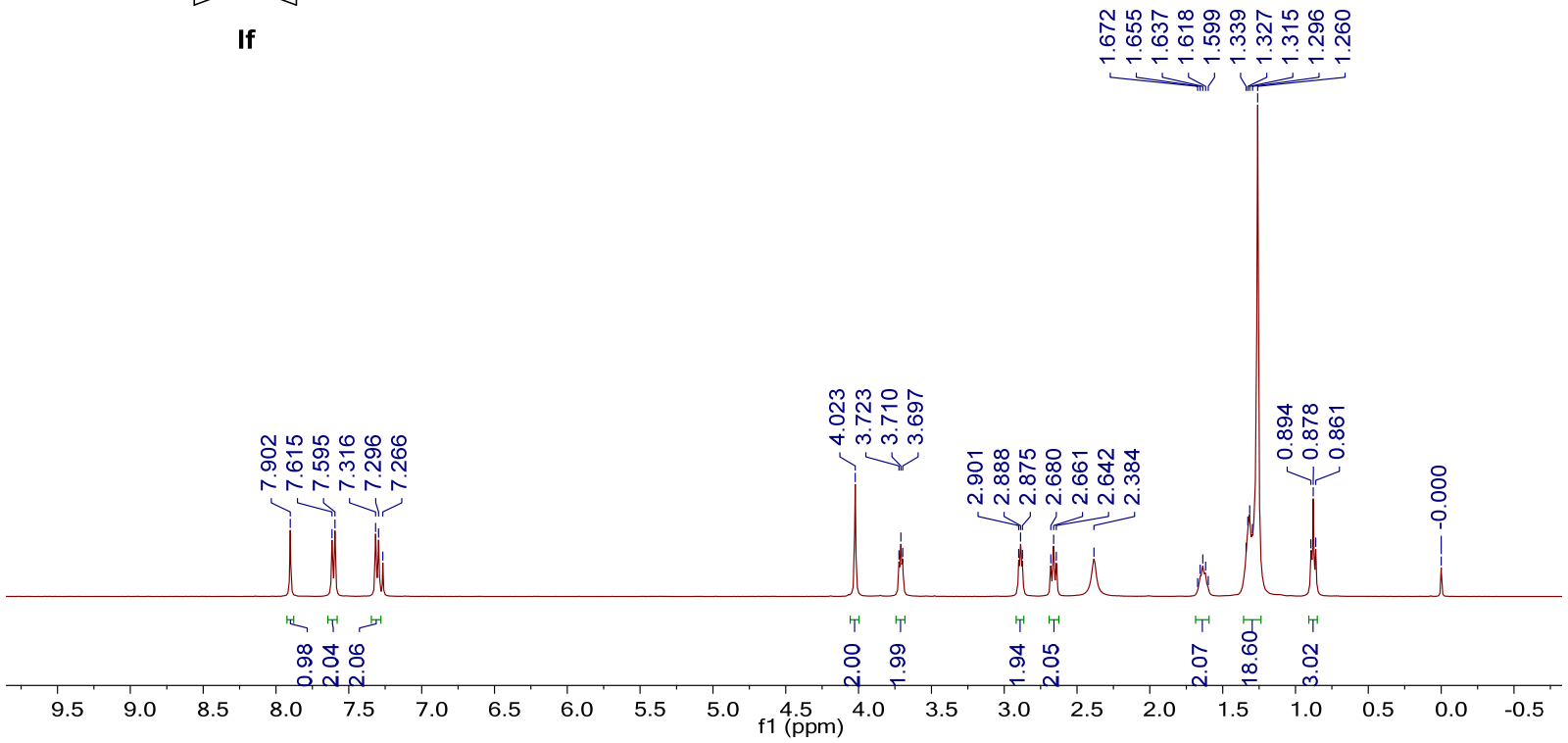

C7H15
HO
H
N
N
N
N
Id
77.315
76.997
76.679
147.164
143.840
134.881
129.559
120.408
119.831
60.962
50.743
44.227
35.450
31.748
31.285
29.121
29.090
22.610
14.051
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

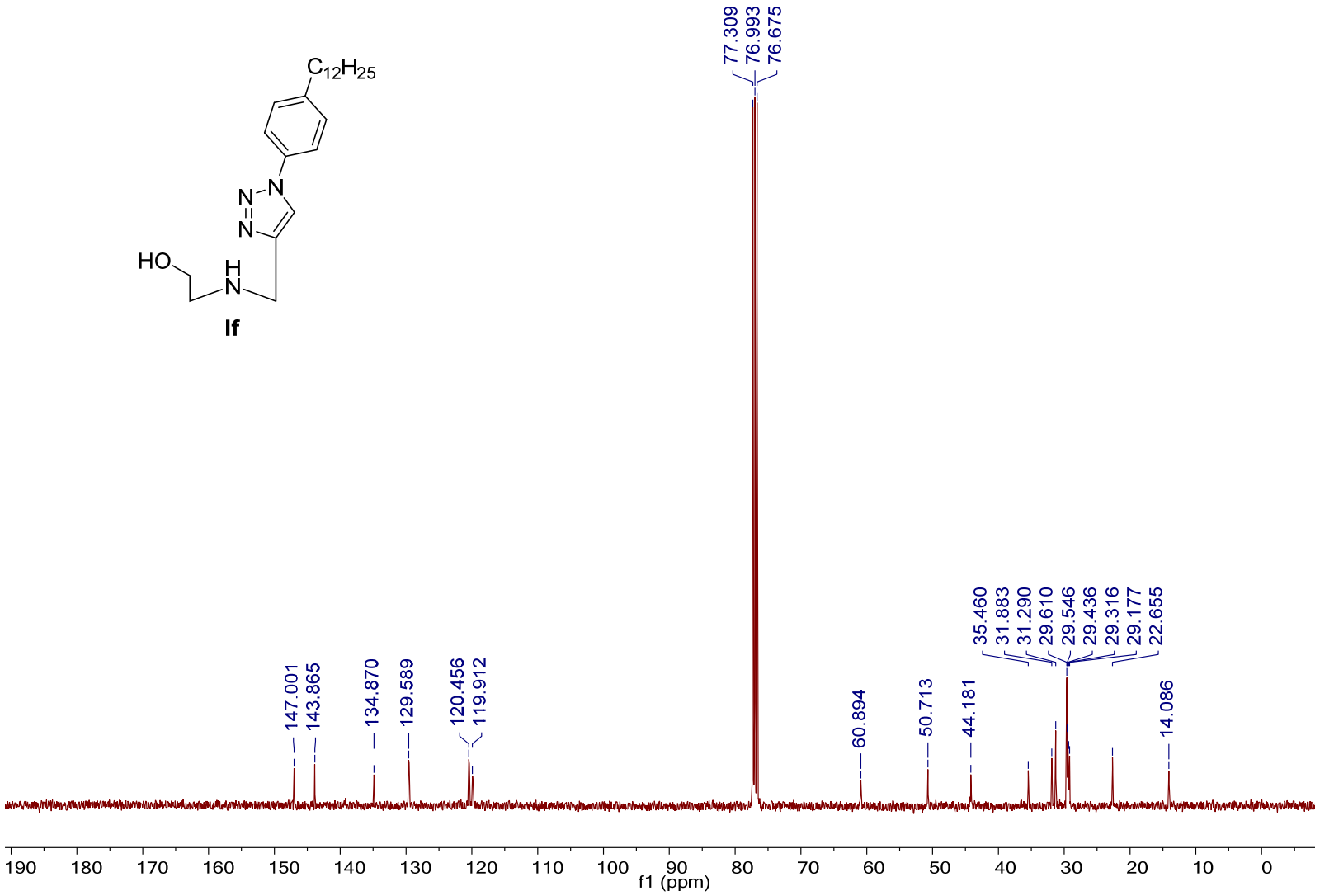

C10H21
HO
H
N
N
N
N
Ie
7.918
7.610
7.590
7.306
7.286
7.277
4.010
3.720
3.708
3.695
2.884
2.872
2.859
2.738
2.675
2.655
2.636
1.652
1.634
1.615
1.327
1.315
1.296
1.265
0.894
0.879
0.861
-0.000
0.95
2.00
1.93
1.99
1.96
2.04
2.07
2.06
14.13
3.00
f1 (ppm)

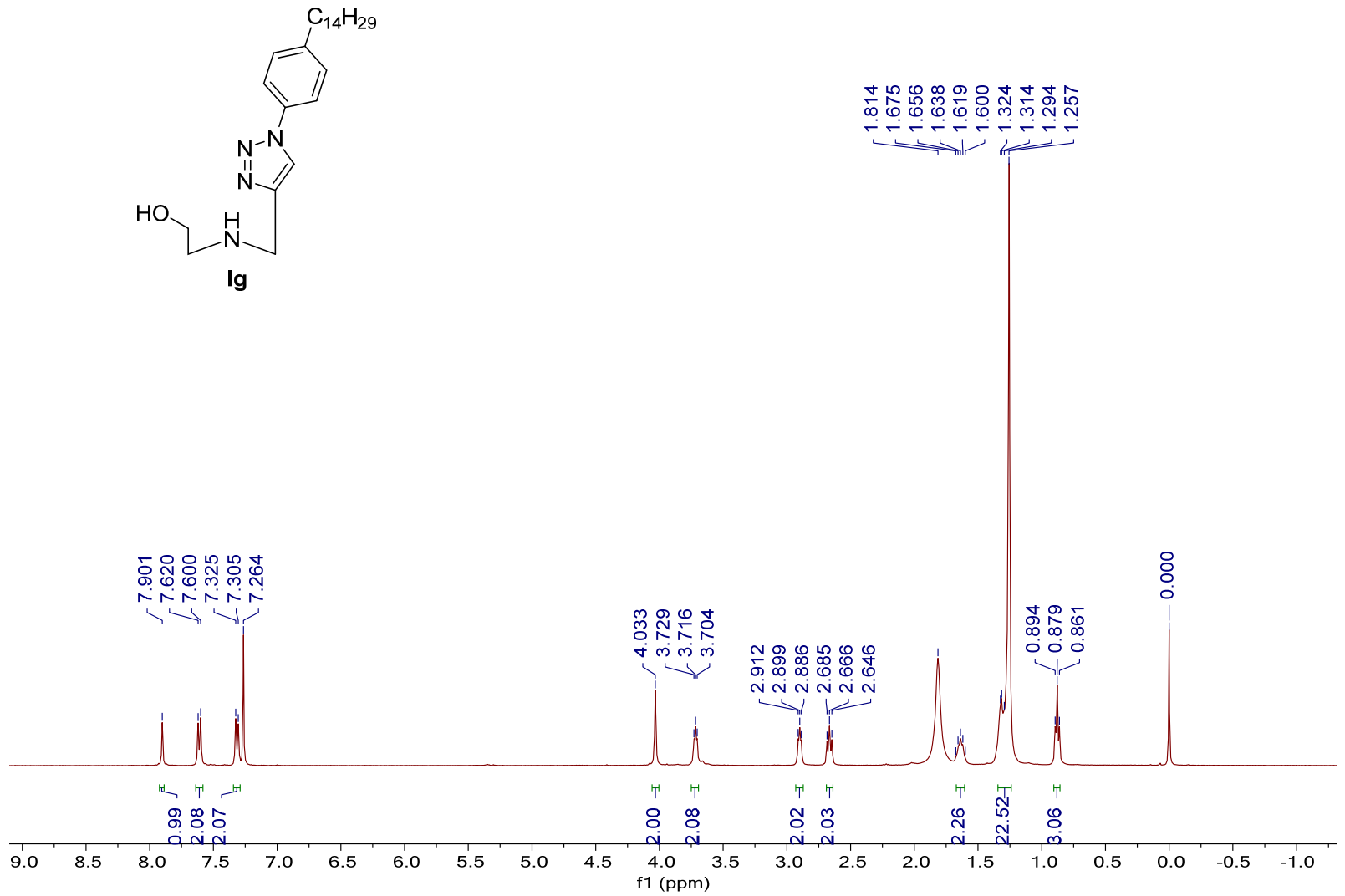

C10H21
HO
H
N
N
N
N
Ie
77.342
77.024
76.706
147.061
143.820
134.859
129.504
120.427
119.934
60.874
50.816
44.215
35.446
31.854
31.278
29.550
29.427
29.279
29.170
22.639
14.072
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

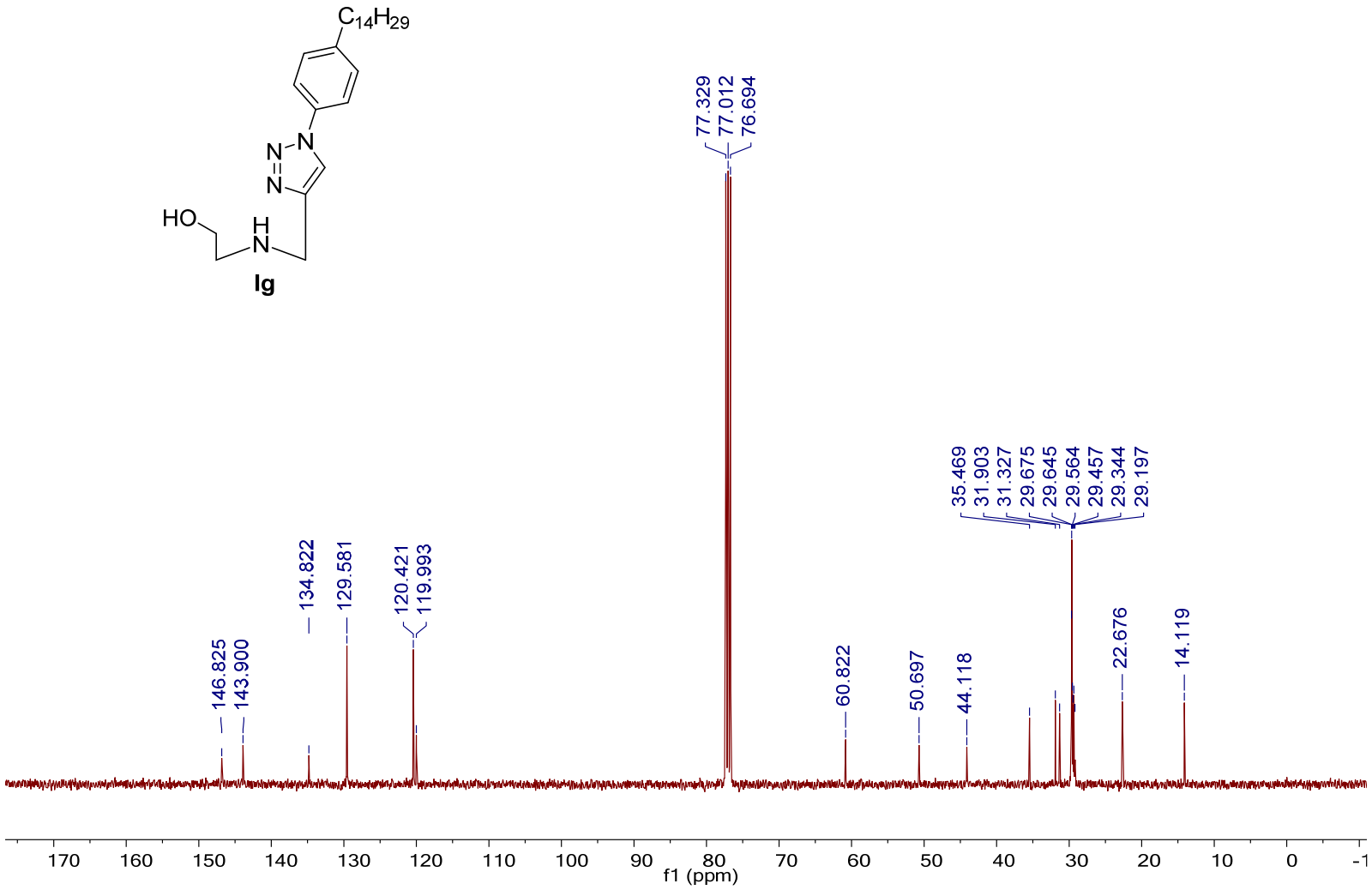

C12H25
N
N
N
HO
H
N

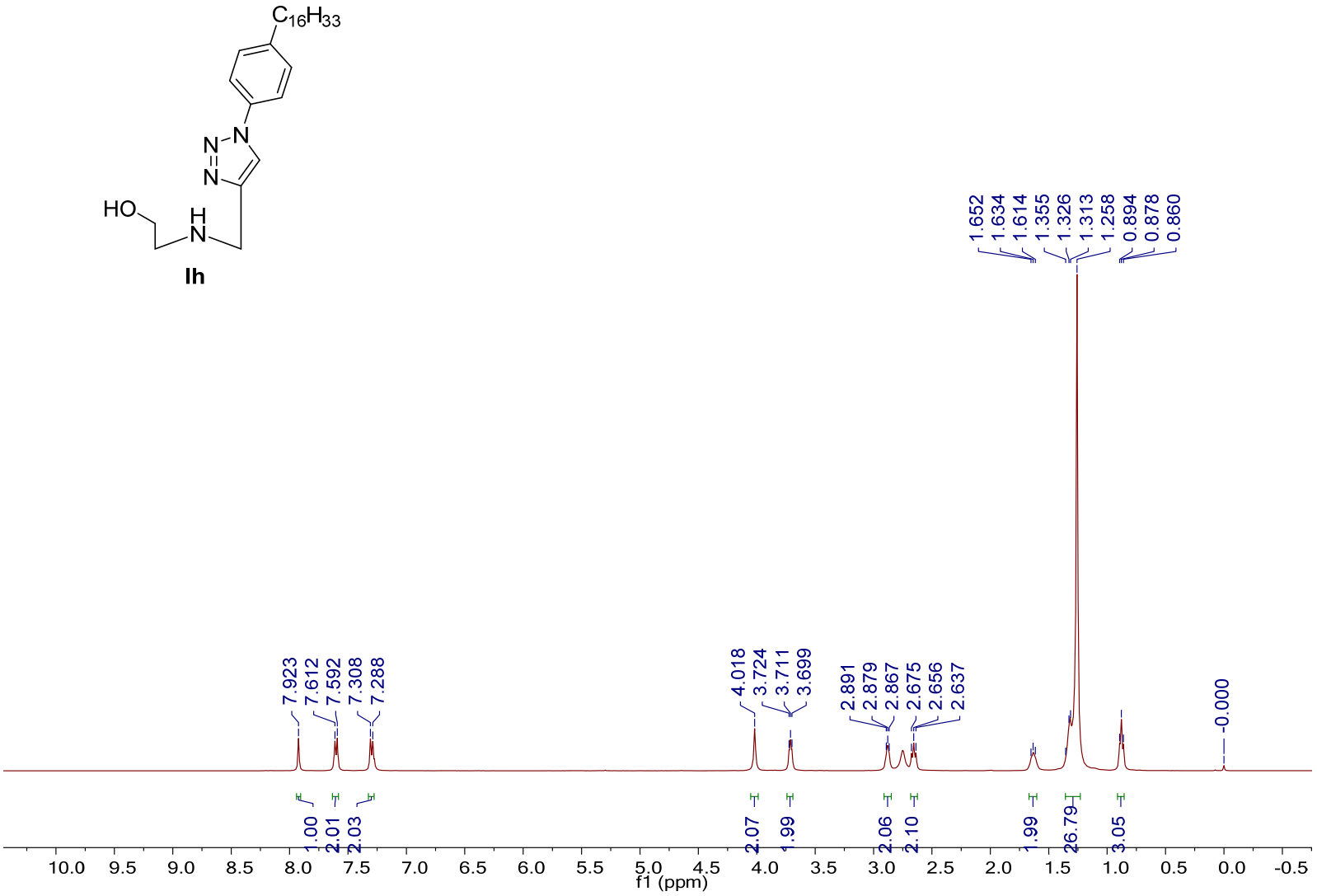
If

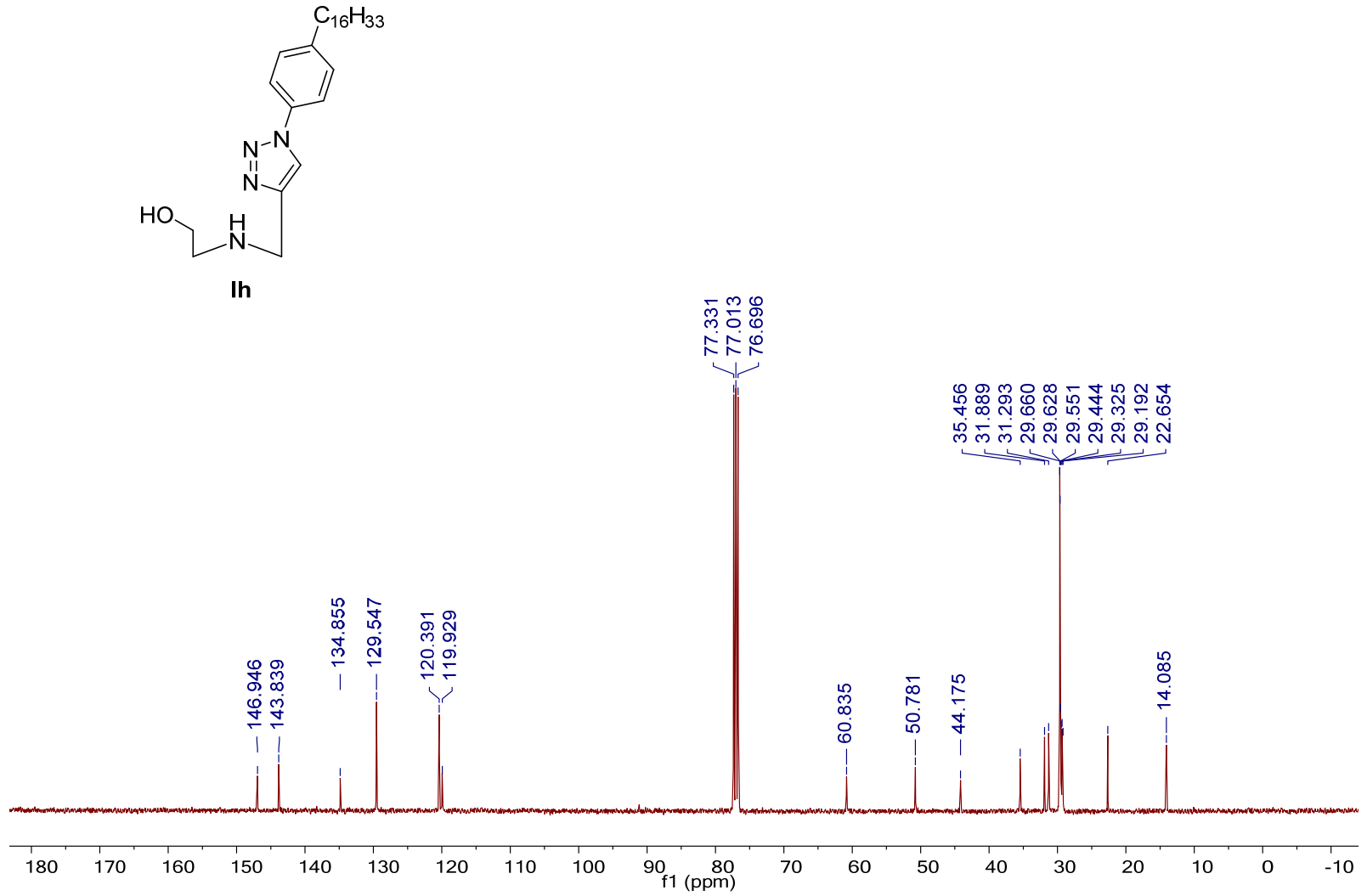

7.902
7.615
7.595
7.316
7.296
7.266
4.023
3.723
3.710
3.697
2.901
2.888
2.875
2.680
2.661
2.642
2.384
1.672
1.655
1.637
1.618
1.599
1.339
1.327
1.315
1.296
1.260
0.894
0.878
0.861
-0.000
0.98
2.04
2.06
2.00
1.99
1.94
2.05
2.07
18.60
3.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

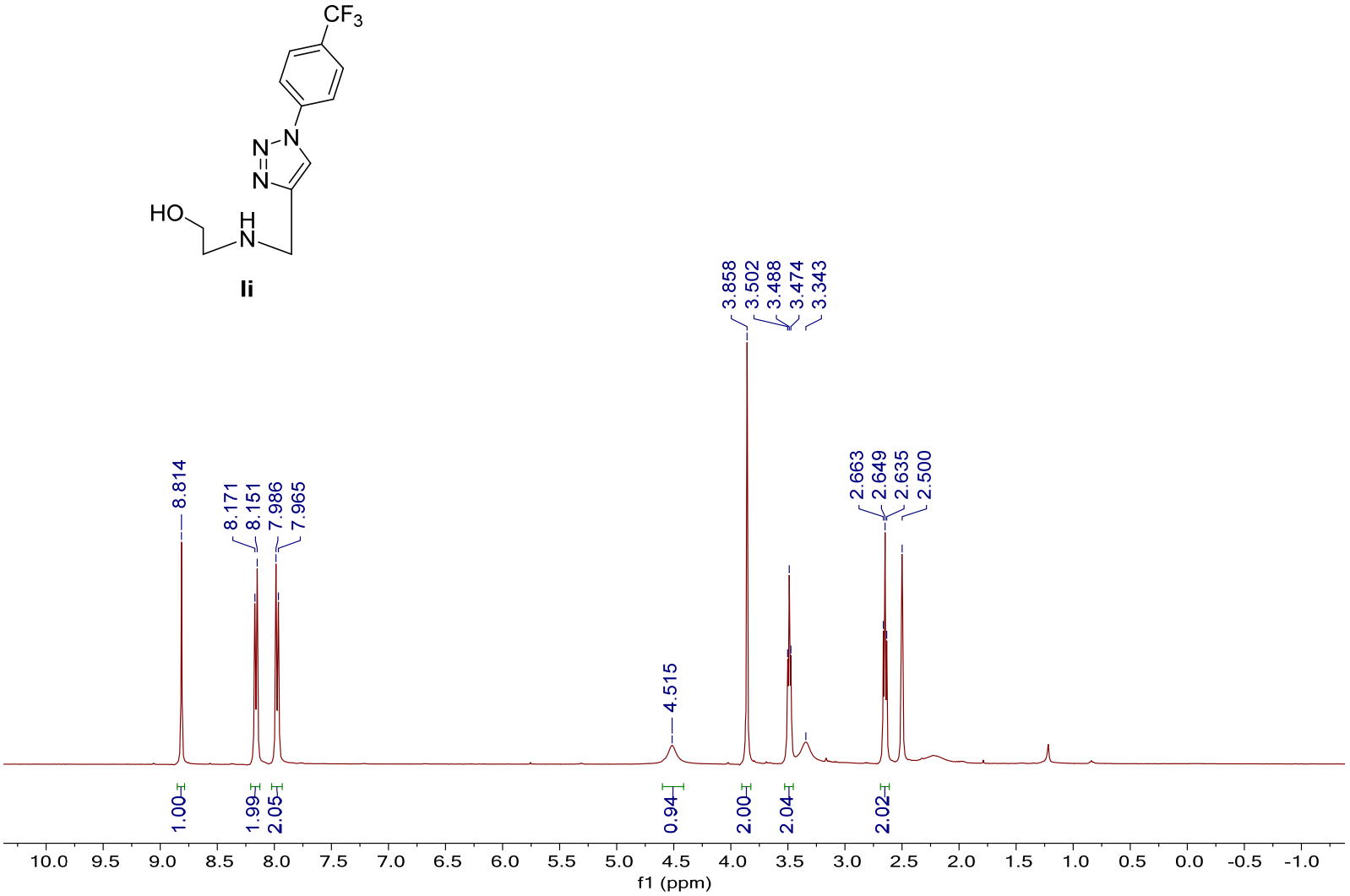

C12H25
N
N
N
HO
H
N
If
77.309
76.993
76.675
147.001
143.865
134.870
129.589
120.456
119.912
60.894
50.713
44.181
35.460
31.883
31.290
29.610
29.546
29.436
29.316
29.177
22.655
14.086
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

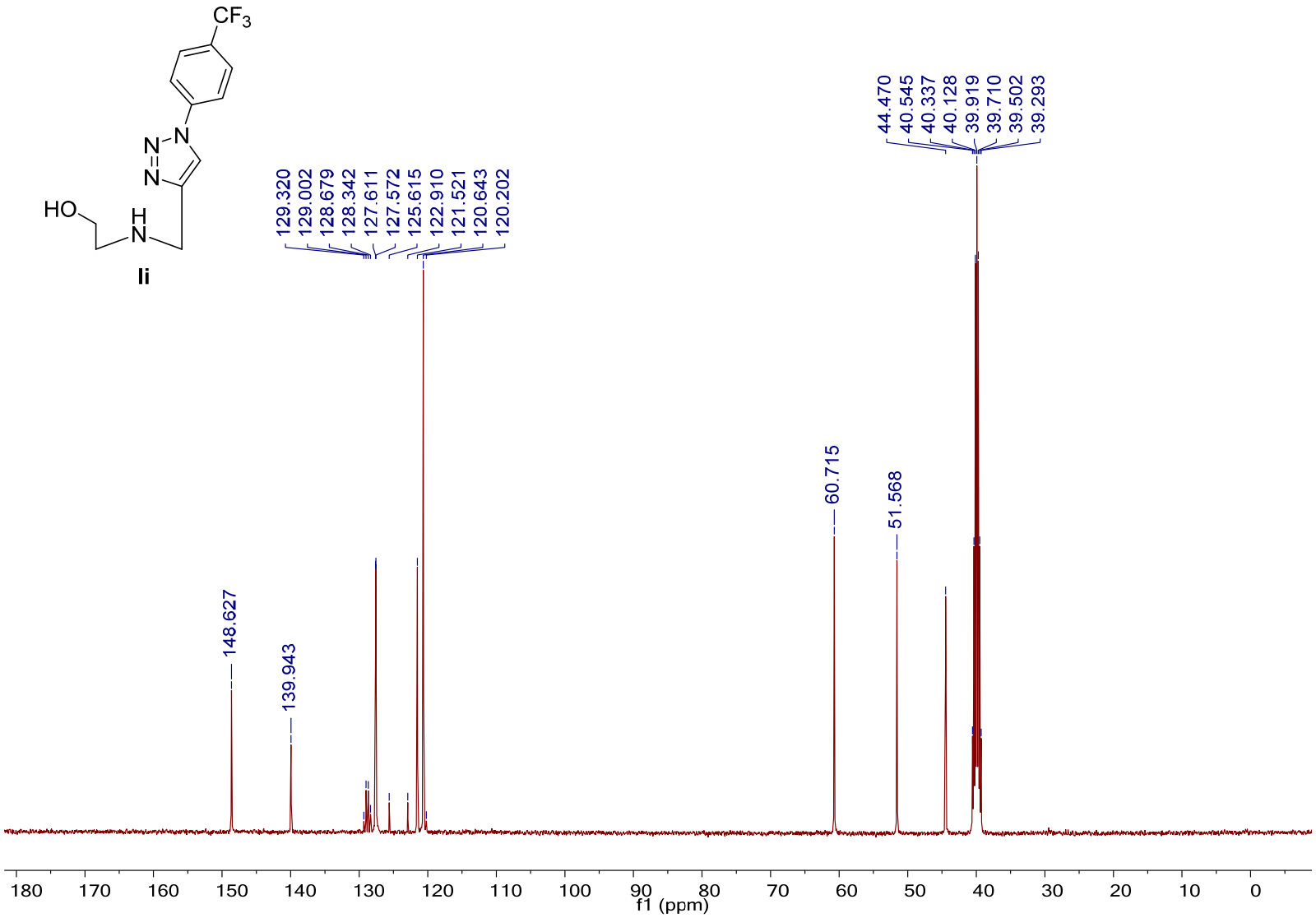

C14H29
HO
H
N
N
N
N
Ig
1.814
1.675
1.656
1.638
1.619
1.600
1.324
1.314
1.294
1.257
7.901
7.620
7.600
7.325
7.305
7.264
4.033
3.729
3.716
3.704
2.912
2.899
2.886
2.685
2.666
2.646
0.894
0.879
0.861
0.000
0.99
2.08
2.07
2.00
2.08
2.02
2.03
2.26
22.52
3.06
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

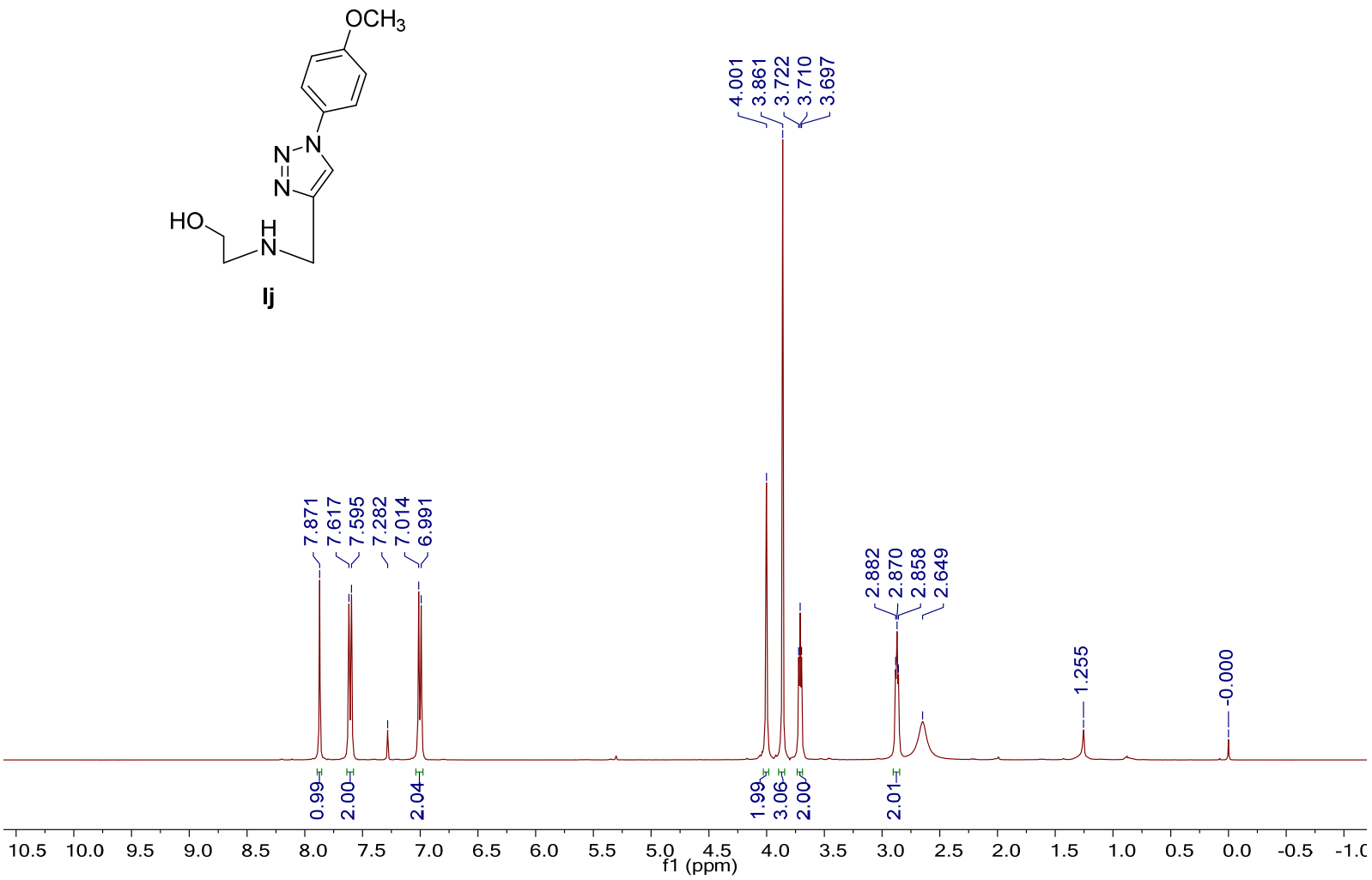

C14H29
HO
H
N
N
N
N
Ig
77.329
77.012
76.694
146.825
143.900
134.822
129.581
120.421
119.993
60.822
50.697
44.118
35.469
31.903
31.327
29.675
29.645
29.564
29.457
29.344
29.197
22.676
14.119
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

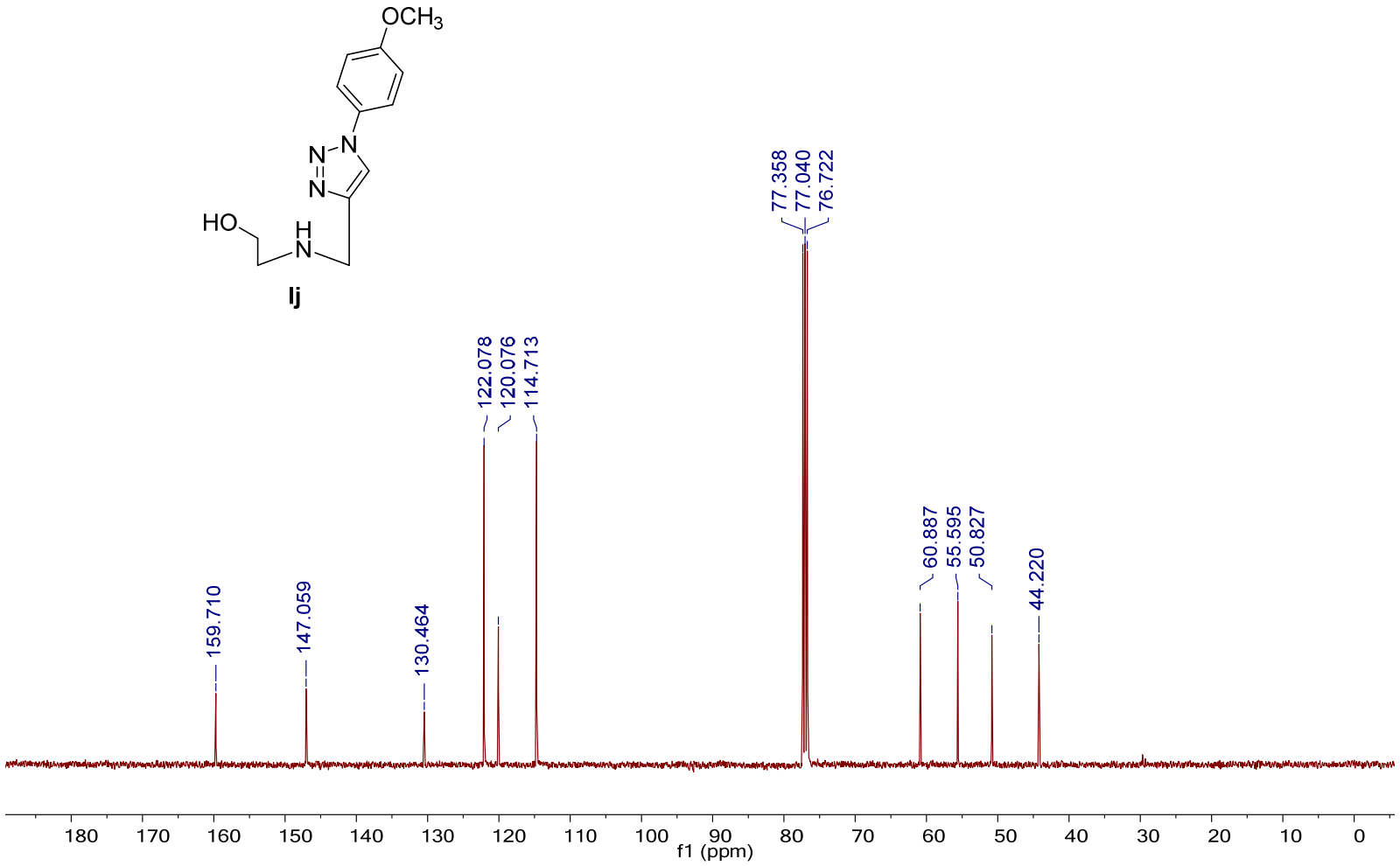

C16H33
HO
H
N
N
N
N
Ih
1.652
1.634
1.614
1.355
1.326
1.313
1.258
0.894
0.878
0.860
7.923
7.612
7.592
7.308
7.288
4.018
3.724
3.711
3.699
2.891
2.879
2.867
2.675
2.656
2.637
-0.000
1.00
2.01
2.03
2.07
1.99
2.06
2.10
1.99
26.79
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

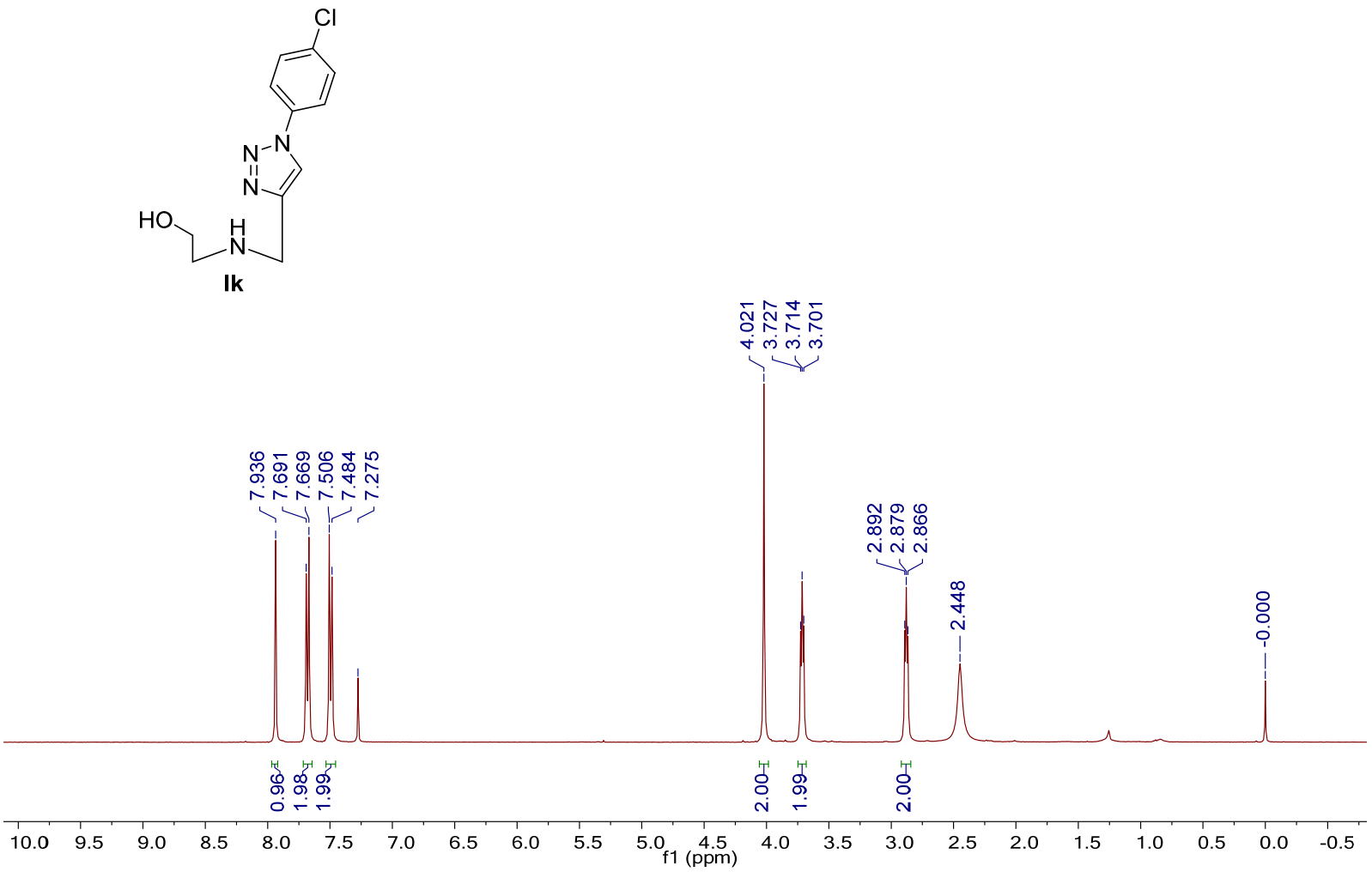

C16H33
HO
H
N
N
N
N
Ih
77.331
77.013
76.696
35.456
31.889
31.293
29.660
29.628
29.551
29.444
29.325
29.192
22.654
146.946
143.839
134.855
129.547
120.391
119.929
60.835
50.781
44.175
14.085
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

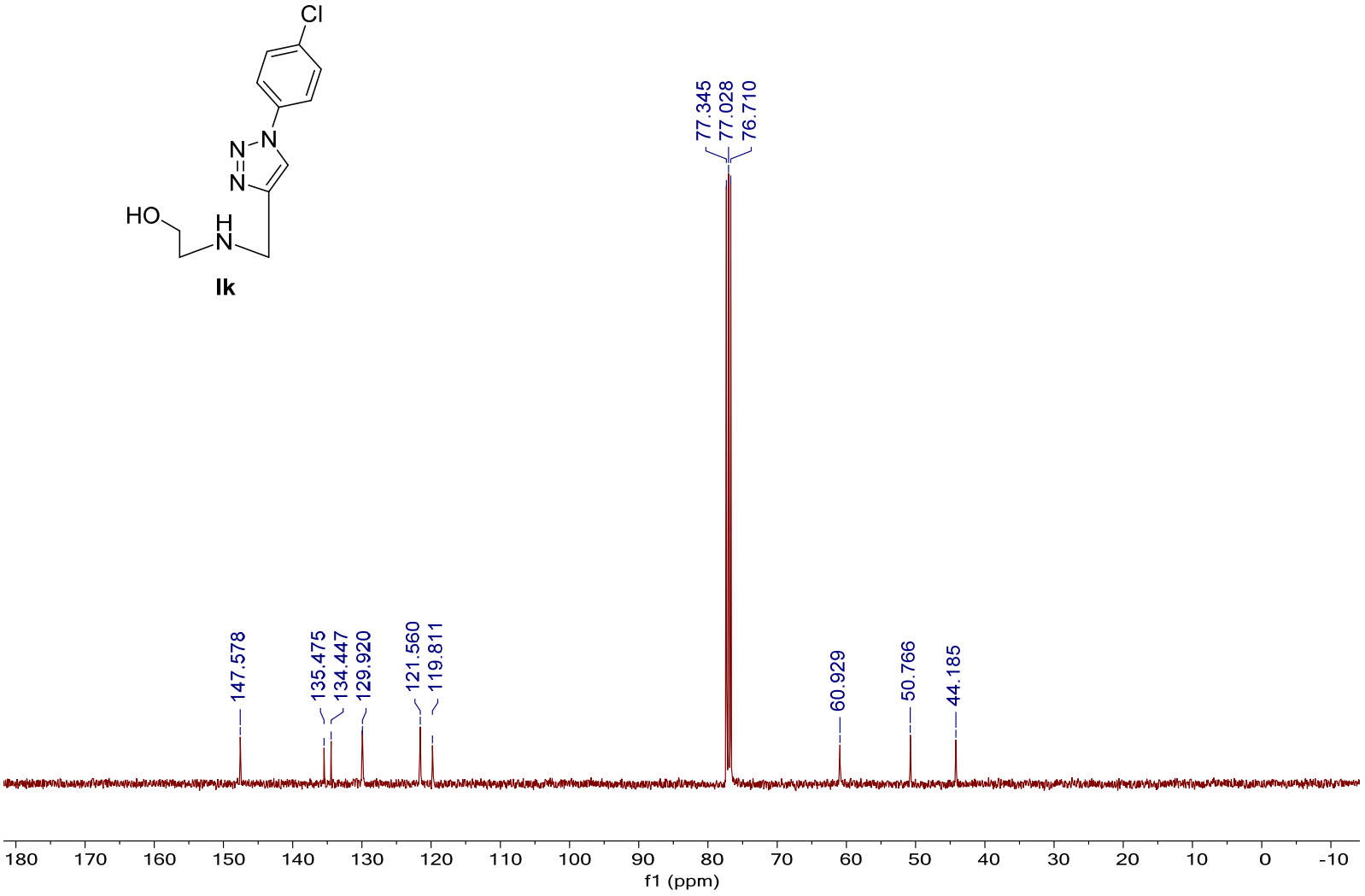

CF3
N
N
N
HO
H
N
Ii
8.814
8.171
8.151
7.986
7.965
4.515
3.858
3.502
3.488
3.474
3.343
2.663
2.649
2.635
2.500
1.00
1.99
2.05
0.94
2.00
2.04
2.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

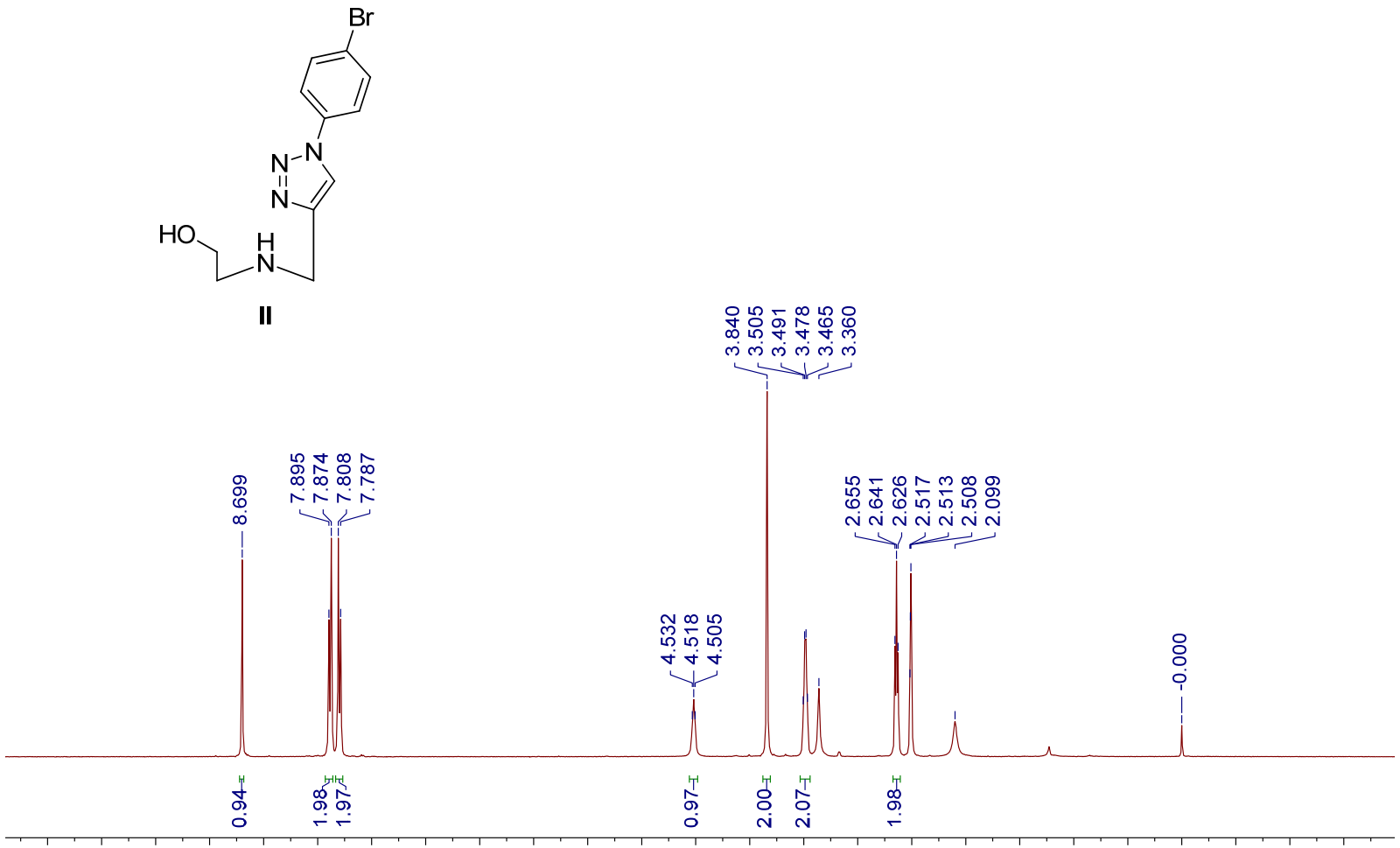

CF3
HO
H
N
N
N
N
li
129.320
129.002
128.679
128.342
127.611
127.572
125.615
122.910
121.521
120.643
120.202
148.627
139.943
60.715
51.568
44.470
40.545
40.337
40.128
39.919
39.710
39.502
39.293
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

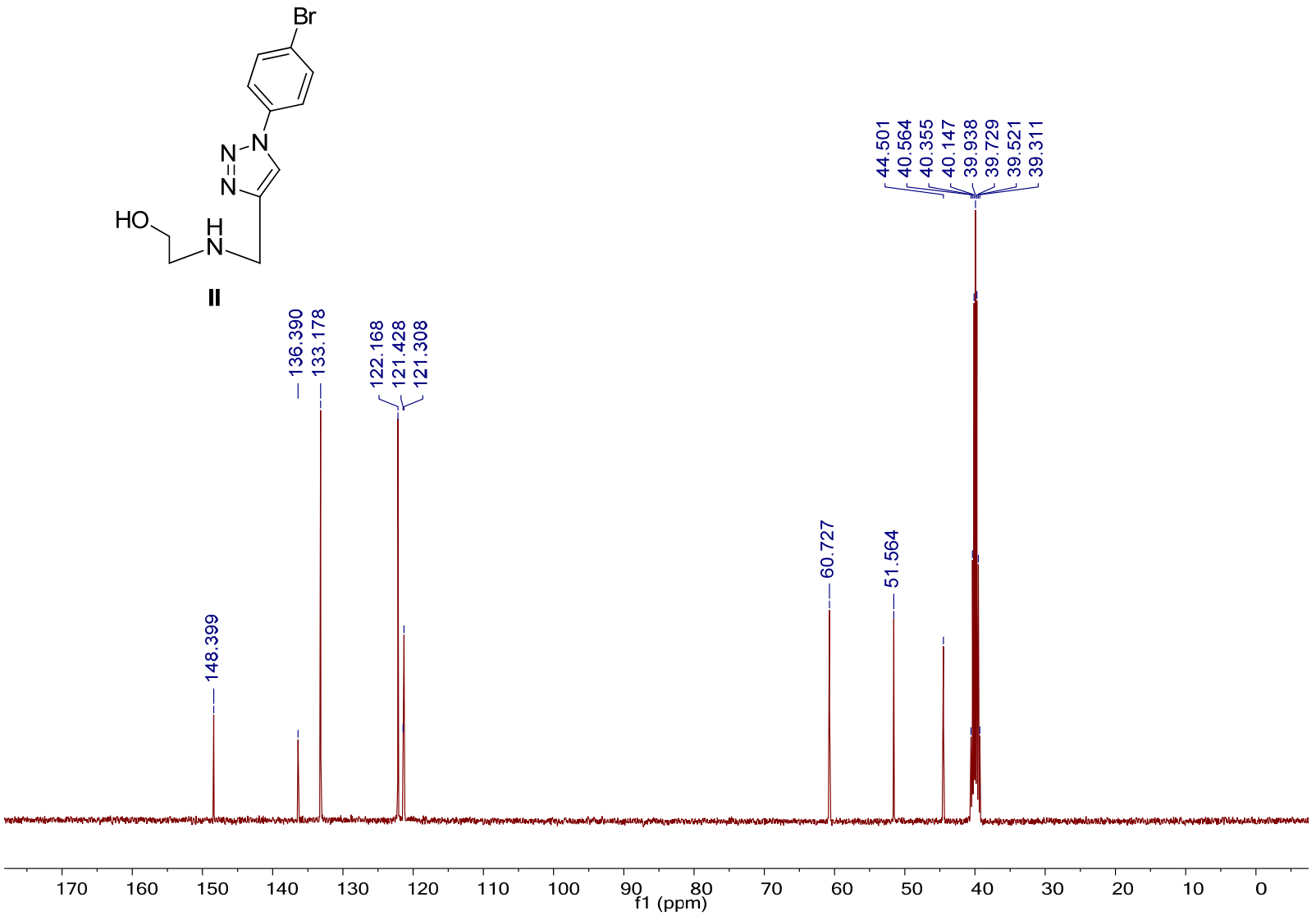

OCH3
N
N
N
HO
H
N
Ij
4.001
3.861
3.722
3.710
3.697
7.871
7.617
7.595
7.282
7.014
6.991
2.882
2.870
2.858
2.649
1.255
-0.000
0.99
2.00
2.04
1.99
3.06
2.00
2.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

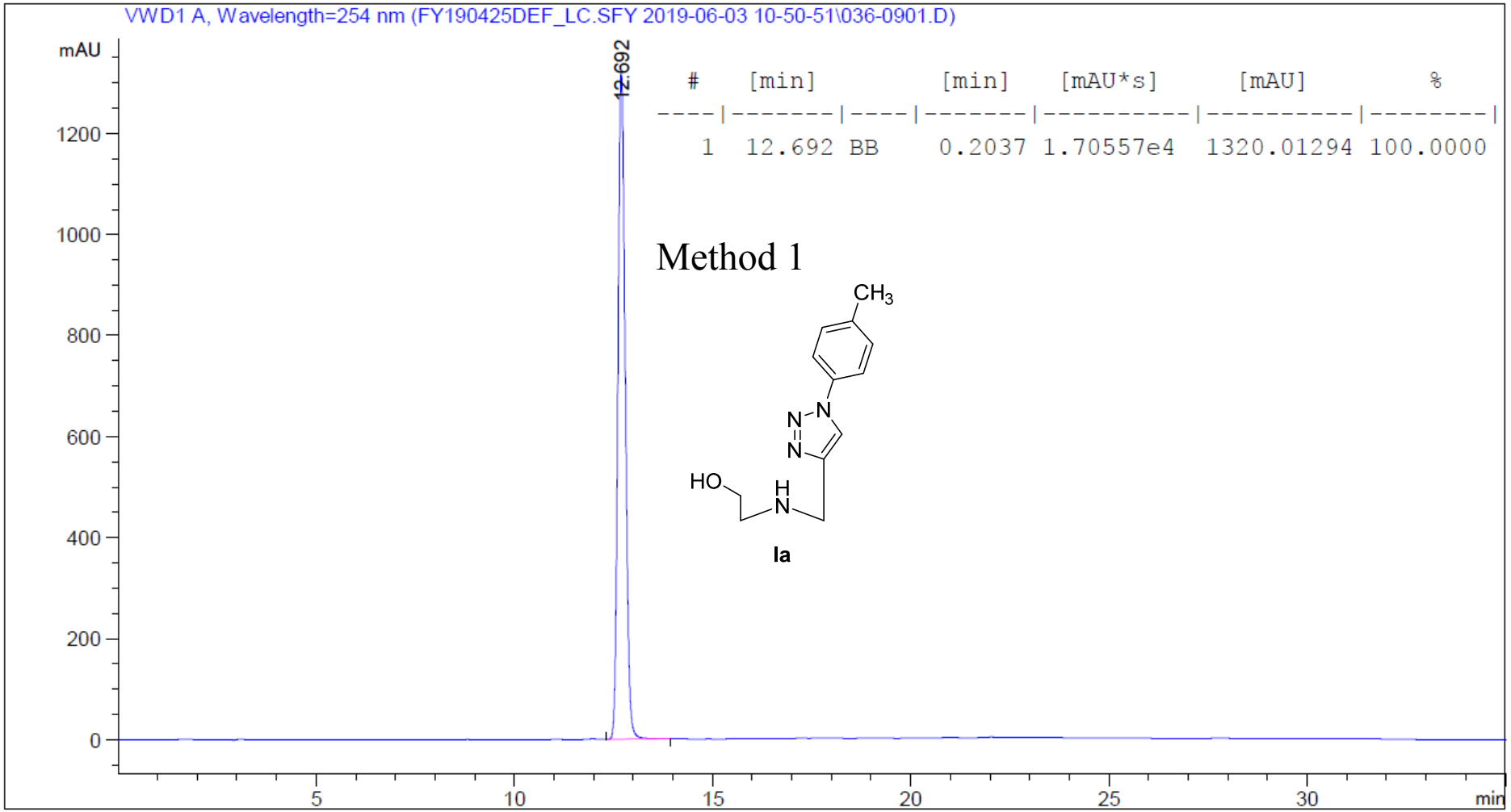

OCH3
N
N
N
HO
H
N
Ij
77.358
77.040
76.722
122.078
120.076
114.713
159.710
147.059
130.464
60.887
55.595
50.827
44.220
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

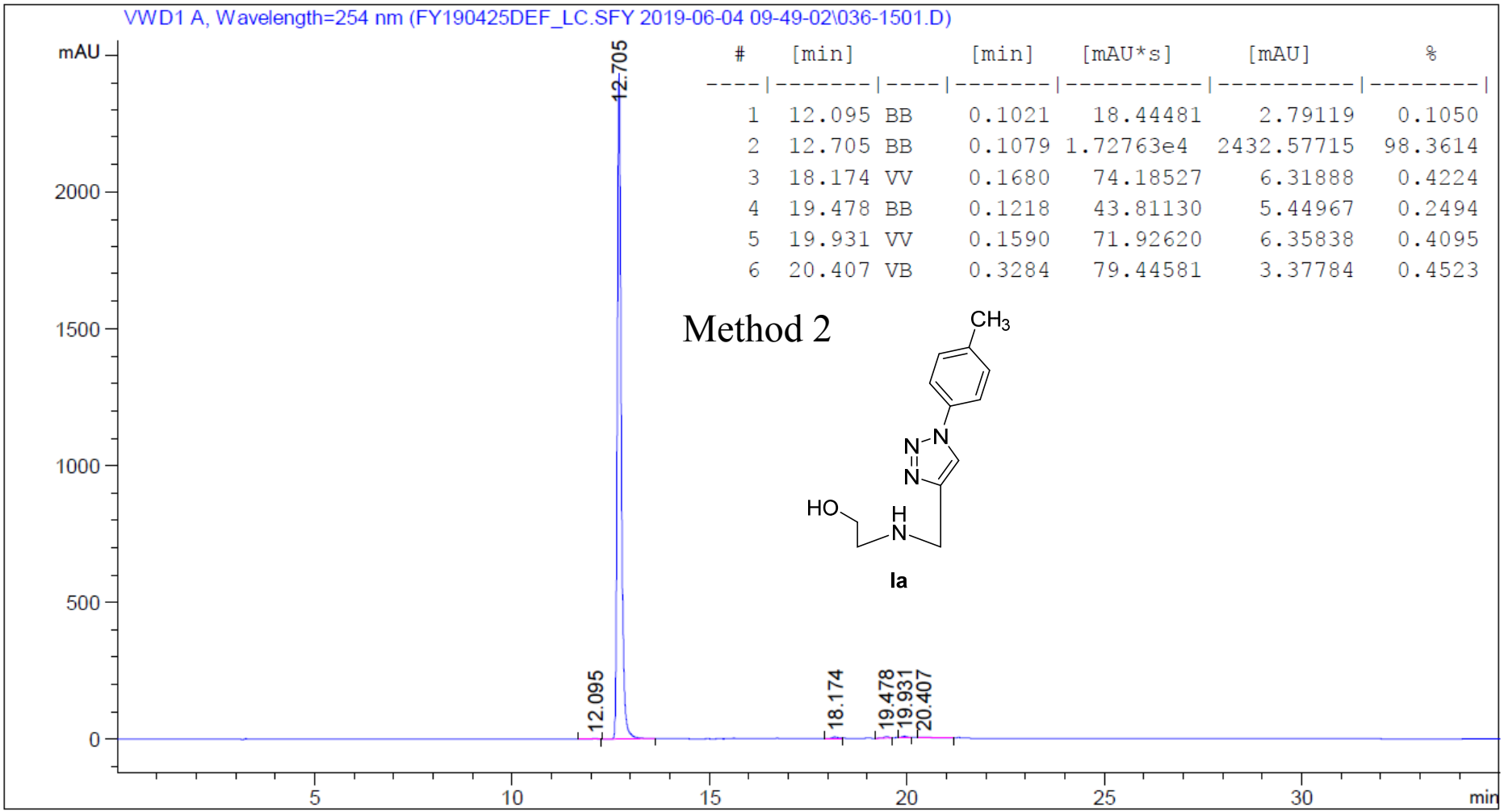

Cl
N
N
N
HO
H
N
Ik
4.021
3.727
3.714
3.701
7.936
7.691
7.669
7.506
7.484
7.275
2.892
2.879
2.866
2.448
-0.000
0.96
1.98
1.99
2.00
1.99
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Cl
N
N
N
HO
H
N
Ik
77.345
77.028
76.710
147.578
135.475
134.447
129.920
121.560
119.811
60.929
50.766
44.185
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Br
N
N
N
HO
H
N
II
8.699
7.895
7.874
7.808
7.787
4.532
4.518
4.505
3.840
3.505
3.491
3.478
3.465
3.360
2.655
2.641
2.626
2.517
2.513
2.508
2.099
-0.000
0.94
1.98
1.97
0.97
2.00
2.07
1.98


Br
N
N
N
HO
H
N
II
44.501
40.564
40.355
40.147
39.938
39.729
39.521
39.311
136.390
133.178
122.168
121.428
121.308
60.727
51.564
148.399
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

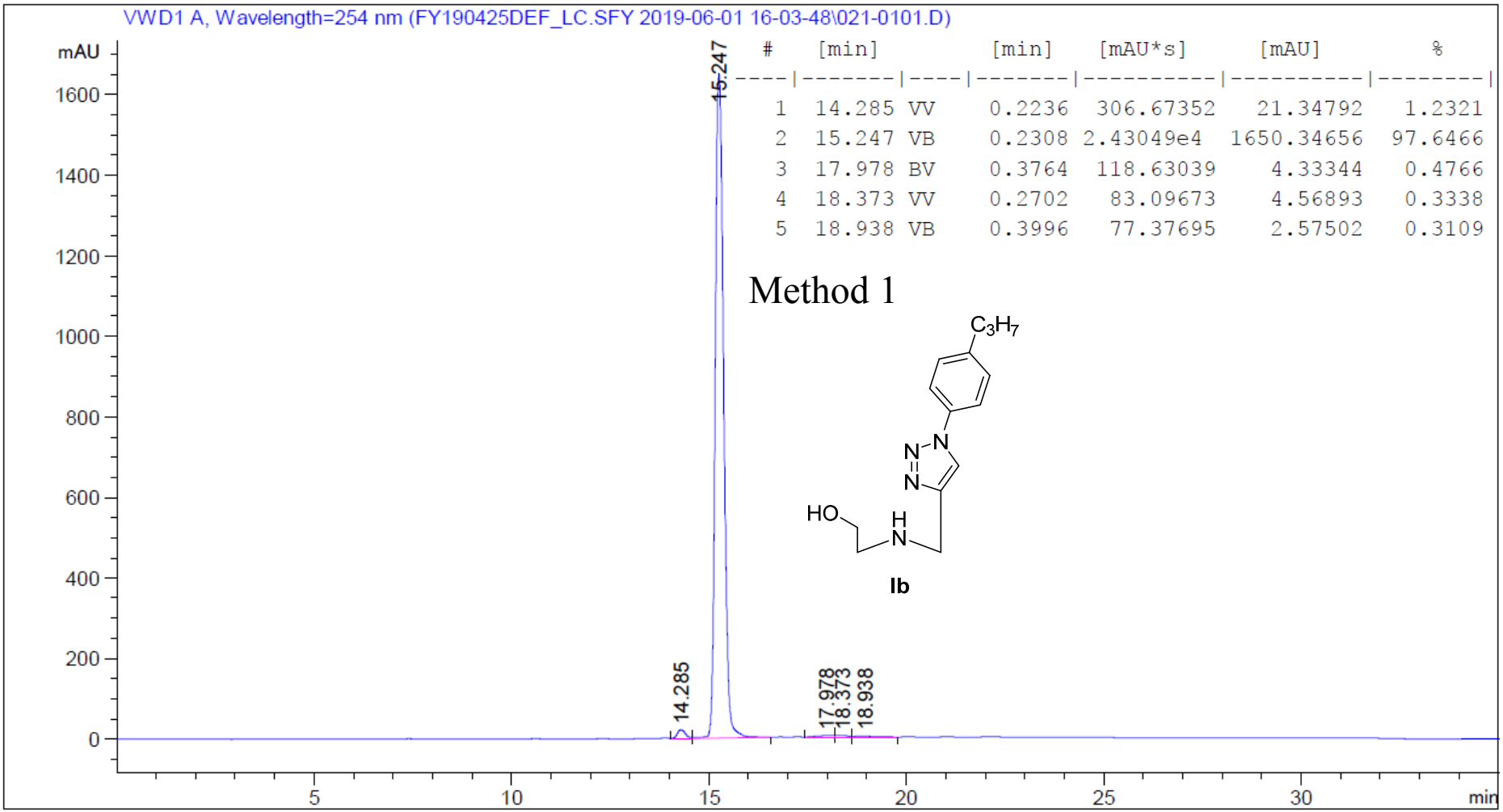

VWD1 A, Wavelength=254 nm (FY190425DEF_LC.SFY 2019-06-03 10-50-51\036-0901.D)
mAU
1200
1000
800
600
400
200
0
12.692
5
10
15
20
25
30
min
[min] [min] [mAU*s] [mAU] %
1 12.692 BB 0.2037 1.70557e4 1320.01294 100.0000
Method 1
CH3
N
N
N
HO
H
N
Ia

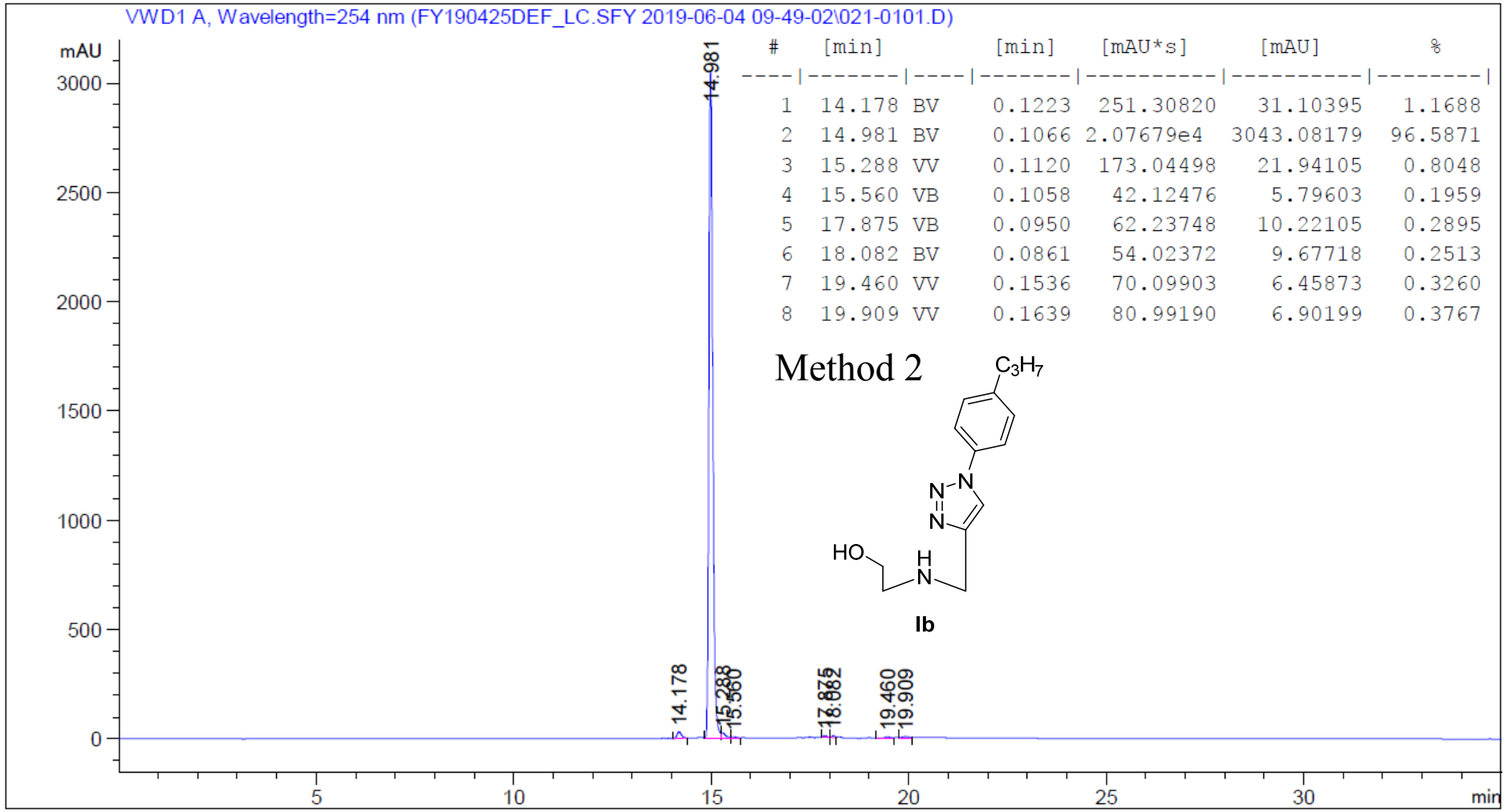


#	[min]		[min]	[mAU*s]	[mAU]	%
1	12.095	BB	0.1021	18.44481	2.79119	0.1050
2	12.705	BB	0.1079	1.72763e4	2432.57715	98.3614
3	18.174	VV	0.1680	74.18527	6.31888	0.4224
4	19.478	BB	0.1218	43.81130	5.44967	0.2494
5	19.931	VV	0.1590	71.92620	6.35838	0.4095
6	20.407	VB	0.3284	79.44581	3.37784	0.4523

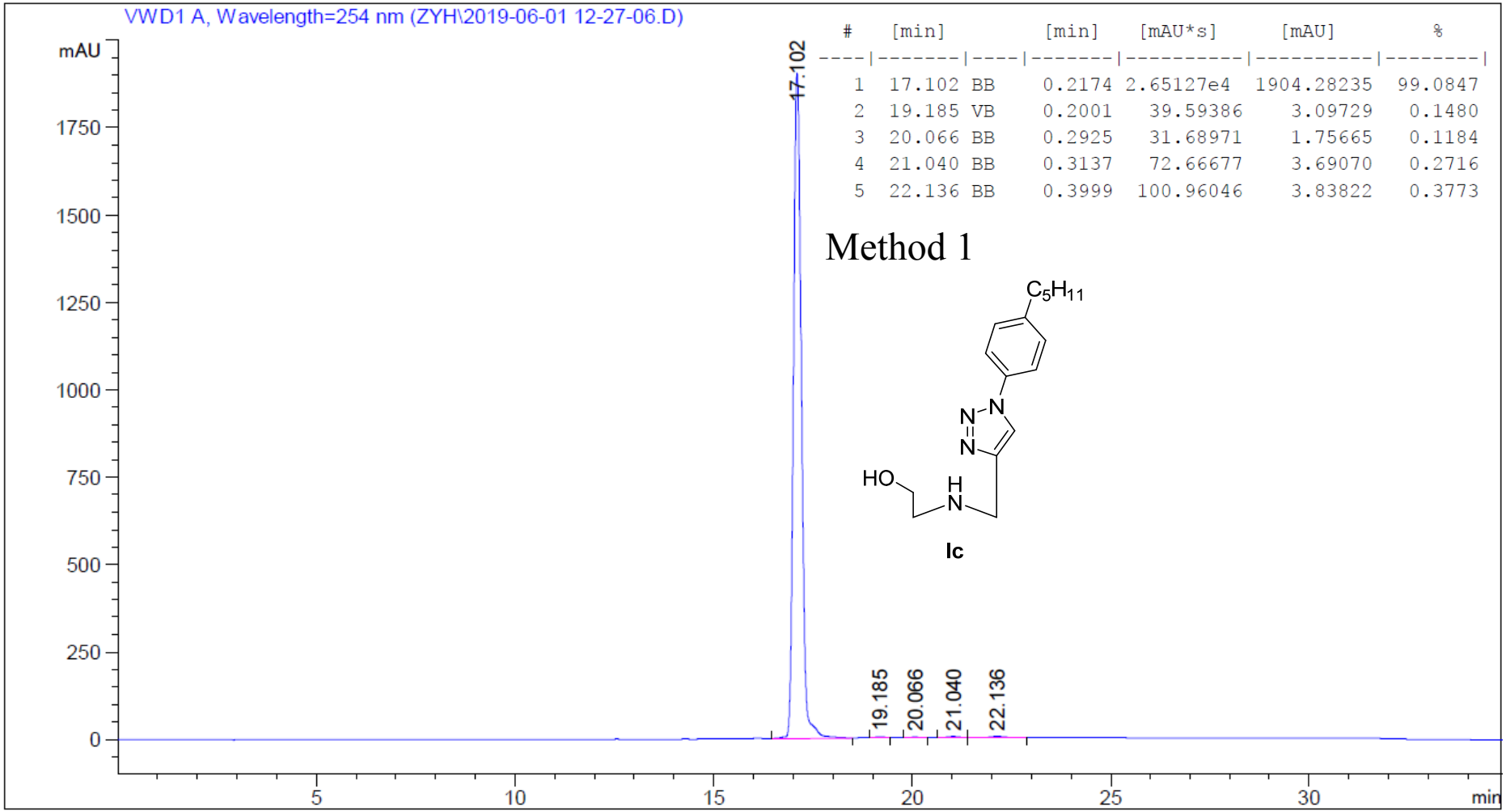
Method 2

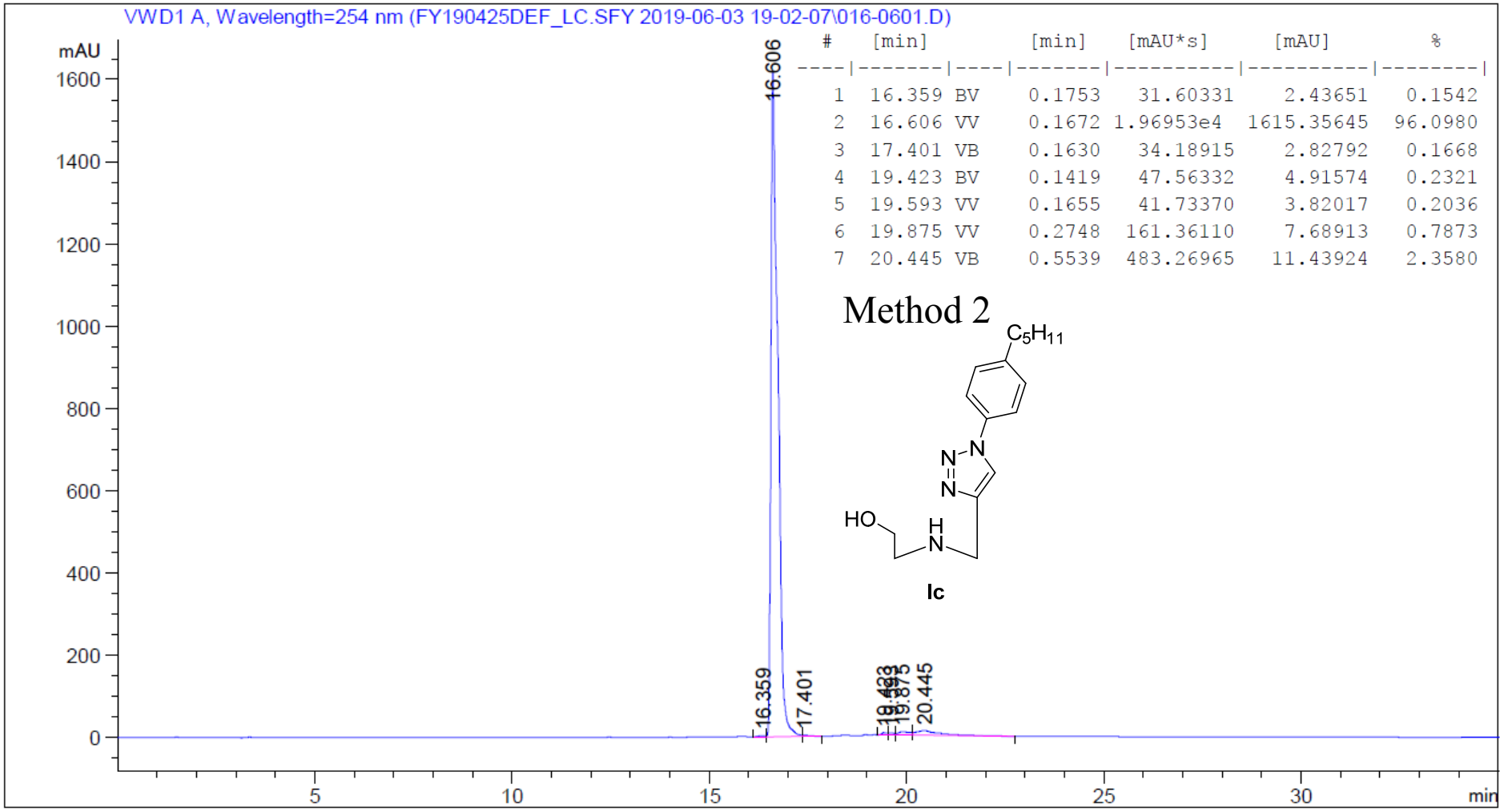
Ia


VWD1 A, Wavelength=254 nm (FY190425DEF_LC.SFY 2019-06-01 16-03-48\021-0101.D)
mAU
1600
1400
1200
1000
800
600
400
200
0
5
10
15
20
25
30
min
15.247
14.285
17.978
18.373
18.938
[min] [min] [mAU*s] [mAU] %
1 14.285 VV 0.2236 306.67352 21.34792 1.2321
2 15.247 VB 0.2308 2.43049e4 1650.34656 97.6466
3 17.978 BV 0.3764 118.63039 4.33344 0.4766
4 18.373 VV 0.2702 83.09673 4.56893 0.3338
5 18.938 VB 0.3996 77.37695 2.57502 0.3109
Method 1
C3H7
N
N
N
HO
H
N
Ib

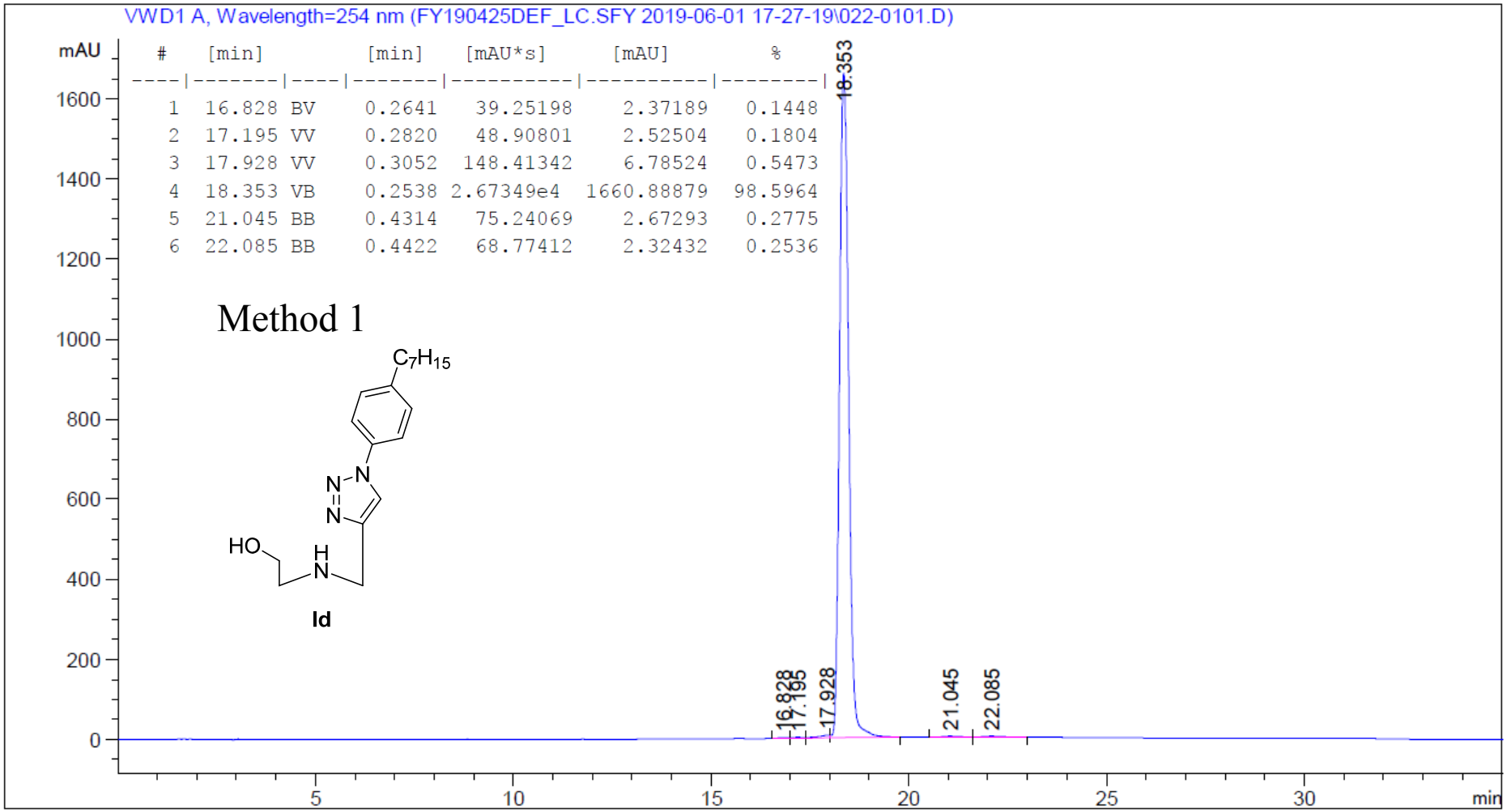


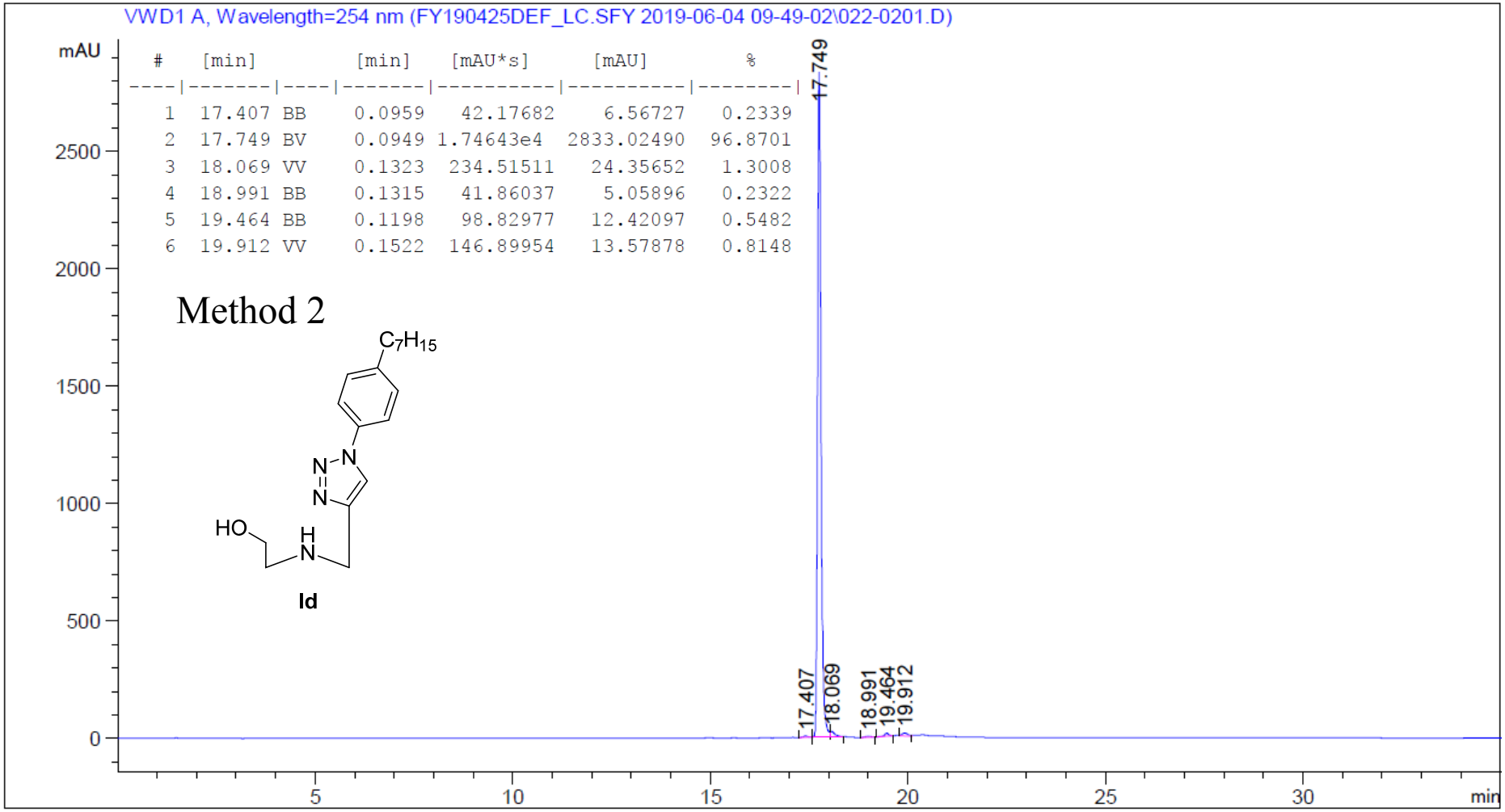
#	[min]		[min]	[mAU*s]	[mAU]	%
1	14.178	BV	0.1223	251.30820	31.10395	1.1688
2	14.981	BV	0.1066	2.07679e4	3043.08179	96.5871
3	15.288	VV	0.1120	173.04498	21.94105	0.8048
4	15.560	VB	0.1058	42.12476	5.79603	0.1959
5	17.875	VB	0.0950	62.23748	10.22105	0.2895
6	18.082	BV	0.0861	54.02372	9.67718	0.2513
7	19.460	VV	0.1536	70.09903	6.45873	0.3260
8	19.909	VV	0.1639	80.99190	6.90199	0.3767


VWD1 A, Wavelength=254 nm (ZYH\2019-06-01 12-27-06.D)
mAU
1750
1500
1250
1000
750
500
250
0
5
10
15
20
25
30
min
17.102
19.185
20.066
21.040
22.136
[min] [min] [mAU*s] [mAU] %
1 17.102 BB 0.2174 2.65127e4 1904.28235 99.0847
2 19.185 VB 0.2001 39.59386 3.09729 0.1480
3 20.066 BB 0.2925 31.68971 1.75665 0.1184
4 21.040 BB 0.3137 72.66677 3.69070 0.2716
5 22.136 BB 0.3999 100.96046 3.83822 0.3773
Method 1
C5H11
N
N
N
HO
H
N
Ic

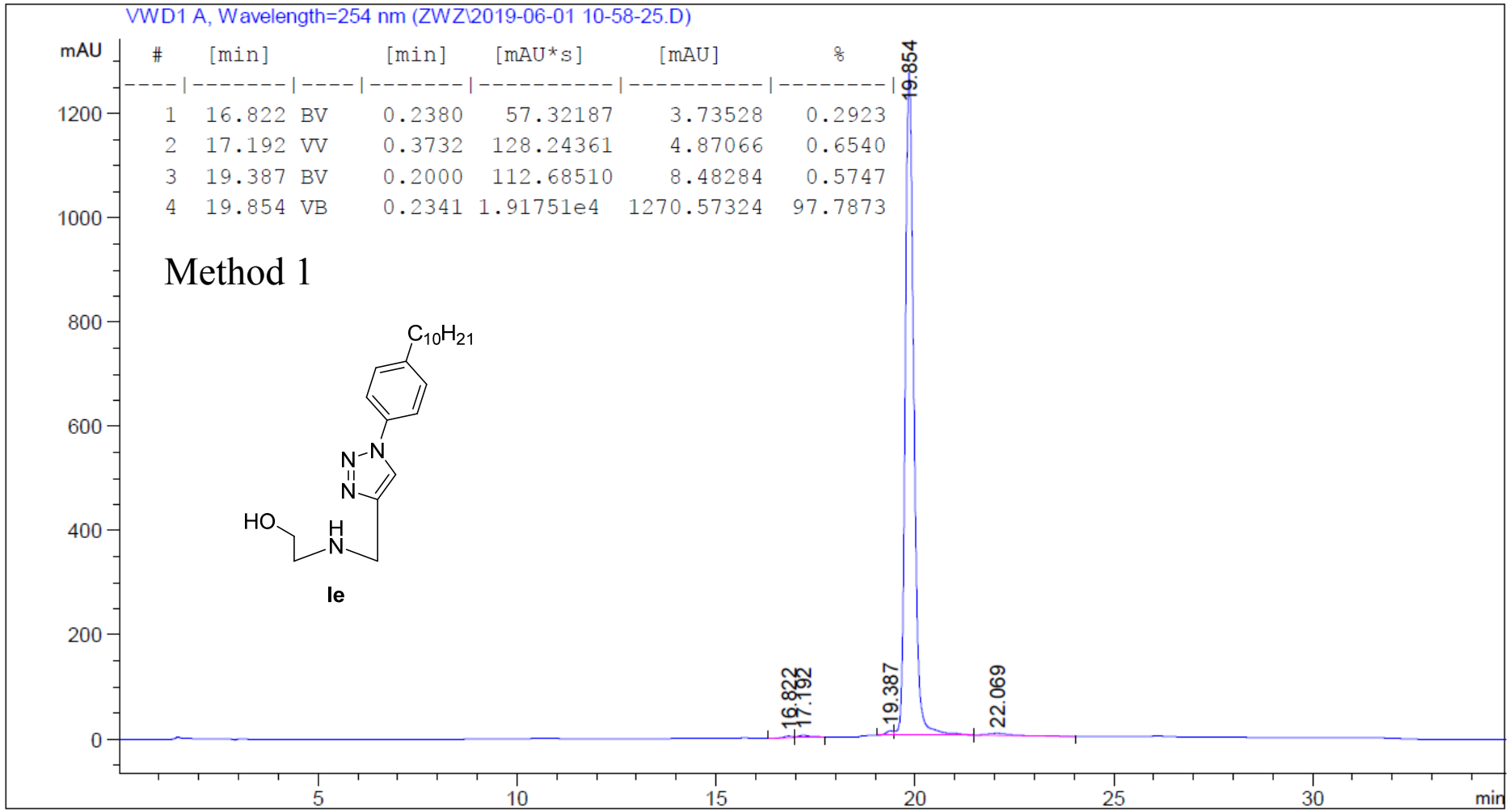


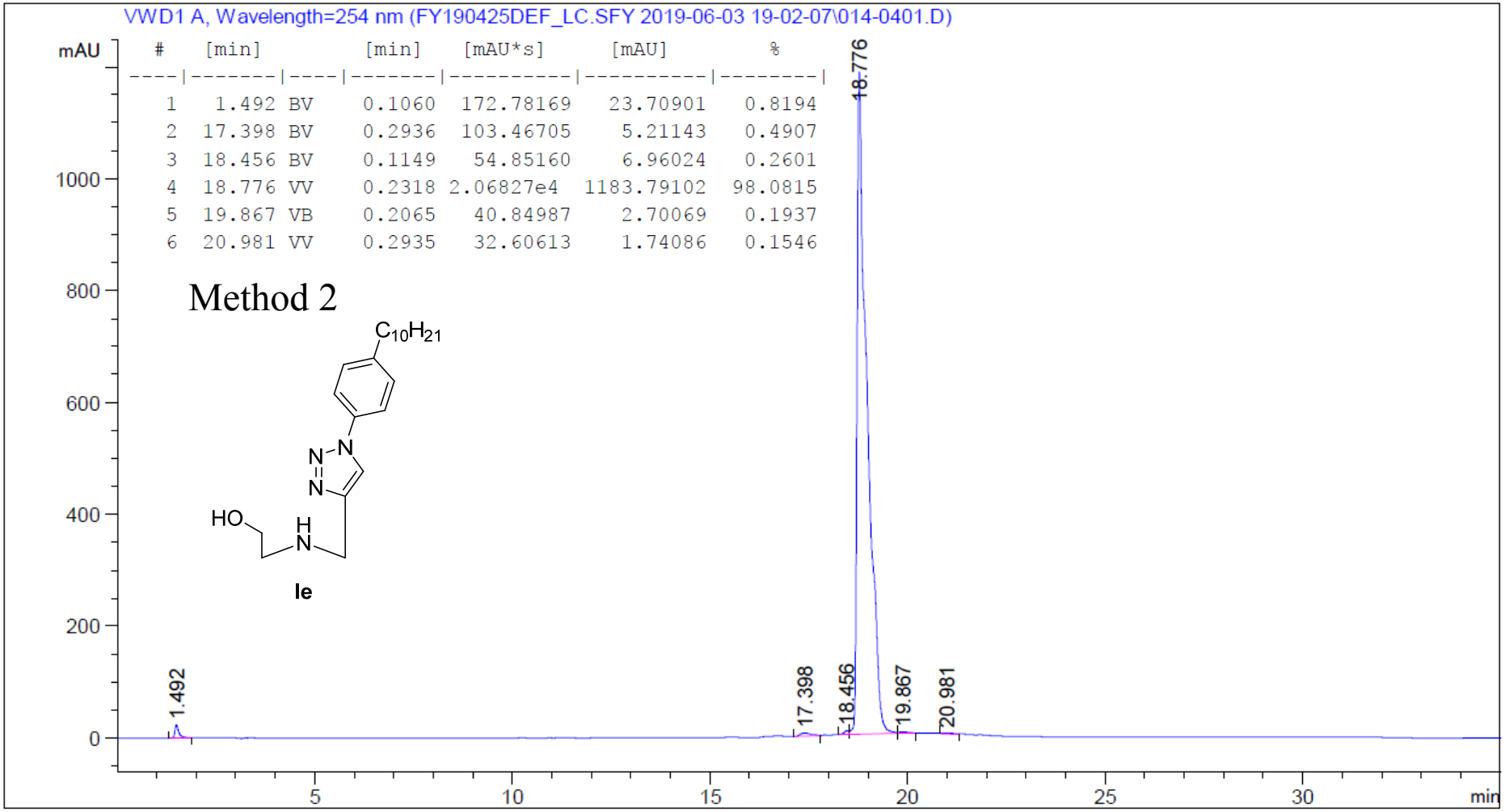
#	[min]		[min]	[mAU*s]	[mAU]	%
1	16.359	BV	0.1753	31.60331	2.43651	0.1542
2	16.606	VV	0.1672	1.96953e4	1615.35645	96.0980
3	17.401	VB	0.1630	34.18915	2.82792	0.1668
4	19.423	BV	0.1419	47.56332	4.91574	0.2321
5	19.593	VV	0.1655	41.73370	3.82017	0.2036
6	19.875	VV	0.2748	161.36110	7.68913	0.7873
7	20.445	VB	0.5539	483.26965	11.43924	2.3580

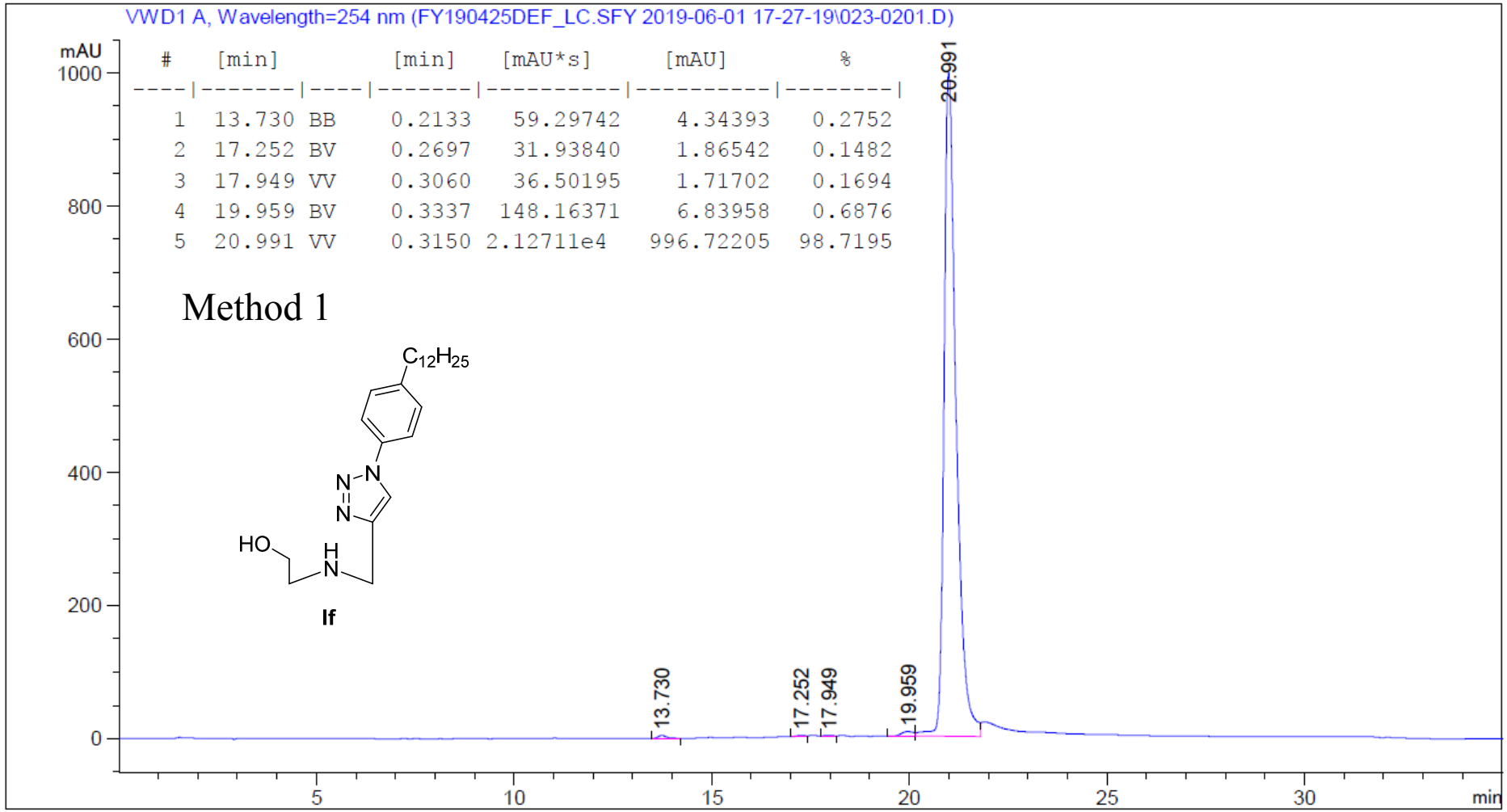

VWD1 A, Wavelength=254 nm (FY190425DEF_LC.SFY 2019-06-01 17-27-19\022-0101.D)
mAU
[min] [min] [mAU*s] [mAU] %
1 16.828 BV 0.2641 39.25198 2.37189 0.1448
2 17.195 VV 0.2820 48.90801 2.52504 0.1804
3 17.928 VV 0.3052 148.41342 6.78524 0.5473
4 18.353 VB 0.2538 2.67349e4 1660.88879 98.5964
5 21.045 BB 0.4314 75.24069 2.67293 0.2775
6 22.085 BB 0.4422 68.77412 2.32432 0.2536
Method 1
C7H15
HO
H
N
Id
16.828
17.195
17.928
18.353
21.045
22.085
min



#	[min]		[min]	[mAU*s]	[mAU]	%
1	17.407	BB	0.0959	42.17682	6.56727	0.2339
2	17.749	BV	0.0949	1.74643e4	2833.02490	96.8701
3	18.069	VV	0.1323	234.51511	24.35652	1.3008
4	18.991	BB	0.1315	41.86037	5.05896	0.2322
5	19.464	BB	0.1198	98.82977	12.42097	0.5482
6	19.912	VV	0.1522	146.89954	13.57878	0.8148


VWD1 A, Wavelength=254 nm (ZWZ\2019-06-01 10-58-25.D)
mAU
[min] [min] [mAU*s] [mAU] %
1 16.822 BV 0.2380 57.32187 3.73528 0.2923
2 17.192 VV 0.3732 128.24361 4.87066 0.6540
3 19.387 BV 0.2000 112.68510 8.48284 0.5747
4 19.854 VB 0.2341 1.91751e4 1270.57324 97.7873
Method 1
C10H21
HO
H
N
Ie
16.822
17.192
19.387
19.854
22.069
1200
1000
800
600
400
200
0
5
10
15
20
25
30
min

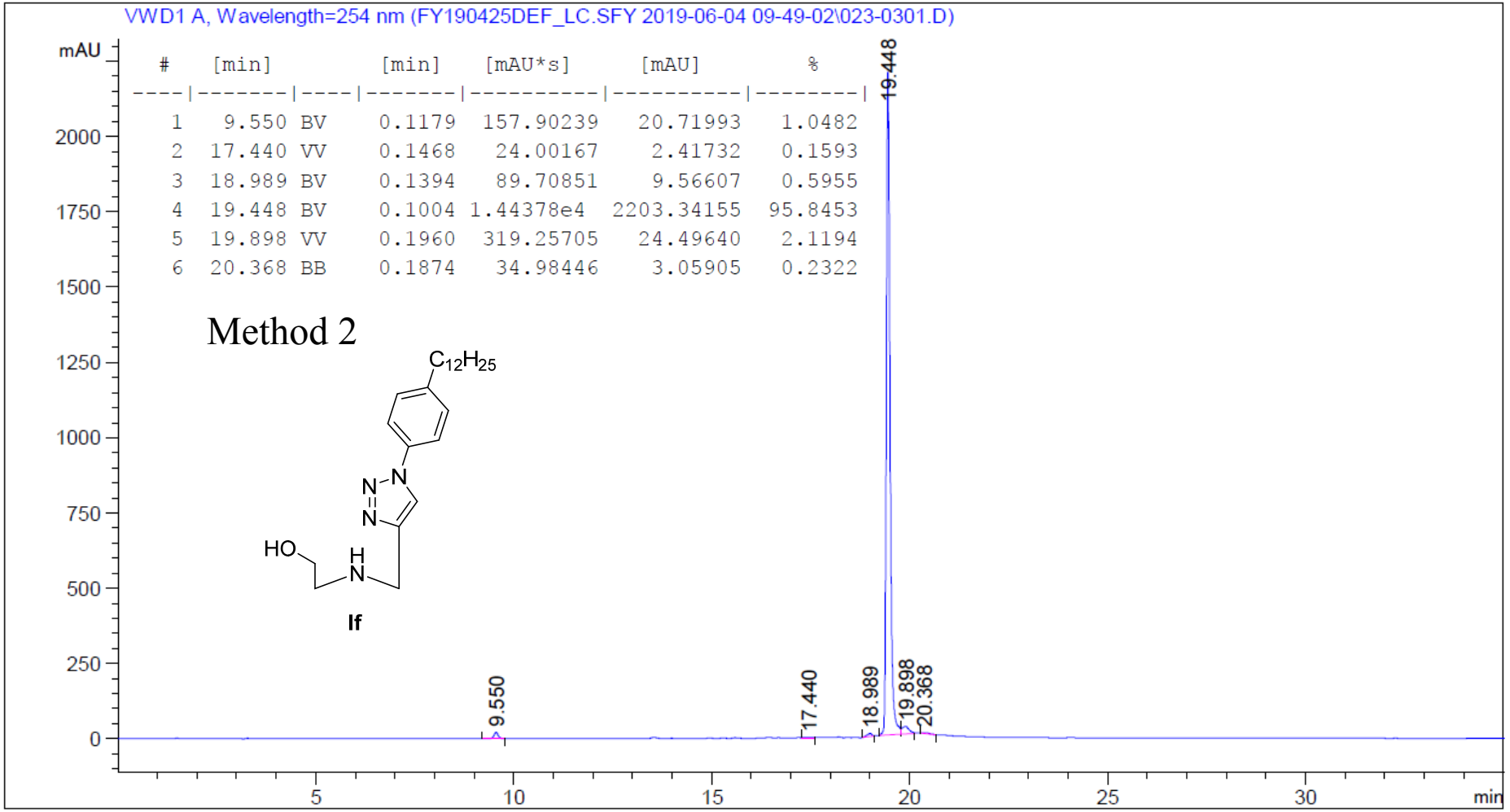

VWD1 A, Wavelength=254 nm (FY190425DEF_LC.SFY 2019-06-03 19-02-07\014-0401.D)
mAU
[min] [min] [mAU*s] [mAU] %
1 1.492 BV 0.1060 172.78169 23.70901 0.8194
2 17.398 BV 0.2936 103.46705 5.21143 0.4907
3 18.456 BV 0.1149 54.85160 6.96024 0.2601
4 18.776 VV 0.2318 2.06827e4 1183.79102 98.0815
5 19.867 VB 0.2065 40.84987 2.70069 0.1937
6 20.981 VV 0.2935 32.60613 1.74086 0.1546
Method 2
C10H21
HO
H
N
Ie
1.492
17.398
18.456
18.776
19.867
20.981
1000
800
600
400
200
0
5
10
15
20
25
30
min



#	[min]		[min]	[mAU*s]	[mAU]	%
1	13.730	BB	0.2133	59.29742	4.34393	0.2752
2	17.252	BV	0.2697	31.93840	1.86542	0.1482
3	17.949	VV	0.3060	36.50195	1.71702	0.1694
4	19.959	BV	0.3337	148.16371	6.83958	0.6876
5	20.991	VV	0.3150	2.12711e4	996.72205	98.7195

Method 1

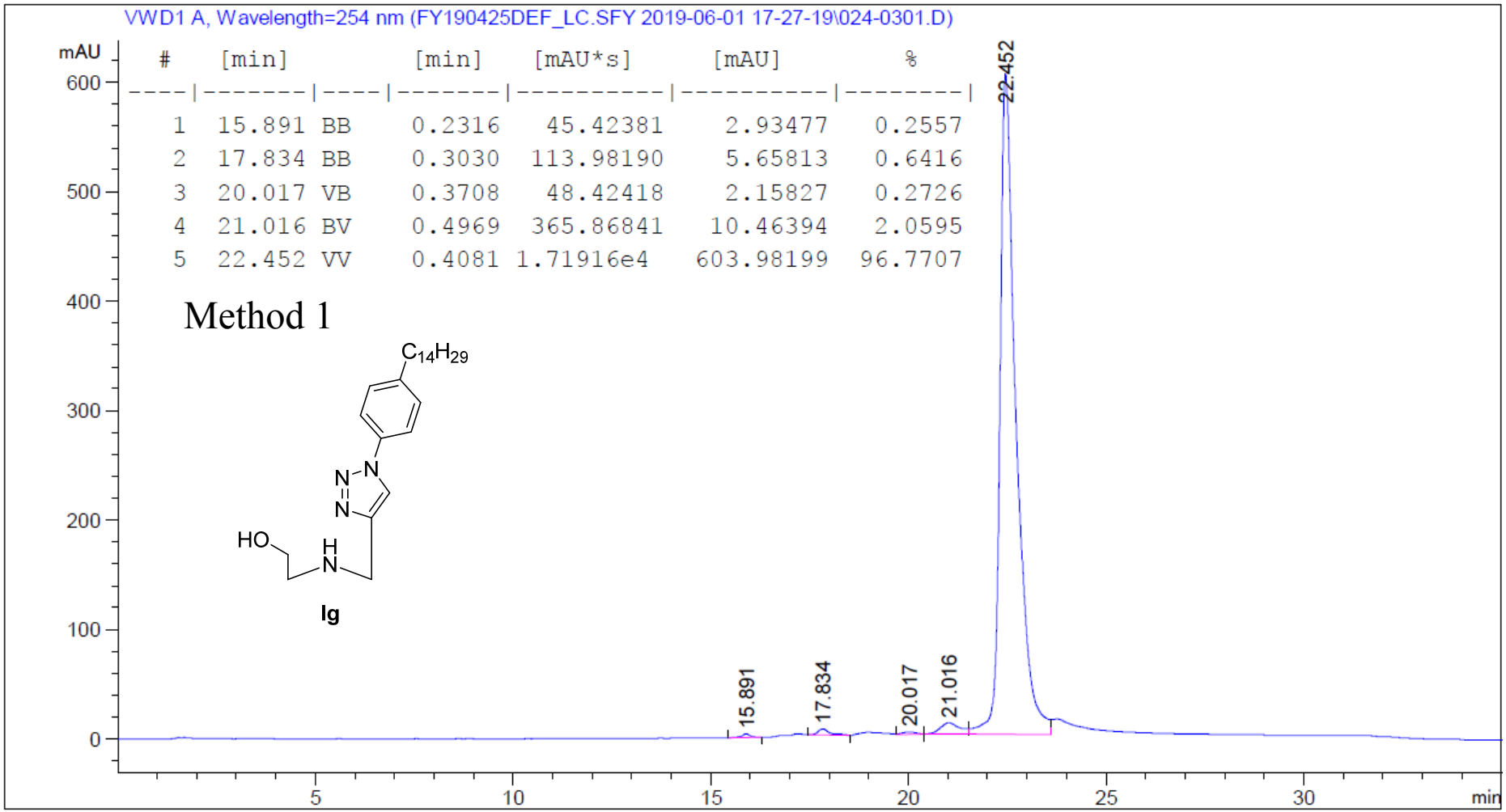
If

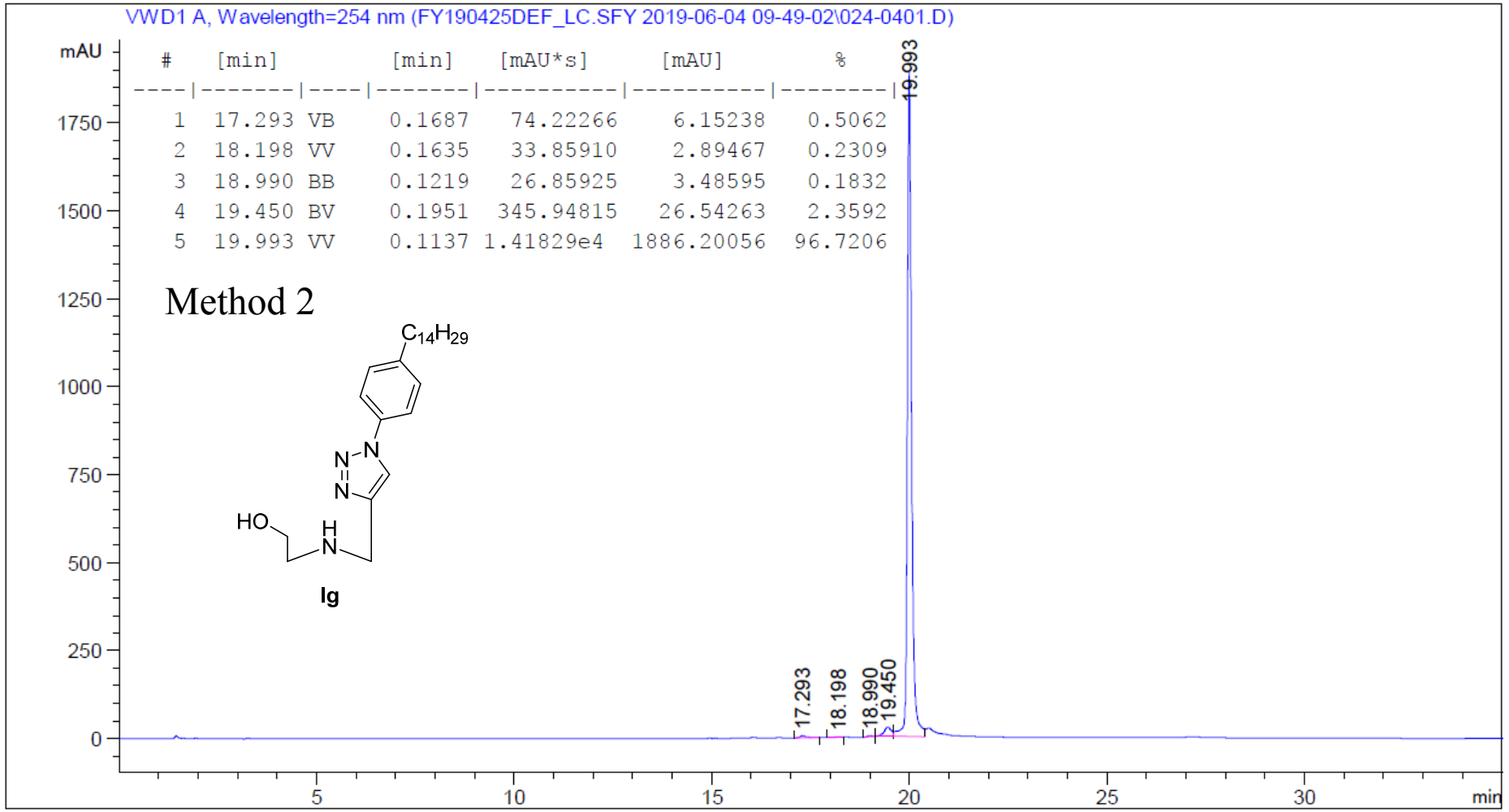


#	[min]		[min]	[mAU*s]	[mAU]	%
1	9.550	BV	0.1179	157.90239	20.71993	1.0482
2	17.440	VV	0.1468	24.00167	2.41732	0.1593
3	18.989	BV	0.1394	89.70851	9.56607	0.5955
4	19.448	BV	0.1004	1.44378e4	2203.34155	95.8453
5	19.898	VV	0.1960	319.25705	24.49640	2.1194
6	20.368	BB	0.1874	34.98446	3.05905	0.2322

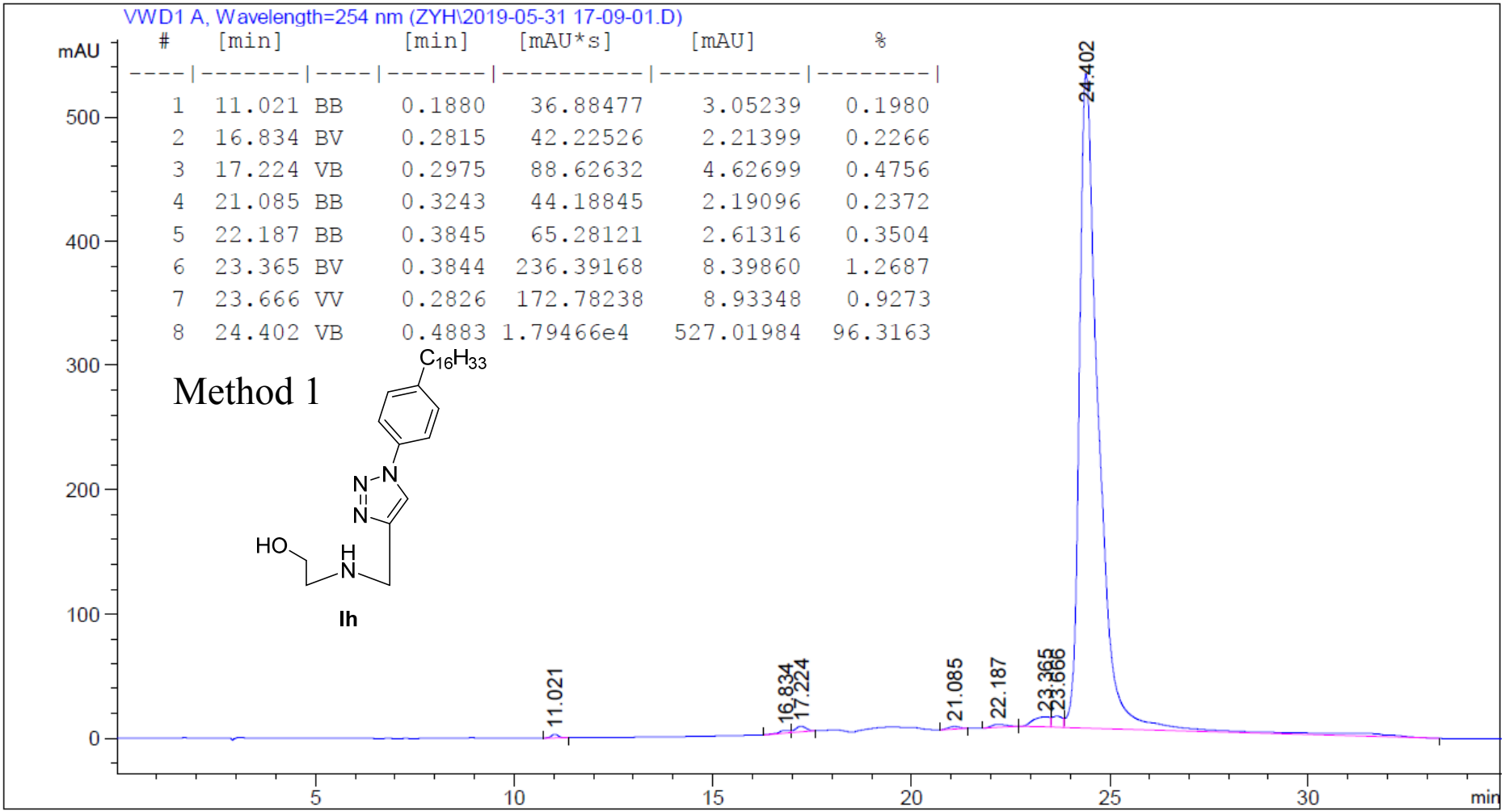
Method 2

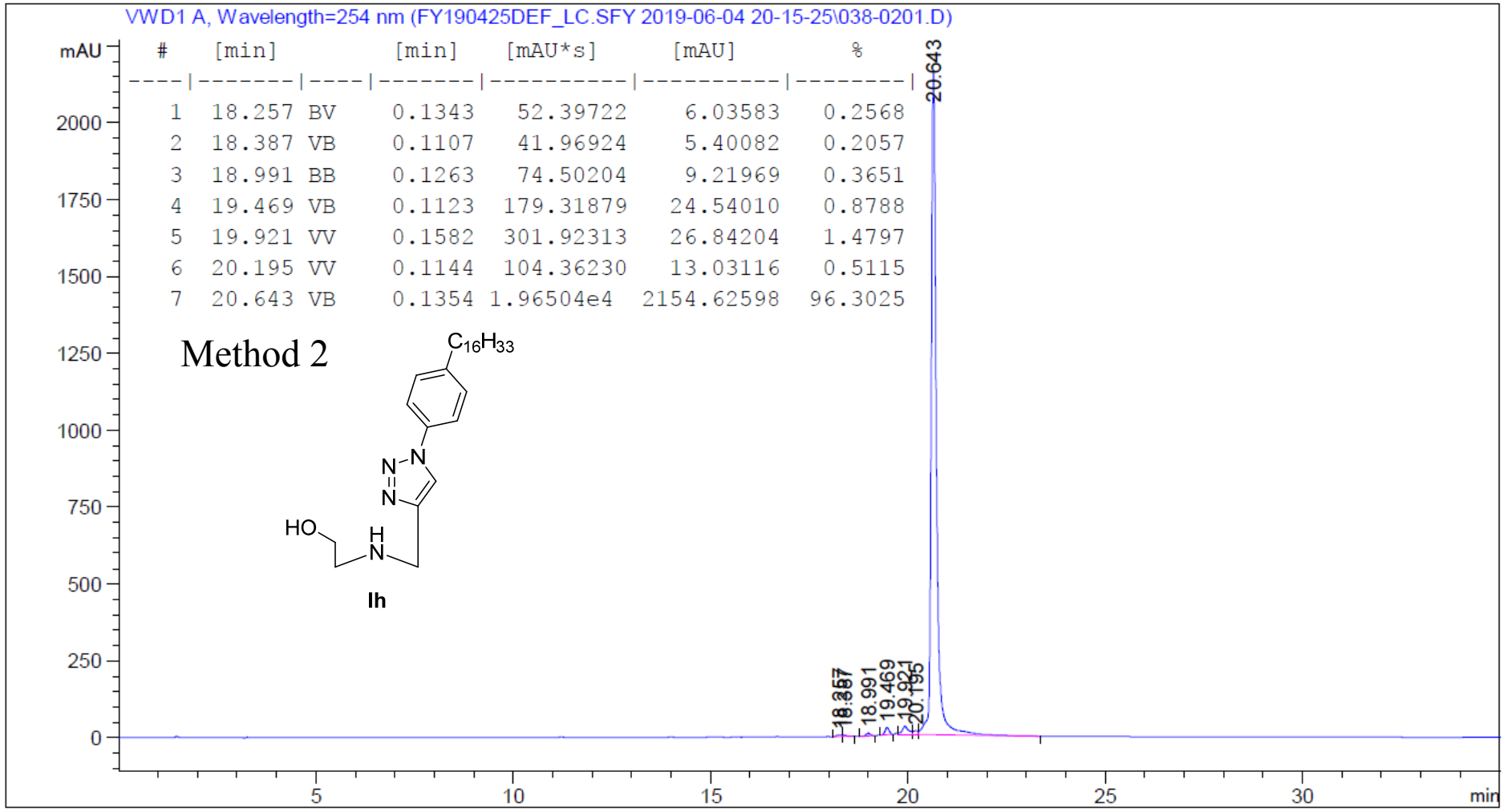
If

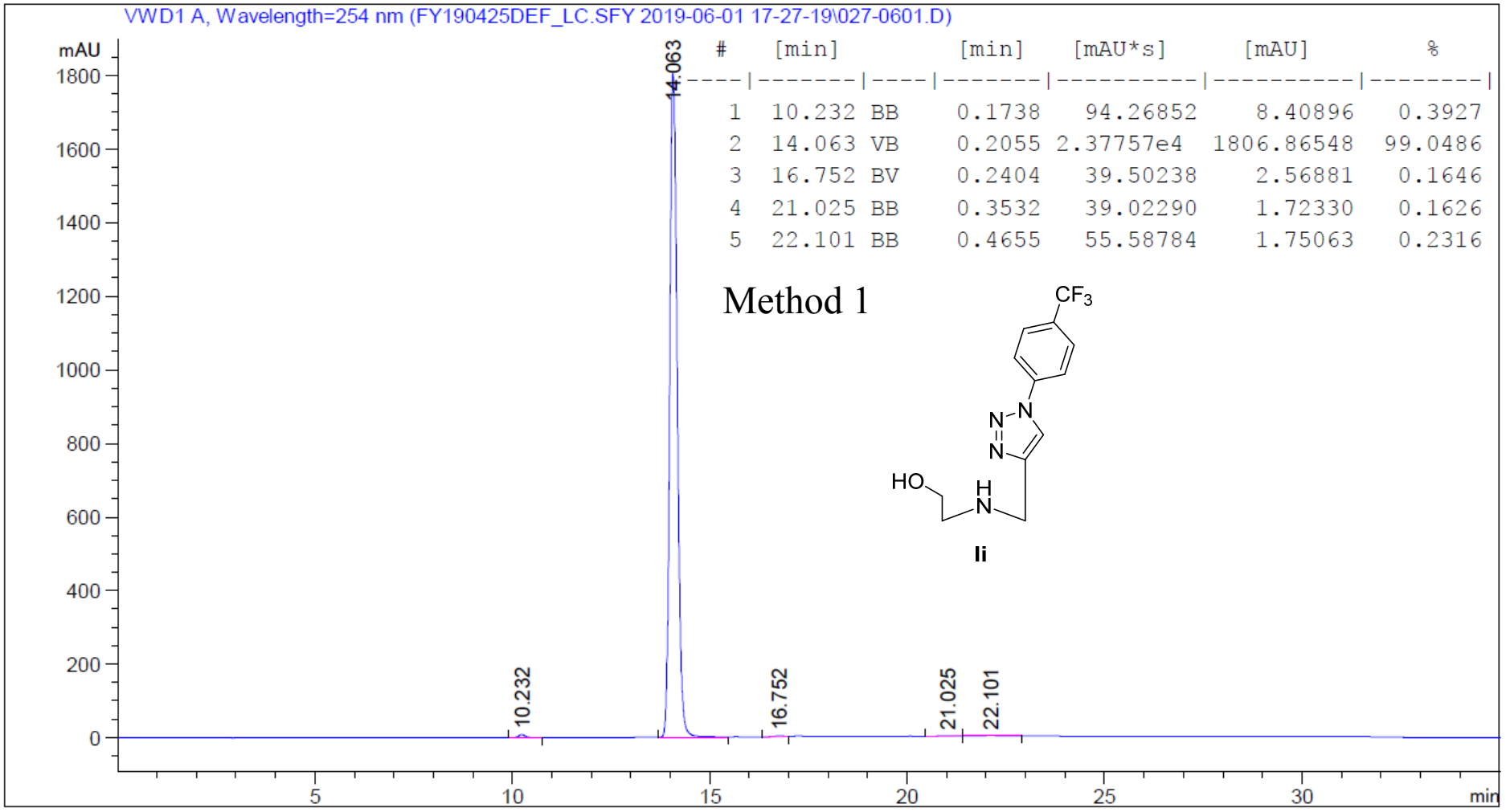

VWD1 A, Wavelength=254 nm (FY190425DEF_LC.SFY 2019-06-01 17-27-19\024-0301.D)
mAU
600
500
400
300
200
100
0
[min] [min] [mAU*s] [mAU] %
1 15.891 BB 0.2316 45.42381 2.93477 0.2557
2 17.834 BB 0.3030 113.98190 5.65813 0.6416
3 20.017 VB 0.3708 48.42418 2.15827 0.2726
4 21.016 BV 0.4969 365.86841 10.46394 2.0595
5 22.452 VV 0.4081 1.71916e4 603.98199 96.7707
Method 1
$C_{14}H_{29}$
HO
H
N
N
N
Ig
15.891
17.834
20.017
21.016
22.452
5
10
15
20
25
30
min



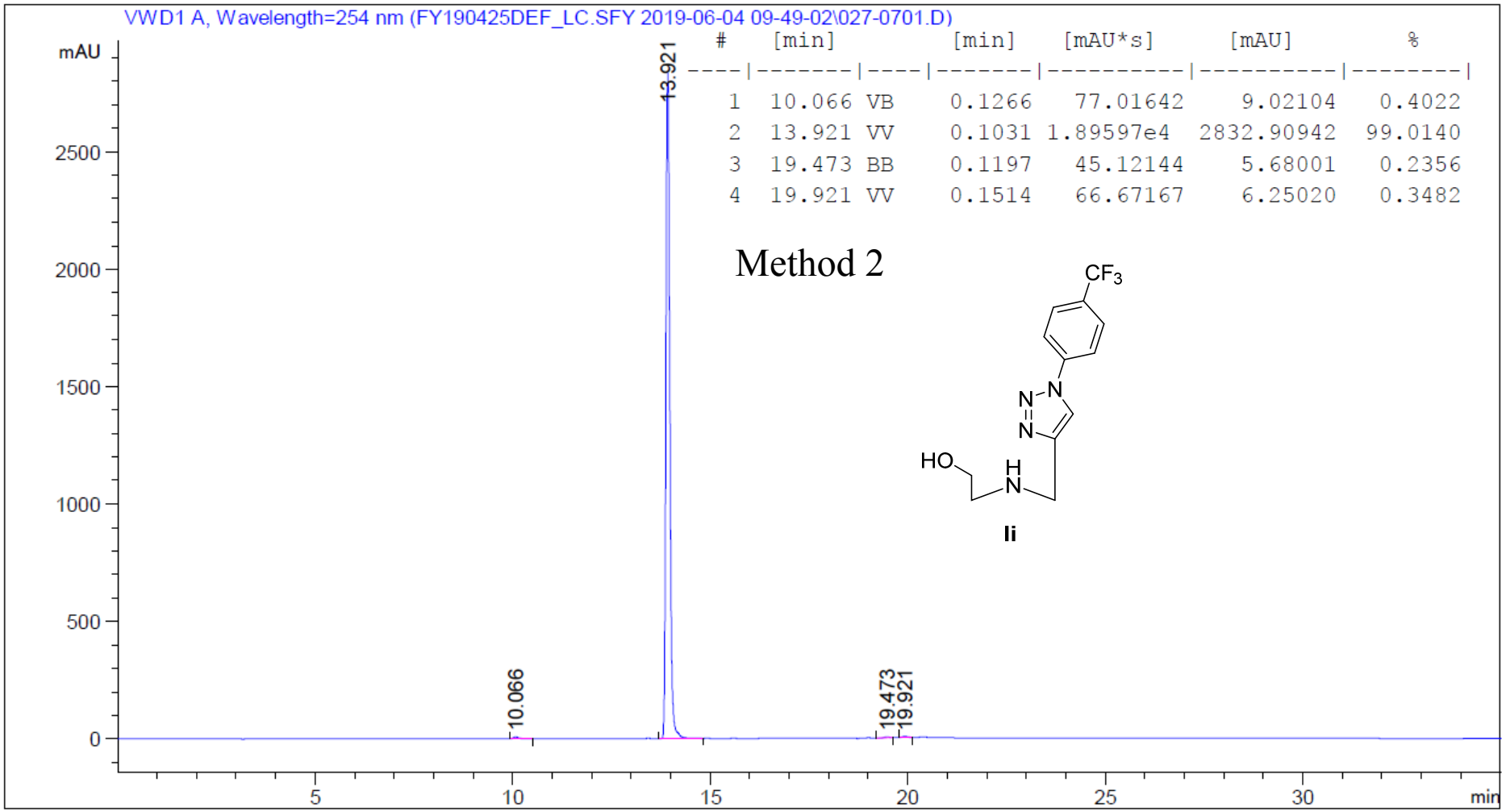
#	[min]		[min]	[mAU*s]	[mAU]	%
1	17.293	VB	0.1687	74.22266	6.15238	0.5062
2	18.198	VV	0.1635	33.85910	2.89467	0.2309
3	18.990	BB	0.1219	26.85925	3.48595	0.1832
4	19.450	BV	0.1951	345.94815	26.54263	2.3592
5	19.993	VV	0.1137	1.41829e4	1886.20056	96.7206


VWD1 A, Wavelength=254 nm (ZYH\2019-05-31 17-09-01.D)
[min] [min] [mAU*s] [mAU] %
1 11.021 BB 0.1880 36.88477 3.05239 0.1980
2 16.834 BV 0.2815 42.22526 2.21399 0.2266
3 17.224 VB 0.2975 88.62632 4.62699 0.4756
4 21.085 BB 0.3243 44.18845 2.19096 0.2372
5 22.187 BB 0.3845 65.28121 2.61316 0.3504
6 23.365 BV 0.3844 236.39168 8.39860 1.2687
7 23.666 VV 0.2826 172.78238 8.93348 0.9273
8 24.402 VB 0.4883 1.79466e4 527.01984 96.3163
Method 1
mAU
500
400
300
200
100
0
11.021
16.834
17.224
21.085
22.187
23.365
23.666
24.402
5
10
15
20
25
30
min
HO
H
N
N
N
N
C16H33
Ih


VWD1 A, Wavelength=254 nm (FY190425DEF_LC.SFY 2019-06-04 20-15-25\038-0201.D)
mAU
[min] [min] [mAU*s] [mAU] %
1 18.257 BV 0.1343 52.39722 6.03583 0.2568
2 18.387 VB 0.1107 41.96924 5.40082 0.2057
3 18.991 BB 0.1263 74.50204 9.21969 0.3651
4 19.469 VB 0.1123 179.31879 24.54010 0.8788
5 19.921 VV 0.1582 301.92313 26.84204 1.4797
6 20.195 VV 0.1144 104.36230 13.03116 0.5115
7 20.643 VB 0.1354 1.96504e4 2154.62598 96.3025
Method 2
C16H33
HO
H
N
N
N
Ih
20.643
18.991
19.469
2000
1750
1500
1250
1000
750
500
250
0
5
10
15
20
25
30
min


VWD1 A, Wavelength=254 nm (FY190425DEF_LC.SFY 2019-06-01 17-27-19\027-0601.D)
mAU
1800
1600
1400
1200
1000
800
600
400
200
0
5
10
15
20
25
30
min
14.063
10.232
16.752
21.025
22.101
[min] [min] [mAU*s] [mAU] %
1 10.232 BB 0.1738 94.26852 8.40896 0.3927
2 14.063 VB 0.2055 2.37757e4 1806.86548 99.0486
3 16.752 BV 0.2404 39.50238 2.56881 0.1646
4 21.025 BB 0.3532 39.02290 1.72330 0.1626
5 22.101 BB 0.4655 55.58784 1.75063 0.2316
Method 1
CF3
N
N
N
HO
H
N

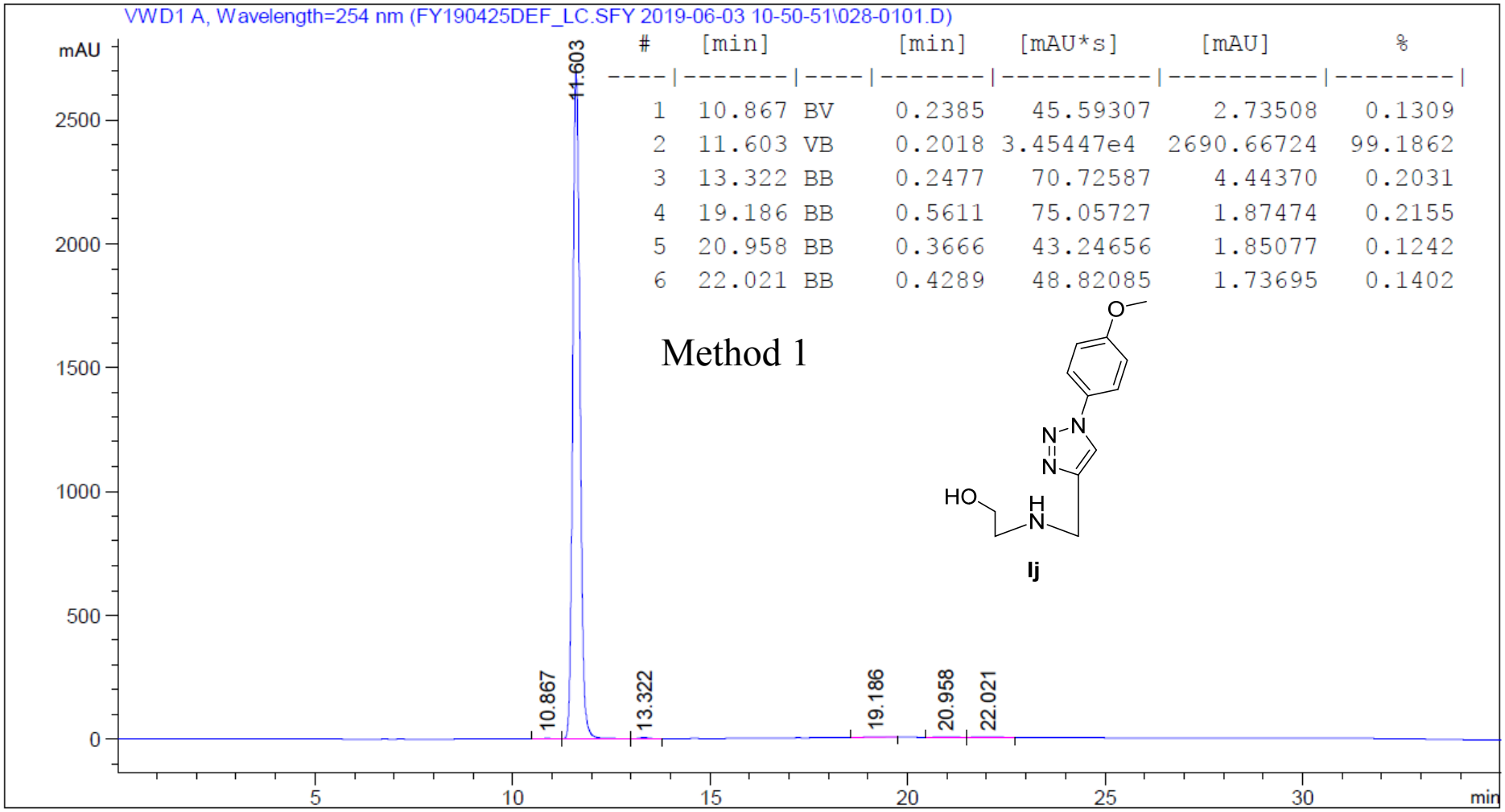
Ii



#	[min]		[min]	[mAU*s]	[mAU]	%
1	10.066	VB	0.1266	77.01642	9.02104	0.4022
2	13.921	VV	0.1031	1.89597e4	2832.90942	99.0140
3	19.473	BB	0.1197	45.12144	5.68001	0.2356
4	19.921	VV	0.1514	66.67167	6.25020	0.3482

Method 2

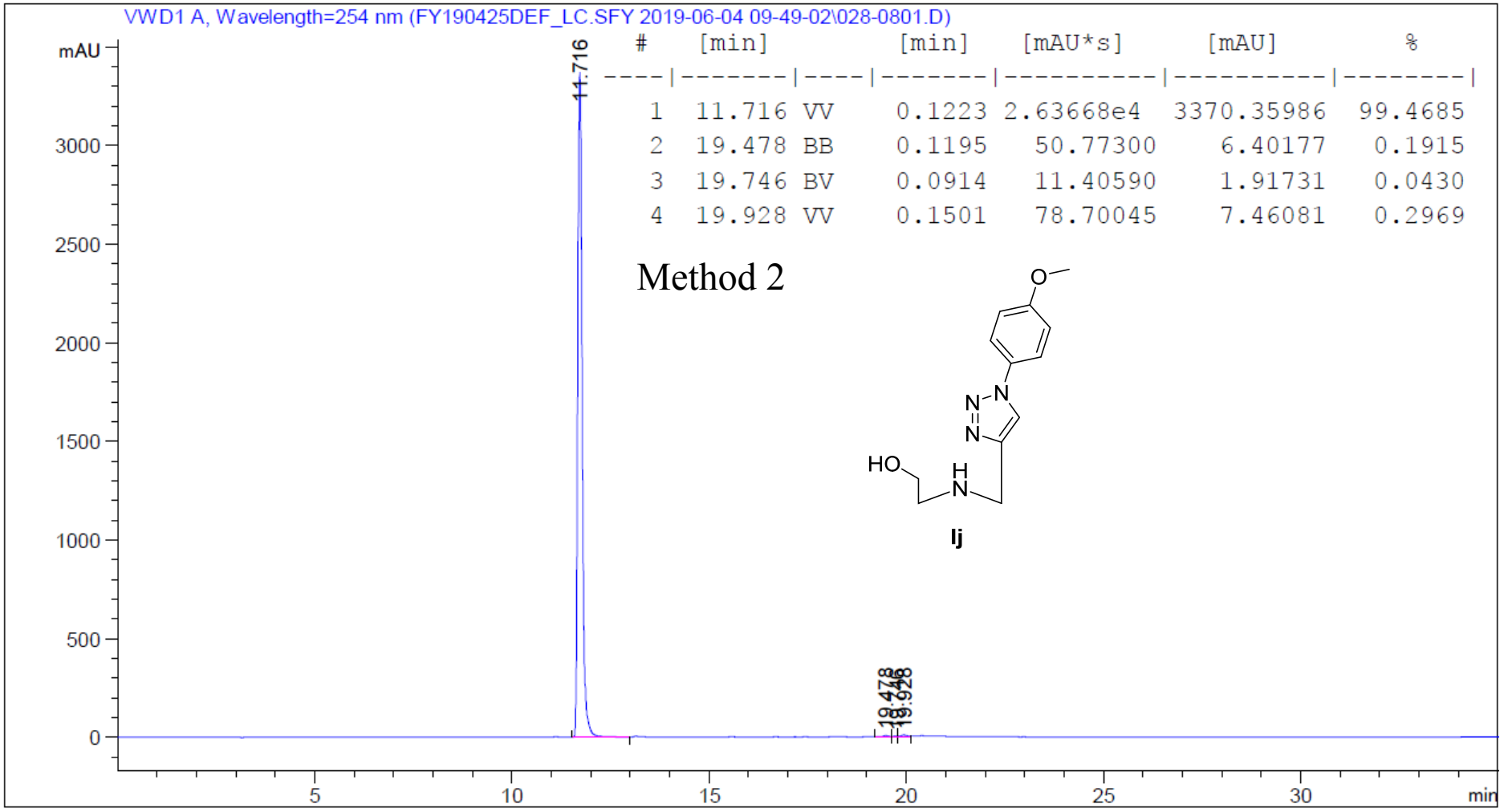
Ii



#	[min]		[min]	[mAU*s]	[mAU]	%
1	10.867	BV	0.2385	45.59307	2.73508	0.1309
2	11.603	VB	0.2018	3.45447e4	2690.66724	99.1862
3	13.322	BB	0.2477	70.72587	4.44370	0.2031
4	19.186	BB	0.5611	75.05727	1.87474	0.2155
5	20.958	BB	0.3666	43.24656	1.85077	0.1242
6	22.021	BB	0.4289	48.82085	1.73695	0.1402

Method 1

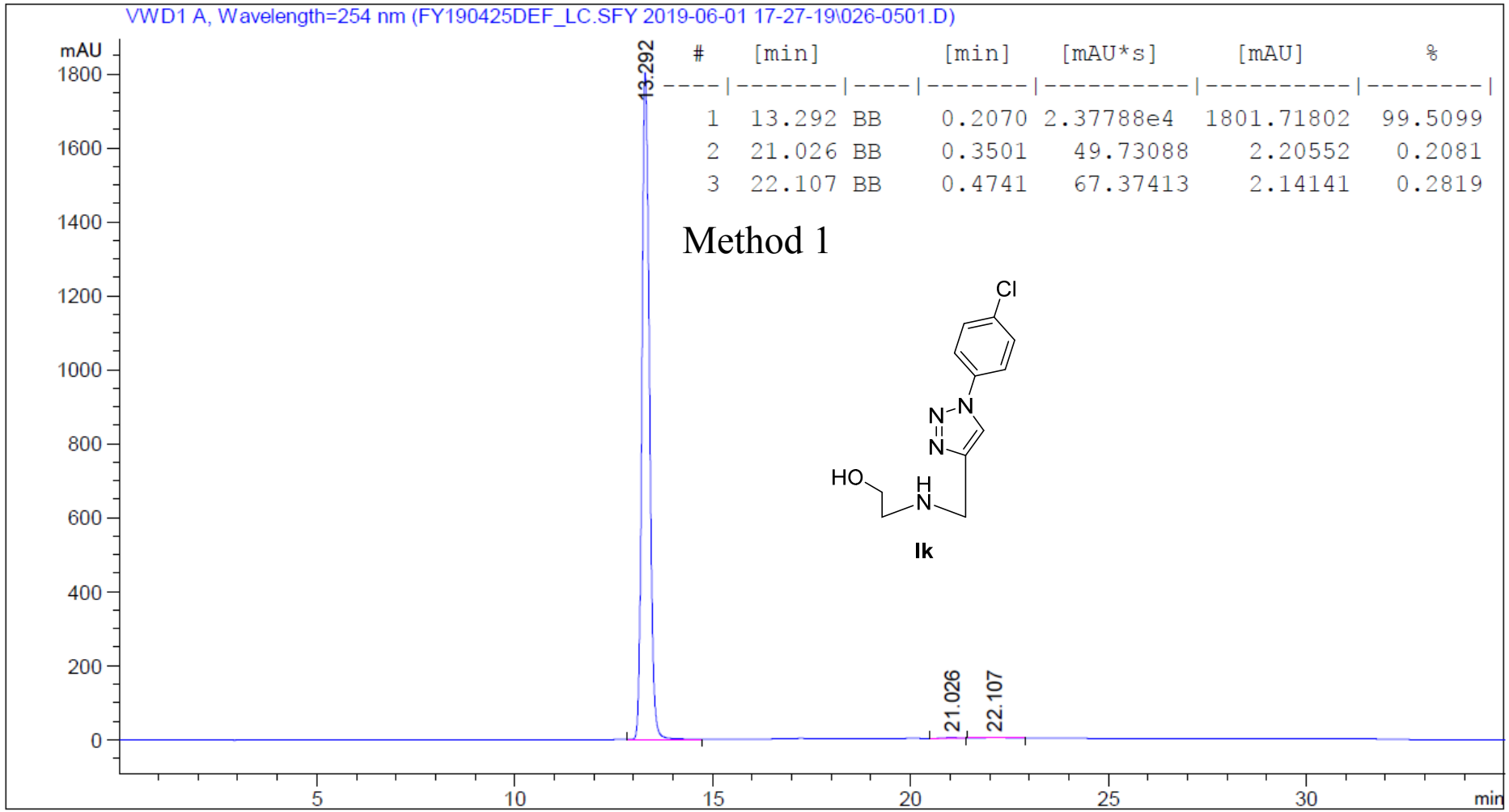
Ij

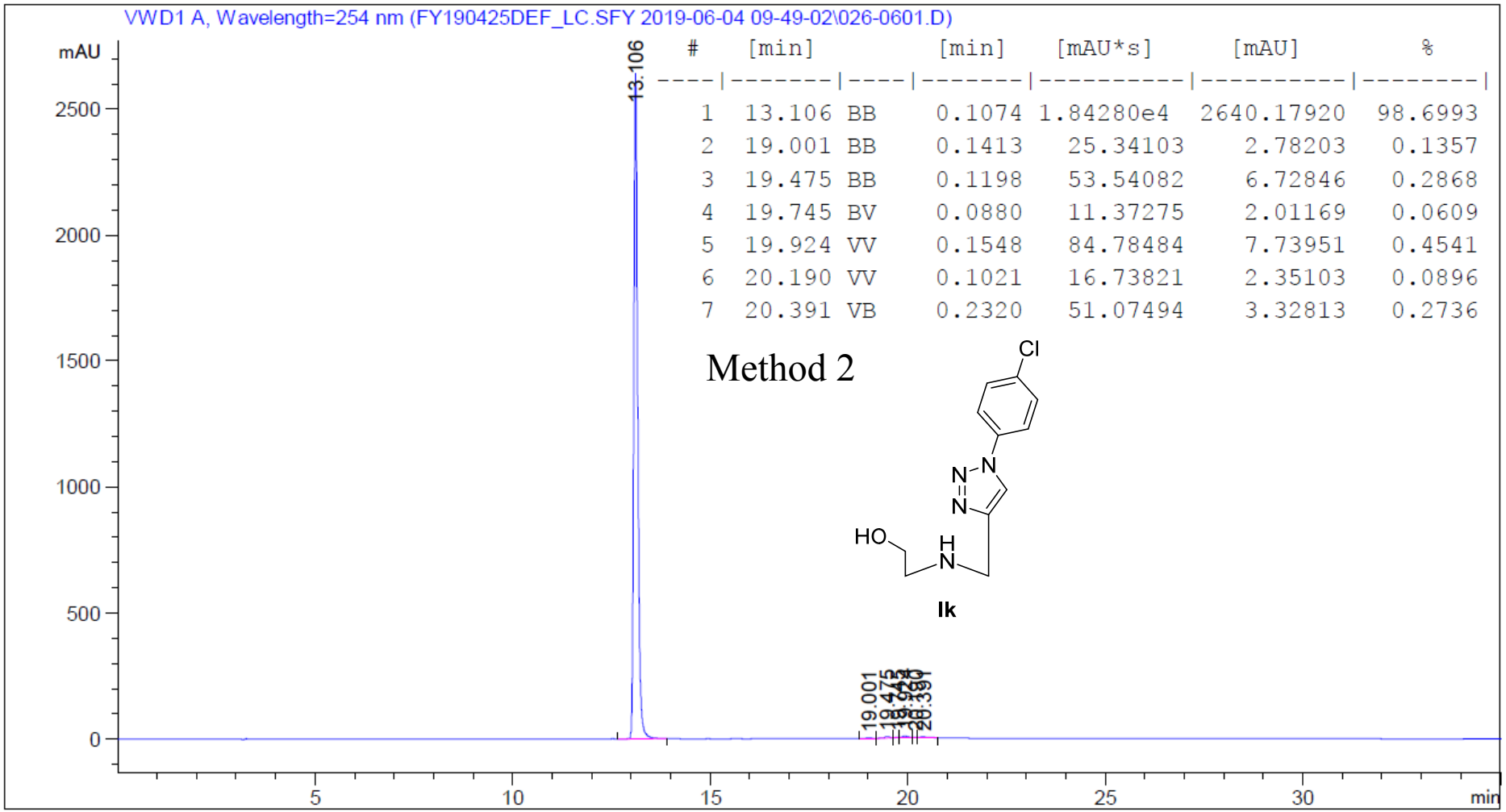


#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.716	VV	0.1223	2.63668e4	3370.35986	99.4685
2	19.478	BB	0.1195	50.77300	6.40177	0.1915
3	19.746	BV	0.0914	11.40590	1.91731	0.0430
4	19.928	VV	0.1501	78.70045	7.46081	0.2969

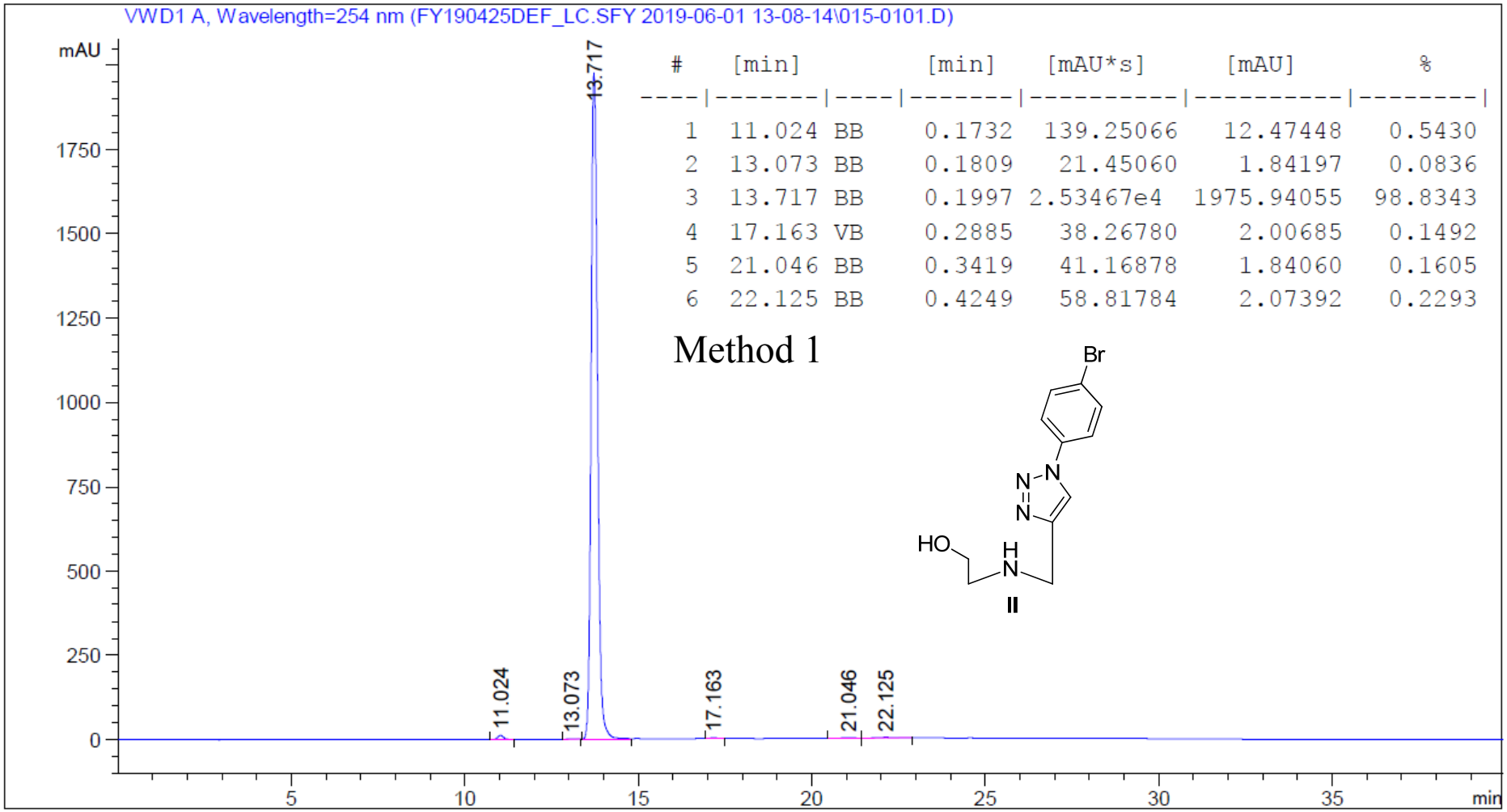
Method 2

Ij

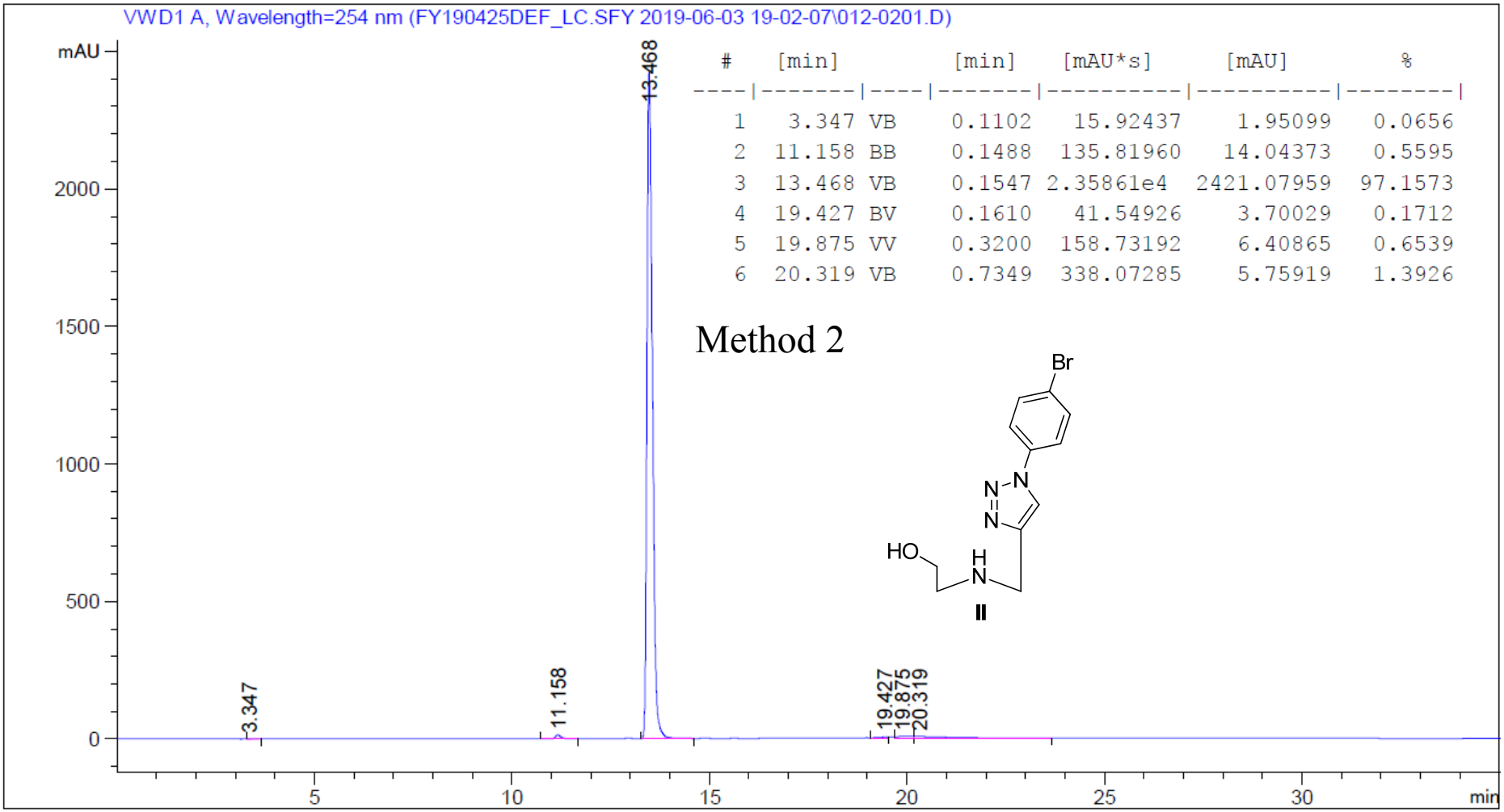

VWD1 A, Wavelength=254 nm (FY190425DEF_LC.SFY 2019-06-01 17-27-19\026-0501.D)
mAU
1800
1600
1400
1200
1000
800
600
400
200
0
13.292
21.026
22.107
5
10
15
20
25
30
min
[min] [min] [mAU*s] [mAU] %
1 13.292 BB 0.2070 2.37788e4 1801.71802 99.5099
2 21.026 BB 0.3501 49.73088 2.20552 0.2081
3 22.107 BB 0.4741 67.37413 2.14141 0.2819
Method 1
Cl
N
N
N
HO
H
N
Ik



#	[min]		[min]	[mAU*s]	[mAU]	%
1	13.106	BB	0.1074	1.84280e4	2640.17920	98.6993
2	19.001	BB	0.1413	25.34103	2.78203	0.1357
3	19.475	BB	0.1198	53.54082	6.72846	0.2868
4	19.745	BV	0.0880	11.37275	2.01169	0.0609
5	19.924	VV	0.1548	84.78484	7.73951	0.4541
6	20.190	VV	0.1021	16.73821	2.35103	0.0896
7	20.391	VB	0.2320	51.07494	3.32813	0.2736



#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.024	BB	0.1732	139.25066	12.47448	0.5430
2	13.073	BB	0.1809	21.45060	1.84197	0.0836
3	13.717	BB	0.1997	2.53467e4	1975.94055	98.8343
4	17.163	VB	0.2885	38.26780	2.00685	0.1492
5	21.046	BB	0.3419	41.16878	1.84060	0.1605
6	22.125	BB	0.4249	58.81784	2.07392	0.2293



#	[min]		[min]	[mAU*s]	[mAU]	%
1	3.347	VB	0.1102	15.92437	1.95099	0.0656
2	11.158	BB	0.1488	135.81960	14.04373	0.5595
3	13.468	VB	0.1547	2.35861e4	2421.07959	97.1573
4	19.427	BV	0.1610	41.54926	3.70029	0.1712
5	19.875	VV	0.3200	158.73192	6.40865	0.6539
6	20.319	VB	0.7349	338.07285	5.75919	1.3926