In Silico Identification of Tripeptides as Lead Compounds for the Design of KOR Ligands

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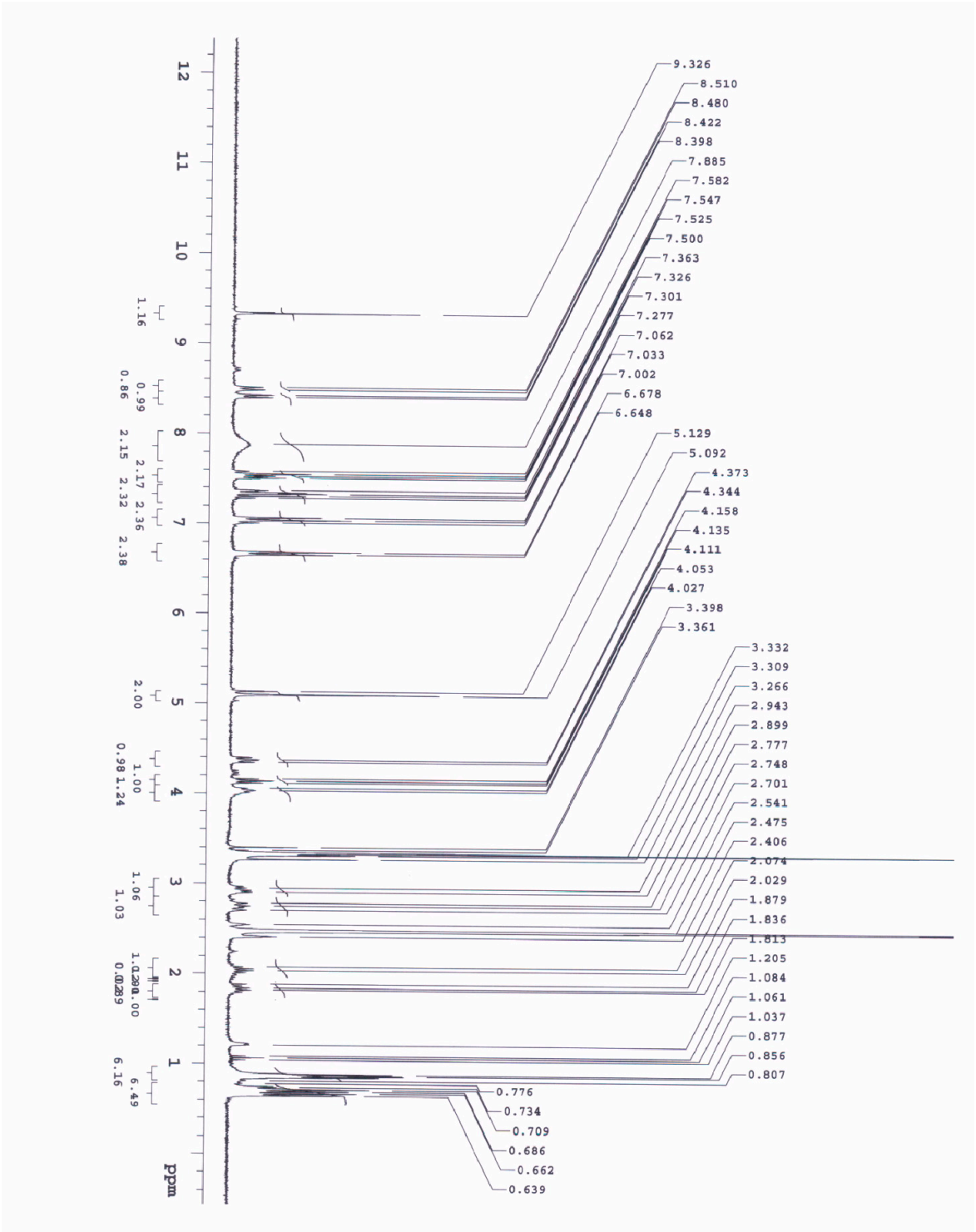
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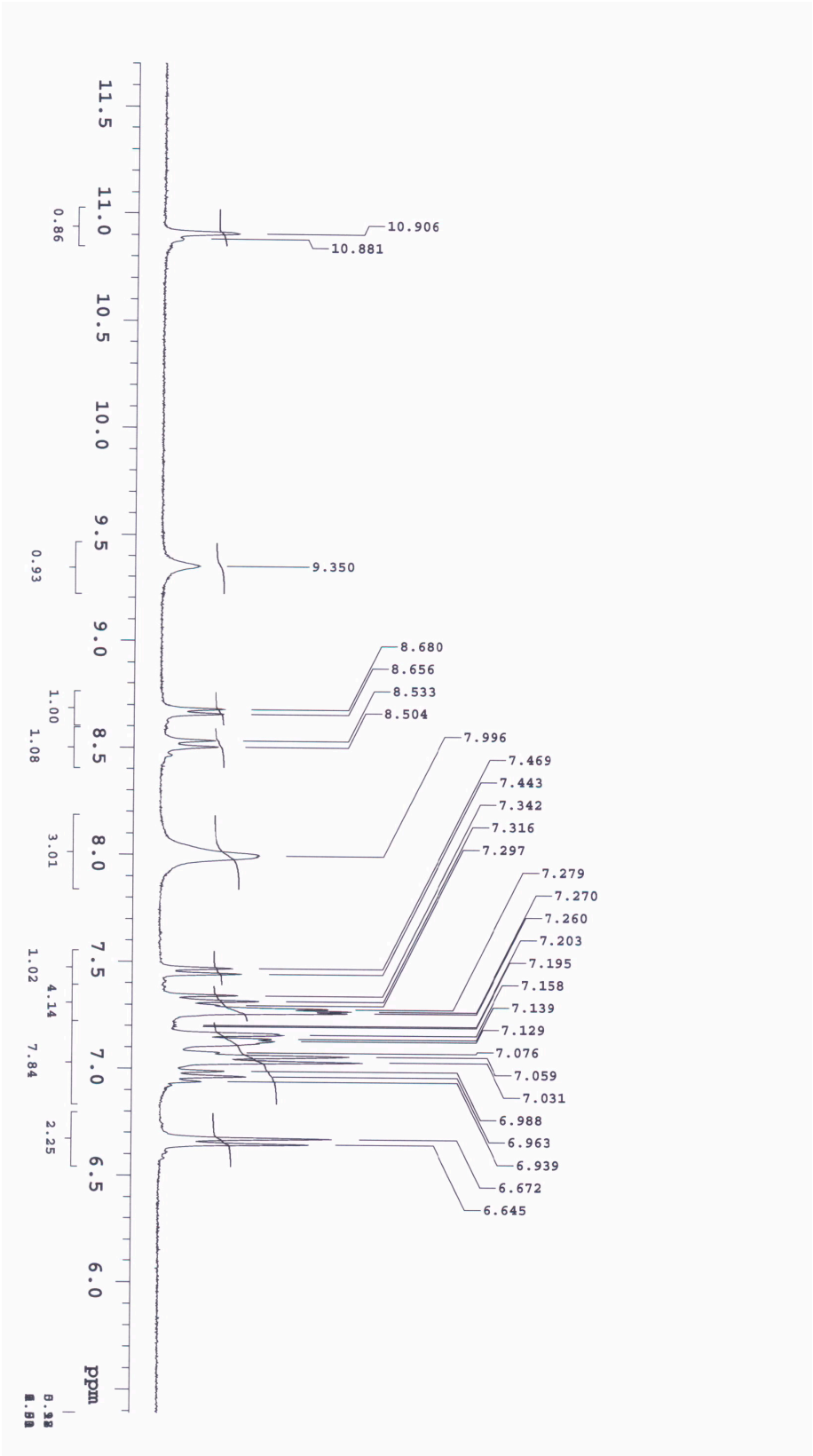
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3.01
1.02
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2.25
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10.881
9.350
8.680
8.656
8.533
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7.316
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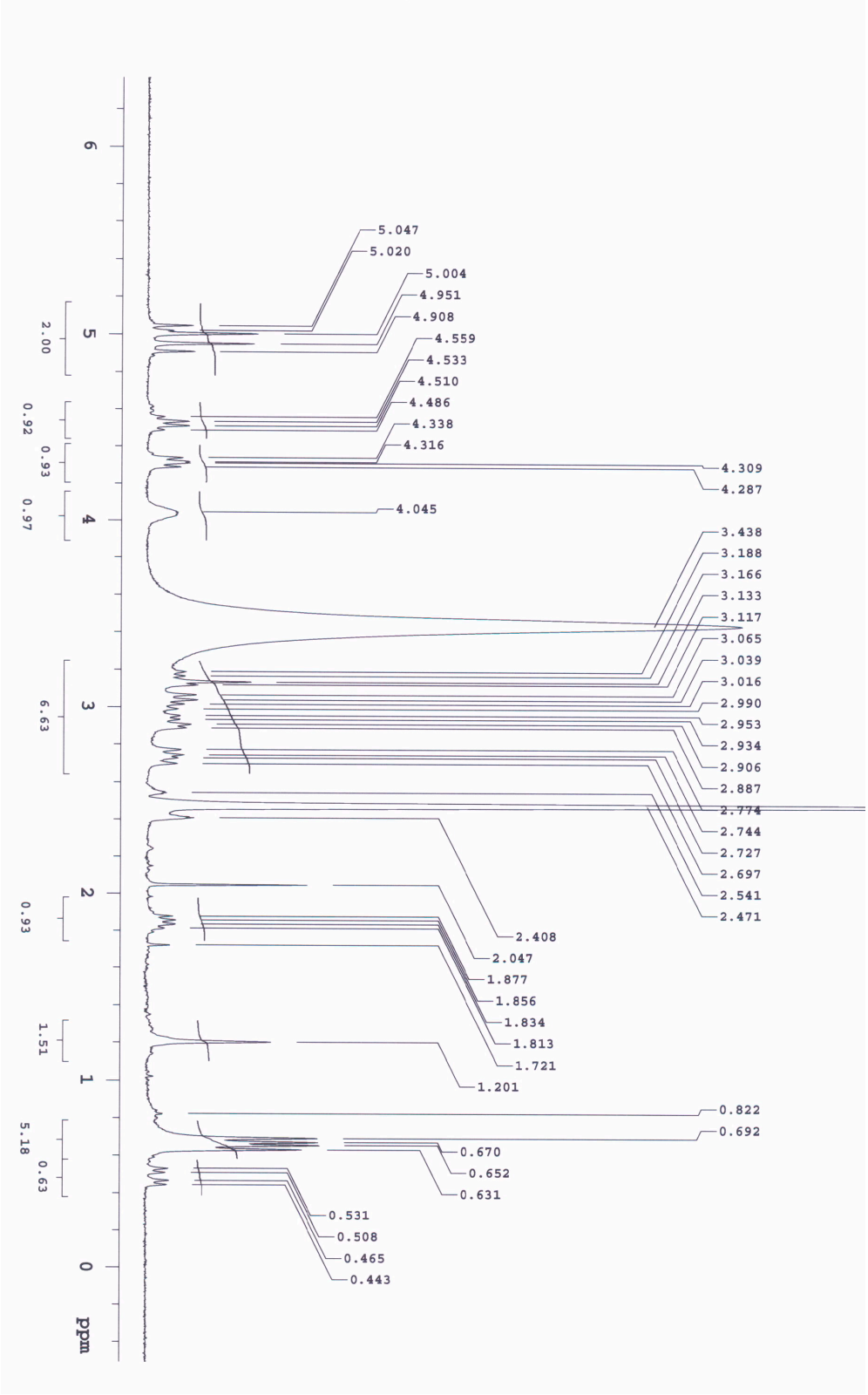


Figure S1. 1H-NMR of peptide **6** in DMSO-d_6.

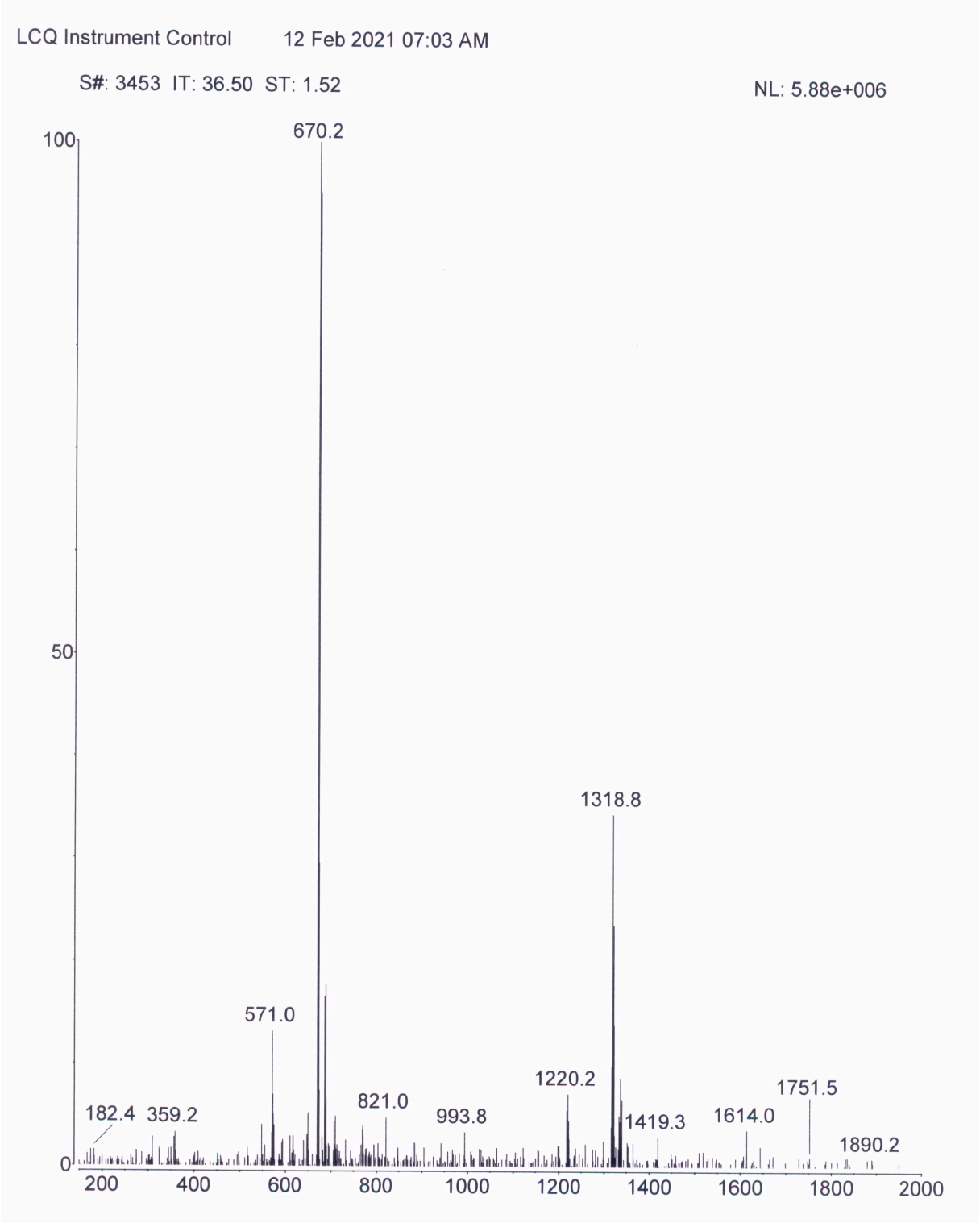
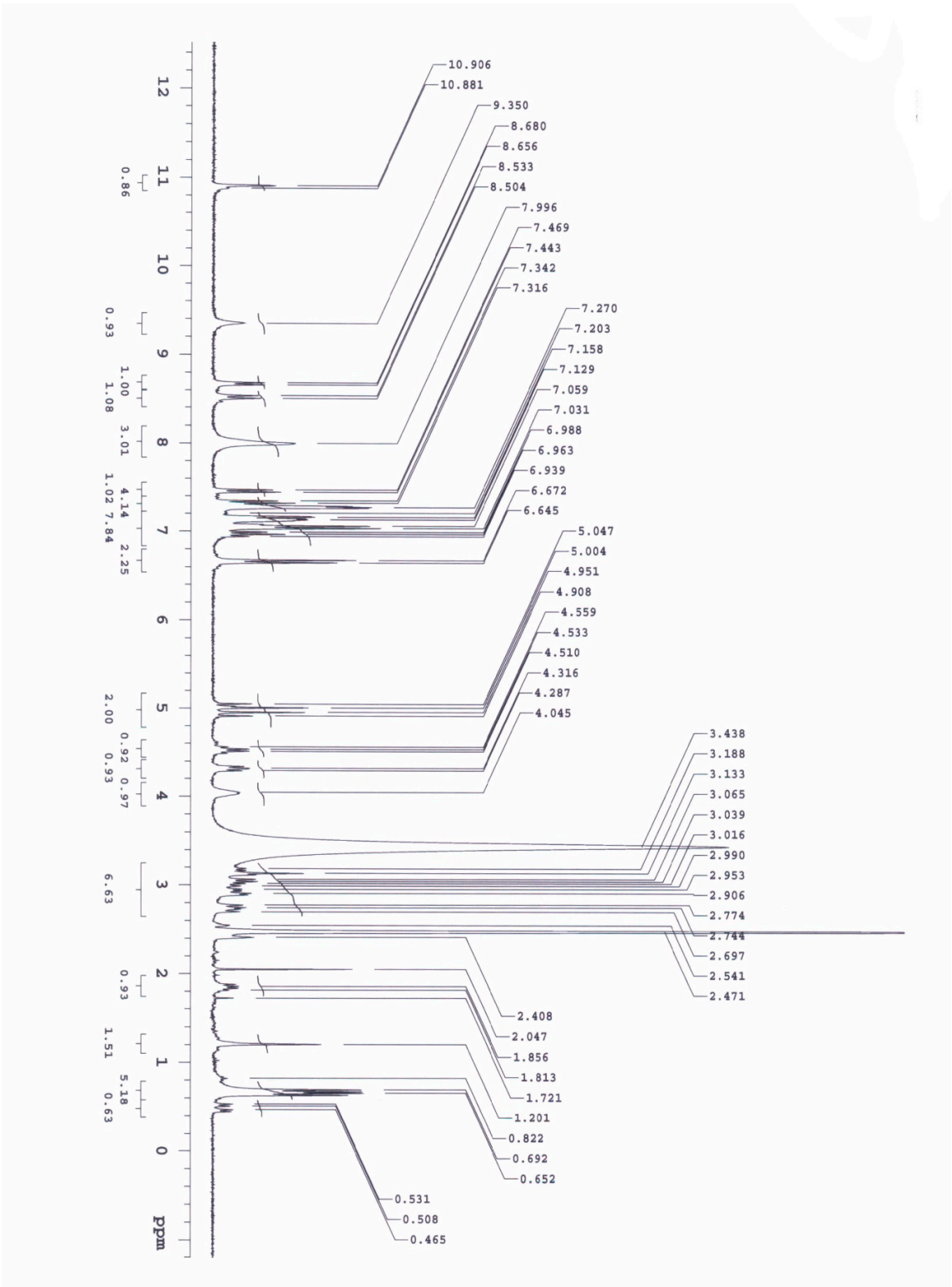


Figure S2. LRMS of peptide **5**.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6.963
6.939
6.672
6.645
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5.004
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4.908
4.559
4.533
4.510
4.316
4.287
4.045
3.438
3.188
3.133
3.065
3.039
3.016
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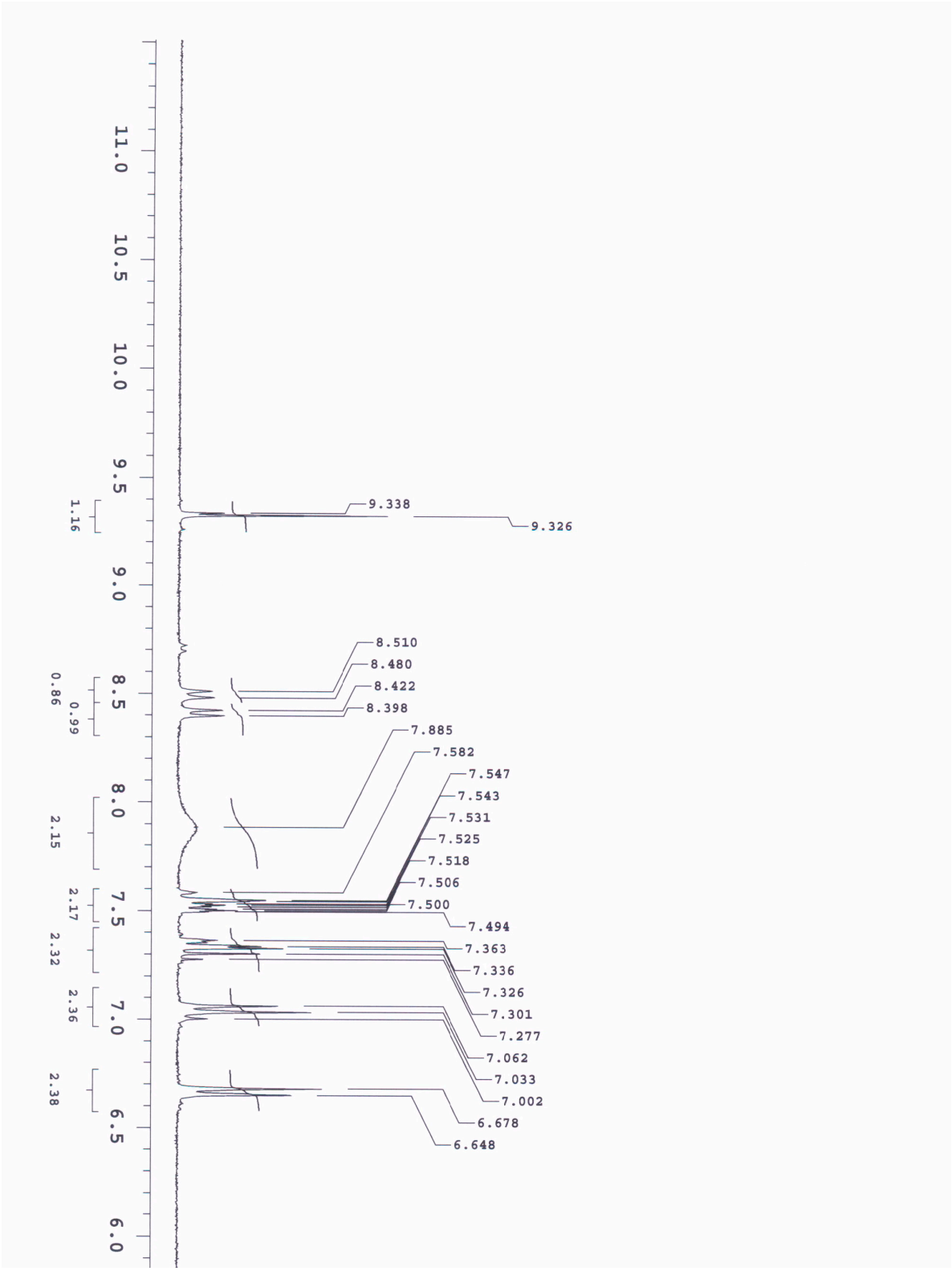
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0.99
2.15
2.17
2.32
2.36
2.38
9.338
9.326
8.510
8.480
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8.398
7.885
7.582
7.547
7.543
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6.678
6.648

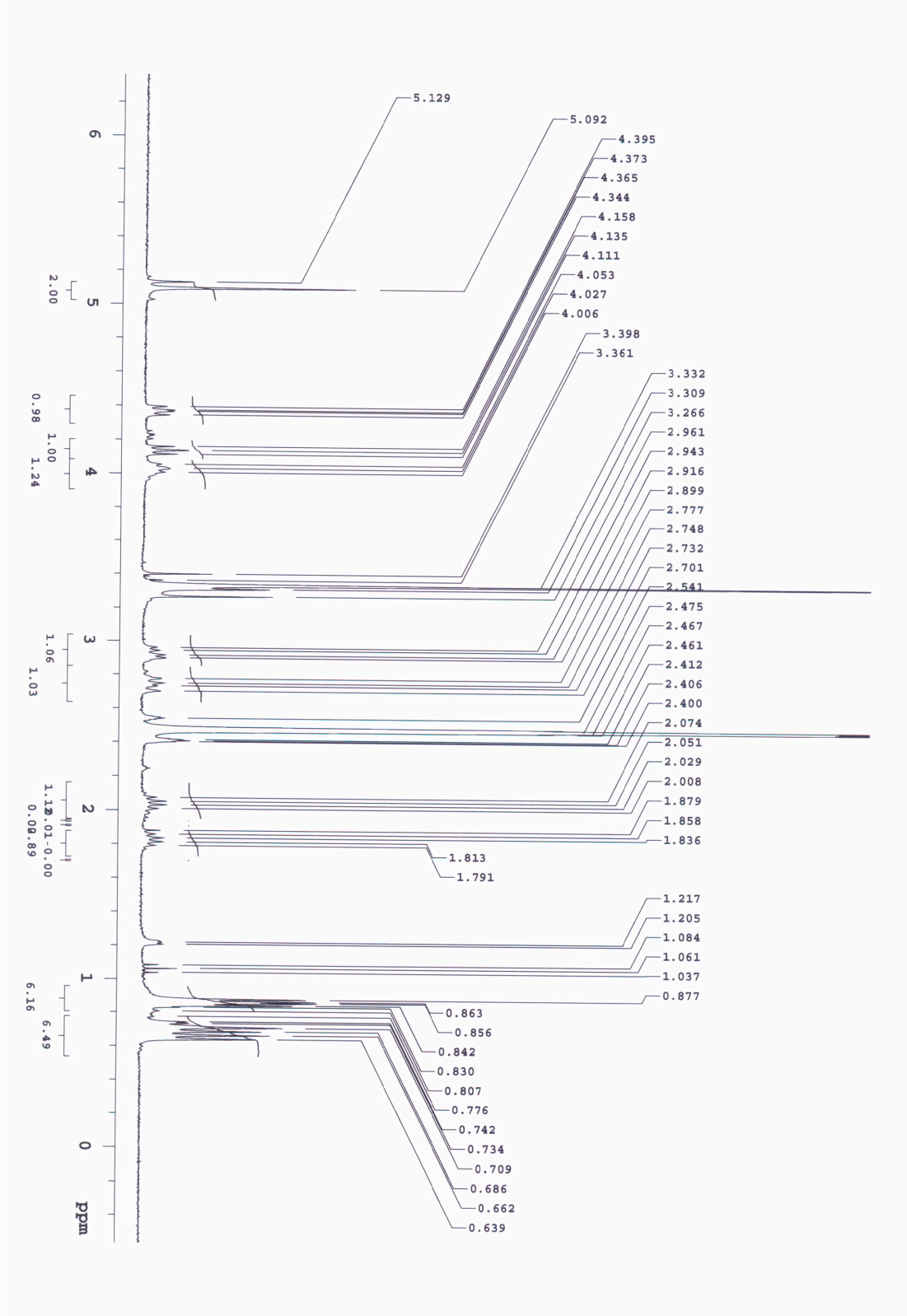

Figure S3. 1H-NMR of peptide **11** in DMSO-d_6.

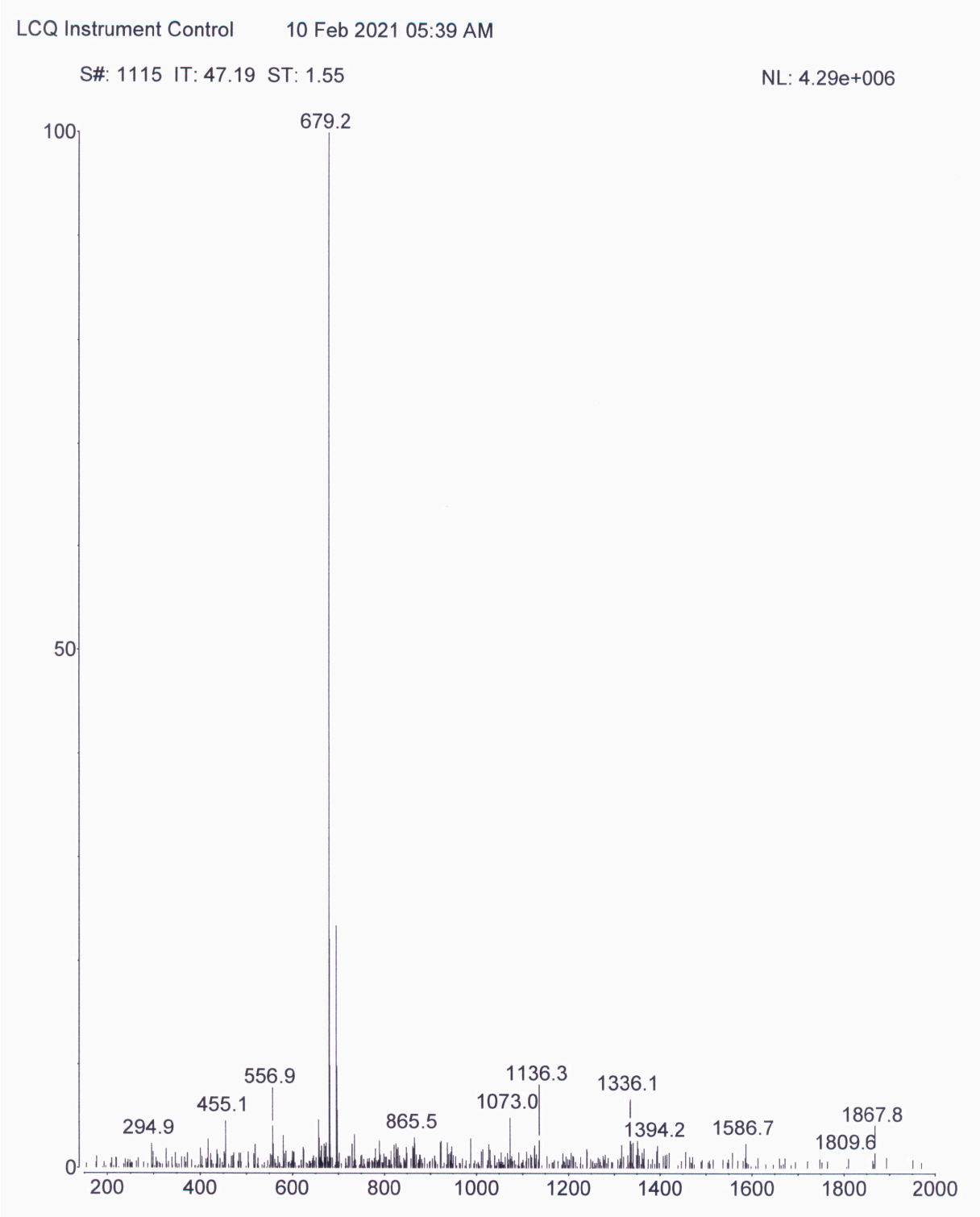

Figure S4. LRMS of peptide **10**.

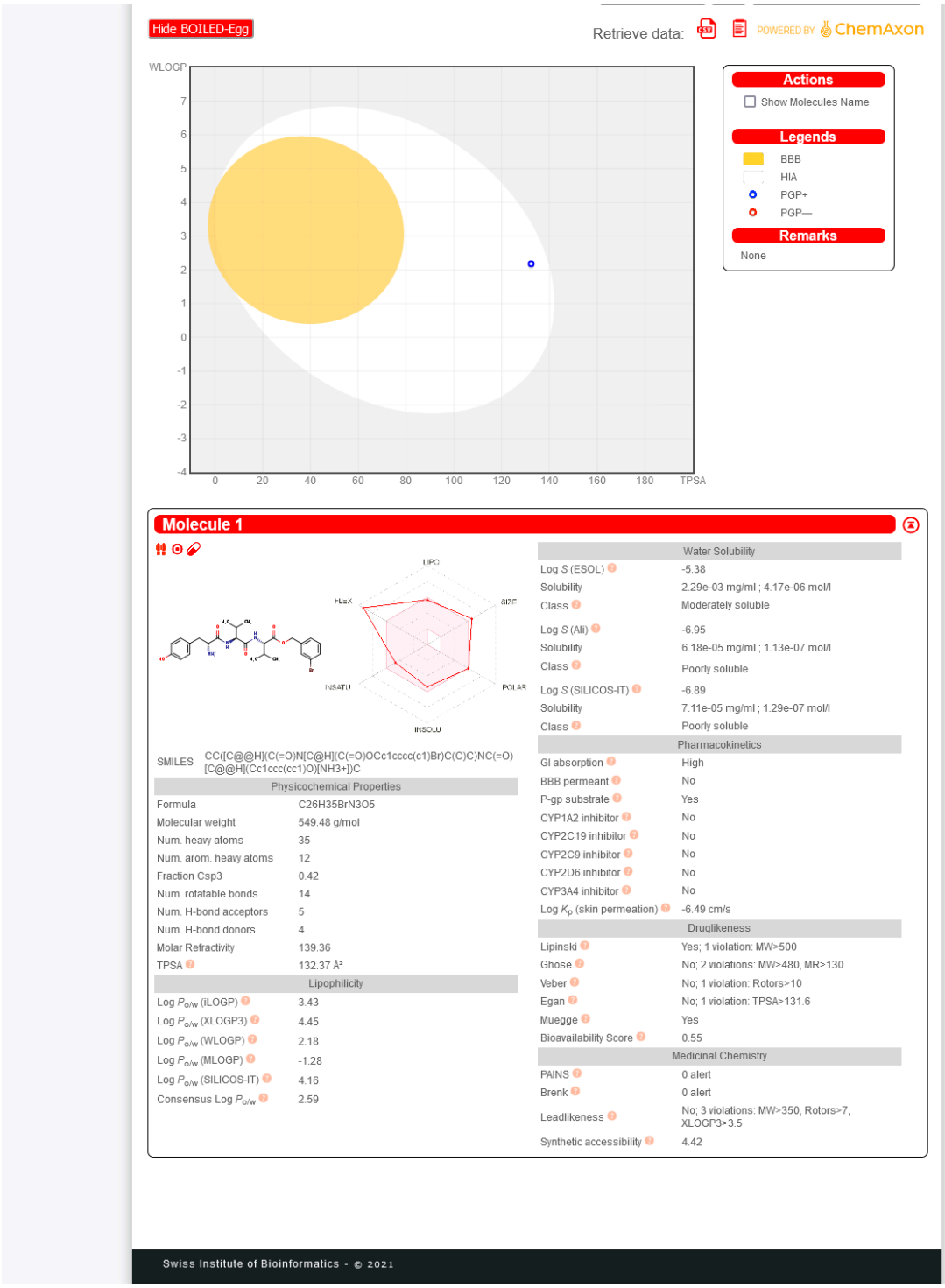

Figure S5. ADME prediction for **6**.

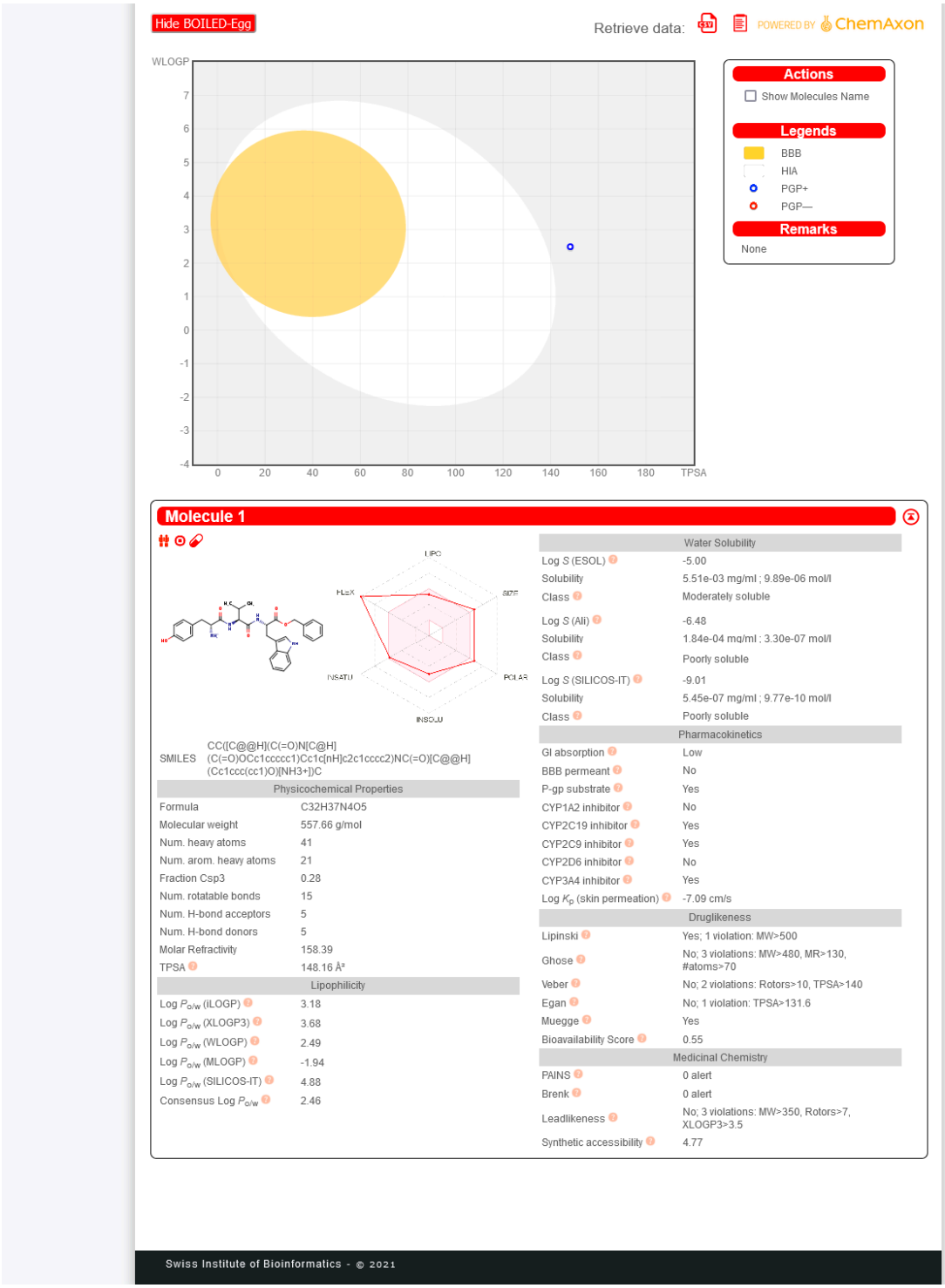

Figure S6. ADME prediction for **11**.