

Supporting Information

Conjugation of oligonucleotides with activated carbamate reagents prepared by the Ugi reaction for oligonucleotide library synthesis

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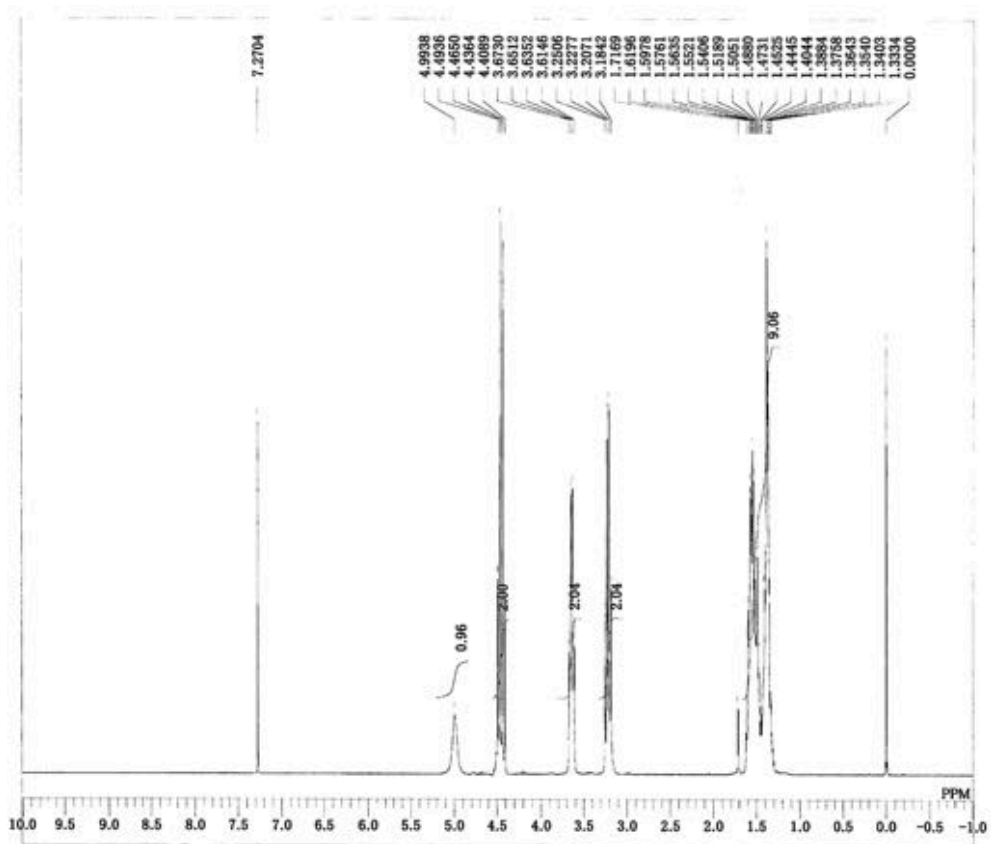
E-mail: obika@phs.osaka-u.ac.jp

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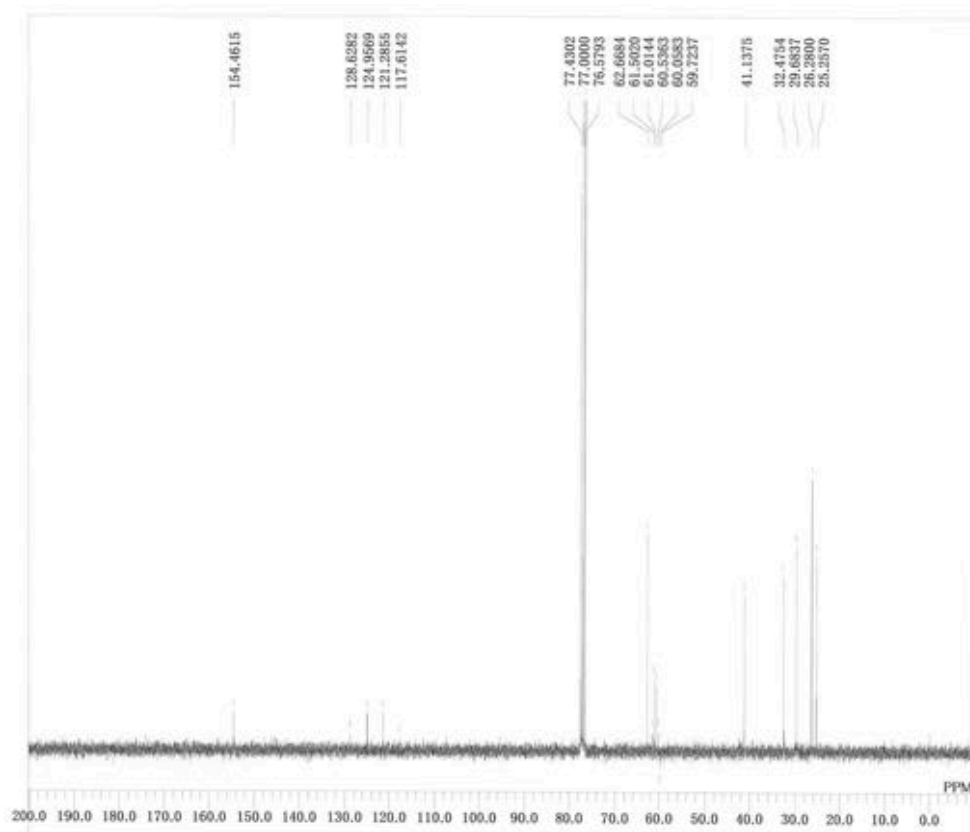
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Figure S1. ^1H NMR, ^{13}C NMR spectra of each compound

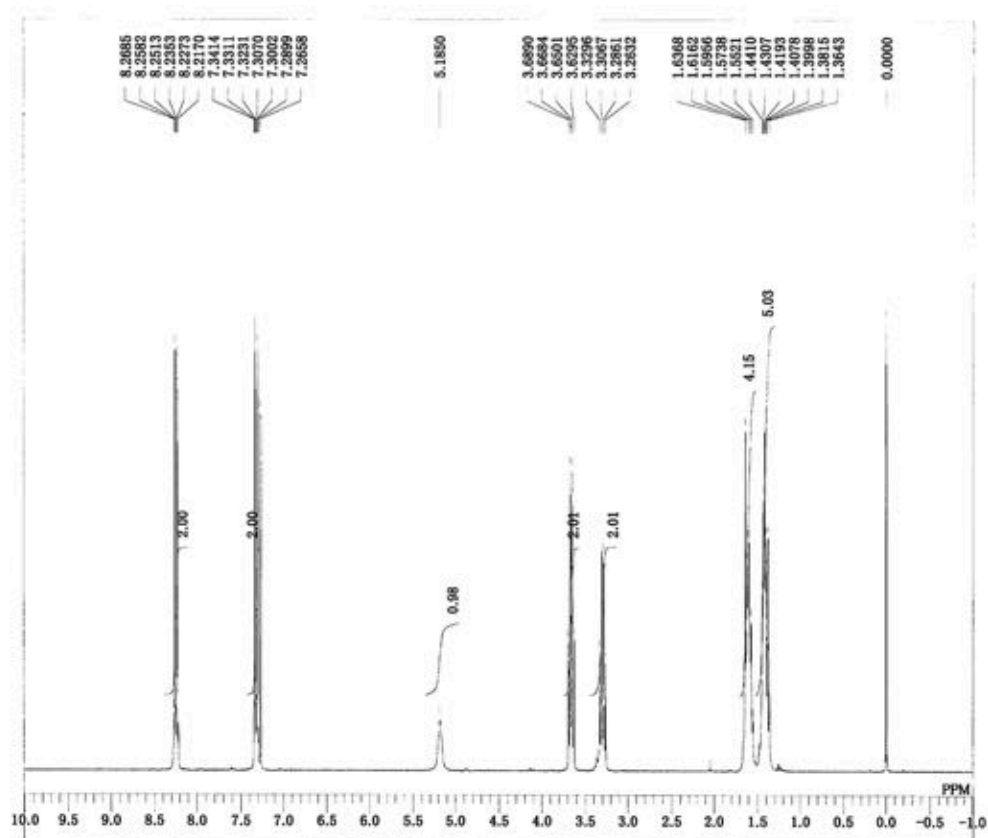
(a) ^1H NMR (CDCl_3) of compound **2**



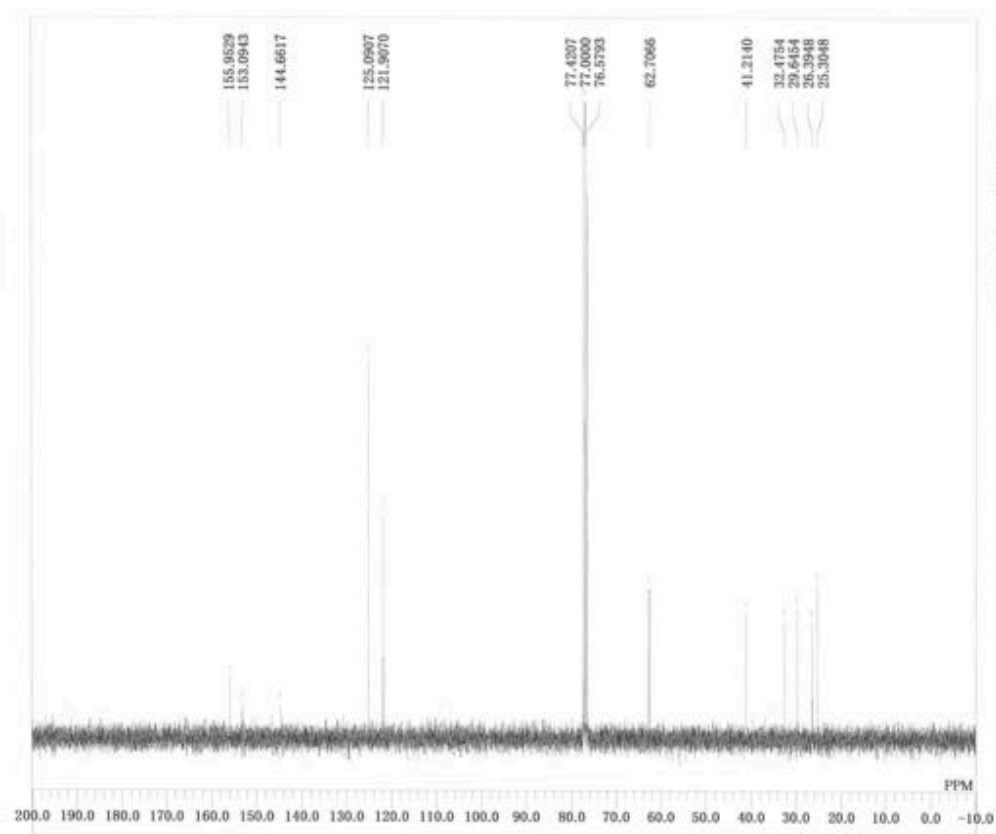
^{13}C NMR (CDCl_3) of compound **2**



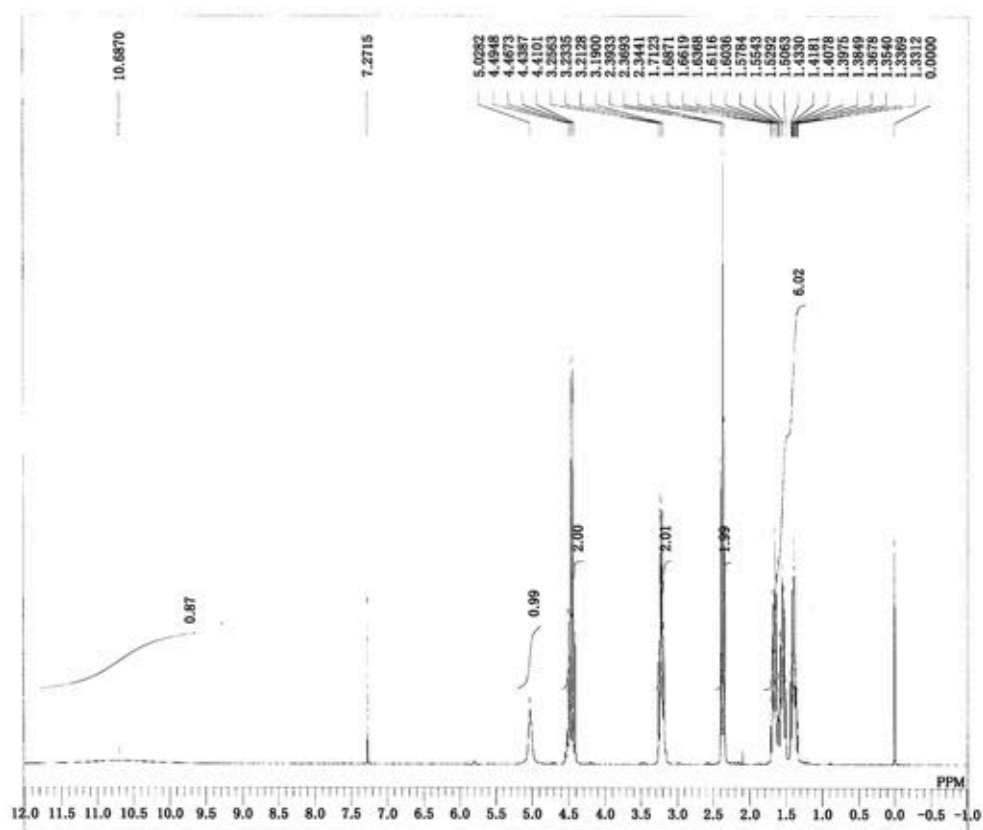
(b) ^1H NMR (CDCl_3) of compound **3**



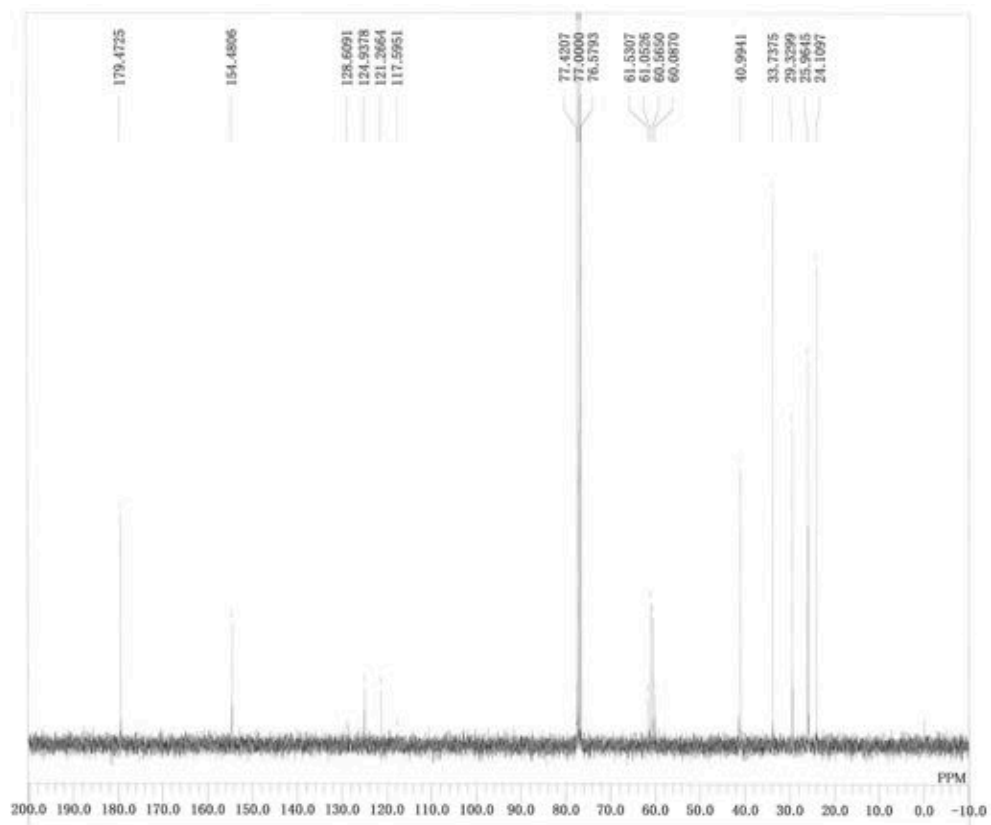
^{13}C NMR (CDCl_3) of compound **3**



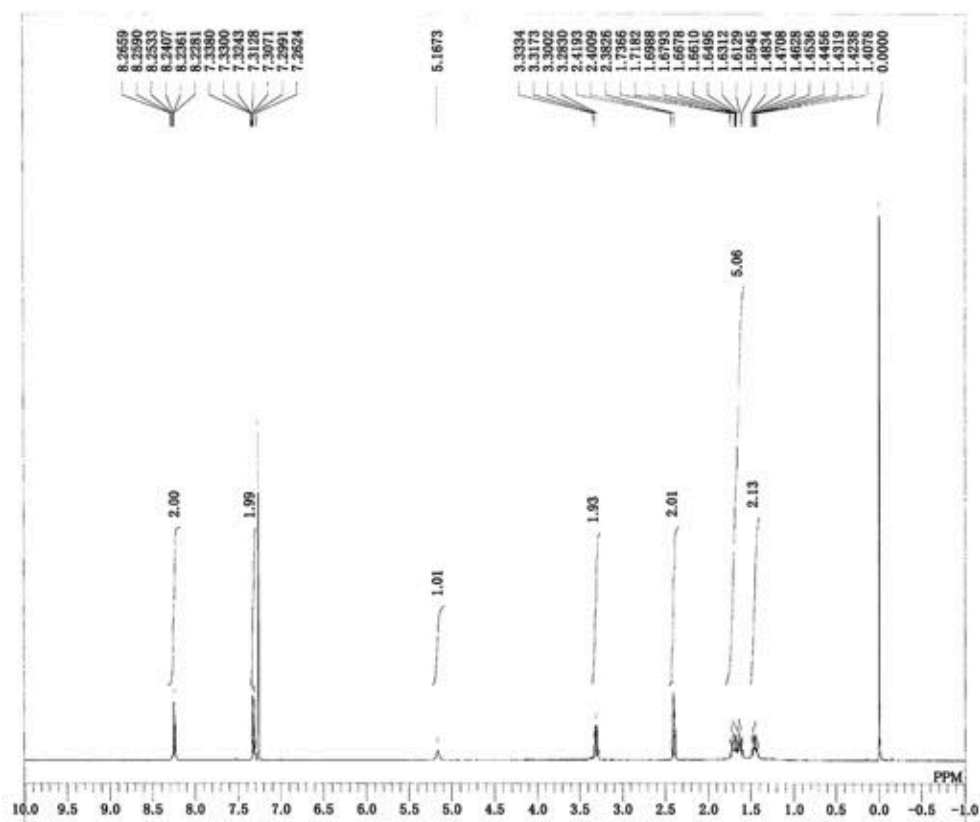
(c) ^1H NMR (CDCl_3) of compound **5**



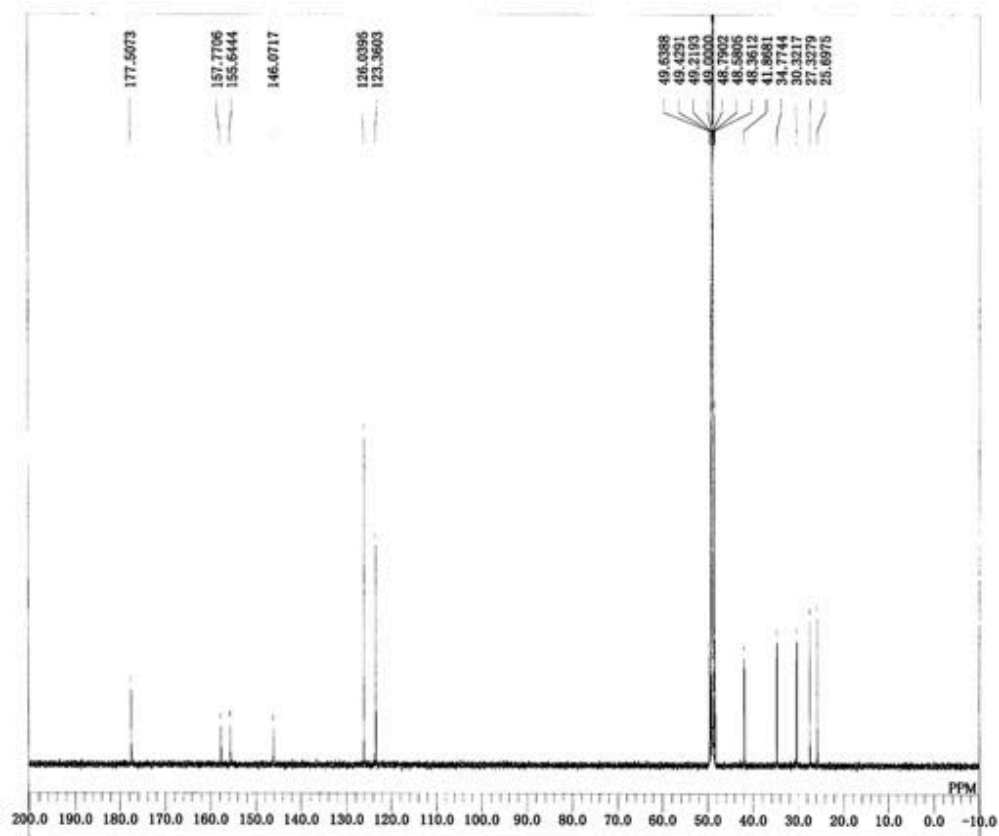
^{13}C NMR (CDCl_3) of compound **5**



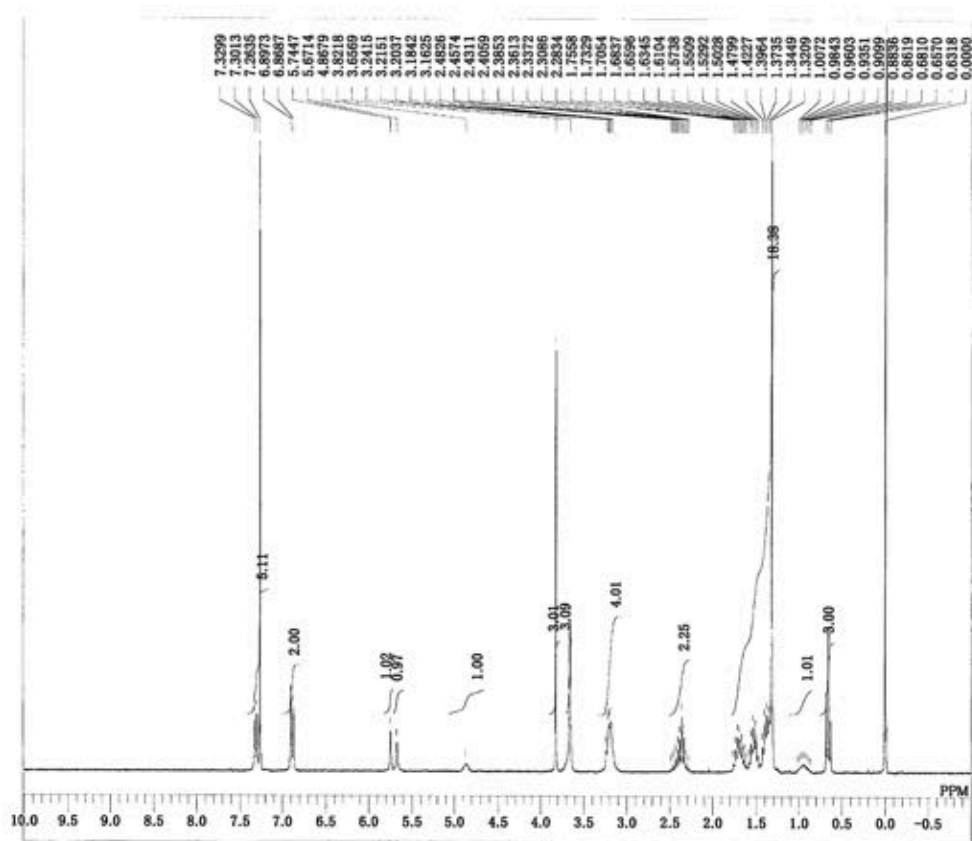
(d) ^1H NMR (CDCl_3) of compound 7



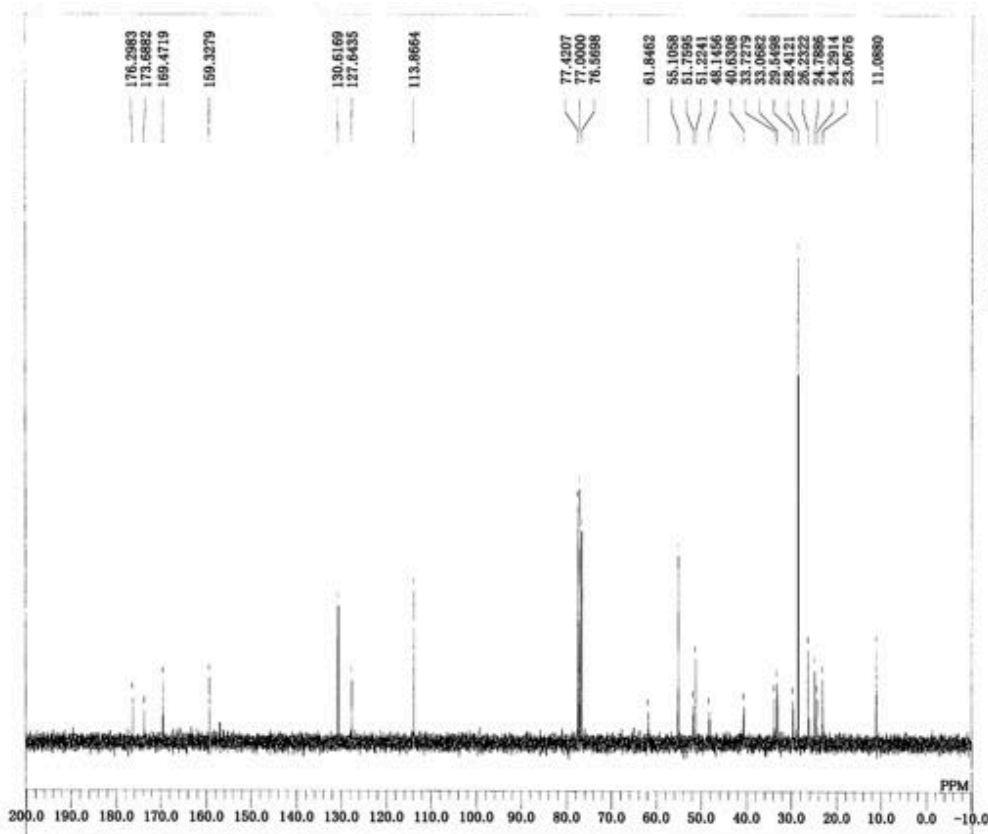
^{13}C NMR (CD_3OD) of compound 7



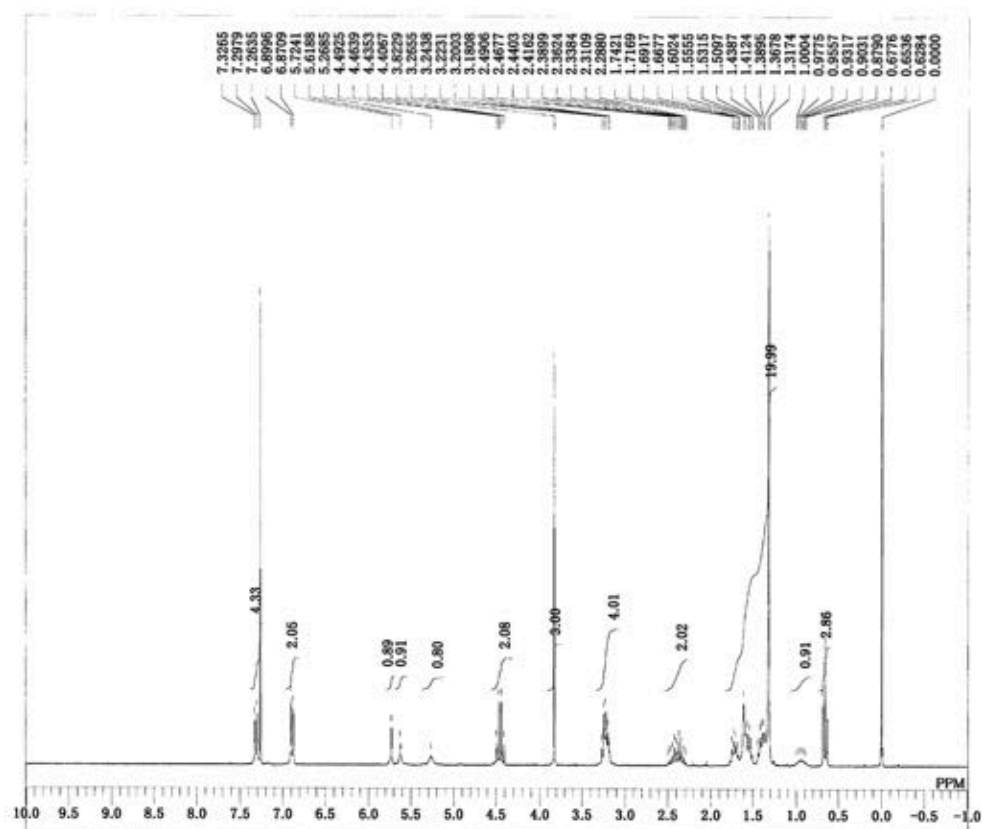
(e) ^1H NMR (CDCl_3) of compound **11**



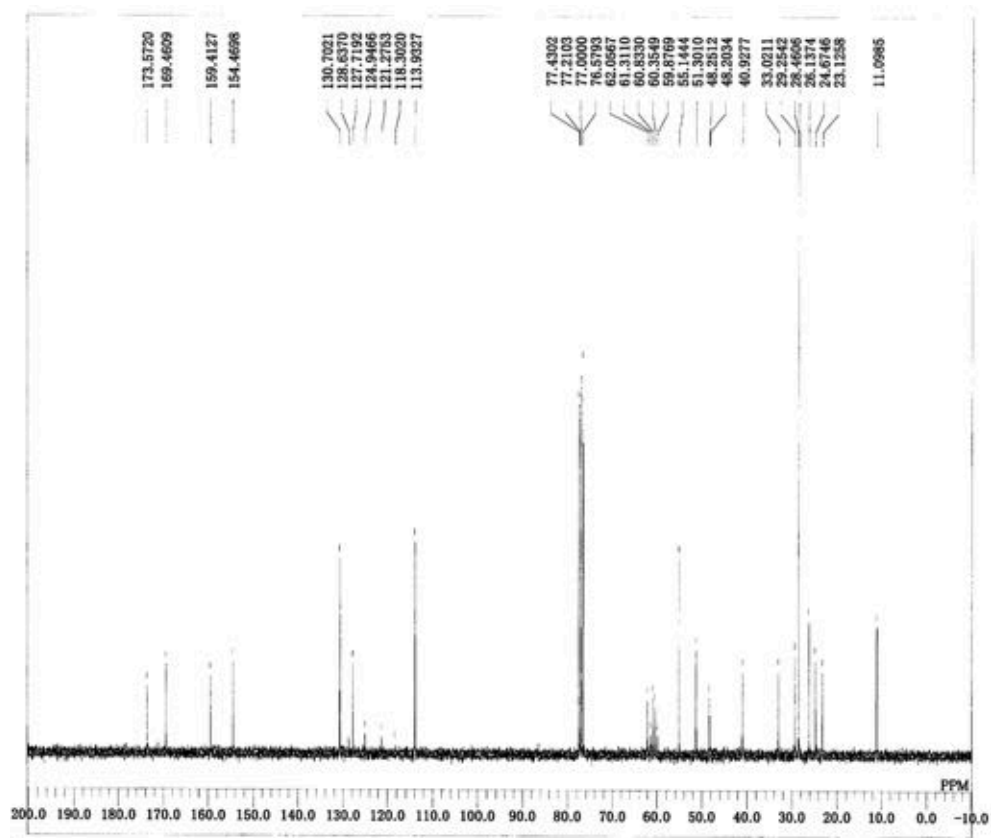
^{13}C NMR (CDCl_3) of compound **11**



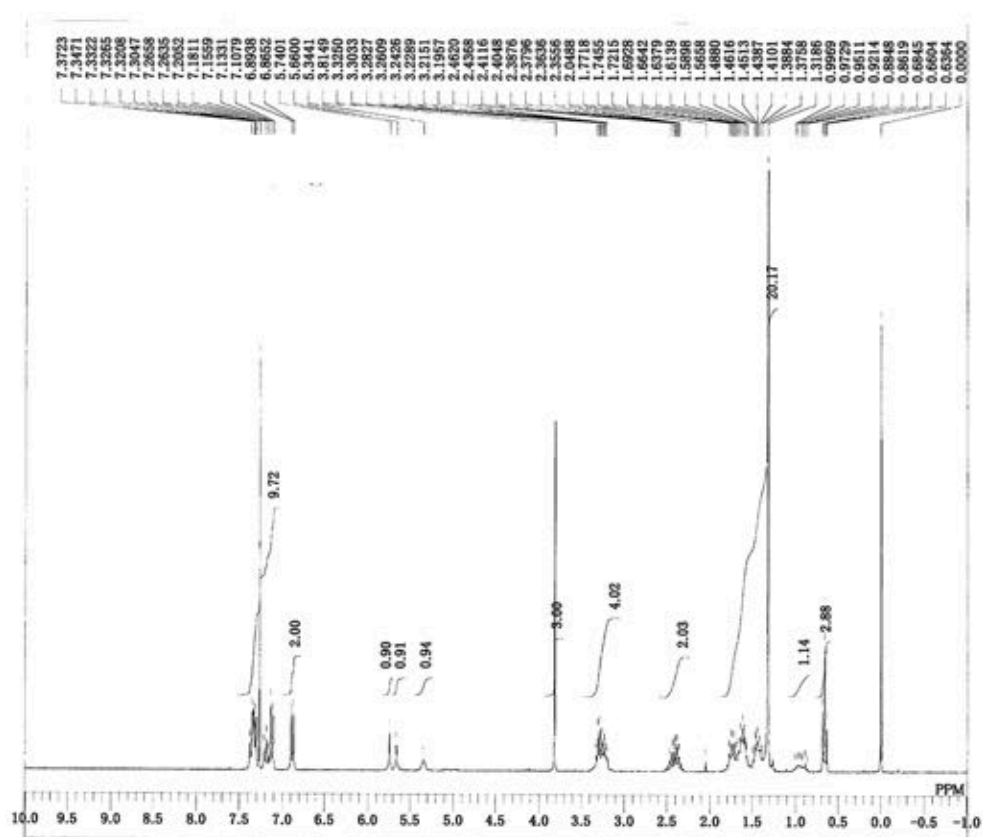
(f) ^1H NMR (CDCl_3) of compound **12**



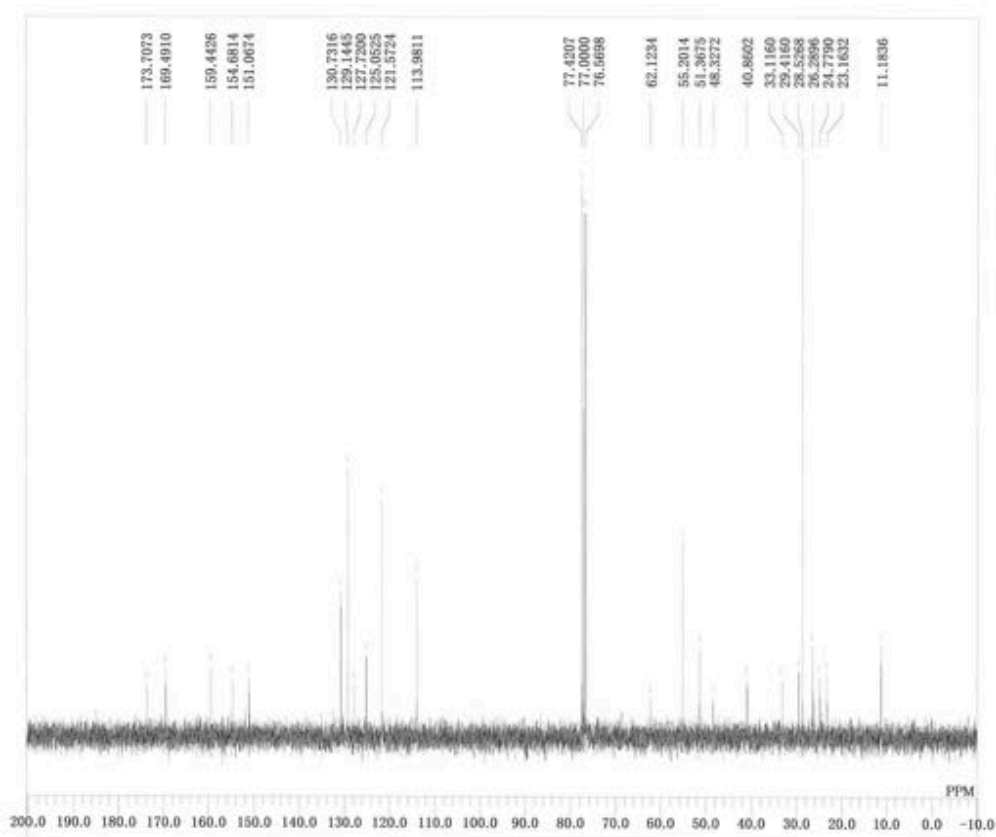
^{13}C NMR (CDCl_3) of compound **12**



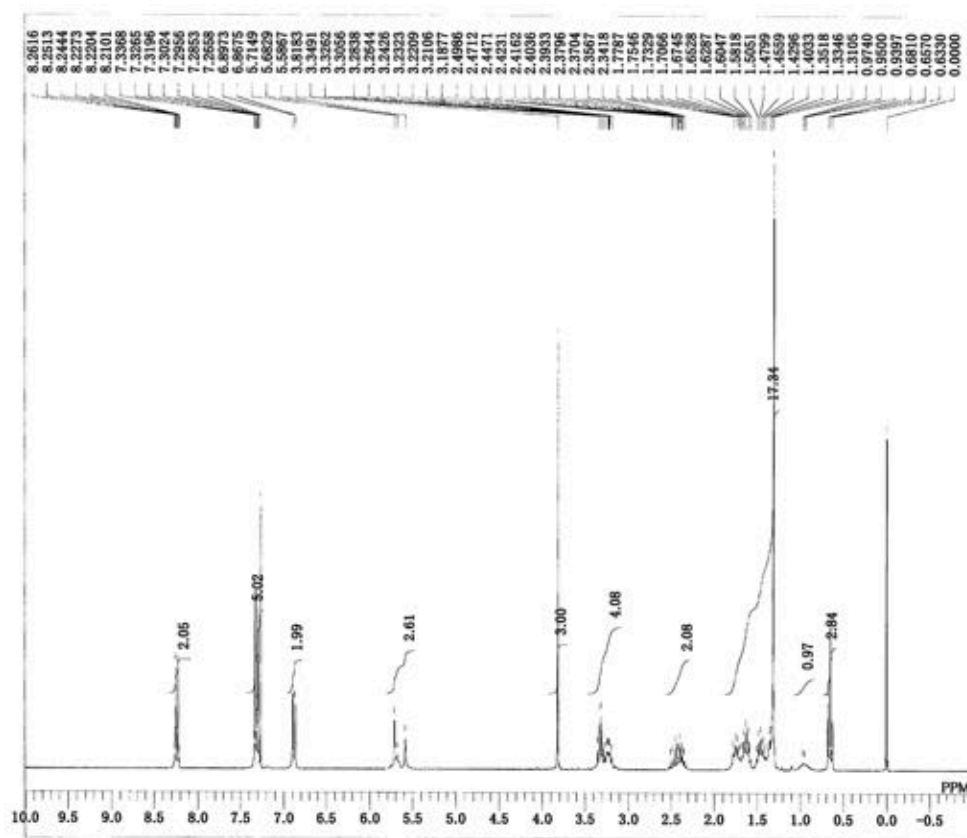
(g) ^1H NMR (CDCl_3) of compound **13**



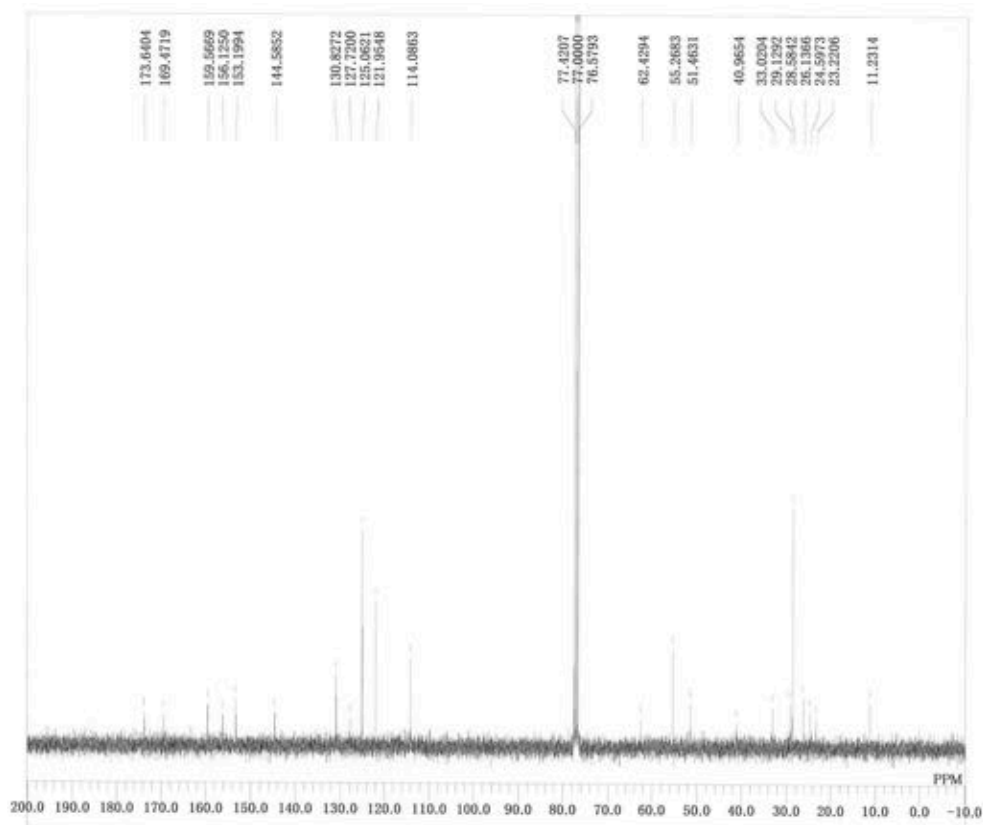
^{13}C NMR (CDCl_3) of compound **13**



(h) ^1H NMR (CDCl_3) of compound **14**



^{13}C NMR (CDCl_3) of compound **14**



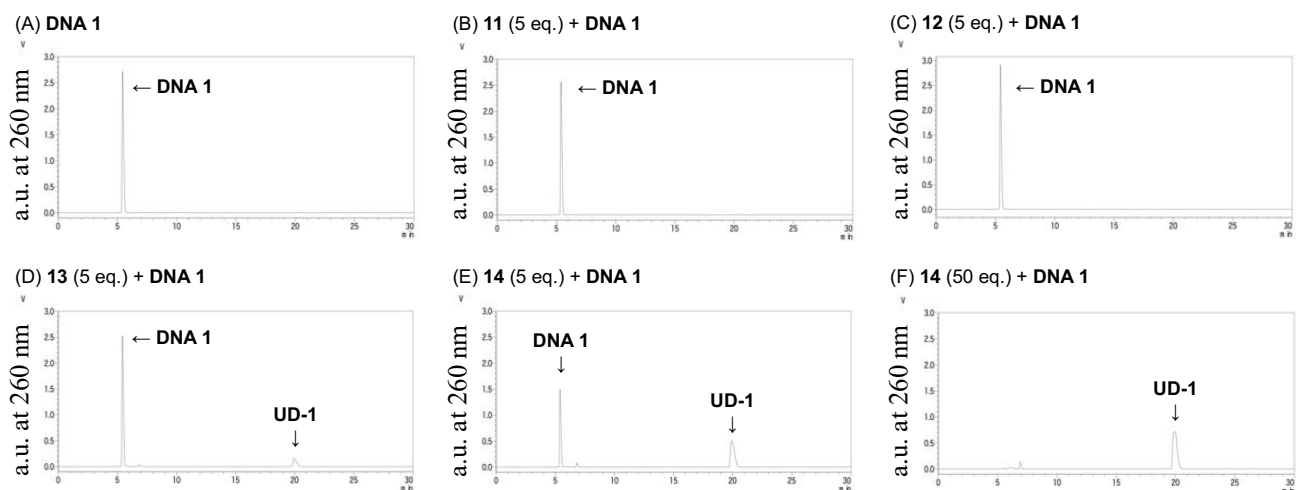


Figure S2. HPLC chromatograms after the conjugation reaction between peptoids 11–14 and DNA 1. The reaction mixtures were analyzed by RP-HPLC with a linear gradient of MeCN (from 7 to 40% over 30 min, 50 °C) in 0.1 M TEAA buffer (pH 7.0).

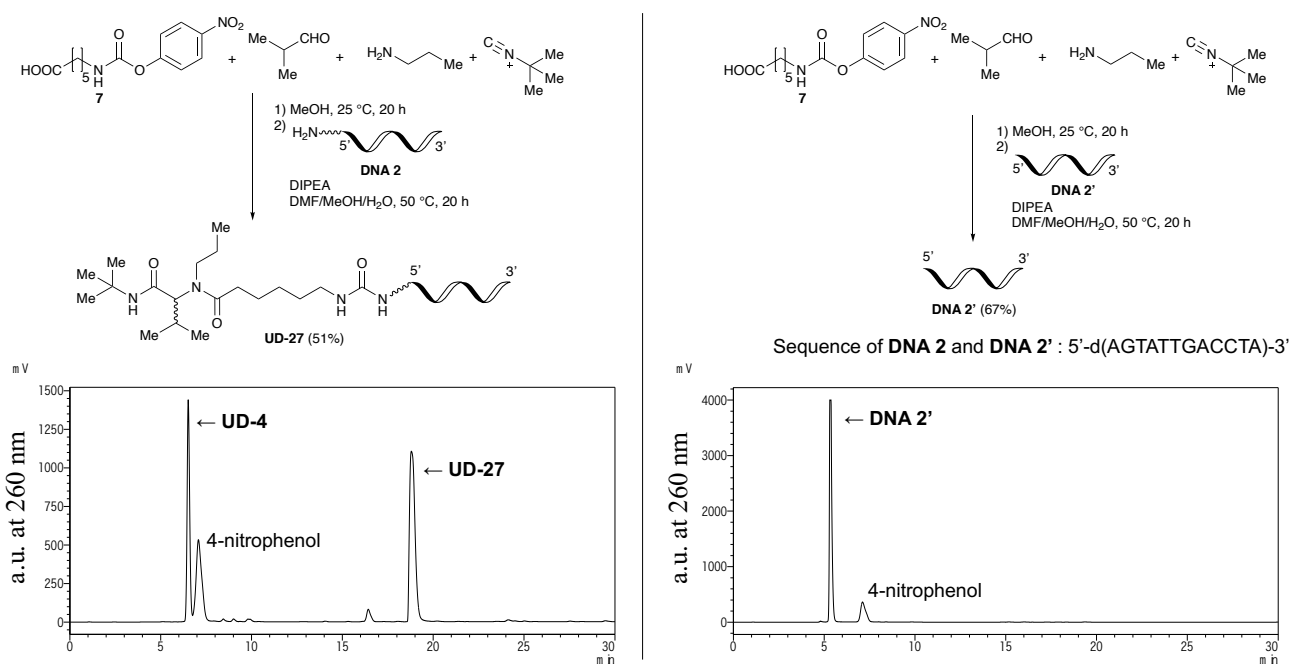


Figure S3. HPLC chromatograms after the conjugation reaction using DNA with or without an aminohexyl linker and the crude peptoid prepared by Ugi reaction. The reaction mixtures were analyzed by RP-HPLC with a linear gradient of MeCN (from 7 to 40% over 30 min, 50 °C) in 0.1 M TEAA buffer (pH 7.0).

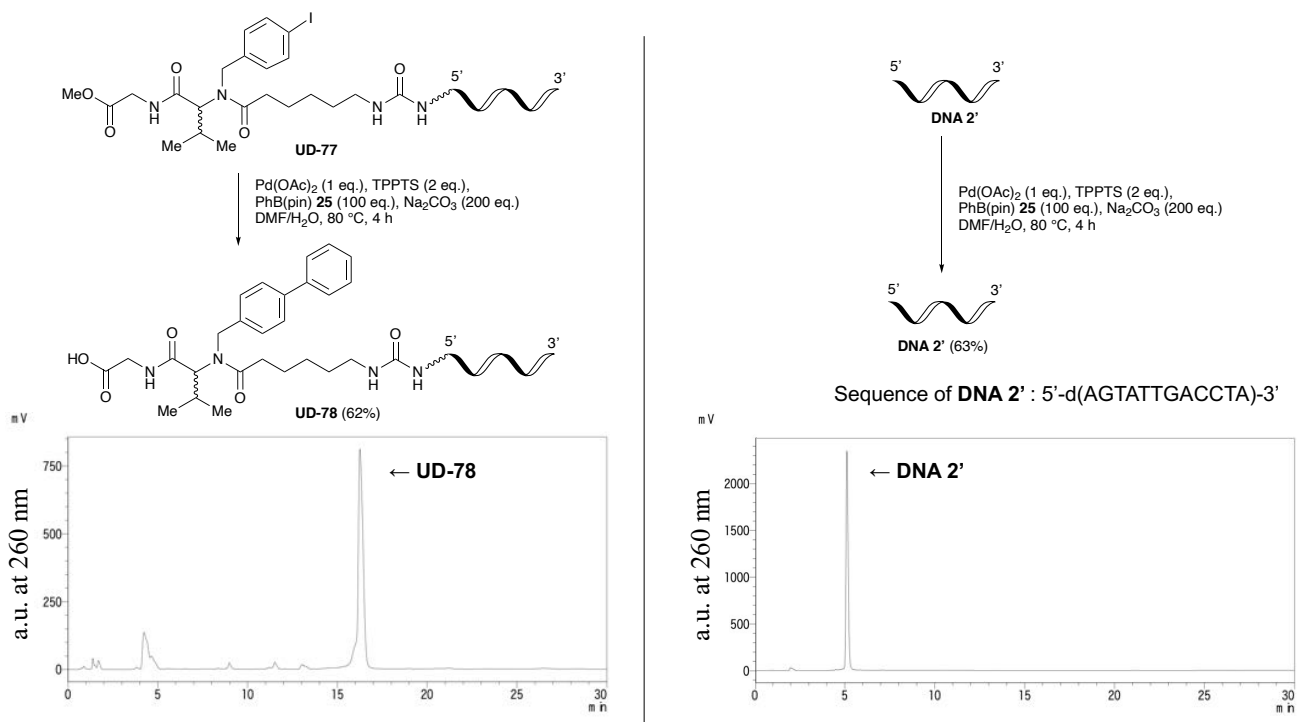


Figure S4. HPLC chromatograms after Suzuki-coupling. The reaction mixtures were analyzed by RP-HPLC with a linear gradient of MeCN (from 7 to 40% over 30 min, 50 °C) in 0.1 M TEAA buffer (pH 7.0).

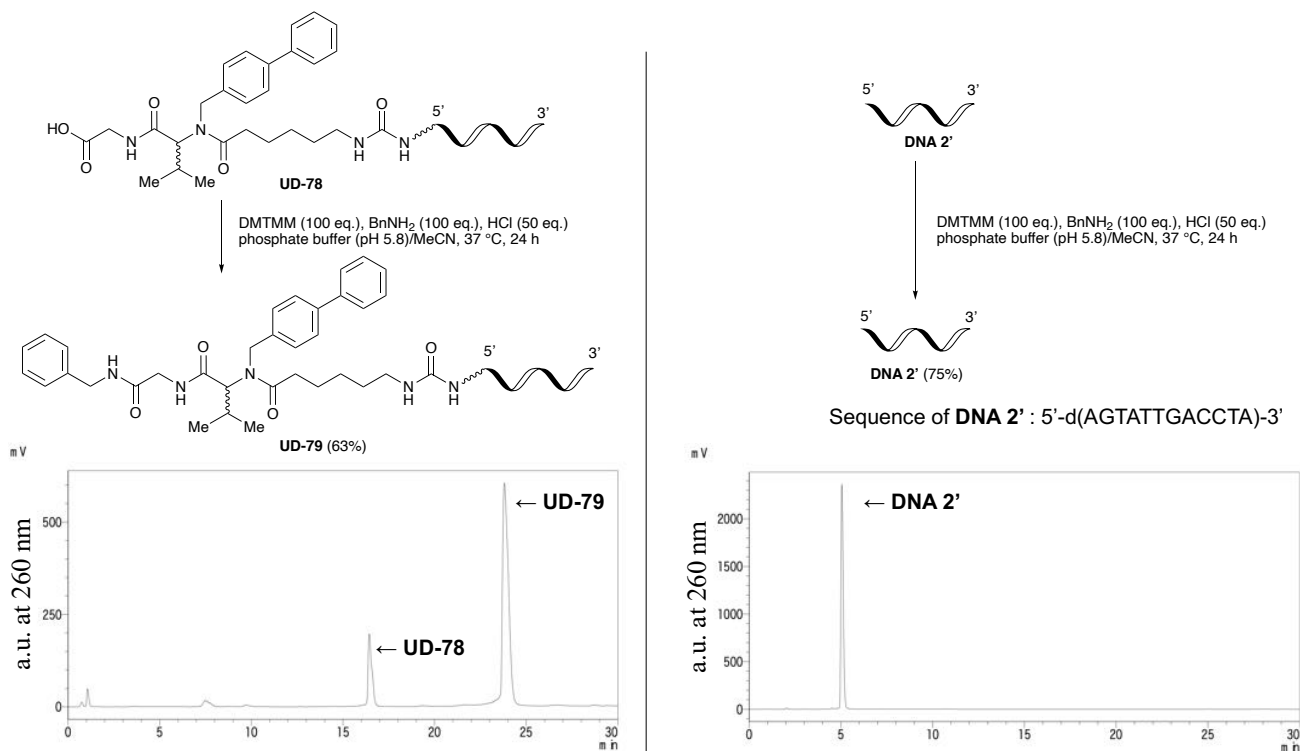
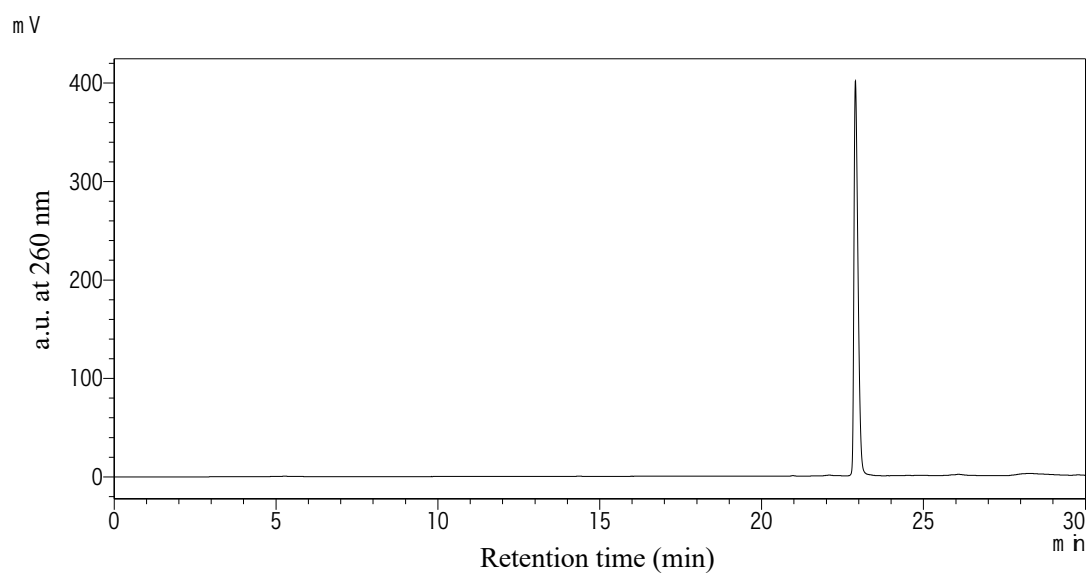


Figure S5. HPLC chromatograms after the amide bond formation reaction. The reaction mixtures were analyzed by RP-HPLC with a linear gradient of MeCN (from 7 to 40% over 30 min, 50 °C) in 0.1 M TEAA buffer (pH 7.0).

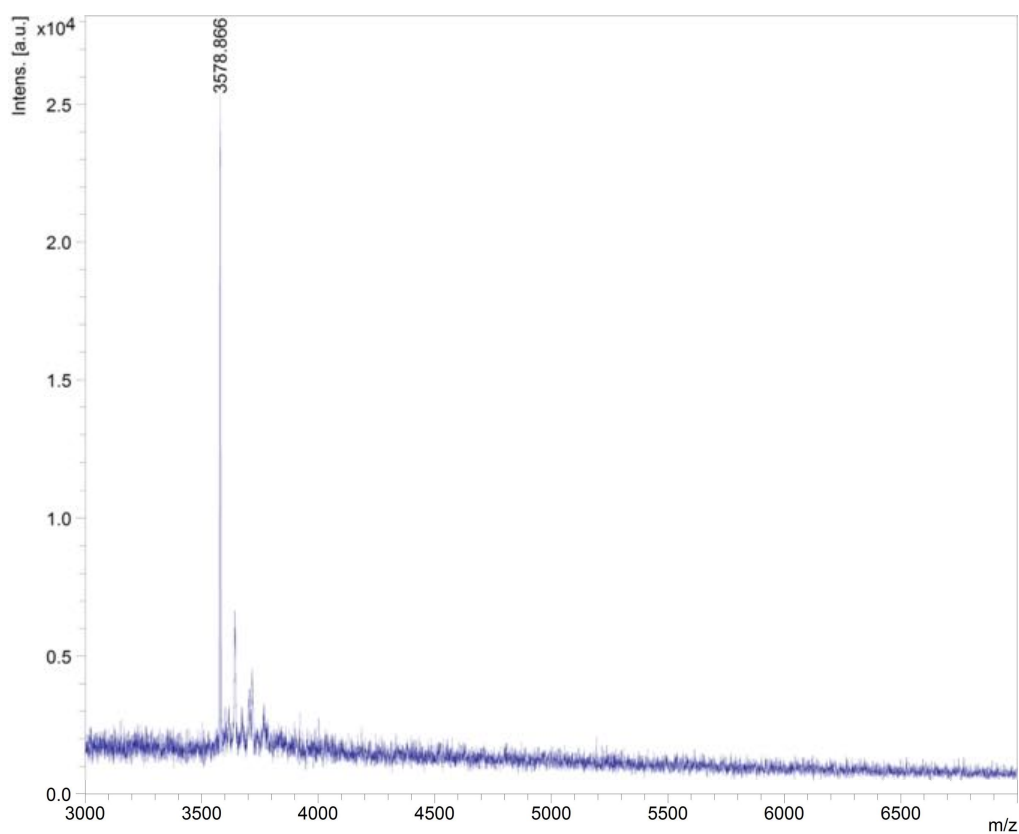
Figure S6. HPLC charts and MALDI-TOF mass spectrometry data of each peptoid-conjugated oligonucleotides
HPLC conditions: Detection: UV 260 nm, flow rate: 1.0 mL/min, mobile phase A: 0.1 M TEAA (pH 7.0), mobile phase B: acetonitrile (MeCN), column: Waters XBridge™ Shield RP18 2.5 μm (4.6×50 mm), temperature: 50 °C

UD-1

[B conc. MeCN: 7-40% (30 min)]



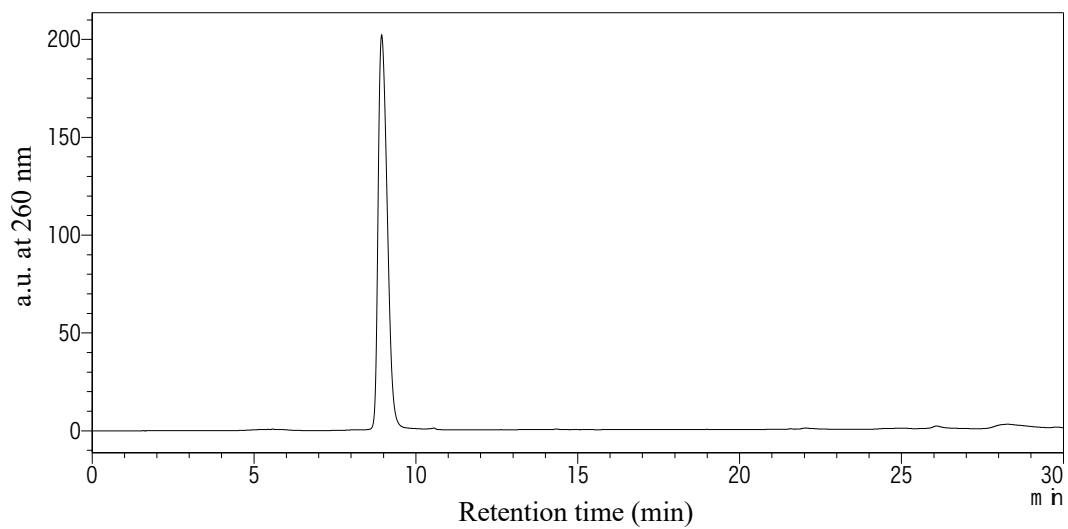
[calcd. (M-H)⁻: 3575.7, found: 3578.9]



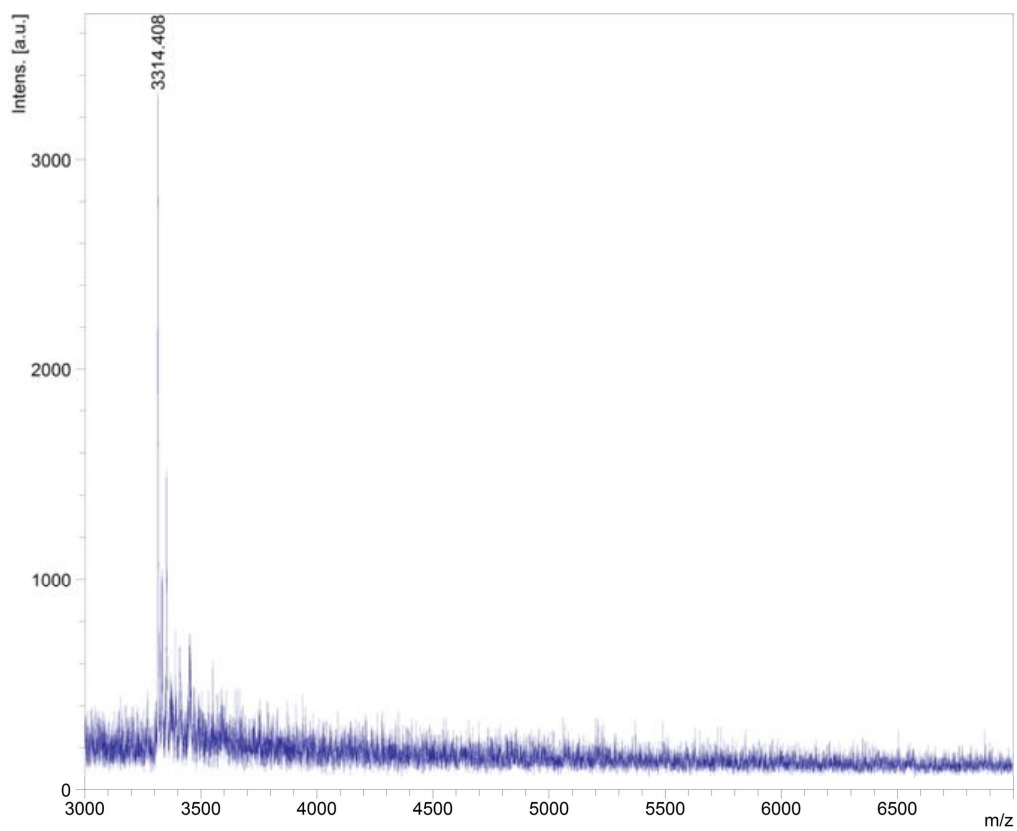
UD-2

[B conc. MeCN: 7-40% (30 min)]

mV



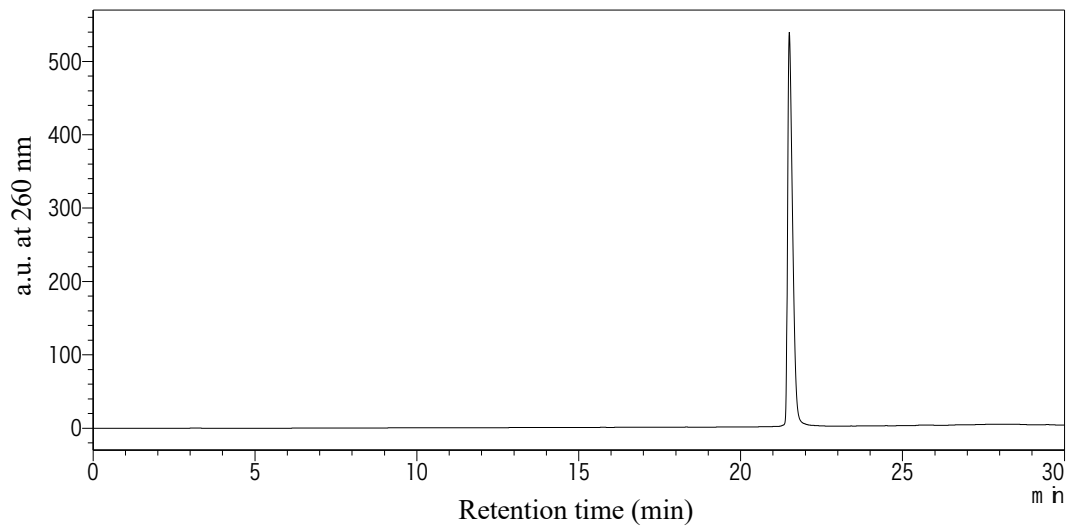
[calcd. (M-H)⁻: 3315.3, found: 3314.4]



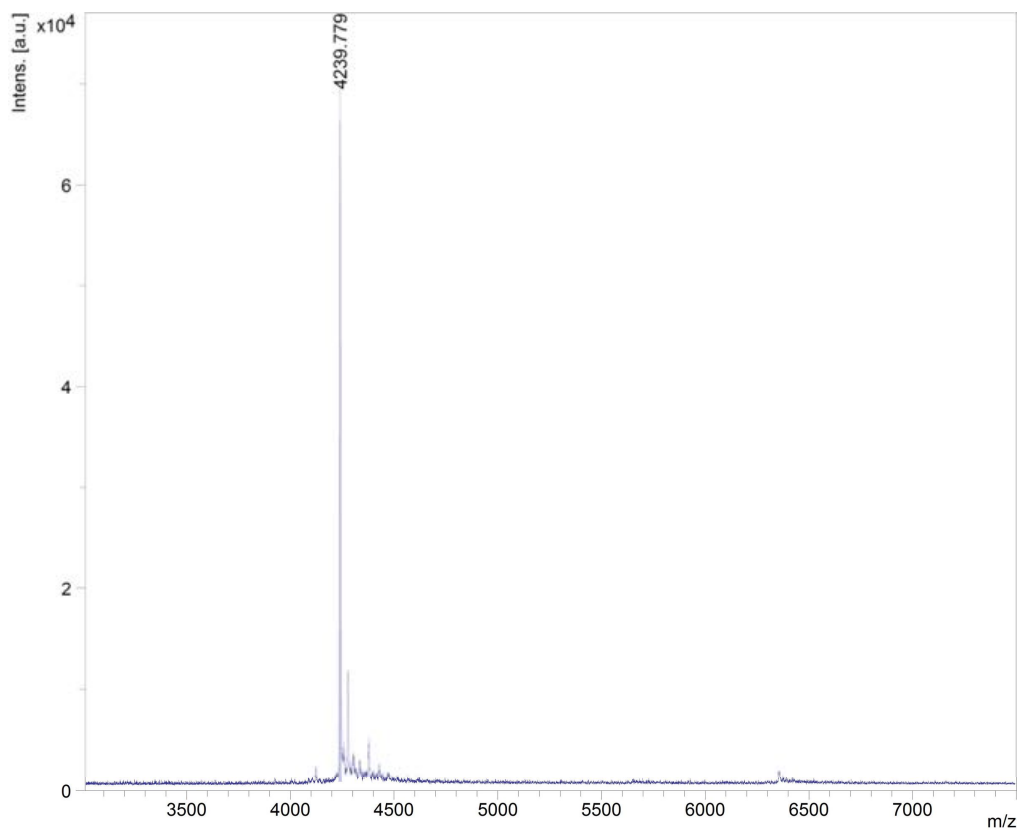
UD-3

[B conc. MeCN: 7-40% (30 min)]

mV



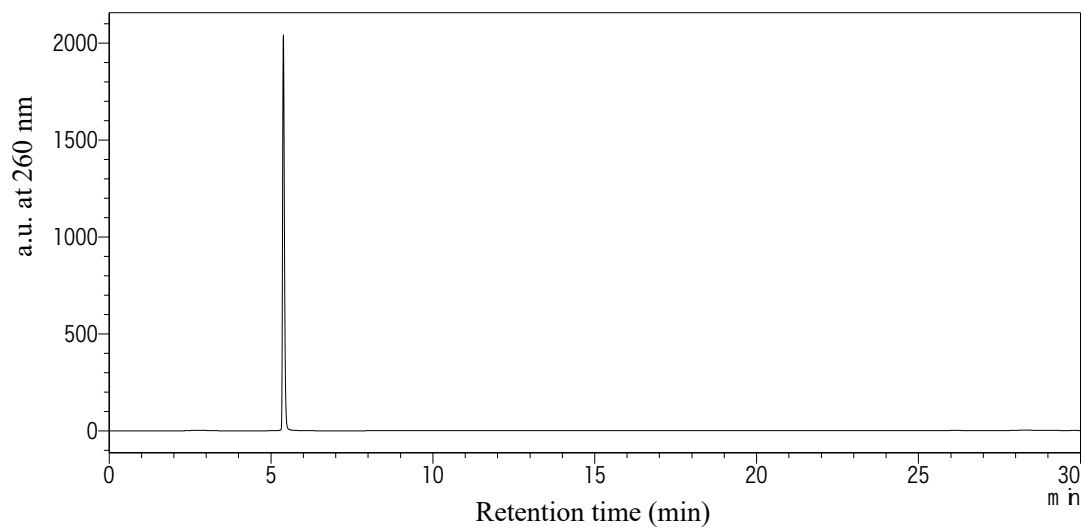
[calcd. (M-H)⁻: 4240.1, found: 4239.8]



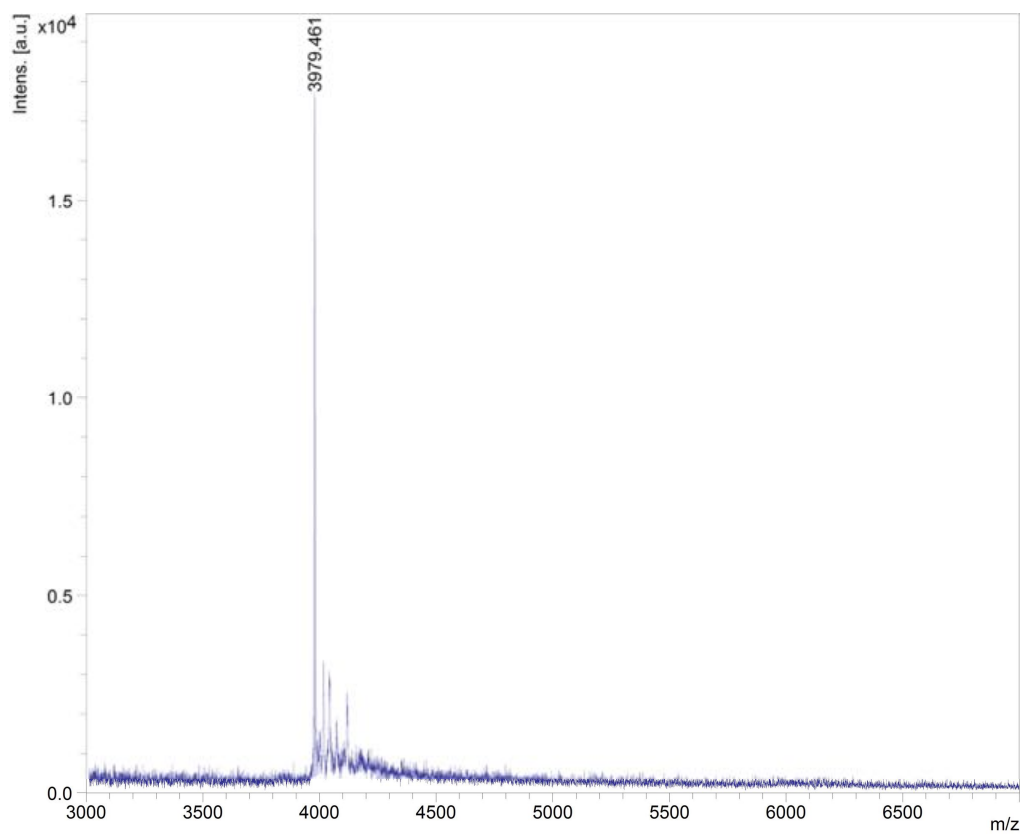
UD-4

[B conc. MeCN: 7-40% (30 min)]

mV



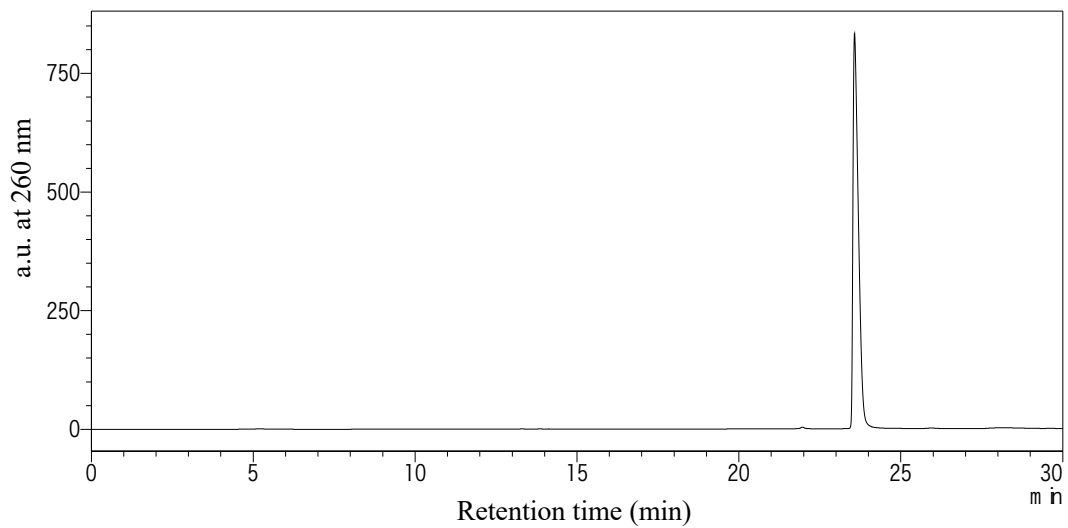
[calcd. (M-H)⁻: 3979.8, found: 3979.5]



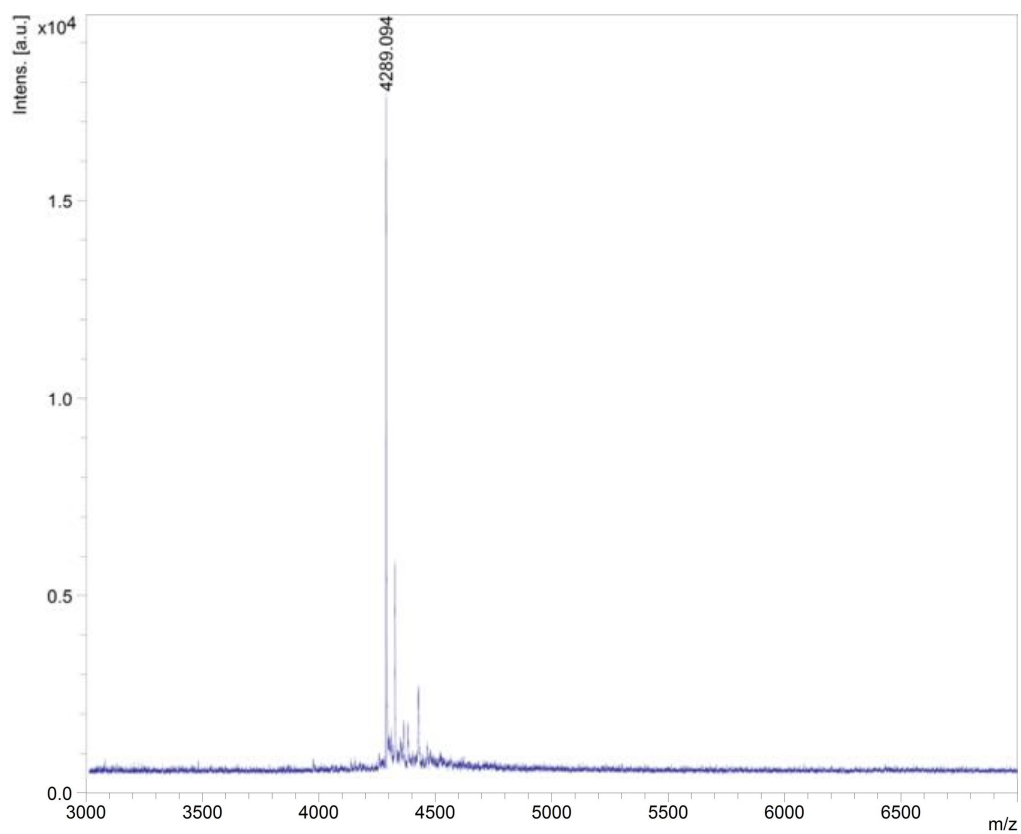
UD-5

[B conc. MeCN: 7-40% (30 min)]

mV



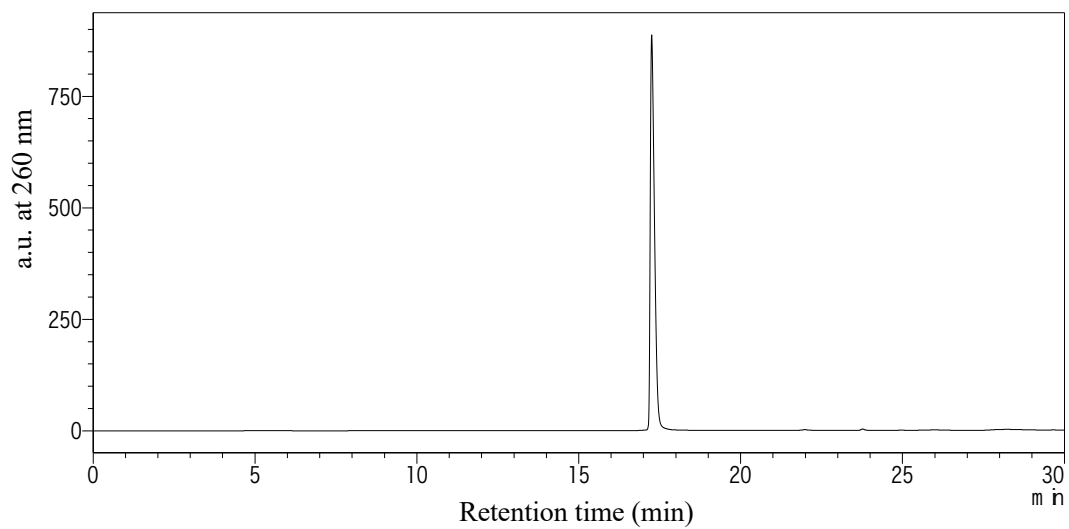
[calcd. (M-H)⁻: 4288.2, found: 4289.1]



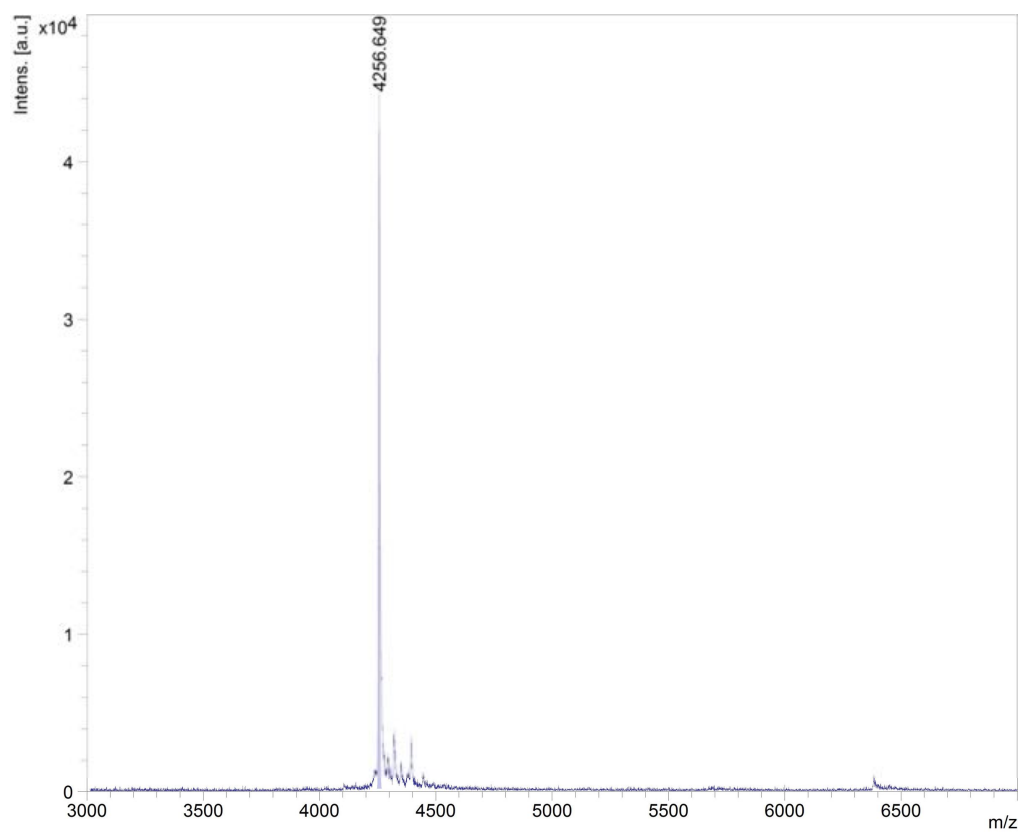
UD-6

[B conc. MeCN: 7-40% (30 min)]

mV



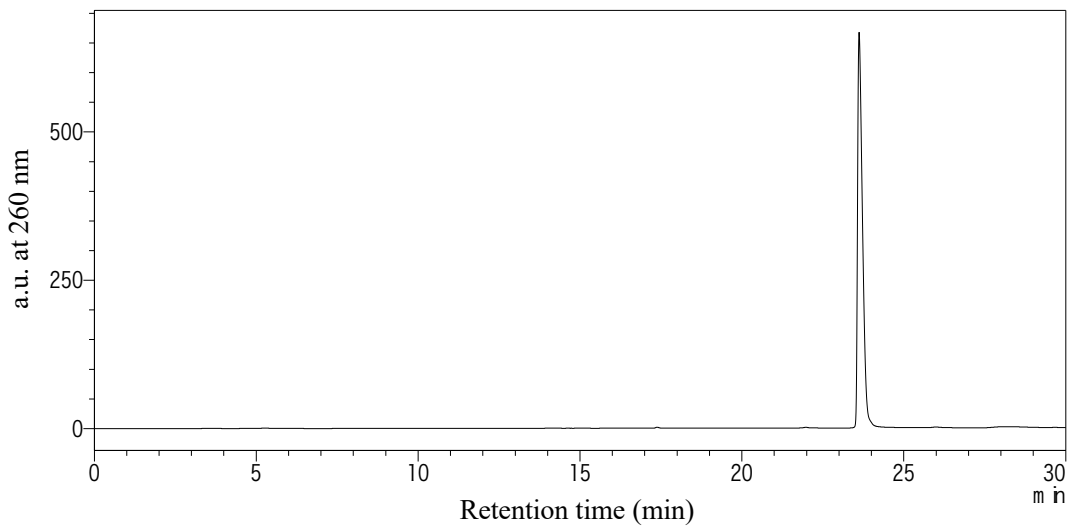
[calcd. (M-H)⁻: 4256.1, found: 4256.6]



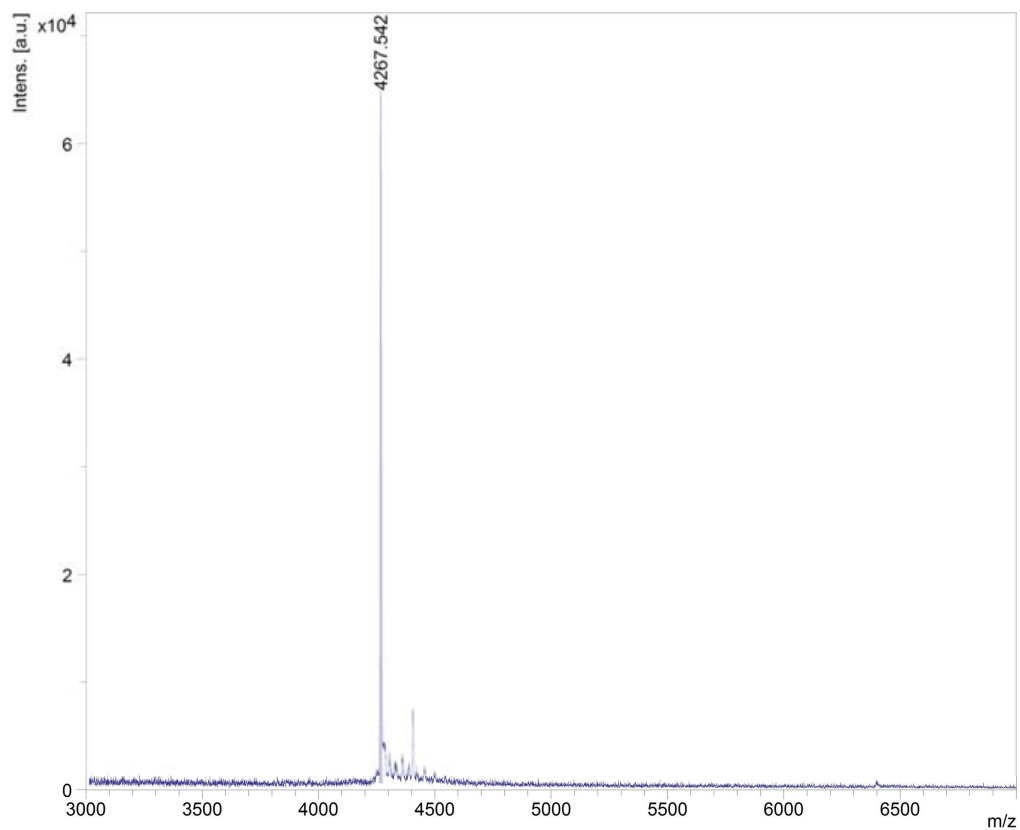
UD-7

[B conc. MeCN: 7-40% (30 min)]

mV



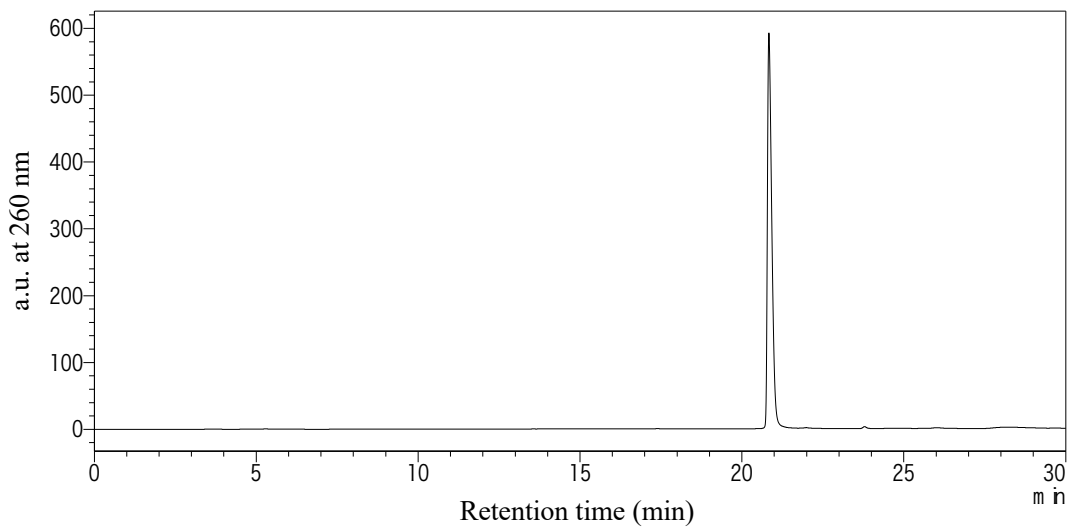
[calcd. (M-H)⁻: 4266.2, found: 4267.5]



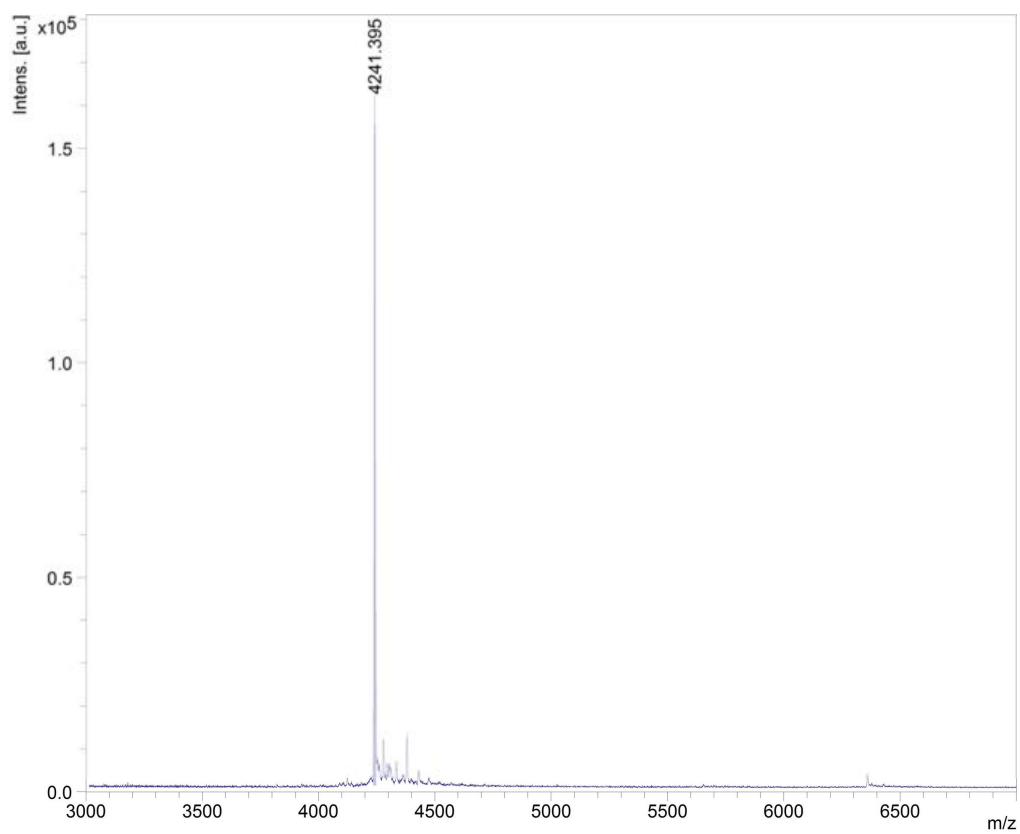
UD-8

[B conc. MeCN: 7-40% (30 min)]

mV



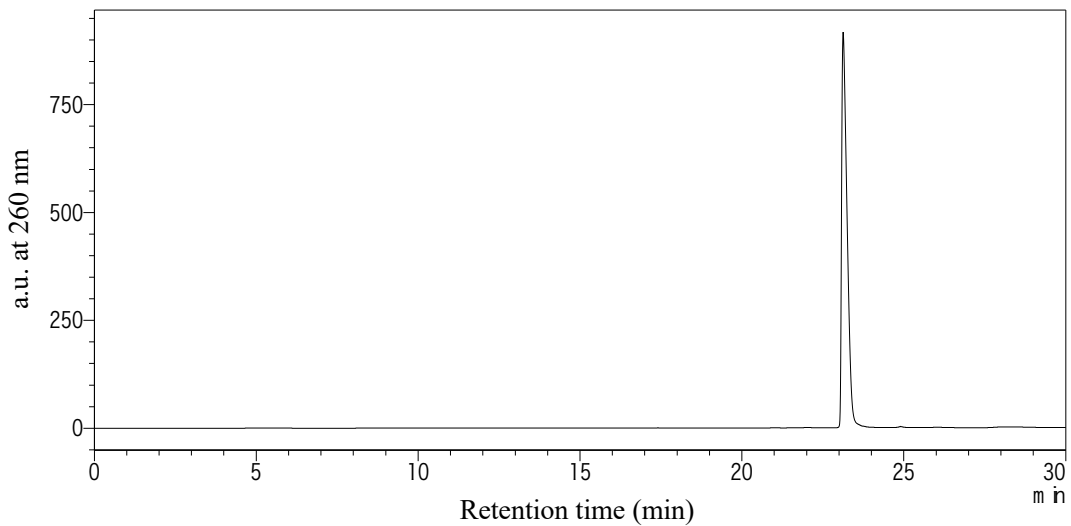
[calcd. (M-H)⁻: 4240.1, found: 4241.4]



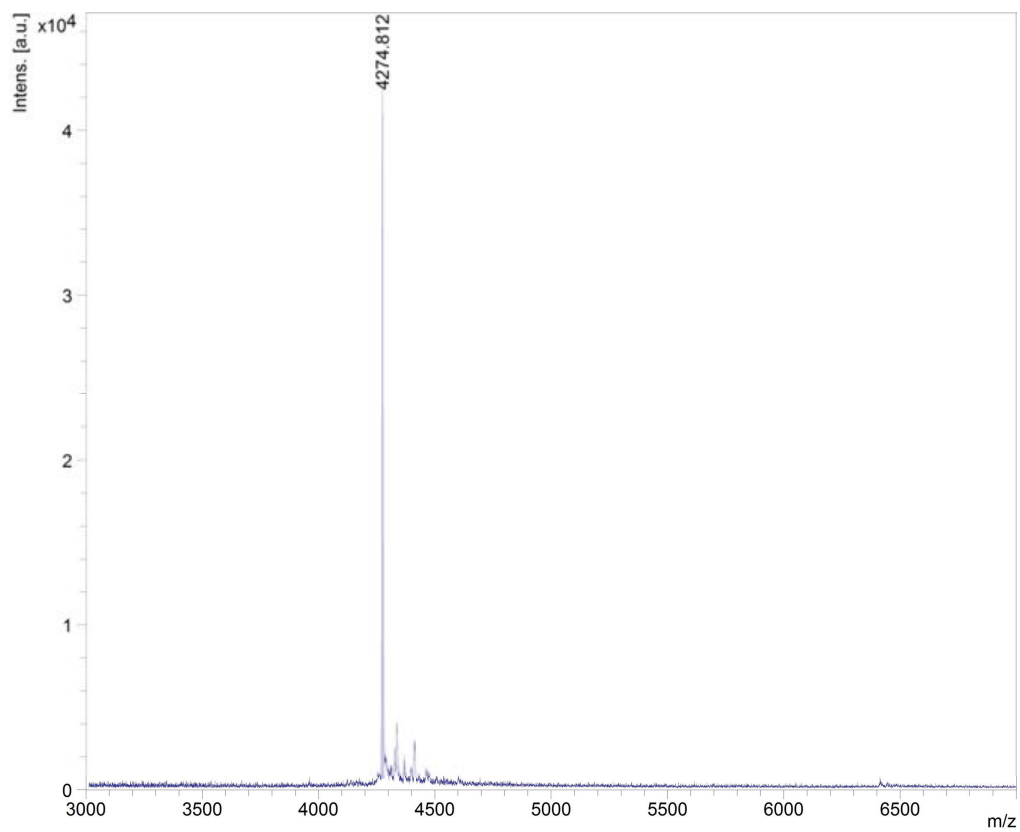
UD-9

[B conc. MeCN: 7-40% (30 min)]

mV



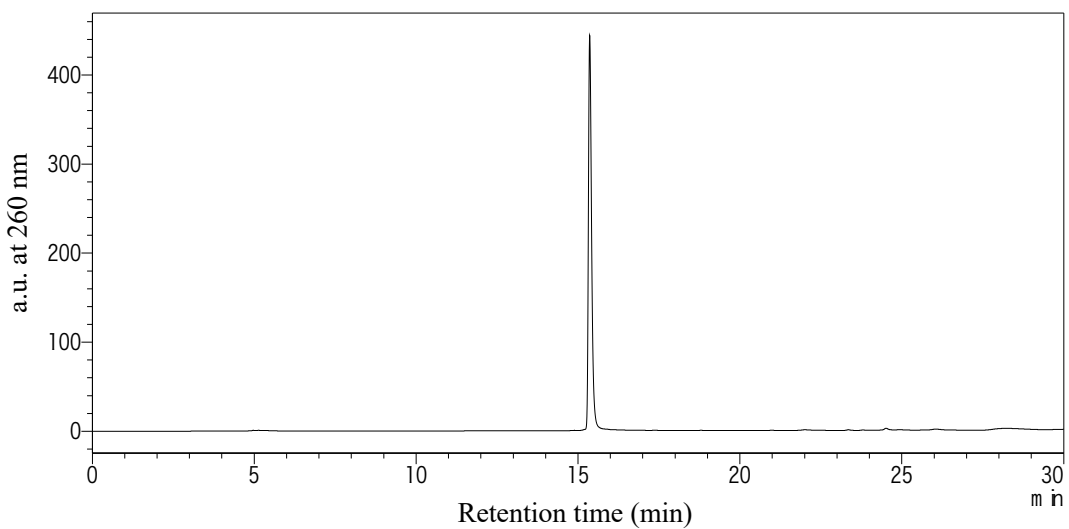
[calcd. (M-H)⁻: 4274.2, found: 4274.8]



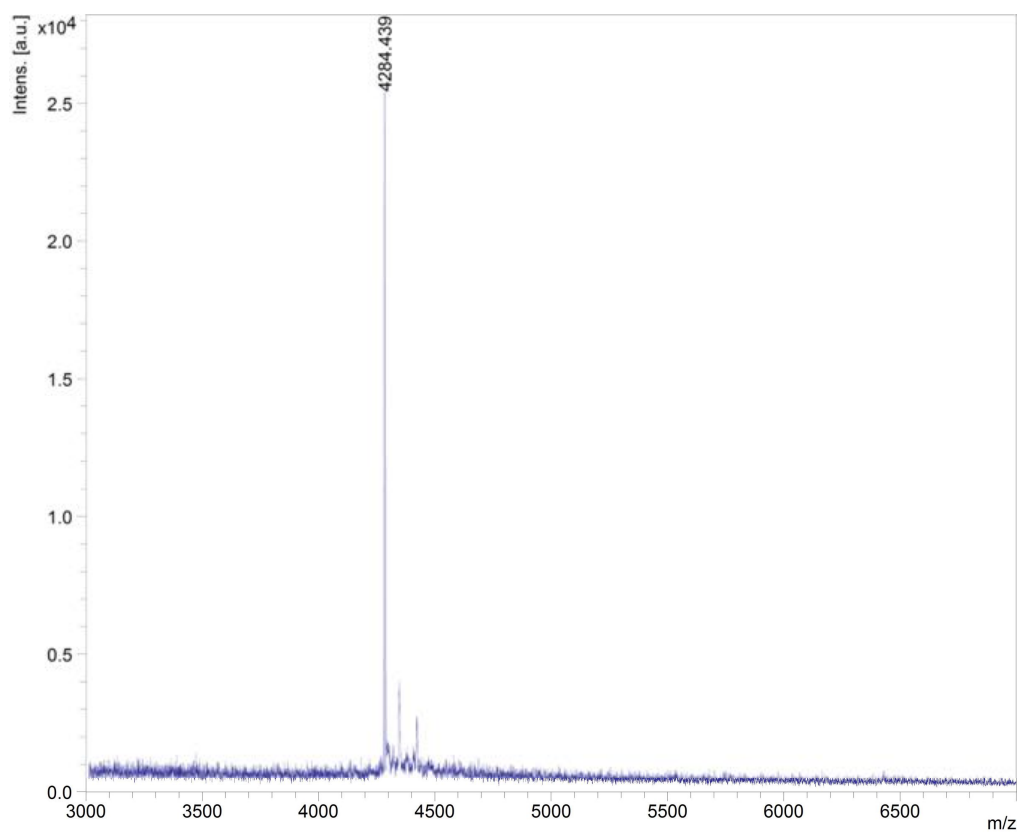
UD-10

[B conc. MeCN: 7-40% (30 min)]

mV



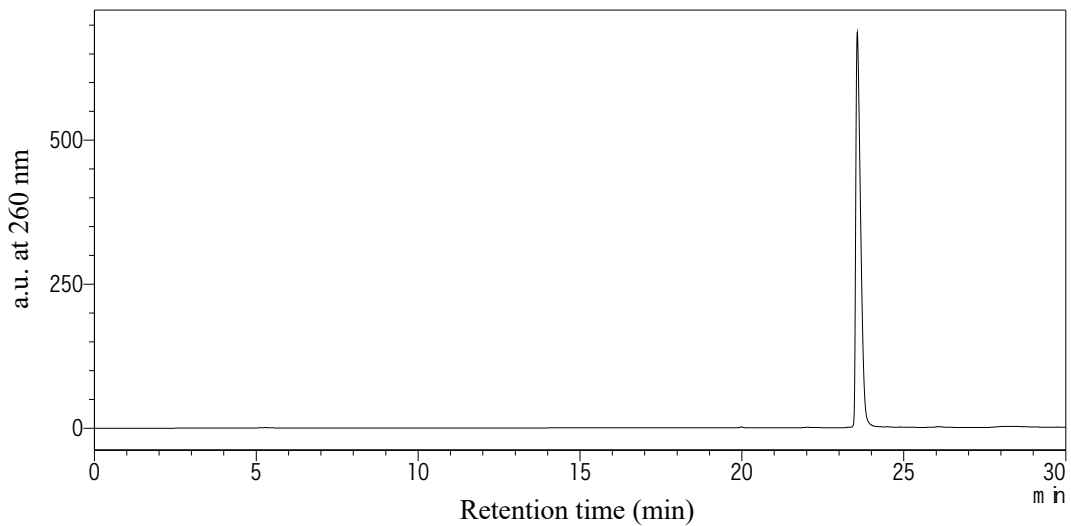
[calcd. (M-H)⁻: 4283.2, found: 4284.4]



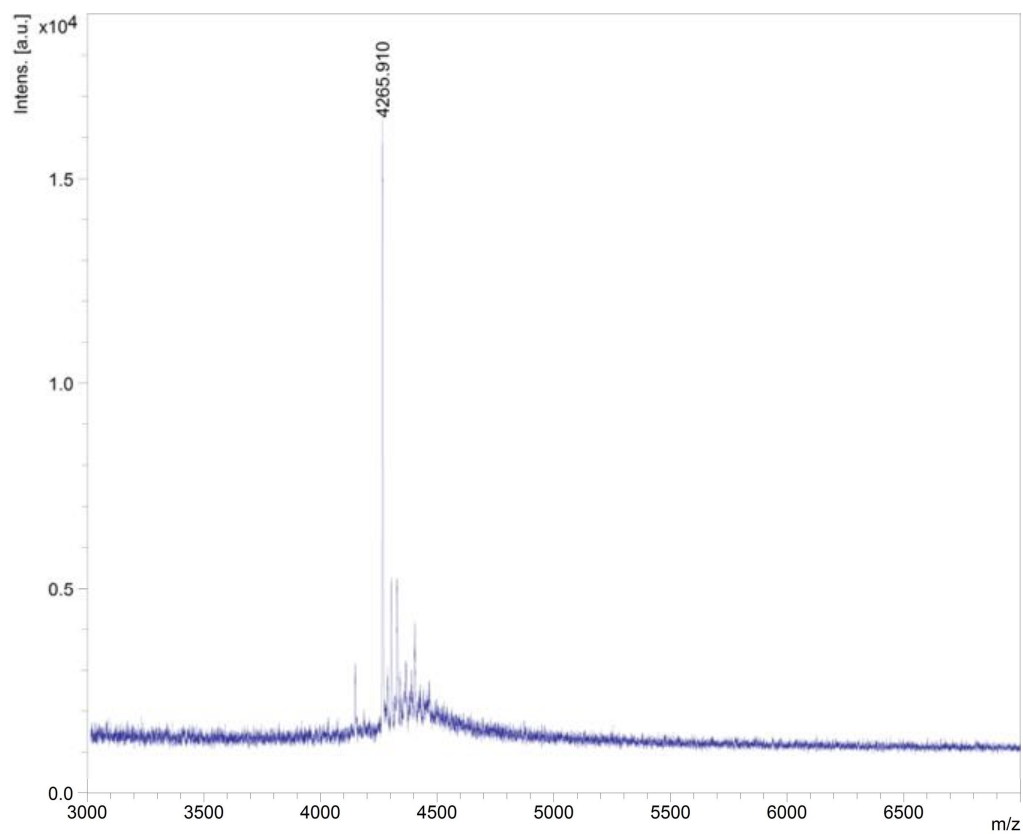
UD-11

[B conc. MeCN: 7-40% (30 min)]

mV



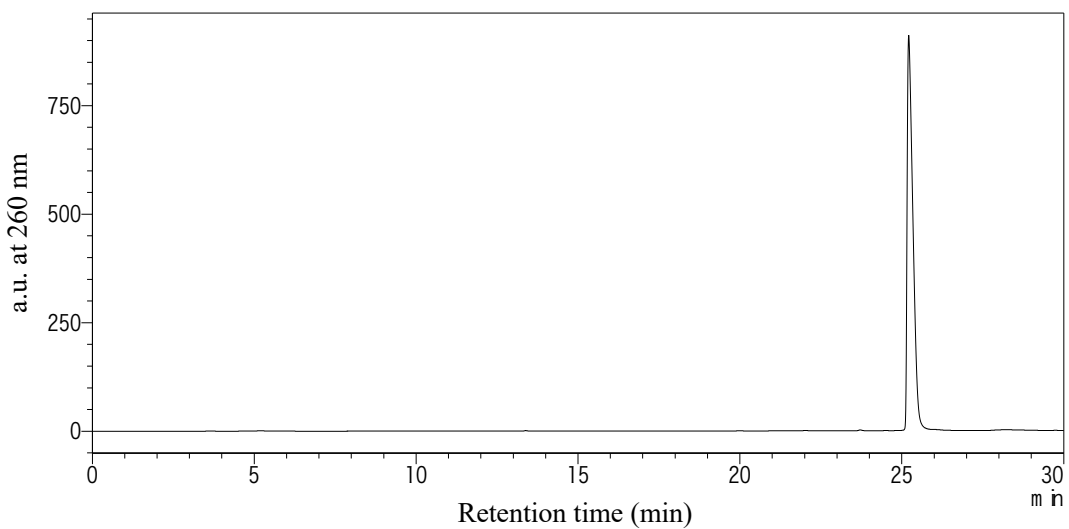
[calcd. (M-H)⁻: 4266.2, found: 4265.9]



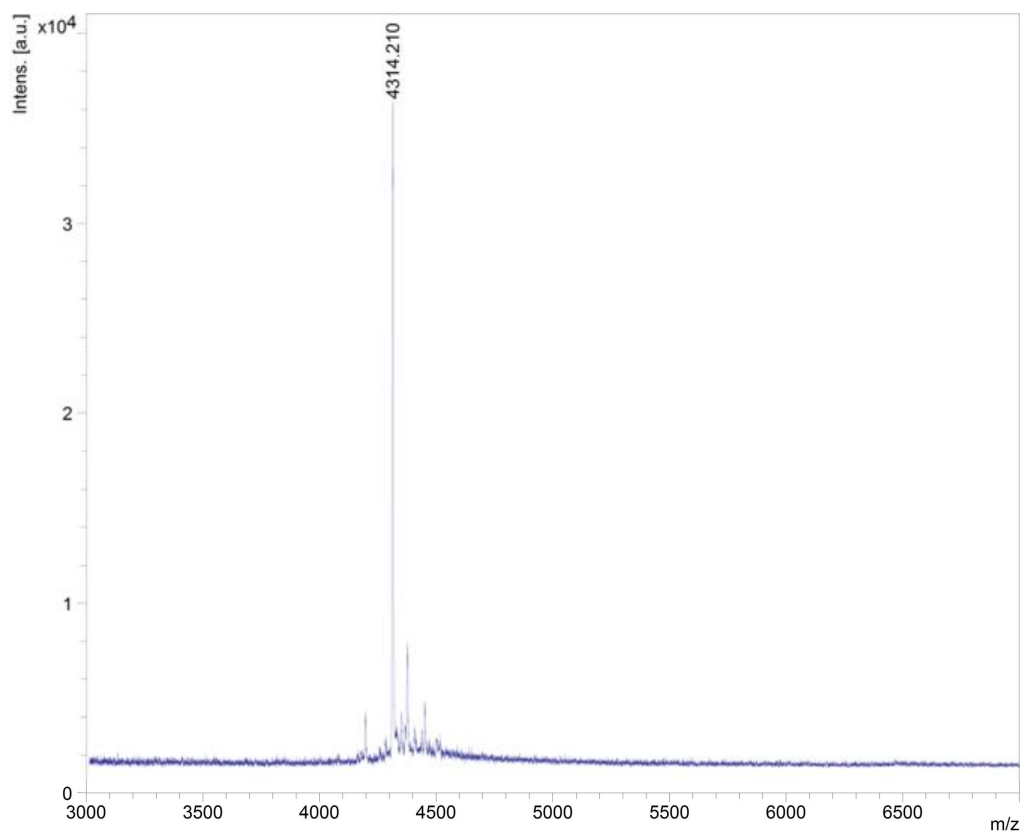
UD-12

[B conc. MeCN: 7-40% (30 min)]

mV



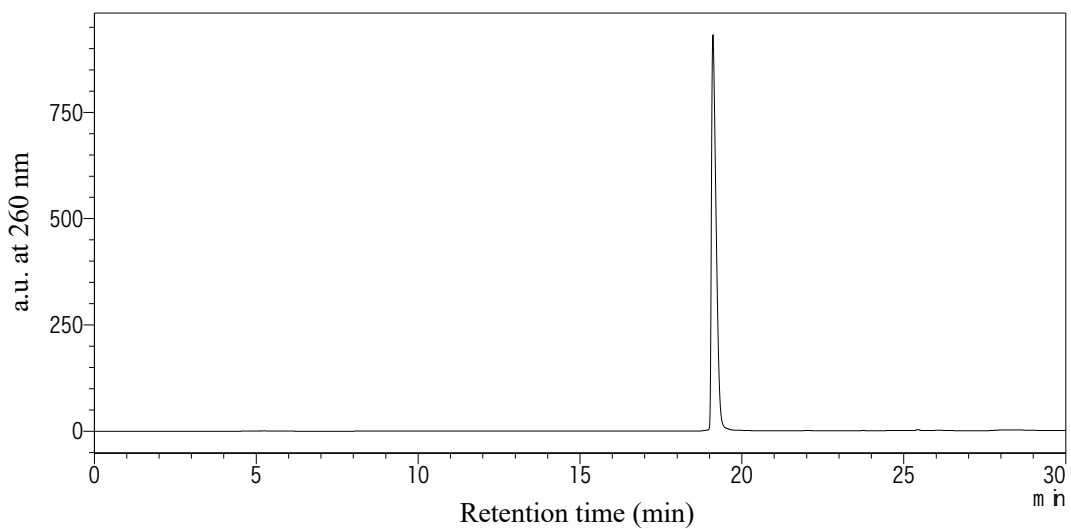
[calcd. (M-H)⁻: 4314.2, found: 4314.2]



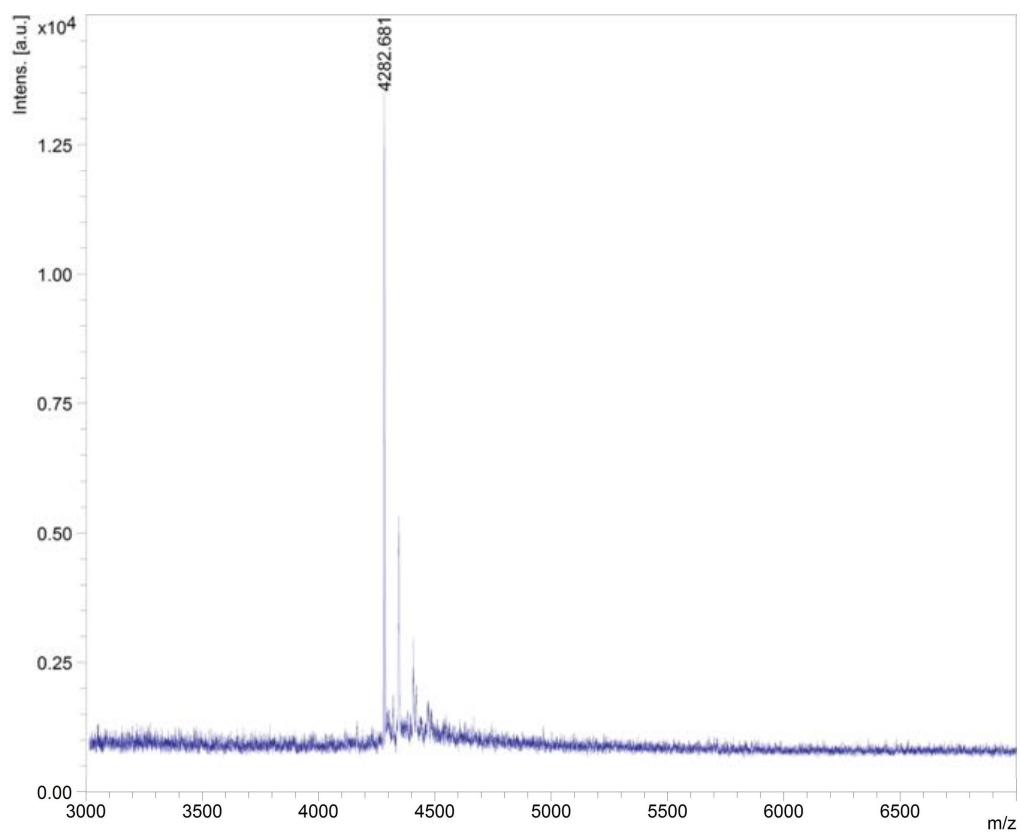
UD-13

[B conc. MeCN: 7-40% (30 min)]

mV



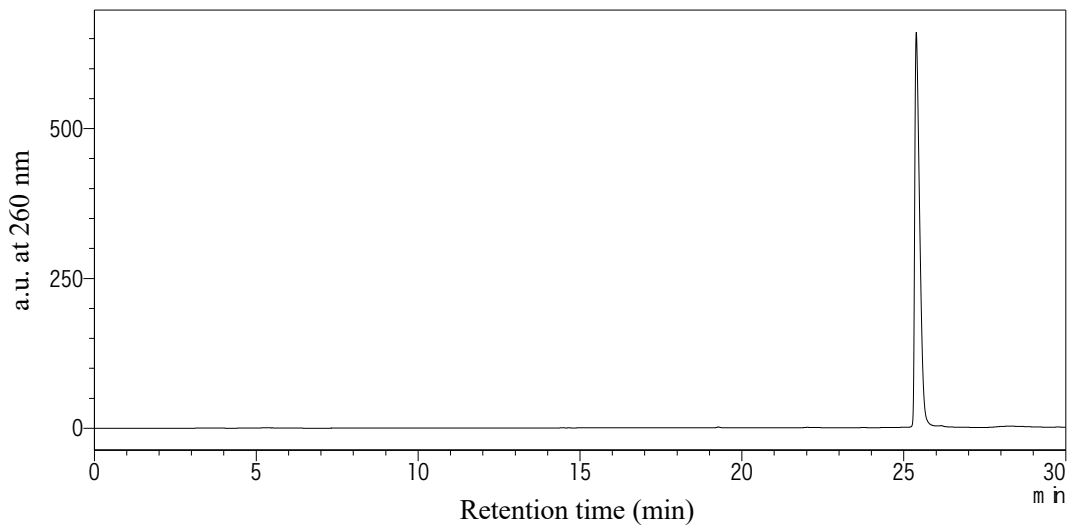
[calcd. (M-H)⁻: 4282.2, found: 4282.7]



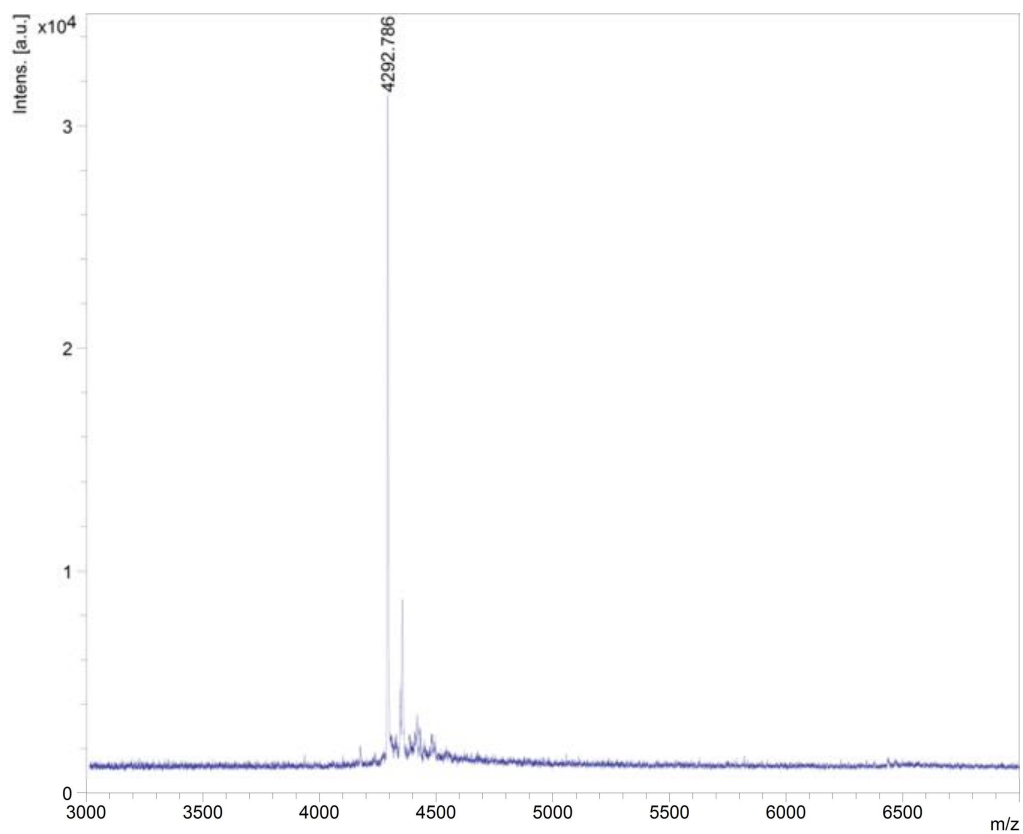
UD-14

[B conc. MeCN: 7-40% (30 min)]

mV



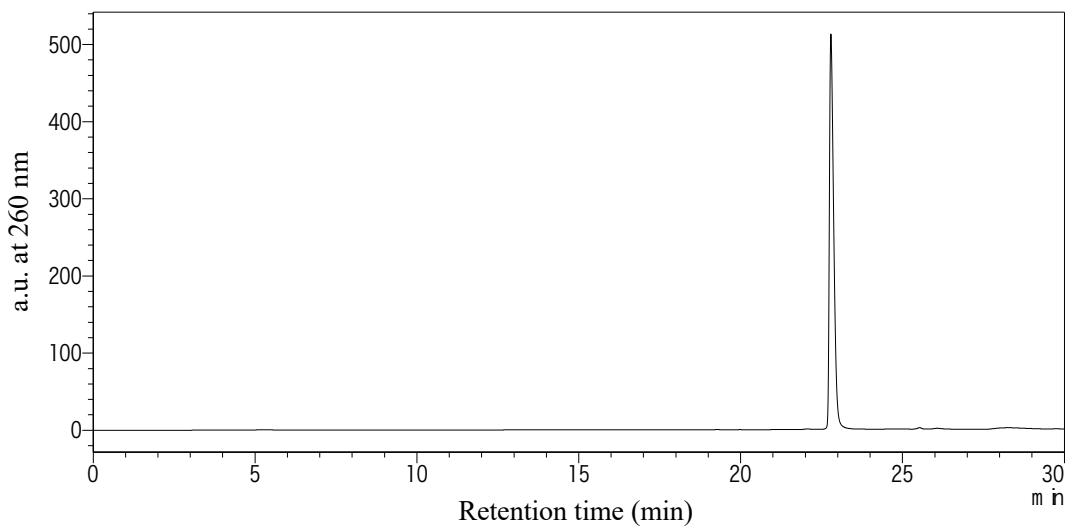
[calcd. (M-H)⁻: 4292.2, found: 4292.8]



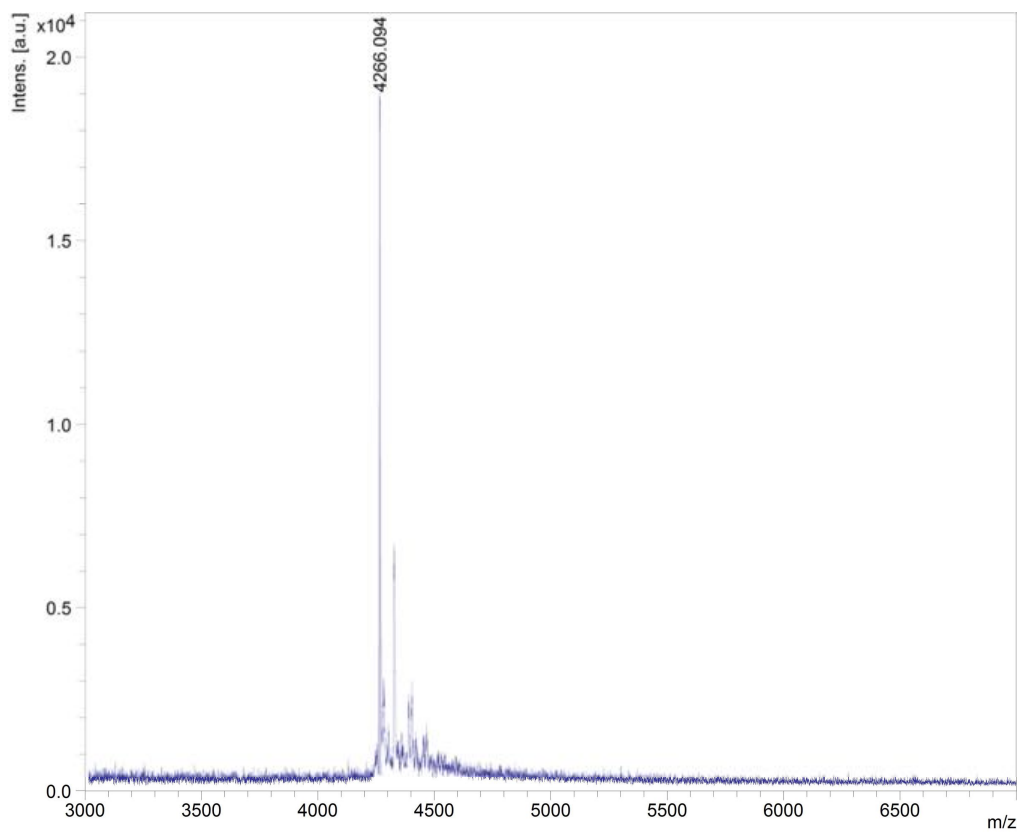
UD-15

[B conc. MeCN: 7-40% (30 min)]

mV



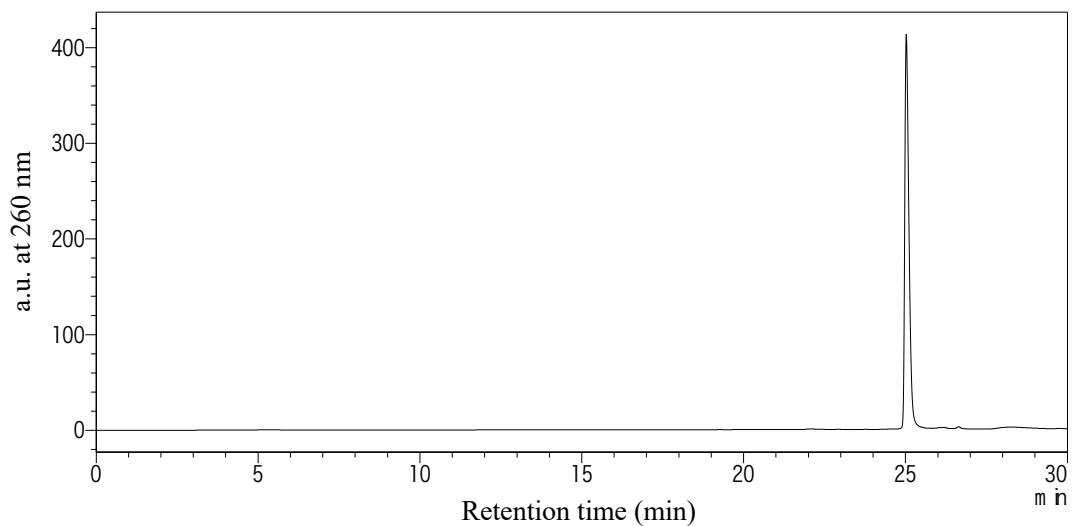
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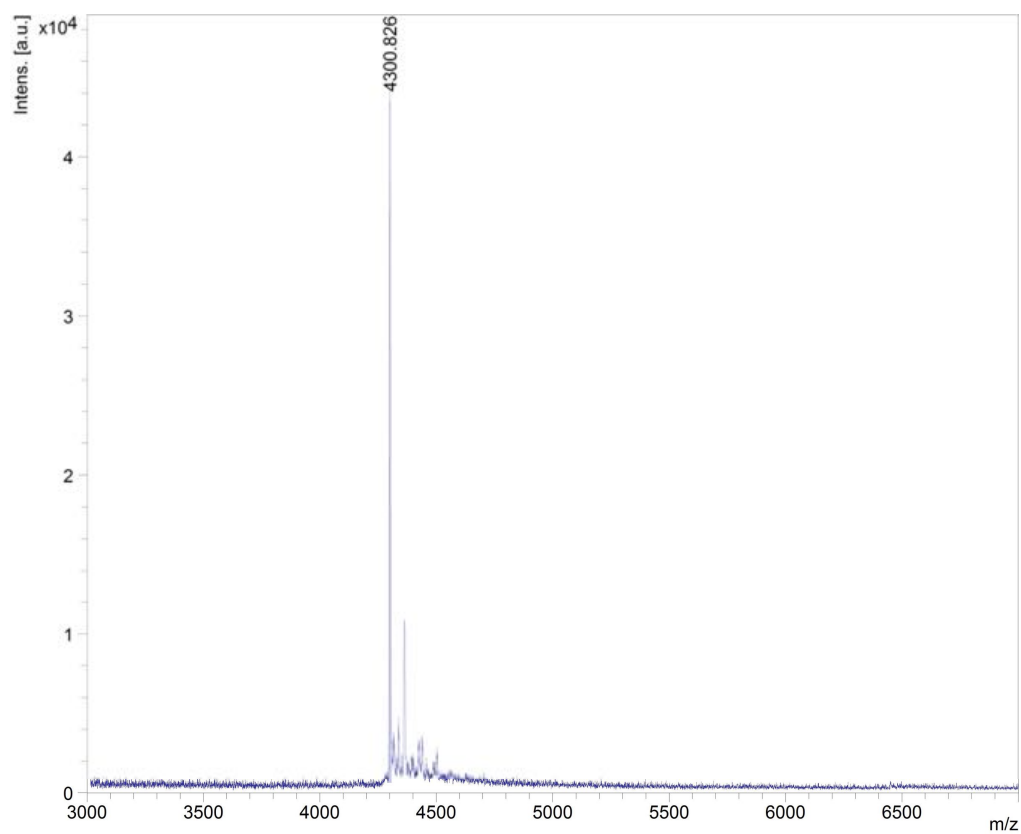
UD-16

[B conc. MeCN: 7-40% (30 min)]

mV



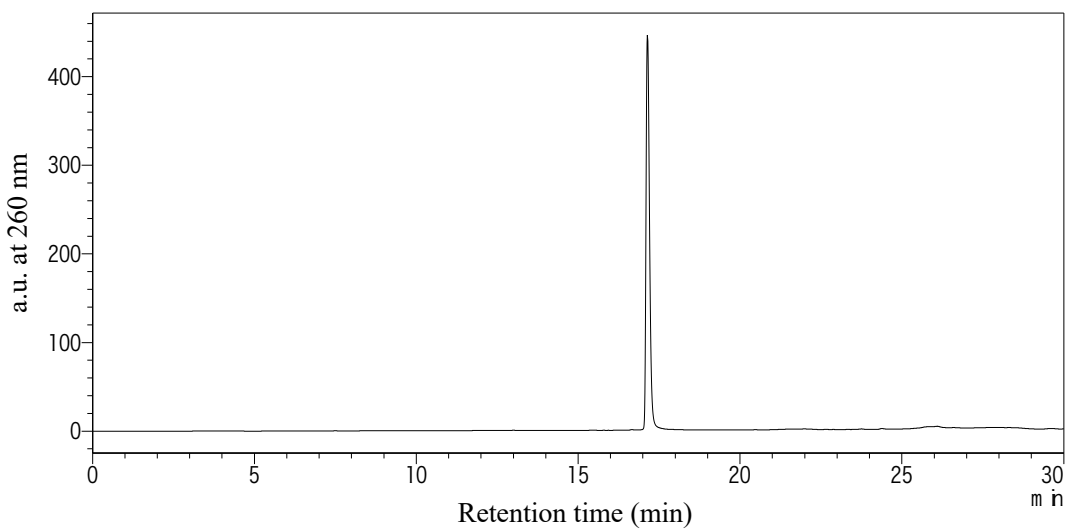
[calcd. (M-H)⁻: 4300.2, found: 4300.8]



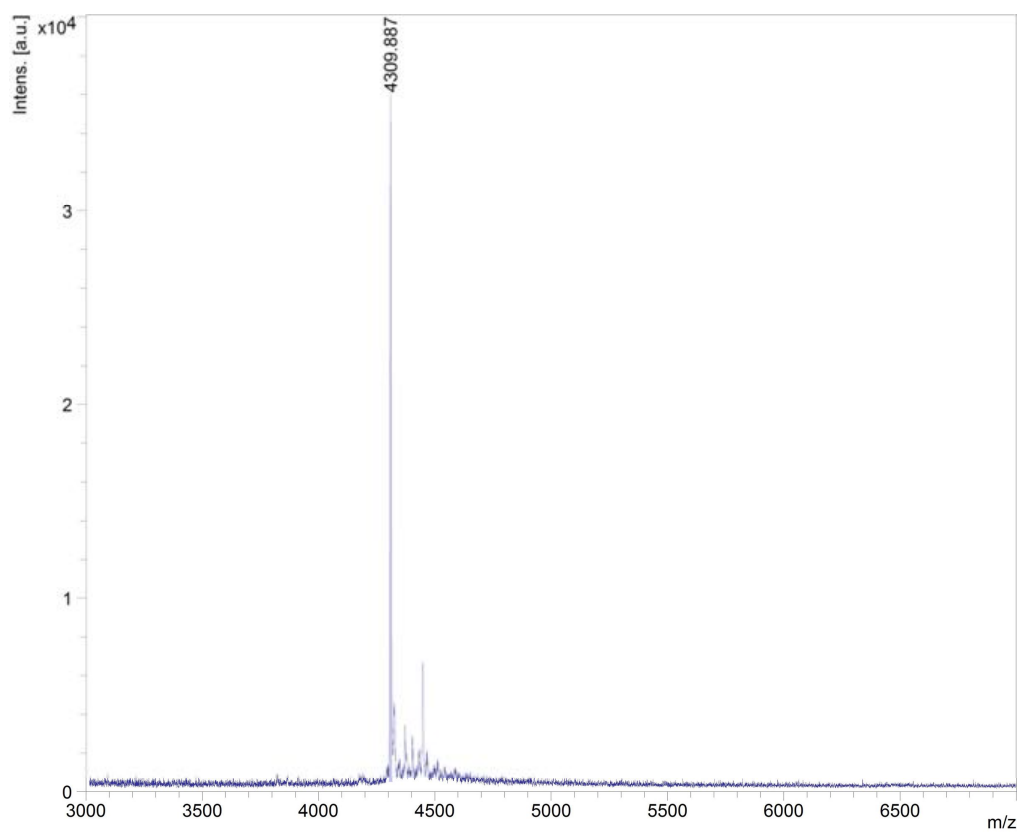
UD-17

[B conc. MeCN: 7-40% (30 min)]

mV



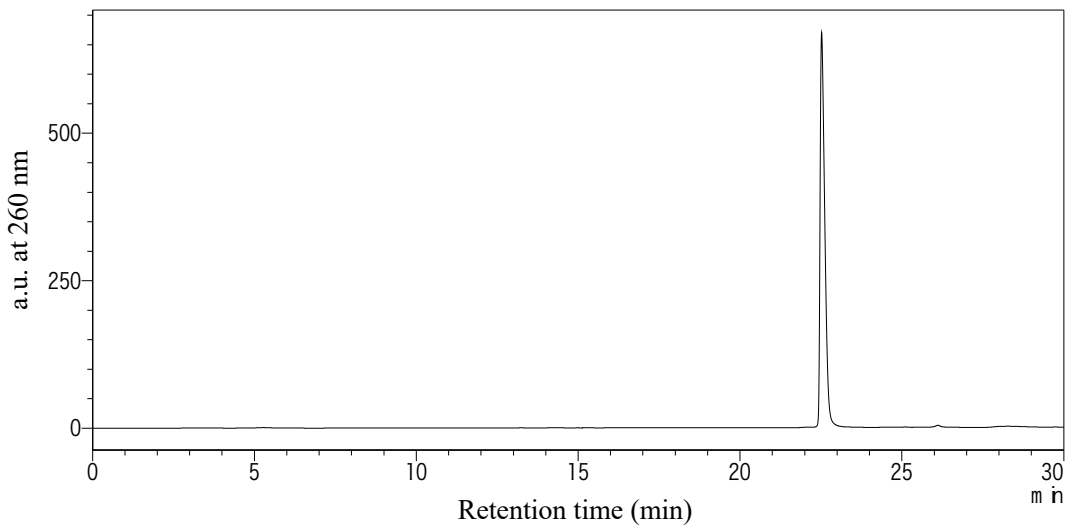
[calcd. (M-H)⁻: 4309.2, found: 4309.9]



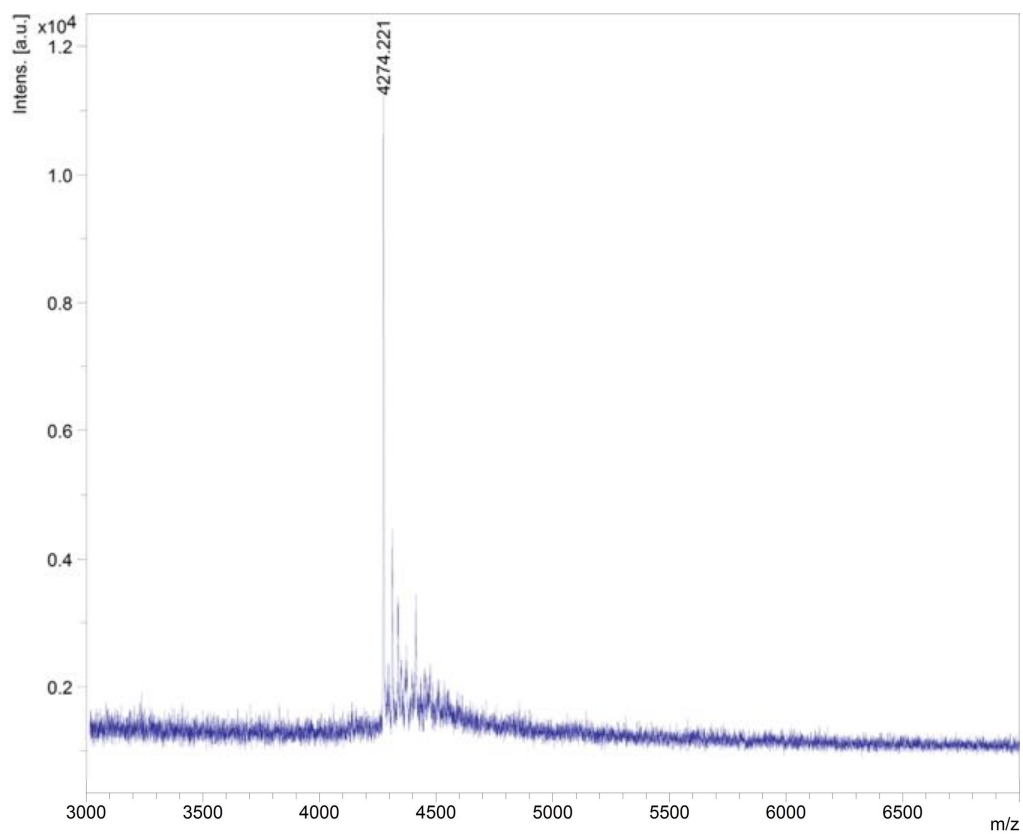
UD-18

[B conc. MeCN: 7-40% (30 min)]

mV



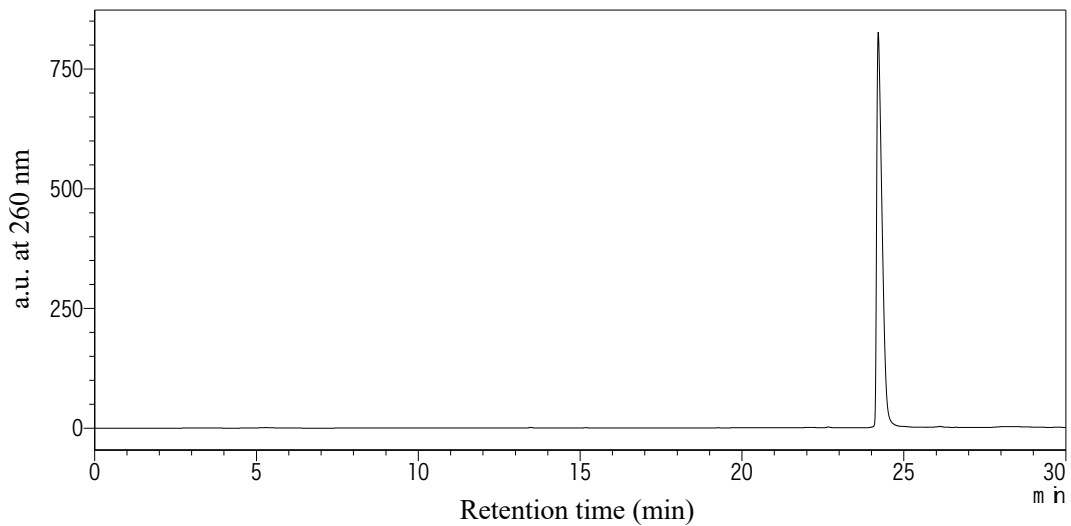
[calcd. (M-H)⁻: 4274.2, found: 4274.2]



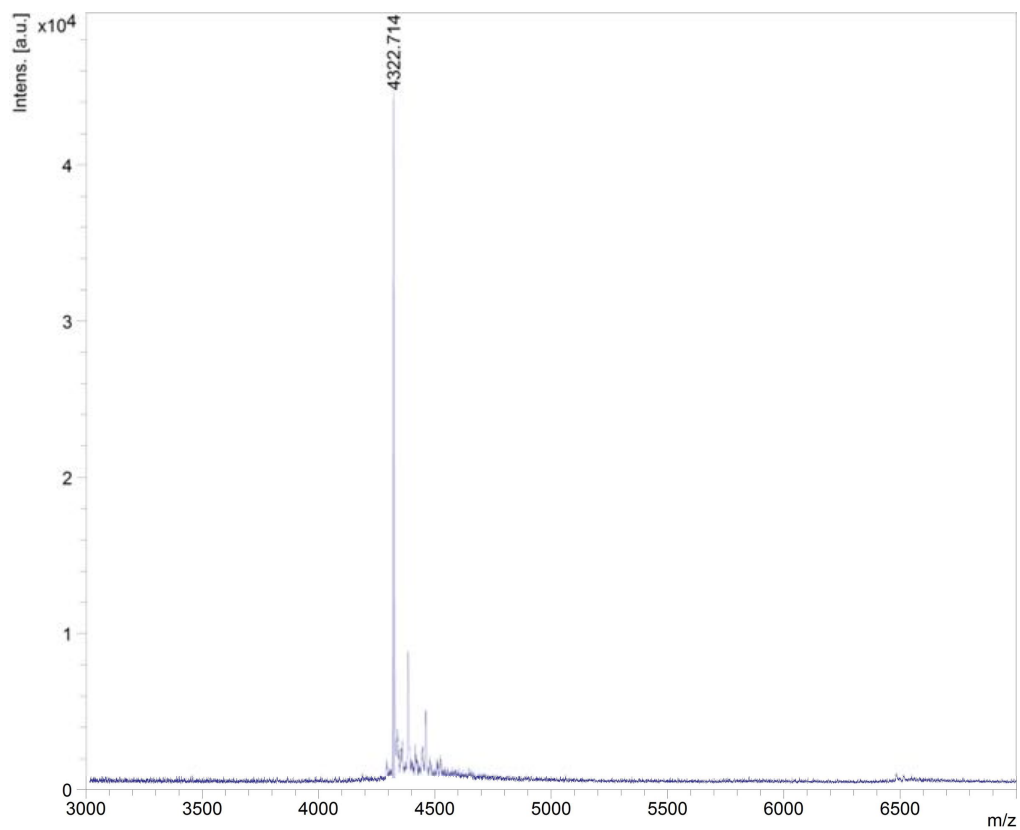
UD-19

[B conc. MeCN: 7-40% (30 min)]

mV



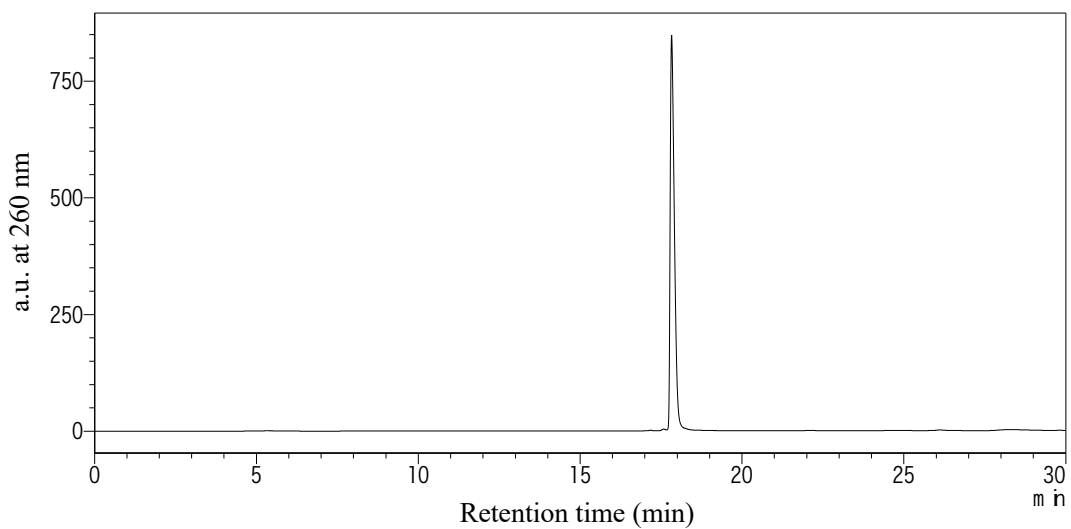
[calcd. (M-H)⁻: 4322.2, found: 4322.7]



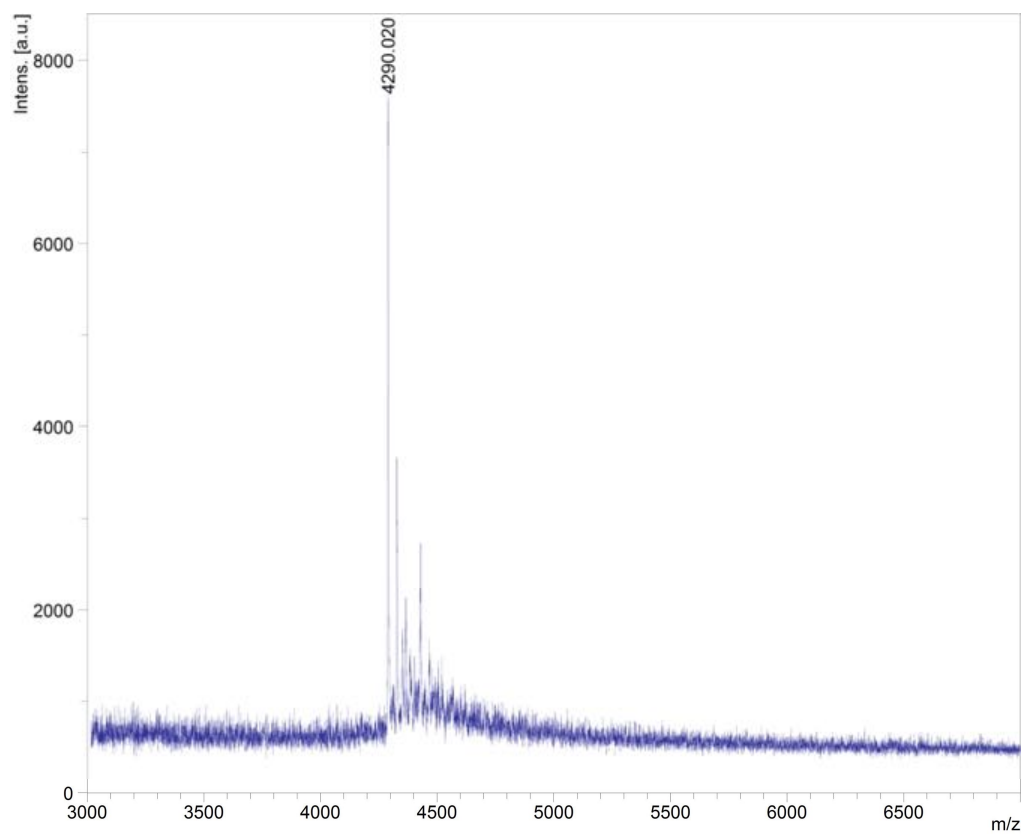
UD-20

[B conc. MeCN: 7-40% (30 min)]

mV



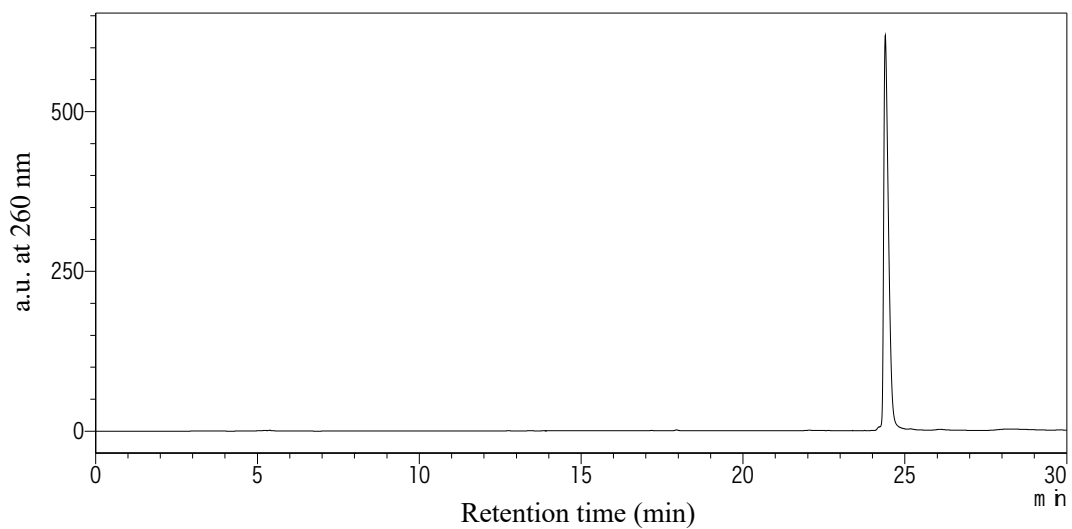
[calcd. (M-H)⁻: 4290.2, found: 4290.0]



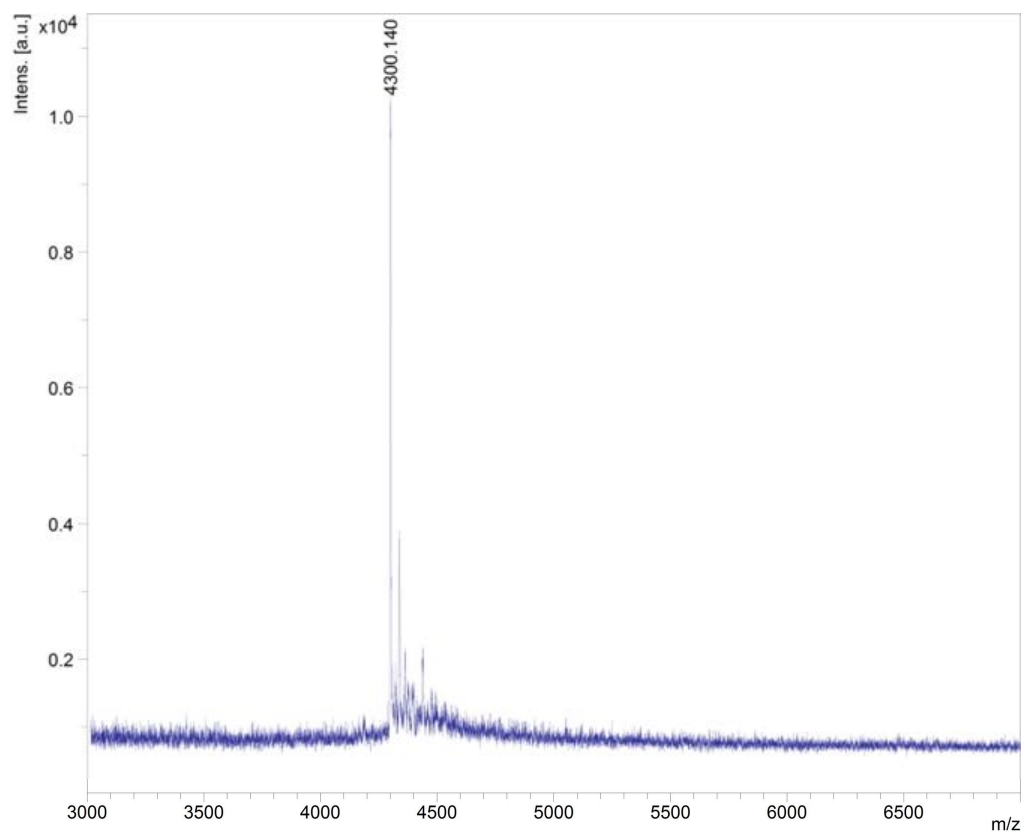
UD-21

[B conc. MeCN: 7-40% (30 min)]

mV



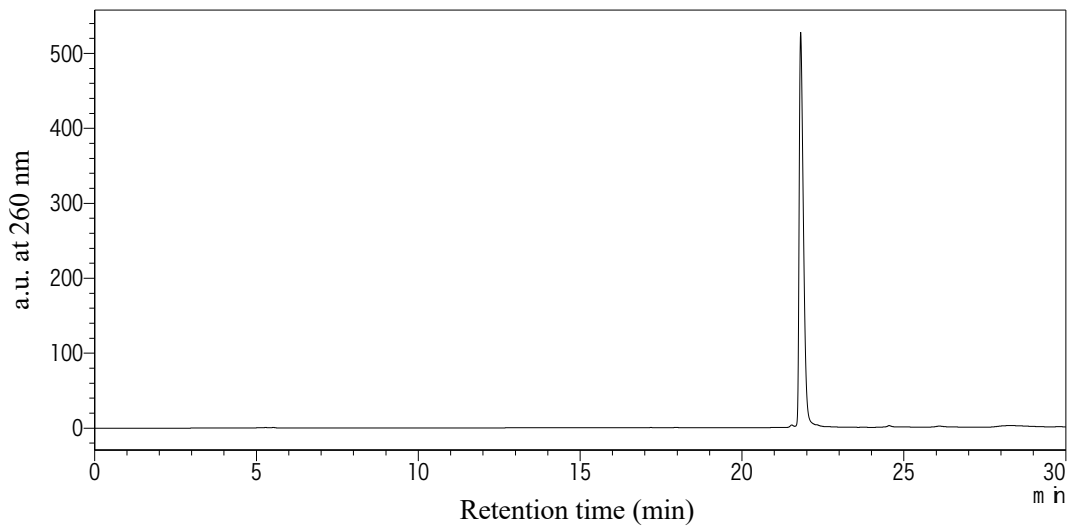
[calcd. (M-H)⁻: 4300.2, found: 4300.1]



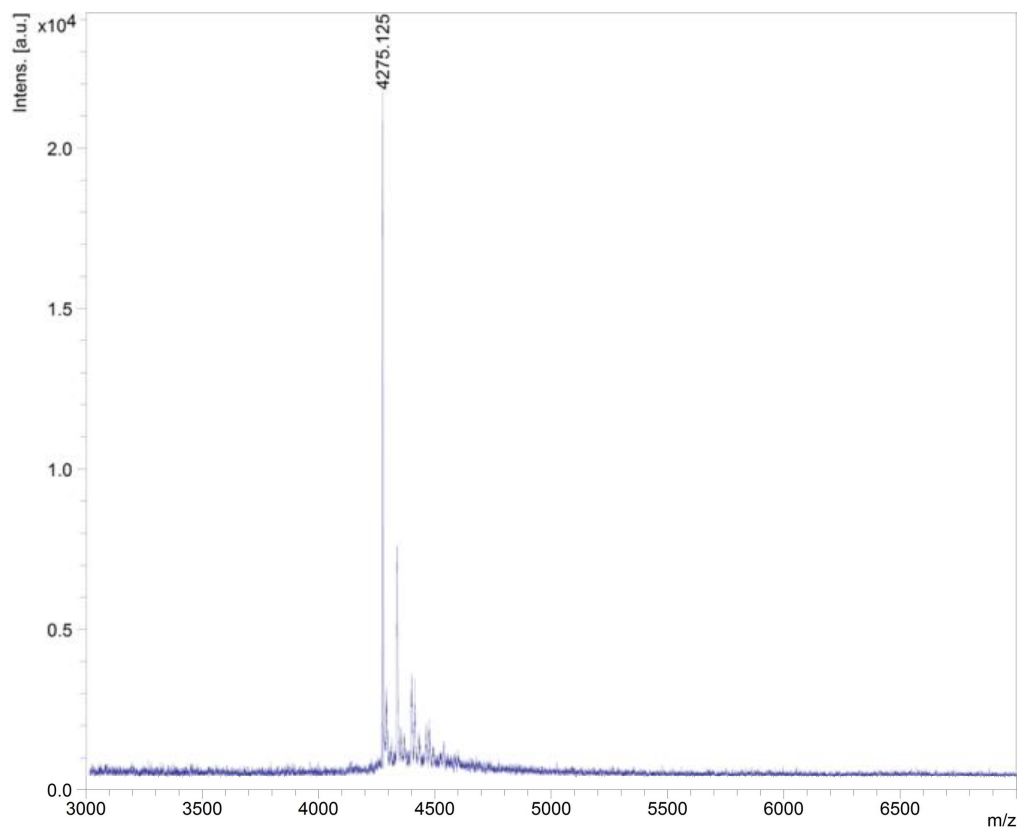
UD-22

[B conc. MeCN: 7-40% (30 min)]

mV



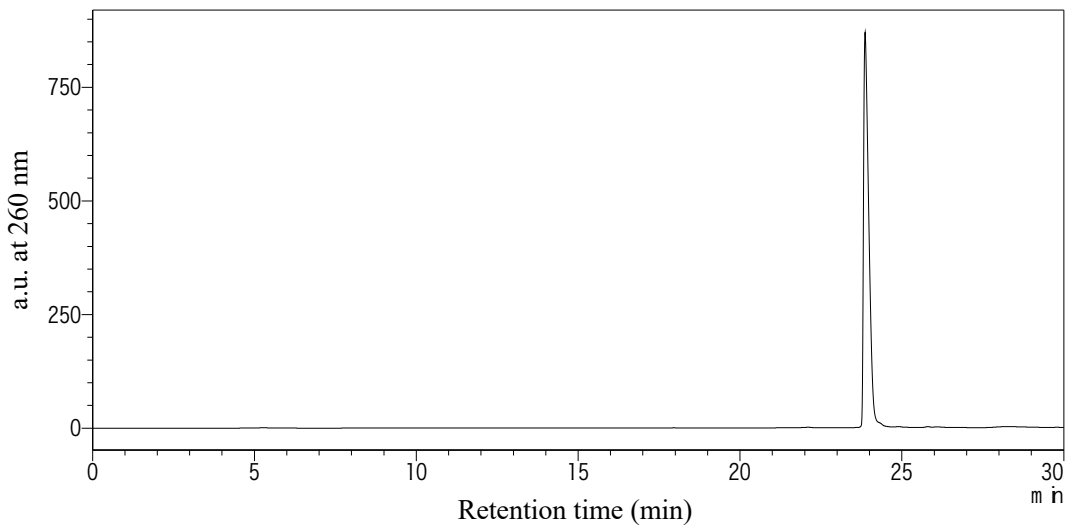
[calcd. (M-H)⁻: 4274.2, found: 4275.1]



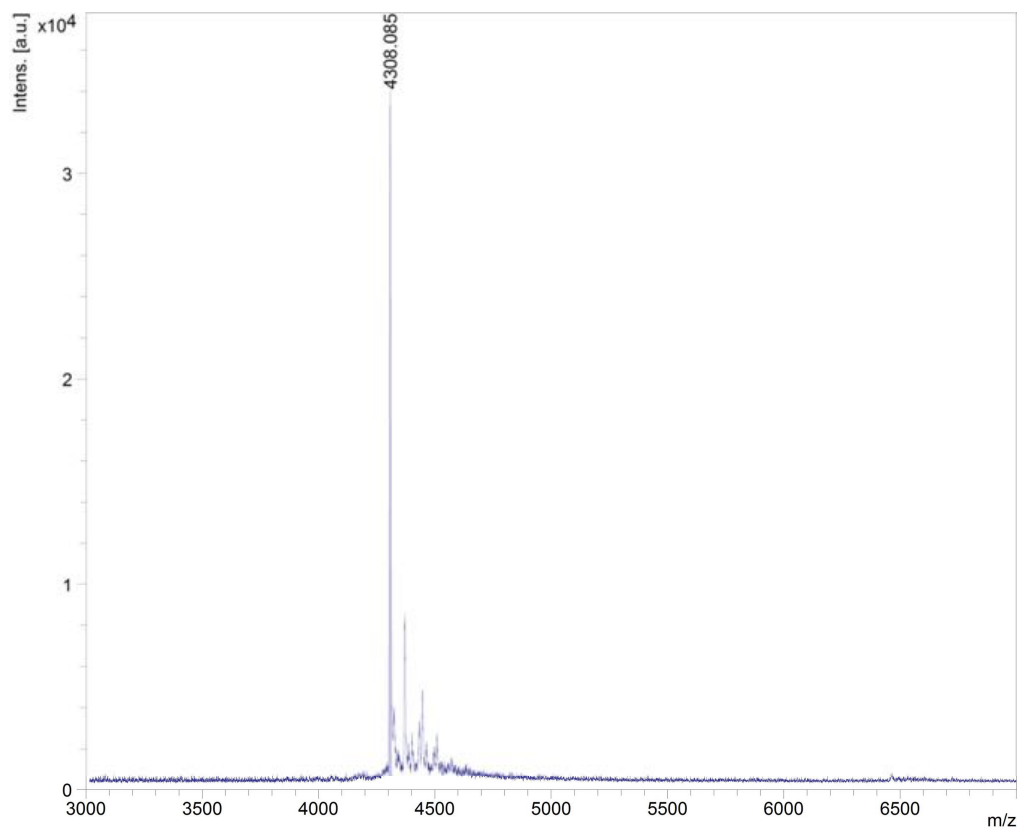
UD-23

[B conc. MeCN: 7-40% (30 min)]

mV



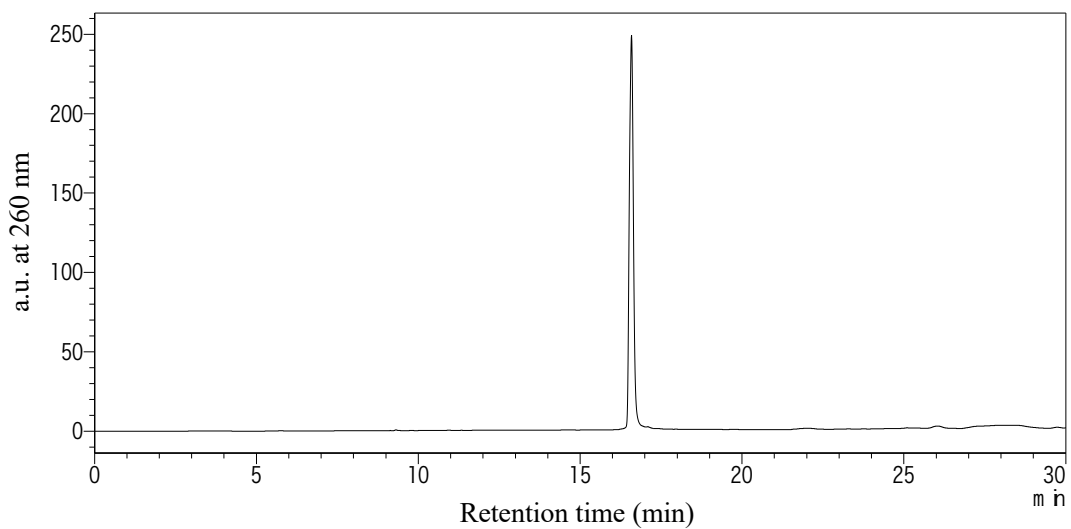
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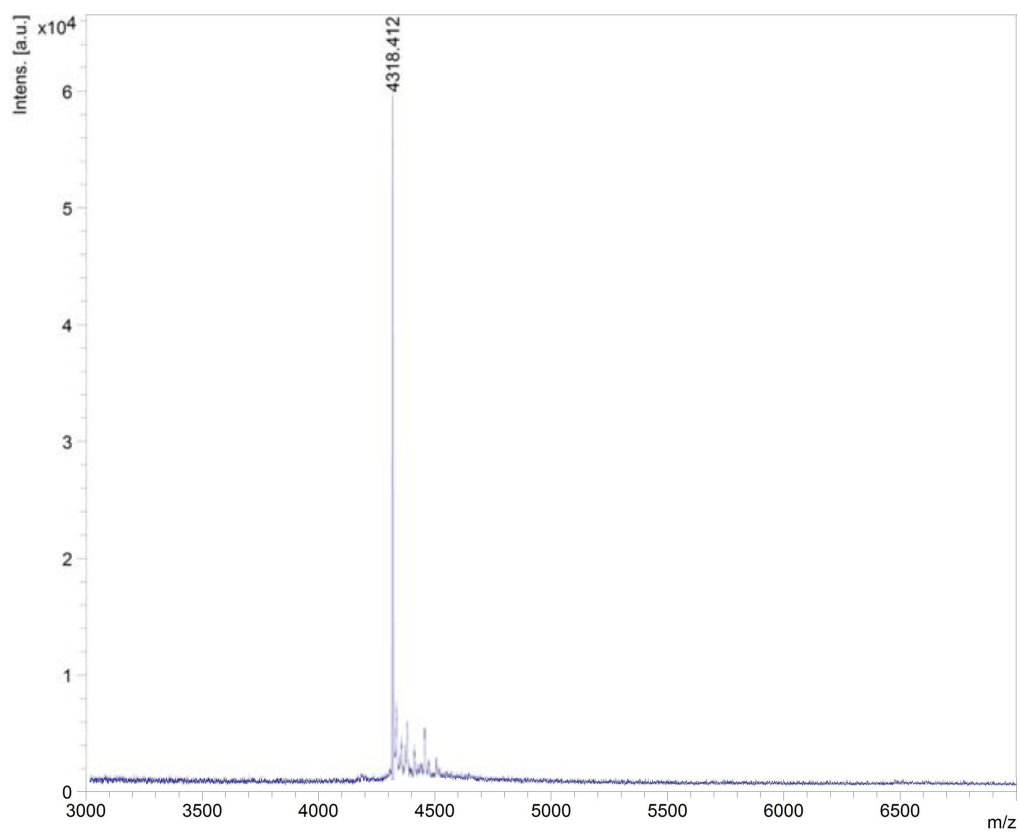
UD-24

[B conc. MeCN: 7-40% (30 min)]

mV



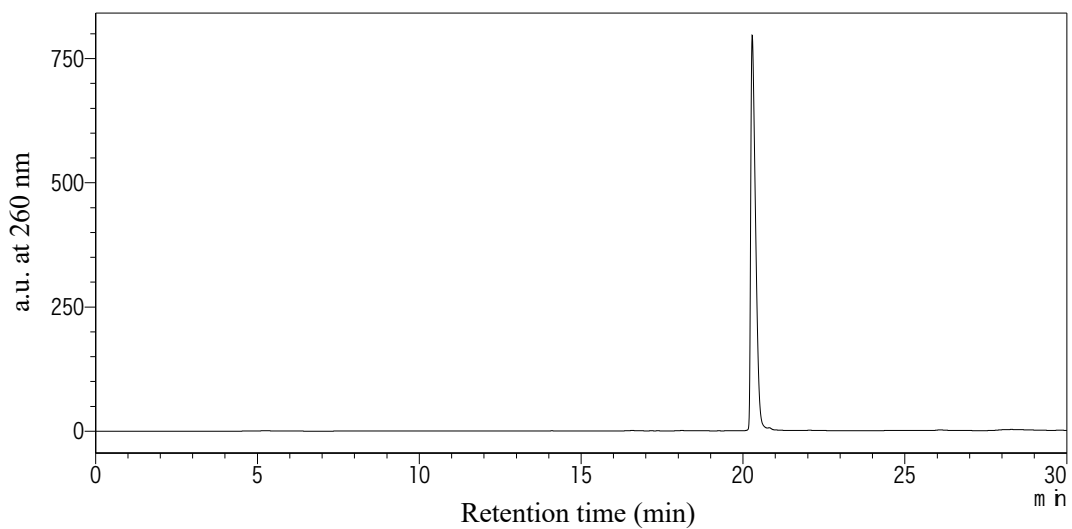
[calcd. (M-H)⁻: 4317.2, found: 4318.4]



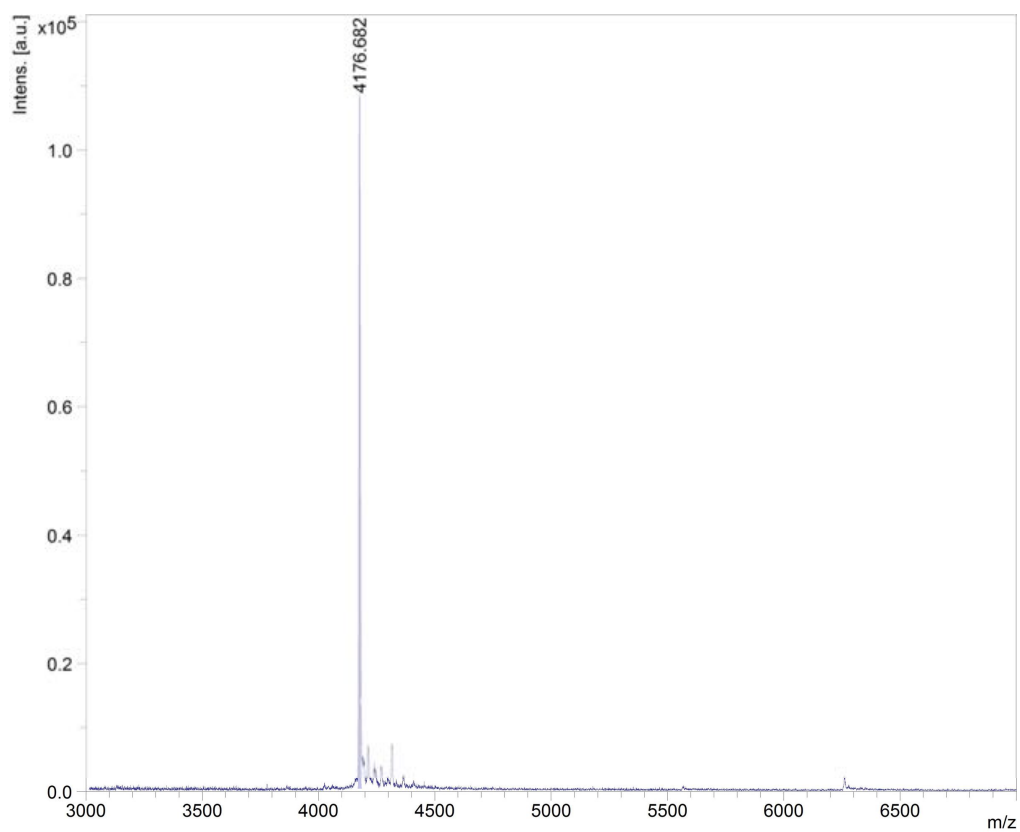
UD-27

[B conc. MeCN: 7-40% (30 min)]

mV



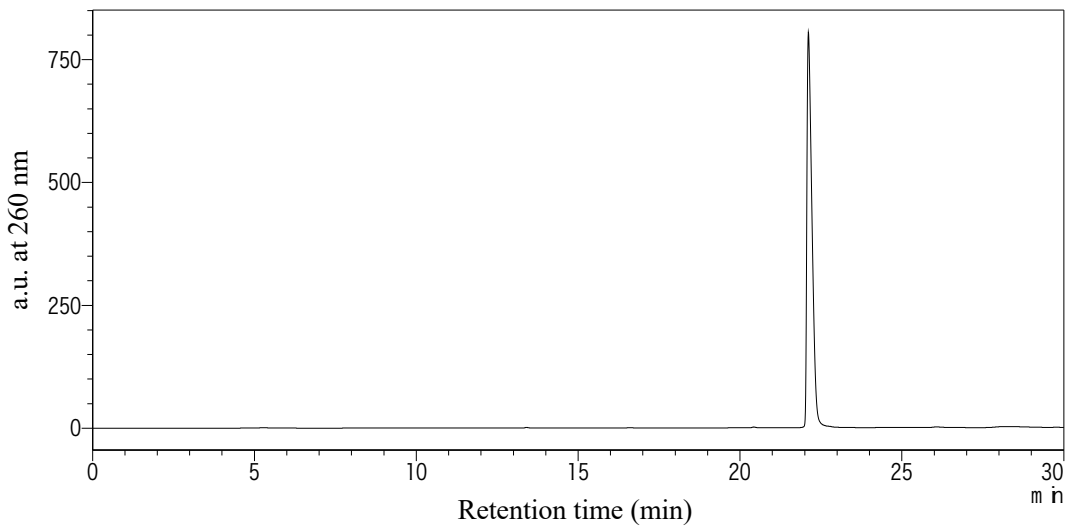
[calcd. (M-H)⁻: 4176.1, found: 4176.7]



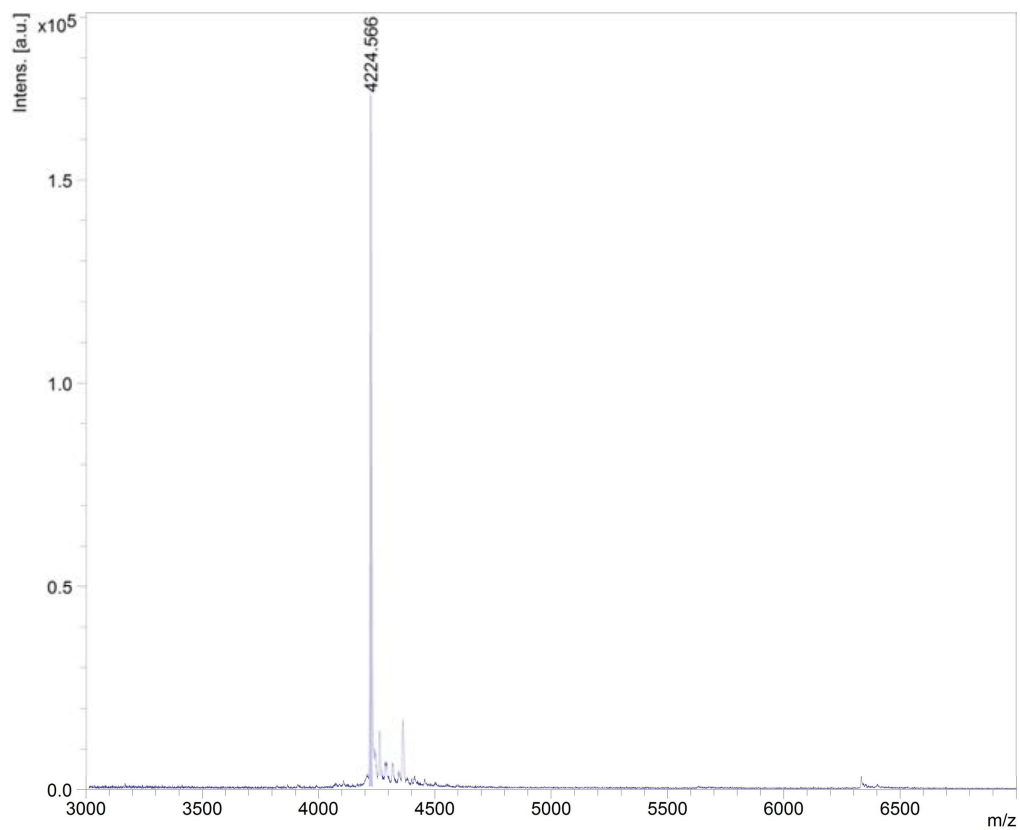
UD-28

[B conc. MeCN: 7-40% (30 min)]

mV



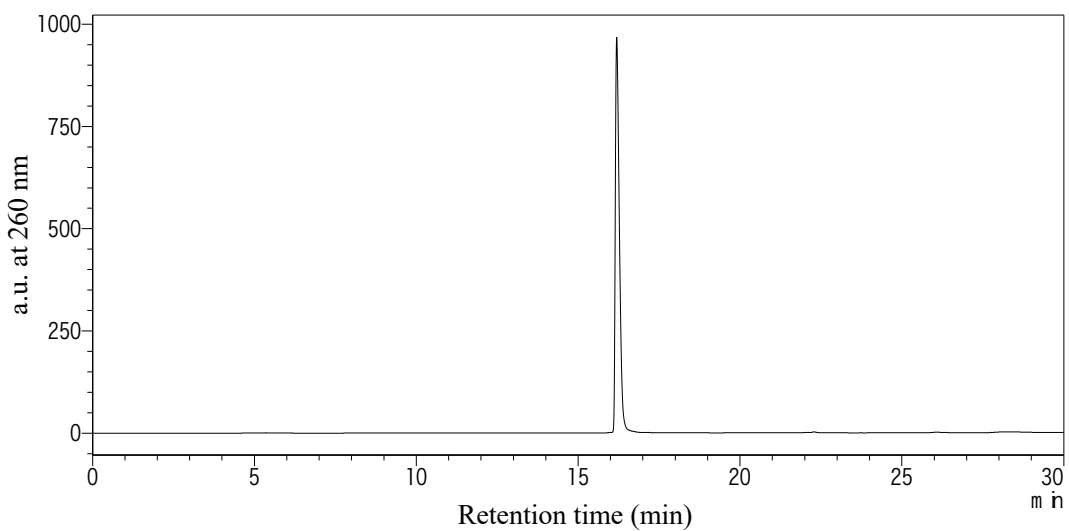
[calcd. (M-H)⁻: 4224.1, found: 4224.6]



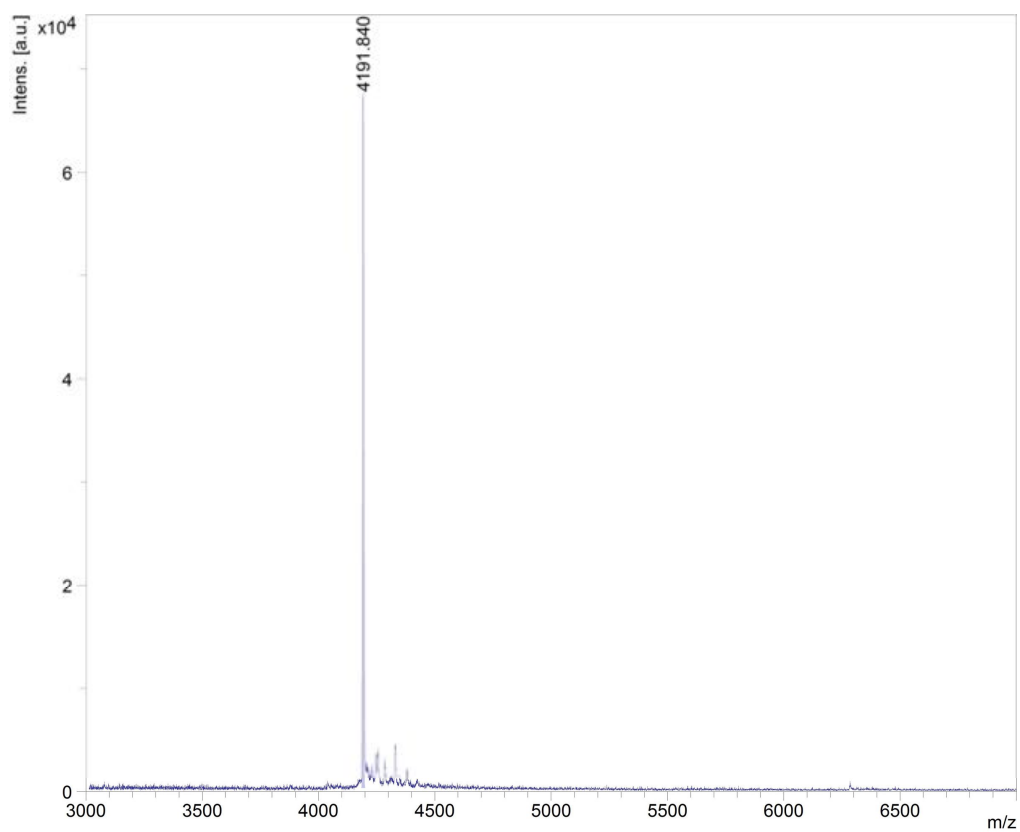
UD-29

[B conc. MeCN: 7-40% (30 min)]

mV



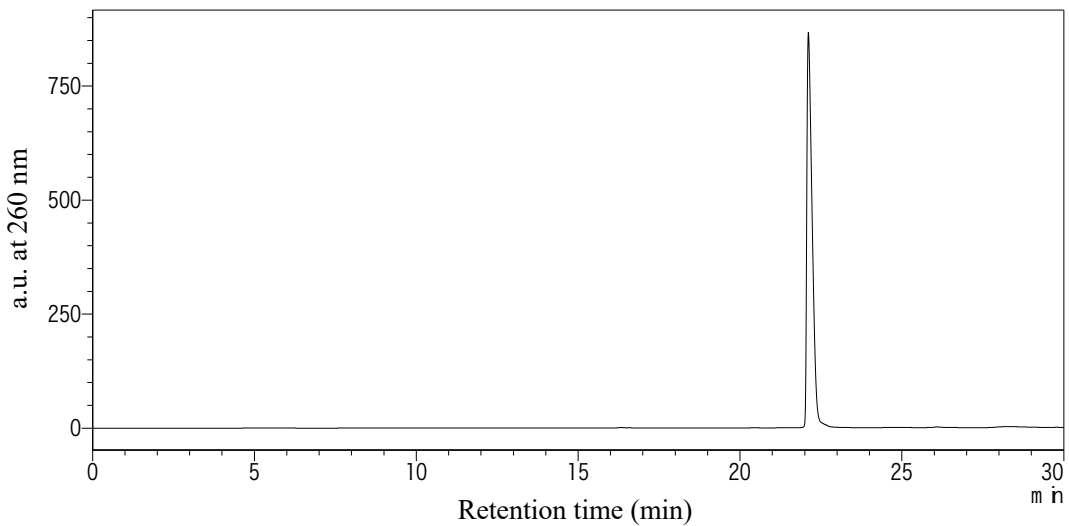
[calcd. (M-H)⁻: 4192.1, found: 4191.8]



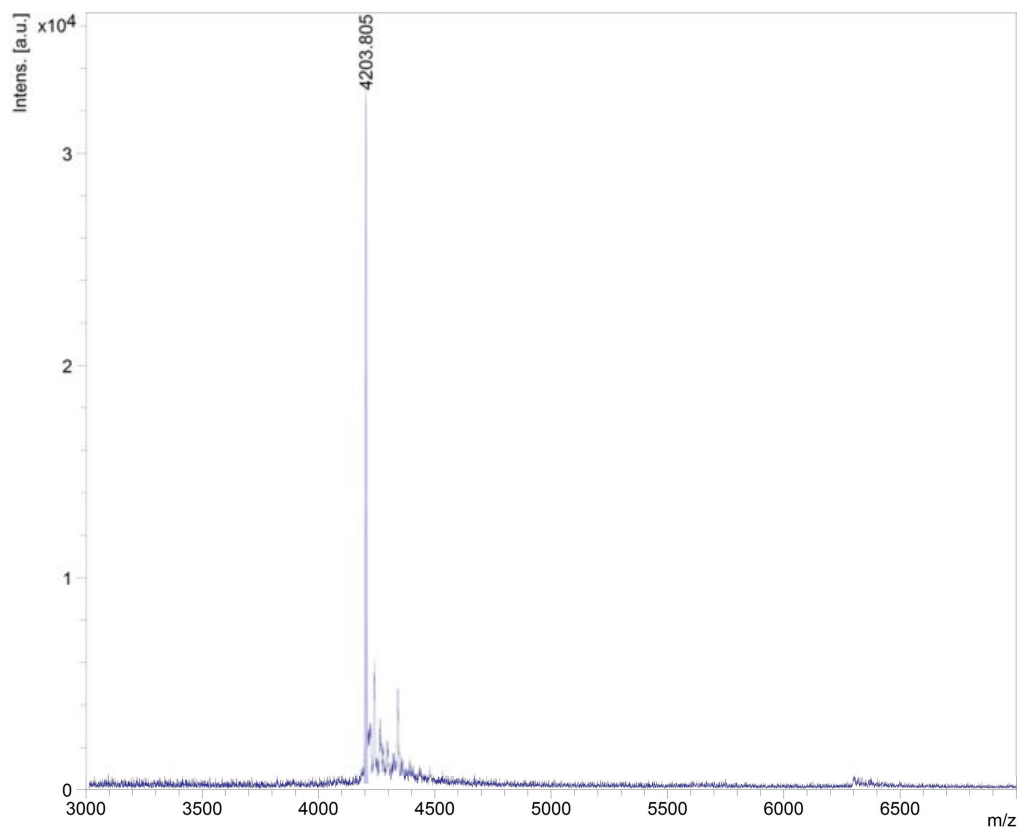
UD-30

[B conc. MeCN: 7-40% (30 min)]

mV



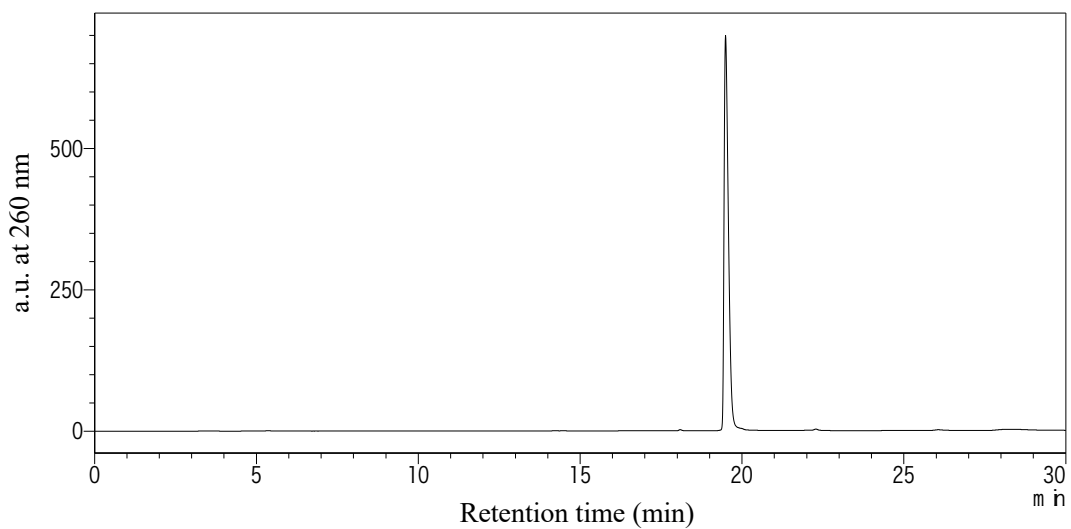
[calcd. (M-H)⁻: 4202.1, found: 4203.8]



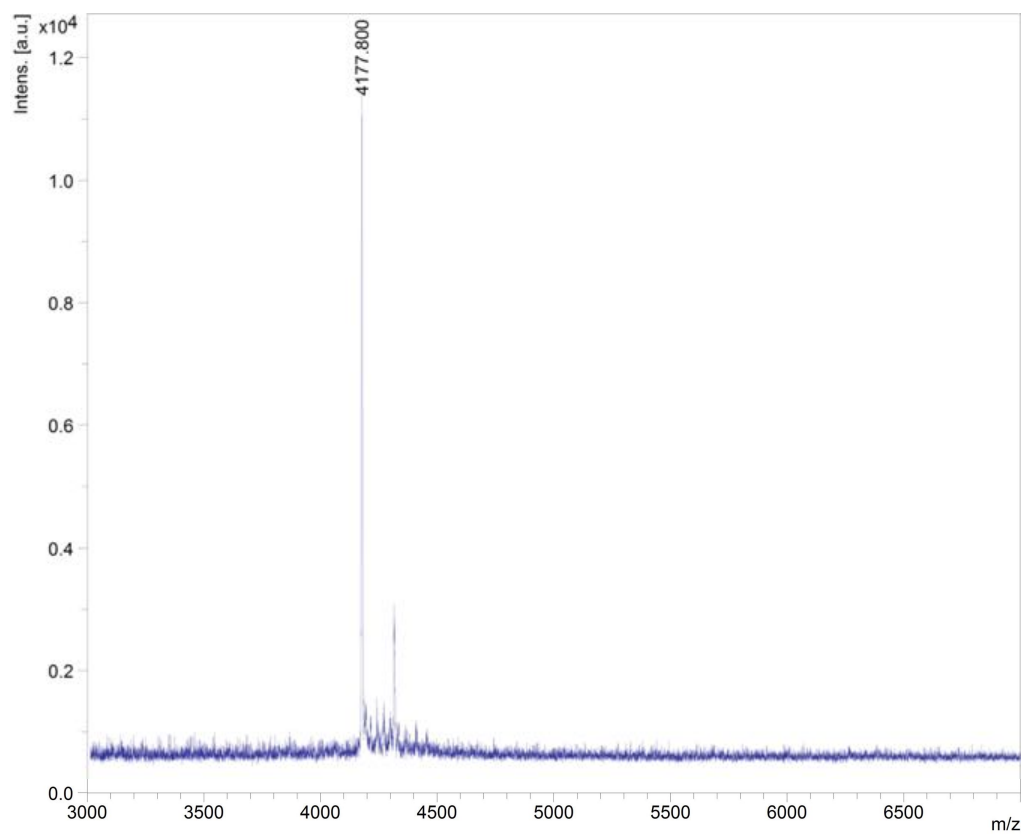
UD-31

[B conc. MeCN: 7-40% (30 min)]

mV



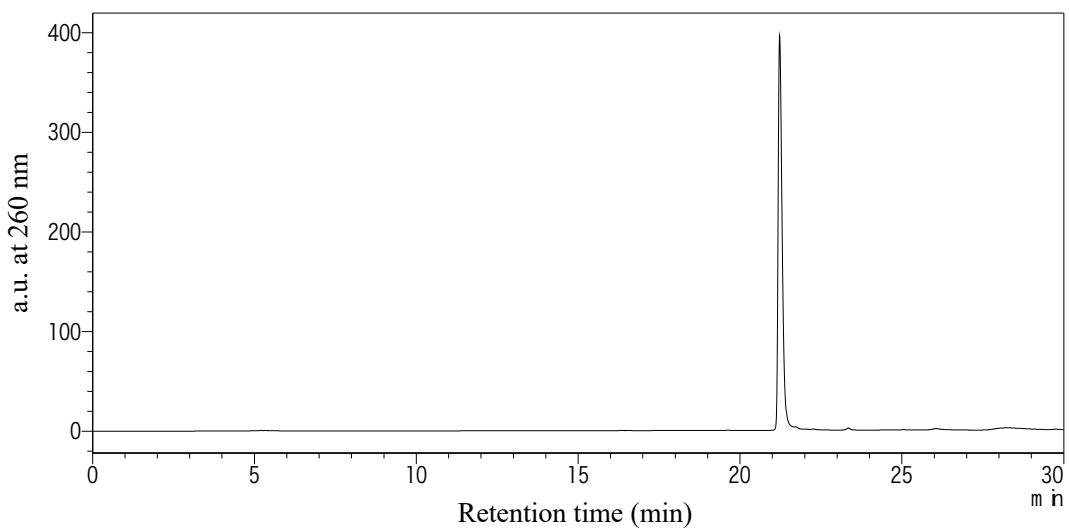
[calcd. (M-H)⁻: 4176.1, found: 4177.8]



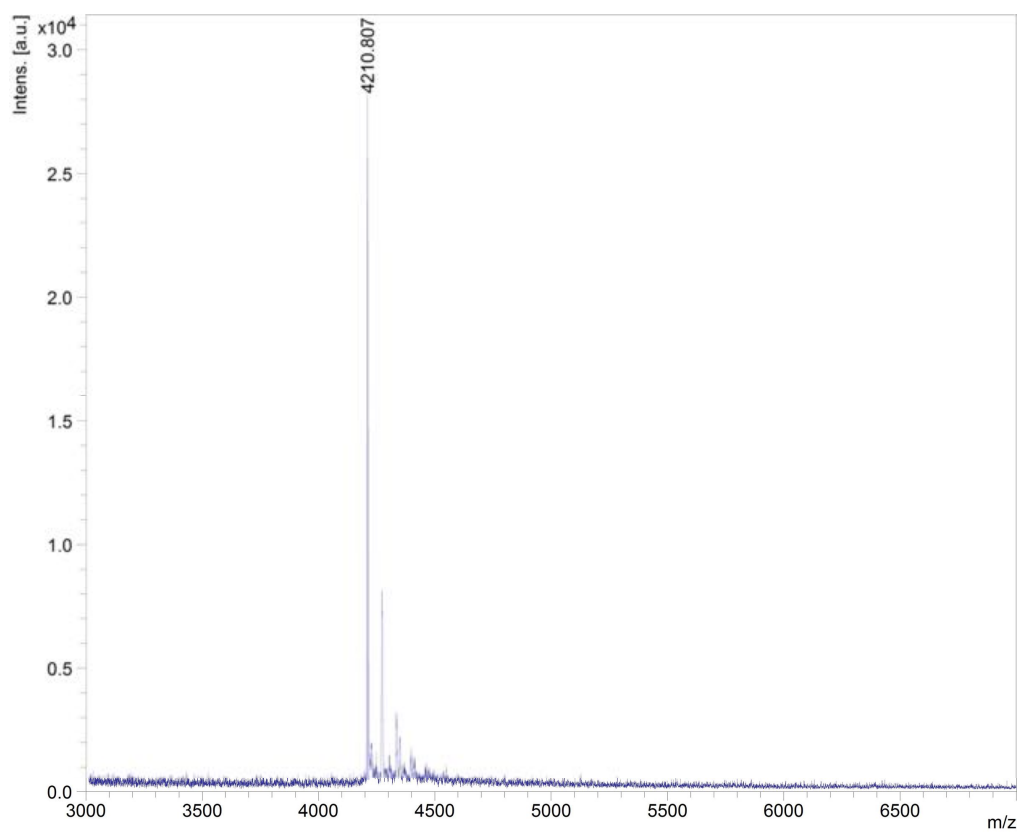
UD-32

[B conc. MeCN: 7-40% (30 min)]

mV



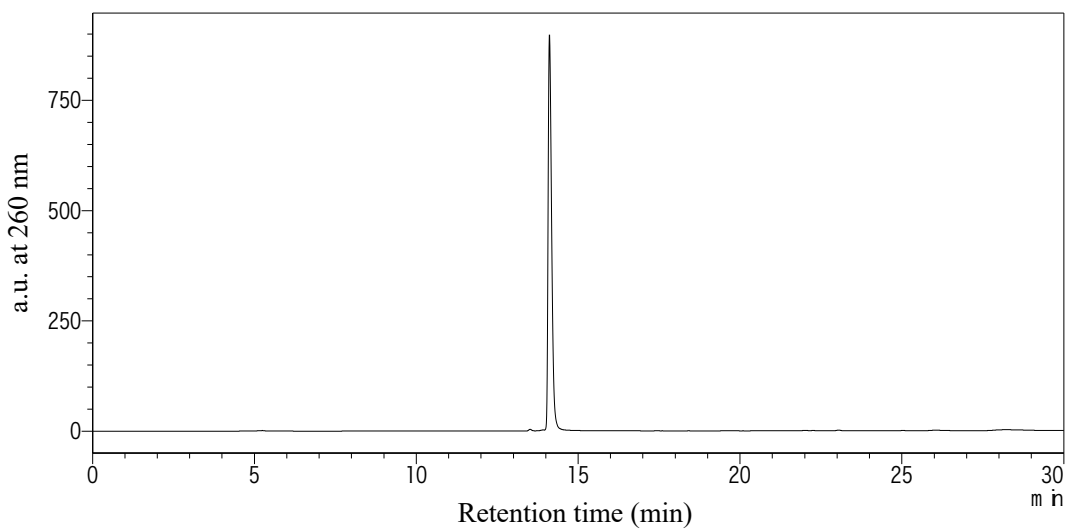
[calcd. (M-H)⁻: 4210.1, found: 4210.8]



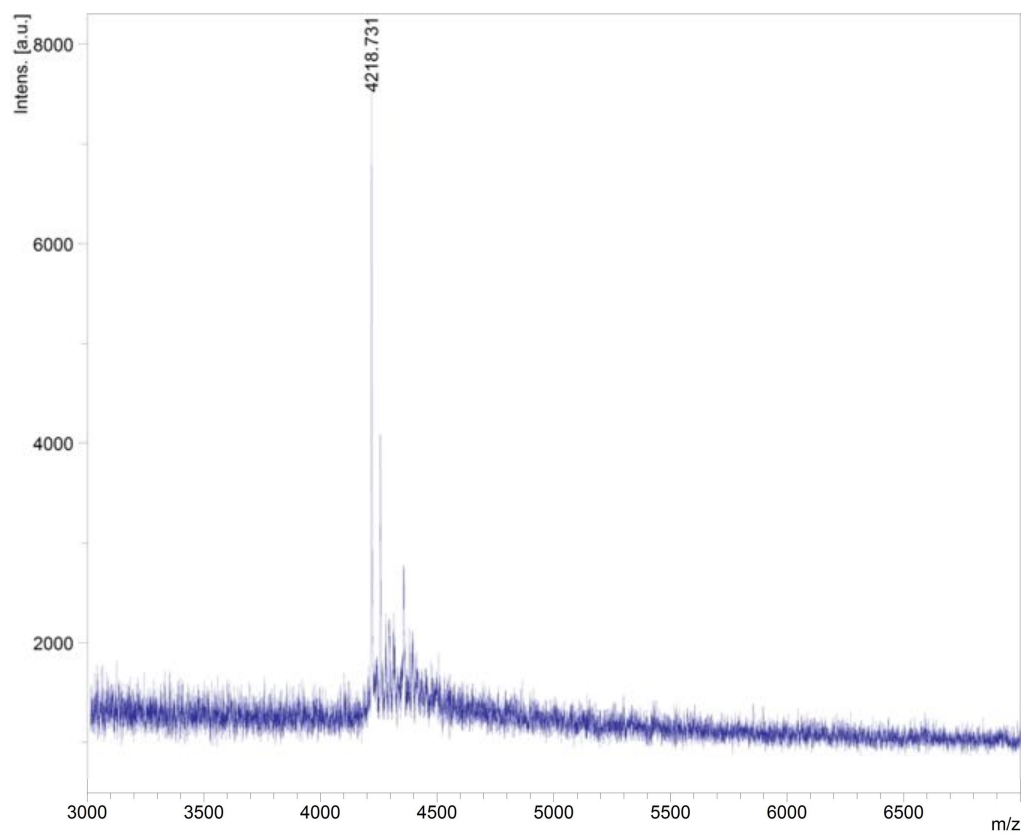
UD-33

[B conc. MeCN: 7-40% (30 min)]

mV



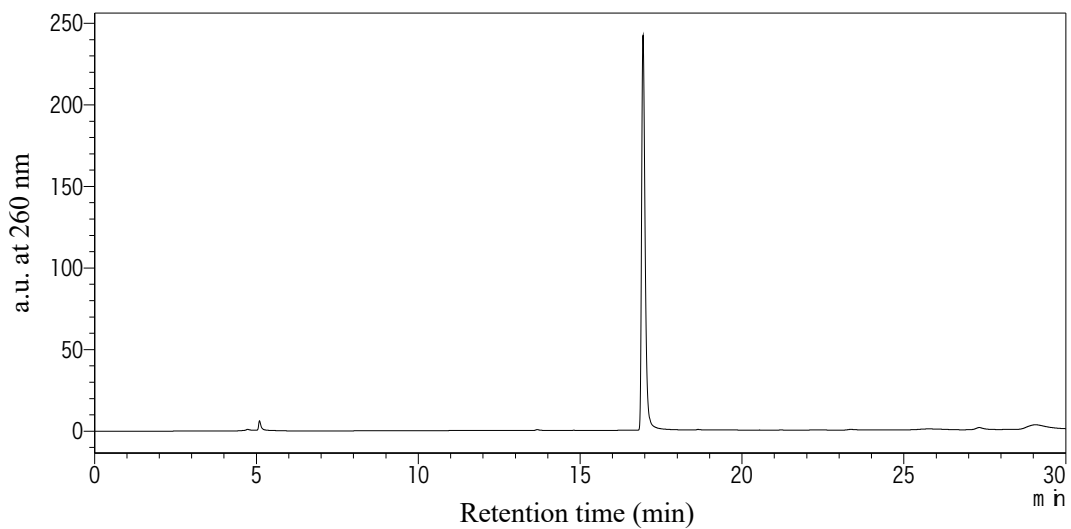
[calcd. (M-H)⁻: 4219.2, found: 4218.7]



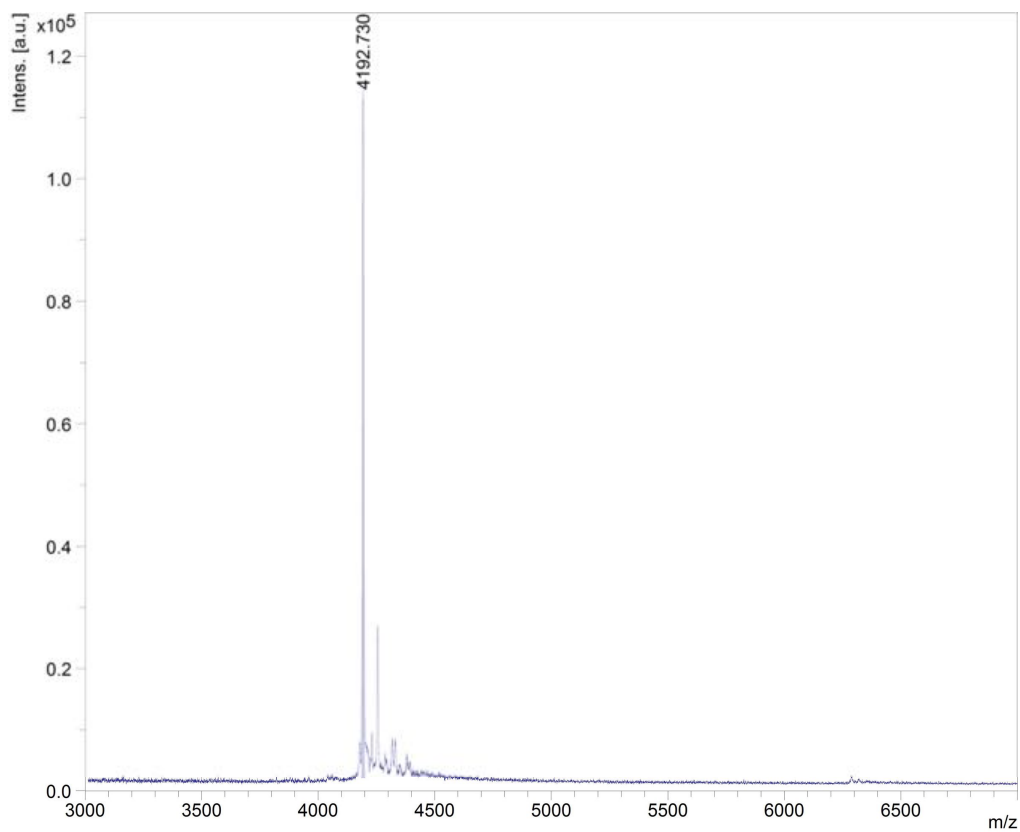
UD-34

[B conc. MeCN: 7-40% (30 min)]

mV



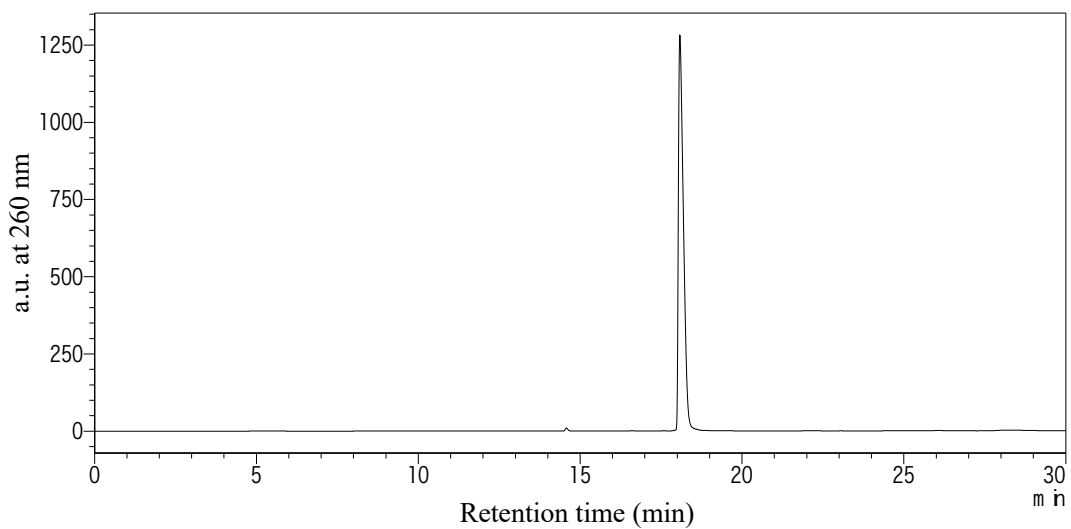
[calcd. (M-H)⁻: 4192.1, found: 4192.7]



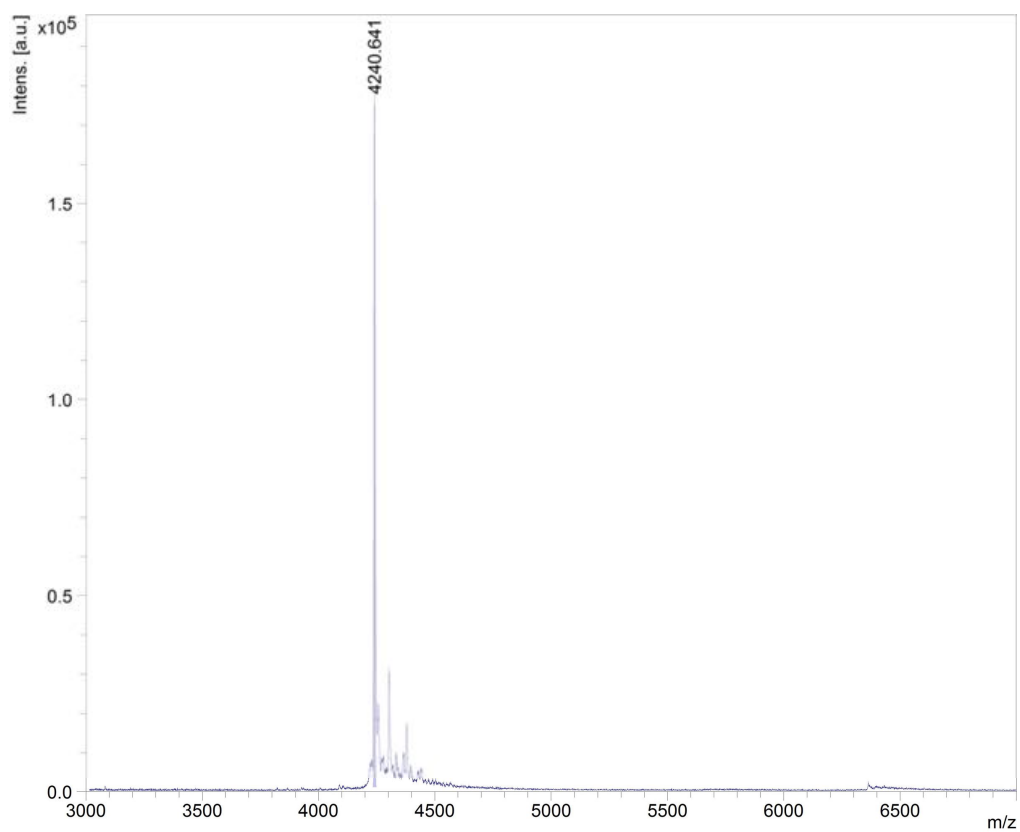
UD-35

[B conc. MeCN: 7-40% (30 min)]

mV



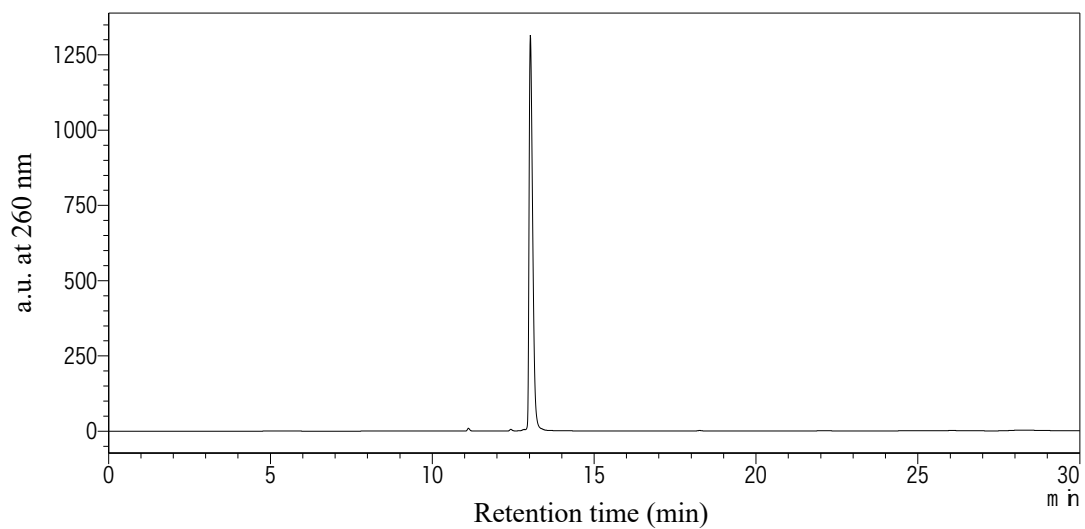
[calcd. (M-H)⁻: 4240.1, found: 4240.6]



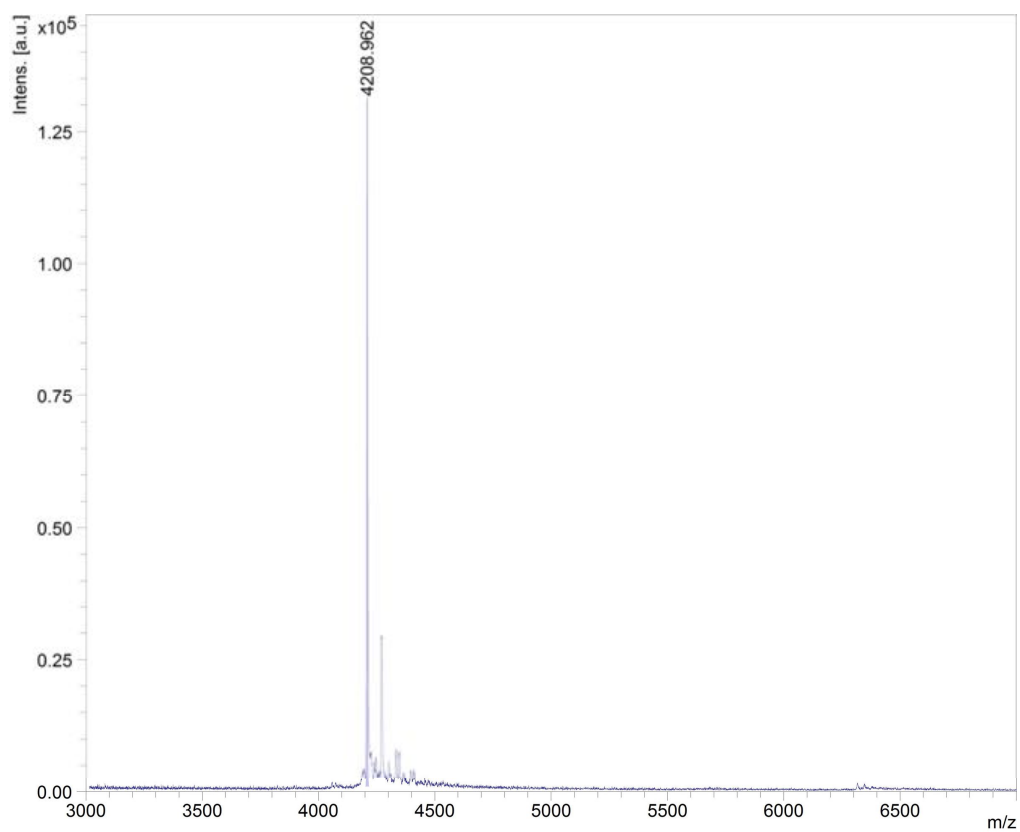
UD-36

[B conc. MeCN: 7-40% (30 min)]

mV



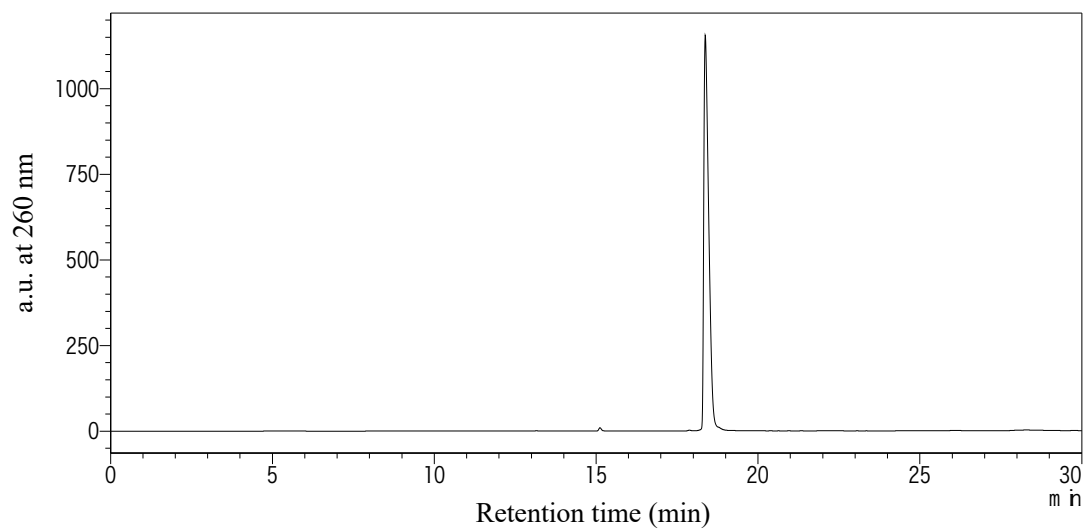
[calcd. (M-H)⁻: 4208.1, found: 4209.0]



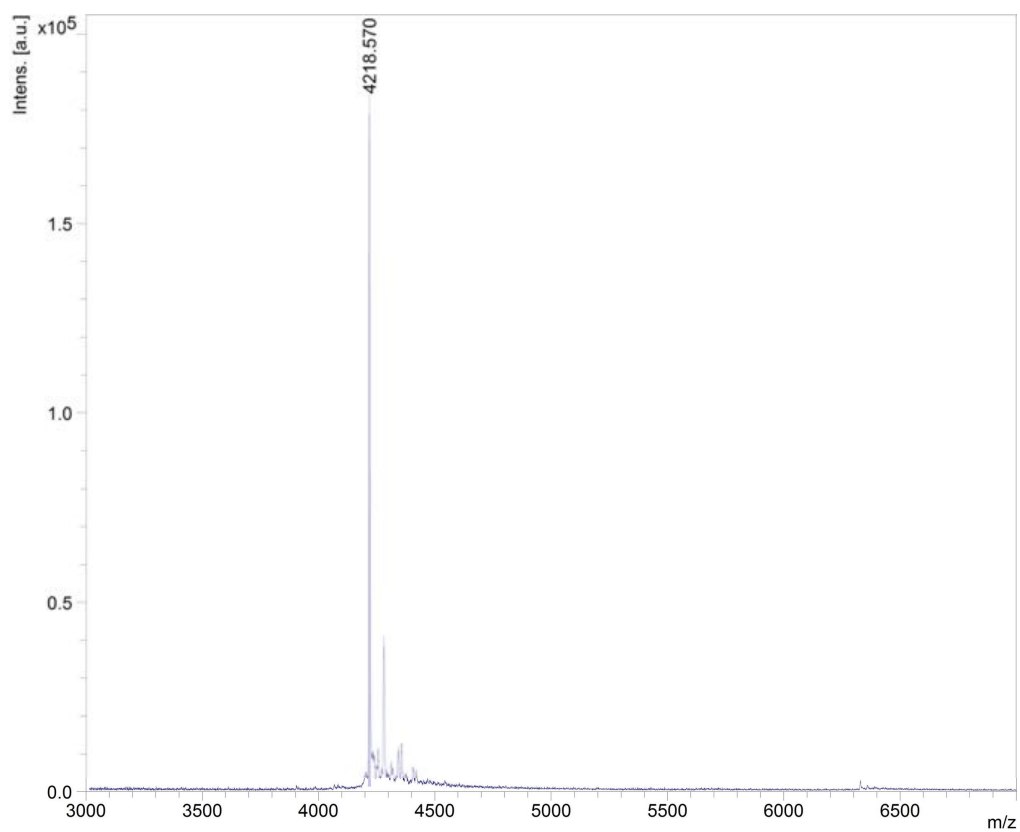
UD-37

[B conc. MeCN: 7-40% (30 min)]

mV



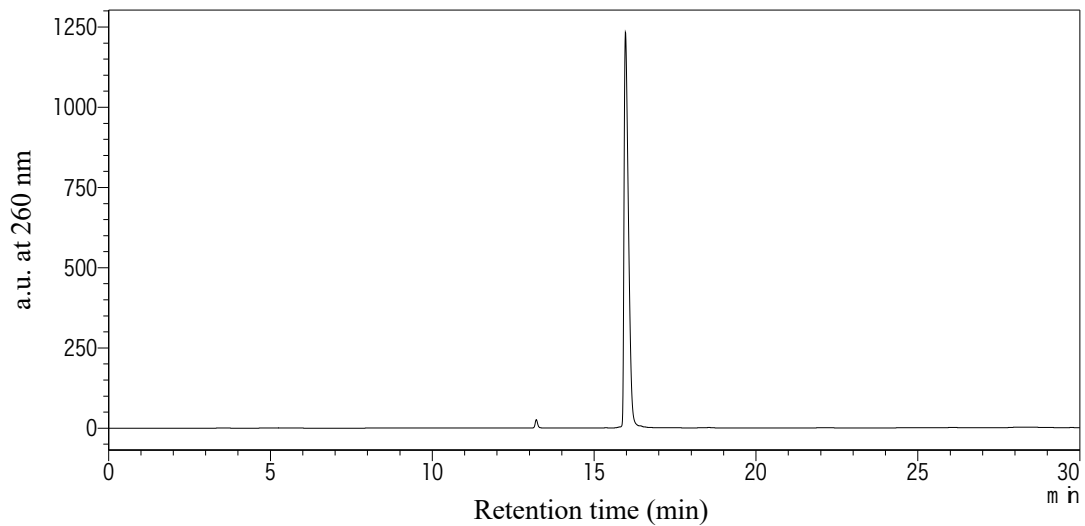
[calcd. (M-H)⁻: 4218.1, found: 4218.6]



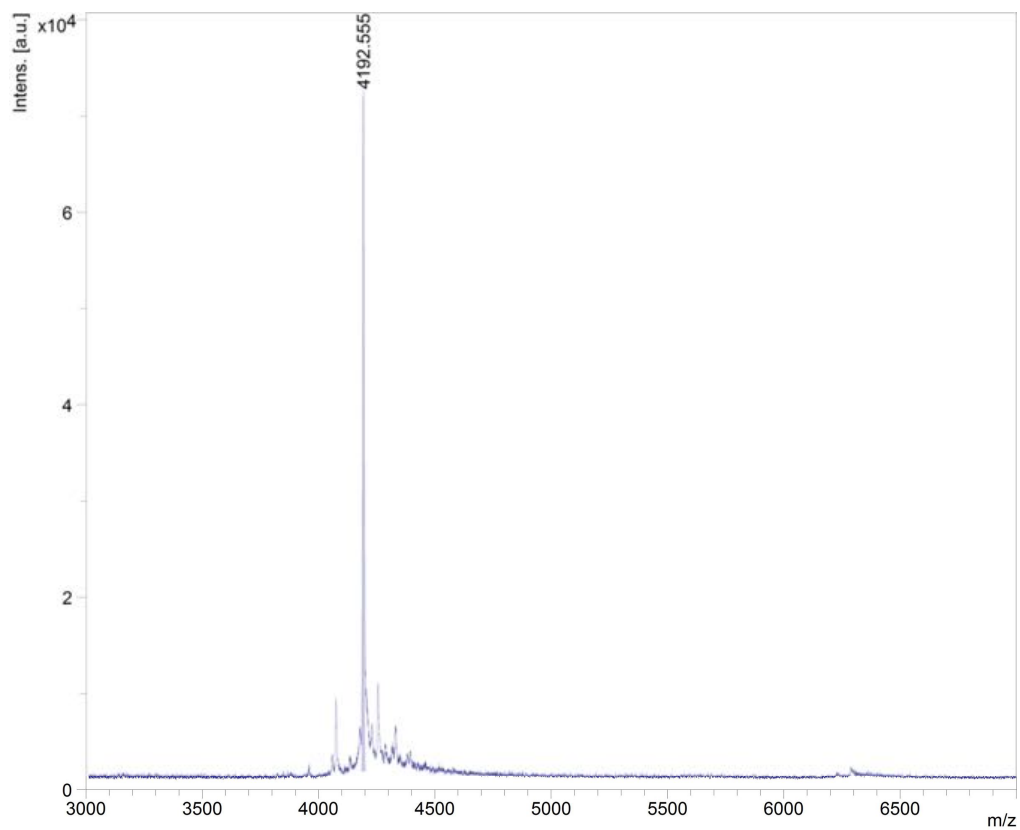
UD-38

[B conc. MeCN: 7-40% (30 min)]

mV



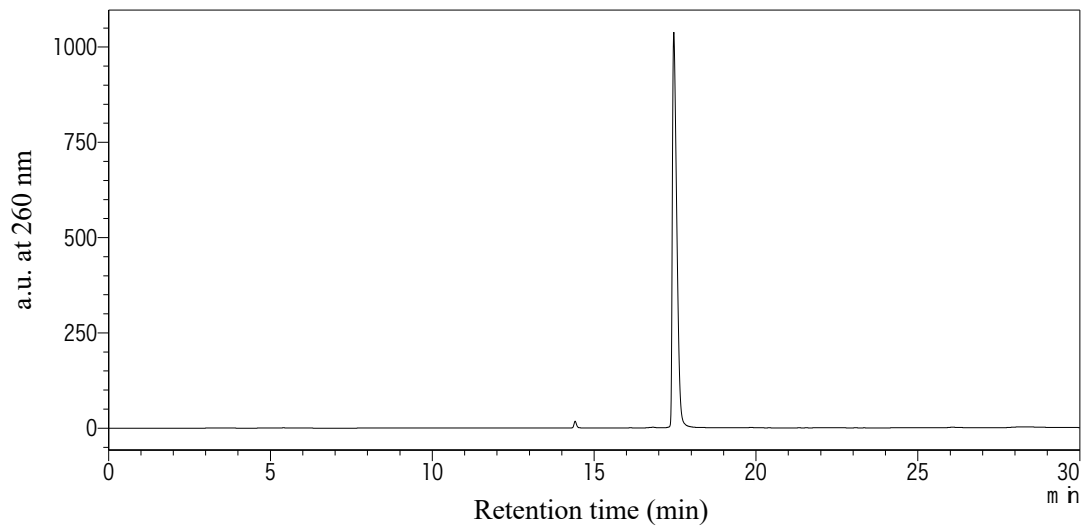
[calcd. (M-H)⁻: 4192.1, found: 4192.6]



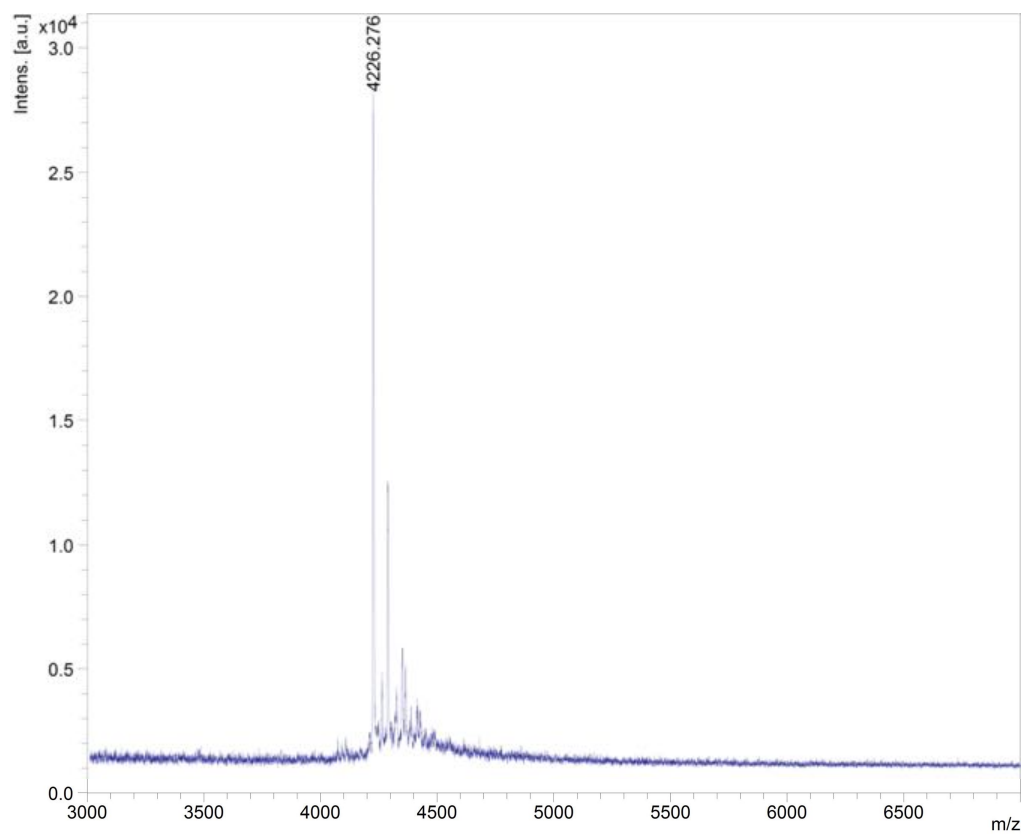
UD-39

[B conc. MeCN: 7-40% (30 min)]

mV



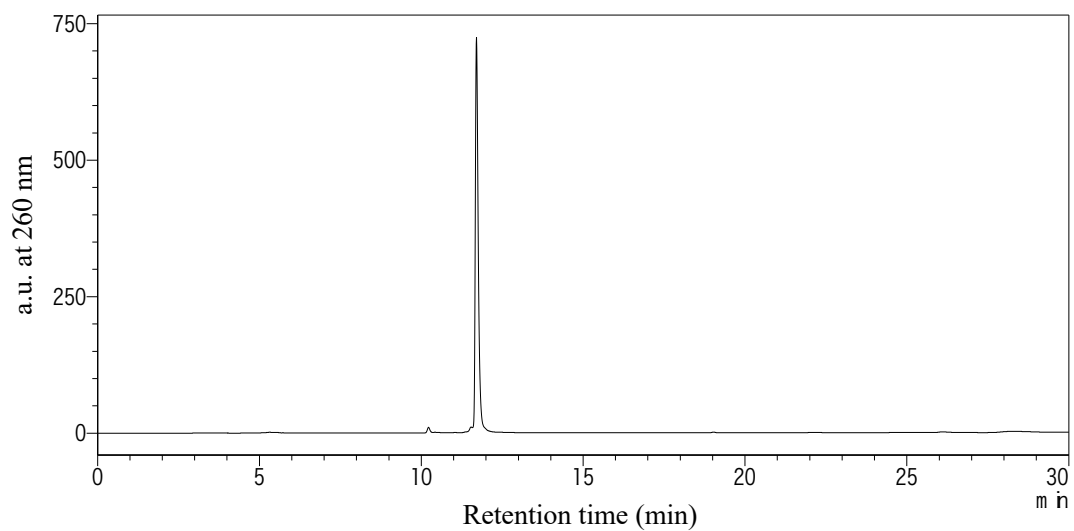
[calcd. (M-H)⁻: 4226.1, found: 4226.3]



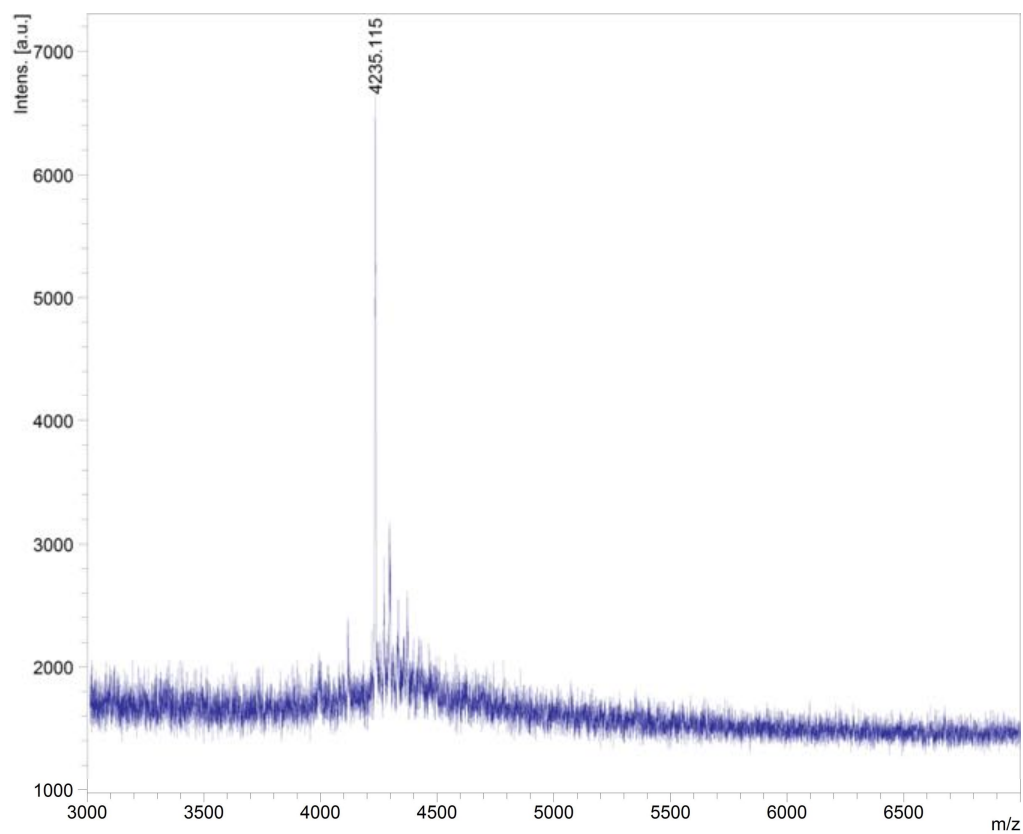
UD-40

[B conc. MeCN: 7-40% (30 min)]

mV



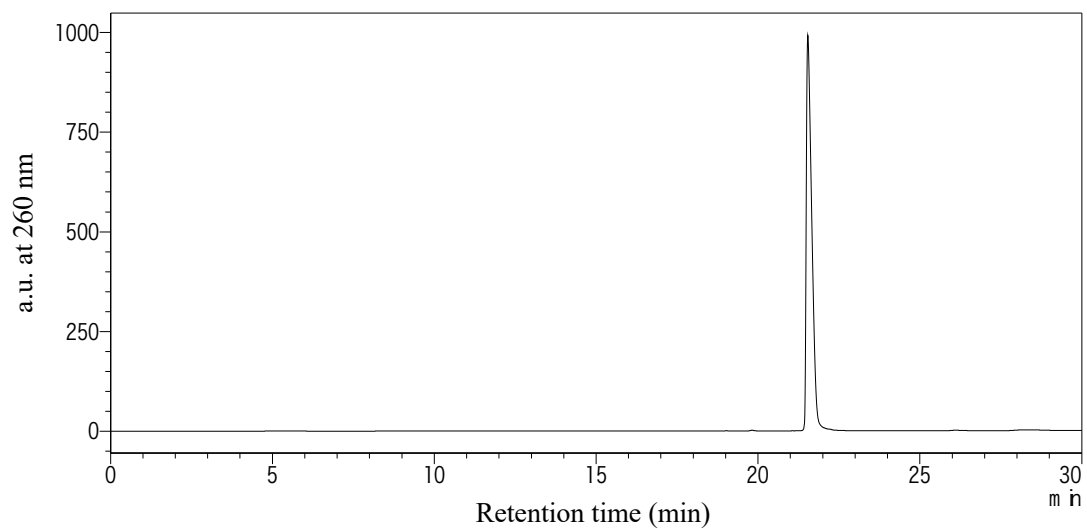
[calcd. (M-H)⁻: 4235.1, found: 4235.1]



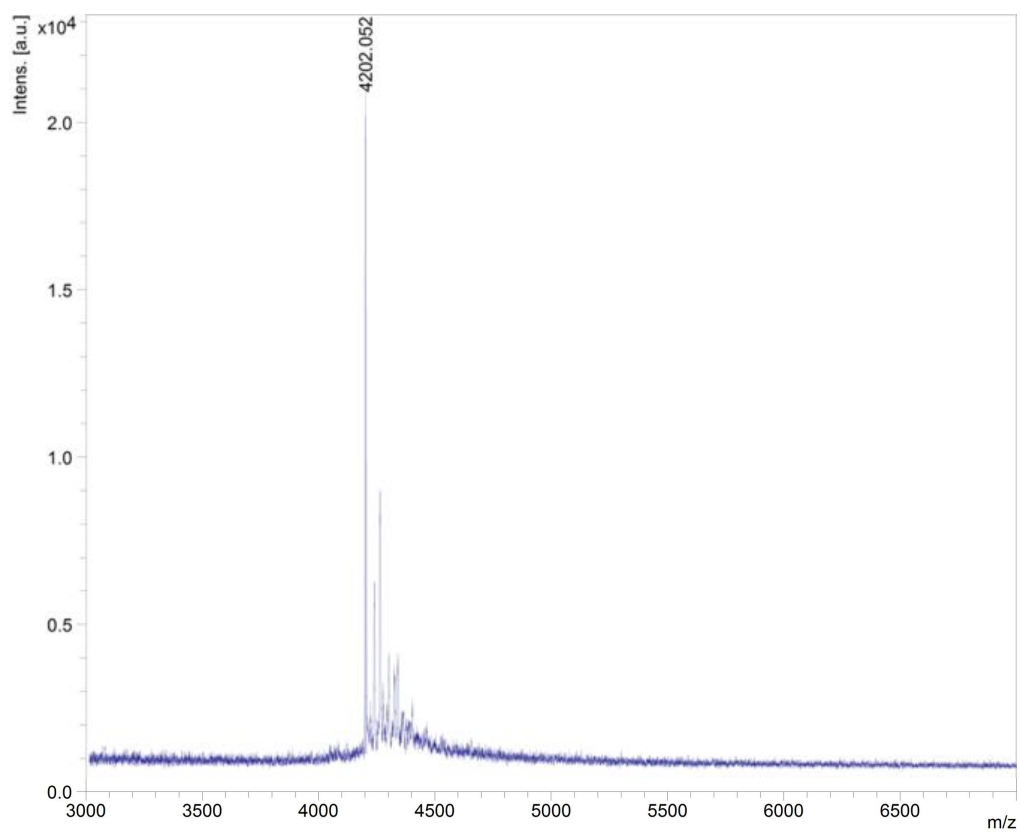
UD-41

[B conc. MeCN: 7-40% (30 min)]

mV



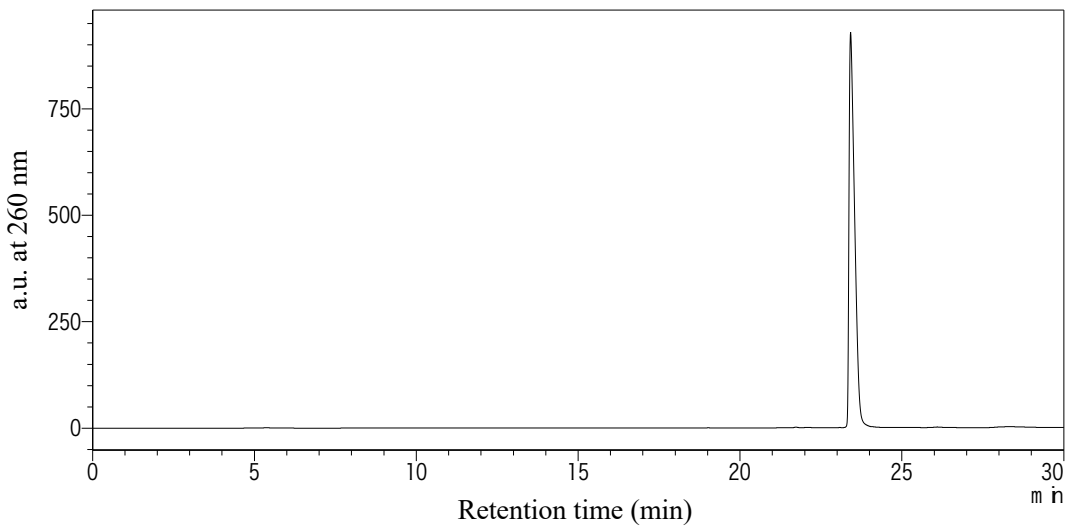
[calcd. (M-H)⁻: 4202.1, found: 4202.1]



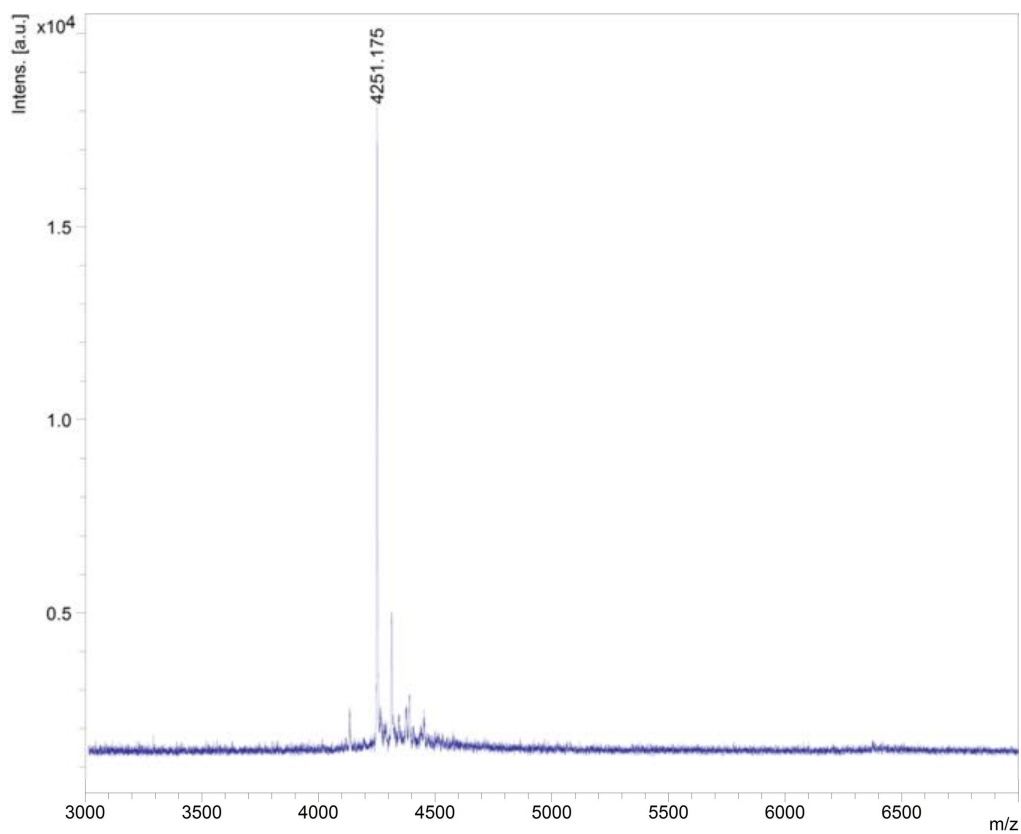
UD-42

[B conc. MeCN: 7-40% (30 min)]

mV



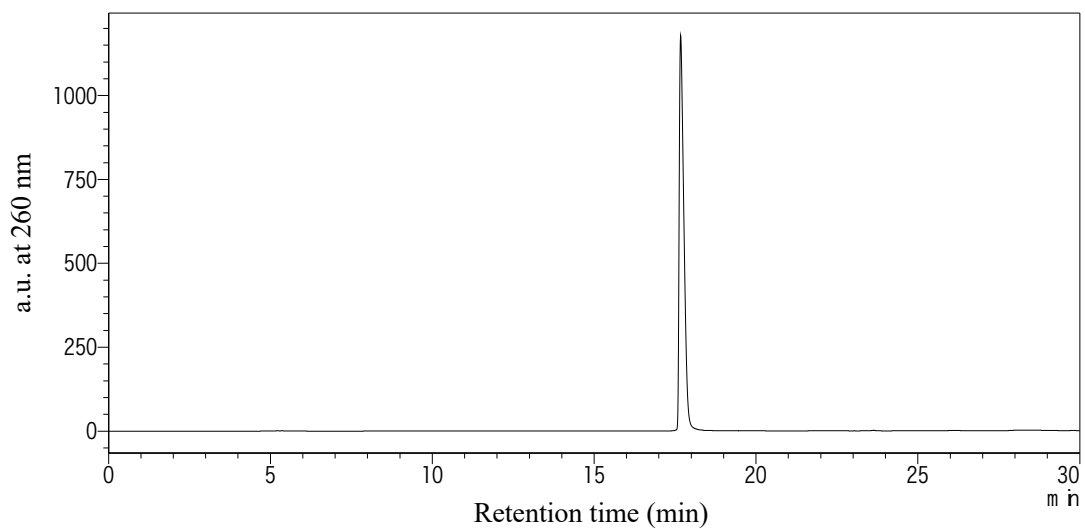
[calcd. (M-H)⁻: 4250.2, found: 4251.2]



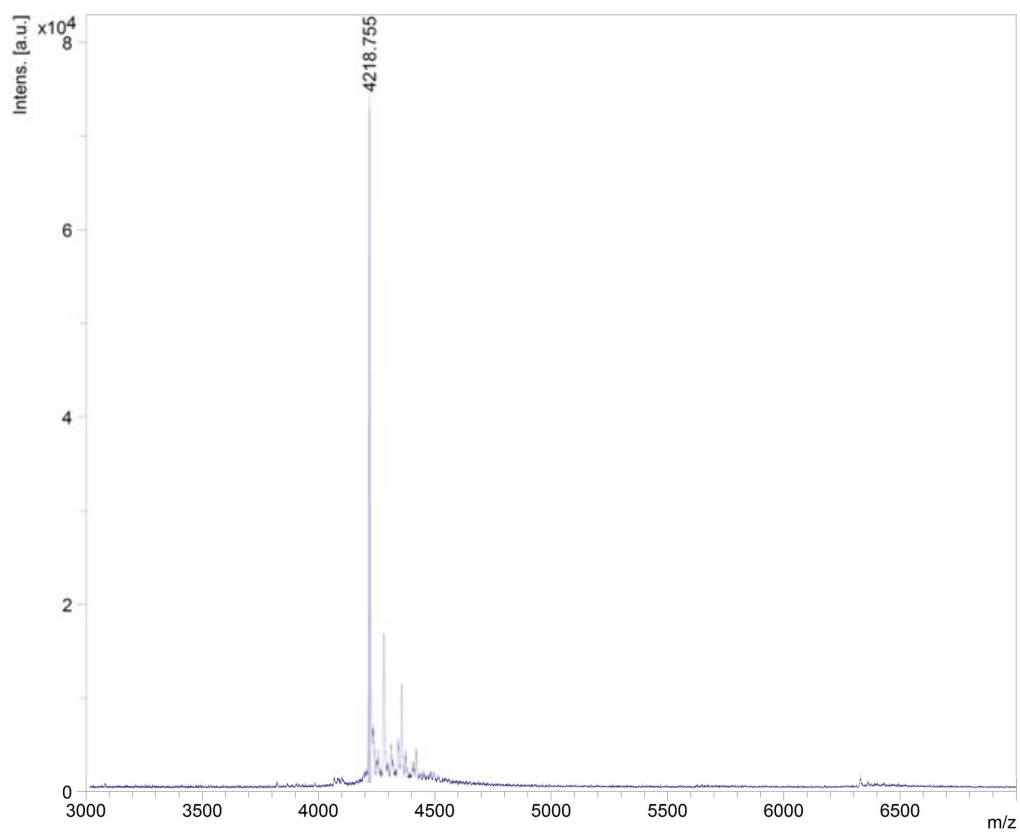
UD-43

[B conc. MeCN: 7-40% (30 min)]

mV



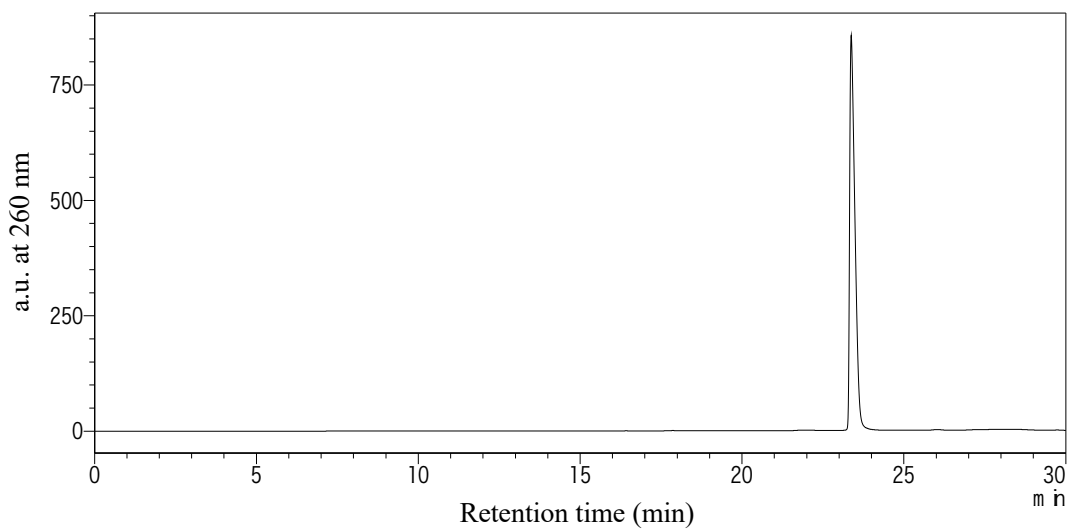
[calcd. (M-H)⁻: 4218.1, found: 4218.8]



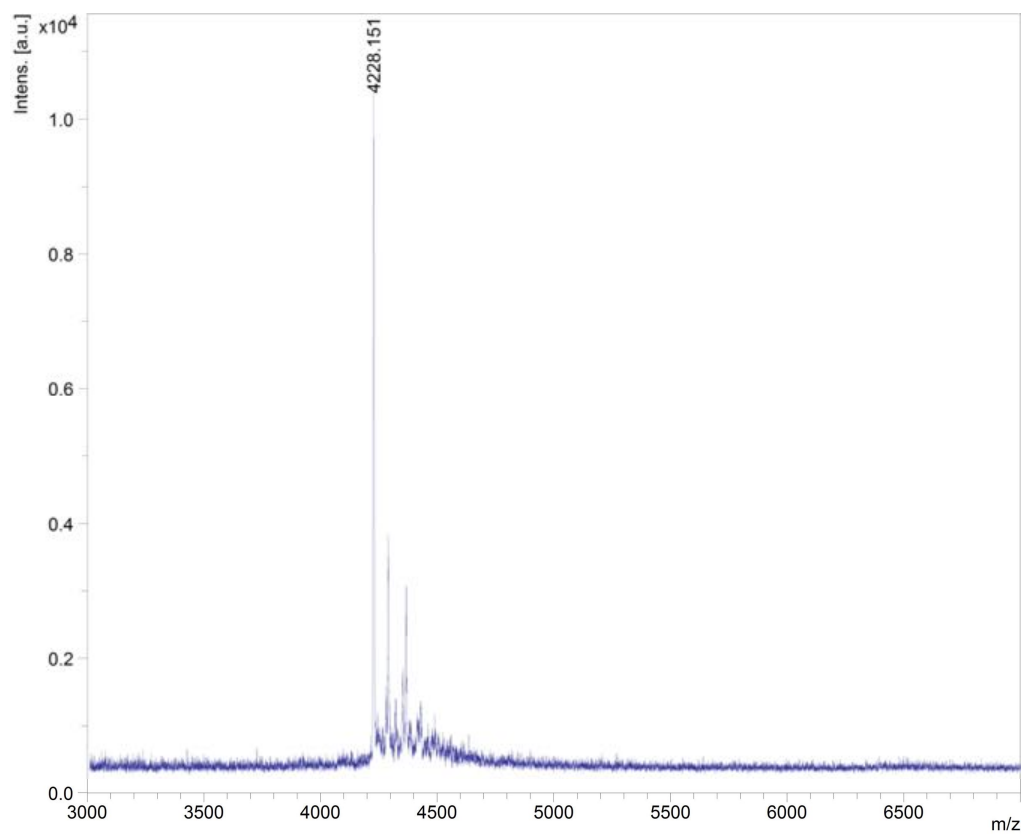
UD-44

[B conc. MeCN: 7-40% (30 min)]

mV



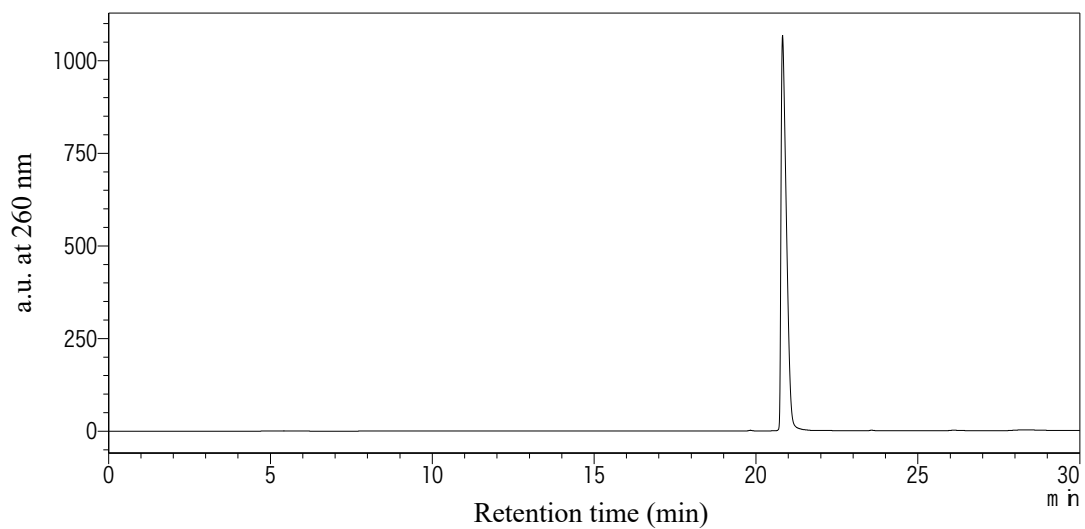
[calcd. (M-H)⁻: 4228.2, found: 4228.2]



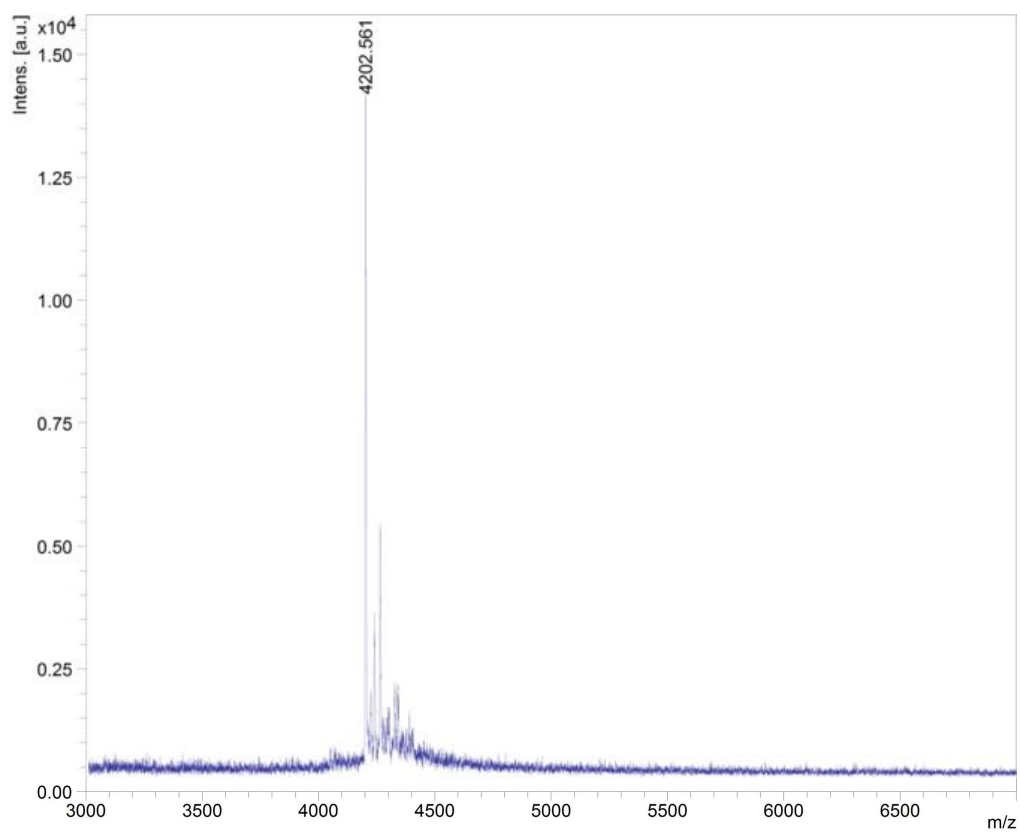
UD-45

[B conc. MeCN: 7-40% (30 min)]

mV



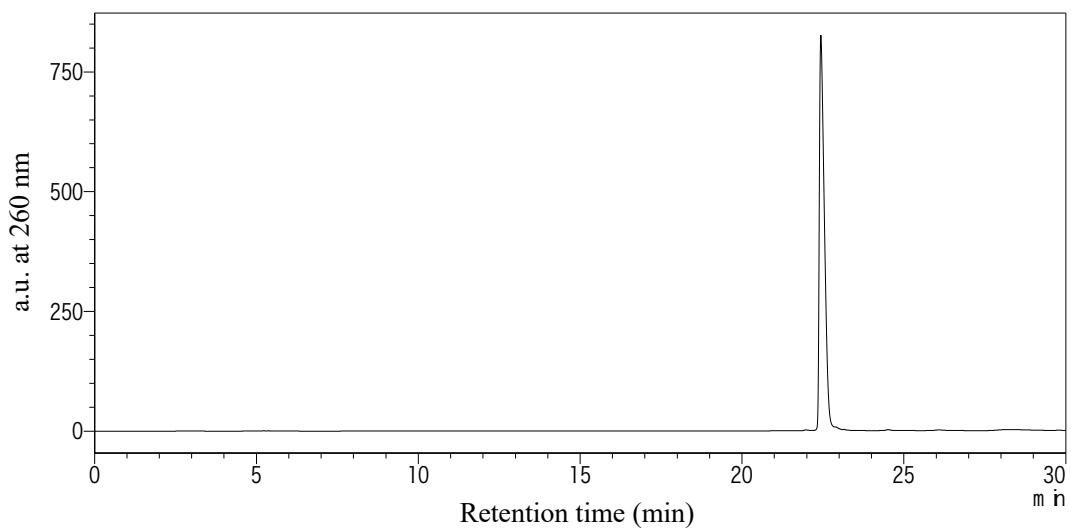
[calcd. (M-H)⁻: 4202.1, found: 4202.6]



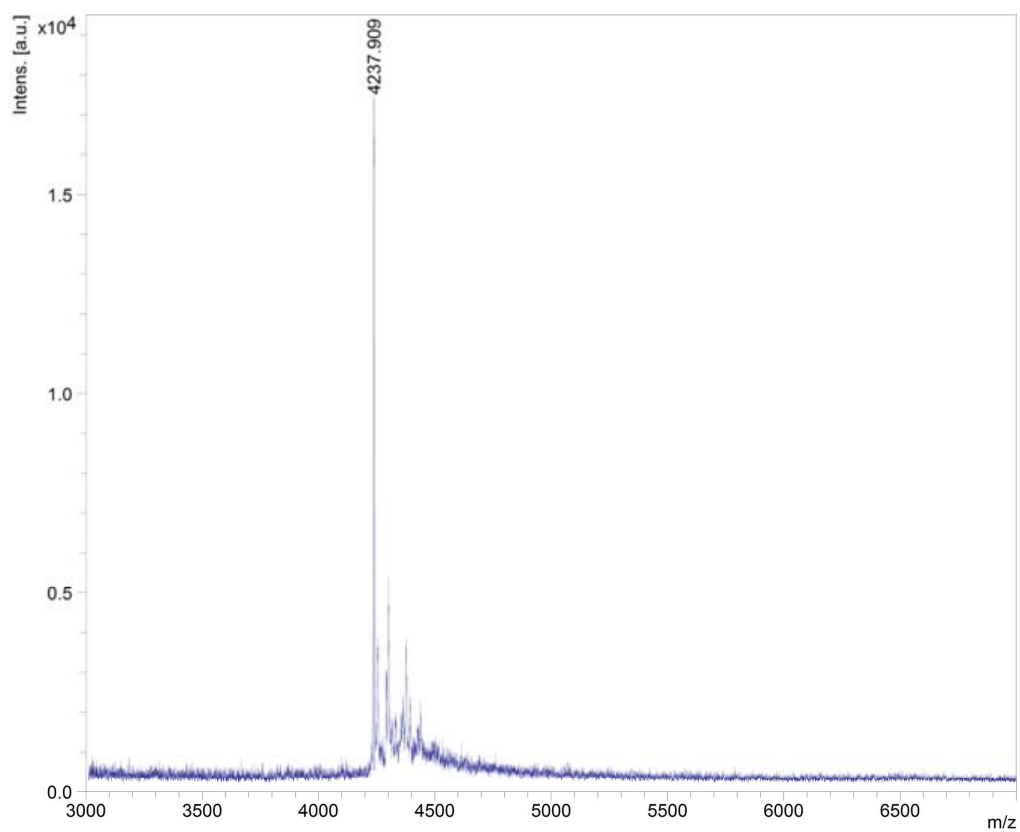
UD-46

[B conc. MeCN: 7-40% (30 min)]

mV



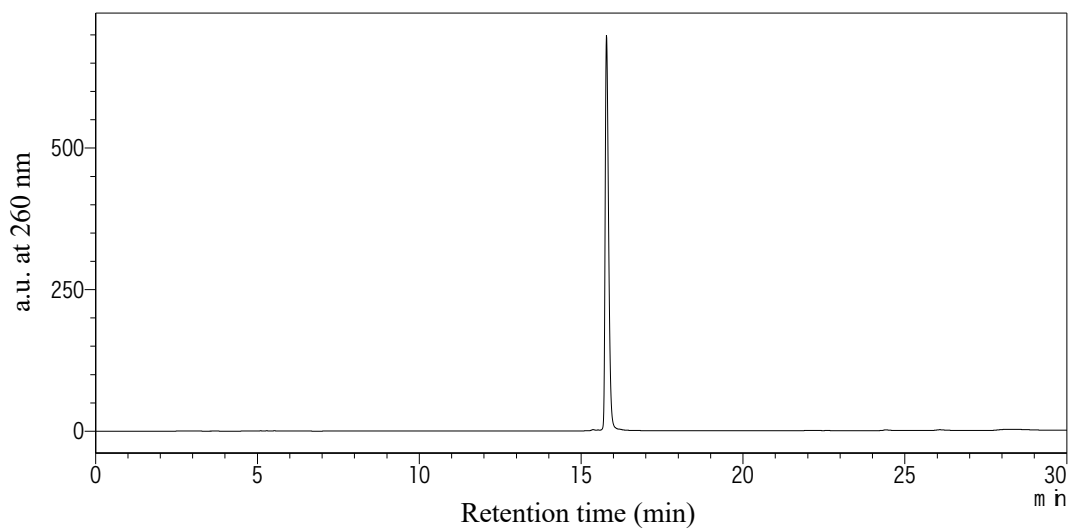
[calcd. (M-H)⁻: 4236.1, found: 4237.9]



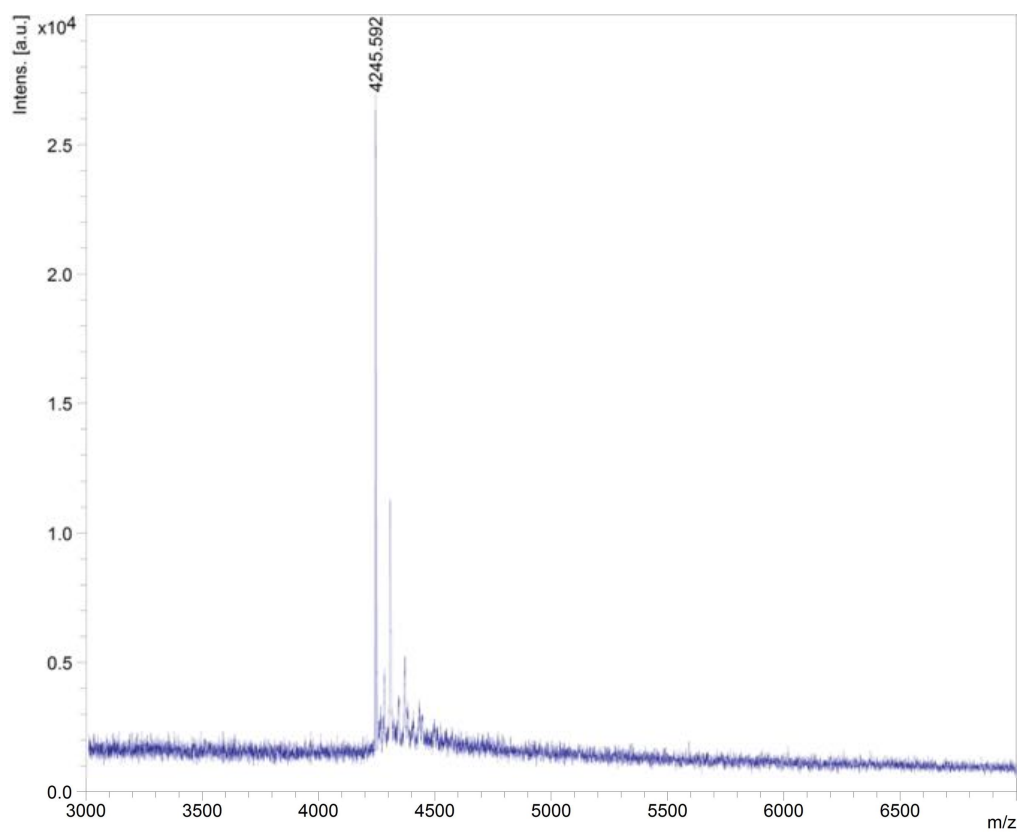
UD-47

[B conc. MeCN: 7-40% (30 min)]

mV



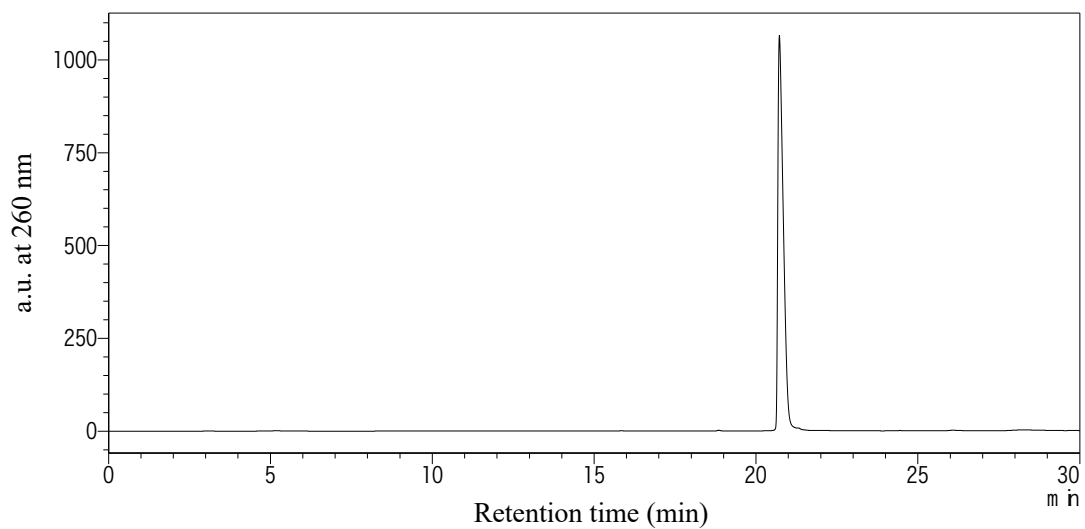
[calcd. (M-H)⁻: 4245.2, found: 4245.6]



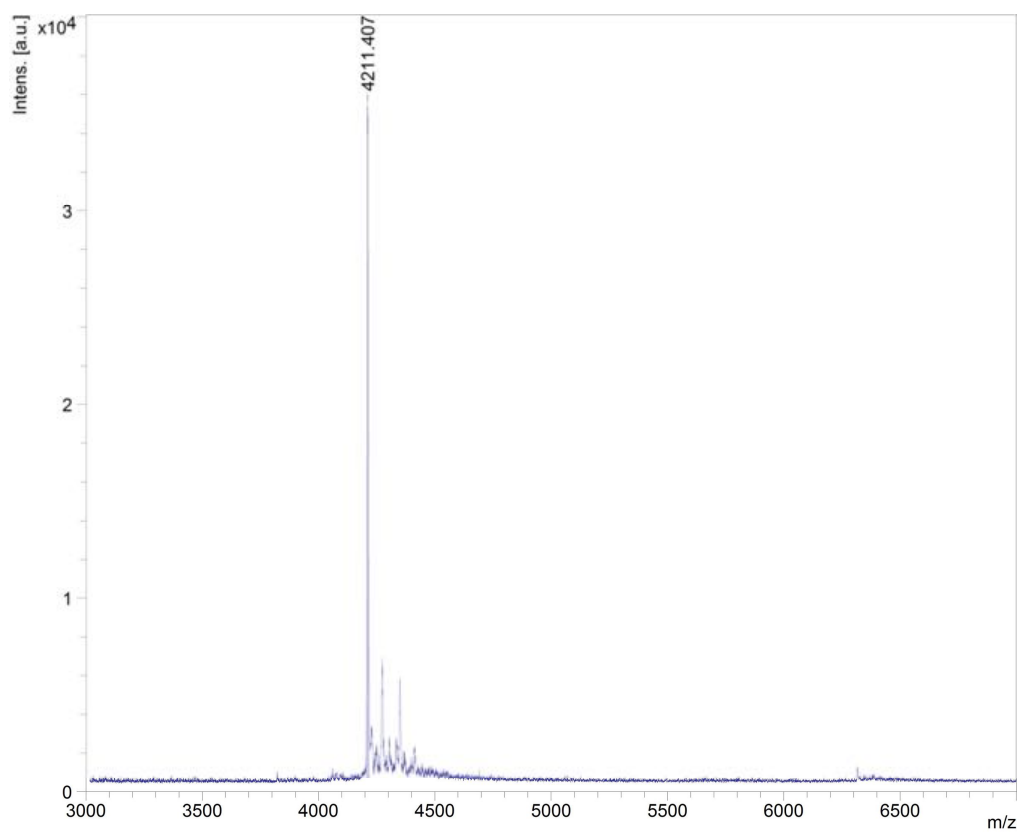
UD-48

[B conc. MeCN: 7-40% (30 min)]

mV



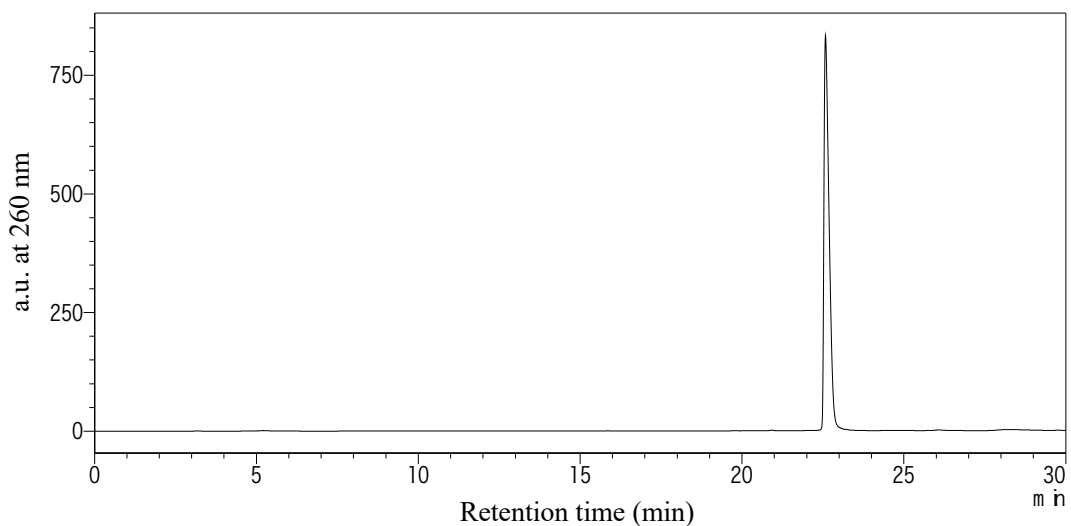
[calcd. (M-H)⁻: 4210.1, found: 4211.4]



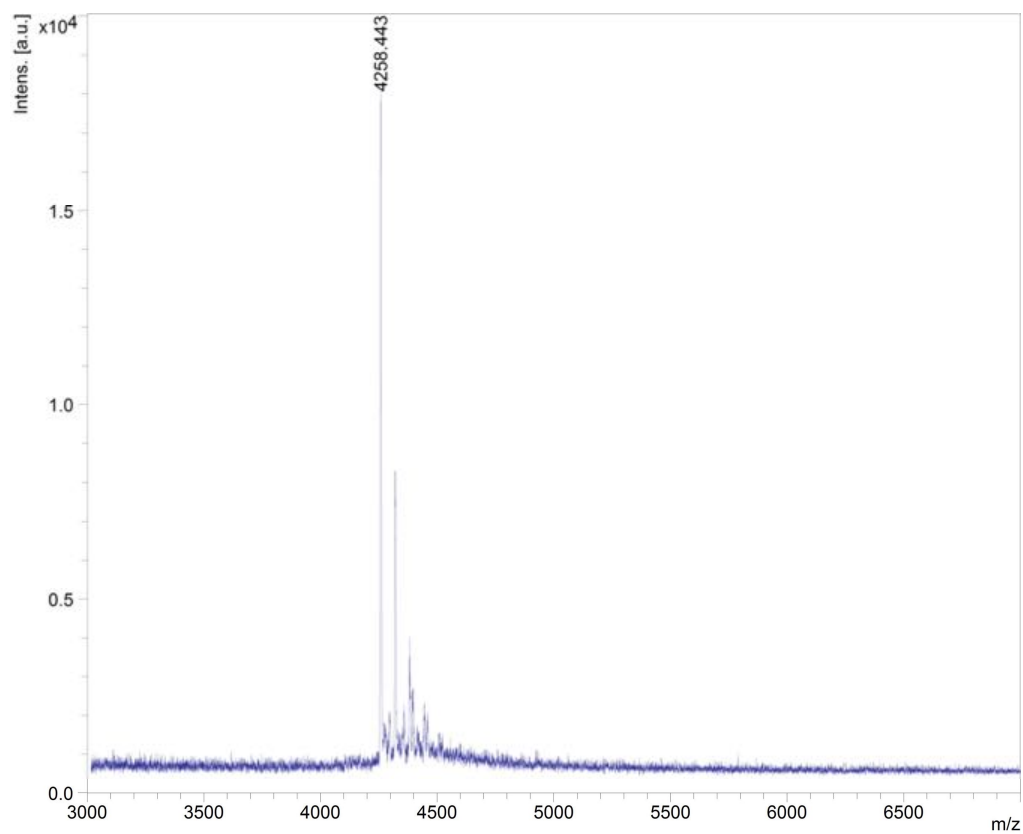
UD-49

[B conc. MeCN: 7-40% (30 min)]

mV



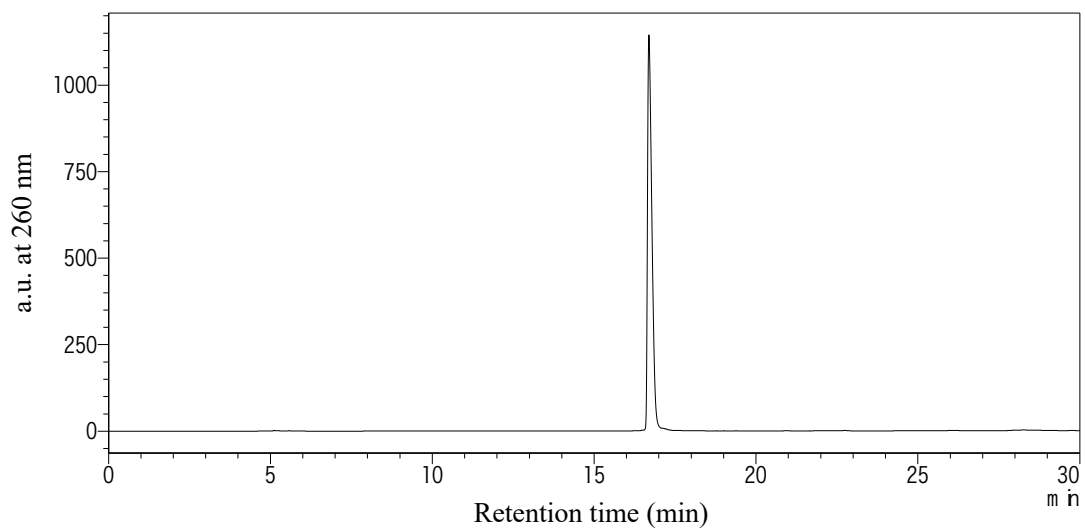
[calcd. (M-H)⁻: 4258.2, found: 4258.4]



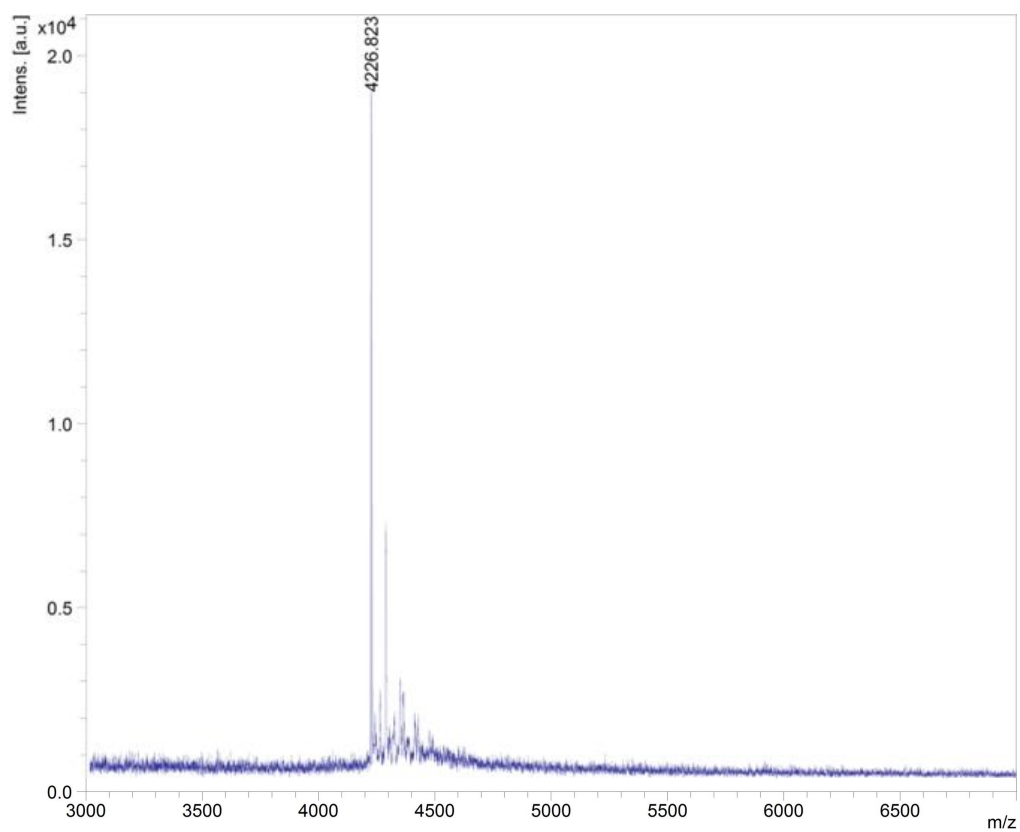
UD-50

[B conc. MeCN: 7-40% (30 min)]

mV



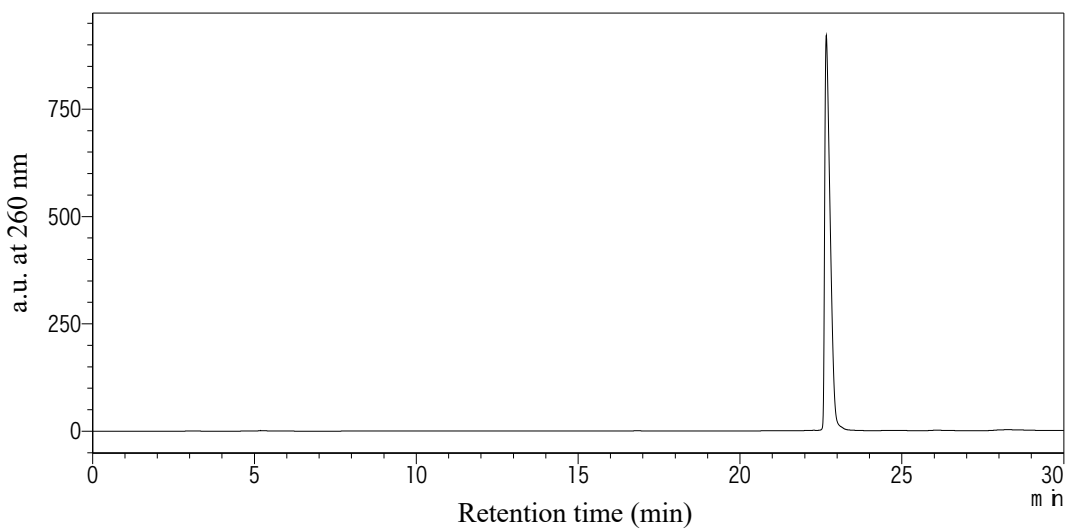
[calcd. (M-H)⁻: 4226.1, found: 4226.8]



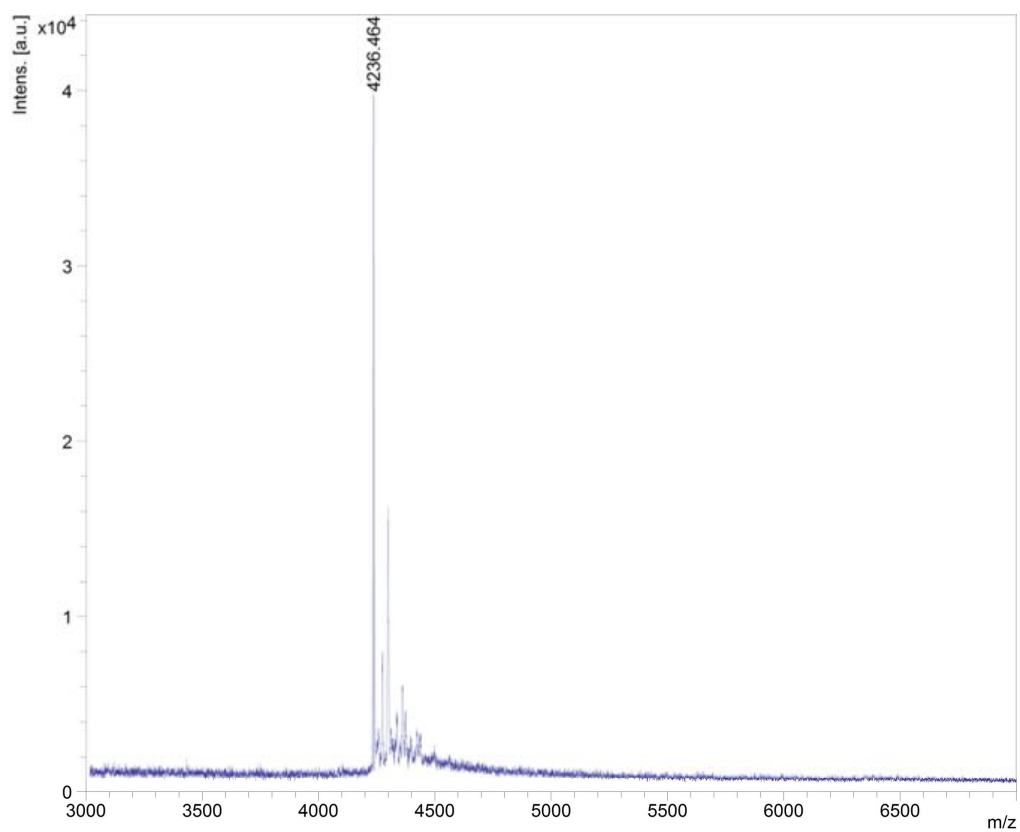
UD-51

[B conc. MeCN: 7-40% (30 min)]

mV



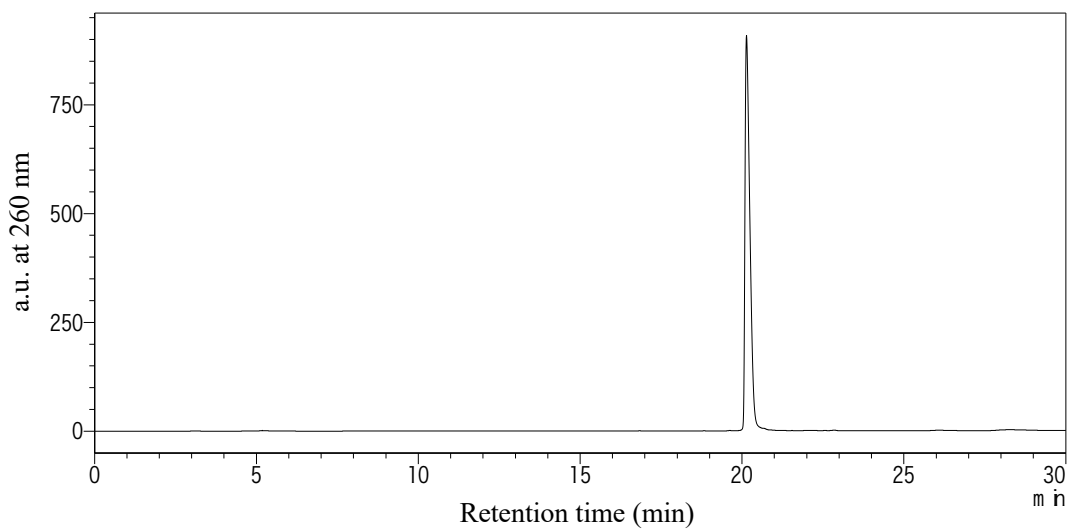
[calcd. (M-H)⁻: 4236.1, found: 4236.5]



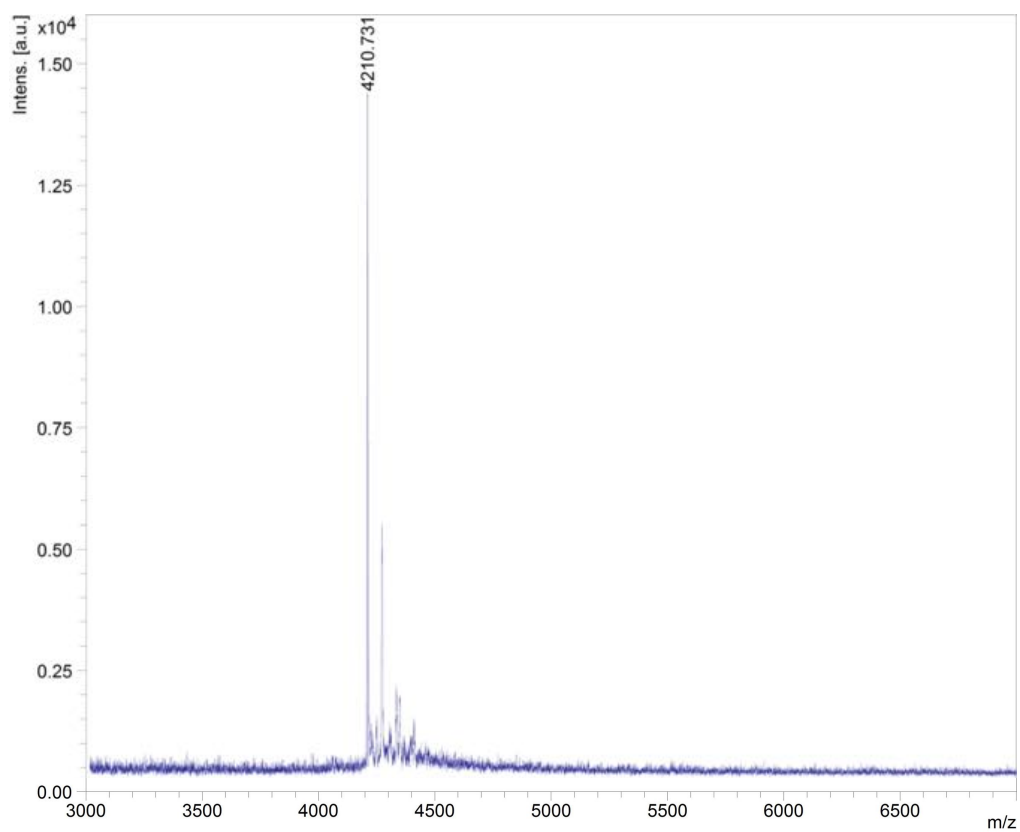
UD-52

[B conc. MeCN: 7-40% (30 min)]

mV



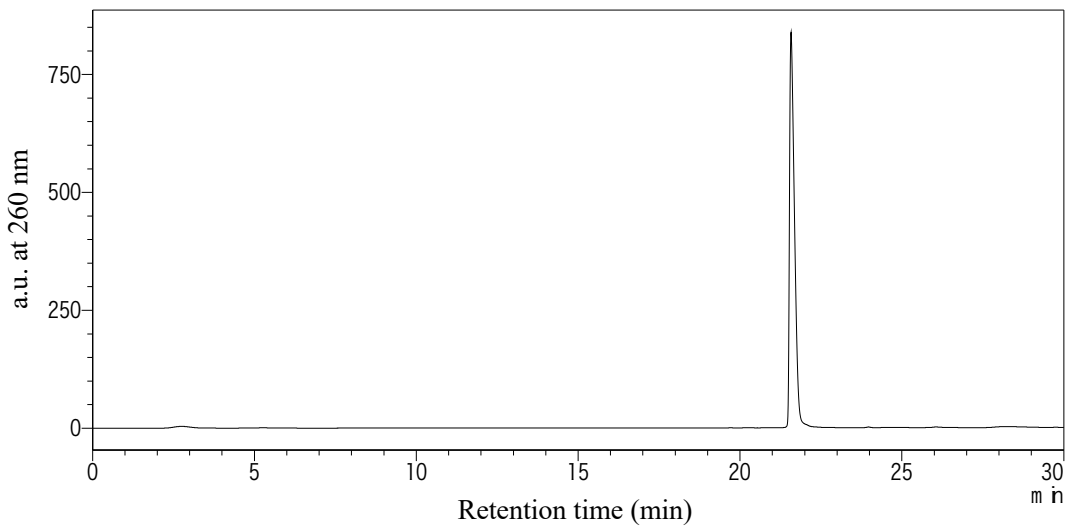
[calcd. (M-H)⁻: 4210.1, found: 4210.7]



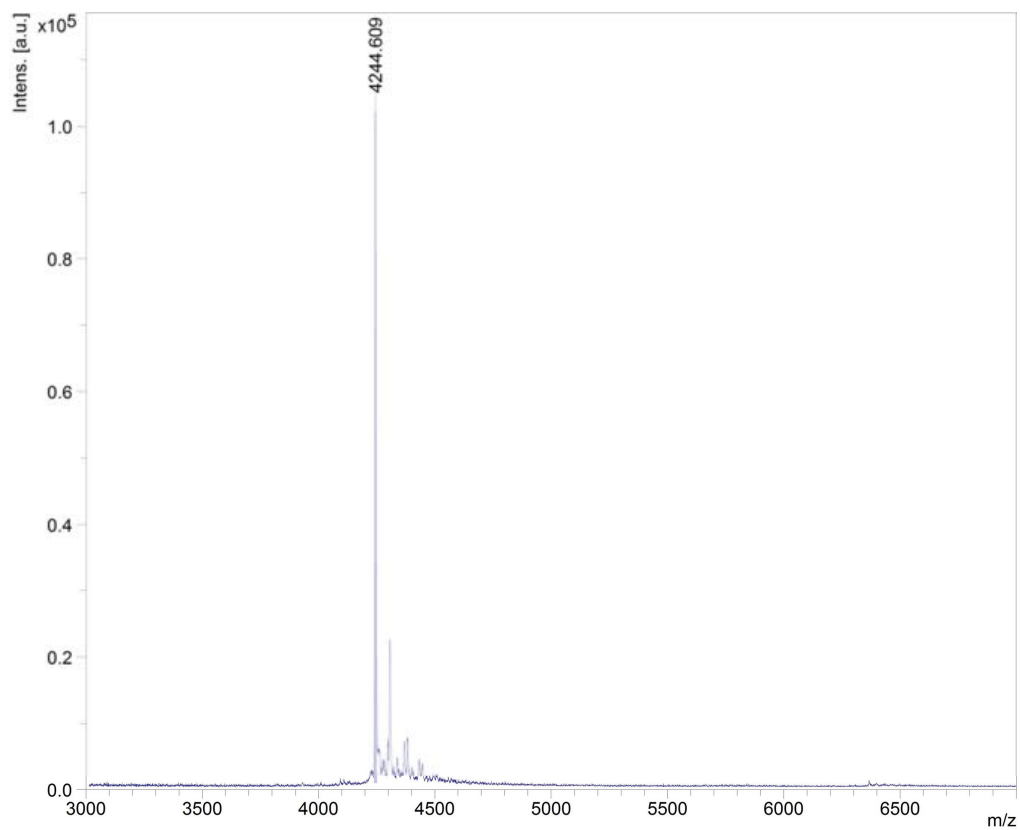
UD-53

[B conc. MeCN: 7-40% (30 min)]

mV



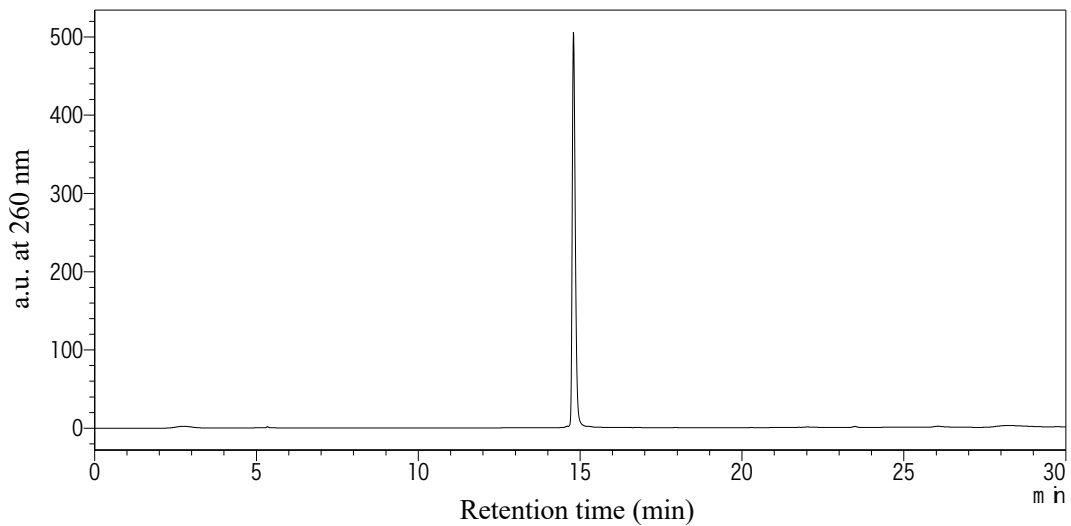
[calcd. (M-H)⁻: 4244.1, found: 4244.6]



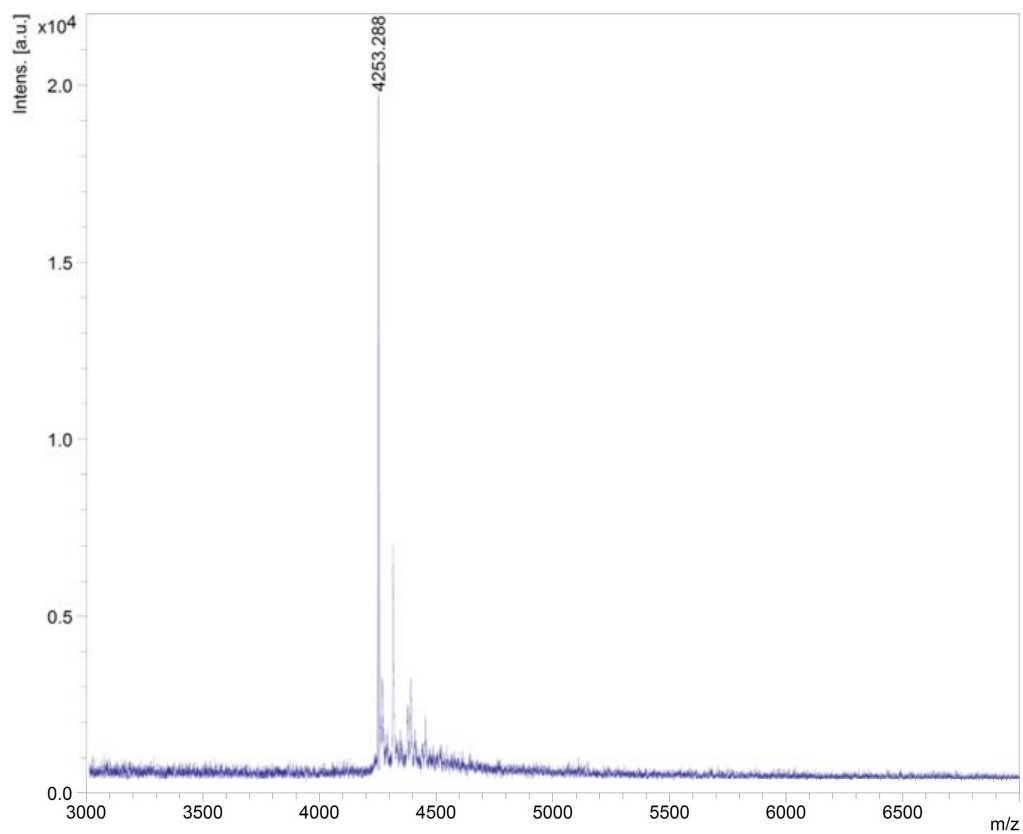
UD-54

[B conc. MeCN: 7-40% (30 min)]

mV



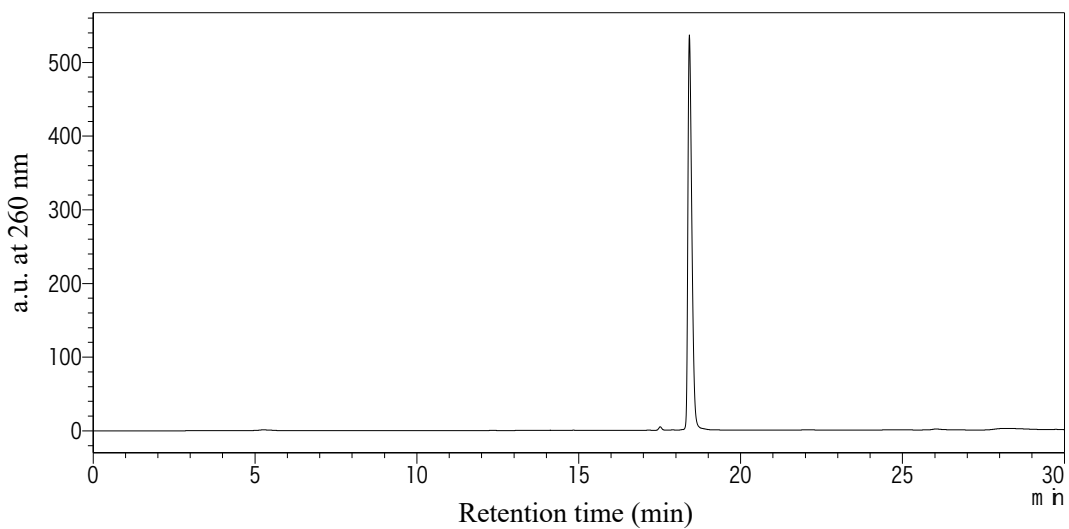
[calcd. (M-H)⁻: 4253.2, found: 4253.3]



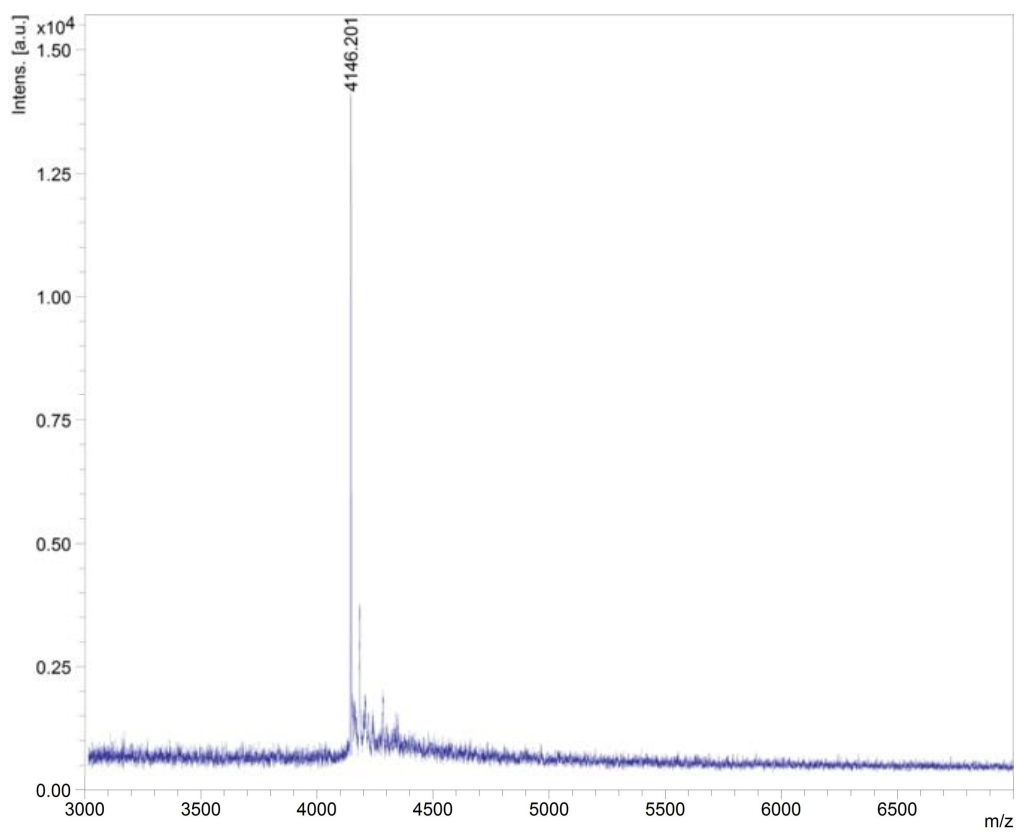
UD-55

[B conc. MeCN: 7-40% (30 min)]

mV



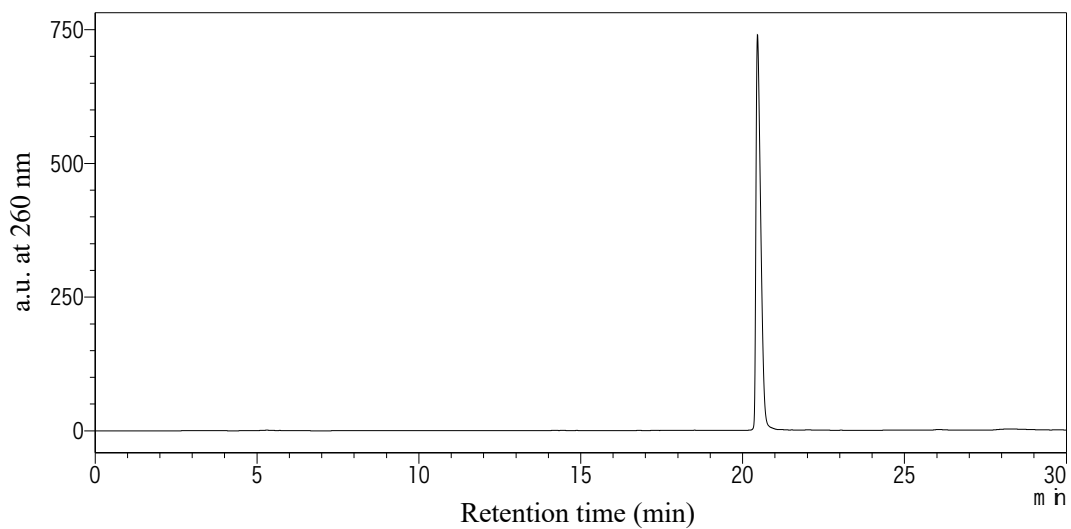
[calcd. (M-H)⁻: 4146.0, found: 4146.2]



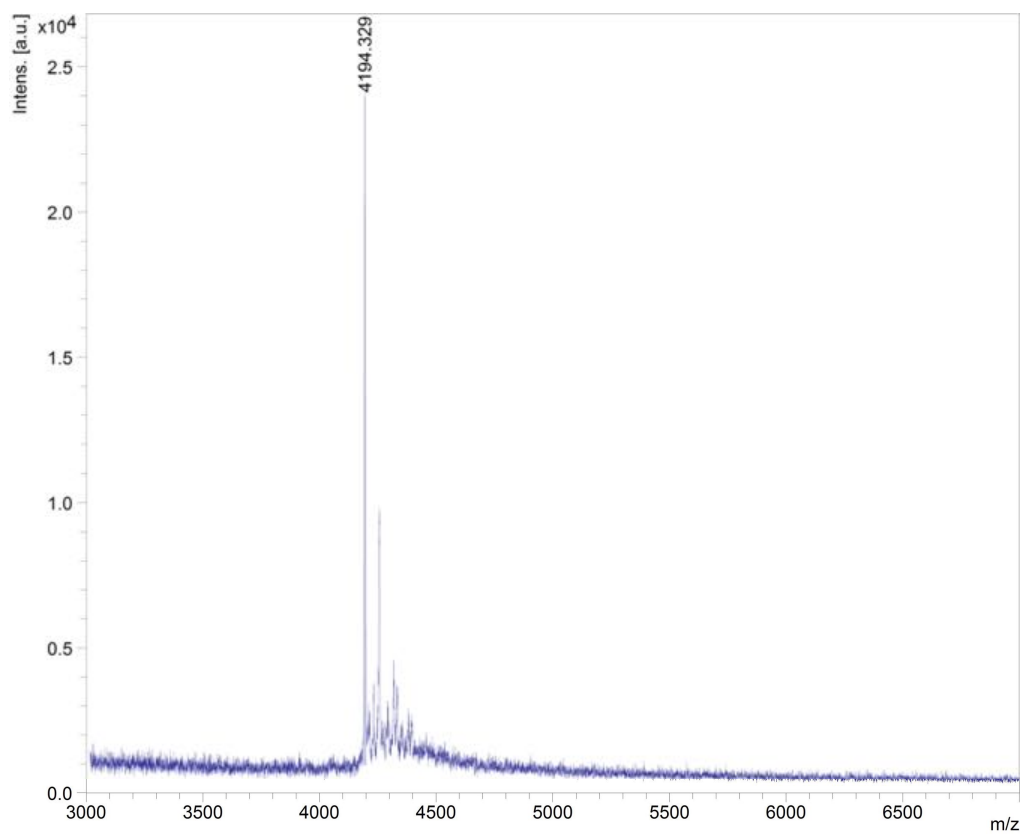
UD-56

[B conc. ACN: 7-40% (30 min)]

mV



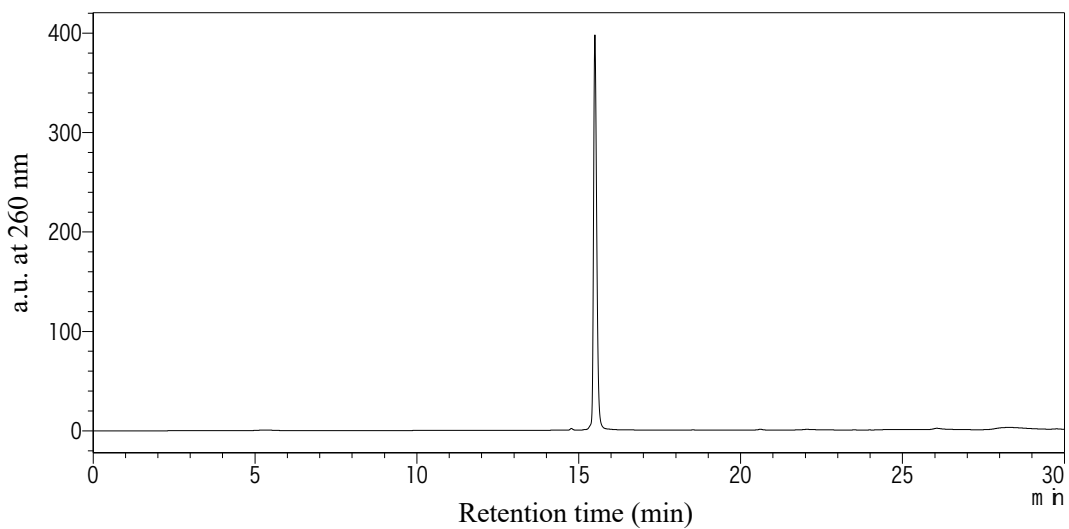
[calcd. (M-H)⁻: 4194.1, found: 4194.3]



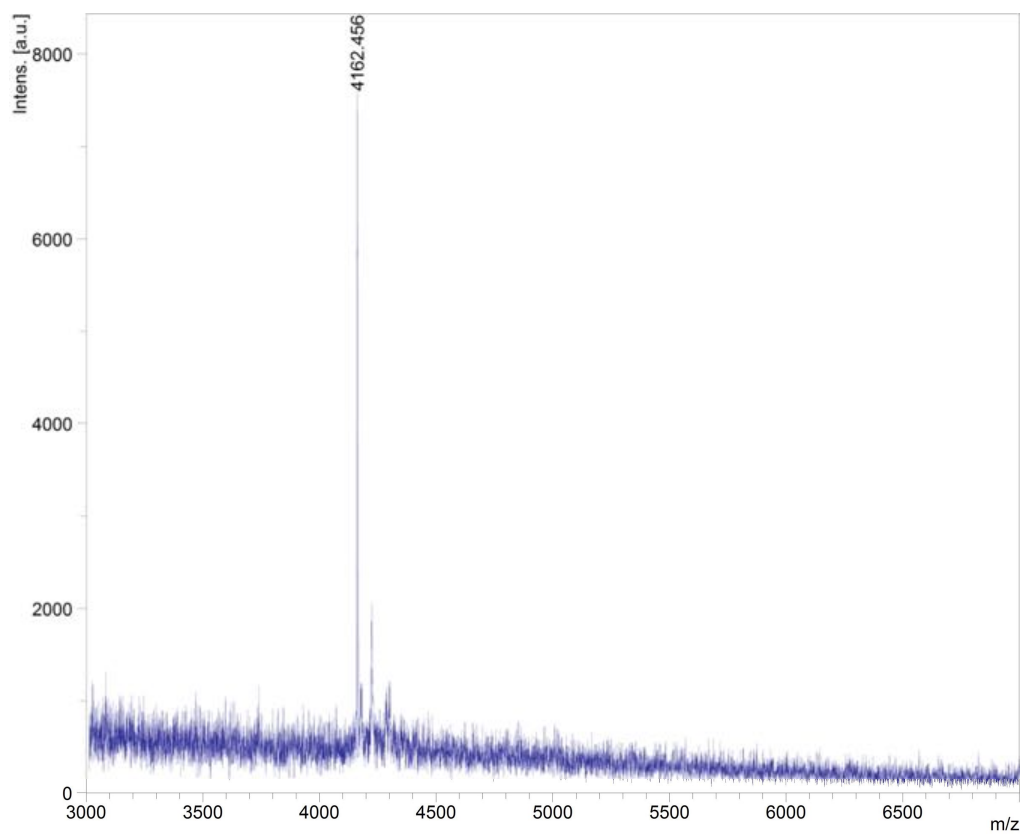
UD-57

[B conc. MeCN: 7-40% (30 min)]

mV

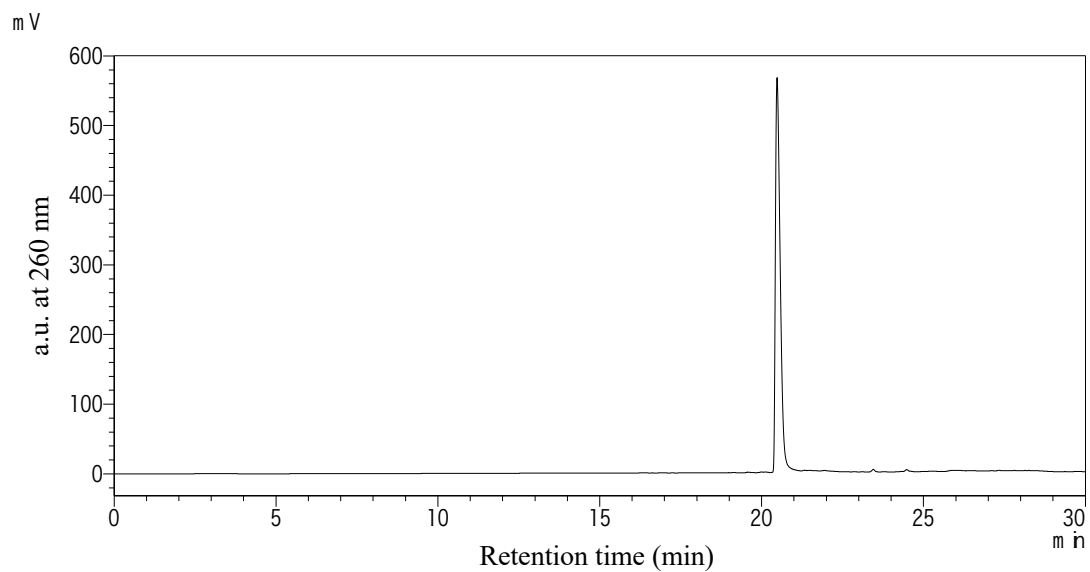


[calcd. (M-H)⁻: 4162.0, found: 4162.5]

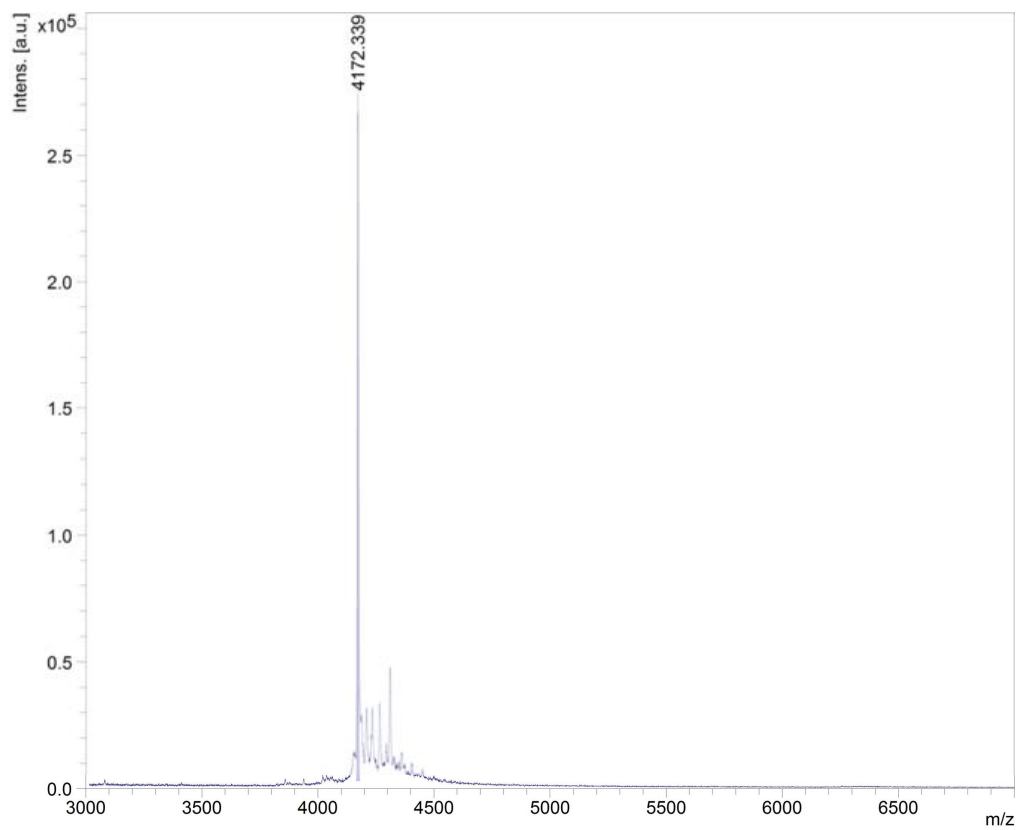


UD-58

[B conc. MeCN: 7-40% (30 min)]



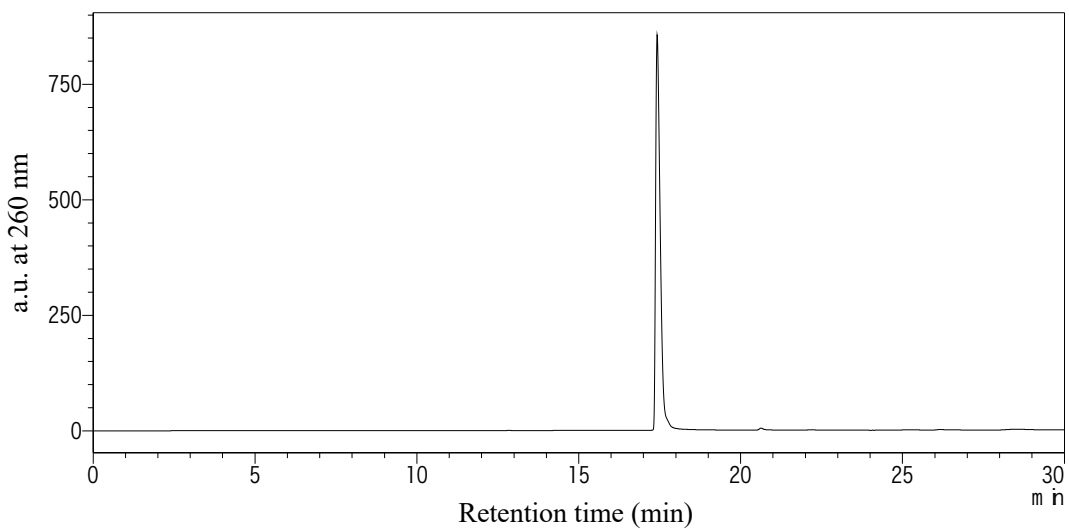
[calcd. (M-H)⁻: 4172.1, found: 4172.3]



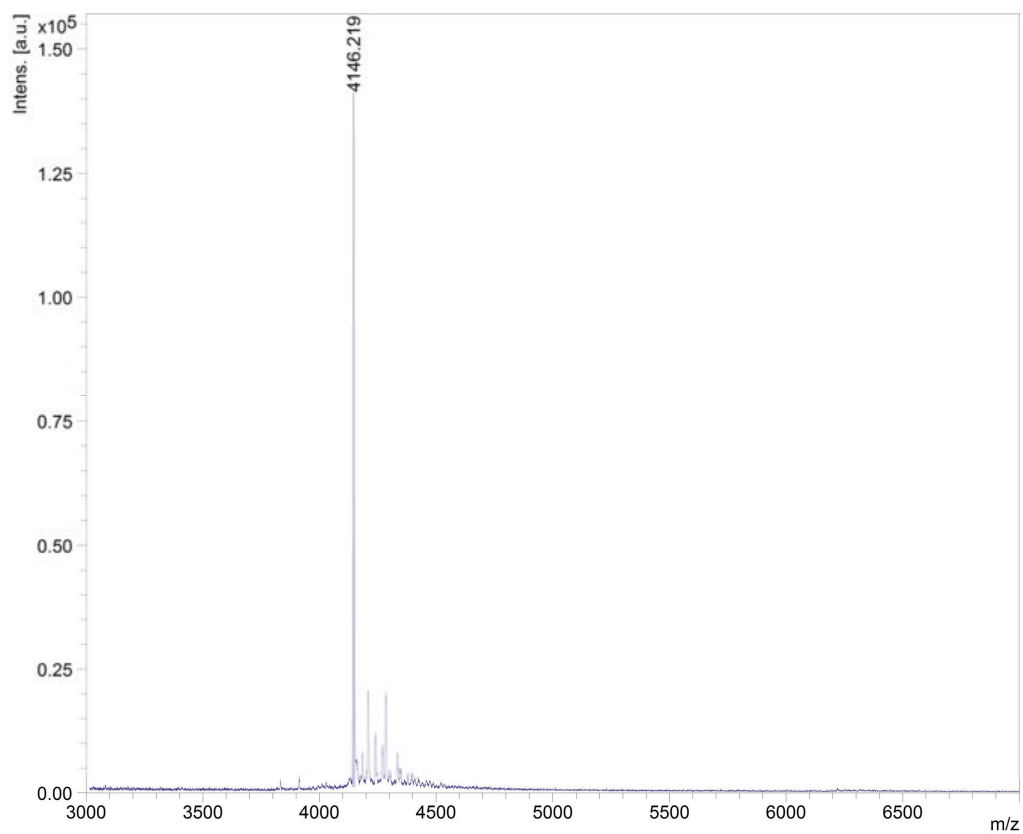
UD-59

[B conc. MeCN: 7-40% (30 min)]

mV



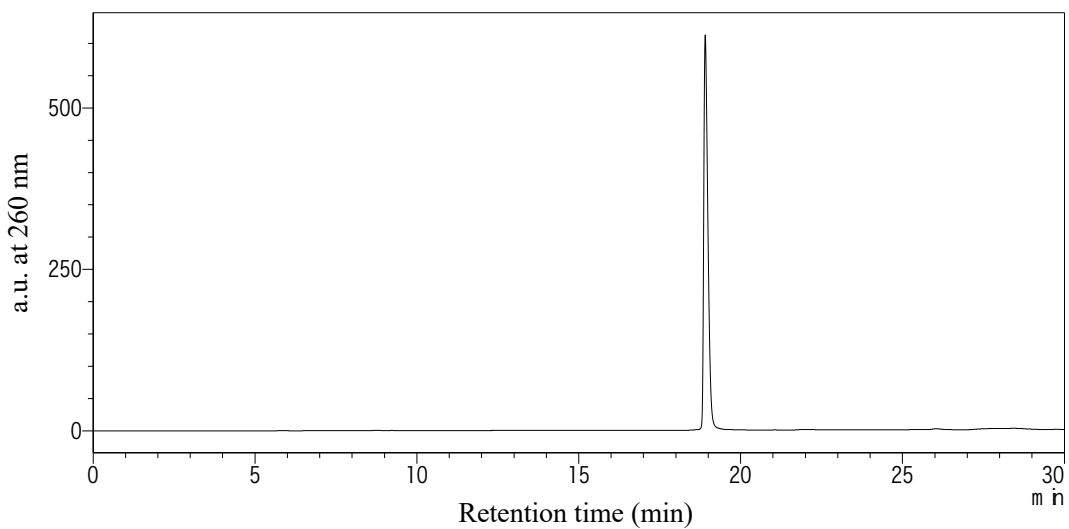
[calcd. (M-H)⁻: 4146.0, found: 4146.2]



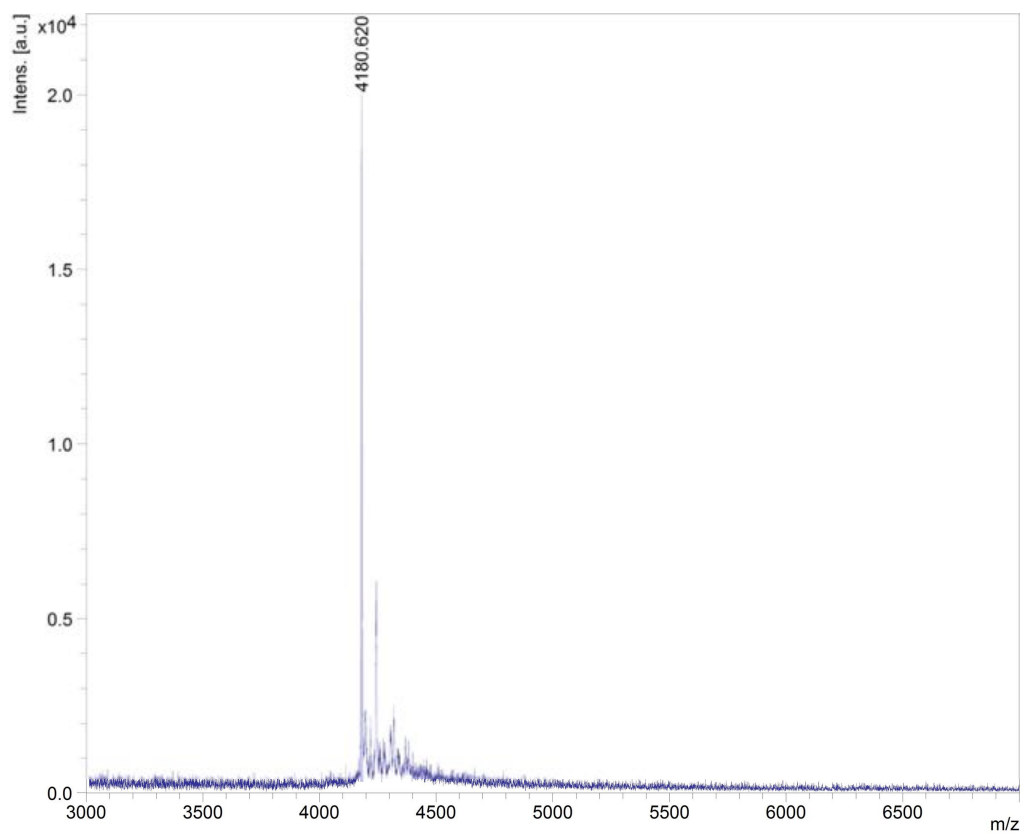
UD-60

[B conc. MeCN: 7-40% (30 min)]

mV



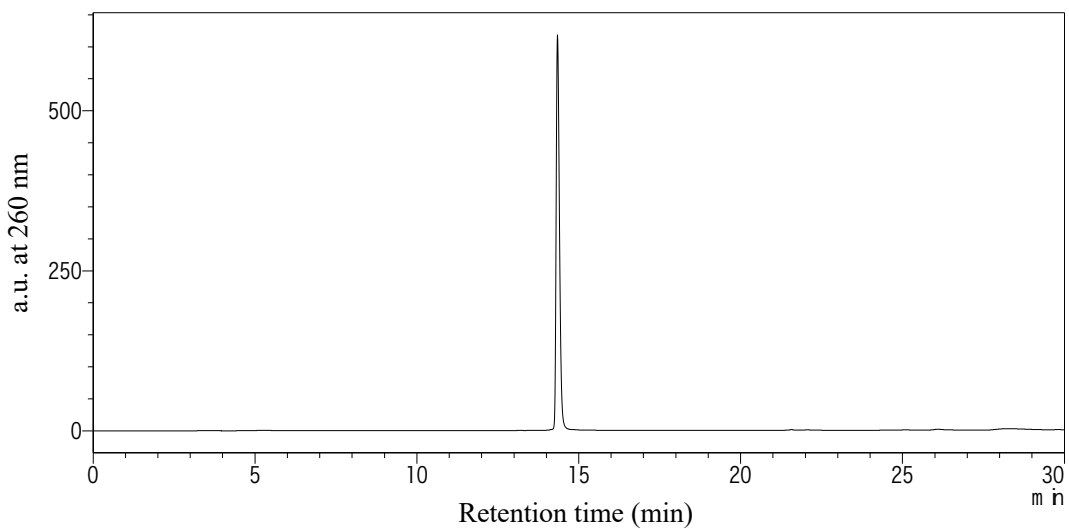
[calcd. (M-H)⁻: 4180.0, found: 4180.6]



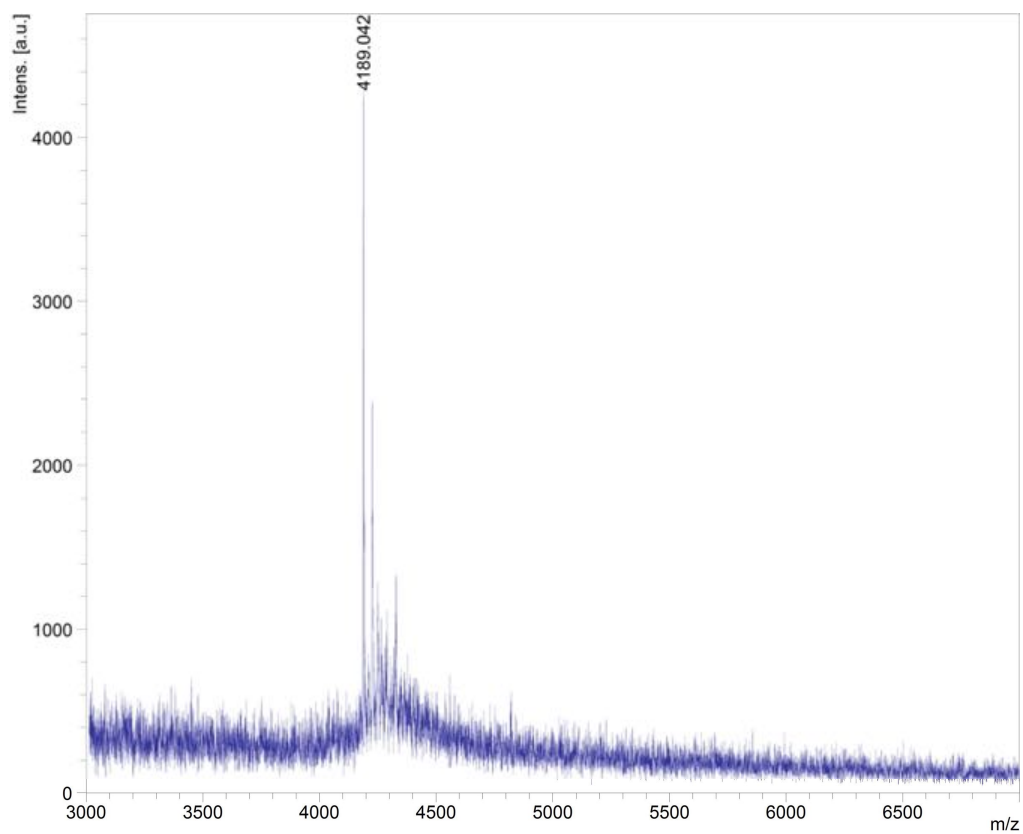
UD-61

[B conc. MeCN: 7-40% (30 min)]

mV



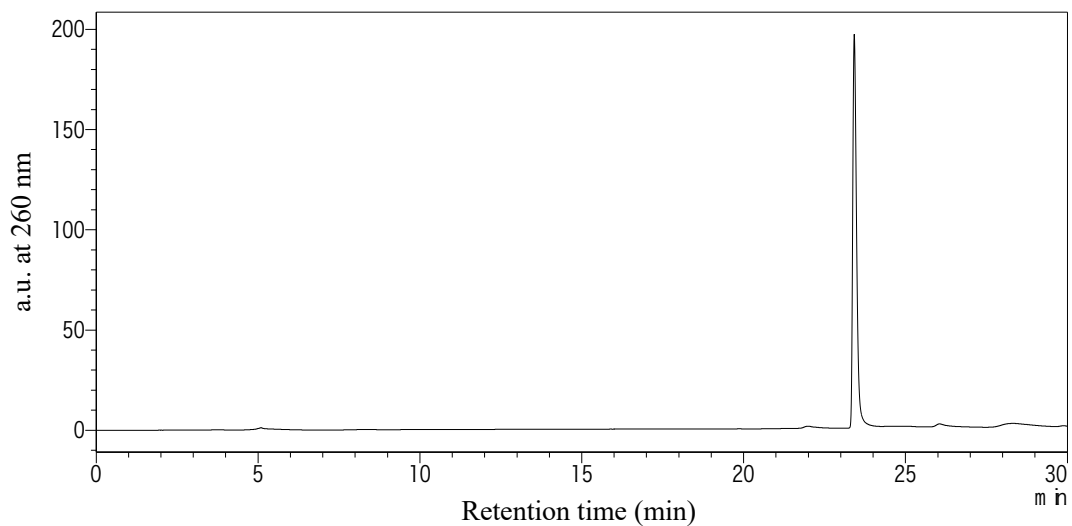
[calcd. (M-H)⁻: 4189.1, found: 4189.0]



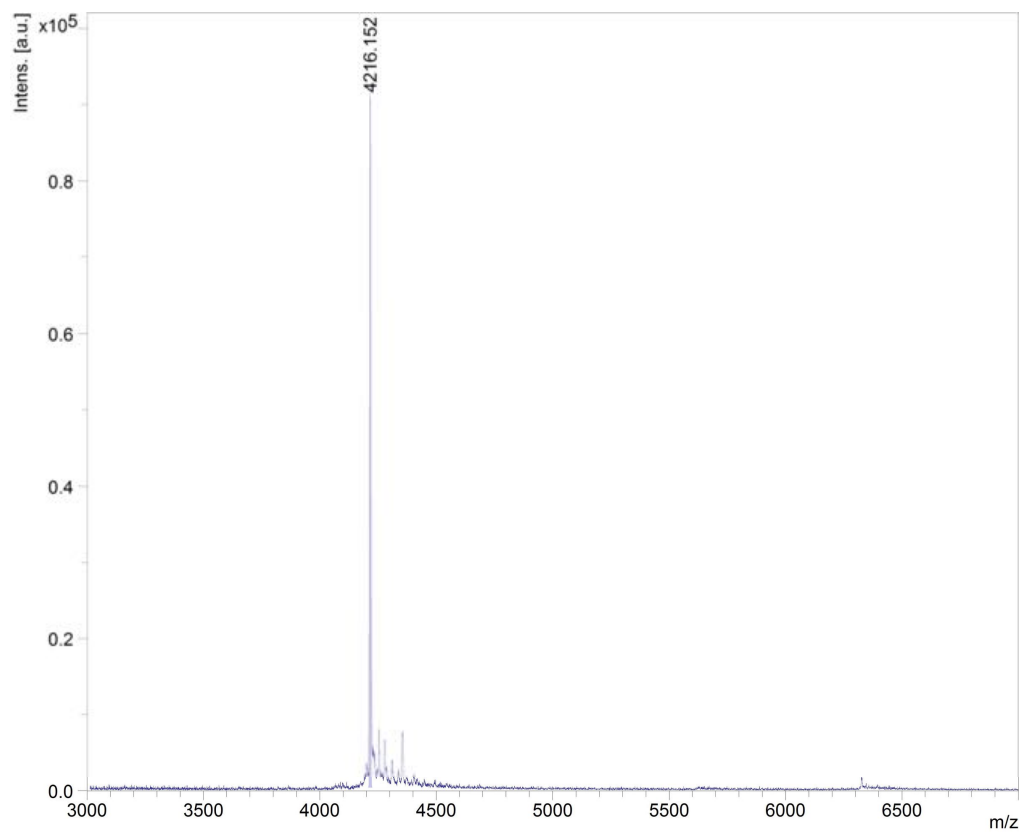
UD-62

[B conc. MeCN: 7-40% (30 min)]

mV



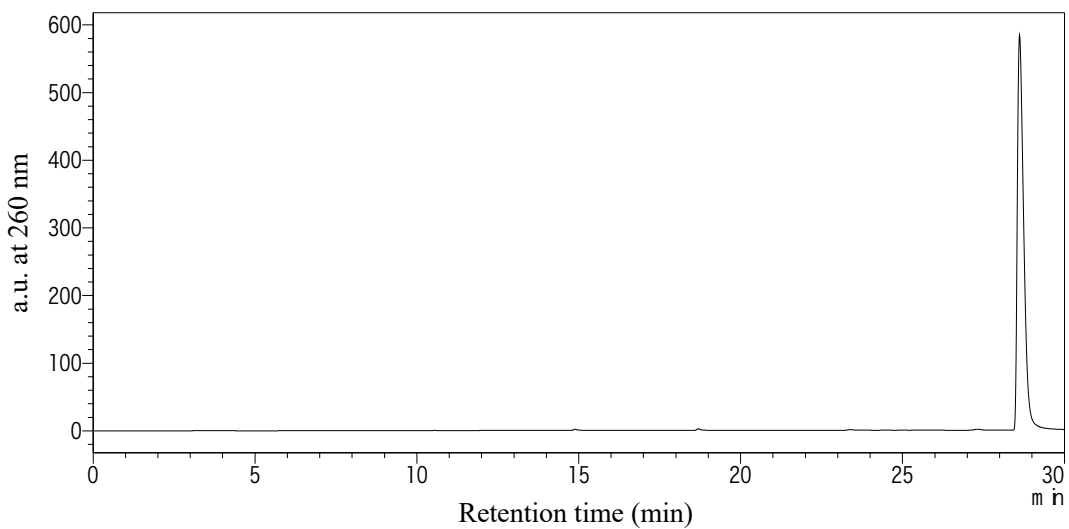
[calcd. (M-H)⁻: 4216.2, found: 4216.2]



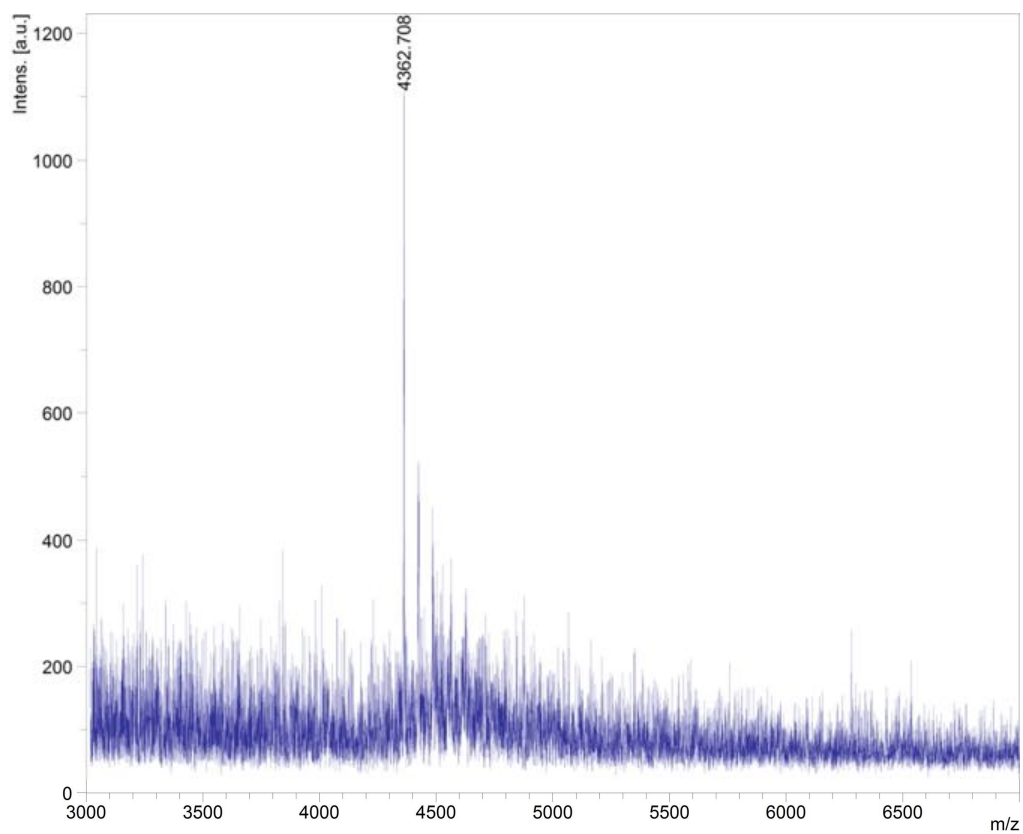
UD-63

[B conc. MeCN: 7-40% (30 min)]

mV



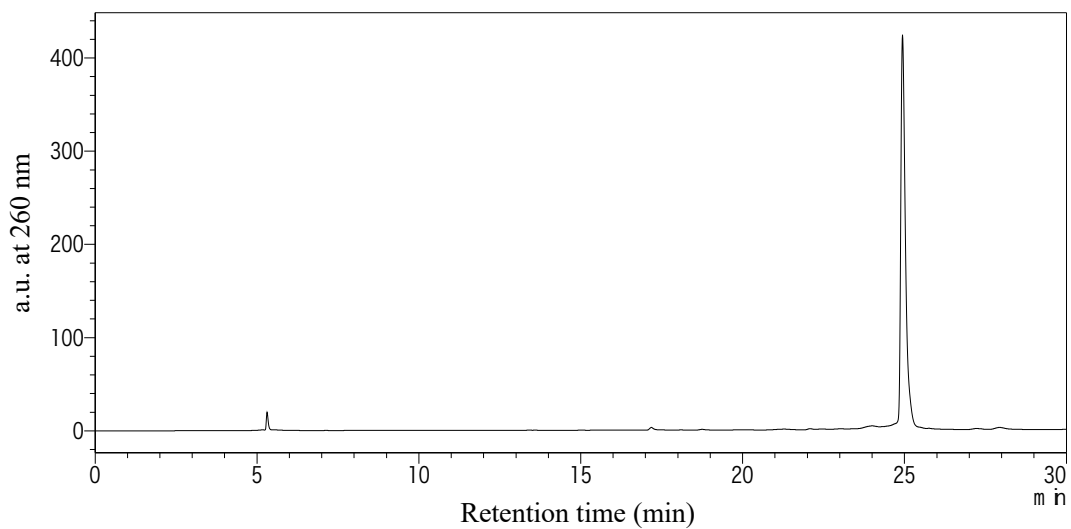
[calcd. (M-H)⁻: 4362.0, found: 4362.7]



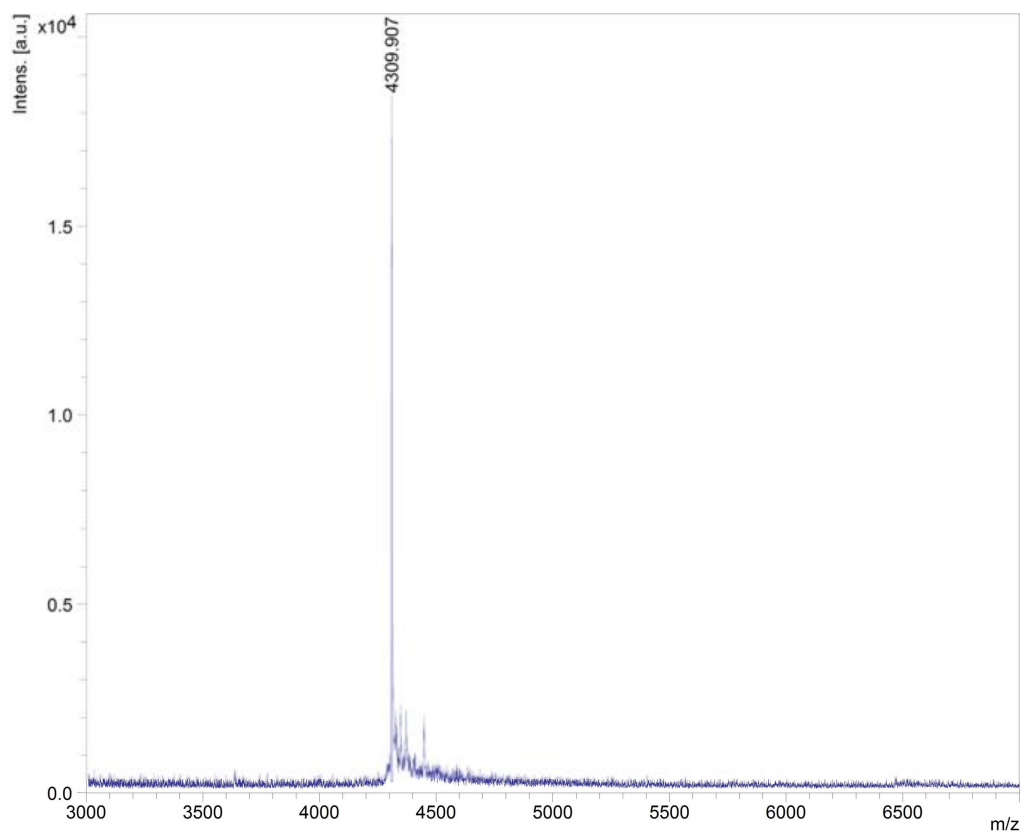
UD-64

[B conc. MeCN: 10-50% (30 min)]

mV



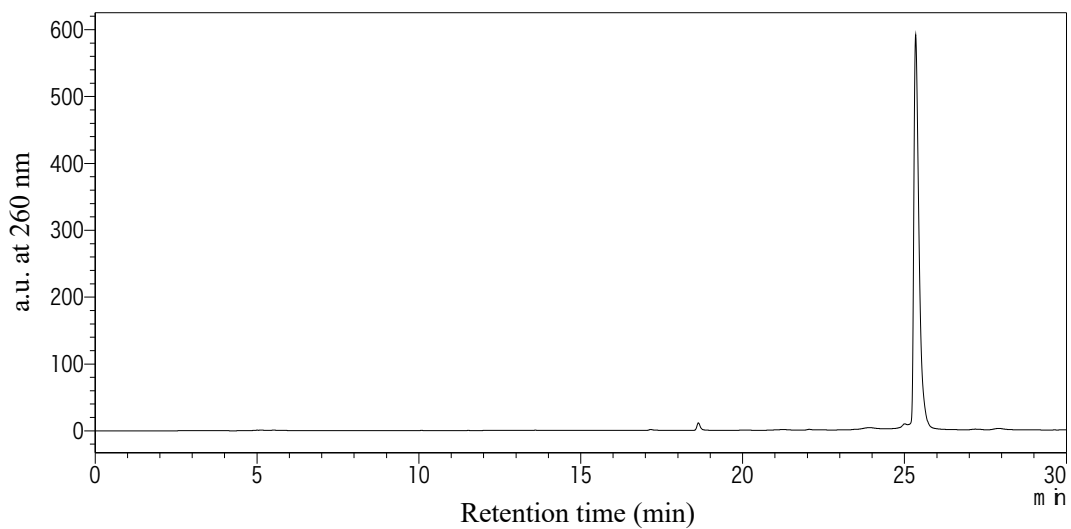
[calcd. (M-H)⁻: 4312.2, found: 4309.9]



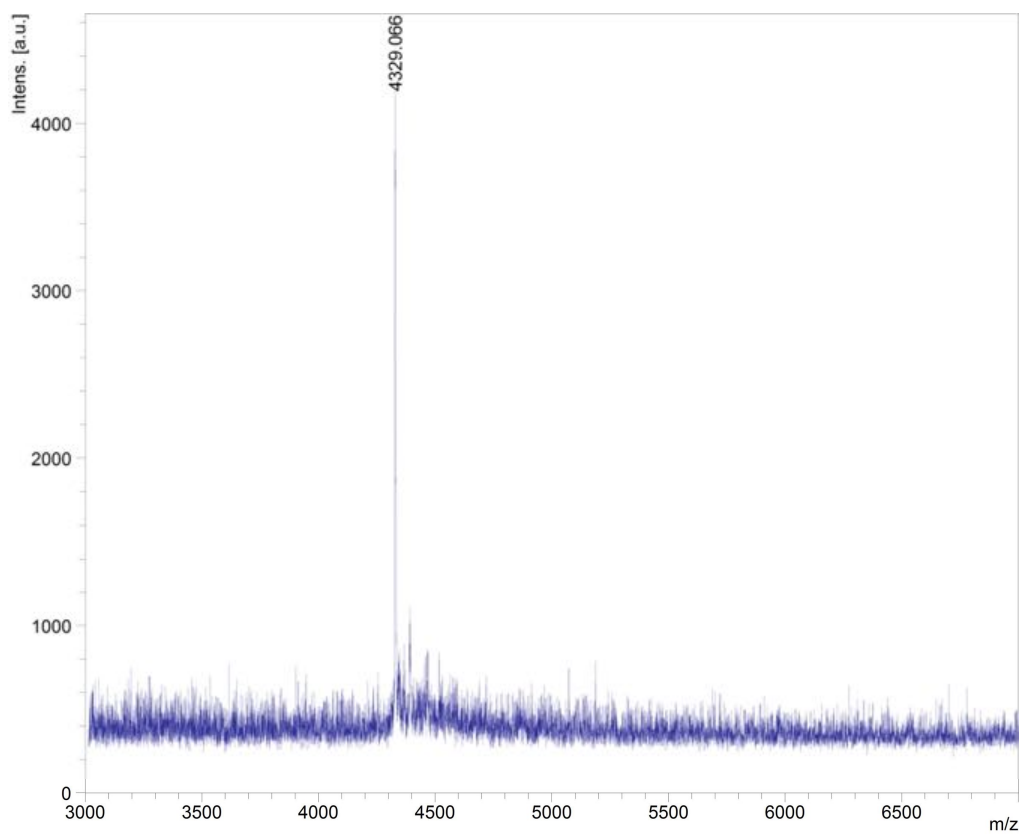
UD-65

[B conc. MeCN: 10-50% (30 min)]

mV



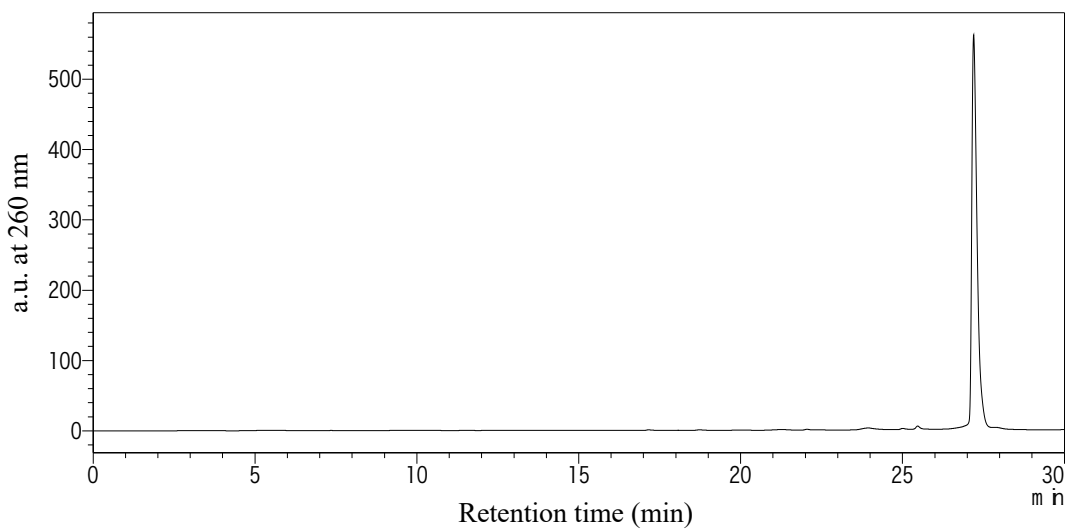
[calcd. (M-H)⁻: 4330.2, found: 4329.1]



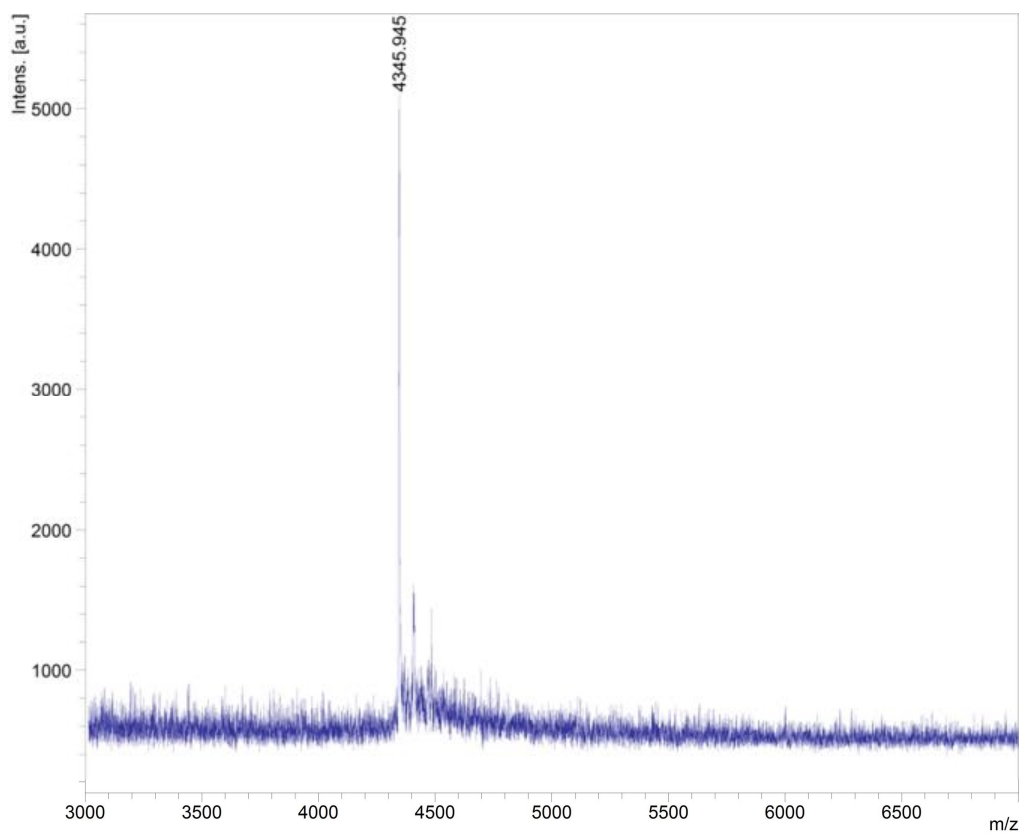
UD-66

[B conc. MeCN: 10-50% (30 min)]

mV



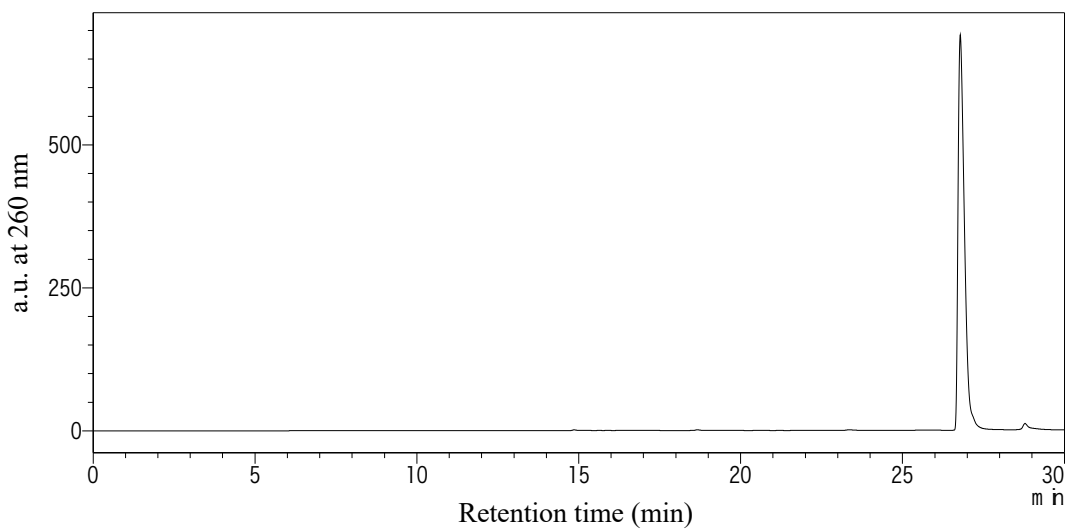
[calcd. (M-H)⁻: 4346.7, found: 4345.9]



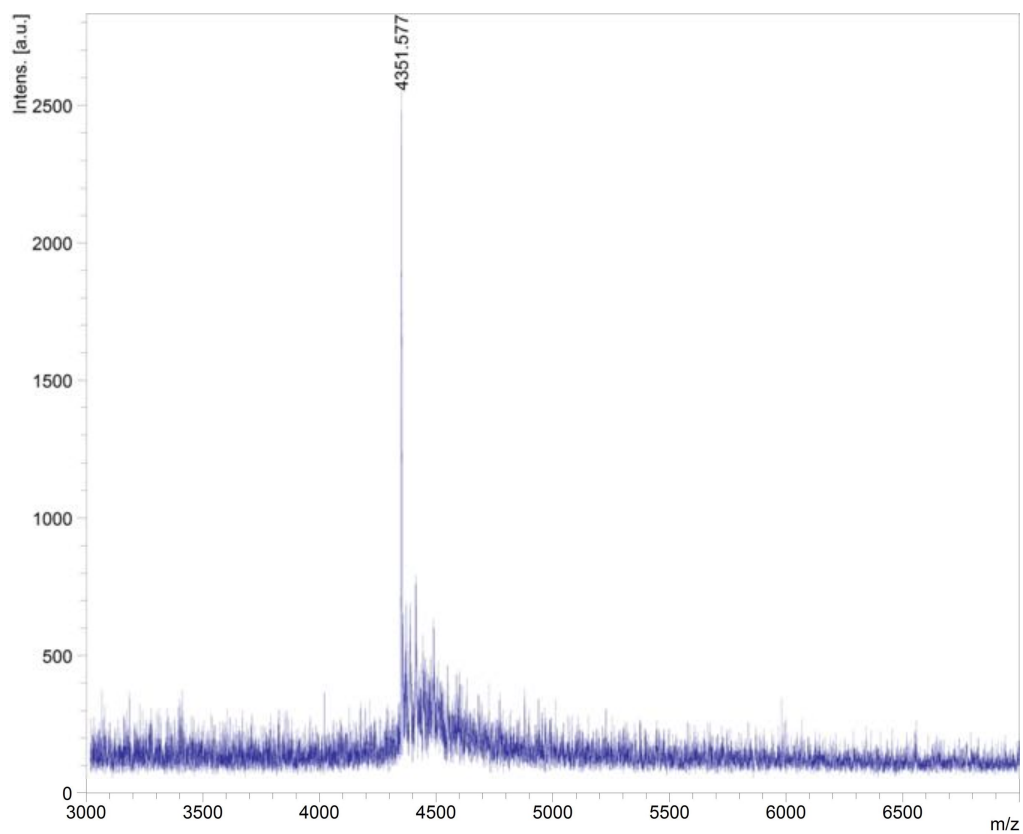
UD-67

[B conc. MeCN: 7-40% (30 min)]

mV



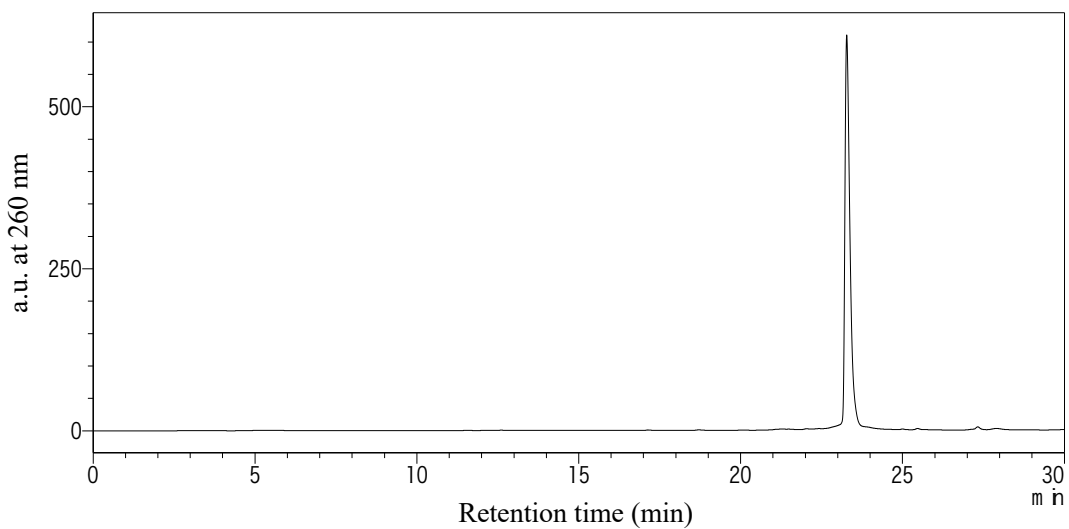
[calcd. (M-H)⁻: 4350.0, found: 4351.6]



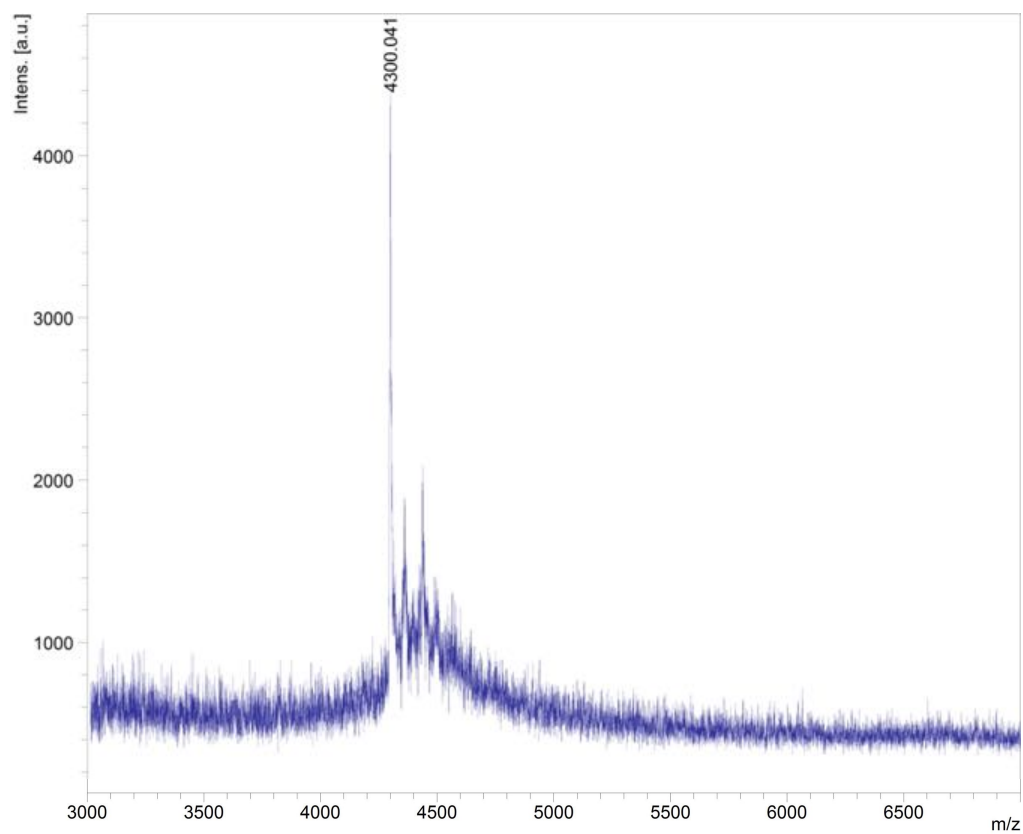
UD-68

[B conc. MeCN: 10-50% (30 min)]

mV



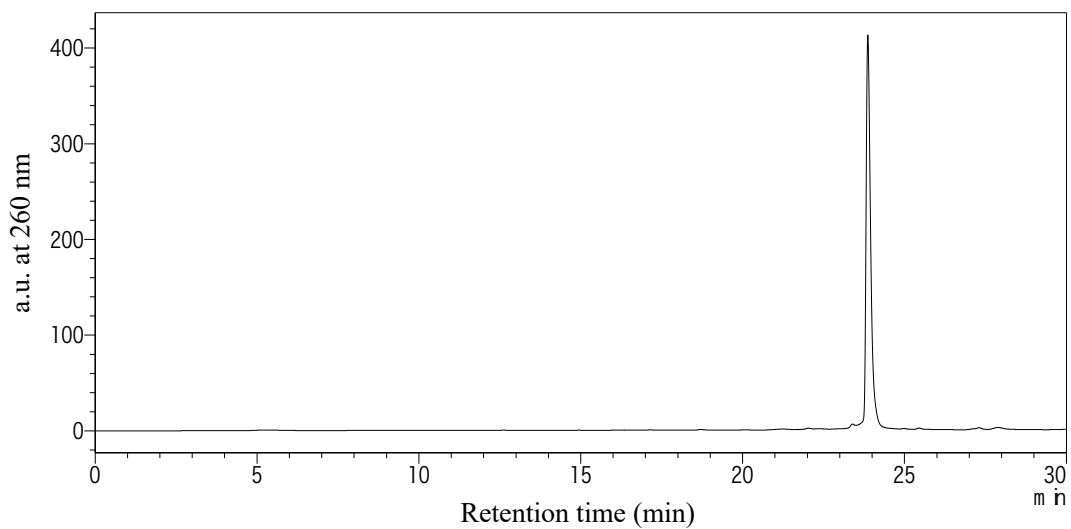
[calcd. (M-H)⁻: 4300.2, found: 4300.0]



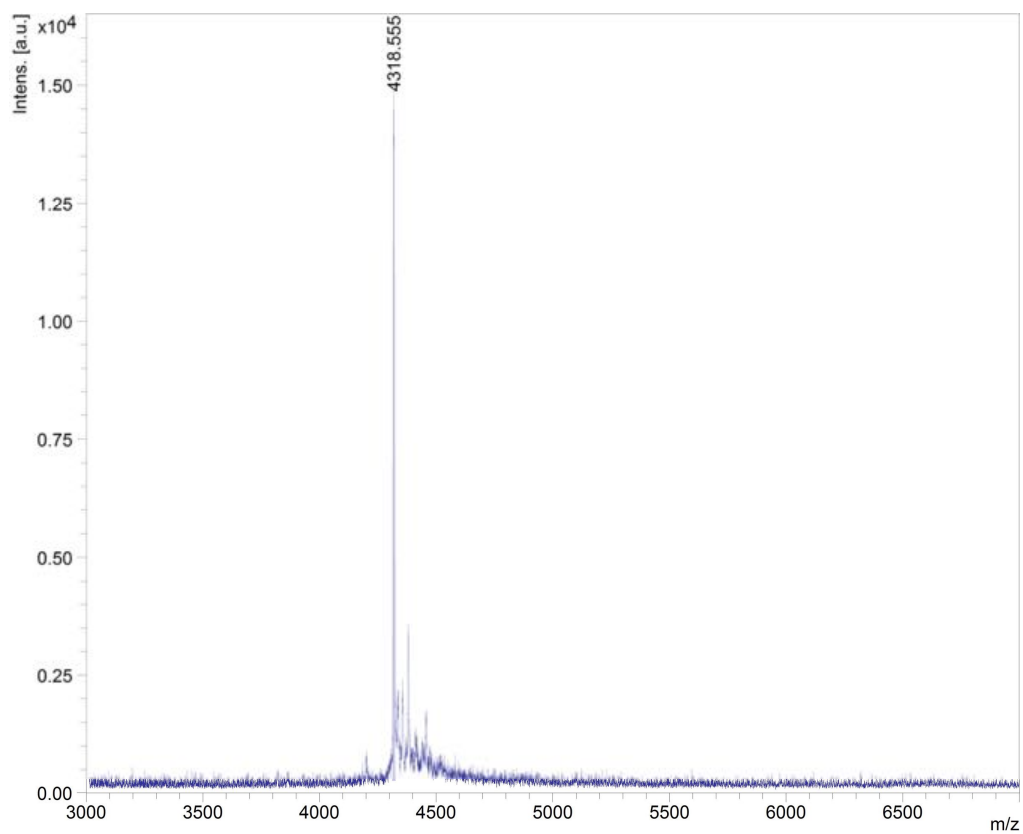
UD-69

[B conc. MeCN: 10-50% (30 min)]

mV



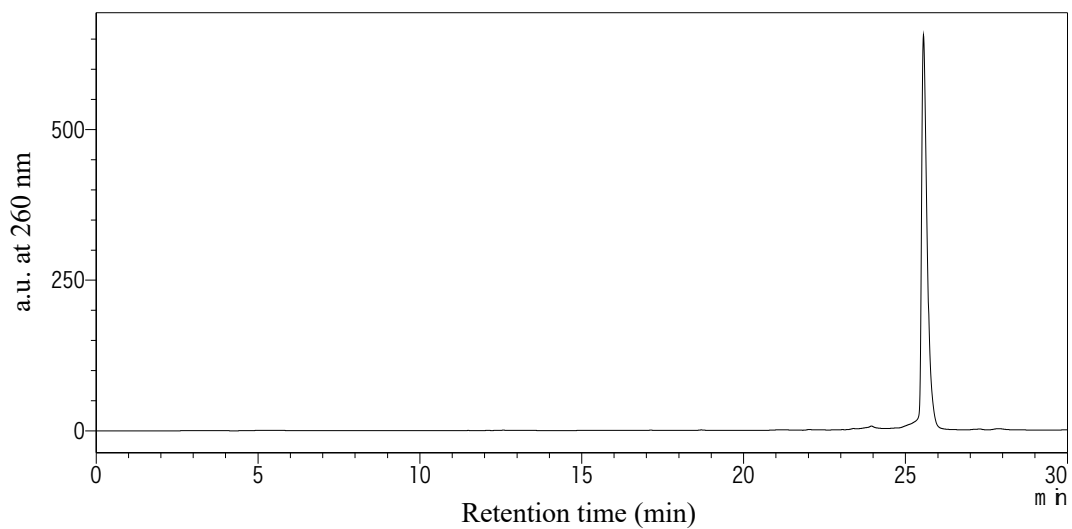
[calcd. (M-H)⁻: 4318.2, found: 4318.6]



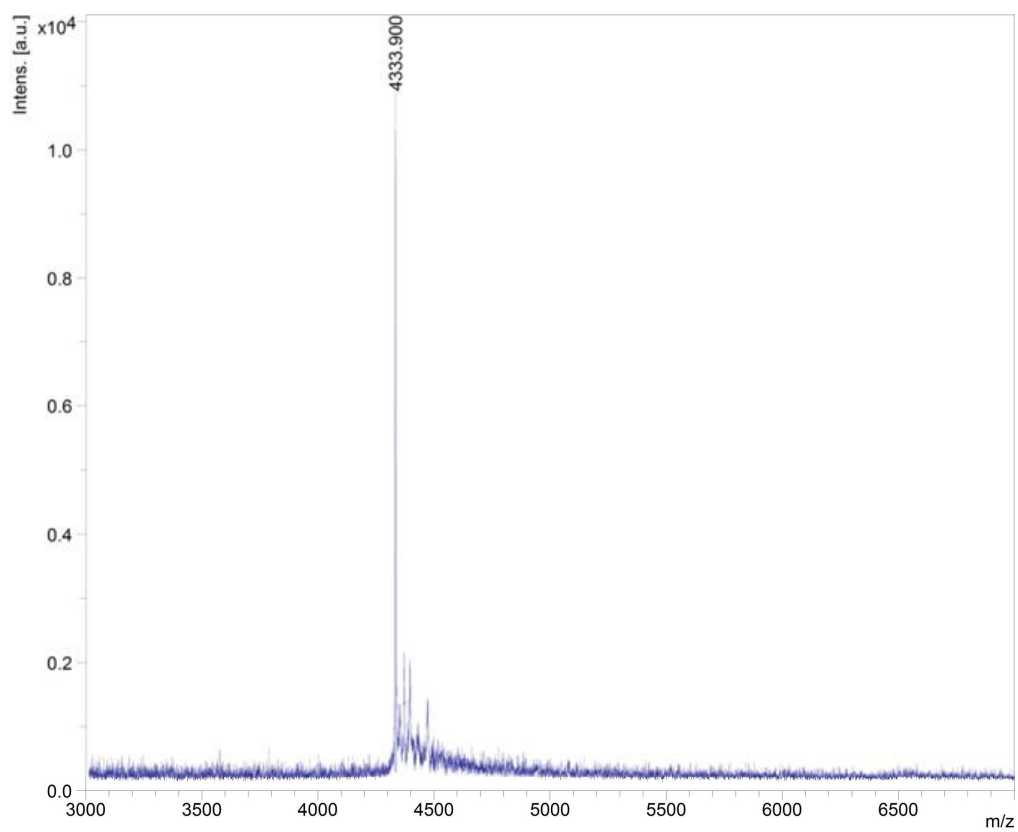
UD-70

[B conc. MeCN: 10-50% (30 min)]

mV



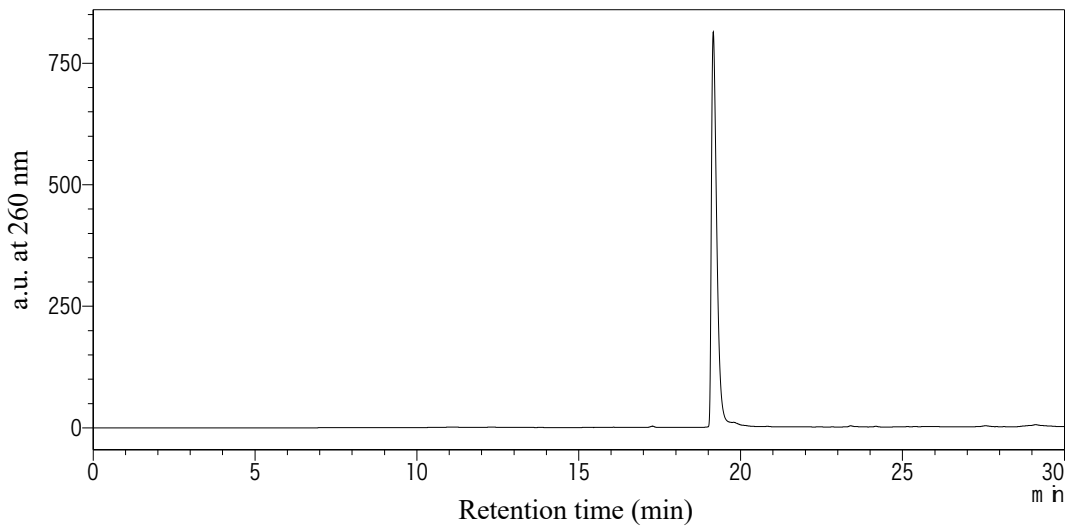
[calcd. (M-H)⁻: 4334.7, found: 4333.9]



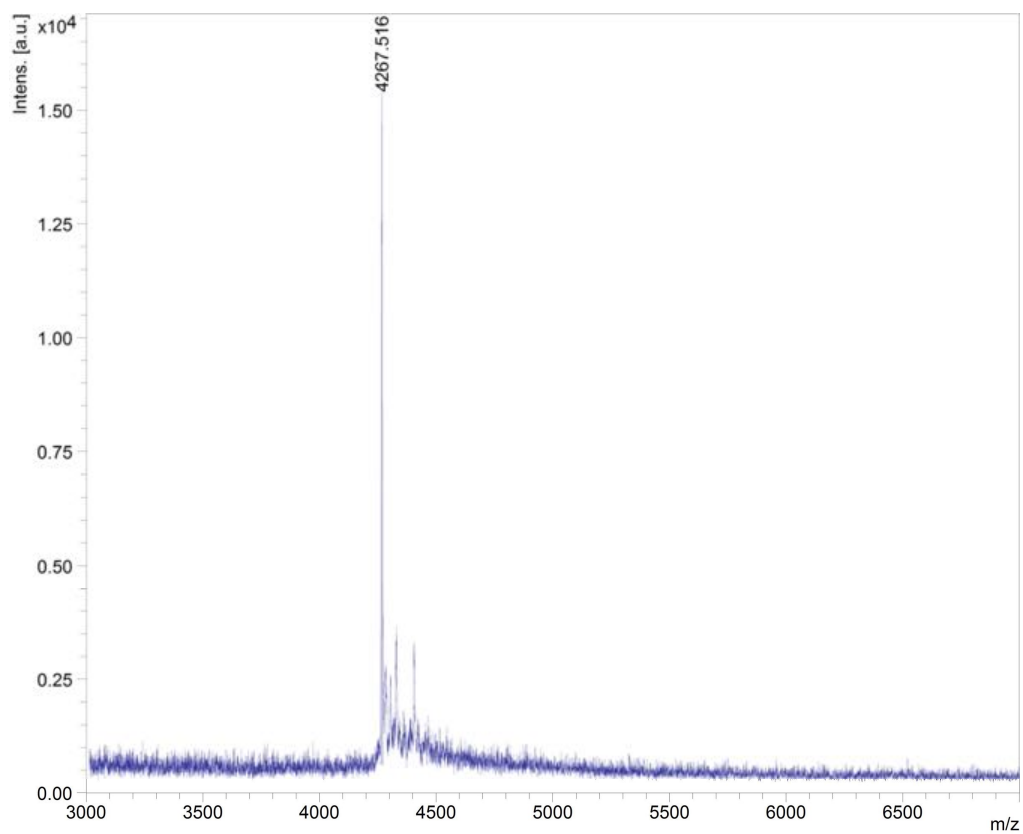
UD-71

[B conc. MeCN: 7-40% (30 min)]

mV



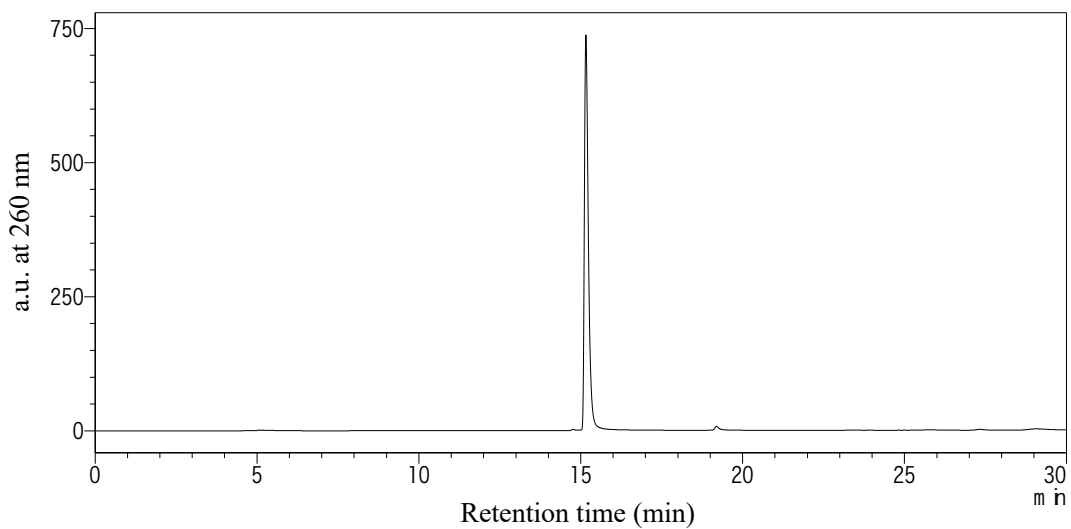
[calcd. (M-H)⁻: 4267.2, found: 4267.5]



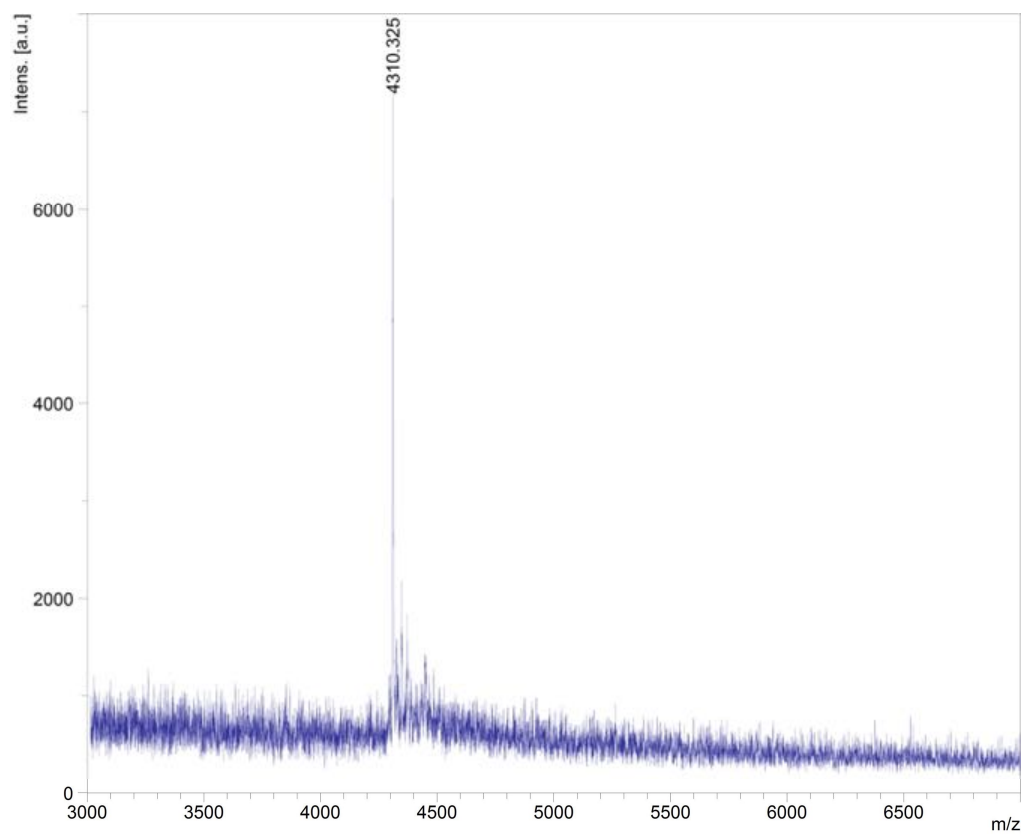
UD-72

[B conc. MeCN: 7-40% (30 min)]

mV



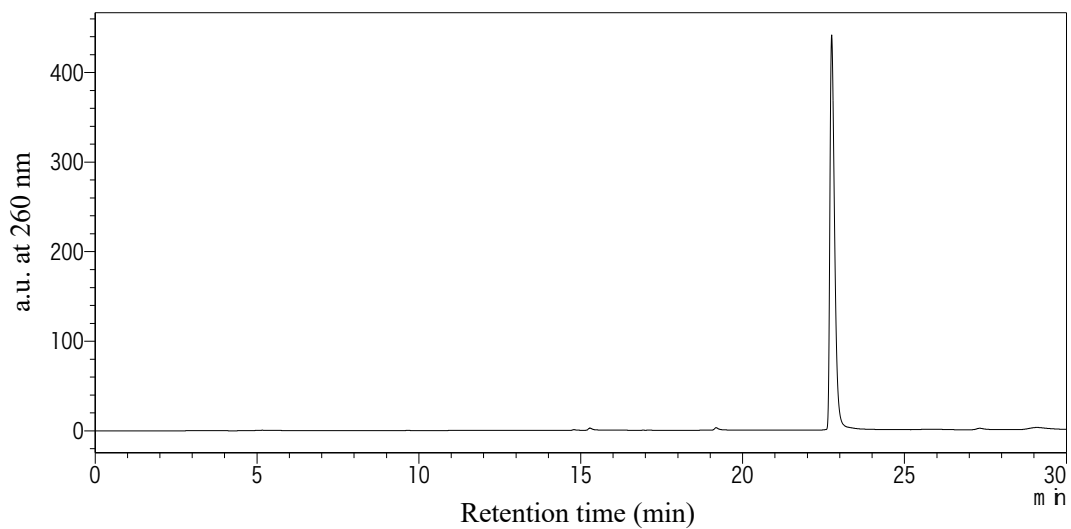
[calcd. (M-H)⁻: 4310.2, found: 4310.3]



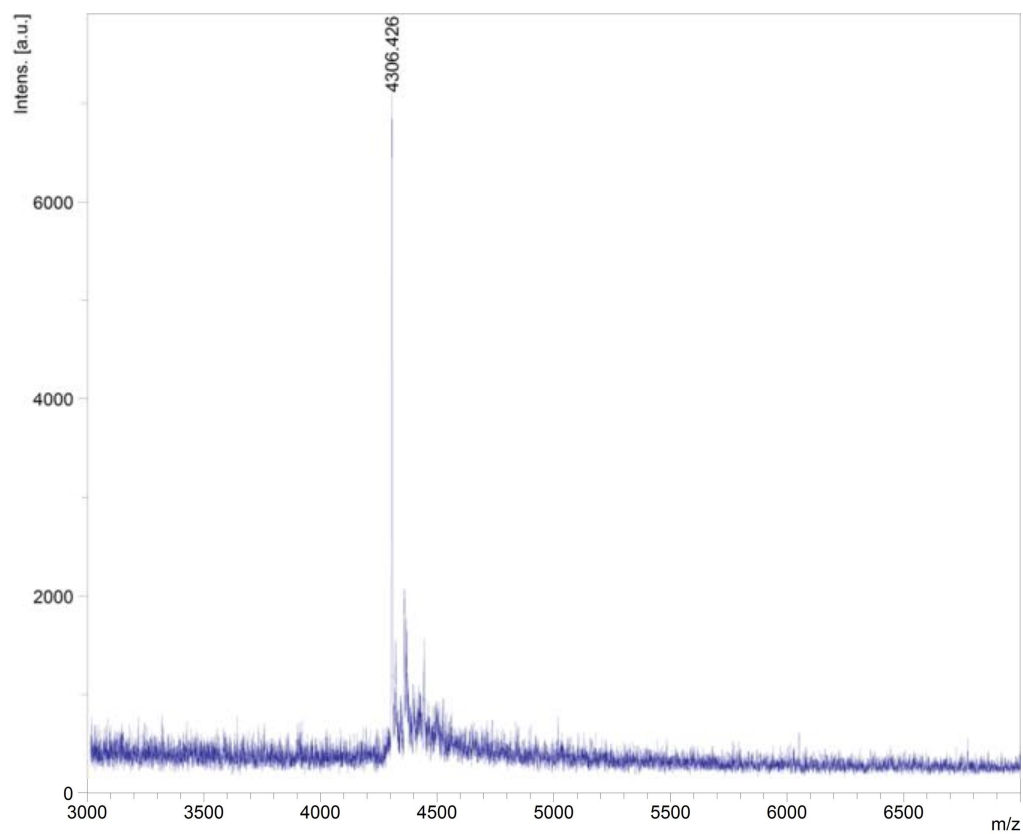
UD-73

[B conc. MeCN: 7-40% (30 min)]

mV



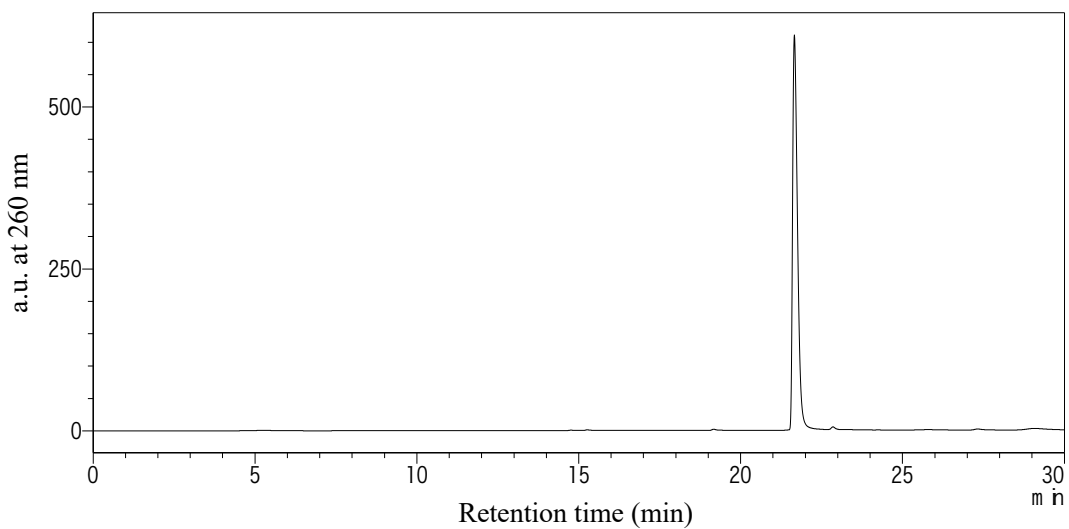
[calcd. (M-H)⁻: 4307.2, found: 4306.4]



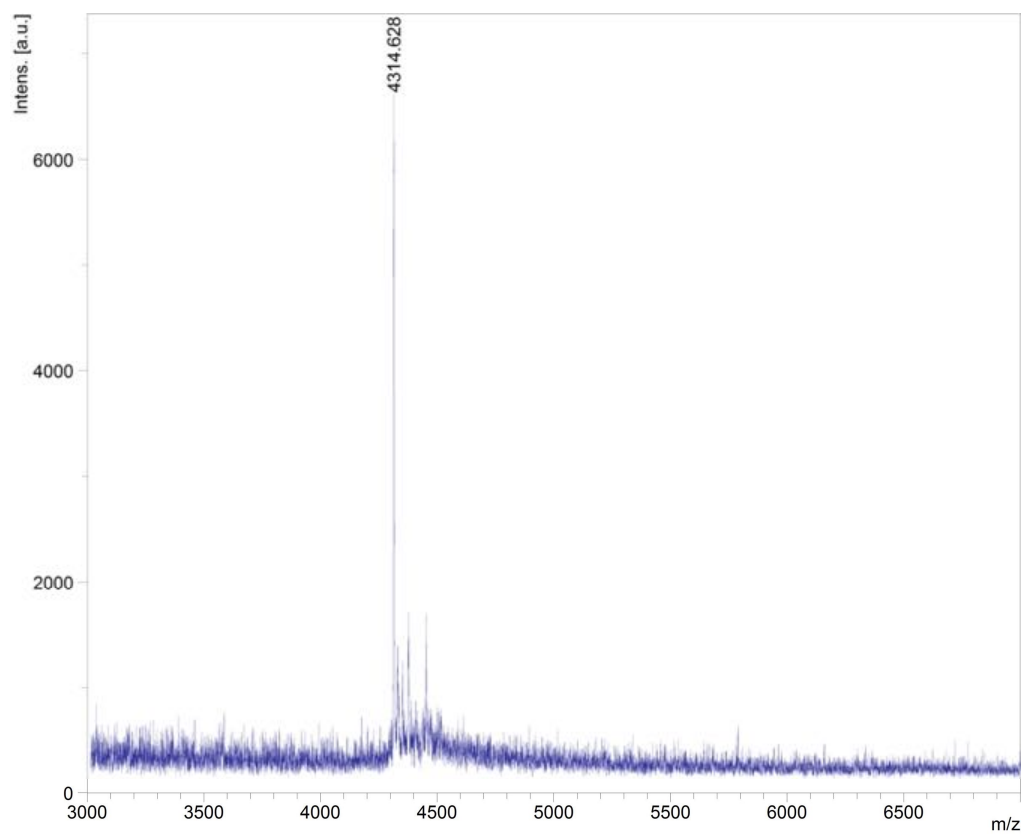
UD-74

[B conc. MeCN: 7-40% (30 min)]

mV

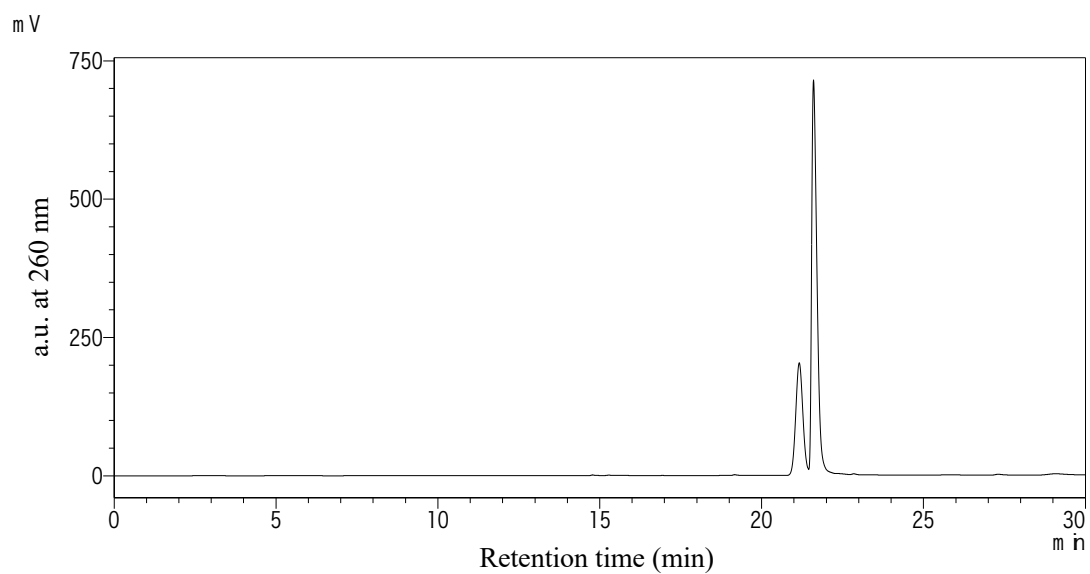


[calcd. (M-H)⁻: 4315.2, found: 4314.6]

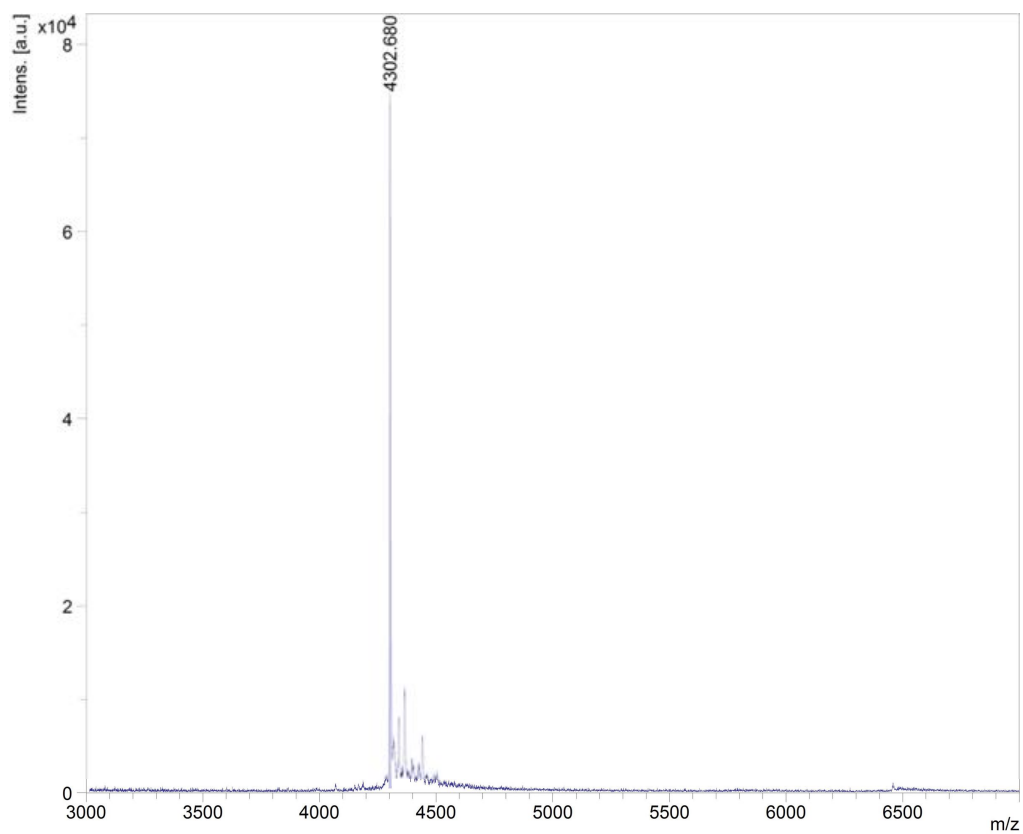


UD-75

[B conc. MeCN: 7-40% (30 min)]



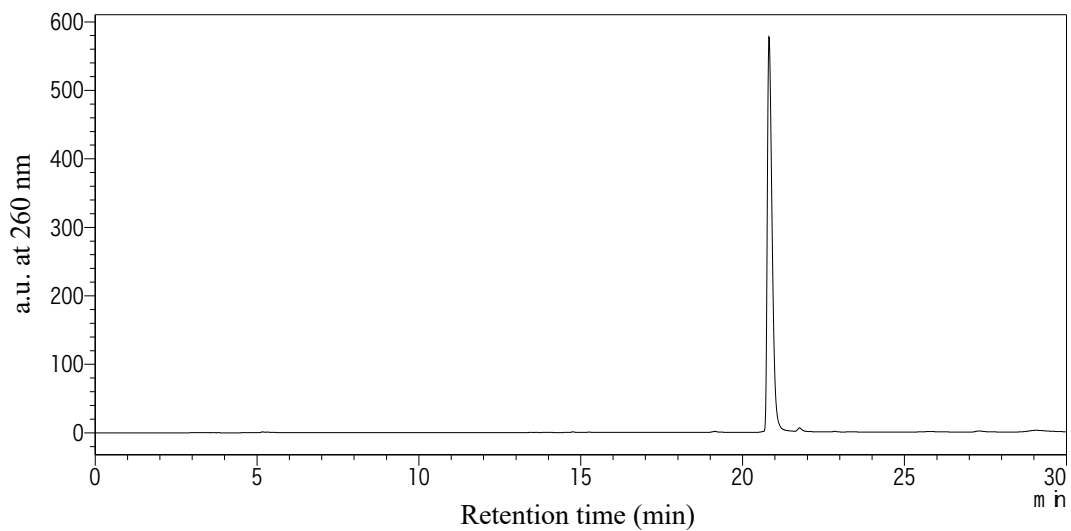
[calcd. (M-H)⁻: 4301.2, found: 4302.7]



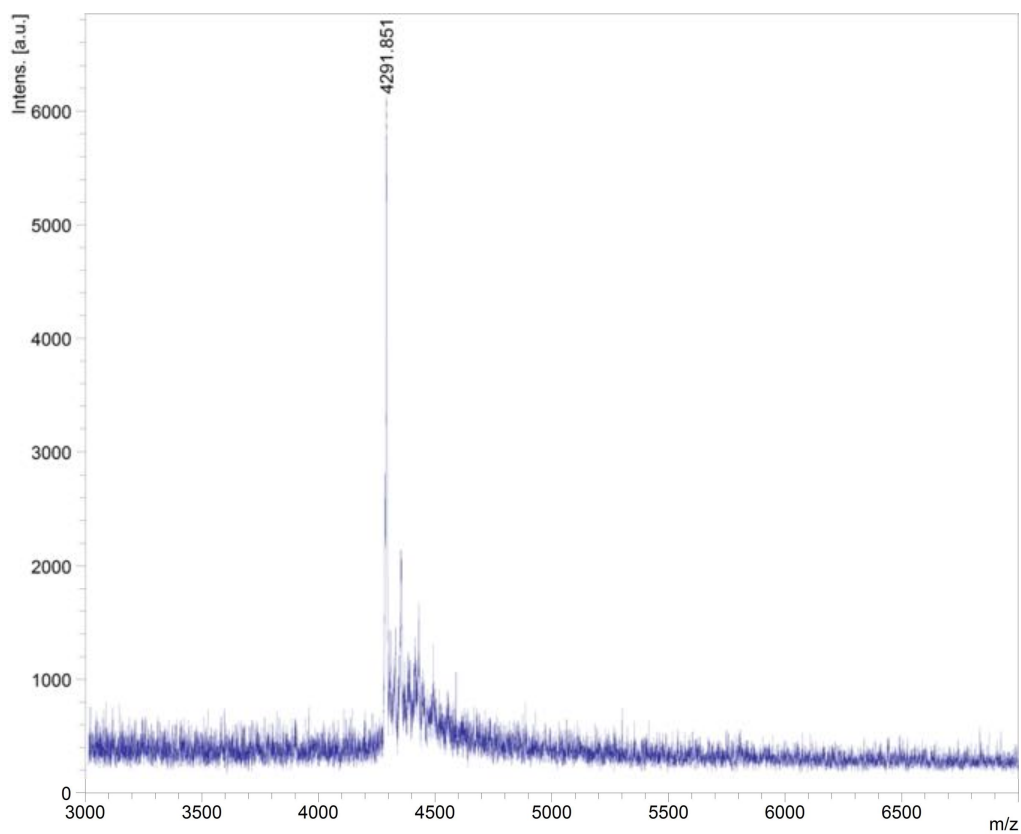
UD-76

[B conc. MeCN: 7-40% (30 min)]

mV



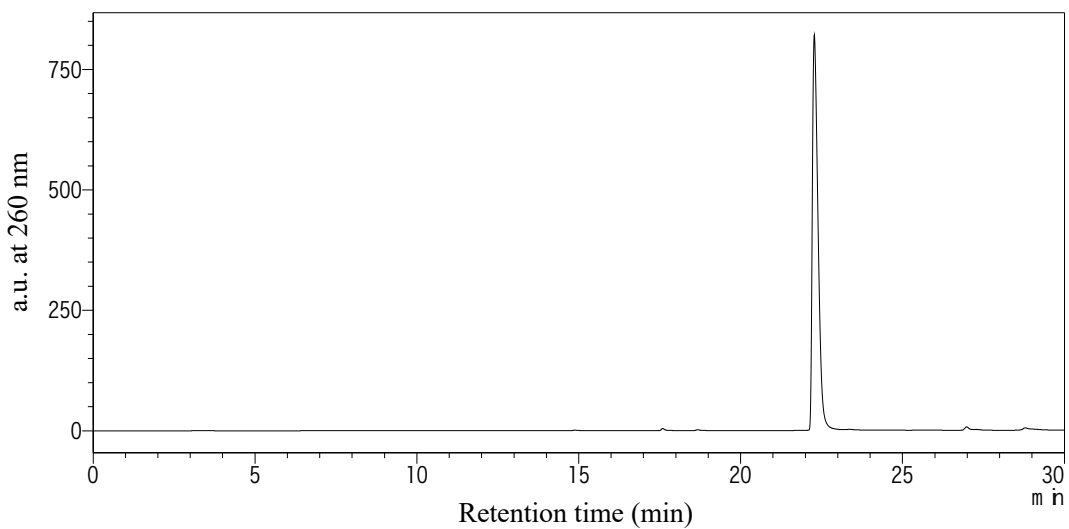
[calcd. (M-H)⁻: 4293.2, found: 4291.9]



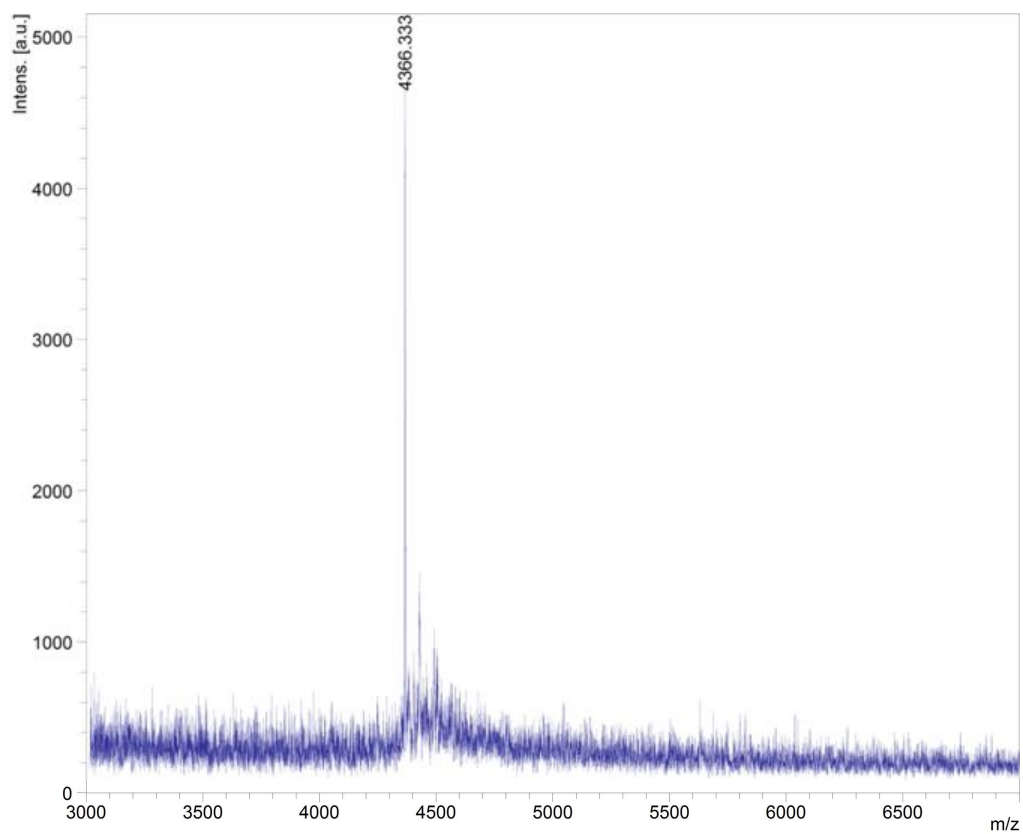
UD-77

[B conc. MeCN: 7-40% (30 min)]

mV



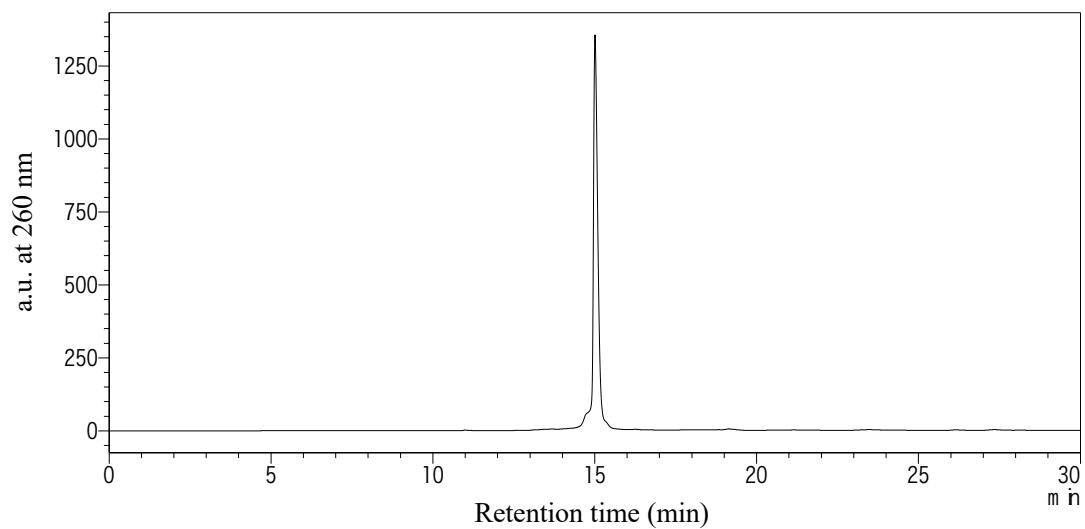
[calcd. (M-H)⁻: 4366.0, found: 4366.3]



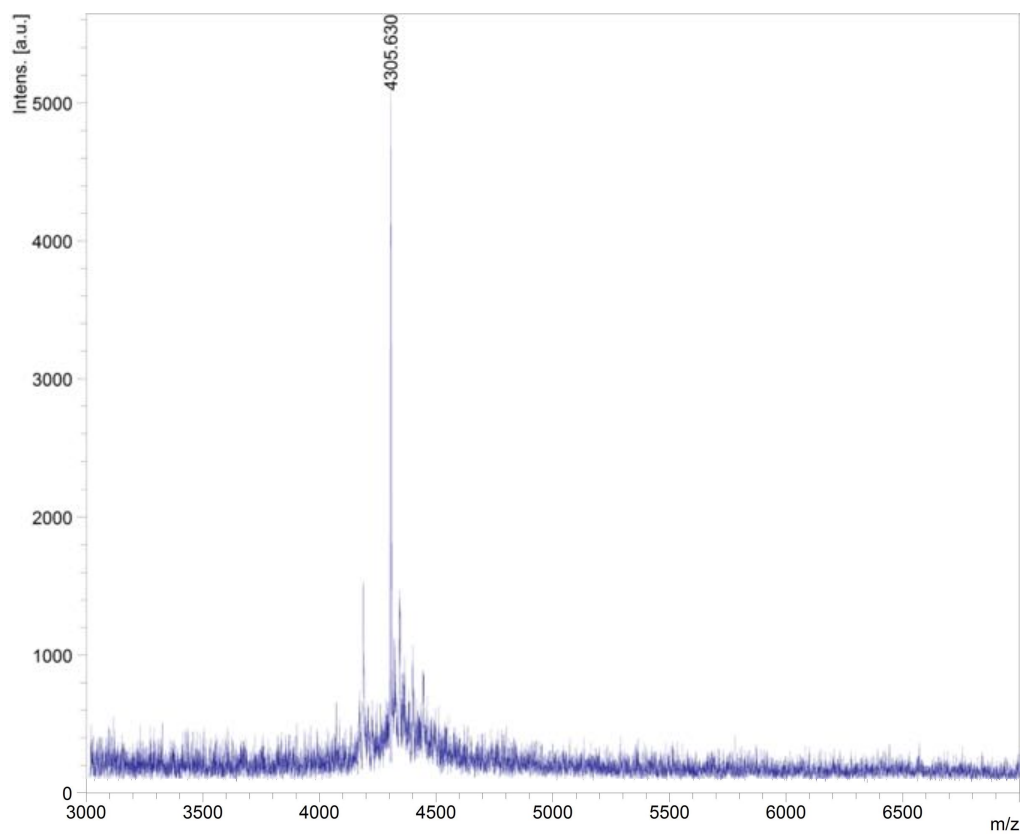
UD-78

[B conc. MeCN: 10-50% (30 min)]

mV



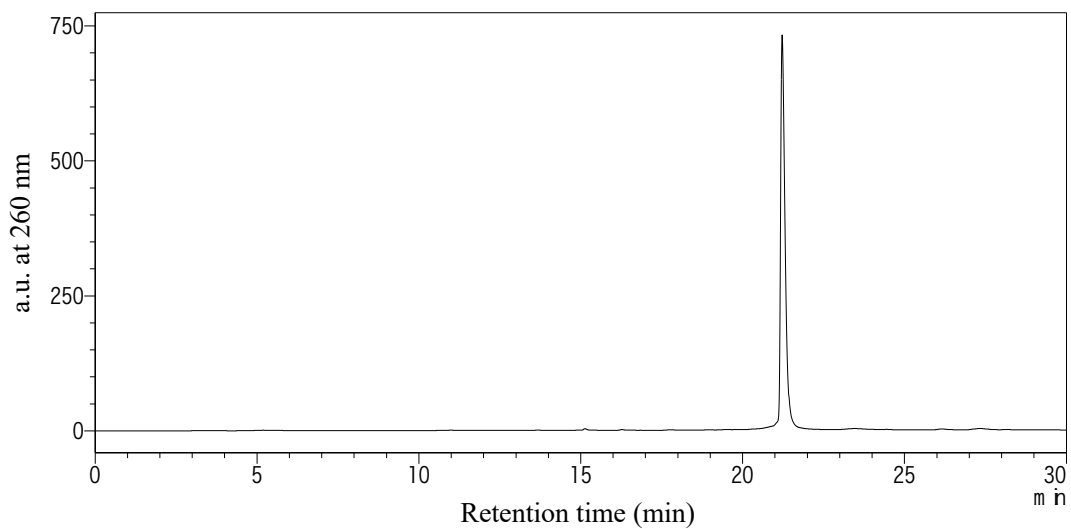
[calcd. (M-H)⁻: 4302.2, found: 4305.6]



UD-79

[B conc. MeCN: 10-50% (30 min)]

mV



[calcd. (M-H)⁻: 4391.3, found: 4390.4]

