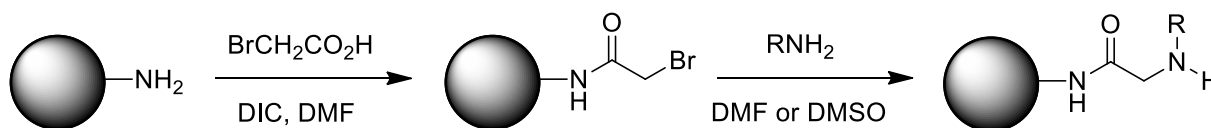


Development of Homo- and Hetero-Multimers of Lung Cancer Specific Peptoids

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1. Basic steps of peptoid synthesis¹

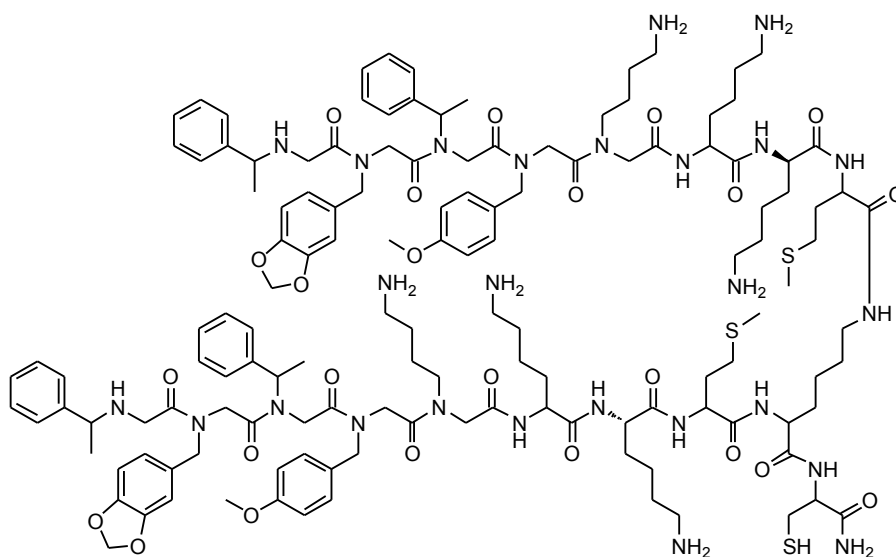


DIC : (Pr)N=C=N(Pr) R : any alkyl group

2. Chemical structures of the multimers synthesized.

2.1 Homo-dimers:

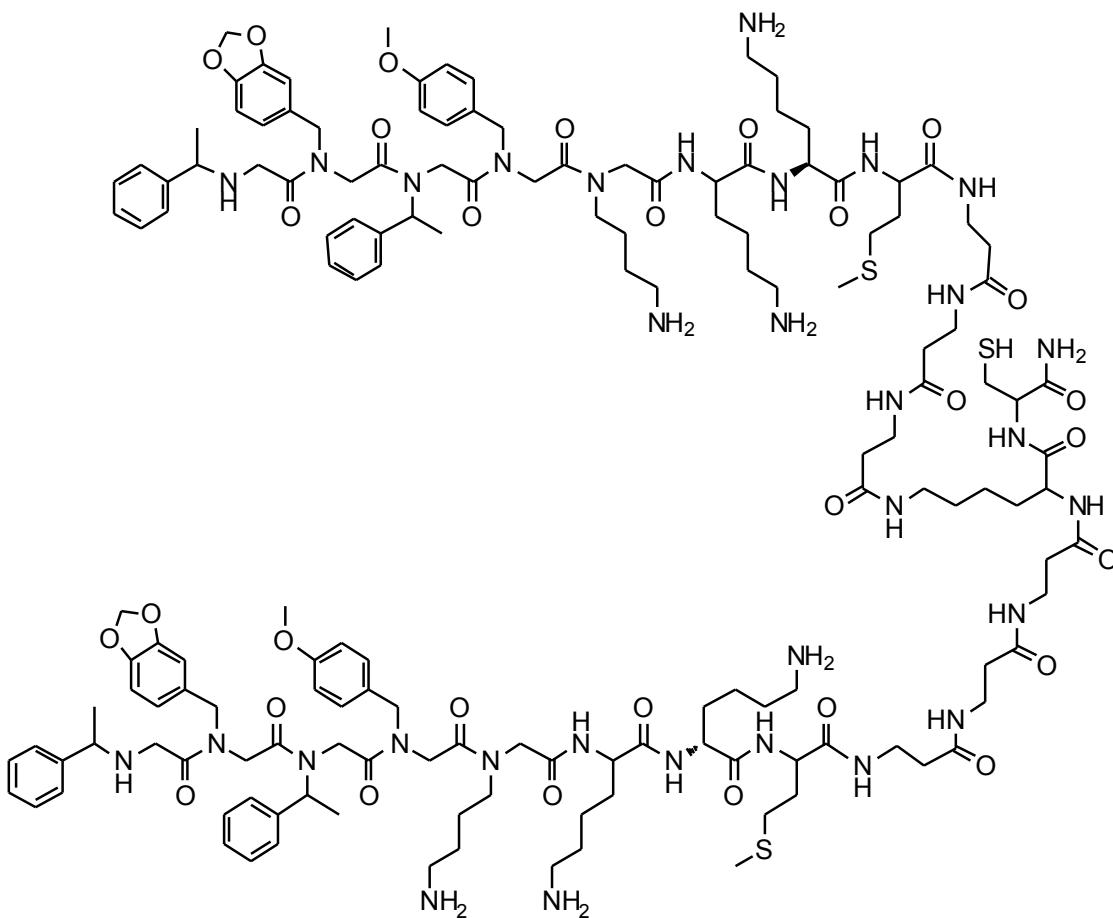
2.1.1 JM79.D1



(MALDI-TOF+) $m/z = 2661.4 [M+H]^+$ (calcd. 2660.4), $2683.2 [M+Na]^+$ (calcd. 2682.4),

HPLC retention time: 27.9 min [40 min 20-50 acetonitrile (0.1% TFA) gradient in H₂O (0.1%TFA)].

2.1.4 JM79.D4

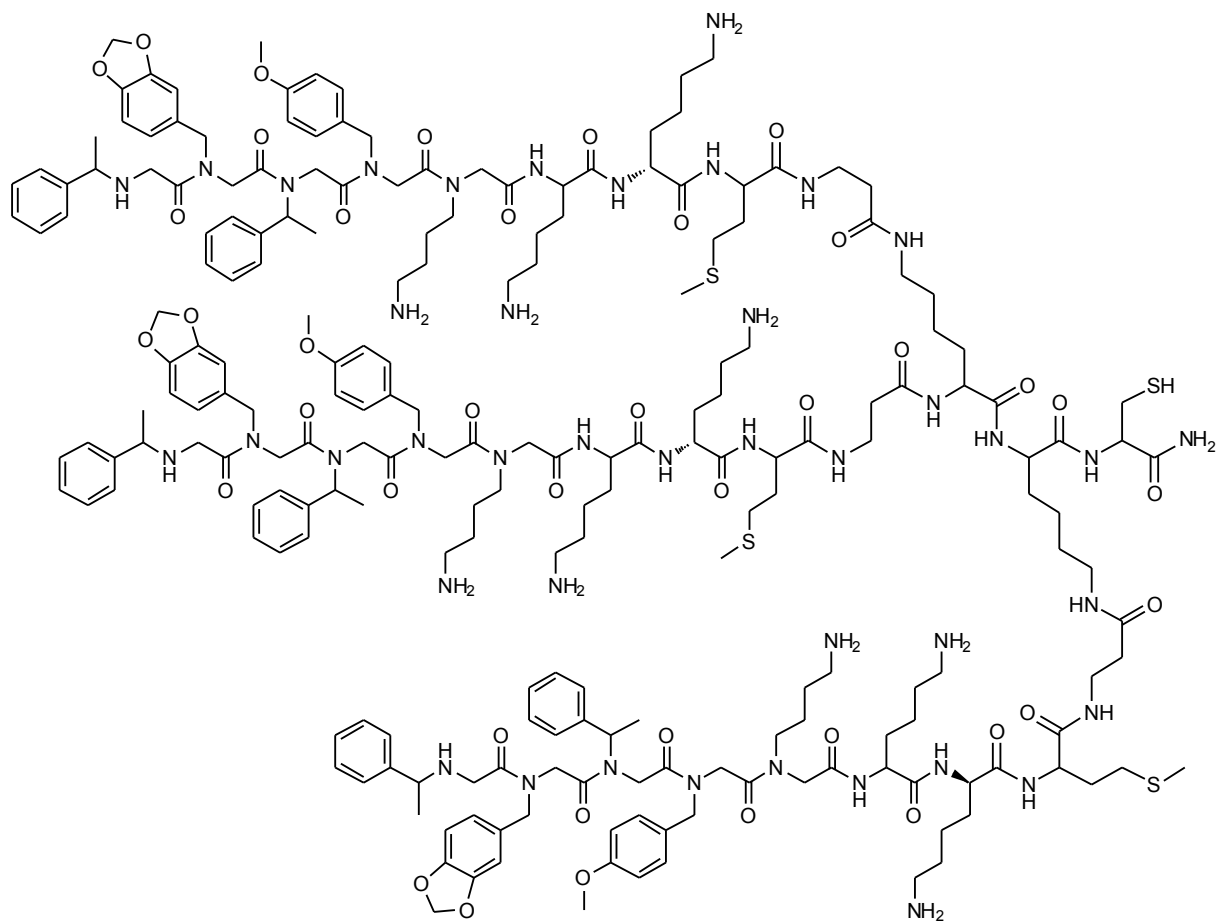


(MALDI-TOF+) $m/z = 3088.1[M+H]^+$ (calcd. 3086.6), $3110.9 [M+Na]^+$ (calcd. 3108.6).

HPLC retention time: 26.2 min [40 min 20-50 acetonitrile (0.1% TFA) gradient in H₂O (0.1%TFA)].

2.2 Homo-Trimers:

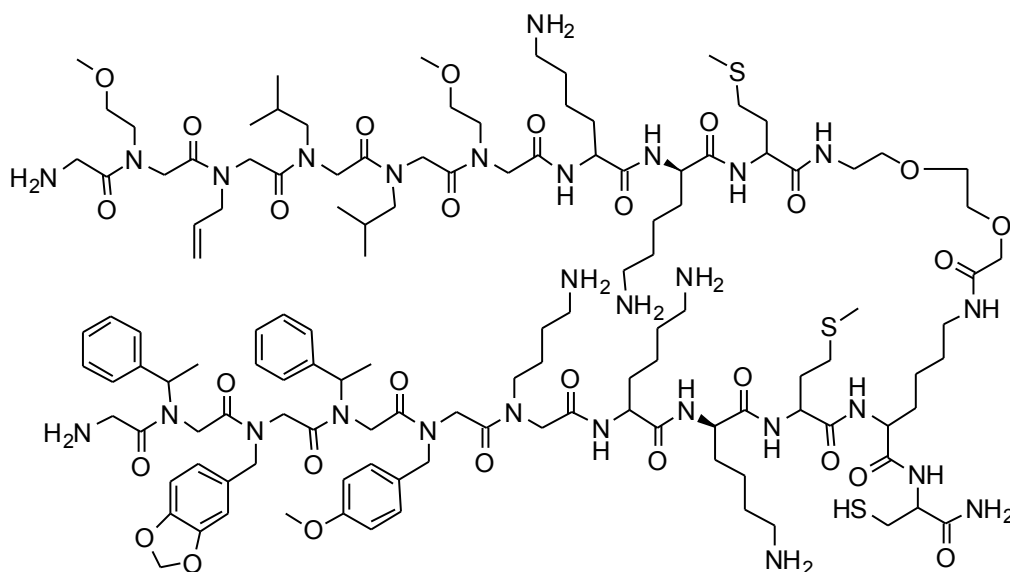
2.2.1 JM79.T1



(MALDI-TOF+) $m/z = 4230.7 [M+Na]^+$ (calcd. 4229.2), $4245.2 [M+K]^+$ (calcd. 4245.2)

2.3 Hetero-drimers:

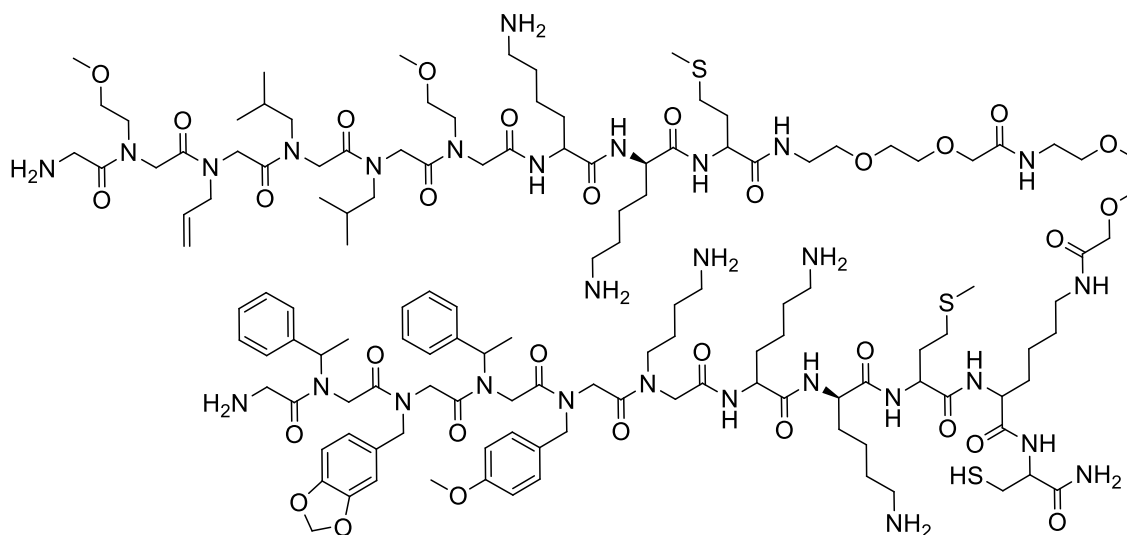
2.3.1 JM79-81.HD1



(MALDI-TOF+) $m/z = 2656.8 [M+H]^+$ (calcd. 2654.5), $2677.7 [M+Na]^+$ (calcd. 2676.5).

HPLC retention time: 18.2 min [30 min 0-75 acetonitrile (0.1% TFA) gradient in H₂O (0.1%TFA)].

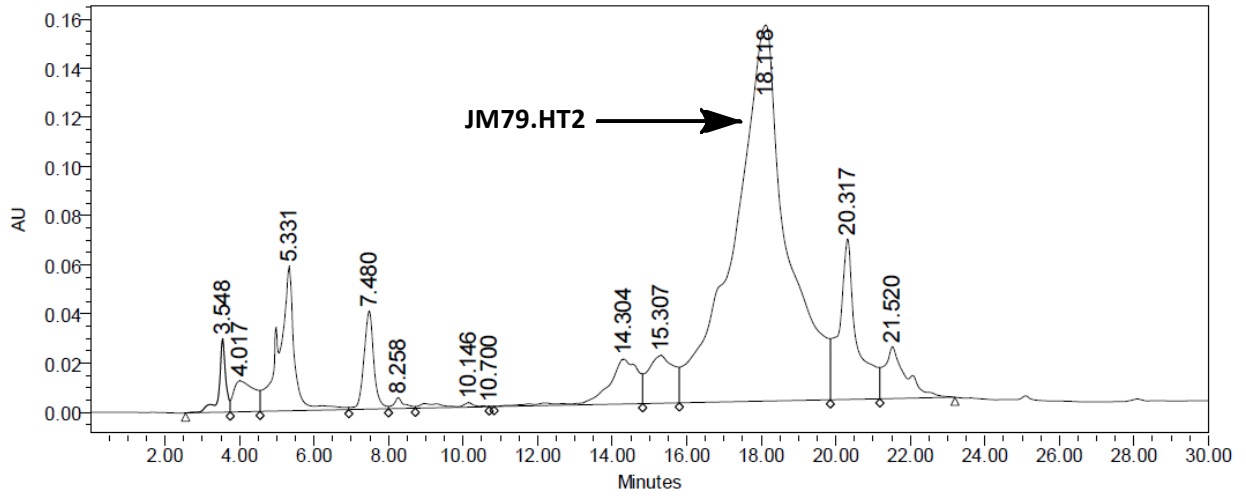
2.3.2 JM79-81.HD2



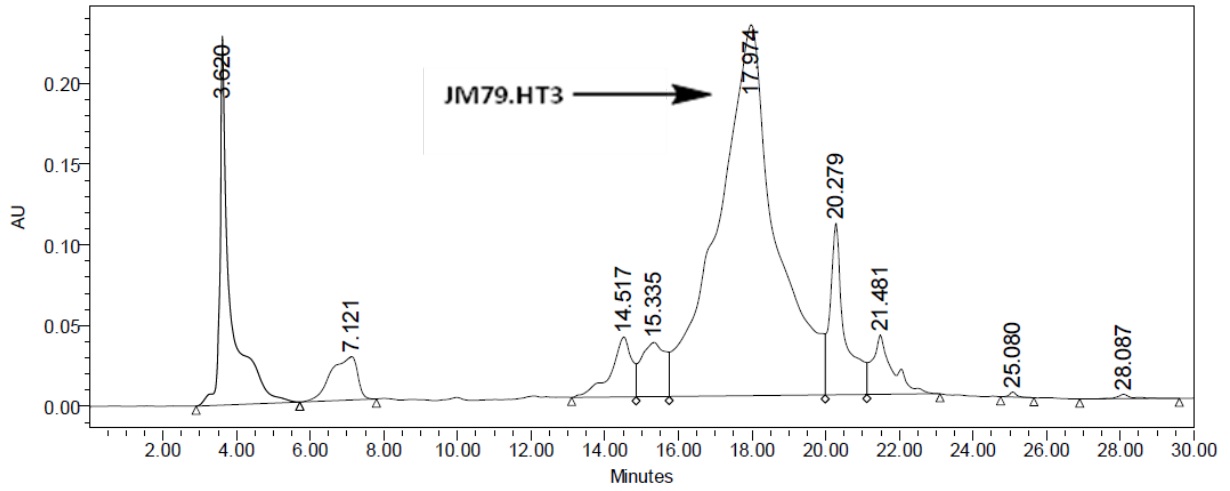
(MALDI-TOF+) $m/z = 2822.3 [M+Na]^+$ (calcd. 2821.5), $2837.1 [M+K]^+$ (calcd. 2837.5).

HPLC retention time: 18.1 min [30 min 0-75 acetonitrile (0.1% TFA) gradient in H₂O (0.1%TFA)]

3.2 JM79-81.HD2



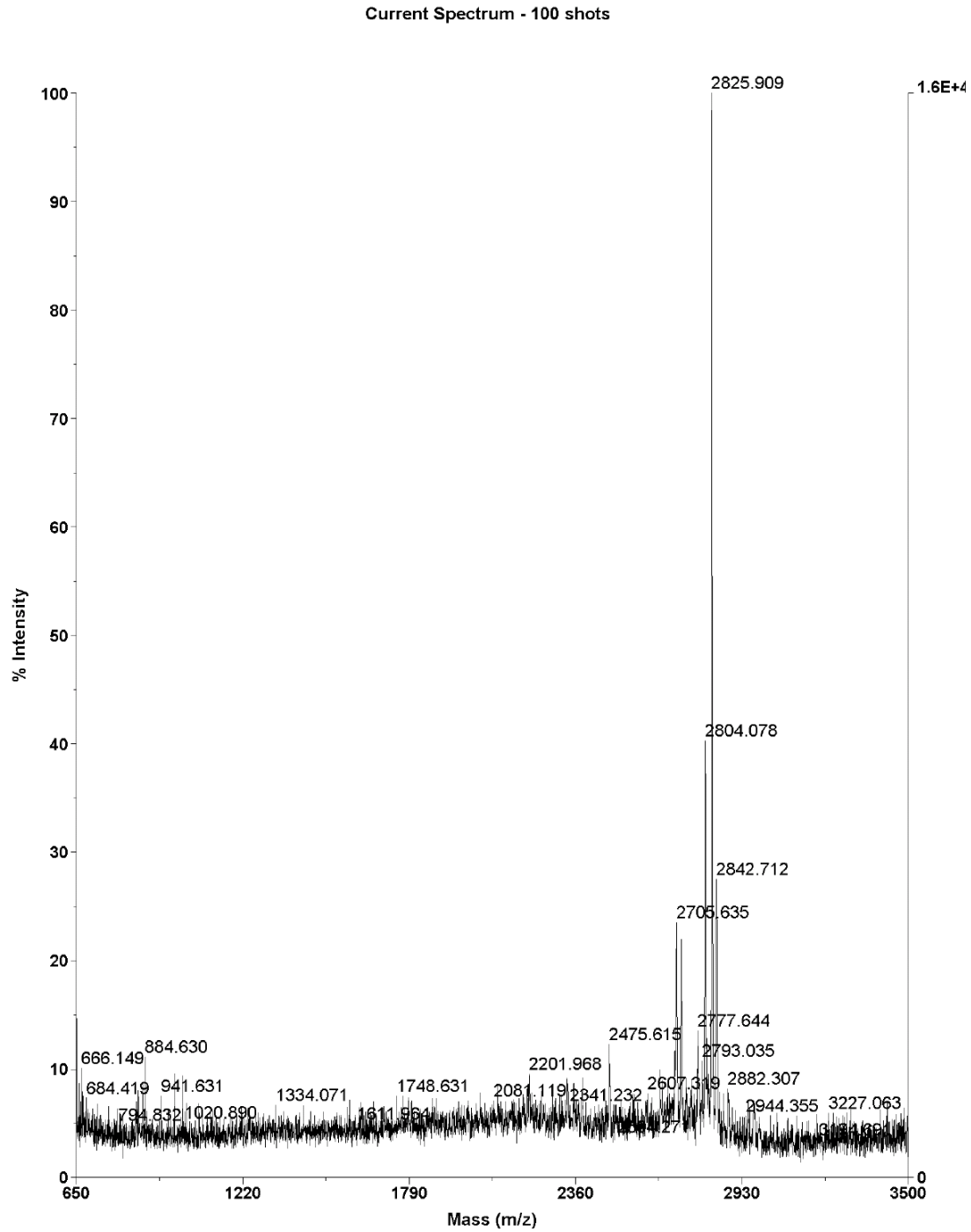
3.3 JM79-81.HD3



4. Representative mass spectrums of for each multimer type:

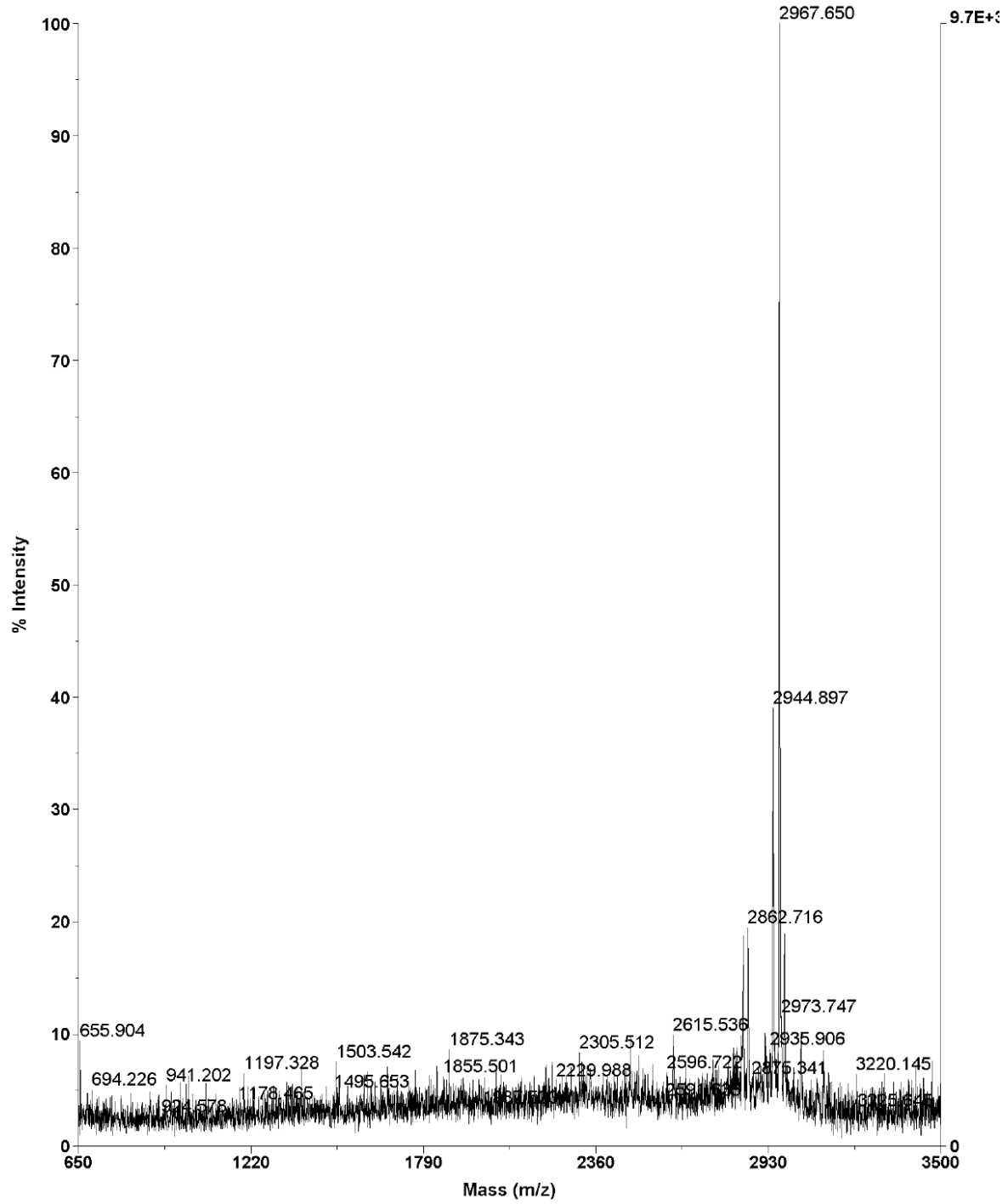
4.1. Homo-dimers:

4.1.1 JM79.D2



4.1.2 JM79.D3

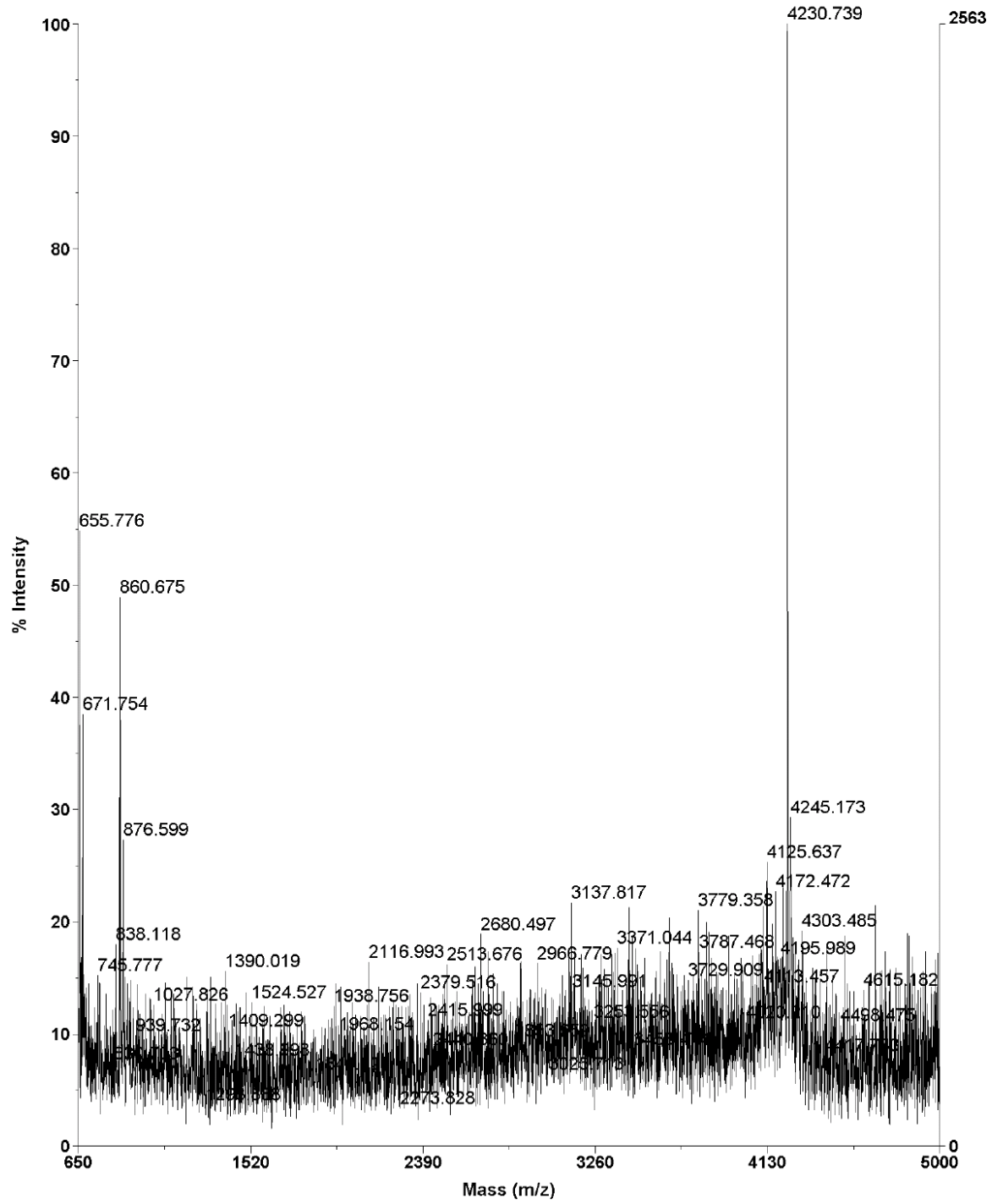
Current Spectrum - 100 shots



4.2 Homo-trimers

4.2.1 JM79.T1

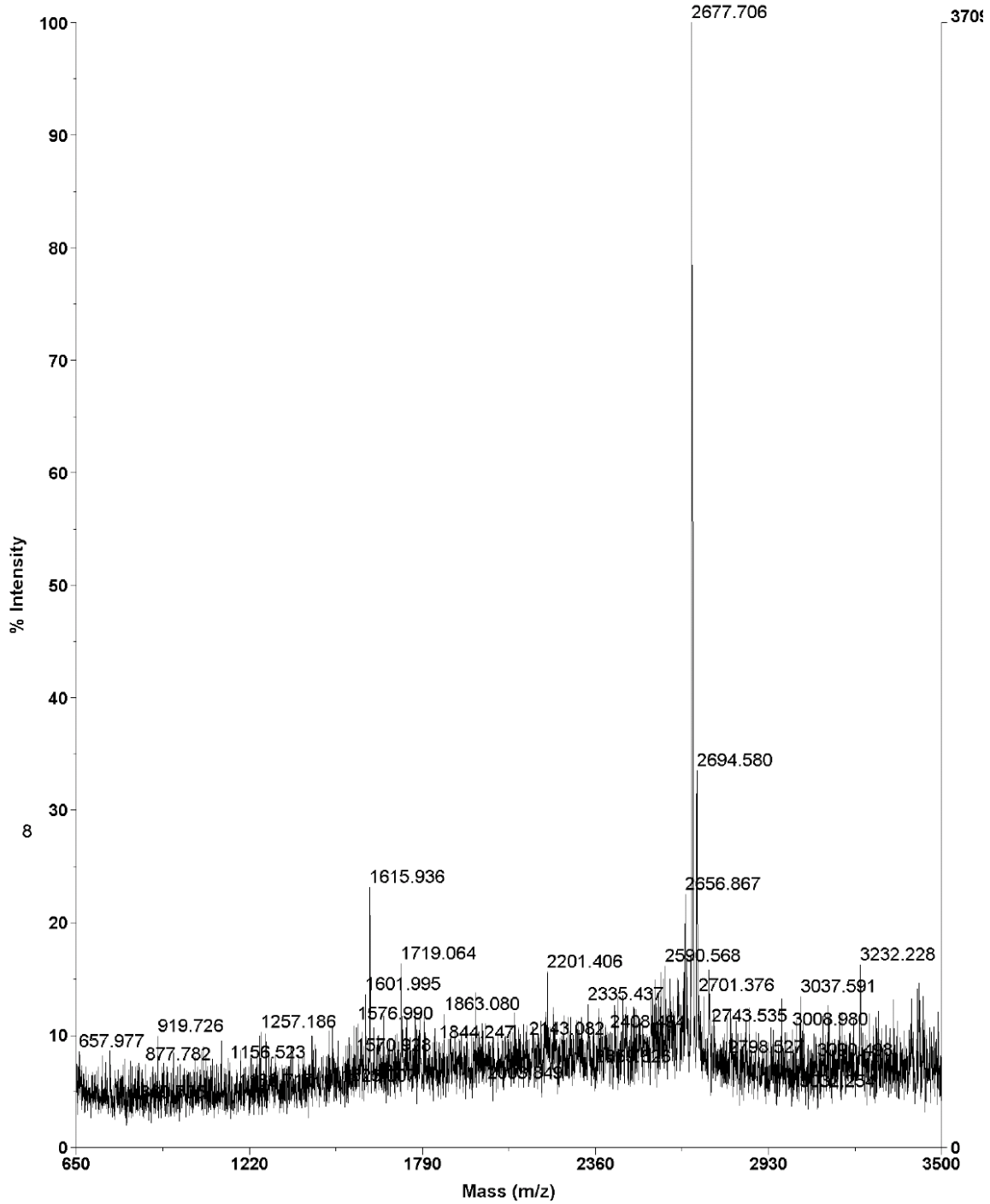
Current Spectrum - 100 shots



4.3 Hetero-dimers

4.3.1 JM79-81.HD1

Current Spectrum - 185 shots



References:

1. Zuckermann, R.N., Kerr, J. M., Kent, S. B. H., Moos, W. H. Efficient method for the preparation of peptoids [oligo(N-substituted glycines)] by submonomer solid-phase synthesis. in *J. Am. Chem. Soc.*, Vol. 114 10646–10647 (1992).