

第七届中国计算蛋白质组学研讨会（CNCP-2023）

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报告题目	<p style="text-align: center;">“Mass+Structure+Knowledge”: A Journey to In-depth Interpretation of Tandem Mass Spectra Derived from RNA Oligonucleotides</p> <p style="text-align: center;">(“质量+结构+知识”：RNA 寡聚核苷酸的质谱深度解析路程)</p>	
个人简历	<p>孙瑞祥 博士</p> <p>北京生命科学研究所一名生物质谱技术的 Superfan，主要从事生物质谱数据的解析研究与软件开发工作：在 ETD 质谱数据、Top-Down 整体蛋白质质谱数据，以及核酸 RNA 的串联质谱数据等方面开展深入的质谱数据解析探索。作为课题负责人，承担了多项国家 863，973 和自然科学基金研究课题。</p> <p>教育经历： 1991-1995 西安交通大学 本科 1995-1996 西安交通大学 硕士 1997-2000 西安交通大学 博士</p> <p>工作经历： 2000-2001 香港科技大学 Research Associate 2002-2004 中国科学院大学 博士后 2004-2018 中国科学院计算技术研究所 副研究员 2016-2017 威斯康星大学（麦迪逊分校）访问学者 2018-至今 北京生命科学研究所 Research Scientist</p> <p>代表论文：</p> <p>(1) Rui-Xiang Sun; Mei-Qing Zuo; Ji-Shuai Zhang; Meng-Qiu Dong; Charge-State-Dependent Collision-Induced Dissociation Behaviors of RNA Oligonucleotides via High-Resolution Mass Spectrometry, Journal of the American Society for Mass Spectrometry, July 18 2023, https://pubs.acs.org/doi/10.1021/jasms.3c00073</p> <p>(2) Rui-Xiang Sun; Rui-Min Wang; Lan Luo; Chao Liu; Hao Chi; Wen-Feng Zeng; Si-Min He; Accurate Proteoform Identification and Quantitation Using pTop 2.0,</p>	

	<p>in Proteoform Identification Methods and Protocols, Springer, 105-129, 2022</p> <p>(3) Rui-Xiang Sun; Lan Luo; Long Wu; Rui-Min Wang; Wen-Feng Zeng; Hao Chi; Chao Liu; Si-Min He; pTop 1.0: A High-Accuracy and High-Efficiency Search Engine for Intact Protein Identification, Analytical Chemistry, 2016, 88(24): 3082-3090</p> <p>(4) Rui-Xiang Sun; Meng-Qiu Dong; Chun-Qing Song; Hao Chi; Bing Yang; Li-Yun Xiu; Li Tao; Zhi-Yi Jing; Chao Liu; Le-Heng Wang; Yan Fu; Si-Min He; Improved Peptide Identification for Proteomic Analysis Based on Comprehensive Characterization of Electron Transfer Dissociation Spectra, Journal of Proteome Research, 2010, 9(12): 6354-6367</p> <p>(5) Mei-Qing Zuo; Rui-Xiang Sun; Meng-Qiu Dong; D/E-rich peptides are less suitable than D/E-deficient peptides for identification by negative-ion HCD due to scarce production of sequencing ions from multiply charged precursors, International Journal of Mass Spectrometry, 2023, 483(116975): 1-11</p>
<p>报告摘要</p>	<p>Mass spectrometry (MS) has been evolving into one of the indispensable tools to elucidate biomolecule structures with widespread applications in biomedical research. Particularly, last decade has witnessed the increasing efforts stretching into DNA and RNA oligonucleotide characterization using tandem mass spectrometry (MS/MS), which includes sequencing RNAs or characterizing their post-transcriptional modifications. However, MS fragmentation behaviors of RNA oligos are so far understood insufficiently. In this talk, I will report our work that characterized the negative-ion-mode fragmentation behaviors of 30 synthetic RNA oligos containing four to eight nucleotides using multiple fragmentation methods, including CID, HCD, UVPD, and EThcD on a high-resolution, accurate-mass instrument. We found that MS/MS spectra derived from RNA oligos were much more complicated than those from peptides or proteins. There are more gas-phase dissociation pathways available for RNAs than for peptides, hence more fragment ions, and dispersed intensities. Moreover, the MS/MS spectra of RNA oligos are greatly affected by their precursor charge states. Among nine types of sequencing ions (<i>a-B</i>, <i>b</i>, <i>c</i>, <i>d</i>, <i>w</i>, <i>x</i>, <i>y</i>, <i>z</i>), we, for the first time, found that the intensity of <i>w</i> ions in CID/HCD spectra is highly correlated to 5'-side nucleotide around the cleavage site and the precursor charge state. Additionally, our analysis revealed that high-charge RNA oligos containing 3'-U, tended to produce precursors with NCO⁻ losses in CID/HCD spectra, which presumably corresponded to cyanate anions. All these findings provide valuable insights for better comprehending the mechanisms behind RNA fragmentation by MS/MS, thereby facilitating future automated identification of RNA oligos based on their MS/MS spectra in a more efficient manner.</p>