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TopSpec

Project Deliverable Report

D8.4 Public Demonstration of TopSpec Technology

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Author: Jan Commandeur (MS)

Contributors: Susanna Lundström (KI)

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CONTENTS

1 Background

In order to promote uptake of the technologies and applications developed in the TopSpec project, various different activities were planned and undertaken. These activities include publication of open access scientific articles, Twitter-, and TopSpec website posts, workshops, videos and contributions at scientific conferences. Each of these activities were targeted at different audiences, ranging from the scientific community to the layman audience. These activities are reported in this document.

2 Public demonstrations of TopSpec technology

2.1 First European Top-Down Proteomics Symposium

The first European Top-Down Proteomics Symposium was organized on February 12-14 2019 at Institut Pasteur, Paris, France, by Julia Chamot-Rooke (Institut Pasteur, TopSpec Consortium Partner) and the Consortium for Top-Down Proteomics. The symposium focused on top-down proteomics, the analysis of intact proteins and protein complexes using high-resolution mass spectrometry. The symposium was attended by several TopSpec Consortium Partners; Julia Chamot-Rooke, Alexander Makarov, Yury Tsybin and Jan Commandeur as well as representatives from Karolinska Institutet and Fasmatech. During the meeting, world-leading experts in top-down proteomics (among those Dr. Chamot-Rooke, Dr. Makarov and Dr. Tsybin) were presenting advances in technologies and approaches within the field. A wide range of topics was covered including the latest developments in instrumentation, sample preparation both in denaturing and native conditions, intact protein fractionation/separation, data analysis as well as applications in life sciences and human health. Additionally, attendees were engaged in discussions on the future directions, challenges, and opportunities for top-down proteomics. During one of the sessions Julia Chamot-Rooke announced the TopSpec initiative (**Figure 1**).

Figure 1. *Julia Chamot-Rooke announcing the TopSpec initiative to an interested audience*

2.2 Former Prime Minister of Greece visits Omnitrap lab in Athens

Dimitris Papanastasiou welcomed the former prime minister of Greece, Alexis Tsipras, to Fasmatech during his visit to Lefkippos Technical Park, Athens, Greece, on March 19, 2019. The Omnitrap was the highlight of the lab visit, and the European collaboration in TopSpec was explicitly mentioned. A video of the visit is available on YouTube, **Figure 2** shows a still from the video.

Figure 2. *Former prime minister of Greece Alexis Tsipras (second from left) is introduced to the Omnitrap by Dimitris Papanastasiou (right) during his visit to Fasmatech.*

2.3 AutoVectis workshop at the Ardgour Symposium

David Kilgour, Nottingham Trent University, held a work shop and presented the latest features and upgrades of AutoVectis v9 (part of WP7), at the 2019 EMSG Ardgour Symposium, held on September 16-20 in the Peak district, UK (**Figure 3**). The Ardgour Symposium is an interdisciplinary scientific meeting centred around the users and developers of scientific instrumentation.

The Symposium structure has been refined over the years to provide an environment that is designed to foster the development of new productive networks. The meeting was attended by 20 scientists from across Europe (countries and nationalities represented: Italy, Netherlands, France, Germany, Romania, Hungary, Sweden and the UK) and the wider world (USA and India) and had a mixture of scientific sessions, group networking sessions, workshops and free discussion time.

In addition to David, Susanna Lundström (KI) attended the meeting and gave a presentation with the title “MS analysis of polyclonal antibodies – the ultimate challenge and reward”. Both David and Susanna acknowledged TopSpec. The project was discussed, and the webpage was also advertised during the meeting.

Figure 3. *David Kilgour presenting the latest features of AutoVectis*

2.4 SMAP 2019

"De Spectrométrie de Masse et Analyse Protéomique" (SMAP) is the annual French mass spectrometry society meeting with up to 350 participants from academia and industry. The 2019 meeting was held on September 16-19 in Strasbourg, France, and was a great opportunity for interdisciplinary networking across different fields with mass spectrometry as the common denominator. Mathieu Dupré (IP) peaked interest in TopSpec following his presentation (**Figure 4**).

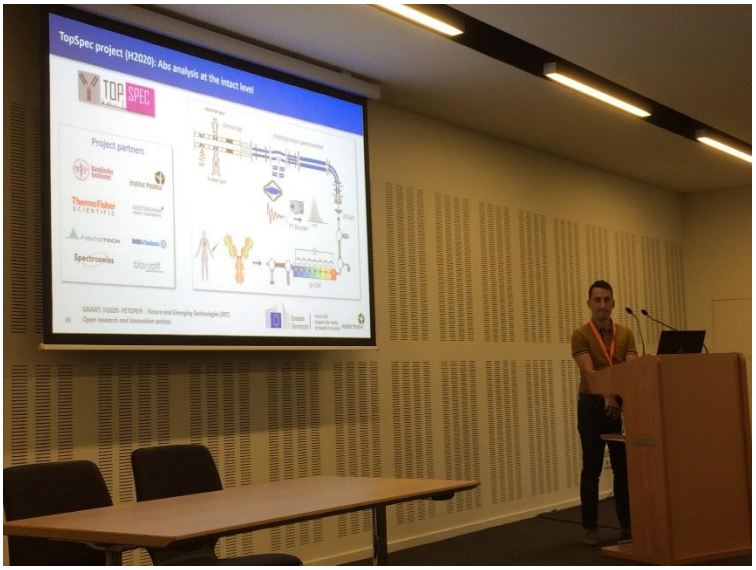

Figure 4. *Mathieu Dupré advertising the TopSpec project*

2.5 IITB Proteomics Bootcamp

David Kilgour (TNTU) travelled to the Indian Institute of Technology Bombay, Mumbai, India, to teach as part of the international faculty at the IITB Proteomics Bootcamp: "Basic and Advanced Proteomics Techniques – Omics Technologies for Life Sciences". This two-week course focused on:

- Proteomics: basic and advanced technologies,
- Other omics technologies – genomics, metabolomics etc

- Big data analysis and bioinformatics

The program also included a mixture of lectures, hands-on workshops and tutorials. It was aimed at life science and medical researchers. Overall, there were more than 50 attendees, who came from across India. The faculty included lecturers from the UK, India and the US.

Dr Kilgour gave lectures on electrospray ionisation, basic Fourier transform mass spectrometry concepts, and an introduction to absorption mode FTMS data processing. The TopSpec project was discussed specifically as an example of the future direction and cutting edge of protein analysis in biomedical research. A picture from the meeting is given in **Figure 5**.

Figure 5. *IITB Proteomics bootcamp participants*

2.6 ASMS 2020 (June 1-12, virtual only)

The Annual Conference on Mass Spectrometry and Allied Topics (ASMS) is the biggest conference in the world for everything mass spectrometry related. It is usually attended by more than 6,500 scientists of the community and with over 3,000 papers presented as posters and talks. Due to COVID, the conference was held electronically in 2020. The TopSpec consortium was represented by Mariangela Kosmopoulou, Fasmatech who presented a poster titled "*Top-down Analysis of Intact Antibodies under Denatured and Native Conditions on the Omnitrap Platform Coupled to an Orbitrap Mass Spectrometer* ". The poster is available on the TopSpec website. Furthermore, Konstantin Nagornov, Spectroswiss presented his poster titled "*Protein-grade FTMS Isotopic Simulator to guide the experiment design and data analysis in top-down proteomics*".

2.7 IMSF focus group on instrumentation

Dimitris Papanastasiou (Fasmatech) and Yury Tsybin (Spectroswiss) held presentations at the first International Mass spectrometry foundation (IMSF) Focus Group in "Instrumentation". The idea behind the focus groups is to make the IMSF community more interactive for members with an aim to create fruitful discussions between young researchers with experts to (as stated in the IMSF webpage) "interlink brains, serve as think tanks, and raise interests for yet unexplored areas." The Webinar series that was held March

9 – 18, 2021, was highlighting the advancement in MS instrument development, showcasing the latest in MS instrument developments. Both the talks from Dimitris Papanastasiou (Fasmatech): "*Multiple-Stage Multidimensional Ion Activation Workflows in the Omnitrap Platform coupled to Ion Mobility and Orbitrap Mass Spectrometry*" and Yury Tsybin (Spectroswis): "*Harnessing the power of the un-reduced data in FTMS*" were advertised on-line (**Figure 6**) by IMSF.

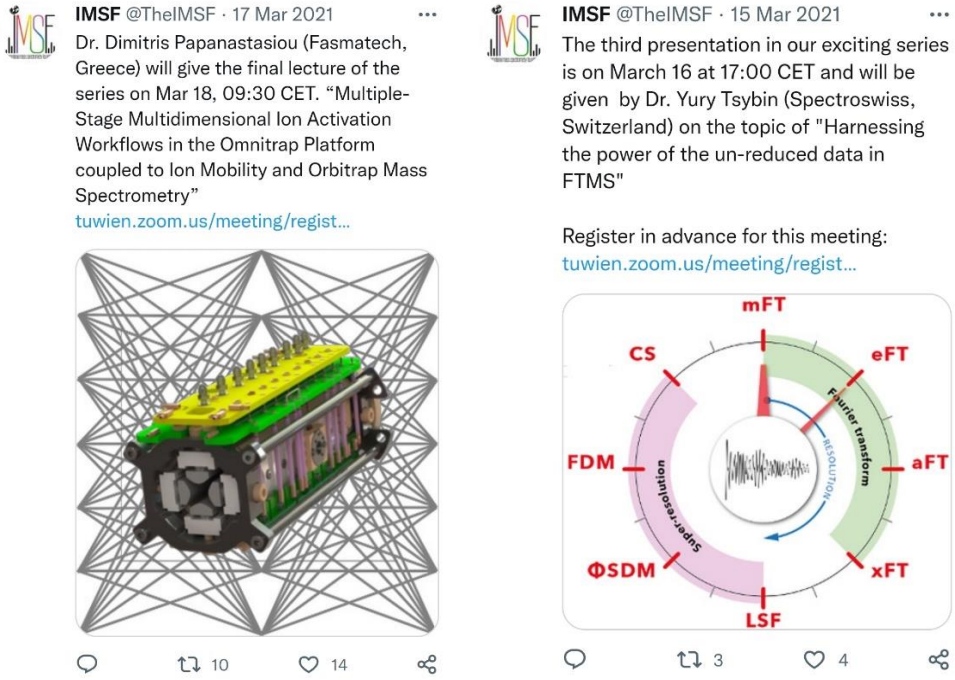

Figure 6. *Tweets from the IMSF twitter page, advertising the talks from TopSpec partners, Fasmatech and Spectroswiss, respectively.*

2.8 ASMS 2021

The Annual Conference on Mass Spectrometry and Allied Topics was held in person in fall 2021 in Pennsylvania, USA. TopSpec partner Spectroswiss was present and had both a presentation talk by Yury Tsybin (Novel data acquisition approaches for enhanced ion detection in FTMS instruments (spectroswiss.ch) and a poster (PP4.pdf (spectroswiss.ch)). In **Figure 7** several tweets from the event are shown.

Figure 7. *Tweets documenting the ASMS 2021 event. In the picture to the left, Yury Tsybin.*

2.9 EuPA 2022

On April 3-7, the 14th annual congress of the European Proteomic Association, EuPA 2022, took place in Leipzig, Germany. This conference is the largest European conference within the proteomics field. The scientific program can be found here: https://www.proteomic-forum.com/programme/scientific-programme. Julia Chamot-Rooke (**Figure 8**) delivered her lecture titled "Expanding the Role of Proteoforms in the Field of Infectious Disease" during the Top-down proteomics & native mass spectrometry session, promoting the TopSpec project when she spoke about future directions.

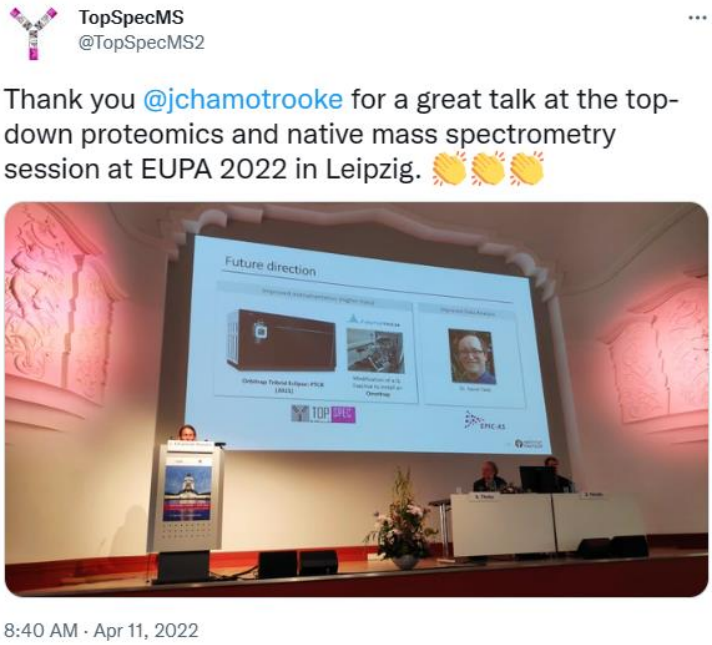

Figure 8. *Julia Chamot-Rooke promoting TopSpec during her presentation at EUPA 2022*

2.10 ASMS 2022

Finally, after two years with a reduced number of participants due to COVID, the Annual Conference on Mass Spectrometry and Allied Topics was back at full capacity at the 70th ASMS conference in Minneapolis, June 5-9, 2022. TopSpec was promoted by Fasmatech, Institut Pasteur, Spectroswiss and MS Vision. A highlight at the conference was the poster from Fasmatech on MS^4 experiments with intact mAbs. A tweet from the TopSpec account is shown in **Figure 9**.

***Figure 9**. Tweet acknowledging contributions by the consortium partners during ASMS 2022.*

2.11 IMSC 2022

During the International Mass Spectrometry Conference (IMSC) 2022, organized August 27 – September 2, in Maastricht, Netherlands several contributions by members of the TopSpec consortium were shared with the community. Fasmatech (**Figure 10**) contributed with oral presentations by Dimitris Papanastasiou on Top-down analysis of intact antibodies and Mariangela Kosmopoulou on EID and ECD on the Omnitrap-Orbitrap system. Furthermore, Athanasios Smyrnakis presented a poster on advanced top-down approaches for intact antibodies with the Omnitrap platform. During the IMSF focus group session on instrumentation Dimitris

Papanastasiou lectured on the arduous road to the finished Omnitrap. David Kilgour, Nottingham Trent University presented two posters on protein fragmentation and analysis. Yury Tsybin, Spectroswiss had an oral presentation on Deconvolution-free feature extraction and annotation via time-domain transient modelling. The full program can be found here https://www.imsc2022.com/programme/general-programme/.

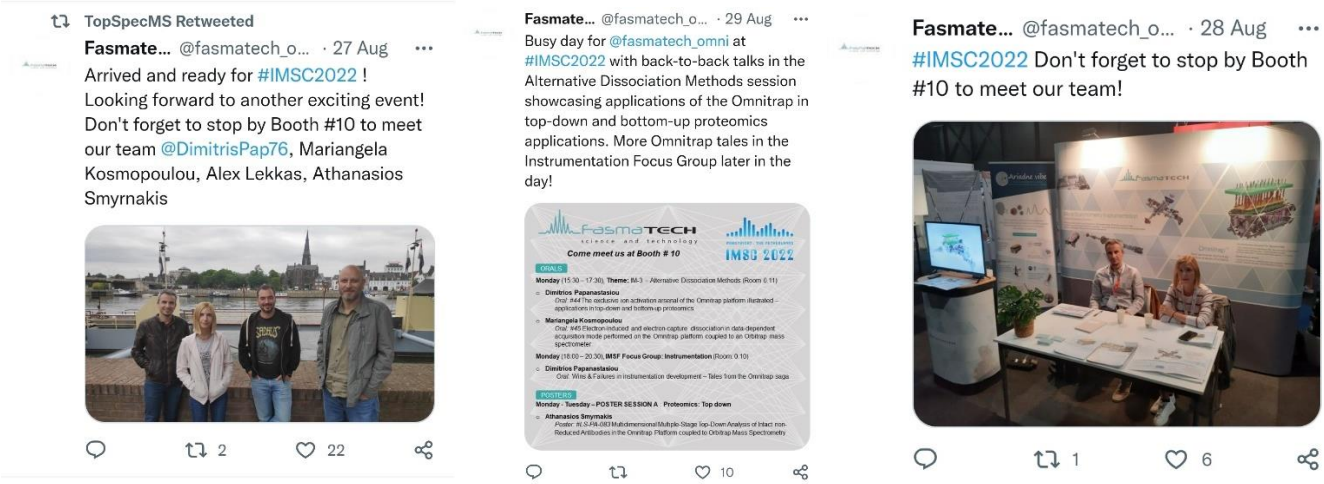

Figure 10. *Tweets showcasing contributions to the scientific program at IMSC2022 by Fasmatech.*

2.12 Omnitrap Workshop and training – KI

In October 2022, the omnitrap was finally installed at Karolinska Institutet. During the installation week (October 10-14), Fasmatech and MS Vision held a crash course in the instrumentation, attended by KI research scientists, staff, visiting researchers and students as well as online attendees (**Figure 11**).

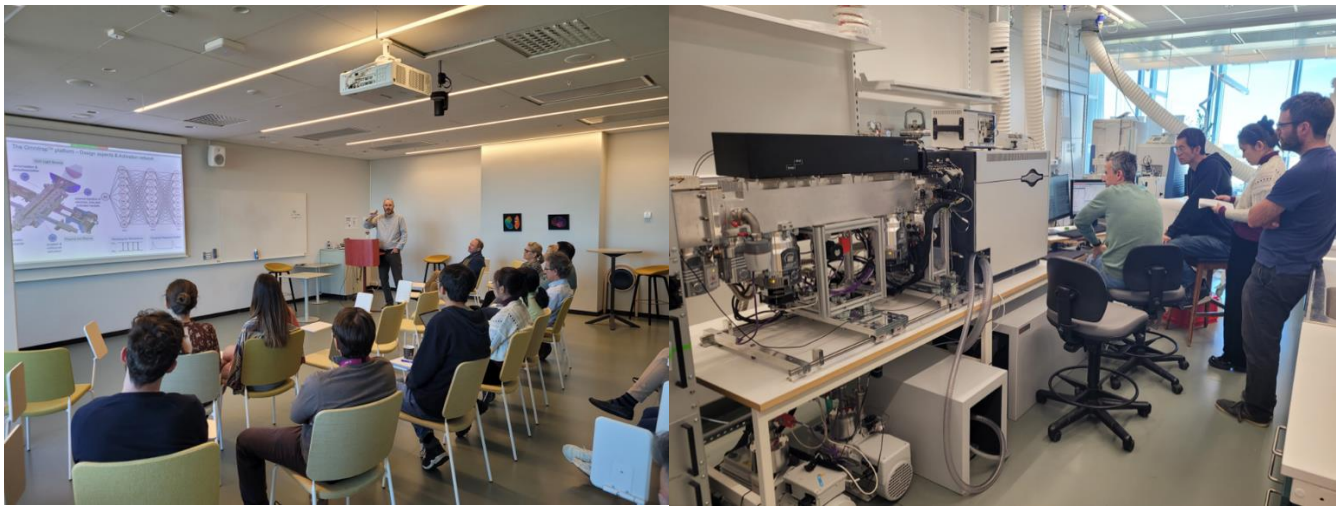

Figure 11. *Activities held during the omnitrap installation week at KI. Attendees were not only representatives from KI, but the online activities were also attended by students and researchers from Stockholm University, University of Helsinki, University of Barcelona, Uppsala University, University of Basel and Xi'an Jiaotong University.*

2.13 Fasmatech lab visit by members of the Greek parliament

In November 2022, two members of the Greek parliament visited Fasmatech, Georgios Koumoutsakos and Christos Tarantilis. Christos Tarantilis is Chairperson of the Hellenic Parliament's Committee on Research and Technology, and Professor at the Athens University of Economics and Business. Mr Koumoutsakos and Professor Tarantilis were given a lab tour by Dimitris Papanastasiou, Fasmatech's R&D Director. During the tour Dr. Papanastasiou showed the Omnitrap connected to a Q Exactive and gave an explanation on its merits and recent achievements with the platform, highlighting the TopSpec project. **Figure 12** shows a Tweet from Prof. Tarantilis which he posted shortly after his visit.

Figure 12. *Tweet by Prof. Tarantilis after his visit to Fasmatech's lab. The left picture on the middle row shows him with Dr. Papanastasiou next to the TopSpec MS platform.*

2.14 KI labtour visit by BioMS platforms

On November 9, 2022, a guided lab tour in the Zubarev lab, KI, for representatives from all BioMS (Swedish National Infrastructure for Biological Mass Spectrometry, https://bioms.se/) platforms in Sweden was given. During the tour the newly installed TopSpec platform peaked extra interest of the attendees which could see the potential in using the instrument in multiple applications ranging from protein structure analysis, glycomics and glycoproteomics, proteogenomics and chemical proteomics.

2.15 MS Booster Workshop and software training – KI

In late November 2022, the MS booster was finally installed at Karolinska Institutet. During the installation week (November 28- December 2), Spectroswiss and NTU held a crash course in the instrumentation and available software, attended by KI research scientists, staff, visiting researchers and students as well as online attendees (**Figure 13**).

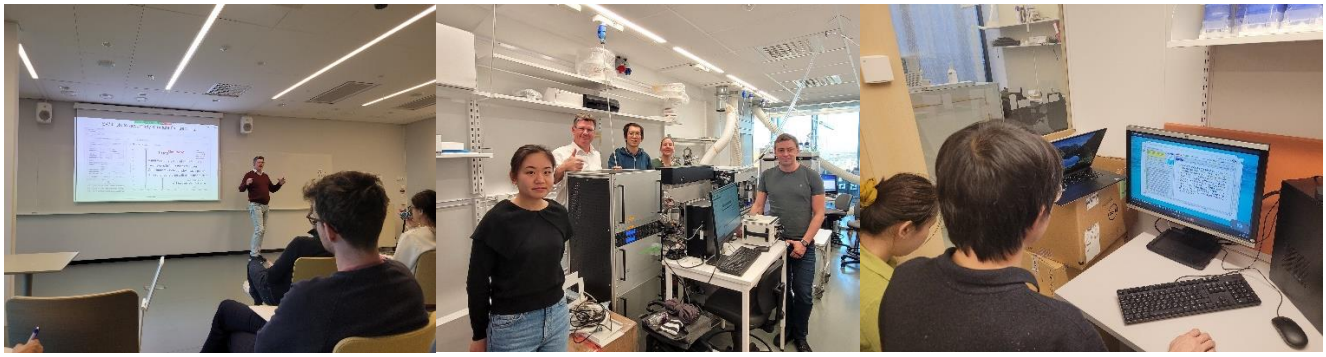

***Figure 13**. Activities held during the MS booster installation and software training at KI. Attendees were not only representatives from KI, but the online activities were also attended by students and researchers from Stockholm University, University of Helsinki, University of Barcelona and Xi'an Jiaotong University.*

2.16 Video

A 3-minute video introducing the TopSpec project to a wider audience is currently in preparation with the aim to have the video finalized by the end of the year or prior the final review meeting (January 26), the latest. The video features comments from all consortium partners, highlighting the various aspects of the project, and shows animations of the system as well as lab footage. The video will be published on YouTube and will be promoted on the websites and media of the consortium partners as well as the TopSpec website. I screenshot of the current version of the video is given in **Figure 14**.

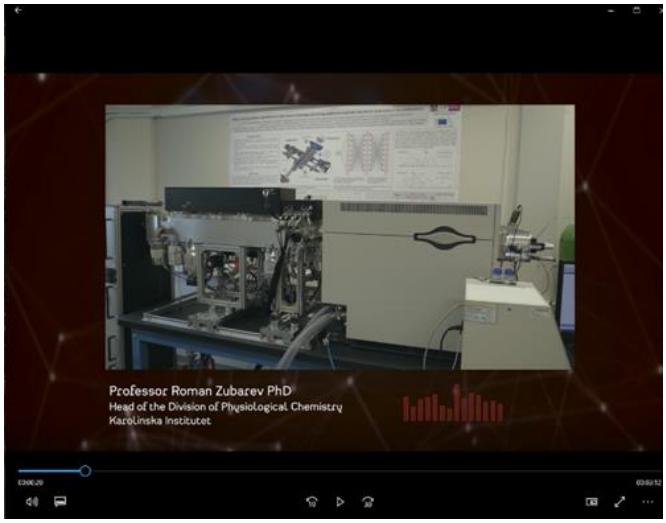

***Figure 14.** Screen shot of the current version of the produced video.*