

## Deep Learning for 'Artefact' Removal in Infrared Spectroscopy

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Table S1. 17 oscillators of the PMMA material, all in unit of  $\text{cm}^{-1}$ .

#	Strength	Damping	Resonance	#	Strength	Damping	Resonance
<b>1</b>	47.0	18.850	750.0	<b>10</b>	100.5	34.071	1263.0
<b>2</b>	51.3	33.890	838.4	<b>11</b>	57.0	28.913	1378.7
<b>3</b>	34.9	32.668	913.2	<b>12</b>	106.3	30.655	1441.8
<b>4</b>	66.7	32.369	960.1	<b>13</b>	72.5	28.471	1475.5
<b>5</b>	53.1	17.328	985.2	<b>14</b>	201.0	17.570	1727.0
<b>6</b>	34.8	17.315	1063.3	<b>15</b>	34.9	32.328	2843.0
<b>7</b>	198.6	37.811	1145.1	<b>16</b>	123.6	62.379	2946.4
<b>8</b>	120.4	27.006	1186.1	<b>17</b>	74.4	34.947	3002.5
<b>9</b>	92.3	23.638	1236.3				

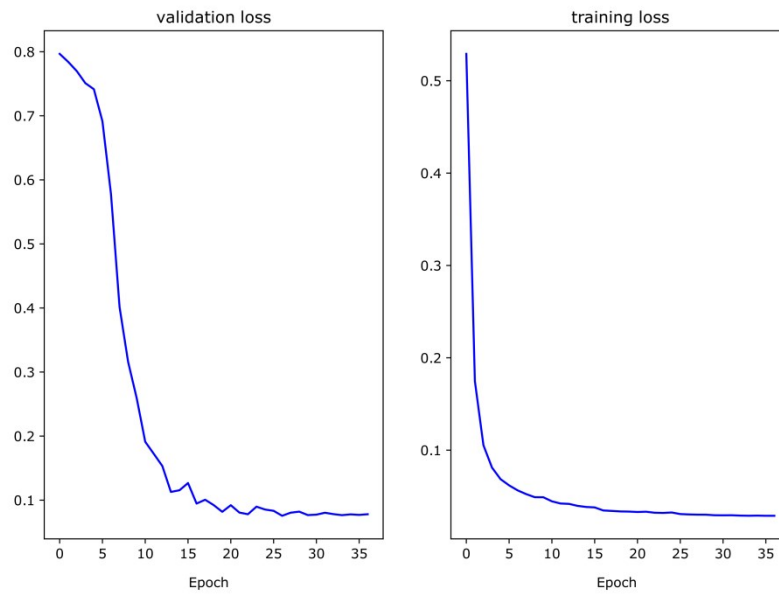
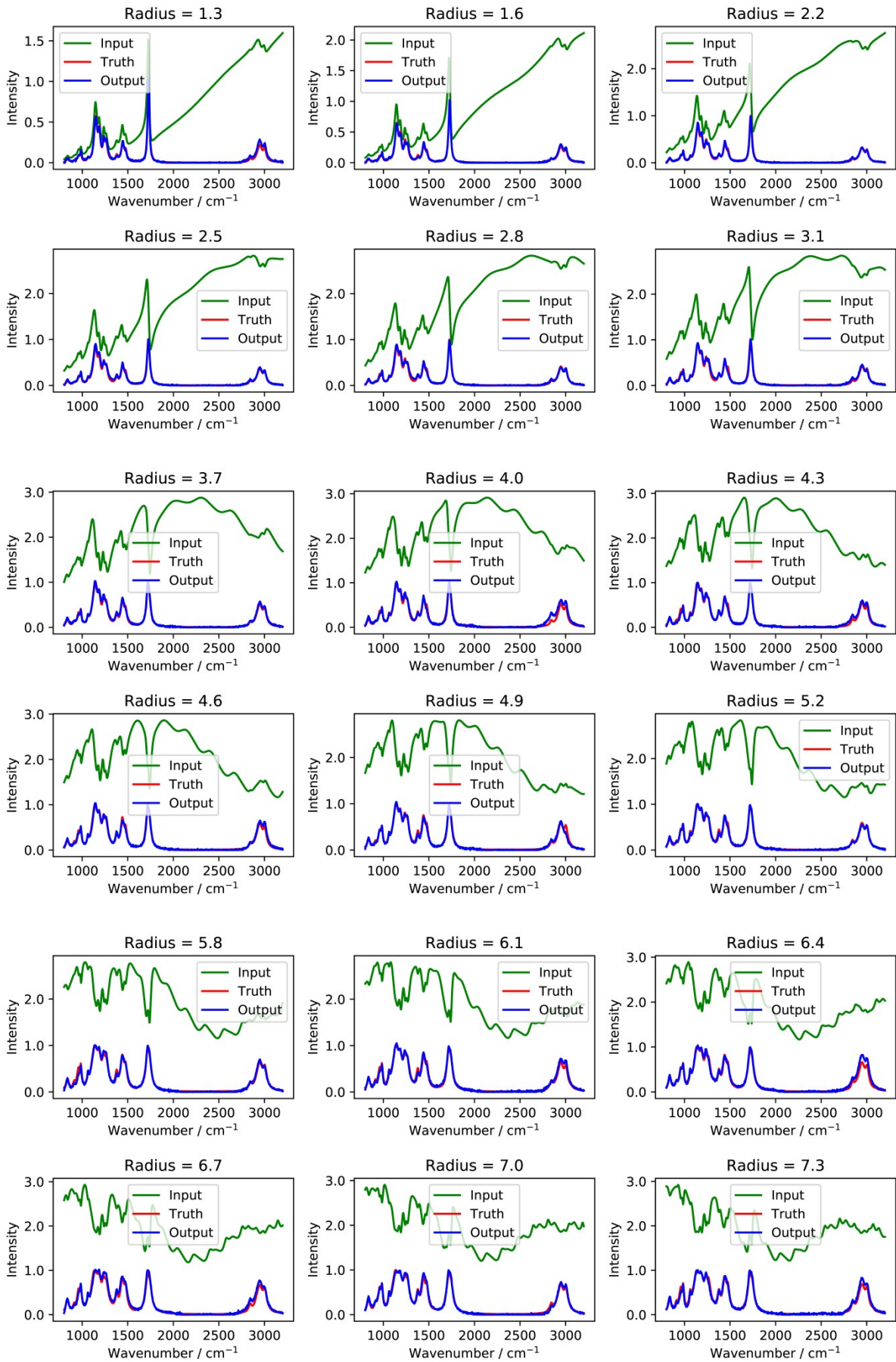


Figure S1 The loss on the validation and training data over the epochs of the training phase. The training was early stopped at 37 epochs, 10 epochs after the validation loss stopped to decrease.



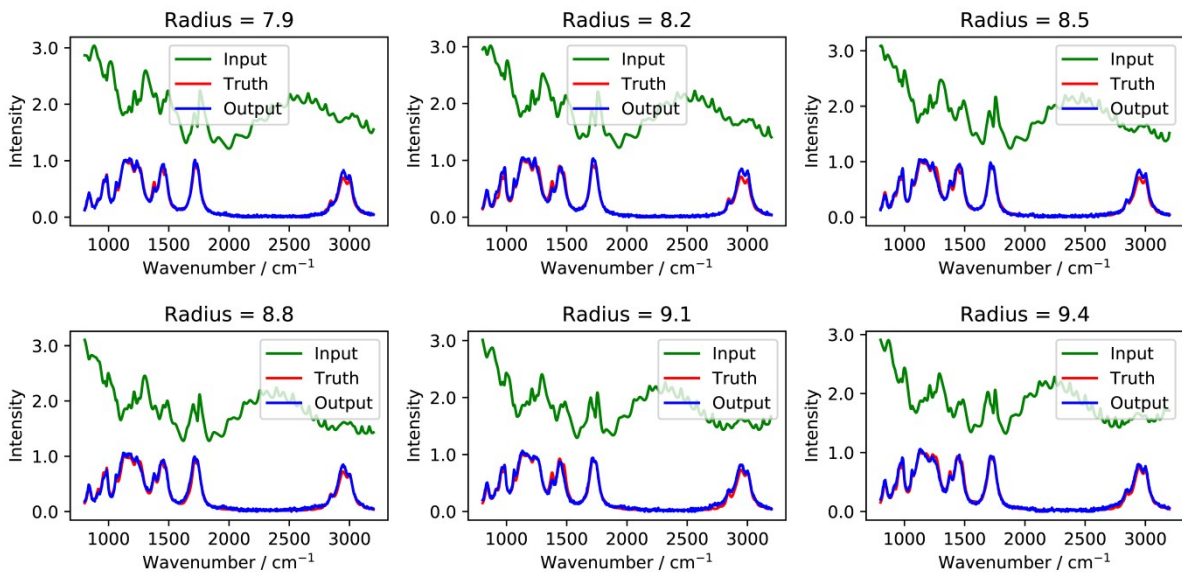


Figure S2 The results of simulated testing data. The results were plotted for every one in three spectra from the whole datasets.

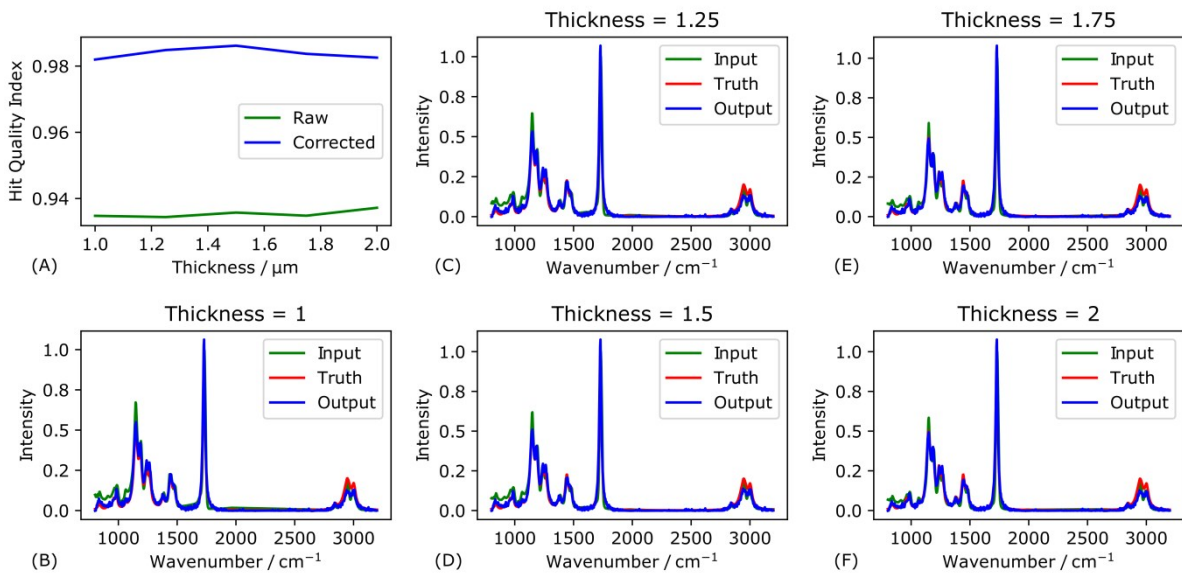


Figure S3 Results from measured PMMA spectra on the substrate CaF<sub>2</sub> of different thickness. (A) The results of the HQI calculated before and after correction. (B-F) The results of the prediction for spectra of different thickness.

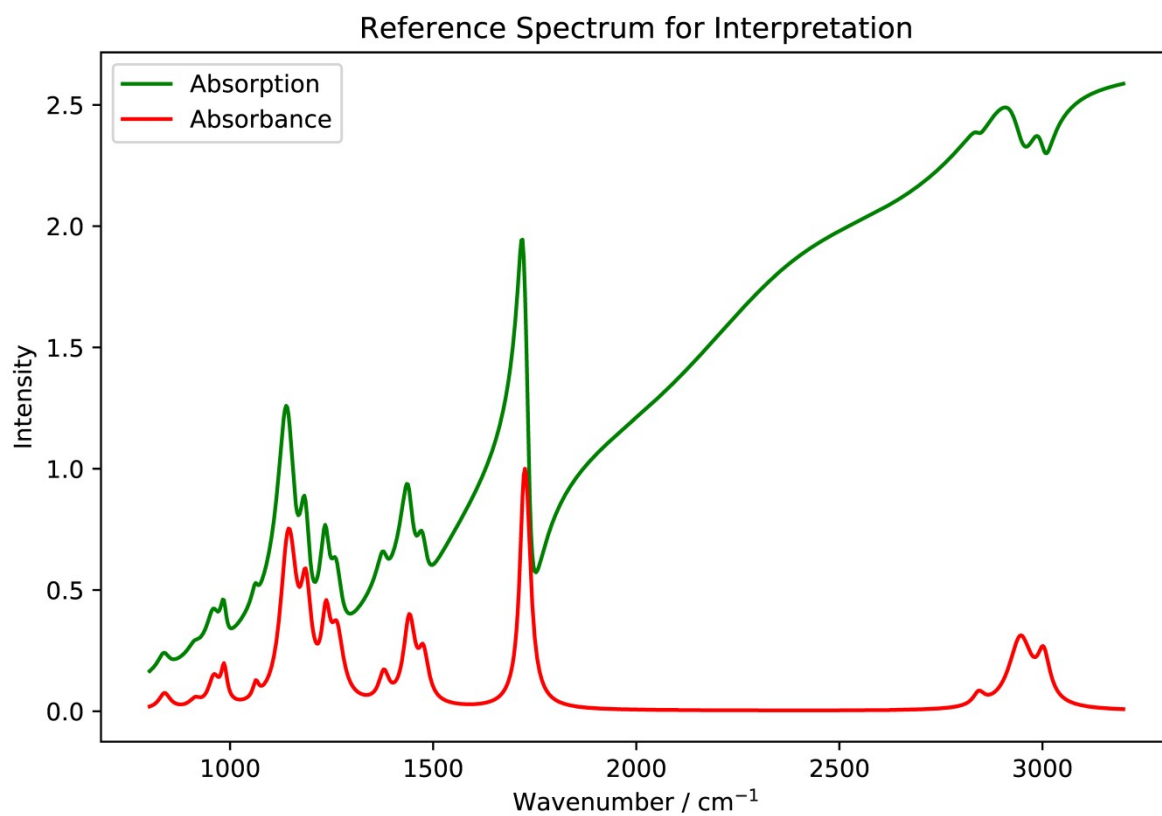


Figure S4. Reference spectrum used for the network interpretation, with apparent absorption in green and the absorbance in red. The apparent absorption was used as the input for the direct visualization, while the absorbance was implemented in the saliency-based method for the calculation of the cost defined in Eq. (4)