Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Energetics of high temperature degradation of fentanyl into primary and secondary products

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Experimental results

Table 1: Propionanilide and phenylethyl pyridinium fragment peak area percentage from pyrolyzed GCxGC-HRMS fentanyl samples at 500 C and 700 C. (*Includes toluene).

Fragment	% Area (500 °C)	% Area (700 °C)
propionanilide	29.24	47.6
phenylethyl pyridinium*	0.0202	0.0111

Analysis of pyrolyzed fentanyl samples identified two fentanyl fragments consistently, propionanilide and phenylethyl pyridinium. Other fragments were not identified. The

phenylethyl pyridinium derivative, toluene, was included due to the instability of phenylethyl pyridinium. No other derivatives were found. Table S1 summarizes the peak area percentages of both propionanilide and phenylethyl pyridinium at 500 and 700 °C.

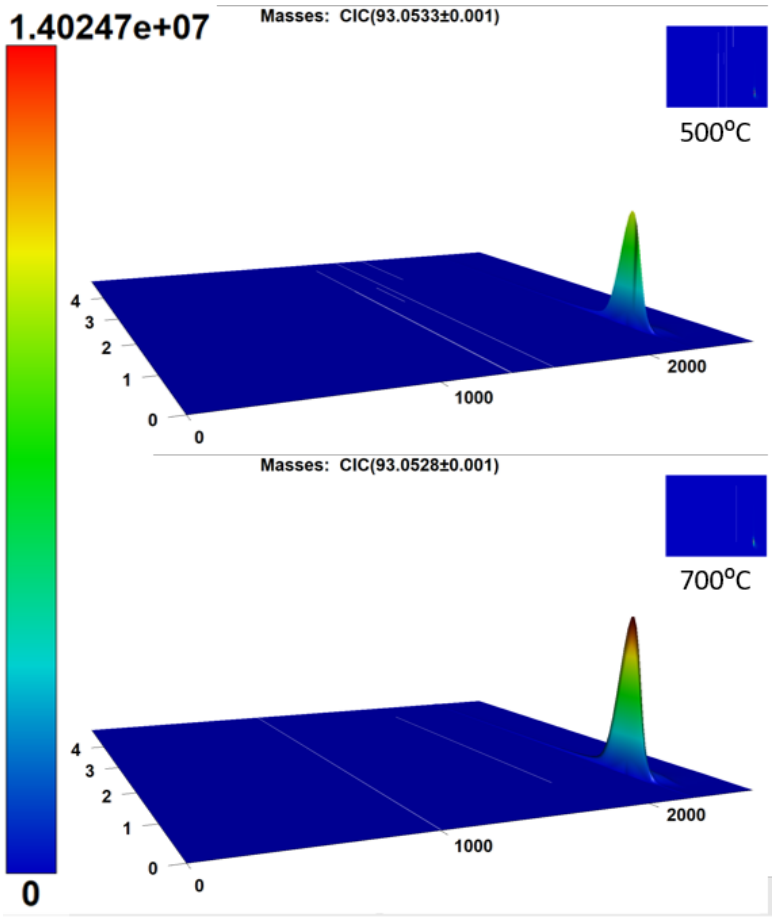

Figure 1: Chromatograms for fentanyl samples pyrolyzed at 500 °C (top) and 700 °C (bottom). Chromatograms are filtered to display mass/charge ratios of 93.0533, Propionanilide's most abundant mass/charge ratio fragment. Propionanilide peaks are at retention times 2500 seconds and 1.1 minutes (right side of chromatograms). Highlighted peaks (white lines along floor of chromatograms) are phenylethyl pyridinium and toluene peaks used for analysis. Gradient bar (left) represents peak area by GCxGC intensity.

Free energy convergence

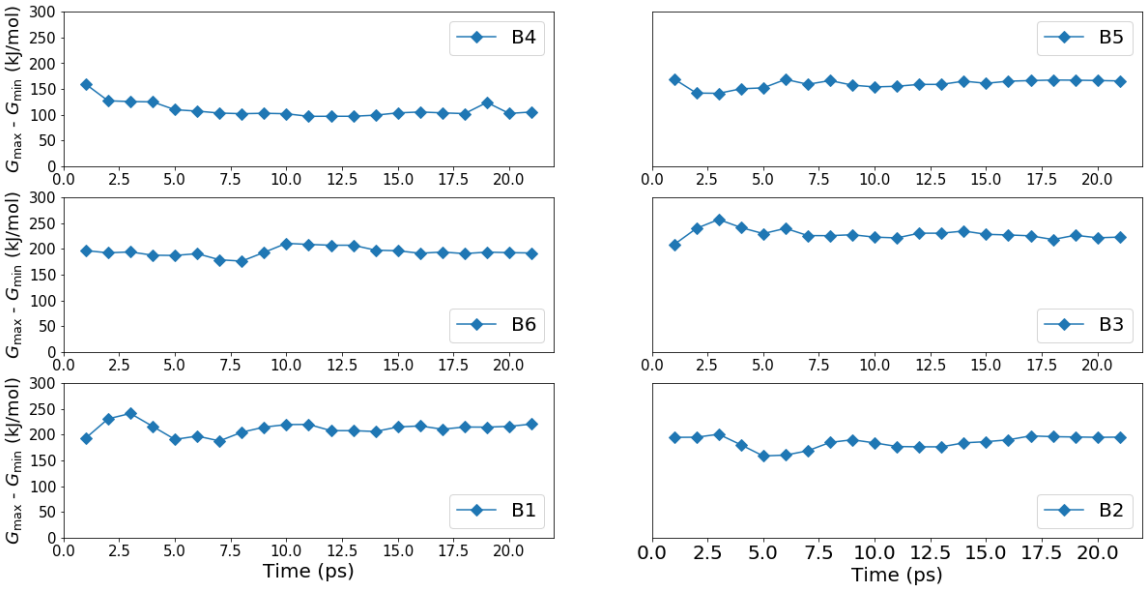

Figure 2: The change in free energy as a function of time throughout the simulation. The G_{max}- G_{min} is the difference in the free energy between the energy barrier and the global minima (which is 0 kJ/mol). This is computed in the interval of every 2 picoseconds. The energy is converged early and suggest us that the simulation is convereged too.

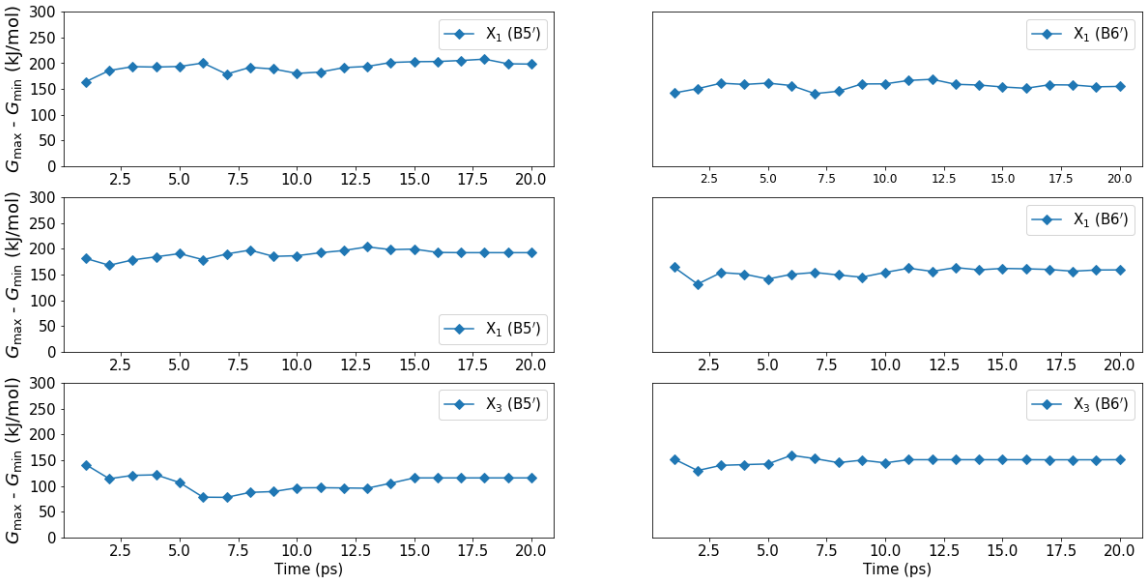

Figure 3: The change in free energy as a function of time throughout the simulation for secondary degradation of bonds B5' and B6'. The G_{max}- G_{min} is the difference in the free energy between the energy barrier and the global minima (which is 0 kJ/mol). This is computed in the interval of every 2 picoseconds. The energy is converged early and suggest us that the simulation is convereged too.