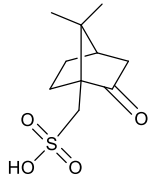
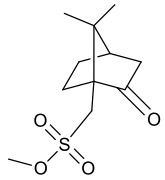
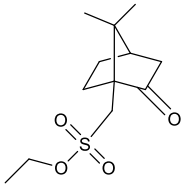
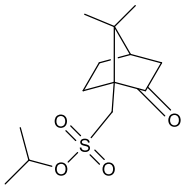
Supporting document for the manuscript 'Determination of 3 alkyl camphorsulfonates as potential genotoxic impurities using GC-FID and GC-MS by analytical QbD"

Table S1. In silico prediction results.

Name	Nexus				Vega				
	Derek assessment	Sarah assessment	Overall assessment	ICH M7 Classification	Caesar assessment	ISS assessment	SarPy assessment	KNN assessment	Overall assessment
 CSA	Negative (Inactive)	Negative (with 42% confidence)	Negative	Class 5	NON-Mutagenic (moderate reliability)	NON-Mutagenic (moderate reliability)	NON-Mutagenic (moderate reliability)	NON-Mutagenic (moderate reliability)	NON-Mutagenic
 MCS	Positive (Plausible)	Negative (with 23% confidence)	Positive	Class 3	NON-Mutagenic (moderate reliability)	Mutagenic (low reliability)	NON-Mutagenic (moderate reliability)	NON-Mutagenic (moderate reliability)	NON-Mutagenic
 ECS	Positive (Plausible)	Equivocal	Positive	Class 3	NON-Mutagenic (moderate reliability	Mutagenic (low reliability)	Mutagenic (low reliability	Mutagenic (moderate reliability	Mutagenic
 ICS	Positive (Plausible)	Positive (with 15% confidence)	Positive	Class 3	NON-Mutagenic (moderate reliability	Mutagenic (low reliability)	Mutagenic (low reliability)	Mutagenic (moderate reliability	Mutagenic

CAESAR: Statistics-based QSAR using a support vector machine, ISS: Rule-based QSAR based on Benigni/Bossa rules, SarPy: Rule-based QSAR based on substructures, KNN: Analogy (read-across) using istKNN.

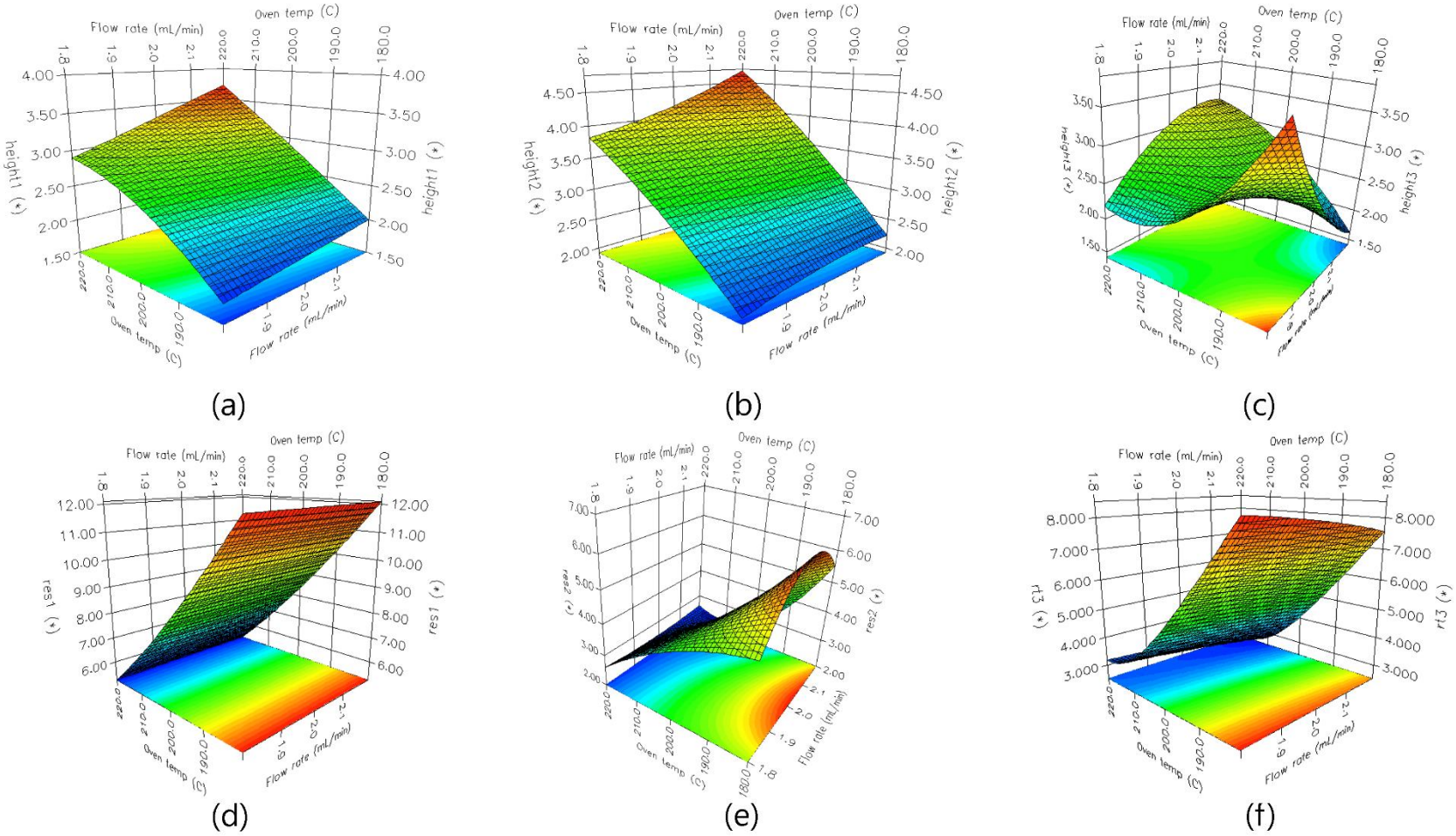


Figure S1. 3D response surface plots for each response as a function of flow rate and column oven temperature at 260℃ of inlet temperature ; (**a**) peak height of MCS, (**b**) peak height of ECS, (**c**) peak height of ICS, (**d**) resolution between MCS and ECS, (**e**) resolution between ECS and ICS and (**f**) retention time of ICS.

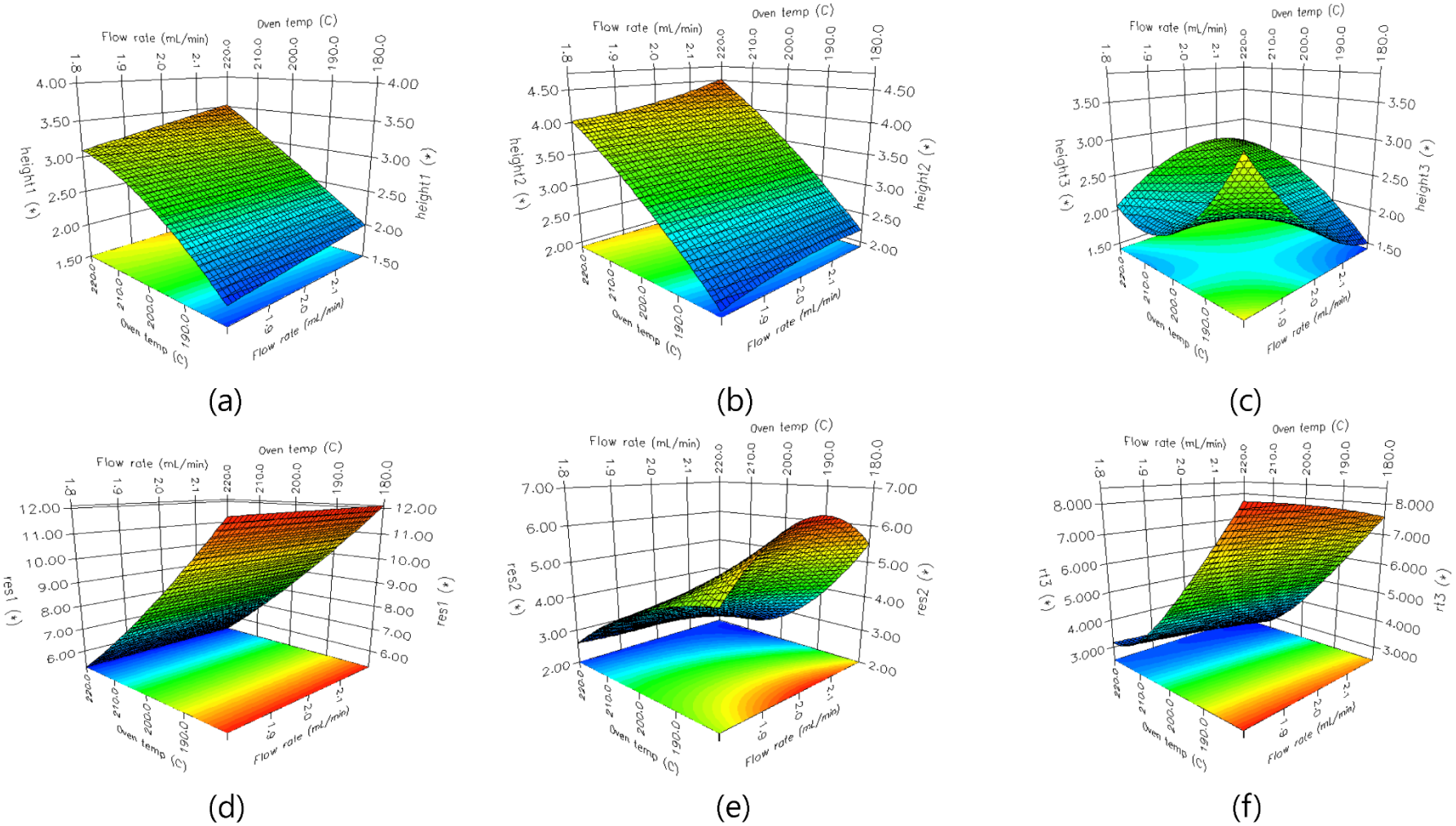


Figure S2. 3D response surface plots for each response as a function of flow rate and column oven temperature at 300℃ of inlet temperature ; (**a**) peak height of MCS, (**b**) peak height of ECS, (**c**) peak height of ICS, (**d**) resolution between MCS and ECS, (**e**) resolution between ECS and ICS and (**f**) retention time of ICS.