

Supporting Information:

A Structural Examination and Collision Cross Section Database for Over 500 Metabolites and Xenobiotics Using Drift Tube Ion Mobility Spectrometry

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Table 1. The DTIMS CCS database generated from this work are in the attached excel Table S1. Chemical information, mass, and CCS values measured for each molecule with relative standard deviation are included.

Instrument settings for direct measurement of DTIMS CCS are listed in Table S2-S4:

Table S2. Front Funnel Settings for the 1700m/z_250 Stable Ions Mode

High Pressure funnel delta (V)	High Pressure Funnel RF (V)	Trap funnel delta (V)	Trap funnel RF (V)	Trap Funnel Exit (V)
150	100	180	100	10

Table S3. Drift Tube Settings for Stepped Field Experiments in Positive Mode

Time Sequence	Time (min)	Drift Tube Entrance (V)	Drift Tube Exit (V)	Rear Funnel Entrance (V)	Rear Funnel Exit (V)
1	0.0 – 0.5	1074	224	217.5	45
2	0.5 – 1.0	1174	224	217.5	45
3	1.0 – 1.5	1274	224	217.5	45
4	1.5 – 2.0	1374	224	217.5	45
5	2.0 – 2.5	1474	224	217.5	45
6	2.5 – 3.0	1574	224	217.5	45
7	3.0 – 3.5	1674	224	217.5	45

Table S4. Drift Tube Settings for Stepped Field Experiments in Negative Mode

Time Sequence	Time (min)	Drift Tube Entrance (V)	Drift Tube Exit (V)	Rear Funnel Entrance (V)	Rear Funnel Exit (V)
1	0.0 – 0.5	-1074	-224	-217.5	-45
2	0.5 – 1.0	-1174	-224	-217.5	-45
3	1.0 – 1.5	-1274	-224	-217.5	-45
4	1.5 – 2.0	-1374	-224	-217.5	-45
5	2.0 – 2.5	-1474	-224	-217.5	-45
6	2.5 – 3.0	-1574	-224	-217.5	-45
7	3.0 – 3.5	-1674	-224	-217.5	-45