M147T296\_POS/hmdbDatabase0.0.1/4-Hydroxycinnamic acid Lab.ID: shen 2388 HMDB02035 Experiment MS2 spectrum 1.0 Compound.name: 4-Hydroxycinnamic acid mz: 164.047344122 CAS.ID: 7400-08-0 HMDB.ID: HMDB02035 KEGG.ID: C00811 0.5 Formula: C9H8O3 SMILES: OC(=O)\C=C\C1=CC=C(O)C=C1 ChemSpider.ID: 553148 Relative intensity METLIN.ID: 6450 Instrument: LC-ESI-QTOF (UPLC Q-Tof Premier, Waters) 0.0 InChikey: InChikey=NGSWKAQJJWE\$NS-ZZXKWVIFSA-N -0.5mz.error: 0.635379495008692 SS: 0.738857696838525 Total.score: 0.836664975 \_1.0 -Adduct: (M+H-H2O)+ Database MS2 spectrum CE; Unknown 1 75 100 125 150 50 Mass to charge ratio (m/z)