

Mass Spectrometry Facility

Sample Submission Form - Small molecules

Mass Spectrometry Facility, Department of Chemistry, University of Cambridge

Service number:	Date:
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Research Group: Duer	Email: mwp37@cam.ac.uk

Sample Information

Sample name:	int2_v3		
Chemical formula:	Varied – multiple products		
Molecular Mass:			
Structural formula:	See next page		
Solvent:	H2O with 19% d6-acetone and 9% D2O		
Sample storage:	Room X	Fridge	Freezer

Experimental requirements and/or preferences

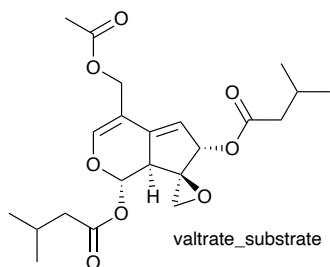
Molecular mass accuracy:	5 ppm, LC/MS
<input type="checkbox"/> Unit Mass	
<input checked="" type="checkbox"/> Accurate mass	<input checked="" type="checkbox"/> Positive ion mode
<input checked="" type="checkbox"/> Accurate mass	<input checked="" type="checkbox"/> Negative ion mode
<input type="checkbox"/> MSMS	Expected fragments:

Safety Information

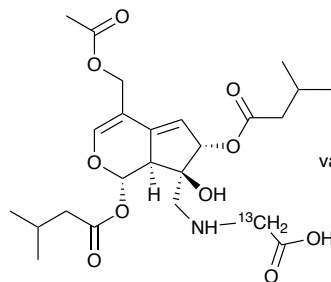
Is your material free from Chemical & Radiological Hazard?	YES / NO
If not, please state nature of the hazard:	

Mass Spectrometry Facility only

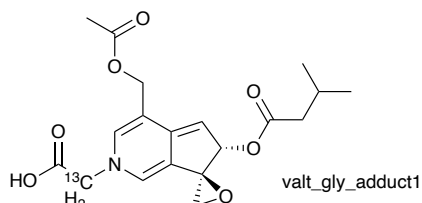
Method:	Name:	Date:



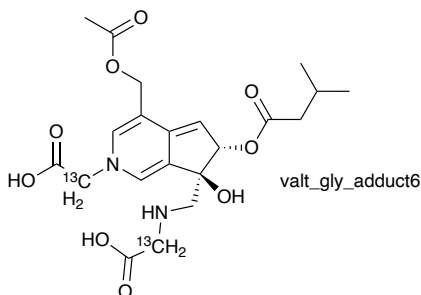
Chemical Formula: $C_{22}H_{30}O_8$
 m/z: 422.1941 (100.0%), 423.1974 (23.8%), 424.2008 (2.7%), 424.1983 (1.6%)



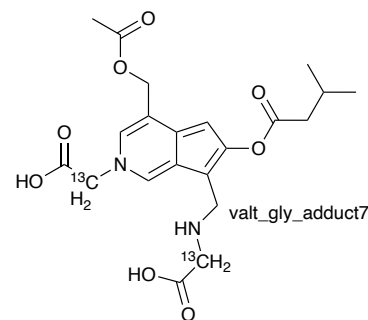
Chemical Formula: $C_{23}^{13}CH_{35}NO_{10}$
 m/z: 498.2295 (100.0%), 499.2328 (24.9%), 500.2362 (3.0%), 500.2337 (2.1%)



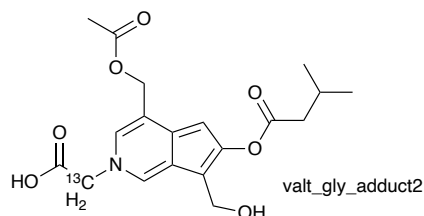
Chemical Formula: $C_{18}^{13}CH_{23}NO_7$
 m/z: 378.1508 (100.0%), 379.1542 (19.5%), 380.1575 (1.8%), 380.1551 (1.4%)



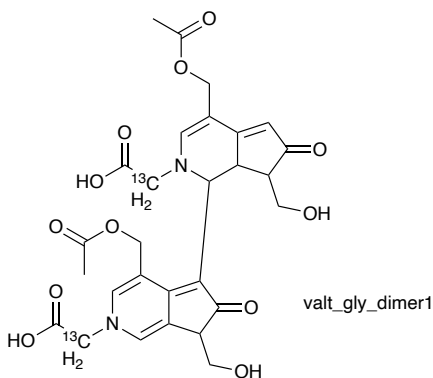
Chemical Formula: $C_{19}^{13}C_2H_{29}N_2O_9$
 m/z: 454.1862 (100.0%), 455.1895 (20.5%), 456.1929 (2.0%), 456.1904 (1.8%)



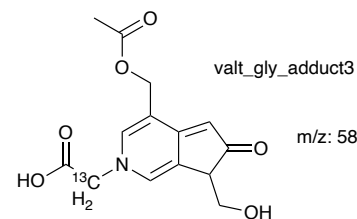
Chemical Formula: $C_{19}^{13}C_2H_{26}N_2O_8$
 m/z: 436.1756 (100.0%), 437.1790 (20.5%), 438.1823 (2.0%), 438.1799 (1.6%)



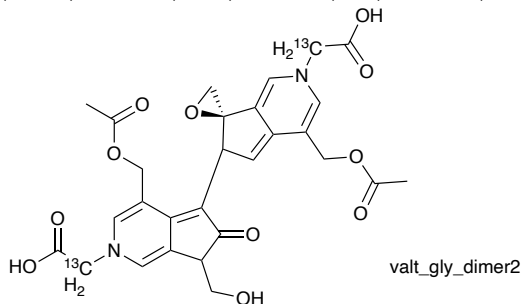
Chemical Formula: $C_{18}^{13}CH_{23}NO_7$
 m/z: 378.1508 (100.0%), 379.1542 (19.5%), 380.1575 (1.8%), 380.1551 (1.4%)



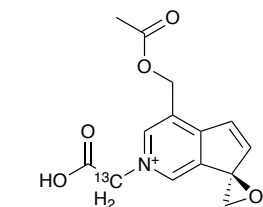
Chemical Formula: $C_{26}^{13}C_2H_{30}N_2O_{12}$
 m/z: 588.1866 (100.0%), 589.1899 (28.1%), 590.1933 (3.8%), 590.1908 (2.5%)



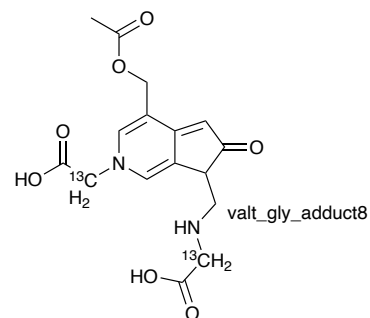
Chemical Formula: $C_{13}^{13}CH_{15}NO_6$
 m/z: 294.0933 (100.0%), 295.0966 (14.1%), 296.0975 (1.2%)



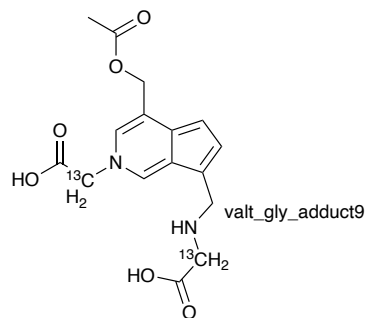
Chemical Formula: $C_{26}^{13}C_2H_{28}N_2O_{11}$
 m/z: 570.1760 (100.0%), 571.1794 (28.1%), 572.1827 (3.8%), 572.1803 (2.3%)



Chemical Formula: $C_{13}^{13}CH_{14}NO_5^+$
 m/z: 277.0901 (100.0%), 278.0934 (14.1%), 279.0943 (1.0%)



Chemical Formula: $C_{14}^{13}C_2H_{18}N_2O_7$
 m/z: 352.1181 (100.0%), 353.1215 (15.1%), 354.1224 (1.4%), 354.1248 (1.1%)



Chemical Formula: $C_{14}^{13}C_2H_{18}N_2O_6$
 m/z: 336.1232 (100.0%), 337.1266 (15.1%), 338.1274 (1.2%), 338.1299 (1.1%)