Mass Spectrometry Facility
Sample Submission Form - Small molecules

Mass Spectrometry Facility, Department of Chemistry, University of Cambridge

Service number:	Date:

Name: Mikolaj Poplawski	
Research Group: Duer	Email: mwp37@cam.ac.uk

Sample Information

Sample name:	**int2_v2**		
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

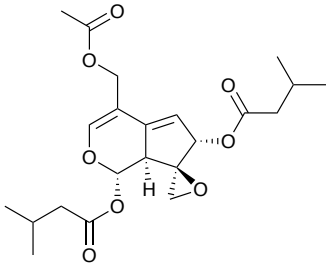
Molecular mass accuracy:	5 ppm, LC/MS
[ ] Unit Mass	
[X] Accurate mass	[X] Positive ion mode
[X] Accurate mass	[X] Negative ion mode
[ ] MSMS	Expected fragments:

Safety Information

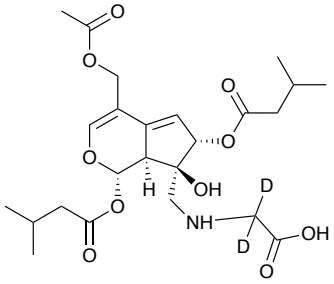
Is your material free from Chemical & Radiological Hazard? YES / NO
If not, please state nature of the hazard:

Mass Spectrometry Facility only

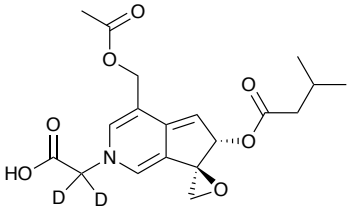
Method:	Name:	Date:



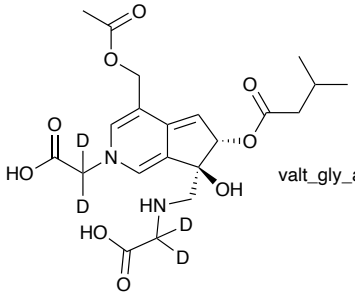
Chemical Formula: $C_{22}H_{30}O_8$
m/z: 422.1941 (100.0%), 423.1974 (23.8%), 424.2008 (2.7%), 424.1983 (1.6%)



Chemical Formula: $C_{24}H_{33}D_2NO_{10}$
m/z: 499.2386 (100.0%), 500.2420 (26.0%), 501.2454 (3.2%), 501.2429 (2.1%)

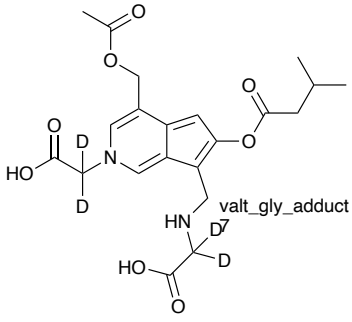


Chemical Formula: $C_{19}H_{21}D_2NO_7$
m/z: 379.1600 (100.0%), 380.1634 (20.5%), 381.1667 (2.0%), 381.1643 (1.4%)



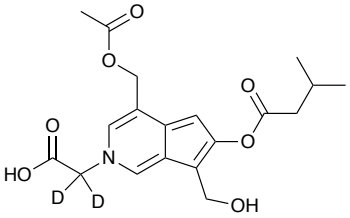
valt_gly_adduct6

Chemical Formula: $C_{21}H_{24}D_4N_2O_9$
m/z: 456.2046 (100.0%), 457.2079 (22.7%), 458.2113 (2.5%), 458.2088 (1.8%)

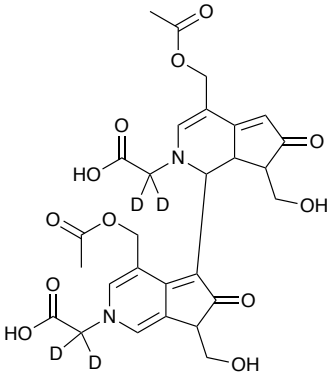


valt_gly_adduct

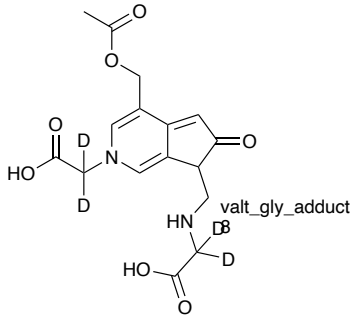
Chemical Formula: $C_{21}H_{22}D_4N_2O_8$
m/z: 438.1940 (100.0%), 439.1974 (22.7%), 440.2007 (2.5%), 440.1983 (1.6%)



Chemical Formula: $C_{19}H_{21}D_2NO_7$
m/z: 379.1600 (100.0%), 380.1634 (20.5%), 381.1667 (2.0%), 381.1643 (1.4%)

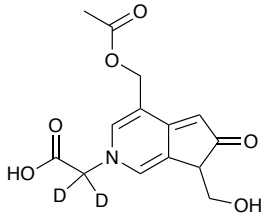


Chemical Formula: $C_{28}H_{26}D_4N_2O_{12}$
m/z: 590.2050 (100.0%), 591.2083 (30.3%), 592.2117 (4.4%), 592.2092 (2.5%)

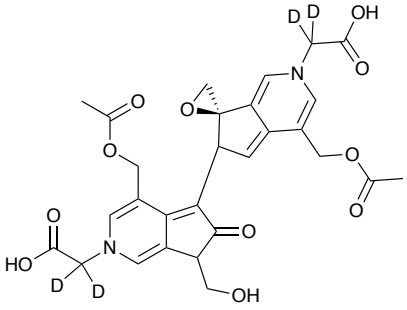


valt_gly_adduct

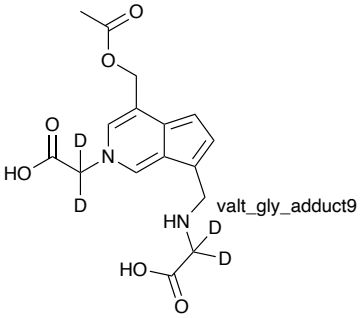
Chemical Formula: $C_{16}H_{14}D_4N_2O_7$
m/z: 354.1365 (100.0%), 355.1399 (17.3%), 356.1408 (1.4%), 356.1432 (1.4%)



Chemical Formula: $C_{14}H_{13}D_2NO_6$
m/z: 295.1025 (100.0%), 296.1058 (15.1%), 297.1067 (1.2%), 297.1092 (1.1%)

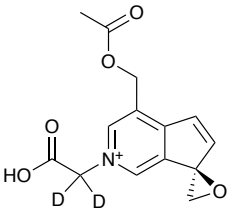


Chemical Formula: $C_{28}H_{24}D_4N_2O_{11}$
m/z: 572.1944 (100.0%), 573.1978 (30.3%), 574.2011 (4.4%), 574.1987 (2.3%)



valt_gly_adduct9

Chemical Formula: $C_{16}H_{14}D_4N_2O_6$
m/z: 338.1416 (100.0%), 339.1449 (17.3%), 340.1483 (1.4%), 340.1458 (1.2%)



Chemical Formula: $C_{14}H_{12}D_2NO_5^+$
m/z: 278.0993 (100.0%), 279.1026 (15.1%), 280.1060 (1.1%), 280.1035 (1.0%)