

Unambiguous stereochemical assignment of cyclo(Phe-Pro), cyclo(Leu-Pro), and cyclo(Val-Pro) by electronic circular dichroic spectroscopy

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GNPS: Global Natural Products Social Molecular Networking

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View Mirror Match USI Links 1 ViewLib	Explore Molecule in 0 Files and 0 Datasets	monolinolein	1855	View Raw Spectra	Bronze	0.79	6	6238.24	509.10	
View Mirror Match USI Links 2 ViewLib	Explore Molecule in 0 Files and 0 Datasets	eudesmin	2039	View Raw Spectra	Bronze	0.84	11	1944.26	663.69	
View Mirror Match USI Links 3 ViewLib	Explore Molecule in 433 Files and 20 Datasets	cyclo(L-Val-L-Pro)	396	View Raw Spectra	Bronze	0.85	6	19110.20	142.71	
View Mirror Match USI Links 4 ViewLib	Explore Molecule in 195 Files and 10 Datasets	cyclo(L-Phe-D-Pro)	711	View Raw Spectra	Bronze	0.83	7	23295.90	220.69	
View Mirror Match USI Links 5 ViewLib	Explore Molecule in 447 Files and 13 Datasets	cyclo(L-Leu-L-Pro)	413	View Raw Spectra	Bronze	0.71	8	41890.50	191.97	
View Mirror Match USI Links 6 ViewLib	Explore Molecule in 0 Files and 0 Datasets	[2,3-dihydroxy-1-(7-methoxy-2-oxochromen-6-yl)-3-methylbutyl] (Z)-2-methylbut-2-enoate	2092	View Raw Spectra	Bronze	0.91	6	4734.26	584.63	
View Mirror Match USI Links 7 ViewLib	Explore Molecule in 0 Files and 0 Datasets	[(2R,3R,4R,5R)-2-(2,4-dioxypyrimidin-1-yl)-4-hydroxy-5-(hydroxymethyl)oxolan-3-yl] 2,4-dimethoxy-6-methylbenzoate	2154	View Raw Spectra	Bronze	0.86	6	14595.00	398.26	
View Mirror Match USI Links 8 ViewLib	Explore Molecule in 0 Files and 0 Datasets	Spectral Match to Phthalic anhydride from NIST14	62	View Raw Spectra	Bronze	0.77	6	51887.30	496.79	

Figure S1. GNPS analysis of metabolites in wheatgrass MMC. A LC/MS/MS dataset of wheatgrass MMC extract was submitted to GNPS, which identified a series of metabolites, including cyclo(L-Val-L-Pro), cyclo(L-Phe-D-Pro), and cyclo(L-Leu-L-Pro) as “Bronze” matches. These DKPs were also observed in the GNPS analyses of other MMCs (not shown).