

Supplementary data for article:

Szwej, E.; Devocelle, M.; Kenny, S.; Guzik, M.; O'Connor, S.; Nikodinović-Runić, J.; Radivojevic, J.; Maslak, V.; Byrne, A. T.; Gallagher, W. M.; et al. The Chain Length of Biologically Produced (R)-3-Hydroxyalkanoic Acid Affects Biological Activity and Structure of Anti-Cancer Peptides. *Journal of Biotechnology* **2015**, *204*, 7–12.

<https://doi.org/10.1016/j.jbiotec.2015.02.036>

Table S1. Characteristic mass peaks used for identification of (*R*)-3-hydroxyalkanoic acids after MSTFA derivatizations.

PHA monomer	First peak (only carboxyl group derivatized)	Second peak (carboxyl and hydroxyl group derivatized)
(<i>R</i>)-3-OH-hexanoic acid	73, 75, 117, 161, 171, 189	73, 145, 147, 219, 233, 261
(<i>R</i>)-3-OH-heptanoic acid	73, 75, 117, 161, 185, 203	73, 147, 159, 233, 275
(<i>R</i>)-3-OH-octanoic acid	73, 75, 117, 161, 199, 217	73, 147, 173, 233, 247, 289
(<i>R</i>)-3-OH-nonanoic acid	73, 75, 117, 161, 213, 231	73, 147, 187, 233, 261, 303
(<i>R</i>)-3-OH-decanoic acid	73, 75, 117, 161, 227, 245	73, 147, 201, 233, 275, 317
(<i>R</i>)-3-OH-undecanoic acid	73, 75, 117, 161, 241, 259	73, 147, 215, 233, 289, 331
(<i>R</i>)-3-OH-dodecanoic acid	73, 75, 117, 161, 255, 273	73, 147, 229, 233, 303, 345

Table S2. Calculated and actual mass of peptide and (*R*)-3-hydroxyalkanoic acid-peptide conjugates used in the current study.

Peptide	Calculated mass	Actual mass
DP18L	2300	2300
DP17L	2186	2188
R6DP18L	2416	2415
R7DP18L	2431	2430
R8DP18L	2443	2442
R9DP18L	2457	2457
R10DP18L	2471	2471
R11DP18L	2485	2485
R12DP18L	2499	2499
R6DP17L	2300	2302
R7DP17L	2314	2316
R8DP17L	2328	2330
R9DP17L	2342	2344
R10DP17L	2356	2356
R11DP17L	2370	2371
R12DP17L	2384	2386
CI10DP18L	2489	2488

Table S3. The anti-proliferation activity the various PHA monomers (R3HAs) and chloro-derivative (C1C10) with fibroblast (MRC5) and cancer (MiaPaCa) cell lines. Values show the micromolar (μM) concentration at which 50% cell growth inhibition occurs (IC50).

Compound	MRC5	MiaPaCa
R6	1750 \pm 15 ^a	1600 \pm 10
R7	1550 \pm 10	1250 \pm 15
R8	2000 \pm 20	2000 \pm 20
R9	1750 \pm 10	1800 \pm 15
R10	2100 \pm 15	2150 \pm 15
R11	1750 \pm 10	1550 \pm 10
R12	2000 \pm 20	1950 \pm 20
C1C10	1250 \pm 20	950 \pm 10

^a Data is an average of three independent determinations performed in triplicate.