5. SUPPLEMENTARY MATERIAL

In Table A are reported the total (SCF) energy, the zero-point vibrational energy (ZPE) and the thermal energy corrections to enthalpy and free energy at 298.15 K and 1 atm for the studied metabolites and the molecules that participate in their isodesmic reactions (Table 2 of main text). These are the source data out of which the data in Tables 4 - 7 were obtained.

Table A: Quantum thermochemical calculations with DFT/B3-LYP/def2TZVP. All quantities are in Hartree units

Compound	SCF	ZPE	Enthalpy Cor., Hv	Free Energy Cor., Gv
Aminoacides / oligopeptides				
Alanine	-323.7246639	0.1074531	0.115242	0.076794
β-Alanine	-323.7254817	0.1081602	0.115802	0.077205
Arginine	-606.4974005	0.2238263	0.237299	0.185763
Asparagine	-492.4312597	0.1355887	0.146111	0.100349
Aspartic acid	-512.3046826	0.1232867	0.133512	0.088067
Cysteine	-721.8869102	0.1079153	0.11693	0.074398
Glutamic acid	-551.6055336	0.1523425	0.163795	0.114374
Glutamine	-531.7323669	0.1645521	0.176247	0.127904
Glycine	-284.4182864	0.0793659	0.085907	0.050558
Histidine	-548.7249403	0.1600383	0.170755	0.124299
Isoleucine	-441.639129	0.1925932	0.204494	0.155813
Leucine	-441.6343596	0.1923098	0.204089	0.155164
Lysine	-496.9782162	0.2105525	0.223669	0.171271
Methionine	-800.4934017	0.1656859	0.17772	0.127241
Ornithine	-457.6746547	0.1821054	0.193891	0.144902
Phenylalanine	-554.7368933	0.1891907	0.201317	0.150618
Proline	-401.1195383	0.1444082	0.152918	0.111172
Sarcosine	-323.7113961	0.1074715	0.115285	0.076265
Serine	-398.9438721	0.1126781	0.12158	0.080219
Serotonine	-572.9364429	0.207006	0.219932	0.168884
Threonine	-438.2502022	0.1408177	0.150877	0.106374
Tryptophan	-686.2875745	0.2176467	0.231922	0.175356
Tyrosine	-629.9595853	0.1930154	0.206327	0.152999
Valine	-402.3335741	0.1641892	0.174674	0.129568
Alanylalanine	-571.0327878	0.1913352	0.204872	0.150435
Alanylglycine	-531.726244	0.163478	0.175518	0.124389
Alanylphenylalanine				
Glycylglycine	-492.4139986	0.1350187	0.145926	0.097543
Glycylphenylalanine				
Glycylvaline	-610.3363537	0.219791	0.234689	0.17767
Leucylglycine				
Prolinylproline				
Valylphenylalanine				
Nucleosides				
Adenosine	-963.4764282	0.2512261	0.26859	0.207275
Deoxyadenosine				
2,3-dideoxyadenosine	-813.0322389	0.2428369	0.25738	0.201879
Inosine	-983.3458504	0.2393569	0.256267	0.194909
Guanosine	-1038.716302	0.2563321	0.274443	0.211754
Deoxyguanosine	-963.4818489	0.2505461	0.268313	0.205063
Uridine	-910.9969722	0.2266014	0.242595	0.183857
Thymidine	-875.0814054	0.2499122	0.266561	0.206643
3-deoxythymidine	-799.8581094	0.2450924	0.26086	0.202338
Cytidine	-891.1046518	0.2376833	0.254523	0.193667
Deoxycytidine	-815.8757081	0.2330047	0.24878	0.190494
Saccharides				
βD-Glucose (glucopyranose)	-687.1538515	0.1969763	0.210224	0.159491
Glucose – chain	-687.1421019	0.1942843	0.208556	0.153959
βD –galactose	-687.1537028	0.1974026	0.210328	0.160272

βD –ribose	-572.6208415	0.1644402	0.175022	0.129964
αD-ribofuranose	-572.6212385	0.1639285	0.174862	0.128911
βD-xylofuranose	-572.6230755	0.1643557	0.174957	0.129913
Fructose-chain	-687.1561832	0.1961478	0.20968	0.157974
βD-fructose (βD-fructofuranose)	-687.1558999	0.1967896	0.210016	0.158884
βD-fructopyranose	-687.1569374	0.197605	0.209943	0.161445
αD-fructopyranose	-687.1586293	0.1977728	0.210396	0.161534
βD –glucofuranose	-687.1479211	0.1969746	0.210244	0.158733
Sucrose	-1297.8859295	0.3722257	0.395466	0.323317
Maltose	-1297.889279	0.3703395	0.394792	0.318095
Auxiliary compounds				
Methane	-56.5505356	0.034158	0.048369	0.026168
Ethane	-213.75366	0.1492909	0.078824	0.051901
Propane	-229.0692794	0.0612661	0.108515	0.07798
Ammonia	-56.5505356	0.034158	0.037974	0.015056
Methylamine	-95.8400592	0.0637473	0.068126	0.040785
Propylamine	-174.45014	0.1208469	0.127489	0.092907
Butylamine	-213.75366	0.1492909	0.157232	0.119008
Pentylamine	-253.0573613	0.1777023	0.186972	0.145147
Acetic acid	-229.0692794	0.0612661	0.066792	0.034293
Propanoic acid	-268.3819198	0.0901658	0.096846	0.060838
butanoic acid	-307.6832621	0.1186126	0.125719	0.088607
Acetamide	-209.2002226	0.0730837	0.079323	0.044144
Propanamide	-248.5040864	0.1018086	0.109177	0.071284
Butanamide	-287.8068568	0.1304908	0.139071	0.097813
Ethylbenzene	-310.8122432	0.1563323	0.164576	0.124168
Isobutane	-158.4134366	0.1310761	0.137736	0.103405
Isopentane	-197.7161856	0.1596491	0.167591	0.129766
Indole	-363.7566449	0.1291352	0.136448	0.098739
Pyrrolidine	-212.5380211	0.1293406	0.135221	0.101271
Guanidine	-205.3536097	0.0749526	0.080817	0.048203
guanine17	-542.5135619	0.1166816	0.125833	0.083659
Adenine	-467.2579145	0.1116188	0.119768	0.079941
Thymine	-454.1067799	0.114706	0.123448	0.08229
Uracil	-414.7970497	0.0869975	0.094091	0.056562
Cytosine 1k	-394.9031544	0.0981528	0.105902	0.067206
Imidazole	-226.1859627	0.0709901	0.075693	0.044691
Tetrahydropyran	-271.7233945	0.1459651	0.152372	0.117341
tetrahydrofuran	-232.4121738	0.1163937	0.12228	0.08802
Ethanol	-155.0213258	0.0796231	0.084878	0.054183
Methanol	-115.7126894	0.0510195	0.055309	0.028217
Isopropanol	-194.3304888	0.1075932	0.113995	0.080156
Acetone	-193.1306794	0.0831496	0.088657	0.056876
Acetaldehyde	-153.8136892	0.0549173	0.059126	0.030535
Ethyleneglycol	-230.2360124	0.0845168	0.090967	0.05729
Dimethylether	-155.005315	0.0793533	0.084633	0.05391
Ethylthiol	-477.9631393	0.0746435	0.080309	0.047813
Methylpropylsulfide	-556.570324	0.1324672	0.140931	0.100642
Glycerol	-344.7710931	0.1193767	0.12715	0.089051
4-ethylphenol	-386.0404505	0.1603522	0.169832	0.126718
p-cresol	-346.736348	0.1314349	0.138936	0.100954