Electronic supplementary information for:

Amino acid hydrogen oxalate quasiracemates – sulfur containing side chains

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Electronic Supplementary Information

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S1. Crystal Growth Experiments

General Considerations. All chemicals and solvents were purchased from the MilliporeSigma, TCI America, or Acros Chemicals and used as received without further purification unless stated otherwise.

Crystal Growth of Racemic Amino Acid Hydrogen Oxalates DL-Nva·HOx and DL-Met·HOx. To a 2-dram vial was added a 1:1:2 molar ratio of the enantiomers (40 – 60 mg total) and oxalic acid dihydrate. The contents of the vial were dissolved in 2 mL of distilled water with the aid of agitation and heat (*ca.* 60 °C) and allowed to crystallize via slow evaporation at room temperature to give needle-like crystals after several days.

Hydrogen Oxalate Quasiracemate Crystal Growth of L-Mecyst·D-Nva·2HOx, L-Met·D-Nva·2HOx, L-Etcyst·D-Nva·2HOx, L-Met·D-Leu·2HOx, L-Met·D-Nle·2HOx, L-Etcyst·D-Leu·2HOx, L-Etcyst·D-Met·2HOx, and L-Etcyst·D-Nle·2HOx. To a 2-dram vial was added a 1:1:2 molar ratio of the quasienantiomers (40 – 60 mg total) and oxalic acid dihydrate. The contents of the vial were dissolved in 2 mL of distilled water with the aid of agitation and heat (*ca.* 60 °C) and allowed to crystallize via slow evaporation at room temperature to give needle-like crystals after several days.

Non-Hydrogen Oxalate Quasiracemate Crystal Growth of L-Etcyst·D-Nle. To a 2-dram vial was added equimolar amounts of L-Etcyst and D-Nle (40 – 60 mg total) and 2 mL of distilled water. The contents of the vial were agitated and heated to ~60°C until dissolution occurred and then placed in the back of a fume hood to allow for slow evaporation at room temperature to give crystals with prism morphology after several days.

Non-Hydrogen Oxalate Quasiracemate Crystal Growth of L-Etcyst·D-Nva and L-Etcyst·D-Met. Crystals of L-Etcyst·D-Nva and L-Etcyst·D-Met were prepared from the vapor diffusion technique by dissolving equimolar ratios of the desired quasienantiomers in a minimal amount of distilled water and using acetone as the diffusion solvent. Crystals with rod (L-Etcyst·D-Nva) and needle (L-Etcyst·D-Met) morphology suitable for crystallographic assessment were retrieved at the interface of the solvent mixture after several days.

S2. X-ray Crystallography

Crystallographic details for each amino acid racemate and quasiracemate are summarized in Table S1. X-ray data were collected on a Bruker Venture D8 or APEX II CCD diffractometers using phi and omega scans with graphite monochromatic Cu $K\alpha$ (λ = 1.54178 Å) radiation. Data sets were corrected for Lorentz and polarization effects as well as absorption. The criterion for observed reflections is $I > 2\sigma(I)$. Lattice parameters were determined from least-squares analysis and reflection data. Empirical absorption corrections were applied using SADABS.[1] Structures were solved by direct methods and refined by full-matrix least-squares analysis on F^2 using X-SEED[2] equipped with SHELXT[3]. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares on F^2 using the SHELXL[4] program. H atoms attached to nitrogen or oxygen were located in difference Fourier synthesis and refined isotropically with independent O/N-H distances or restrained to 0.85(2) Å. The remaining H atoms were included in idealized geometric

1. SADABS-2016/2 (Bruker AXS). L. Krause, R. Herbst-Irmer, G. M. Sheldrick and D. Stalke, *J. Appl. Cryst.,* 2015, **48**, 3-10.
2. L. J. Barbour, *J. Appl. Cryst*., 2020, **53***,* 1141.
3. G. M. Sheldrick, *Acta Cryst*., 2015, **A71**, 3-8.
4. G. M. Sheldrick, *Acta Cryst*., 2015, **C71**, 3-8.

positions with U_{iso}=1.2U_{eq} of the atom to which they were attached (U_{iso}=1.5U_{eq} for methyl groups). Molecular configurations were compared to both the known chirality of the amino acid and estimated Flack parameters[5] and where applicable, atomic coordinates were inverted to achieve correct structural configurations. Hydrogen bond parameters are given in Table S2.

Table S1. Crystallographic Data for Hydrogen Oxalate Amino Acids.

	DL-Nva·HOx	DL-Leu·HOx[6]	DL-Nle·HOx[7]	DL-Met·HOx
Crystal data				
CCDC deposit no.	2017249	2017256	2105696	2017258
Empirical formula	$C_7H_{13}NO_6$	$C_8H_{15}NO_6$	$C_8H_{15}NO_6$	$C_7H_{13}NO_6S$
Crystal System, space group	Triclinic *P*-1	Monoclinic *P*-1	Triclinic *P*-1	Triclinic *P*-1
M_r	207.18	221.21	221.21	293.24
a, Å	5.7278(2)	5.6792(4)	5.6270(5)	5.5359(8)
b, Å	9.4026(3)	9.5687(7)	9.4327(9)	9.4406(14)
c, Å	9.8028(2)	9.9416(8)	10.4431(10)	10.6027(15)
α, deg	77.211(2)	84.722(3)	88.922(4)	90.156(6)
β, deg	78.253(2)	74.876(3)	75.976(4)	103.956(6)
γ, deg	78.876(2)	82.793(3)	83.757(4)	103.969(6)
V, (Å^3)	497.98(3)	516.43(7)	534.57(9)	520.77(13)
Z, *Z'*	2, 1	2, 1	2, 1	2, 1
D_{calc} (g cm^{-3})	1.382	1.423	1.374	1.526
μ (mm^{-1}), rad. type	1.058			2.921
F_{000}	220			252
temp (K)	100(2)			100(2)
Crystal form, color	needle, colorless			needle, colorless
Crystal size, mm	0.052x0.131x0.197			0.062x0.095x0.341
Data collection				
Diffractometer	Bruker D8 Venture CCD			Bruker D8 Venture CCD
T_{min}/ T_{max}	0.6102/0.7530			0.5734, 0.7536
No. of refls. (meas., uniq., and obs.)	5325/1802/1545			6746/2029/1957
R_{int}	0.0288			0.0258
ϑ_{max} (°)	68.282			72.395
Refinement				
R/R^2_ω (obs data)	0.0340/0.0825			0.0287/0.0868
R/R^2_ω (all data)	0.0416/0.0870			0.0295/0.0874
S	1.058			1.145
No. of refls.	1802			2029
No. of parameters	143			152
$\Delta\rho_{max/min}$ (e·Å^{-3})	0.226/-0.206			0.452/-0.311
flack	-			-

5. H. D. Flack, *Acta Crystallogr.,* 1983, **39**¸ 876-881.
6. K. Manoj, H. Takahashi, Y. Morita, R. G. Gonnade, S. Iwama, H. Tsue and R. Tamura, *Chirality*, 2015, **27**, 405 – 410. DL-Leu·HOx (WIPQOE).
7. R. G. Wells, K. D. Sahlstrom, F. I. Ekelem and K. A. Wheeler, *CrystEngComm*, 2021, DOI: 10.1039/D1CE01213D.

Table S1. Crystallographic Data for Hydrogen Oxalate Amino Acids. (Continued)

	L-Mecyst·D-Nva·2HOx	L-Met·D-Nva·2HOx	L-Etcyst·D-Nva·2HOx	L-Met·D-Leu·2HOx
Crystal data				
CCDC deposit no.	2051774	2017257	2017248	2017250
Empirical formula	$C_{13}H_{24}N_2O_{12}S$	$C_{14}H_{26}N_2O_{12}S$	$C_{14}H_{26}N_2O_{12}S$	$C_{15}H_{28}N_2O_{12}S$
Crystal System, space group	Triclinic *P*1	Monoclinic $P2_1$	Triclinic *P*1	Triclinic *P*1
M_r	432.40	446.43	446.43	460.45
a, Å	5.6975(4)	5.6669(3)	5.6937(3)	5.6972(2)
b, Å	9.3292(8)	19.0508(9)	9.8104(5)	9.4773(3)
c, Å	9.9228(7)	9.7996(5)	10.3950(5)	10.1212(4)
α, deg	109.364(5)	90	66.609(2)	90.857(2)
β, deg	102.250(4)	101.181(1)	87.445(2)	104.853(2)
γ, deg	101.496(5)	90	78.329(2)	97.275(2)
V, (Å^3)	465.00(6)	1037.87(9)	521.49(5)	523.33(3)
Z, *Z′*	1, 1	2, 1	1, 1	1, 1
D_{calc} (g cm^{-3})	1.544	1.429	1.422	1.461
μ (mm^{-1}), rad. type	2.182	1.973	1.964	1.974
F_{000}	228	472	236	244
temp (K)	100(2)	100(2)	100(2)	100(2)
Crystal form, color	needle, colorless	needle, colorless	needle, colorless	needle, colorless
Crystal size, mm	0.024x0.069x0.269	0.074x0.107x0.246	0.033x0.072x0.357	0.046x0.081x0.301
Data collection				
Diffractometer	Bruker D8 Venture CCD	Bruker D8 Venture CCD	Bruker D8 Venture CCD	Bruker D8 Venture CCD
T_{min}/ T_{max}	0.2949 / 0.5137	0.6555/ 0.7538	0.4116/0.7534	0.6349/0.7536
No. of refls. (meas., uniq., and obs.)	9527/3172/2836	17076/4136/4079	12781/3907/3831	12515/3899/3624
R_{int}	0.0739	0.0365	0.0343	0.0480
ϑ_{max} (°)	68.466	74.698	72.322	72.419
Refinement				
R/R^2_ω (obs data)	0.0588/0.1539	0.0320/ 0.0814	0.0300/0.0794	0.0341/0.0796
R/R^2_ω (all data)	0.0660/0.1619	0.0324/ 0.0818	0.0305/0.0800	0.0389/0.0841
S	1.045	1.073	1.039	1.064
No. of refls.	3172	4136	3907	3899
No. of parameters	285	295	295	304
$\Delta\rho_{max/min}$ (e·Å^{-3})	0.675/-0.337	0.604/-0.455	0.417/-0.180	0.317/-0.233
flack	0.16(2)	0.06(2)	0.088(19)	0.089(11)

Table S1. Crystallographic Data for Hydrogen Oxalate Amino Acids. (Continued)

	L-Met·D-Nle·2HOx	L-Etcyst·D-Leu·2HOx	L-Etcyst·D-Met·2HOx	L-Etcyst·D-Nle·2HOx
Crystal data				
CCDC deposit no.	2017260	2054514	2017246	2051775
Empirical formula	$C_{15}H_{28}N_2O_{12}S$	$C_{15}H_{28}N_2O_{12}S$	$C_{14}H_{26}N_2O_{12}S_2$	$C_{15}H_{28}N_2O_{12}S$
Crystal System, space group	Triclinic *P*1	Monoclinic $P2_1$	Monoclinic $P2_1$	Monoclinic $P2_1$
M_r	460.45	460.45	478.49	460.45
a, Å	5.6692(2)	5.6805(3)	5.6622(2)	5.6798(3)
b, Å	9.4991(3)	19.7087(9)	19.4329(7)	19.5782(9)
c, Å	10.2324(3)	9.7095(4)	9.8324(3)	9.7982(5)
α, deg	93.406(2)	90	90	90
β, deg	101.269(2)	99.848(3)	101.810(2)	101.642(2)
γ, deg	97.714(2)	90	90	90
V, (Å^3)	533.44(3)	1071.01(9)	1058.99(6)	1067.15(9)
Z, *Z'*	1, 1	2, 1	2, 1	2, 1
D_{calc} (g cm^{-3})	1.433	1.428	1.501	1.433
μ (mm^{-1}), rad. type	1.937	1.929	2.872	1.936
F_{000}	244	488	504	488
temp (K)	100(2)	100(2)	100(2)	100(2)
Crystal form, color	needle, colorless	needle, colorless	needle, colorless	needle, colorless
Crystal size, mm	0.290x0.240x0.180	0.061x0.07x0.28	0.035x0.093x0.477	0.042x0.097x0.398
Data collection				
Diffractometer	Bruker APEX II CCD	Bruker D8 Venture CCD	Bruker D8 Venture CCD	Bruker D8 Venture CCD
T_{min}/ T_{max}	0.604/0.722	0.6273/0.7536	0.5527/0.7538	0.5999/0.7535
No. of refls. (meas., uniq., and obs.)	13001/3684/3654	12103/3885/3599	15724/4222/3484	17194/4135/4021
R_{int}	0.0233	0.0578	0.0861	0.0490
ϑ_{max} (°)	68.333	68.303	74.496	72.418
Refinement				
R/R^2_ω (obs data)	0.0241/0.0664	0.0618/0.0618	0.0475/0.1167	0.0372/0.0975
R/R^2_ω (all data)	0.0243/0.0666	0.0661/0.1761	0.0637/0.1258	0.0382/0.0986
S	1.061	1.136	1.041	1.001
No. of refls.	3684	3885	4222	4135
No. of parameters	281	304	303	340
$\Delta\rho_{max/min}$ (e·Å^{-3})	0.258/-0.210	1.001/-0.387	0.439/-0.419	0.328/-0.221
flack	-0.004(7)	0.100(13)	0.053(14)	0.144(10)

Table S2. Crystallographic data for Non-Hydrogen Oxalate Amino Acids.

	L-Etcyst·D-Nva	L-Etcyst·D-Met	L-Etcyst·D-Nle
Crystal data			
CCDC deposit no.	2051777	2017252	2051776
Empirical formula	$C_{10}H_{22}N_2O_4S$	$C_{10}H_{22}N_2O_4S_2$	$C_{11}H_{24}N_2O_4S$
Crystal System, space group	Monoclinic $P2_1$	Monoclinic $P2_1$	Triclinic $P1$
M_r	266.35	298.41	280.38
a, Å	9.9251(9)	16.4457(10)	5.1451(4)
b, Å	4.7178(4)	4.6941(3)	10.0555(7)
c, Å	14.9823(13)	29.1646(16)	13.4606(10)
α, deg	90	90	85.184(2)
β, deg	105.286(4)	104.877(3)	86.278(2)
γ, deg	90	90	84.585(2)
V, (Å^3)	676.72(10)	2176.0(2)	689.71(9)
Z, *Z'*	2, 1	6, 3	2, 1
D_{calc} (g cm^{-3})	1.307	1.366	1.350
μ (mm^{-1}), rad. type	2.200	3.423	2.185
F_{000}	288	960	304
temp (K)	100(2)	100(2)	100(2)
Crystal form, color	rod, colorless	needle, colorless	prism, colorless
Crystal size, mm	0.066x0.185x0.329	0.042x0.345x0.424	0.138x0.253x0.331
Data collection			
Diffractometer	Bruker D8 Venture CCD	Bruker D8 Venture CCD	Bruker D8 Venture CCD
T_{min}/ T_{max}	0.6314/0.7500	0.5616/0.7531	0.6099/0.7536
No. of refls. (meas., uniq., and obs.)	26867/2669/2625	37344/7845/7334	17337/5137/5071
R_{int}	0.2716	0.0667	0.0217
ϑ_{max} (°)	72.951	68.521	72.307
Refinement			
R/R^2_ω (obs data)	0.0485/0.1350	0.0442/0.1158	0.0214/0.0594
R/R^2_ω (all data)	0.0489/0.1356	0.0477/0.1188	0.0217/0.0597
S	1.061	1.065	1.048
No. of refls.	2669	7845	5137
No. of parameters	174	565	365
$\Delta\rho_{max/min}$ (e·Å^{-3})	0.565/-0.570	0.496/-0.347	0.277/-0.190
flack	0.004(16)	0.093(7)	0.080(3)

Table S3. Hydrogen Bond Parameters for Racemic and Quasiracemic Amino Acids.

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
DL-Nva·HOx	O1–H1···O6^{v}	0.88(2)	1.73(2)	2.5771(14)	161.6(19)
	O3–H3···O5^{i}	0.89(2)	1.75(2)	2.6348(14)	173.8(18)
	N1–H1A···O6^{ii}	0.92(2)	1.95(2)	2.8529(17)	166.4(16)
	N1–H1B···O2^{iii}	0.93(2)	1.94(2)	2.8408(16)	161.9(17)
	N1–H1C···O5^{iv}	0.92(2)	1.94(2)	2.8082(16)	157.7(17)

Symmetry codes: (i) *x*-1, *y*, *z;* (ii) 1-*x*, 2-*y,* 1-*z*; (iii) -*x*, 2-*y,* 1-*z*; (iv) *x*-1, *y,* 1+*z*; (v) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
DL-Leu·HOx	O1–H1···O6^{iv}	0.87(2)	1.72(2)	2.5736(10)	166.7(15)
	O3–H3···O5^{v}	0.91(2)	1.69(2)	2.5920(10)	174.9(14)
	N1–H1A···O6^{ii}	0.92(2)	1.93(2)	2.8278(12)	165.6(13)
	N1–H1B···O2^{iii}	0.90(2)	1.99(2)	2.8542(12)	162.3(13)
	N1–H1C···O5^{i}	0.91(2)	2.00(2)	2.8509(11)	155.0(13)

Symmetry codes: (i) *x, y*-1, *z;* (ii) -*x*+1.5, *y*+0.5*, -z*+1.5; (iii) 1-*x*, -*y,* 1-*z*; (iv) *x*-0.5*, -y*-3.5*, z*-0.5; (v) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
DL-Met·HOx	O1–H1···O6^{i}	0.87(2)	1.76(2)	2.6175(14)	171.7(19)
	O3–H3···O5^{ii}	0.97(2)	1.52(2)	2.4837(13)	175.1(18)
	N1–H1A···O2^{ii}	0.90(2)	2.07(2)	2.8790(15)	149.0(16)
	N1–H1B···O6^{iii}	0.86(2)	2.12(2)	2.8796(15)	146.5(17)
	N1–H1C···O4^{iv}	0.90(2)	1.98(2)	2.8435(15)	161.8(17)

Symmetry codes: (i) 1-*x,* 1+*y*, *z;* (ii) *x*-1, *y, z*; (iii) -*x*, -*y, -z*; (iv) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-Met·D-Nva·2HOx	O1–H1···O8^{i}	0.96(4)	1.63(4)	2.571(2)	166(4)
	O3–H3···O12^{ii}	0.88(4)	1.72(4)	2.557(2)	158(4)
	O5–H5···O7^{iii}	0.88(4)	1.73(4)	2.607(2)	174(4)
	O9–H9···O11^{iv}	0.74(4)	1.86(4)	2.602(2)	177(4)
	N1–H1B···O12^{v}	0.87(4)	2.00(4)	2.859(3)	166(3)
	N1–H1A···O4^{vii}	0.86(4)	2.00(4)	2.813(3)	156(3)
	N1–H1C···O7^{vii}	0.82(4)	2.03(4)	2.811(3)	159(3)
	N2–H2A···O2^{vii}	0.89(4)	2.02(4)	2.835(3)	151(3)
	N2–H2B···O8^{vi}	0.89(4)	1.98(4)	2.833(3)	160(3)
	N2–H2C···O11^{vii}	0.85(4)	2.00(4)	2.802(3)	156(3)

Symmetry codes: (i) 1+*x, y*, 1+*z;* (ii) *x*-1, *y, z*-1; (iii) *x*-1, *y, z*; (iv) 1+*x, y, z*; (v) *x, y, z*-1; (vi) *x, y*, 1+*z;* (vii) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-Mecyst·D-Nva·2HOx	O1–H1···O8^{i}	0.85(3)	1.76(4)	2.569(6)	158(9)
	O3–H3···O12^{ii}	0.86(3)	1.76(4)	2.578(6)	160(10)
	O5–H5···O7^{iii}	0.85(3)	1.79(3)	2.632(5)	179(9)
	O9–H9···O11^{iv}	0.86(3)	1.78(3)	2.628(6)	169(10)
	N1–H1A···O7^{v}	0.85(3)	2.00(4)	2.827(7)	166(8)
	N1–H1B···O12^{ii}	0.86(3)	2.02(4)	2.847(7)	162(9)
	N1–H1C···O4^{iii}	0.86(3)	2.05(5)	2.859(7)	156(9)
	N2–H2A···O11^{v}	0.85(3)	2.09(5)	2.824(7)	144(7)
	N2–H2B···O8^{i}	0.86(3)	2.00(4)	2.813(7)	158(8)
	N2–H2C···O2^{iv}	0.85(3)	2.06(5)	2.859(7)	156(9)

Symmetry codes: (i) *x*-1, *y*, *z*-1; (ii) 1+*x*, *y*, 1+*z*; (iii) 1+*x*, *y*, *z*; (iv) *x*-1, *y*, *z*; (v) *x*, *y*, *z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-Etcyst·D-Nva·2HOx	O1–H1···O8^{v}	0.74(4)	1.83(4)	2.554(2)	167(4)
	O3–H3···O12^{vi}	0.93(4)	1.71(4)	2.592(2)	158(4)
	O5–H5···O7^{iii}	0.79(4)	1.84(4)	2.631(2)	174(4)
	O9–H9···O11^{iv}	0.80(4)	1.81(4)	2.610(2)	174(4)
	N1–H1C···O4^{vii}	0.90(4)	1.99(4)	2.847(3)	159(3)
	N1–H1B···O7^{vii}	0.77(4)	2.11(4)	2.829(3)	155(4)
	N1–H1A···O12^{ii}	0.82(4)	2.08(4)	2.858(3)	159(4)
	N2–H2A···O8^{i}	0.93(4)	1.91(4)	2.827(3)	167(3)
	N2–H2B···O11^{vii}	0.85(4)	2.00(4)	2.799(3)	156(3)
	N2–H2C···O2^{vii}	0.82(4)	2.05(4)	2.827(3)	159(3)

Symmetry codes: (i) *x*, 1+*y*, *z*; (ii) *x*, *y*-1, *z*; (iii) 1+*x*, *y*, *z*; (iv) *x*-1, *y*, *z*; (v) *x*-1, 1+*y*, *z*; (vi) 1+*x*, *y*-1, *z*; (vii) *x*, *y*, *z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-Met·D-Leu·2HOx	O1–H1···O8^{i}	0.85(3)	1.74(3)	2.568(4)	166(5)
	O3–H3···O12^{ii}	0.85(3)	1.72(3)	2.568(4)	172(5)
	O5–H5···O7^{iii}	0.85(3)	1.77(3)	2.618(3)	173(5)
	O9–H9···O11^{iv}	0.83(3)	1.80(3)	2.624(3)	170(5)
	N1–H1A···O7^{vii}	0.86(3)	1.95(3)	2.790(4)	166(5)
	N1–H1B···O12^{v}	0.87(3)	2.03(3)	2.899(4)	174(5)
	N1–H1C···O4^{vii}	0.88(3)	1.98(3)	2.797(4)	154(5)
	N2–H2B···O8^{vi}	0.88(3)	1.95(3)	2.776(4)	156(4)
	N2–H2A···O11^{vii}	0.87(7)	2.02(7)	2.878(5)	171(4)
	N2–H2C···O2^{vii}	0.86(3)	1.99(3)	2.795(4)	155(5)

Symmetry codes: (i) 1+*x*, 1+*y*, *z*; (ii) *x*-1, *y*-1, *z*; (iii) *x*-1, *y*, *z*; (iv) 1+*x*, *y*, *z*; (v) *x*, *y*-1, *z*; (vi) *x*, 1+*y*, *z*; (vii) *x*, *y*, *z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-Etcyst·D-Leu·2HOx	O1–H1···O8^{i}	0.83(2)	1.75(2)	2.572(2)	169(3)
	O3–H3···O12^{ii}	0.86(2)	1.73(2)	2.567(2)	163(3)
	O5–H5···O7^{iii}	0.81(2)	1.79(2)	2.6009(19)	176(3)
	O9–H9···O11^{iv}	0.85(2)	1.75(2)	2.5972(19)	176(3)
	N1–H1A···O7^{vii}	0.88(2)	1.94(2)	2.781(2)	160(3)
	N1–H1B···O4^{v}	0.87(2)	1.98(2)	2.791(2)	154(3)
	N1–H1C···O12^{vii}	0.88(2)	2.01(2)	2.883(2)	173(3)
	N2–H2A···O8^{vi}	0.84(2)	2.03(2)	2.867(2)	175(3)
	N2–H2B···O2^{vii}	0.85(2)	2.01(2)	2.803(2)	154(3)
	N2–H2C···O11^{vii}	0.88(2)	1.92(2)	2.774(2)	162(3)

Symmetry codes: (i) 1+*x*, 1+*y, z;* (ii) *x*-1, *y*-1*, z*; (iii) *x*-1, *y, z*; (iv) 1+*x, y, z*; (v) *x, y*-1*, z*; (vi) *x,* 1+*y*, *z;* (vii) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-Met·D-Nle·2HOx	O1–H1···O8^{i}	0.83(2)	1.75(2)	2.572(2)	169(3)
	O3–H3···O12^{ii}	0.86(2)	1.73(2)	2.567(2)	163(3)
	O5–H5···O7^{iii}	0.81(2)	1.79(2)	2.6009(19)	176(3)
	O9–H9···O11^{iv}	0.85(2)	1.75(2)	2.5972(19)	176(3)
	N1–H1A···O7^{vii}	0.88(2)	1.94(2)	2.781(2)	160(3)
	N1–H1B···O4^{vii}	0.87(2)	1.98(2)	2.791(2)	154(3)
	N1–H1C···O12^{v}	0.88(2)	2.01(2)	2.883(2)	173(3)
	N2–H2A···O8^{vi}	0.84(2)	2.03(2)	2.867(2)	175(3)
	N2–H2B···O2^{vii}	0.85(2)	2.01(2)	2.803(2)	154(3)
	N2–H2C···O11^{vii}	0.88(2)	1.92(2)	2.774(2)	162(3)

Symmetry codes: (i) 1+*x*, 1+*y, z;* (ii) *x*-1, *y*-1*, z*; (iii) *x*-1, *y, z*; (iv) 1+*x, y, z*; (v) *x, y*-1*, z*; (vi) *x,* 1+*y*, *z;* (vii) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-Etcyst·D-Nle·2HOx	O1–H1···O8^{i}	0.86(3)	1.75(3)	2.576(12)	159(5)
	O3–H3···O12^{ii}	0.85(3)	1.79(3)	2.617(11)	166(5)
	O5–H5···O7^{iii}	0.85(3)	1.78(3)	2.617(12)	169(5)
	O9–H9···O11^{iv}	0.86(3)	1.76(3)	2.619(12)	176(5)
	N1–H1C···O7^{vii}	0.83(3)	2.04(3)	2.856(12)	165(4)
	N1–H1A···O12^{v}	0.84(3)	1.99(3)	2.782(14)	157(5)
	N1–H1B···O4^{vii}	0.85(3)	2.06(3)	2.836(4)	153(4)
	N2–H2A···O8^{vi}	0.87(3)	1.92(3)	2.773(14)	166(4)
	N2–H2B···O11^{vii}	0.85(3)	2.05(3)	2.838(11)	154(4)
	N2–H2C···O2^{vii}	0.86(3)	2.00(3)	2.825(4)	162(4)

Symmetry codes: (i) *x*-1, *y, z*-1*;* (ii) 1+*x*, *y,* 1+*z*; (iii) 1+*x*, *y, z*; (iv) *x*-1*, y, z*; (v) *x, y,* 1+*z*; (vi) *x, y*, *z*-1*;* (vii) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-Etcyst·D-Met·2HOx	O1–H1···O8^{i}	0.86(3)	1.76(4)	2.586(5)	160(7)
	O3–H3···O12^{ii}	0.86(3)	1.75(4)	2.550(5)	154(7)
	O5–H5···O7^{iii}	0.84(3)	1.77(3)	2.601(5)	171(7)
	O9–H9···O11^{iv}	0.84(3)	1.76(3)	2.599(5)	172(7)
	N1–H1A···O7^{vii}	0.94(7)	1.98(7)	2.825(6)	148(6)
	N1–H1B···O12^{v}	0.93(7)	1.93(7)	2.860(6)	176(6)
	N1–H1C···O4^{vii}	0.96(7)	1.92(7)	2.831(6)	157(6)
	N2–H2B···O8^{vi}	0.73(7)	2.18(7)	2.873(6)	159(7)
	N2–H2C···O2^{vii}	0.76(7)	2.14(7)	2.849(6)	156(7)
	N2–H2A···O11^{vii}	0.97(7)	1.83(7)	2.783(6)	166(6)

Symmetry codes: (i) *x*-1, *y, z*-1*;* (ii) 1+*x*, *y,* 1+*z*; (iii) 1+*x*, *y, z*; (iv) *x*-1*, y, z*; (v) *x, y,* 1+*z*; (vi) *x, y*, *z*-1*;* (vii) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
(DL)-Met	N1–H1C···O2^{i}	0.92(2)	1.90(2)	2.8073(18)	169(2)
	N1–H1A···O2^{ii}	0.98(2)	1.83(2)	2.7847(18)	166.4(19)
	N1–H1B···O1^{iii}	0.93(2)	1.85(2)	2.7753(17)	173(2)

Symmetry codes: (i) *x,* 1-*y*, 1/2+*z;* (ii) *x*, 2-*y,* 1/2+*z*; (iii) 3/2-*x*, 1/2+*y,* 1/2-*z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-EtCys·D-Met	N1A–H11A···O4B^{vii}	0.78(7)	2.04(8)	2.802(5)	167(7)
	N1C–H12C···O3C^{i}	0.88(3)	1.95(3)	2.811(4)	168(4)
	N1C–H11C···O3C^{ii}	0.89(7)	1.92(7)	2.800(4)	167(6)
	N1C–H13C···O2C^{ii}	0.84(5)	1.92(5)	2.751(4)	171(4)
	N1A–H12A···O4B^{iii}	0.85(6)	1.95(6)	2.802(5)	173(4)
	N1B–H13B···O3A^{vii}	0.83(6)	2.00(6)	2.822(5)	170(5)
	N1A–H13B···O1B^{vii}	0.91(5)	1.87(5)	2.776(4)	173(5)
	N1B–H11B···O2A^{iv}	0.91(5)	1.84(5)	2.741(4)	168(5)
	N2B–H16B···O1C^{iv}	0.92(6)	1.84(6)	2.753(4)	171(5)
	N2B–H14B···O4C^{vii}	0.79(6)	1.99(6)	2.774(4)	171(6)
	N2A–H14A···O4A^{v}	0.84(5)	1.94(5)	2.785(4)	177(4)
	N2C–H16C···O2B^{iii}	0.84(6)	1.98(6)	2.810(5)	168(4)
	N2A–H15A···O1A^{vi}	0.88(6)	1.89(6)	2.764(4)	174(5)
	N2C–H15C···O2B^{vii}	0.94(5)	1.92(5)	2.853(5)	171(4)
	N2B–H15B···O1C^{vii}	0.91(6)	1.91(6)	2.762(4)	156(5)
	N1B–H12B···O3A^{iv}	0.80(6)	2.05(6)	2.812(5)	158(5)
	N2A–H16A···O1A^{v}	0.92(5)	1.88(5)	2.750(4)	157(4)
	N2C–H14C···O3B^{iii}	0.88(5)	1.96(5)	2.831(4)	166(4)

Symmetry codes: (i) 2-*x,* -1-*y*, 1-*z;* (ii) 2-*x*, *y,* 1-*z*; (iii) *x*, *y*-1*, z*; (iv) *x, y*+1*, z*; (v) 1-*x,* -1-*y, -z*; (vi) 1-*x, -y, -z*; (vii) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-EtCys·D-Nle	N1A–H1A···O1B^{v}	0.92(2)	1.86(3)	2.7620(17)	167(2)
	N1A–H2A···O3A^{v}	0.89(2)	2.32(2)	2.9464(17)	127.7(19)
	N1A–H2A···O4A^{i}	0.89(2)	2.25(2)	3.0146(18)	144(2)
	N1A–H3A···O2A^{ii}	0.90(2)	1.98(2)	2.8339(18)	158.6(19)
	N1B–H4A···O4A^{iii}	0.93(2)	1.84(3)	2.7599(17)	168(2)
	N1B–H5A···O2B^{ii}	0.90(2)	1.99(2)	2.8536(18)	159(2)
	N1B–H6A···O3B^{v}	0.88(2)	2.36(2)	3.0007(17)	130.6(19)
	N1B–H6A···O4B^{i}	0.88(2)	2.24(2)	2.9857(18)	143(2)
	N2A–H7B···O3B^{iv}	0.87(3)	1.90(3)	2.7605(18)	173(2)
	N2A–H9B···O4A^{i}	0.87(2)	1.94(2)	2.8125(18)	172(2)
	N2A–H8B···O1A^{v}	0.89(3)	2.42(2)	2.9116(17)	115.0(18)
	N2A–H8B···O2A^{ii}	0.89(3)	2.08(3)	2.9241(19)	157(2)
	N2B–H2···O3A^{v}	0.88(3)	1.88(3)	2.7542(18)	172(2)
	N2B–H3···O1B^{v}	0.91(2)	2.37(2)	2.9420(17)	120.7(18)
	N2B–H3···O2B^{ii}	0.91(2)	2.11(3)	2.9345(19)	151(2)
	N2B–H12B···O4B^{i}	0.87(2)	1.98(2)	2.8265(18)	166(2)

Symmetry codes: (i) *x*-1*, y, z;* (ii) *x*+1, *y, z*; (iii) *x*+1, *y*-1*, z*; (iv) *x*-1*, y*+1*, z*; (v) *x, y, z*

S3. Conformational and Symmetry Assessments

Conformational Assessments (χ_{RMS}). Each quasiracemic hydrogen oxalate amino acid structure was processed using X-SEED[2] where each amino acid component was isolated, configuration inverted to L if necessary, and saved as an individual file. These structure files were then loaded into CCDC-Mercury[8] and processed using the structure overlay feature. Hydrogen atoms were omitted from the assessments. The initial overlay process involved matching common atoms from the core N-C(C)-CO_2 fragments to determine the root-mean-squared best fit value (χ_{RMS}). Additional overlay calculations were performed on the two molecules by including the core fragments and the next atom associated with the side chain *R* group. These sequential assessments provided a range of χ_{RMS} values that shows the dependency of molecular conformations to chain length.

Inversion Symmetry Assessments (C_i). The quasiracemic crystal structures were initially processed using X-SEED[2]. The hydrogen oxalate fragments, hydrogen atoms, and non-hydrogen atoms lacking an equivalent partner were omitted. Each quasienantiomeric pair was organized with the same packing motifs – *i.e.,* $R_2^2(10)$ patterns – to provide consistent processing of the structures. A series of structure files were then generated that differed by the length of the *R* groups. These files containing near inversion related quasiracemate fragments and were assessed using Avnir's *Continuous Symmetry Measures* online tools.[9] The output from this process gave a quantitative measure (C_i values) of the degree of inversion symmetry for each structural fragment as a function of side chain length.

Table S4. Symmetry (C_i values) and Conformation (χ_{RMS} values) Data for the Quasiracemates

Compound	Molecular section	χ_{RMS} L-Mecyst·D-Nva·2HOx	C_i L-Metcyst·D-Nva·2HOx
L-Mecyst·D-Nva·2HOx	1	0.0194	0.0065
	2	0.0769	0.0312
	3	0.116	0.0513

Compound	Molecular section	χ_{RMS} L-Etcyst·D-Nva·2HOx	C_i L-Etcyst·D-Nva·2HOx
L-Etcyst·D-Nva·2HOx	1	0.035	0.0453
	2	0.118	0.830
	3	0.610	1.3336

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Compound	Molecular section	χ_{RMS} L-Etcyst·D-Leu·2HOx	C_i L-Etcyst·D-Leu·2HOx
L-Etcyst·D-Leu·2HOx	1	0.189	0.4585
	2	0.609	1.1924
	3	0.881	2.5009

Compound	Molecular section	χ_{RMS} L-Etcyst·D-Nle·2HOx	C_i L-Etcyst·D-Nle·2HOx
L-Etcyst·D-Nle·2HOx	1	0.058	0.0322
	2	0.099	0.475
	3	0.578	1.3527
	4	0.886	3.6913

Compound	Molecular section	χ_{RMS} L-Met·D-Nva·2HOx	χ_{RMS} URODIP	C_i L-Met·D-Nva·2HOx	C_i URODIP
L-Met·D-Nva·2HOx	1	0.063	0.0144	0.0848	0.0007
	2	0.629	0.0282	1.2585	0.0031
	3	0.904	0.0946	2.6933	0.0186

Compound	Molecular section	χ_{RMS} L-Met·D-Leu·2HOx	χ_{RMS} BERNIV	C_i L-Met·D-Leu·2HOx	C_i BERNIV
L-Met·D-Leu·2HOx	1	0.031	0.109	0.0074	0.1432
	2	0.074	0.168	0.0493	0.4149
	3	0.136	0.251	0.1404	0.7938

Compound	Molecular section	χ_{RMS} L-Met·D-Nle·2HOx	χ_{RMS} GOLVOS	C_i L-Met·D-Nle·2HOx	C_i GOLVOS
L-Met·D-Nle·2HOx	1	0.027	0.0082	0.0236	0.0009
	2	0.059	0.00918	0.0355	0.0009
	3	0.623	0.0861	1.2465	0.0157
	4	0.987	0.124	3.578	0.0172

Compound	Molecular section	χ_{RMS} L-Etcyst·D-Nva	C_i L-Etcyst·D-Nva
L-Etcyst·D-Nva	1	0.0531	0.1993
	2	0.166	0.3818
	3	0.595	0.4329

Compound	Molecular section	χ_{RMS} L-Etcyst·D-Nle	C_i L-Etcyst·Nle
L-Etcyst·D-Nle			
Quasiracemate A	1	0.172	0.067
	2	0.654	1.7635
	3	1.08	3.0163
	4	1.29	3.2735
Quasiracemate B	1	0.0649	0.3137
	2	0.718	1.2735
	3	0.915	3.7358
	4	1.03	6.2681

Compound	Molecular section	χ_{RMS} L-Etcyst·D-Met	C_i L-Etcyst·Met
L-Etcyst·D-Met			
Quasiracemate A	1	0.0282	0.0222
	2	0.114	0.0429
	3	0.110	0.0315
	4	0.184	0.0341
Quasiracemate B	1	0.0444	0.0256
	2	0.117	0.0507
	3	0.110	0.0444
	4	0.161	0.0657
Quasiracemate C	1	0.0862	0.0194
	2	0.183	0.0955
	3	0.6	0.6396
	4	0.578	0.4927

S4. Cambridge Crystallographic Database (CSD) Searches

A search for methyl cysteinium, ethyl cysteinium, and methioninium cations in the *CCDC-Cambridge Structural Database* (CSD, version 5.42, update 2) produced 15 hits with 19 fragments. The CSD refcodes are provided below.

CSD Refcode (number of fragments)
BANPUC (1)
CONZIO01 (1)
FAPMAL (1)
FAPMEP (1)
FONJAU (1)
LUDHEX (2)
METHCL01 (1)
MOCXUX (1)
REMSUX (2)
REMSUX01 (1)
VICZEN (2)
WOYVIP (1)
XAZNAO (1)
YIGMEI (1)
YUDDIM (1)

A CSD search (version 5.42, update 2) for the methionyl, methyl cysteinyl, ethyl cysteinyl, and norleucinyl fragments retrieved 292, 35, 12, and 69 entries, respectively. When necessary, the stereochemistry of the retrieved molecular fragments was inverted to the L isomer [*S* stereochemical configuration for (methionyl and norleucinyl or the *R* isomer for methyl and ethyl cysteine]. The dihedral angles were converted to values between 0 and 360 °.

CSD Structure Code	Fragment	ϕ_1 (°)	ϕ_2 (°)	ϕ_3 (°)
Methionyl				
2051773	1	186.335	180.791	185.081
2017246	1	299.277	186.61	73.282
2017250	1	168.846	308.436	306.316
2017252	1	188.925	180.778	189.402
2017252	2	188.543	181.983	191.315
2017252	3	185.385	181.019	185.18
2017257	1	75.031	47.367	63.419
2017258	1	155.851	184.293	273.885
2017260	1	163.492	304.371	304.221
ACMETM	1	175.358	177.456	181.389
ACMTDE	1	62.125	176.033	285.479
ALAMET01	1	306.45	178.036	188.156

ALAMET10	1	303.765	175.001	186.229
ALAMET11	1	306.421	178.044	188.241
ANUPOQ	1	68.698	168.468	178.225
ANUPOQ	2	69.317	195.984	300.025
ANUPOQ	3	72.334	69.062	72.748
ANUPOQ	4	312.977	176.442	289.669
ANUPOQ01	1	304.546	180.392	284.734
AVIKIA	1	148.354	68.174	77.359
BANPUC	1	304.595	179.42	289.811
BCMEGL	1	165.576	175.295	174.866
BERNIV	1	81.97	183.924	296.331
BERQIY	1	70.951	187.374	296.15
BIDLOQ	1	183.946	301.006	268.341
BIDLOQ	2	167.529	291.71	89.166
BOXFUS	1	183.091	177.867	163.203
BUYXEY10	1	179.692	175.94	71.674
CAQTOD	1	68.717	183.993	290.751
CAQTOD	2	69.714	181.606	290.254
CAWKIU	1	308.495	189.826	77.745
CONZIO01	1	182.575	193.176	75.513
DACXUA	1	178.031	287.954	160.111
DACXUA10	1	178.004	287.976	160.12
DADGUK	1	172.877	300.901	300.64
DADNEB	1	180.209	179.036	292.019
DADNEB	2	175.363	169.615	282.562
DAXLEU	1	60.697	177.833	88.897
DAXLIY	1	174.116	186.031	327.608
DAXLIY	2	178.107	175.978	330.378
DAXLOE	1	181.628	195.04	299.759
DEHFAA	1	170.399	276.567	87.348
DEHFAA	2	170.452	290.252	101.85
DEHFAA	3	170.731	182.181	293.392
DEHFAA	4	172.098	175.053	284.669
DENNUF	1	62.301	181.353	288.276
DEQJOY	1	304.438	289.991	295.598
DIWREH	1	167.644	179.441	70.404
DIZHAV	1	167.665	287.215	275.983
DLMETA05	1	186.435	180.764	184.985
DLMETA07	1	181.988	176.652	69.339
DLMETA08	1	186.454	180.767	184.982
DLMETA09	1	184.977	180.84	185.454
DLMETA10	1	179.302	175.814	74.832
DLMETA11	1	179.343	176.43	75.837

DUMCET	1	58.279	177.036	289.877
DUVSAR	1	174.932	175.061	172.618
EBESEM	1	174.467	173.862	62.351
EBESEM	2	175.493	173.48	62.85
EGUVOU	1	172.702	183.392	281.027
EMIPAR	1	303.303	152.825	178.663
EMIPAR	2	164.817	71.808	182.682
EMIREX	1	175.104	161.338	282.539
EMIREX	2	191.537	138.798	271.2
EROGEY	1	304.071	182.353	100.925
ETUTES	1	55.319	174.282	121.271
ETUTES	2	55.484	172.171	95.208
ETUTES	3	57.144	169.106	80.147
ETUTES	4	58.304	171.367	76.057
EVIPII	1	172.642	295.72	290.644
EYIKEC	1	174.39	186.553	300.581
FABPAB	1	176.239	204.549	117.568
FABPAB01	1	159.695	172.882	74.587
FABPIJ	1	165.114	199.758	189.179
FABPOP	1	159.088	177.347	73.311
FAPMAL	1	78.34	182.172	284.602
FAPMEP	1	296.222	178.463	157.362
FEMFOS	1	291.719	177.744	281.684
FEYHIA	1	308.846	173.548	71.55
FEYHIA	2	304.134	178.014	70.161
FITLID	1	185.753	178.076	79.108
FIYMUX	1	139.27	304.705	296.988
FIYMUX	2	286.371	174.048	297.472
FIYMUX	3	167.118	179.522	71.34
FOCGOU	1	295.076	180.127	169.704
FOCGOU	2	164.505	290.504	288.381
FOCGOU	3	170.561	292.432	172.814
FOCGOU	4	176.987	181.82	185.173
FOKNIC	1	307.352	175.663	286.59
FONJAU	1	306.567	177.821	174.933
GADBEV	1	305.47	179.47	71.835
GADBEV	2	301.48	177.543	72.256
GAKZIC	1	290.914	196.892	289.964
GAKZIC	2	176.034	180.64	291.033
GASTRN10	1	174.972	195.516	194.365
GASTRN10	2	179.214	178.092	81.064
GEQMEW	1	172.393	296.485	281.525
GIMDOW	1	88.822	70.766	164.923

GIMFAK	1	169.87	295.45	174.99
GIMFAK	2	173.671	170.92	56.902
GIPHUJ	1	165.326	198.659	298.104
GOLVOS	1	187.596	180.577	189.223
GUKNEF	1	71.4	179.641	282.094
GUMXIX	1	170.412	186.868	183.879
GUMXIX	2	65.588	168.329	283.828
HAFKUU	1	65.497	183.765	87.591
HEYRAH	1	163.021	182.13	63.638
HEZCOE	1	190.707	189.328	311.846
HUCYUA	1	173.92	174.667	69.903
HUKQEL	1	57.565	176.189	176.629
HURXUP	1	191.029	64.352	59.722
HUSJEK	1	165.432	297.273	293.31
HUSJEK	2	170.521	177.962	66.14
IBUDUF	1	294.32	165.936	276.253
IBUDUF	2	301.311	177.55	65.234
IDIHEI	1	165.366	152.43	282.511
IDIHEI	2	78.995	179.394	296.032
IPISAB	1	177.162	194.475	181.323
IPISEF	1	159.518	176.17	169.709
IPISIJ	1	158.603	176.006	170.26
JAQHUH	1	169.911	185.354	63.73
JAQJAP	1	169.283	181.808	58.59
JAQJET	1	63.441	64.672	76.026
JAQJIX	1	60.919	65.393	76.061
JAQJIX01	1	64.33	63.318	80.895
JAQJUJ	1	59.53	69.362	81.387
JUKMIL	1	160.748	174.549	289.572
KAFBUP	1	293.898	180.238	172.213
KAFBUP	2	164.069	290.636	289.299
KAFBUP	3	171.506	292.599	172.035
KAFBUP	4	178.263	183.081	184.548
LARBEO	1	192.607	186.458	197.155
LARBIS	1	190.398	184.866	195.929
LEQFIZ	1	161.886	174.007	282.36
LEQFIZ	2	167.746	178.82	293.179
LEQFIZ	3	174.879	177.714	296.295
LIMZIT	1	296.829	169.666	60.349
LIMZIT	2	62.649	73.474	62.098
LMETON02	1	71.827	171.599	181.473
LMETON02	2	74.103	71.521	72.374
LMETON11	1	71.704	171.878	181.637

LMETON11	2	74.096	71.706	72.242
LMETON12	1	74.895	72.557	72.723
LMETON12	2	76.687	172.718	182.465
LMETON13	1	75.832	73.359	76.87
LMETON13	2	82.599	167.075	164.981
LMETON14	1	179.277	171.766	59.192
LMETON14	2	78.67	173.978	181.871
LMETZN	1	59.377	182.721	175.988
LMETZN	2	59.377	182.721	175.988
LMETZN01	1	56.839	181.758	177.094
LOVQUI	1	158.529	297.803	297.592
LOVQUI	2	148.685	301.158	301.102
LUDHEX	1	167.079	181.694	274.27
LUDHEX	2	173.452	181.524	175.973
LUHBUL	1	171.658	302.282	295.02
LUHBUL	2	171.987	169.417	62.537
MAKLIU	1	172.272	298.101	294.147
MAKLIU	2	178.584	306.993	291.321
MAZYES	1	175.672	186.149	281.983
MAZYES	2	66.372	176.302	286.243
MEGNAO	1	177.303	182.398	71.902
METHCL	1	299.15	181.815	68.739
METHCL01	1	296.138	180.267	70.145
METMET	1	74.629	191.711	178.387
METMET	2	302.353	189.503	302.347
MOCXUX	1	85.661	73.845	73.464
NEQYIR	1	172.819	181.675	286.491
NOHMON	1	182.489	304.791	291.257
NOHMON	2	177.467	311.606	303.332
NOHMON	3	174.835	295.34	169.248
NOHMON	4	177.872	304.834	300.087
OBAVUI	1	170.067	191.919	181.125
OBAVUI	2	170.64	299.547	292.764
OHELOE	1	71.363	179.104	277.428
OLOGEB	1	193.301	304.171	290.426
OLOGEB	2	190.914	305.611	287.201
OLOGEB	3	308.974	184.475	154.365
OLOGEB	4	161.034	191.197	177.644
OLOGEB	5	173.795	184.134	285.345
OLOGEB	6	178.745	178.454	283.977
OLOGEB	7	62.659	186.352	294.501
POVYOP	1	183.925	173.881	78.251
QOYJEU	1	190.628	186.568	280.897

RAVZAQ	1	303.768	166.052	288.54
REMSUX	1	80.205	161.506	277.449
REMSUX	2	84.482	63.087	70.797
REMSUX01	1	70.914	153.197	292.479
RIBTAA	1	165.844	286.649	282.669
RICKIA	1	60.053	181.945	187.388
RIFVAF	1	164.625	276.512	168.49
RIFVAF	2	171.221	193.157	299.238
RIFVAF	3	171.57	190.56	75.411
RIFVAF	4	174.595	188.564	294.939
SAFVOM	1	179.929	308.284	306.371
SEGYUA	1	169.134	190.35	171.92
SEGYUA	2	173.23	183.657	177.787
SEGZAH	1	168.215	180.572	185.216
SEGZAH	2	173.515	185.592	186.517
SEGZAH	3	175.373	181.502	161.639
SIKWEO01	1	163.815	300.633	290.536
SIKWEO01	2	307.675	195.441	182.272
SUSZIP01	1	177.336	303.803	288.73
SUSZIP01	2	158.206	168.95	63.098
TBLMCU	1	57.556	180.463	174.767
TBLMCU	2	171.019	296.391	289.253
TIBZUA	1	155.172	162.56	78.001
TICKAS	1	170.315	194.899	181.017
TOPSID	1	78.939	186.529	296.991
TOPSOJ	1	54.745	160.484	76.97
TOPSUP	1	165.206	169.186	290.121
TOPSUP	2	173.975	187	185.129
TOPSUP	3	175.656	200.797	84.536
TOPSUP	4	177.042	199.608	83.902
TOPSUP	5	157.885	188.871	68.15
TOPSUP	6	158.568	167.946	71.646
TOPSUP	7	159.803	181.1	64.254
TOPSUP	8	168.835	174.369	293.935
TOPSUP	9	149.885	181.959	63.426
TOPSUP	10	150.19	184.335	62.213
TOPSUP	11	158.737	297.568	288.984
TOPSUP	12	171.119	186.523	182.296
TOPSUP	13	155.757	295.851	279.981
TOPSUP	14	84.978	188.33	285.997
TOPSUP	15	166.49	169.008	292.732
TOPSUP	16	174.998	178.965	285.007
TOPSUP	17	153.012	182.347	171.193

TOPSUP	18	155.766	182.686	172.842
TOPSUP	19	163.614	173.464	77.128
TOPSUP	20	168.468	294.21	291.121
UCAJIT	1	165.047	289.458	273.045
UJEJEY	1	161.713	280.381	280.156
UJEJEY	2	168.607	296.305	286.386
ULEWIT	1	169.999	293.886	285.646
UMUBIN	1	158.227	302.577	293.999
URODIP	1	184.324	174.422	67.846
URODIP01	1	183.754	175.001	68.475
URODIP02	1	184.422	174.177	68.085
URODIP03	1	184.158	174.342	67.761
URODIP04	1	184.044	174.521	67.652
URODIP05	1	184.386	180.57	67.669
URODIP06	1	72.766	181.875	296.871
URODIP06	2	183.971	174.785	64.301
URODIP07	1	74.351	183.605	288.575
UZIPUP	1	163.818	291.21	301.835
VALDIX	1	179.601	299.613	278.978
VENXOB	1	63.27	182.622	290.184
VEPDOK	1	305.129	179.713	67.784
VICZEN	1	176.123	181.672	282.843
VICZEN	2	81.657	174.743	290.843
VOYNUS	1	170.869	198.108	72.825
VOYNUS	2	56.218	176.114	286.807
VUKHAK	1	174.612	185.199	185.543
VUQNAY	1	187.577	180.456	189.201
VUQNAY01	1	186.639	180.769	188.112
VUQNAY02	1	181.578	180.583	196.507
VUQNAY03	1	177.634	174.91	183.219
VUQNAY03	2	188.021	175.301	60.108
VUQNAY04	1	191.758	195.311	152.463
WAHSAA	1	174.629	292.17	281.032
WAHSEE	1	172.621	193.83	295.025
WEKVAK	1	164.457	183.298	288.719
WEKVAK	2	184.624	296.975	279.966
WEKVAK	3	181.383	190.056	305.223
WEKVAK	4	68.391	60.386	69.491
WIFSIQ	1	173.651	314.623	291.127
WIFSIQ	2	173.772	182.474	70.748
WOYVIP	1	155.345	171.841	58.747
WOYVIP	2	85.161	65.581	67.024
XABNAQ	1	166.334	172.914	273.469

XAZNAO	1	157.195	69.448	74.355
XAZNAO	2	98.11	172.069	317.223
XECLUN	1	163.312	299.327	301.65
XEZSOK	1	298.931	291.486	300.968
XEZTIF	1	182.984	173.397	294.968
XEZTOL	1	176.557	178.695	296.364
XIJPUB	1	170.158	181.036	289.753
XIMNIR	1	150.01	170.303	186.173
XIMNIR	2	179.528	294.469	193.647
XOVQOR	1	181.685	307.468	293.539
XOVQOR	2	168.416	296.324	292.57
YAJFOG	1	174.332	295.292	180.728
YIGMEI	1	310.246	176.29	75.054
YIGMEI	2	176.146	191.07	290.012
YOSKAU	1	173.279	171.498	75.881
YOSKAU	2	182.822	199.445	87.293
YOTVAF	1	170.964	183.941	290.243
YUDDIM	1	307.286	179.667	285.866
YUNTUY	1	178.733	302.914	285.978
YUNTUY	2	176.761	295.805	282.206
ZEHDEV	1	176.269	185.028	284.699
ZUHNUL	1	172.927	183.729	182.634

Methyl Cysteinyl

2051774	1	290.771	79.278
CICROY	1	46.581	63.388
EBEQUA	1	288.508	189.379
EYOBUP	1	183.13	294.484
EYOCAW	1	183.203	292.718
EYOCEA	1	175.582	287.681
FIYBUK	1	172.094	289.644
KACQIR	1	187.211	295.681
KACQIR	2	54.785	52.882
KACQIR	3	185.17	274.428
KACQIR	4	165.341	272.576
MCYSCD	1	174.193	275.159
MCYSCD	2	167.774	292.825
MCYSZN	1	173.8	284.987
MCYSZN	2	169.842	284.364
MCYSZN	3	173.8	284.987
NIDXIJ	1	183.06	303.836
NIDXIJ	2	321.833	293.428

NIDXIJ	3	301.862	88.346	
NIDXIJ	4	164.292	287.638	
NOHMUT	1	167.952	265.461	
NOHMUT	2	169.777	275.189	
NOHMUT	3	178.376	301.923	
NOHMUT	4	178.836	287.756	
NOHMUT	5	161.646	261.697	
NOHMUT	6	174.222	287.467	
NOHMUT	7	65.165	77.724	
NOHMUT	8	67.297	79.961	
TIJZAN	1	184.332	291.178	
WEXYII	1	290.102	85.223	
WEXYII	2	284.398	91.534	
WEXYOO	1	180.807	289.076	
WEXYOO	2	165.854	81.962	
WUTPIM	1	161.75	285.618	
WUTPOS	1	307.567	279.167	

Ethyl Cysteinyl

2054514	1	292.022	86.448	58.088
2051775	1	297.675	99.959	157.049
2051776	1	287.625	80.73	63.517
2051776	2	287.054	80.276	172.691
2051777	1	168.708	90.329	161.38
2017246	1	295.929	91.476	152.808
2017248	1	292.222	82.468	58.097
2017251	1	169.278	90.1	161.689
2017252	1	182.586	179.257	188.65
2017252	2	182.079	177.989	189.809
2017252	3	173.245	89.586	158.597
FAXLUL	1	177.685	100.472	181.134

Norleucinyl

2105696	1	179.470	178.050	-172.450
2017260	1	-172.300	168.280	66.250
2051775	1	59.140	174.490	-66.220
KUZNIF	1	172.526	175.849	-175.186
NAJDAH	1	-47.842	-177.528	-176.010
NAJDUB	1	45.810	167.048	173.854
NAJFAJ	1	-45.281	-169.490	-173.800
CITXEI10	1	-152.845	174.813	66.947
CITXEI10	2	-162.743	-170.800	77.827

DLNLIT	1	-175.614	178.773	70.483
DLNLUA01	1	174.068	177.760	174.296
DLNLUA02	1	-172.283	-177.903	-174.639
DLNLUA03	1	176.228	178.393	175.281
DLNLUA04	1	-172.669	-178.050	-174.641
DLNLUA05	1	-67.920	-175.828	167.858
DLNLUA06	1	-172.648	-177.949	-174.504
FITLEZ	1	-73.196	175.499	59.905
FITLEZ	2	175.791	172.526	172.609
GOLVIM	1	171.065	175.929	174.034
GOLVIM01	1	170.331	175.481	174.504
GOLVIM02	1	171.413	175.771	174.093
GOLVIM03	1	172.551	175.701	172.035
GOLVIM04	1	173.151	175.543	170.901
GOLVIM04	2	175.761	-177.572	179.613
GOLVIM05	1	177.649	179.619	173.676
GOLVOS	1	172.429	177.031	174.302
GOLVUY	1	-179.865	176.989	-62.138
GOLWAF	1	179.297	173.070	-65.466
GOLWEJ	1	-73.141	-172.158	176.028
LNLEUC11	1	70.172	171.340	-176.377
LNLEUC11	2	70.602	171.803	-177.353
LNLEUC11	3	71.554	72.263	175.259
LNLEUC11	4	72.665	171.907	-177.408
LNLEUC11	5	73.307	173.195	-176.202
LNLEUC11	6	74.972	70.785	174.935
LNLEUC12	1	71.390	170.492	-176.867
LNLEUC13	1	70.304	175.880	-173.478
LNLEUC14	1	67.977	173.908	-174.718
LNLEUC15	1	63.733	178.770	46.204
MITDUR	1	55.270	-159.080	-60.916
NAXNOS	1	-176.336	-59.109	-58.719
QIHSEI	1	-179.788	171.493	-170.867
QUBVOA	1	176.130	-60.779	-173.831
TOWDAN	1	44.821	178.627	169.798
TOWDAN	2	55.788	-169.141	174.293
UHEPUS	1	-179.475	178.092	-175.887
UHEPUS	2	-62.895	-148.766	-179.388
URODOV	1	-74.267	-171.803	178.031
VOXHUL	1	170.247	-176.372	-170.853
VOXHUL01	1	170.951	-178.708	-175.590
VUQNAY	1	-172.527	-177.152	-174.266
VUQNAY01	1	-177.413	-176.123	-174.185
VUQNAY02	1	-175.750	175.218	149.880
VUQNAY03	1	175.506	179.350	53.033

VUQNAY03	2	177.724	178.851	58.294
VUQNAY04	1	179.290	173.267	163.598
YAPJEG	1	-62.957	177.594	-178.455
YAPJEG	2	174.209	-78.094	-174.067
ZUHPAT	1	172.169	177.128	178.697
IBADUO	1	-178.245	-176.226	-172.406
IBAFAW	1	163.314	-171.574	178.250
IBAFAW	2	163.603	-177.945	168.702
IBAFAW	3	164.040	174.677	172.117
IBAFAW	4	164.122	-60.055	-160.907
IBAFAW	5	172.585	169.437	63.928
IBAFEA	1	-177.320	-58.531	-57.645
IBAFEA	2	-177.384	-58.484	-61.655
IBAFEA	3	-178.909	-57.714	-59.551
IBAFUQ	1	166.609	-80.941	177.527
IBAFUQ	2	172.285	171.240	175.108
IBAFUQ	3	177.426	177.218	178.025
IBAFUQ	4	60.103	65.648	172.699