

Table S1

| Peptide | Bioactive |
|---------|-----------|
| CW | 0.99581 |
| MW | 0.995312 |
| GF | 0.994712 |
| CMW | 0.993837 |
| GW | 0.993164 |
| PW | 0.992911 |
| LF | 0.986934 |
| LW | 0.985244 |
| LMF | 0.979926 |
| RPF | 0.977766 |
| PFPY | 0.969077 |
| APW | 0.966955 |
| CPPSF | 0.96497 |
| WMA | 0.961852 |
| AGW | 0.959298 |
| MDF | 0.959246 |
| CPCR | 0.949732 |
| IF | 0.949173 |
| SF | 0.948796 |
| QF | 0.946135 |
| IW | 0.944175 |
| NF | 0.941145 |
| DGF | 0.939426 |
| HGF | 0.938552 |
| PDF | 0.934107 |
| SW | 0.93391 |
| DW | 0.933025 |
| CG | 0.931922 |
| QW | 0.928524 |
| GP | 0.905487 |
| HPIW | 0.896869 |
| ML | 0.894564 |
| GG | 0.88736 |
| PP | 0.886915 |
| LMP | 0.886515 |
| WPVL | 0.880808 |
| EGCW | 0.876556 |
| HPNF | 0.875719 |
| CR | 0.865233 |

| | |
|--------|----------|
| PGL | 0.855192 |
| ADPNF | 0.852384 |
| MR | 0.849148 |
| GGL | 0.838635 |
| CY | 0.831032 |
| MDSF | 0.829954 |
| EMW | 0.82038 |
| SHW | 0.816324 |
| VF | 0.815398 |
| NGDW | 0.815121 |
| TW | 0.814447 |
| GGR | 0.81127 |
| GL | 0.808777 |
| SIF | 0.805497 |
| MEW | 0.801147 |
| PR | 0.787626 |
| LGP | 0.786814 |
| DSWPSL | 0.785783 |
| DNF | 0.775374 |
| GR | 0.766288 |
| ISW | 0.757343 |
| INPYPR | 0.756391 |
| YPR | 0.754834 |
| QNCMY | 0.75044 |
| INF | 0.749347 |
| AM | 0.74549 |
| SQF | 0.743007 |
| GSM | 0.742395 |
| GY | 0.741592 |
| PPA | 0.738574 |
| SSW | 0.731445 |
| GSMGY | 0.728079 |
| CDGY | 0.719177 |
| RPY | 0.716662 |
| HGVF | 0.702486 |
| APAP | 0.70062 |
| SML | 0.696547 |
| CSGHP | 0.695588 |
| QWME | 0.691206 |
| AMR | 0.688815 |
| SSAMM | 0.68653 |

| | |
|--------|----------|
| LDMGP | 0.684233 |
| SSIW | 0.68172 |
| LIGC | 0.676497 |
| DML | 0.667515 |
| LISW | 0.665913 |
| AANW | 0.66488 |
| NPG | 0.664548 |
| LYPR | 0.663945 |
| CH | 0.660567 |
| CI | 0.660168 |
| LGL | 0.652338 |
| HSILMP | 0.649456 |
| DCY | 0.64835 |
| CPK | 0.648049 |
| MGD | 0.644133 |
| IGG | 0.642808 |
| AVW | 0.63114 |
| CGGT | 0.631018 |
| SC | 0.620334 |
| LL | 0.618551 |
| LKPTW | 0.615503 |
| LHM | 0.614823 |
| SGG | 0.611845 |
| NM | 0.604672 |
| CGGQR | 0.603286 |
| TIGCAW | 0.601279 |
| CSL | 0.601262 |
| NGMIR | 0.599087 |
| CGSR | 0.59867 |
| LHPGR | 0.594419 |
| GDMDY | 0.589397 |
| CSGHR | 0.589257 |
| EW | 0.585631 |
| LNMY | 0.585134 |
| SGNIPY | 0.580003 |
| IVF | 0.57343 |
| SVF | 0.573302 |
| LAC | 0.571138 |
| LR | 0.569984 |
| MD | 0.569594 |
| HP | 0.566647 |

| | |
|--------|----------|
| GLPK | 0.561671 |
| DVF | 0.551408 |
| DLP | 0.549727 |
| VDW | 0.548779 |
| CQR | 0.546227 |
| AMQL | 0.545898 |
| NTW | 0.543895 |
| CQ | 0.540359 |
| AGY | 0.540291 |
| SHHPR | 0.538536 |
| PA | 0.53447 |
| RPIR | 0.532517 |
| IGR | 0.532161 |
| NGNC | 0.53085 |
| GH | 0.530477 |
| HPNL | 0.523186 |
| LGPK | 0.516678 |
| LY | 0.516639 |
| MTPR | 0.515171 |
| SP | 0.514894 |
| LQPY | 0.51421 |
| CS | 0.513886 |
| LAP | 0.512708 |
| TCIC | 0.510885 |
| SGR | 0.508729 |
| ISCR | 0.504779 |
| SAC | 0.503776 |
| ACSY | 0.501397 |
| LIPAIP | 0.500751 |

Table S2

| pepcalc | Sequence |
|---------|----------|
| 0 | SW |
| 0 | SSIW |
| 1 | SC |
| 0 | SSW |
| 1 | CS |
| 0 | ACSY |
| 1 | SP |
| 0 | CY |
| 0 | SAC |
| 0 | SHW |
| 0 | SSAMM |
| 0 | GSMGY |
| 0 | APW |
| 0 | GSM |
| 0 | SGNIPY |
| 1 | CQ |
| 0 | AANW |
| 1 | GDMDY |
| 0 | SML |
| 0 | CG |
| 0 | QW |
| 1 | CPK |
| 0 | HSILMP |
| 0 | CSL |
| 0 | CSGHP |
| 0 | CPPSF |
| 1 | CGSR |
| 1 | GLPK |
| 0 | APAP |
| 0 | SQF |
| 0 | AMQL |
| 1 | SHHPR |
| 1 | ADPNF |
| 1 | DSWPSL |
| 0 | NGNC |
| 1 | SGR |
| 1 | CGGQR |
| 0 | AM |
| 1 | EGCW |

| | |
|---|--------|
| 1 | CPCR |
| 0 | SF |
| 0 | CMW |
| 0 | AGW |
| 1 | CSGHR |
| 0 | GW |
| 1 | SGG |
| 0 | GP |
| 0 | TW |
| 0 | CGGT |
| 0 | LKPTW |
| 0 | AGY |
| 0 | NTW |
| 0 | NM |
| 1 | NGDW |
| 1 | GR |
| 1 | LGPK |
| 0 | GH |
| 1 | GGR |
| 1 | INPYPR |
| 1 | CQR |
| 1 | NGMIR |
| 1 | QWME |
| 1 | YPR |
| 0 | SIF |
| 0 | GGL |
| 0 | CI |
| 1 | DW |
| 1 | CDGY |
| 0 | PW |
| 0 | LAC |
| 0 | GF |
| 0 | GG |
| 0 | AVW |
| 1 | ISCR |
| 0 | PA |
| 0 | NPG |
| 0 | TIGCAW |
| 0 | GL |
| 0 | PGL |
| 1 | DGF |

| | |
|---|--------|
| 1 | EW |
| 0 | LAP |
| 0 | TCIC |
| 0 | HPNL |
| 1 | CR |
| 1 | VDW |
| 0 | IGG |
| 0 | SVF |
| 0 | LGP |
| 1 | RPY |
| 1 | IGR |
| 1 | PDF |
| 0 | PPA |
| 0 | HGVF |
| 1 | LDMGP |
| 1 | DCY |
| 1 | DNF |
| 0 | WPVL |
| 0 | LIGC |
| 0 | ISW |
| 1 | AMR |
| 0 | LIPAIP |
| 0 | HGF |
| 1 | DLP |
| 1 | EMW |
| 1 | MGD |
| 1 | LHPGR |
| 0 | WMA |
| 1 | DVF |
| 0 | VF |
| 1 | LYPR |
| 0 | QNCMY |
| 0 | LISW |
| 1 | DML |
| 0 | NF |
| 0 | LGL |
| 1 | RPIR |
| 0 | GY |
| 1 | PR |
| 0 | LL |
| 1 | MD |

| | |
|---|------|
| 0 | LW |
| 1 | LR |
| 0 | IVF |
| 0 | ML |
| 0 | HPIW |
| 0 | PP |
| 0 | IW |
| 0 | LQPY |
| 0 | HPNF |
| 0 | LHM |
| 0 | LMP |
| 0 | CH |
| 1 | MEW |
| 1 | MTPR |
| 0 | IF |
| 1 | MDF |
| 0 | INF |
| 0 | LF |
| 0 | RPF |
| 0 | HP |
| 0 | LMF |
| 1 | MDSF |
| 0 | LY |
| 0 | MR |
| 0 | LNMY |
| 0 | QF |
| 0 | MW |
| 0 | PFPY |

Table S3

| P | | H | W | Att | Gr |
|----|---|----|-----|--------|---------|
| e | | G | L | en | ap |
| pt | SMILES | N | N | tiv | hS |
| id | | | | eF | AG |
| e | | | | P | E |
| S | | S | B | | |
| C | N[C@@H](CO)C(=O)N[C@@H](CS)C(=O)O | w | 0 0 | it 0 0 | Sw 0 0 |
| | | e | . | . | . |
| | | e | 6 3 | t 2 7 | ee 9 0 |
| | | e | 8 2 | e 2 8 | t 7 3 |
| | | t | r | | t |
| | | S | B | | |
| C | N[C@@H](CS)C(=O)N[C@@H](CO)C(=O)O | w | 0 0 | it 0 0 | Sw 0 0 |
| S | | e | . | . | . |
| | | e | 6 3 | t 4 5 | ee 9 0 |
| | | e | 8 2 | e 8 2 | t 7 3 |
| | | t | r | | t |
| | | B | B | | |
| S | N[C@@H](CO)C(=O)N1CCC[C@H]1C(=O)O | it | | | 0 0 |
| P | | t | 0 1 | t 0 9 | Bit 0 1 |
| | | e | | | ter 4 5 |
| | | r | 1 9 | | |
| | | B | S | | |
| C | NC(=O)CC[C@H](NC(=O)[C@@H](N)CS)C(=O)O | it | 0 0 | w 0 0 | Sw 0 0 |
| Q | O)O | t | . | e . | ee . |
| | | e | 2 7 | e 7 2 | t 8 1 |
| | | r | 5 5 | e 7 3 | t 1 9 |
| | | t | | | t |
| | | B | B | | |
| G | | it | | | 0 0 |
| D | CSCC[C@H](NC(=O)[C@H](CC(=O)O)NC(=O)CN)C(=O)N[C@@H](CC(=O)O)C(=O)N[C@H](Cc1ccc(O)cc1)C(=O)O | t | 0 1 | t 0 1 | Bit 0 0 |
| M | | e | | | ter . . |
| D | | r | 0 1 | e | ee 9 0 |
| Y | | t | | | t 2 8 |
| | | B | B | | |
| C | NCCCC[C@H](NC(=O)[C@@H]1CCCCN1C(=O)O)[C@@H](N)CS)C(=O)O | it | 0 1 | t 0 1 | Bit 0 1 |
| P | | e | | | ter 0 9 |
| K | | r | 0 1 | | |
| | | t | | | 6 4 |
| | | B | B | | |
| C | | it | | | 0 0 |
| G | N=C(N)NCCCC[C@H](NC(=O)[C@H](CO)NC(=O)CNC(=O)[C@@H](N)CS)C(=O)O | t | . | t . | Bit . |
| S | | e | 0 9 | e 0 9 | ter 1 8 |
| R | | r | 6 4 | r 1 9 | ter 2 8 |
| | | t | | | 2 8 |
| | | B | B | | |
| G | CC(C)C[C@H](NC(=O)CN)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCCCN)C(=O)O | it | 0 1 | it 0 1 | Bit 0 1 |
| L | | t | | | ter 0 1 |
| P | | | | | |

| | | | | | | | | |
|----|---------------------------------------|---------|---------|------------|------------|------------|------------|-----|
| K | | e r | e r | | | | | |
| S | N=C(N)NCCC[C@H](NC(=O)[C@@H]1CCCN | B it | B it | 0 0 | 0 0 | | | |
| H | 1C(=O)[C@H](Cc1c[nH]cn1)NC(=O)[C@H](| t 0 1 | t 0 1 | Bit ter | . . | Bit ter | 0 1 | |
| H | Cc1c[nH]cn1)NC(=O)[C@@H](N)CO)C(=O) | e | e | | 0 9 | ter | | |
| P | O | r | r | | 1 9 | | | |
| R | | | | | | | | |
| A | | | | | | | | |
| D | C[C@H](N)C(=O)N[C@@H](CC(=O)O)C(=O) | B it | B it | 0 0 | 0 0 | 0 0 | 0 0 | |
| P | N1CCC[C@H]1C(=O)N[C@@H](CC(N)=O)C(| t 0 1 | t 0 1 | . . | Bit ter | . . | Bit ter | . . |
| N | =O)N[C@@H](Cc1ccccc1)C(=O)O | e | e | 0 9 | ter | 0 9 | ter | 0 9 |
| F | | r | r | 3 7 | 1 9 | | 2 8 | |
| D | CC(C)C[C@H](NC(=O)[C@H](CO)NC(=O)[C | B it | B it | | | | 0 0 | |
| S | @@H]1CCCN1C(=O)[C@H](Cc1c[nH]c2ccc | t 0 1 | t 0 1 | Bit ter | 0 1 | Bit ter | . . | |
| W | cc12)NC(=O)[C@H](CO)NC(=O)[C@@H](N) | e | e | | | | 0 9 | |
| P | CC(=O)O)C(=O)O | r | r | | | | 7 3 | |
| SL | | | | | | | | |
| S | N=C(N)NCCC[C@H](NC(=O)CNC(=O)[C@@ | B it | B it | 0 0 | 0 0 | 0 0 | 0 0 | |
| G | H](N)CO)C(=O)O | t 0 9 | t 0 9 | . . | Bit ter | . . | ter | 0 9 |
| R | | e 9 1 | e 3 7 | | 4 6 | | | 1 9 |
| C | | r | | | | | | |
| G | N=C(N)NCCC[C@H](NC(=O)[C@H](CCC(N)= | B it | B it | 0 0 | 0 0 | 0 0 | 0 0 | |
| G | O)NC(=O)CNC(=O)CNC(=O)[C@@H](N)CS) | t 0 9 | t 0 9 | . . | Bit ter | . . | Bit ter | . . |
| Q | C(=O)O | e 1 9 | e 1 9 | 0 9 | ter | 1 8 | ter | 0 9 |
| R | | r | r | 1 9 | 9 1 | | 3 7 | |
| E | | | | | | | | |
| G | N[C@@H](CCC(=O)O)C(=O)NCC(=O)N[C@ | B it | B it | 0 0 | 0 0 | 0 0 | 0 0 | |
| C | @H](CS)C(=O)N[C@@H](Cc1c[nH]c2cccc1 | t 0 9 | t 0 9 | . 1 | Bit ter | . . | Bit ter | . . |
| W | 2)C(=O)O | e 1 9 | e 1 9 | | 0 9 | ter | 0 9 | |
| C | | r | | | 4 6 | | 5 5 | |
| P | | | | | | | | |
| C | N=C(N)NCCC[C@H](NC(=O)[C@H](CS)NC(= | B it | B it | 0 1 | 0 1 | 0 1 | 0 1 | |
| C | O)[C@@H]1CCCN1C(=O)[C@@H](N)CS)C(=O)O | t 0 1 | t 0 1 | Bit ter | 0 1 | Bit ter | 0 1 | |
| R | | e | e | | | | | |
| C | | r | | | | | | |
| S | N=C(N)NCCC[C@H](NC(=O)[C@H](Cc1c[nH] | B it | B it | 0 0 | 0 0 | 0 0 | 0 0 | |
| G |]cn1)NC(=O)CNC(=O)[C@H](CO)NC(=O)[C | t 0 9 | t 0 9 | . 1 | Bit ter | . . | Bit ter | . . |
| H | @@H](N)CS)C(=O)O | e 1 9 | e 1 9 | 0 9 | ter | 1 9 | ter | 0 9 |
| R | | r | r | | | | 1 9 | |
| S | | | | | | | | |
| G | N[C@@H](CO)C(=O)NCC(=O)NCC(=O)O | S 0 0 | S 1 0 | Sw ee | 0 0 | Sw ee | 0 0 | |
| | | w . . | w . . | | | | | |

| | | | | |
|----|--------------------------------------|---------------|---------|---------|
| G | | e 9 0 e | t 9 0 t | 9 0 |
| | | e 8 2 e | t 3 7 | 3 7 |
| | | t t | | |
| N | NC(=O)C[C@H](N)C(=O)NCC(=O)N[C@@H] | B B | 0 0 | |
| G | (CC(=O)O)C(=O)N[C@@H](Cc1c[nH]c2cccc | it it | . . | Bit 0 0 |
| D | c12)C(=O)O | t 0 1 t 0 1 | ter 0 9 | ter . . |
| W | | e e | 9 1 | 4 6 |
| | | r r | | |
| | | B B | | |
| G | N=C(N)NCCC[C@H](NC(=O)CN)C(=O)O | it 0 0 it 0 0 | Sw 0 0 | |
| R | | t . . t . . | ee . . | Bit 0 1 |
| | | e 0 9 e 0 9 | t 7 2 | ter |
| | | r 3 7 r 6 4 | 4 6 | |
| L | | B B | | |
| G | CC(C)C[C@H](N)C(=O)NCC(=O)N1CCC[C@ | it it | | |
| P | H]1C(=O)N[C@@H](CCCCN)C(=O)O | t 0 1 t 0 1 | Bit 0 1 | Bit 0 1 |
| K | | e e | ter | ter |
| | | r r | | |
| G | | B B | | |
| G | N=C(N)NCCC[C@H](NC(=O)CNC(=O)CN)C(= | it 0 0 it 0 0 | Sw 0 0 | 0 0 |
| R | O)O | t . . t . . | ee . . | Bit . . |
| | | e 0 9 e 0 9 | t 6 3 | ter 0 9 |
| | | r 1 9 r 7 3 | 4 6 | 1 9 |
| IN | | B B | | |
| P | CC[C@H](C)[C@H](N)C(=O)N[C@@H](CC(| it it | 0 0 | |
| Y | N)=O)C(=O)N1CCC[C@H]1C(=O)N[C@@H] | t 0 1 t 0 1 | Bit . . | Bit 0 1 |
| P | (Cc1ccc(O)cc1)C(=O)N1CCC[C@H]1C(=O)N | e e | ter 0 9 | ter |
| R | [C@@H](CCCNC(=N)N)C(=O)O | r r | 1 9 | |
| C | | B B | | |
| Q | N=C(N)NCCC[C@H](NC(=O)[C@H](CCC(N)= | it 0 0 it 0 0 | 0 0 | 0 0 |
| R | O)NC(=O)[C@@H](N)CS)C(=O)O | t . . t . . | Bit . . | Bit . . |
| | | e 1 9 e 0 9 | ter 2 7 | ter 0 9 |
| | | r 4 6 r 7 3 | 7 3 | 6 4 |
| N | | B B | | |
| G | CC[C@H](C)[C@H](NC(=O)[C@H](CCSC)NC | it 0 0 it 0 0 | 0 0 | 0 0 |
| M | (=O)CNC(=O)[C@@H](N)CC(N)=O)C(=O)N[| t . . t . . | Bit . . | Bit . . |
| IR | C@@H](CCCNC(=N)N)C(=O)O | e 0 9 e 0 9 | ter 2 7 | ter 0 9 |
| | | r 2 8 r 2 8 | 6 4 | 1 9 |
| Q | | B B | | |
| W | CSCC[C@H](NC(=O)[C@H](Cc1c[nH]c2cccc | it it | 0 0 | 0 0 |
| M | c12)NC(=O)[C@@H](N)CCC(N)=O)C(=O)N[| t 0 1 t 0 1 | Bit . . | Bit . . |
| E | C@@H](CCC(=O)O)C(=O)O | e e | ter 1 8 | ter 0 9 |
| | | r r | 5 5 | 9 1 |
| Y | N=C(N)NCCC[C@H](NC(=O)[C@@H]1CCCN | B 0 1 B 0 1 | Bit 0 0 | Bit 0 1 |

| | | | | | | | |
|----|--------------------------------------|----------|-------|-----|-----|-----|-----|
| P | 1C(=O)[C@@@H](N)Cc1ccc(O)cc1C(=O)O | it | it | ter | . | . | ter |
| R | | t | t | | 0 | 9 | |
| | | e | e | | 1 | 9 | |
| | | r | r | | | | |
| | | B | B | | | | |
| D | N[C@@H](CC(=O)O)C(=O)N[C@@H](Cc1c[| it | 0 0 | 0 0 | | | 0 0 |
| W | nH]c2cccc12)C(=O)O | t 0 1 | . | Bit | . | . | Bit |
| | | t | 3 6 | ter | 1 8 | ter | 3 6 |
| | | e | 9 1 | | 6 4 | | 5 5 |
| | | r | | | | | |
| C | N[C@@H](CS)C(=O)N[C@@H](CC(=O)O)C(| B 0 0 | | 0 0 | | | 0 0 |
| D | =O)NCC(=O)N[C@@H](Cc1ccc(O)cc1)C(=O) | it . . | t 0 1 | Bit | . | . | Bit |
| G | O | t 1 8 | . | ter | 1 8 | ter | 4 5 |
| Y | | e 5 5 | | | 5 5 | | 9 1 |
| | | r | | | | | |
| IS | CC[C@H](C)[C@H](N)C(=O)N[C@@H](CO) | B 0 0 | | 0 0 | | | |
| C | C(=O)N[C@@H](CS)C(=O)N[C@@H](CCCN | it . . | t 0 1 | Bit | . | . | Bit |
| R | R C(=N)N)C(=O)O | t 0 9 | e | ter | 0 9 | ter | 0 1 |
| | | r 7 3 | | | 4 6 | | |
| | | | | | | | |
| D | N[C@@H](CC(=O)O)C(=O)NCC(=O)N[C@@ | B 0 0 S | 0 0 | 0 0 | | | 0 0 |
| G | H](Cc1cccc1)C(=O)O | it . . w | . | Bit | . | . | Sw |
| F | | t 2 7 e | 8 1 | ter | 3 6 | ee | . |
| | | e 8 2 e | 2 8 | | 9 1 | t | 6 3 |
| | | r 8 2 t | | | | 9 1 | 9 1 |
| | | | | | | | |
| E | N[C@@H](CCC(=O)O)C(=O)N[C@@H](Cc1 | B 0 0 | 0 0 | 0 0 | | | 0 0 |
| W | c[nH]c2cccc12)C(=O)O | it . . | t . . | Bit | . | . | Bit |
| | | t 0 9 e | 0 9 | ter | 1 8 | ter | 2 7 |
| | | r 2 8 r | 3 7 | | 1 9 | | 6 4 |
| | | | | | | | |
| C | N=C(N)NCCC[C@H](NC(=O)[C@@H](N)CS) | B 0 0 | 0 0 | 0 0 | | | 0 0 |
| R | R C(=O)O | it . . | t . . | Sw | . | . | Bit |
| | | t 0 9 e | 2 7 | ee | 6 3 | ter | . |
| | | e 8 2 e | 8 2 | t | 9 1 | | 0 9 |
| | | r 8 2 r | | | | | 2 8 |
| | | | | | | | |
| V | CC(C)[C@H](N)C(=O)N[C@@H](CC(=O)O)C | B 0 0 | | 0 0 | | | 0 0 |
| D | (=O)N[C@@H](Cc1c[nH]c2cccc12)C(=O)O | it 0 1 | t 0 1 | Bit | . | . | Bit |
| W | | e | | ter | 0 9 | ter | 1 8 |
| | | r | | | 3 7 | | 4 6 |
| | | | | | | | |
| R | N=C(N)NCCC[C@H](N)C(=O)N1CCC[C@H]1 | B 0 0 | | 0 0 | | | 0 0 |
| P | C(=O)N[C@@H](Cc1ccc(O)cc1)C(=O)O | it 0 1 | t 0 1 | Bit | . | . | Bit |
| Y | | e | | ter | 0 9 | ter | 0 1 |
| | | r | | | 1 9 | | |

| | | | | | | | | | |
|----|--|----|-------|-----|-----|-----|-----|-----|-----|
| | | B | 0 0 | B | 0 0 | Sw | 0 0 | | |
| IG | CC[C@H](C)[C@H](N)C(=O)NCC(=O)N[C@H](CCCNC(=N)N)C(=O)O | it | . | it | . | ee | . | Bit | 0 1 |
| R | | t | . | t | . | | 5 4 | ter | |
| | | e | 0 9 | e | 1 9 | t | 4 6 | | |
| | | r | 1 9 | r | | | | | |
| P | O=C(O)C[C@H](NC(=O)[C@@H]1CCCN1)C(=O)N[C@@H](Cc1ccccc1)C(=O)O | B | 0 0 | B | 0 0 | 0 0 | 0 0 | 0 0 | |
| D | | it | . | it | . | Bit | . | Bit | . |
| F | | t | . | t | 4 5 | ter | 0 9 | ter | 4 5 |
| | | e | 2 8 | e | 7 3 | | 3 7 | | 9 1 |
| L | | r | | | | | | | |
| D | CSCC[C@H](NC(=O)[C@H](CC(=O)O)NC(=O))[C@@H](N)CC(C)C(=O)NCC(=O)N1CCC[| B | 0 0 | B | 0 0 | | | 0 0 | |
| M | G C@H]1C(=O)O | it | . | it | . | Bit | 0 1 | Bit | . |
| P | | t | 0 1 | t | 0 9 | ter | | ter | 0 9 |
| | | e | | e | 2 8 | | | | 6 4 |
| R | | r | | | | | | | |
| D | N[C@@H](CC(=O)O)C(=O)N[C@@H](CS)C(=O)N[C@@H](Cc1ccc(O)cc1)C(=O)O | B | 0 0 | B | 0 0 | 0 0 | Sw | 0 0 | |
| C | | it | . | it | . | Bit | . | ee | . |
| Y | | t | 4 5 | t | 0 9 | ter | 1 8 | t | 6 3 |
| | | e | 1 9 | e | 6 4 | | 9 1 | | 4 6 |
| R | | r | | | | | | | |
| D | NC(=O)C[C@H](NC(=O)[C@@H](N)CC(=O)O)C(=O)N[C@@H](Cc1ccccc1)C(=O)O | B | 0 0 | B | 0 0 | 0 0 | 0 0 | 0 0 | |
| N | | it | . | it | . | Bit | . | Bit | . |
| F | | t | 0 9 | t | 2 7 | ter | 2 7 | ter | 3 6 |
| | | e | 1 9 | e | 1 9 | | 6 4 | | 2 8 |
| R | | r | | | | | | | |
| A | CSCC[C@H](NC(=O)[C@H](C)N)C(=O)N[C@H](CCCNC(=N)N)C(=O)O | B | 0 0 | B | 0 0 | 0 0 | 0 0 | 0 0 | |
| M | | it | . | it | 0 1 | Bit | . | Bit | . |
| R | | t | 0 9 | t | | ter | 3 6 | ter | 0 9 |
| | | e | 4 6 | e | | | 9 1 | | 1 9 |
| R | | r | | | | | | | |
| D | CC(C)C[C@H](NC(=O)[C@@H](N)CC(=O)O)C(=O)N1CCC[C@H]1C(=O)O | B | 0 0 | B | 0 0 | | | 0 0 | |
| L | | it | . | it | . | Bit | 0 1 | Bit | . |
| P | C(=O)N1CCC[C@H]1C(=O)O | t | 0 1 | t | 0 9 | ter | | ter | 0 9 |
| | | e | | e | 4 6 | | | | 4 6 |
| R | | r | | | | | | | |
| E | CSCC[C@H](NC(=O)[C@@H](N)CCC(=O)O)C(=O)N[C@@H](Cc1c[nH]c2cccc12)C(=O)O | B | 0 0 | B | 0 0 | 0 0 | 0 0 | 0 0 | |
| M | | it | . | it | . | Bit | . | Bit | . |
| W | O | t | 0 9 | t | 0 9 | ter | 1 8 | ter | 1 9 |
| | | e | 2 8 | e | 1 9 | | 5 5 | | |
| R | | r | | | | | | | |
| M | CSCC[C@H](N)C(=O)NCC(=O)N[C@@H](CC(=O)O)C(=O)O | B | 0 0 S | 0 0 | Sw | 0 0 | Sw | 0 0 | |
| G | | it | . | w | . | ee | . | ee | . |
| D | | t | 2 7 | e | 6 3 | t | 9 0 | t | 8 1 |
| | | e | 9 1 | e | 2 8 | | 4 6 | | 5 5 |

| | | | | | | | | |
|----|--|--------|--------|---------|---------|---------|-----|--|
| | | r | t | | | | | |
| L | | B | B | | | | | |
| H | CC(C)C[C@H](N)C(=O)N[C@@H](Cc1c[nH]1 | it | it | | 0 0 | | | |
| P | cn1)C(=O)N1CCC[C@H]1C(=O)NCC(=O)N[C@H](@@H](CCCNC(=N)N)C(=O)O | t 0 1 | t 0 1 | Bit ter | . . 0 9 | Bit ter | 0 1 | |
| R | | e | e | | 1 9 | | | |
| D | | r | r | | | | | |
| V | CC(C)[C@H](NC(=O)[C@@H](N)CC(=O)O)C(=O)N[C@@H](Cc1cccc1)C(=O)O | B 0 0 | B 0 0 | | 0 0 | | 0 0 | |
| F | | it . . | it . . | Bit | . . | Bit | . . | |
| LY | | t 0 9 | t 1 8 | ter | 0 9 | ter | 2 7 | |
| P | CC(C)C[C@H](N)C(=O)N[C@@H](Cc1ccc(O)c1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCCNC(=N)N)C(=O)O | e 3 7 | e 3 7 | | 8 2 | | 8 2 | |
| R | | r | r | | | | | |
| D | | B | B | | | | | |
| M | CSCC[C@H](NC(=O)[C@@H](N)CC(=O)O)C(=O)N[C@@H](CC(C)C)C(=O)O | it 0 0 | it 0 0 | | 0 0 | | 0 0 | |
| L | | it . . | it . . | Bit | . . | Bit | . . | |
| R | CC[C@H](C)[C@H](NC(=O)[C@@H]1CCCN1C(=O)[C@@H](N)CCNC(=N)N)C(=O)N[C@@H](CCCNC(=N)N)C(=O)O | t 0 9 | t 2 7 | ter | 1 8 | ter | 4 5 | |
| PI | | e 6 4 | e 5 5 | | 5 5 | | 1 9 | |
| R | | r | r | | | | | |
| P | | B | B | | 0 0 | | | |
| R | N=C(N)NCCC[C@H](NC(=O)[C@@H]1CCCN1)C(=O)O | it 0 1 | it 0 1 | Bit | . . 0 9 | Bit ter | 0 1 | |
| PI | | t e | t e | | 1 9 | | | |
| R | | r | r | | | | | |
| P | | B | B | | 0 0 | | 0 0 | |
| R | | it . . | it . . | Bit | . . | Bit | . . | |
| P | | t 0 9 | t 0 9 | ter | 1 8 | ter | 0 9 | |
| R | | e 7 3 | e 3 7 | | 3 7 | | 2 8 | |
| S | | r | r | | | | | |
| M | CSCC[C@H](N)C(=O)N[C@@H](CC(=O)O)C(=O)O | S 0 0 | S 0 0 | | 0 0 | | 0 0 | |
| D | | it . . | it . . | Bit | . . | Bit | . . | |
| E | | t 5 4 | t 8 1 | ee | 9 0 | ee t | 9 0 | |
| W | | e 4 6 | e 6 4 | t | 7 3 | t | 1 9 | |
| L | | t | t | | | | | |
| R | CC(C)C[C@H](N)C(=O)N[C@@H](CCCNC(=N)N)C(=O)O | B 0 0 | B 0 0 | | 0 0 | | | |
| M | CSCC[C@H](N)C(=O)N[C@@H](CCC(=O)O)C(=O)O | it . . | it . . | Bit | . . | Bit | 0 1 | |
| E | | t 0 9 | t 0 9 | ter | 3 6 | ter | | |
| W | O | e 2 8 | e 3 7 | | 3 7 | | | |
| M | | r | r | | | | | |
| E | | B 0 0 | B 0 0 | | 0 0 | | 0 0 | |
| W | | it . . | it . . | Bit | . . | Bit ter | . . | |
| T | | t 0 9 | t 0 9 | ter | 1 8 | ter | 1 9 | |

| | | | | | | | | | | |
|----|-------------------------------------|----|---|---|----|---|---|-----|---|-----|
| | | e | 2 | 8 | e | 1 | 9 | | 5 | 5 |
| | | r | | | r | | | | | |
| M | CSCC[C@H](N)C(=O)N[C@H](C(=O)N1CCC[| B | | | B | | | | | |
| T | C@H]1C(=O)N[C@@H](CCCNC(=N)N)C(=O | it | | | it | | | | | |
| P |)O)[C@@H](C)O | t | 0 | 1 | t | 0 | 1 | Bit | 0 | 1 |
| R | | e | | | e | | | ter | | Bit |
| | | r | | | r | | | ter | 0 | 1 |
| M | CSCC[C@H](N)C(=O)N[C@@H](CC(=O)O)C(| B | 0 | 0 | B | 0 | 0 | | 0 | 0 |
| D | =O)N[C@@H](Cc1ccccc1)C(=O)O | it | . | . | it | . | . | Bit | . | . |
| F | | t | 3 | 6 | t | 2 | 7 | ter | . | ee |
| | | e | 9 | 1 | e | 3 | 7 | | 4 | 6 |
| R | N=C(N)NCCCC[C@H](N)C(=O)N1CCC[C@H]1 | r | | | r | | | t | 6 | 3 |
| P | C(=O)N[C@@H](Cc1ccccc1)C(=O)O | B | | | B | | | | 1 | 9 |
| F | | it | | | it | | | 0 | 0 | |
| | | t | 0 | 1 | t | 0 | 1 | Bit | . | Bit |
| | | e | | | e | | | ter | 0 | 1 |
| | | r | | | r | | | ter | | |
| M | CSCC[C@H](N)C(=O)N[C@@H](CC(=O)O)C(| B | 0 | 0 | B | 0 | 0 | | 0 | 0 |
| D | =O)N[C@@H](CO)C(=O)N[C@@H](Cc1cccc | it | . | . | it | . | . | Bit | . | . |
| SF | c1)C(=O)O | t | 2 | 7 | t | 0 | 9 | ter | 1 | 8 |
| | | e | 3 | 7 | e | 8 | 2 | | 4 | 6 |
| | | r | | | r | | | t | 5 | 5 |

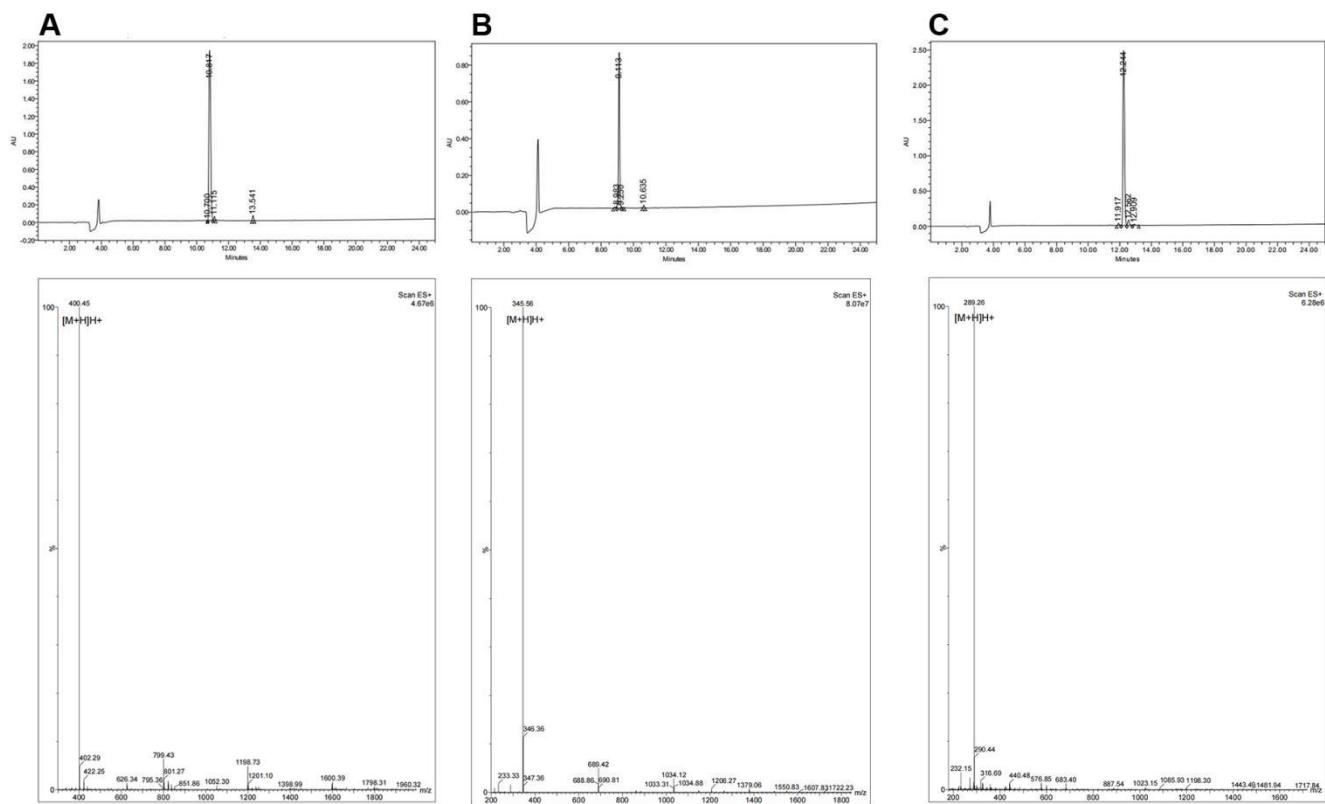
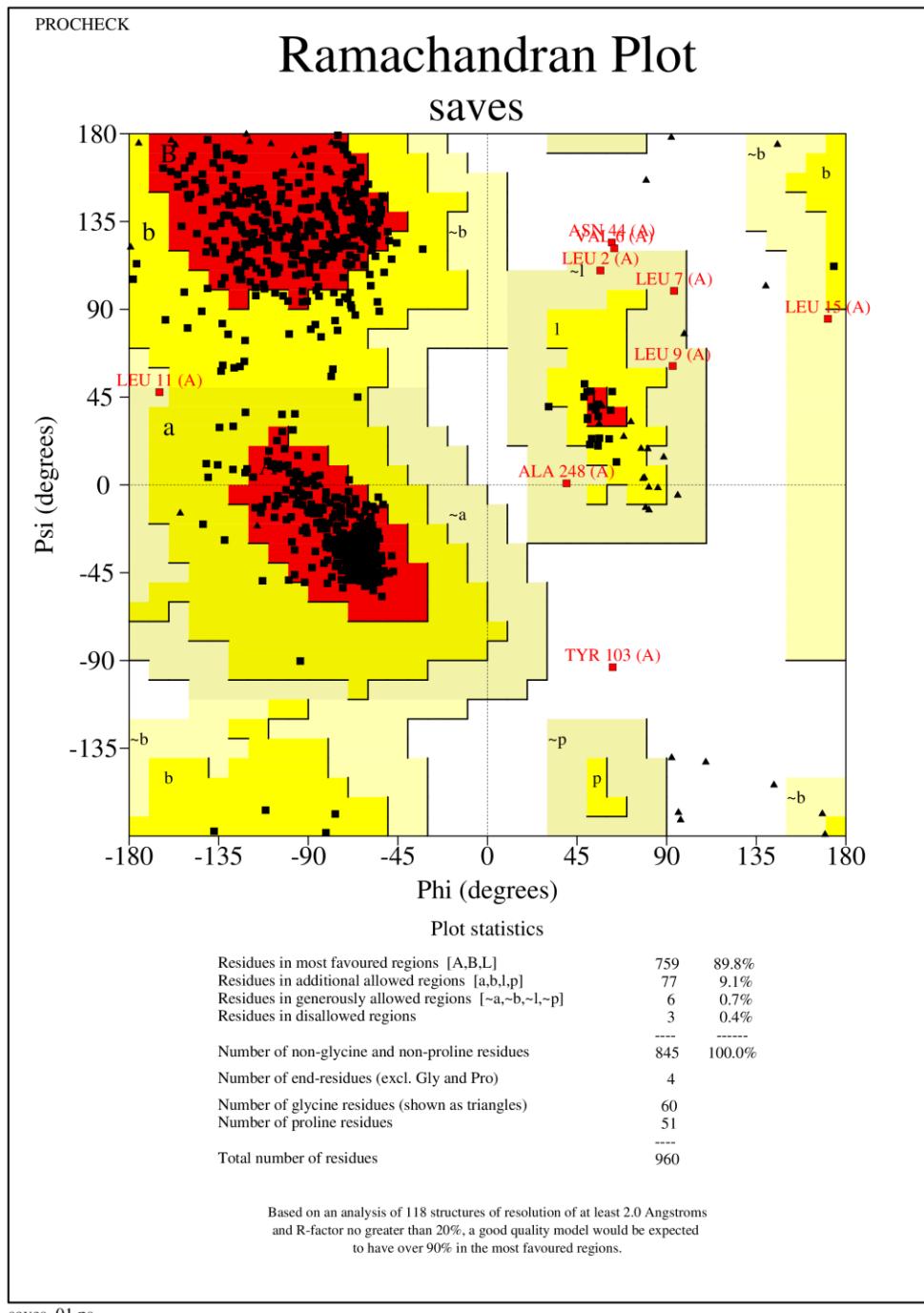


Figure S1 The results of HPLC-MS. A:DCY B: IGR C:GGR.



saves_01.ps

Figure S2 The Ramachandran plot validation of the developed structures.