

## iACP: a sequence-based tool for identifying anticancer peptides

### Supplementary Materials

**Supporting Information S1: The benchmark dataset contains 138 anticancer peptides and 206 non-anticancer peptides (see Eq.1)**

#### I. 138 anticancer peptides

> ACP_1
GLWSKIKEVVGKEAAKAAAKAAGKAALGAVSEAV
> ACP_2
GLFDIIKKIAESI
> ACP_3
GLLDIVKKVVGAFGSL
> ACP_4
GLFDIVKKVVGALGSL
> ACP_5
GLFDIVKKVVGTLAGL
> ACP_6
GLFDIAKKVIGVIGSL
> ACP_7
GLFDIVKKIAGHIAGSI
> ACP_8
GLFDIVKKIAGHIVSSI
> ACP_9
AACARFIDDFCDLTPNIYRPRDNGQRCYAVNGHRCDFTVFNTNNGGNPIRASTPN CKTVLRTAANRCPTGGRGKINPNAPFLFAIDPNDGDCSTNF
> ACP_10
HGVSGHGQHG VHG
> ACP_11
FKCRRWQWRMCKLGAPSITCVRRAF
> ACP_12
KWKLFKKIKFLHSAKKF
> ACP_13
KSSAYSLQMGATAIKQVKKLFKKWGW
> ACP_14
GIGTKILGGVKTALKGALKELASTYAN
> ACP_15
GIGGKILSGLKTALKGAAKELASTYLH
> ACP_16
GIGGVLLSAGKAALKGLAKVLAEKYAN
> ACP_17
SIGAKILGGVKTFFKGALKELASTYLQ
> ACP_18
FLPLLAGLAANFLPTIICKISYKC

> ACP_19
FVQWFSKFLGRIL
> ACP_20
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> ACP_21
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> ACP_22
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> ACP_23
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> ACP_24
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> ACP_25
GIGAVLKVLTTGLPALISWIKRKRQQ
> ACP_26
ALWKNMLKGIGKLAGQAALGAVKTLVGAE
> ACP_27
ACYCRIPACIAGERRYGTICIYQGRWAFCC
> ACP_28
ECRRLCYKQRCVTYCRGR
> ACP_29
LKLKSIVSWAKKVL
> ACP_30
KWCFRVCYRGICYRRCR
> ACP_31
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> ACP_32
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> ACP_33
GLLSVLGSAKHVLPVVPVIAEHL
> ACP_34
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> ACP_35
GLFGVLGSAKHVLPVVPVIAEK
> ACP_36
GLFVGLAKVAAHVPAIAEHF
> ACP_37
GLFVGLAKVAAHNPVIAEHFQA
> ACP_38
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> ACP_39
GLLQTIKESLESLESLAKGIVSGIQA
> ACP_40
TRSSRAGLQFPVGRVHLLRK
> ACP_41
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> ACP_42

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> ACP_43
GLFDIIKKVASVVGGL
> ACP_44
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> ACP_45
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> ACP_46
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> ACP_47
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> ACP_73
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> ACP_75
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> ACP_106
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<b>II. 206 non-anticancer peptides</b>
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> non-ACP_184
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> non-ACP_185
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> non-ACP_186
ENWRKQKRERWEKIQADKERRARLQAEAQE
> non-ACP_187
LKEERQRQKKEARIAAMASAEGQDSAEAQD
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> non-ACP_206
QTLVHNGGRLPPDLQLSAEDSSSTPS

**Supporting Information S2: The Independent dataset contains 150 anticancer peptides and 150 non-anticancer peptides (see Eq.2)**

**I. 150 anticancer peptides**

> ACP_1
AAKKWAKAKWAKAKKWAKAA
> ACP_2
AAVPIVNLKDELLFPSWEALFSGSE
> ACP_3
AAWKWAWAKKWAKAKKWAKAA
> ACP_4
AIGSILGALAKGLPTLISWIKNR
> ACP_5
AKRHHGYKRKFH
> ACP_6
ALSKALSKALSKALSKALSK
> ACP_7
ALWKDILKNVGAAGKAVLNTVTDMVNQ
> ACP_8
ALWKTMLKKLGTMALHAGKAALGAAADTISQGTQ
> ACP_9
AWKKWAKAWKWAKAKWWAKAA
> ACP_10
FAFAKIIAKIAKKII
> ACP_11
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> ACP_12
FAKAIAKIAFGKGIGKVGKKLL
> ACP_13
FAKALAKLAKKLL
> ACP_14
FAKFLAKFLKKAL
> ACP_15
FAKIIAKIAKIAKKIL
> ACP_16
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> ACP_17
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> ACP_18
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> ACP_19
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> ACP_20
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> ACP_21
FAKKLAKLAKKALAL
> ACP_22



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> ACP_23
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> ACP_96
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> ACP_97
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> ACP_98
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> ACP_99
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> ACP_100
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> ACP_103
ILRWPWWPWRRK
> ACP_104
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> ACP_105
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> ACP_107
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> ACP_108
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> ACP_110
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> ACP_112
KNWKKILKKIIKVVK
> ACP_113
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> ACP_114
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> ACP_115
KWFKKIPKFLHLAKKF

> ACP_116
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> ACP_133
LLGDFKRIVQRIKDF
> ACP_134
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> ACP_135
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> ACP_136
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> ACP_137
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> ACP_138
MPRWLFRRIDRVGKQIKQGILRAGPAIALVGDARAVG
> ACP_139

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> ACP_140
MWKEFHNVLSSGQLLADKRWARWYNRW
> ACP_141
MWKWFHNVLSSGQLLADKWWAWWYNWW
> ACP_142
MWKWFHNVLSSWQLLADKRPARDYNRK
> ACP_143
NKWKKILGKIKVVK
> ACP_144
NYHNRTVEVRTLKSFSTLANNFVLIVSQLQPSQENEMFSIRGDSAHRRLFFRAFKQLDVEAAL
> ACP_145
PDEDAINDALNKVCSTGRRQRSICKQLLKK
> ACP_146
PEWFKCRRWQWRMKKLGA
> ACP_147
RGDLLRHVVKILEKYL
> ACP_148
RKAFRWAWRMLKKAAPSITCVR
> ACP_149
RWGKWFKKATHVKGKHVGAALAYL
> ACP_150
SWLSKTAKKLENSAKKRISSEGIAIAIQGGPR
<b>II. 150 non-anticancer peptides</b>
> non-ACP_1
AAEFPDFYDSEEQMGPHQEADEKDRADQRVLTREEKKELENLAAMDLELQKIAEKFSQR
> non-ACP_2
AAKPMGITCDLLSLWKVGHAAACAHLVLDVGGYCTKEGLCVCKE
> non-ACP_3
ACNFQSCWATCQAQHSIYFRAFCDRSQCKCVFVRG
> non-ACP_4
ACYCRIGACVSGERLTGACGLNGRIYRLCCR
> non-ACP_5
AEVAPAPAAAAPAKAPKKKAAAKPKKAGPS
> non-ACP_6
AFPPPNVPGPRFPPPNFPGPRFPPPNFPGPRFPPPNFPGPRFPPPNFPGPPFPPPIFPGPWFPFPPFRPPPFPPPRFP
> non-ACP_7
AGANDLCQECEDIVHLLTKMTKEDAFQDTIRKFLEQECDILPLKLLVPCRQVLDVYLPVIDYFQGQIKPKA ICSHVGLC
> non-ACP_8
AGDPLADPNSQIVRQIMSNAAWGPPLVPERFRGMAVGAAGGVTQTVLQGAHMPVNVPIPKVPMGPSWNGSKG
> non-ACP_9
ALPKKLYLNLFDGFNYMGVV
> non-ACP_10
ALSILKGLEKLAKMGIALTNCKATKCC
> non-ACP_11
ALWKDILKNAGKAALNEINQLVNQ
> non-ACP_12

ANTAFVSSAHNTQKIPAGAPFNRNLRAMLADLRQNAAFAG
> non-ACP_13
APPGARPPPGPPPPGPPPPGP
> non-ACP_14
AQRCGDQARGAKCPNCLCCGKYGFCGSGDAYCGAGSCQSQCRGCR
> non-ACP_15
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> non-ACP_16
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> non-ACP_17
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> non-ACP_18
ATCDLLSGTGINHSACAAHCLLRGNRGGYCNGKAVCVCRN
> non-ACP_19
ATCDLLSMWNVNHSACAAHCLLLGKSGGRCNDDAVCVCRK
> non-ACP_20
ATCYCRTGRCATRESLSGVCEISGRLYRLCCR
> non-ACP_21
ATPATPTVAQFVIQGSTICLVC
> non-ACP_22
ATRVVYCNRRSGSVVGGDDTVYYEG
> non-ACP_23
AVDFSSCARMDVPGLSKVAQGLCISSCKFQNCGTGHCEKRGGRPTCVCDRCGRGGGEWPSVPMKGRSS RGRRH
> non-ACP_24
AVTCNTVSSSLAPCVFFAGSAAQPTAACCGVRSLSAARTTPDRRTACNCIKSSASSIGLNYNKAAKLPSRCT VNVTVPIPSVNCAT
> non-ACP_25
CAWYNISCR LGNK GAYCTLTVECMPCSN
> non-ACP_26
CLAGRLDKQCTCRRSQPSRRSGHEVGRPSPHCGPSRQCGCHMD
> non-ACP_27
CSCRTSSCRFGERLSGACRLNGRIYRLCC
> non-ACP_28
DAPGHPGKHYLQVNVPSDVRTIGVAGGGVQQCFRVTPGAWNDTRALVSNGAQVEVWGYTVADCA NRTTANQKYDCAAAPSDSSTYFWFTLKNLRV
> non-ACP_29
DDMTMKPTPPPQYPLNLQGGGGGGSGDGFQGHQKQVWTSNDRHEIGLNGGYGQHLGGPYGNSE PSWKVGSTYTYRFPNF
> non-ACP_30
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> non-ACP_31
DHHHDHGHDDHEHEELTLEKIKEKIKDYADKTPVDQLTERVQAGRDYLLGKGARPSHLPARVDRHLSKLTA AEKQELADYLLTFLH
> non-ACP_32
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> non-ACP_33
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> non-ACP_34
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> non-ACP_35
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> non-ACP_36
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> non-ACP_37
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> non-ACP_38
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> non-ACP_39
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> non-ACP_40
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> non-ACP_41
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> non-ACP_42
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> non-ACP_43
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> non-ACP_44
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> non-ACP_45
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> non-ACP_46
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> non-ACP_47
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> non-ACP_48
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> non-ACP_49
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> non-ACP_50
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> non-ACP_51
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> non-ACP_52
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> non-ACP_53
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> non-ACP_54
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> non-ACP_55
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> non-ACP_56
GILDSFKQFAKGVGKDLIKGAAQGVVLTMSCKLAKTC
> non-ACP_57



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> non-ACP_58
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> non-ACP_59
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> non-ACP_60
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> non-ACP_61
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> non-ACP_62
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> non-ACP_63
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> non-ACP_64
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> non-ACP_65
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> non-ACP_66
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> non-ACP_67
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> non-ACP_68
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> non-ACP_69
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> non-ACP_70
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> non-ACP_71
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> non-ACP_72
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> non-ACP_73
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> non-ACP_75
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> non-ACP_76
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> non-ACP_77
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> non-ACP_78
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> non-ACP_79
GRPNPVNTKPTPYPR L
> non-ACP_80
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> non-ACP_81
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> non-ACP_82
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> non-ACP_83
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> non-ACP_84
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> non-ACP_87
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> non-ACP_91
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> non-ACP_95
GVVDILKGAGKDLLAHLVGKISEKV
> non-ACP_96
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> non-ACP_97
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> non-ACP_98
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> non-ACP_99
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> non-ACP_100
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> non-ACP_101
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> non-ACP_102
IIEKLVNTALGLLSGL
> non-ACP_103
IIGLVSKGTCVLVKTVCCKVLKQG

> non-ACP_104
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> non-ACP_105
ILENLLARSTNEDREGSIFDTGPIRRPKPRPRRPEG
> non-ACP_106
ITCQQVTSELGPCVPYLTGQGIP
> non-ACP_107
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> non-ACP_108
KCKWWNISCDLGNNGHVCTLSHECQVSCN
> non-ACP_109
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> non-ACP_110
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> non-ACP_111
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> non-ACP_112
KRFGRLAKSFLMRILLPRRKILLAS
> non-ACP_113
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> non-ACP_114
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> non-ACP_115
KRRHWFPLSFQEFLEQLRRFRDQLPFP
> non-ACP_116
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> non-ACP_117
LCLDQKPEMEPFRKDAQALEPSRQRRWLHRRCLSGRGFCRAICSI FEEPVRGNIDCYFGYNCCRRMF SHYRTS
> non-ACP_118
LIDHLGAPRWAVDTILGAIAVGNLASWVLALVPGPGWAVKAGLATAAAIVKHQGKAAAAAW
> non-ACP_119
LLGRCKVKS NR FHGPCLTDTHCSTVCRGEGYKGGDCHGLRRRCMCLC
> non-ACP_120
LPVNEAQRQVGGYCGLRICNFPSRFLGLCTR NHPCCSR VVW
> non-ACP_121
LQDAALGWRRCPQCPRCPCPCPCPRCPCPRCKCNPK
> non-ACP_122
LRVRLASHLRKLRKRLLRDADDLQKRLAVY
> non-ACP_123
LSCKRG TCHFGRCPSHLIKGSCSGG
> non-ACP_124
LTCEIDRSLCLLHCRLKGYL RAYCSQQKVCRCVQ
> non-ACP_125
MDSNKDERAYAQWV III LHN V GSSPFKIANLGLSWGKLYADGNKDKEV
> non-ACP_126
MHDFWVLWV LLEYIYNSACSVLSATSSVSSRVLNRSLQVKVVKITN
> non-ACP_127

MINRTDCNENSYLEIHNNEGRDTLCFANAGTMPVAIYGVNWVESGNNVVTLQFQRNLSDPRL ETITLQKWGSWNPGHIHEILSIRIY
> non-ACP_128
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> non-ACP_129
MKTFSVAVAVAVVLAFICTQESSALPVTGIEELVEPVSSDNNNDNHQGLPVELRERLVNIRKKRAP TDCIPYCYPTGDGFHCGVTCRF
> non-ACP_130
MLAKIKAMIKKFPNPYTLAAKLTTYEINWYKQYGRYPWERPVA
> non-ACP_131
MNFNKLFFVVALVLAFCIGQSEAGWLKIGKIKIERVQGHTRDATIQTIGVAQ
> non-ACP_132
MRILYLLFSVLFVLVQVSPGLSLPQRDMFLCRIGSCHFGRCPIHLVRVGSFCGFRSCCKSPWDV
> non-ACP_133
PDEDAINDALNKVCSTGRRQRSICKQLLKK
> non-ACP_134
SKRNTWTPSGSNTKWMVEWVGQNLDSGALGTITVDVLRKGN
> non-ACP_135
SKYGGECVSVEHNTCTYLKGGKDHIVSCPSAANLRCKTERHHCEYDEHHKTVDCQTPV
> non-ACP_136
SLQGGAPNFPQPSQQNGGWQVSPDLGRDDKGNTRGQIEIQNKGDHDFNAGWGKVIRGPNKA KPTWHVGGTYRR
> non-ACP_137
SLQPGAPNVNNDQPWQVSPHISRDDSGNTRTDINVQRHGENNDFEAGWSKVVRGPNKAKP TWHIGGTHRW
> non-ACP_138
TYMPVEEGEYIVNISYADQPKKNSPFTAKKQPGPKVDLSGVKAYGPG
> non-ACP_139
VLLFLFQAAPGSADAPFADTAACRSQGNFCRAGACPPTFAASGSCHGGLLNCCA
> non-ACP_140
VNYGNGVSCSKTKCSVNWGQAFQERYTAGINSFVSGVASGAGSIGRRP
> non-ACP_141
VQETQKLAKTVGANLEETNKKLAPQIKSAYDDFVKQAQEVQKKLHEAASKQ
> non-ACP_142
VSCTCRRFSCGFGERASGCTVNGVRHTLCCRR
> non-ACP_143
VTCDILSVEAKGVKLNDAACAAHCLFRGRSGGYCNGKRVCVCR
> non-ACP_144
VTCDLLSFEAKGFAANHSLCAAHCLAIGRRGGSCERGVCICRR
> non-ACP_145
VTCYCRTRCGFRERLSGACGYRGRIYRLCCR
> non-ACP_146
VTSWSLCTPGCTSPGGGSNCSFCC
> non-ACP_147

WNPFKELERAGQRVRDAIISAGPAVATVAQATALAK
> non-ACP_148
YPSDYNGKTVGPDEKIQINSCGRENASSGTEGSFDIVDPNDGNKTIRHFYWECPWG
> non-ACP_149
YRQSMNMFQGLRSFGCRFGTCTVQKLAHQIQFTDKDKDNVAPRSKISPOGY
> non-ACP_150
YVPLPNVPQPGRRPFPTFPGQGFNPKIKWPQGY

None of the peptides in the independent dataset occurs in Supporting Information S1.

**Supporting Information S3: The predictive results of iACP and Tyagi et al.’s models based on the same independent dataset given in Supporting Information S2**

Peptide ID <sup>a</sup>	Experimental annotations	Predictive results		iACP
		Tyagi et al.’s method		
		Module 1	Module 2	
ACP_1	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_2	Anticancer peptide	Anticancer peptide	Non-Anticancer peptide	Non-Anticancer peptide
ACP_3	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_4	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_5	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_6	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_7	Anticancer peptide	Anticancer peptide	Non-Anticancer peptide	Anticancer peptide
ACP_8	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_9	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_10	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_11	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_12	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_13	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_14	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_15	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_16	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_17	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_18	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_19	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_20	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_21	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_22	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_23	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_24	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_25	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_26	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_27	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_28	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_29	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide
ACP_30	Anticancer peptide	Anticancer peptide	Anticancer peptide	Anticancer peptide















**Supporting Information S4: List of the 126 optimal one-gap dipeptides and their *F*-scores**

Dipeptide	F-score	Dipeptide	F-score	Dipeptide	F-score	Dipeptide	F-score	Dipeptide	F-score
AK	38.03	CN	16.30	LP	8.93	EL	6.19	NV	4.61
KC	34.43	AR	15.79	VL	8.59	EQ	6.19	YP	4.47
EC	34.14	CS	15.32	VG	8.56	PK	6.10	MI	4.45
CE	34.02	FI	14.96	EP	8.31	PN	6.08	HV	4.43
IK	31.22	GR	14.79	QE	7.93	LN	6.07	IY	4.41
KF	30.09	CK	14.75	VI	7.89	DM	6.06	VN	4.41
PI	28.37	PP	14.04	AL	7.84	RQ	5.91	FV	4.30
KI	28.01	GS	13.78	LE	7.80	NS	5.83	YC	4.28
LL	27.60	YN	13.75	QP	7.62	CI	5.81	NR	4.22
VY	27.37	AA	13.65	RT	7.58	EN	5.78	WQ	4.17
IC	27.16	CW	13.00	AQ	7.58	SC	5.62	RS	4.14
CC	26.86	QQ	12.99	ES	7.52	NL	5.48	MV	4.11
SK	25.78	CT	12.83	IA	7.49	ND	5.45	CL	4.08
KK	25.58	LR	12.80	LA	7.42	SI	5.43	LF	4.03
FK	22.53	QS	12.66	PC	7.41	WP	5.43	QT	4.01
IG	20.92	IS	12.56	PQ	7.15	EA	5.42	EE	4.01
GF	20.88	KV	12.50	AE	7.01	VM	5.29	GV	3.90
GI	20.75	QR	11.10	LV	6.98	QK	5.15	RM	3.88
KA	19.65	SY	10.61	MA	6.97	PD	4.92		
VK	19.55	FG	10.36	DQ	6.95	GL	4.89		
SV	19.37	TQ	10.01	AM	6.88	QV	4.83		
AP	18.56	RR	9.98	CR	6.82	SR	4.83		
LK	18.10	CF	9.86	AH	6.70	ER	4.83		
KL	18.04	FP	9.70	SQ	6.46	TE	4.81		
RA	17.34	WK	9.42	PT	6.43	QL	4.76		
RL	17.17	FC	9.15	TP	6.39	GD	4.74		
LQ	17.15	PA	9.07	RD	6.29	DD	4.70		