Supporting Information

for

Identification and Optimization of Short Helical Peptides with Novel Reactive Functionality as Catalysts for Acyl Transfer by Reactive Tagging

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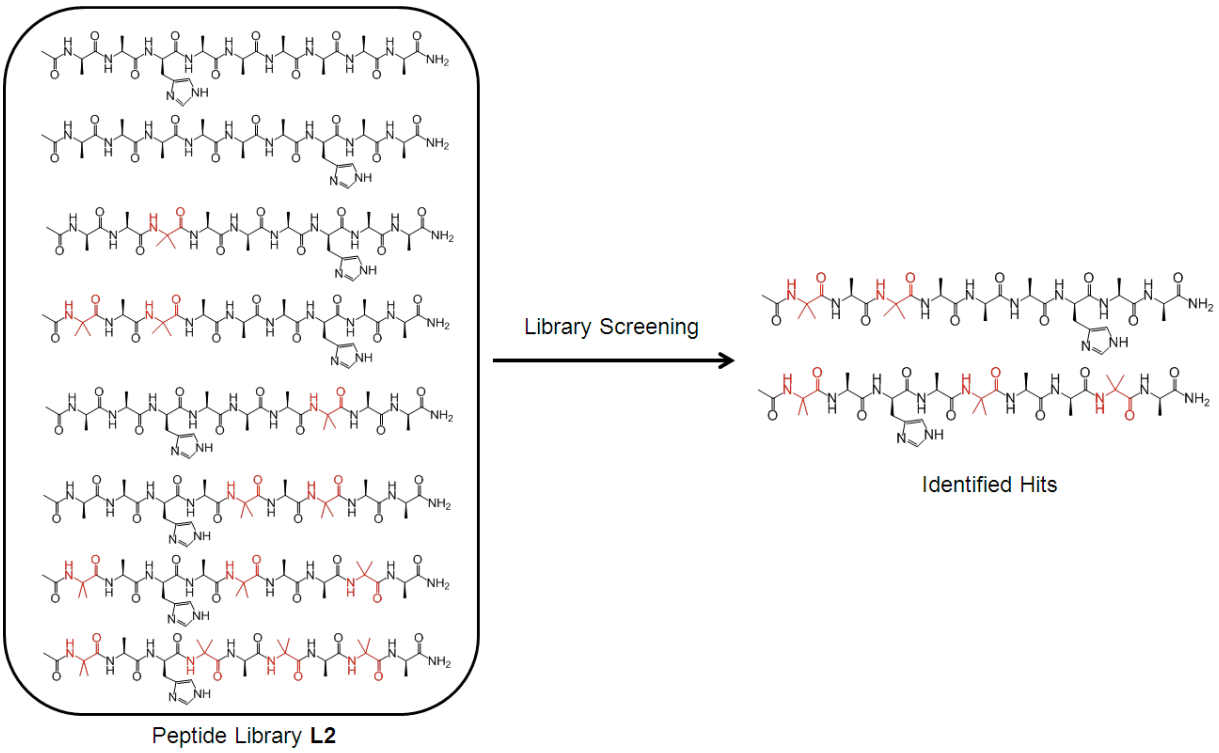
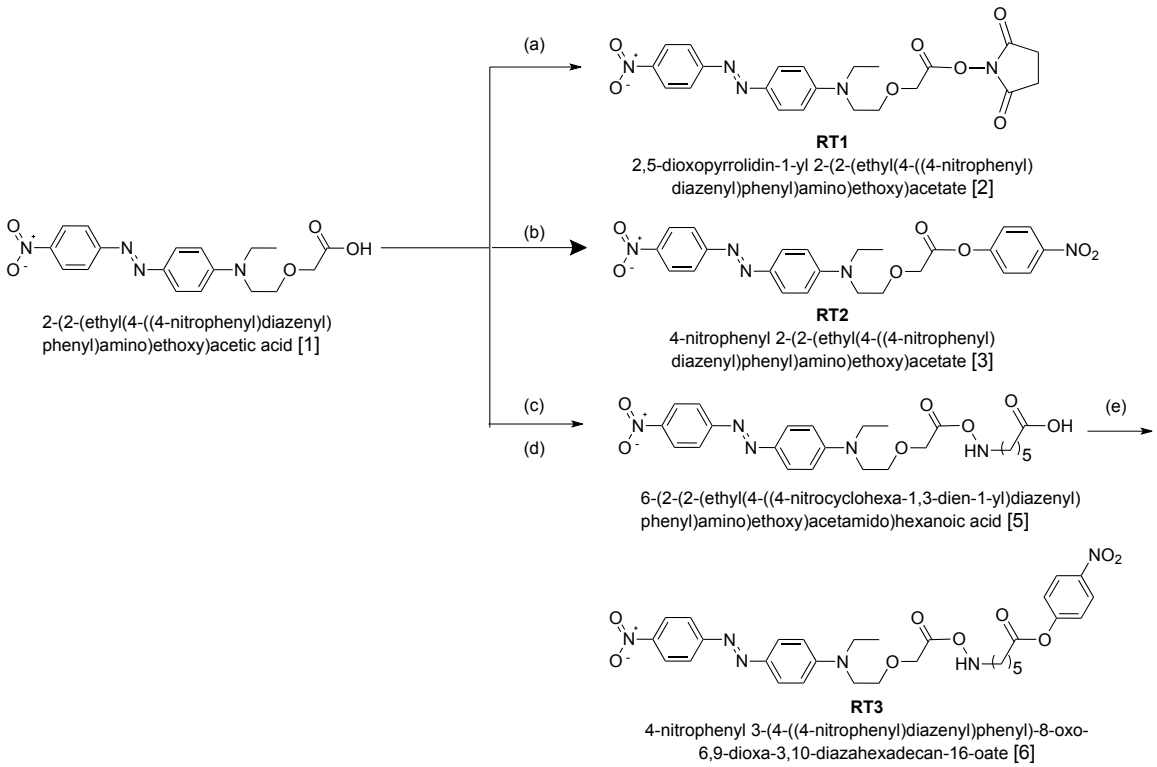
Peptide Synthesis. Peptides were synthesized by automated solid-phase peptide synthesis on CEM Liberty 1 microwave peptide synthesizer using Fmoc-protected amino acids on a Tentagel (library peptides) or CLEAR-Amide (individual peptides) resin.[1] Activation of amino acids was performed with PyClock in the presence of DIPEA in DMF. Peptide deprotection was carried out in 20% piperidine in DMF. All peptides where acetylated at the N-terminus with 5% acetic anhydride and 6% lutidine in DMF. For the peptide libraries on Tentagel resin, the peptides were first washed with 95:2.5:2.5 trifluoroacetic acid (TFA) and triisopropylsilane (TIPS)/water for 1h to remove trityl group protecting imidazole. Cleavage of the peptide from the resin was performed in: (a) for the peptides on Tentagel resin – in methanol irradiated with UV light; (b) for the peptides on CLEAR-Amide resin - 95:2.5:2.5 trifluoroacetic acid (TFA) and triisopropylsilane (TIPS)/water for 3 h. TFA was evaporated and cleavage products were precipitated with cold ether. The precipitate was washed with ether for five times and dried under N_2. It was then purified by reverse-phase HPLC using an Atlantis C-18 semipreparative column and a gradient of 0 to 100% B over 45 min, where solvent A was 95 : 5 water : acetonitrile with 0.1% TFA and solvent B was 95 : 5 acetonitrile : water with 0.1% TFA. After purification, the peptides were lyophilized to a powder and treated with Amberlist 21 in methanol for residual TFA removal.[2]

Split-and-mix synthesis. The peptide libraries were synthesized on Tentagel resin up to a specific length, then split in n portions (For **L1** n=X=34, for **L3**, n=Y=17) coupling a different amino acid to each portion followed by mixing of all portions. The cycle was repeated for **L3**, with the library splitting in 25 portions coupling different amino acids and mixed again to continue with the scaffold synthesis. For **L1**, X=[1]-[34] in Scheme S1. For **L3**, X=[1]-[7], [9], [11]-[12], [16], [18]-[25], [27], [29]-[30], [32]-[34] in Scheme S1; Y= [1]-[7], [9], [11], [13], [16], [20], [22], [24]-[25], [27], [32].



Scheme S1. Cartoon representation of screening process for library **L2** in presence of 10 mM reactive tag **RT3** in DCM (reaction time 1.5 h).

Reactive tag synthesis. All reagents were obtained from commercially available sources as analytical grade and were used without further purification. All reactions were monitored by TLC on SiO_2. Reactive tag **RT 4**, which represents a succinimide ester of Bodipy (Bodipy-630/650-X) was commercially available (*Life Technologies*). The precursor compound **[1]** for the synthesis of reactive tags **RT 1-3** and compound **[3]** (**RT2**) were prepared according to published procedures.[3]



Scheme S2. Synthetic scheme of the reactive dyes **RT1-3**: (a) **[1]**, N-hydroxysuccinimide, $POCl_3$, pyridine, at -15 ºC, (Yield, 67%); (b) **[1]**, p-nitrophenol, $POCl_3$, pyridine, at -15 ºC. (Yield 81%); (c) **[1]**, HBTU, HOBT, Et_3N, in DMF, (Yield, 65%); (d) **[4]**, KOH in MeOH:Toluene, reflux, (Yield, 79%); (e) **[5]**, p-nitrophenol, $POCl_3$, pyridine, at -15 ºC. (Yield 41%).

(a) RT1 Synthesis. 2,5-dioxopyrrolidin-1-yl 2-(2-(ethyl(4-((4-nitrophenyl)diazenyl)phenyl) amino)ethoxy)acetate [2] (RT1): Compound **[2]** was synthesized according to modified published procedure,[3] with a yield of 79 %. ^{1}H- NMR (400MHz, $CDCl_3$): δ, 1.21-1.25 (t, 3H, J = 7.2 Hz), 2.82 (s, 4H), 3.52-3.57 (q, 2H, J = 7.2 Hz), 3.67-3.7 (t, 2H, J = 6 Hz), 3.83-3.86 (t, 2H, J = 6 Hz), 4.44 (s, 2H), 6.74-6.77 (d, 2H, J = 9.2 Hz), 7.87-7.91 (m, 4H), 8.29-8.31 (d, 2H, J = 8.8 Hz).

(b) RT2 Synthesis. RT2 (Compound **[3]**) was synthesized according to modified published procedure.[3]

RT3 Synthesis.

(c) Methyl 6-(2-(2-(ethyl(4-((4-nitrophenyl)diazenyl)phenyl)amino) ethoxy)acetamido) hexanoate [4]: To a solution of compound **[1]** (0.5 g, 1.3 mmol) in 5mL DMF was added a solution of triethylamine (0.36 mL, 2.6 mmol) in 5mL DMF and a solution of HBTU (0.42 g, 1.1 mmol) and HOBT (0.15 g, 1.1 mmol) in 5mL DMF. After stirring the mixture for one hour, a solution of methyl 6-aminohexanoate (0.2 g, 1.1 mmol) and triethylamine (0.36 mL, 2.6 mmol) in 5 mL DMF was added and the reaction mixture was stirred over night at room temperature. The DMF was removed and the crude product was dissolved in water followed by an extraction with EtOAc (3×150 mL) of the final product resulting in a dark-red solid **[4]** (0.42 g, Yield 65 %). ^{1}H- NMR (400MHz, $CDCl_3$): δ, 1.20-1.25 (m, 2H), 1.28-1.31 (t, 3H, *J* = 7.0 Hz), 1.33-1.40 (p, 2H, *J* = 14.7 Hz), 1.53-1.60 (p, 2H, *J* = 15.2 Hz), 2.25-2.3 (t, 2H, *J* = 7.4 Hz), 3.14-3.20 (q, 2H, *J* = 6.8 Hz), 3.55-3.60 (q, 2H, *J* = 7.1 Hz), 3.65 (s, 3H), 3.72-3.78 (m, 4H), 3.99 (s, 2H), 6.85-6.87 (d, 2H, *J* = 9.2 Hz), 7.92-7.96 (m 4H), 8.34-8.36 (d, 2H, *J* = 9 Hz). ESI-MS (m/z): mass calcd for ($C_{25}H_{33}N_5O_6$ +Na^+) 522.23, found 522.20.

(d) 6-(2-(2-(ethyl(4-((4-nitrophenyl)diazenyl)phenyl)amino)ethoxy)acetamido)hexanoic acid [5]: Compound **[4]** (0.25 g, 0.5 mmol), without any further purification, was dissolved in 15 mL MeOH and 3.5 mL toluene. KOH (0.2 g, 3.6 mmol) was added to the solution and the resulting mixture was refluxed for 3h. After the solvent removal, the crud product was dissolved in water and the solution was adjusted to pH=5 with HCl (3M) and compound **[5]** was extracted with EtOAc (3×100 mL) to afford a dark-red powder (0.19 g, Yield 79%). ^{1}H-NMR (400MHz, $CDCl_3$): δ, 1.20-1.25 (m, 2H), 1.27-1.31 (t, 2H, *J* = 7.1 Hz), 1.31-1.39 (m, 2H), 1.52-1.59 (p, 2H, *J* = 15.2 Hz), 2.25-2.28 (t, 2H, *J* = 7.4 Hz), 3.14-3.19 (q, 2H, *J* = 6.6 Hz), 3.55-3.60 (q, 2H, *J* = 7 Hz), 3.70-3.79 (m, 4H), 4.0 (s, 2H), 6.85-6.88 (d, 2H, *J* = 9.2 Hz), 7.91-7.95 (m 4H), 8.33-8.35 d, 2H, *J* = 9.1 Hz).

(e) 4-nitrophenyl 6-(2-(2-(ethyl(4-((4-nitrophenyl)diazenyl)phenyl)amino)ethoxy) acetamido) hexaneate [6] (RT3): Compound **[6]** was synthesized according to published procedure, with a yield of 79 %. ^{1}H- NMR (400MHz, $CDCl_3$): δ, 0.88-0.92 (m, 2H), 1.27-1.31 (t, 3H, *J* = 7.1 Hz), 1.38-1.43 (m, 2H), 1.65-1.73 (p, 2H, *J* = 15 Hz), 2.5-2.54 (t, 2H, *J* = 7.4 Hz), 3.17-3.22 (q, 2H, *J* = 6.6 Hz), 3.55-3.6 (q, 2H, *J* = 6.8 Hz), 3.7-3.8 (m, 4H), 3.99 (s, 2H), 6.85-6.88 (d, 2H, *J* = 9.2 Hz), 7.24-7.27 (d, 2H, *J* = 9.1 Hz), 7.92-7.95 (m 4H), 8.26-8.28 (d, 2H, *J* = 9.1 Hz), 8.32-8.34 (d, 2H, *J* = 9 Hz).

Mass Spectrometry. Mass spectrometry of the peptides was performed using either MALDI-FT on IonSpec spectrometer using 2,5-dihydroxybenzoic acid as the matrix or MALDI-ToF on a Applied Biosystems spectrometer using alpha cyanocinnamic acid.

Circular Dichroism (CD). Peptide concentrations of ≈ 60 mM stock solution in TFE were determined by weight with a 0.1mg error. CD spectra were recorded on a Chirascan Plus spectrometer using a 1mm path length cell. Data were normalized to give mean residue ellipticity (degrees square centimeters per decimole). Spectra were collected from 180 to 300 nm with 3 *s* scanning at 4 °C or 25 °C. A concentration dependence study was performed to confirm that the peptides do not aggregate under the conditions studied. Peptide solutions were measured at four different concentrations ranging from 0.2-2 mM and $[\Theta]_{222}$ for each solution by CD and was found to be independent in this concentration range.

UV-Vis measurements. The peptide activities were determined spectrophotometrically with *p*-nitrophenyl 4-methoxyacetate[4] (20 mM) as substrate at 25 °C in TFE-d3 using a HP 845x UV-Vis spectrophotometer. Measurements were made at 340 nm corresponding to *p*-nitrophenol (ε = 5,852 $cm^{-1}M^{-1}$) and 425 nm corresponding to *p*-nitrophenolate ion (ε = 7,589 $cm^{-1}M^{-1}$). The substrate solution was prepared fresh each day. Peptide concentrations of ≈ 60 mM stock solution in TFE-d3 were determined by weight with a 0.1mg error. For measuring the catalytic activity: in a 1 mm pathlength spectrophotometric cuvette, the absorbance for the substrate solution was recorded and corrected. Upon addition of 10 mol% peptide catalyst, the increase in absorption at 340 nm and 425 nm was measured every 30 seconds. Initial rates (repeated three times) were determined from linear fits of plots of product formation versus time measured for 7-10% substrate conversion.

NMR Measurements. For measuring peptide catalytic activity and imidazole protonation state, a solution of 500 μL in TFE-d3 containing 20mM *p*-nitrophenyl 4-methoxyacetate and 2mM peptide was prepared and investigated at 25 °C using 500 MHz Bruker spectrometer. The spectrum was taken at 16 scans every 20 minutes until the transesterification reaction was complete. The progress of reaction was investigated by monitoring the changes in p-nitrophenol integrations by

^{I}H-NMR. The protonation state of imidazole over the course of the reaction was determined using the following formulae:

$$\% \text{ protonated imidazole} = 100\% * (\delta CH_n - \delta CH_{initial}) / (\delta CH_{final} - \delta CH_{initial})$$

where, δCH_{final}-chemical shift for 100% protonated imidazole (full protonation of imidazole was determined by adding 10mL of TFA to the imidazole-containing peptide solution)

$\delta CH_{initial}$-chemical shift for non-protonated imidazole

δCH_n- chemical shift for each protonation step

The nuclear Overhauser effect spectroscopy (NOESY) spectrum is taken with 48 scans in the direct dimension with 256 increments in the indirect dimension. The mixing time for the NOESY spectra is 300 ms.[5, 6]

Library Screening Procedure Using Reactive Tags.

Library **L1** and **L3**: Approximately 40 mg of resin (corresponding to ca 12 μmol of peptide) was added to a DCM (TFE) solution of reactive dye. The resulting suspension was shaken at room temperature for a specific time. When 1% of the beads got colored (acylated), beads were washed with DCM (6×10 mL), then transferred to a small glass plate and inspected under the microscope. For a two-step screening, the library was allowed to react with the reactive tag in DCM until 10% of the beads got acylated, then washed with DCM (6×10 mL), and 2 mL TFE solution was added until 1% of the beads got discolored (deacylated). Library **L2**: Each peptide was synthesized on 50 mg Tentagel resin and was reacted individually with a DCM solution of **RT3** (10 mM, 1 mL) until the most reactive one was visually identified.

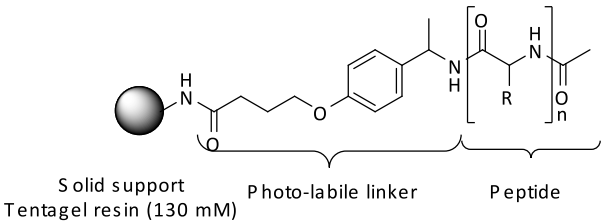


Figure S1. Schematic representation of the peptide attached to the solid support through the photo-labile linker.

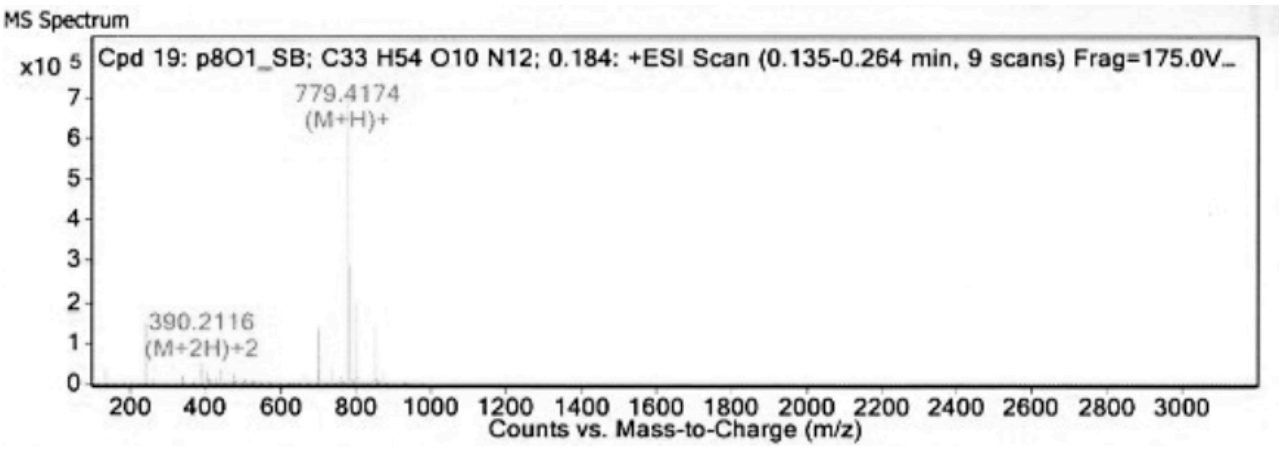


Figure S2a. Mass spectrum for the hits identified in library **L1**. Peak at 779.4174 corresponds to **Hit 1** (**Ala7HisAib)**.

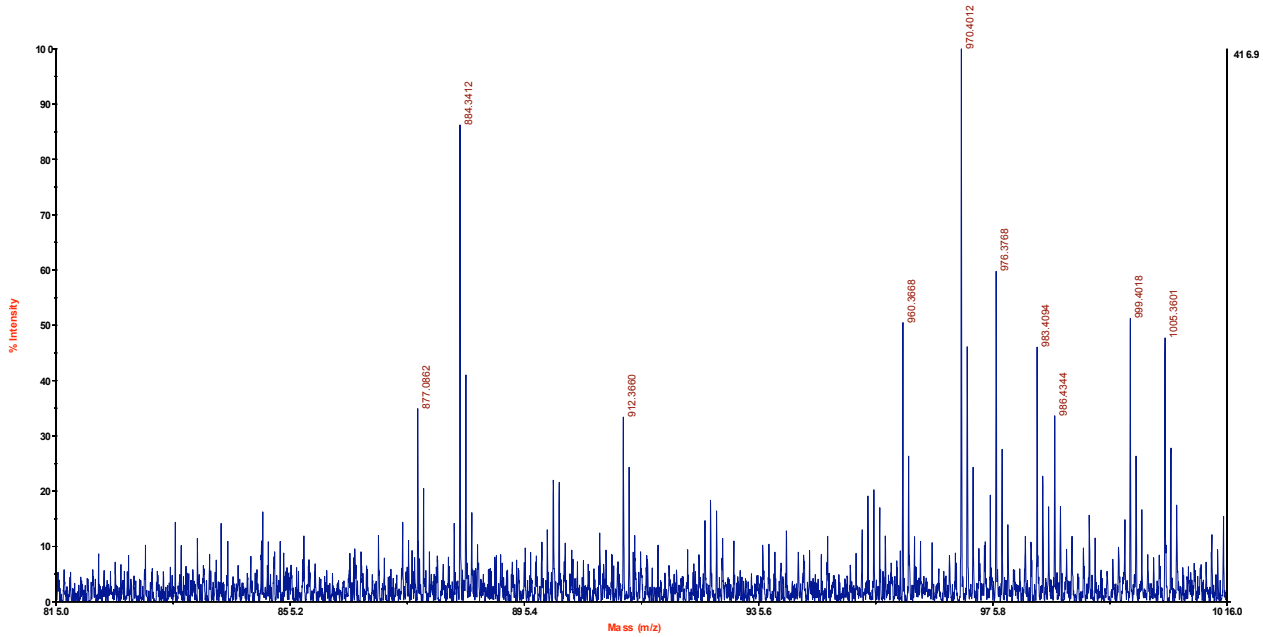


Figure S2b. Mass spectrum for the hits identified in library **L3** upon screening with **RT2** in DCM.

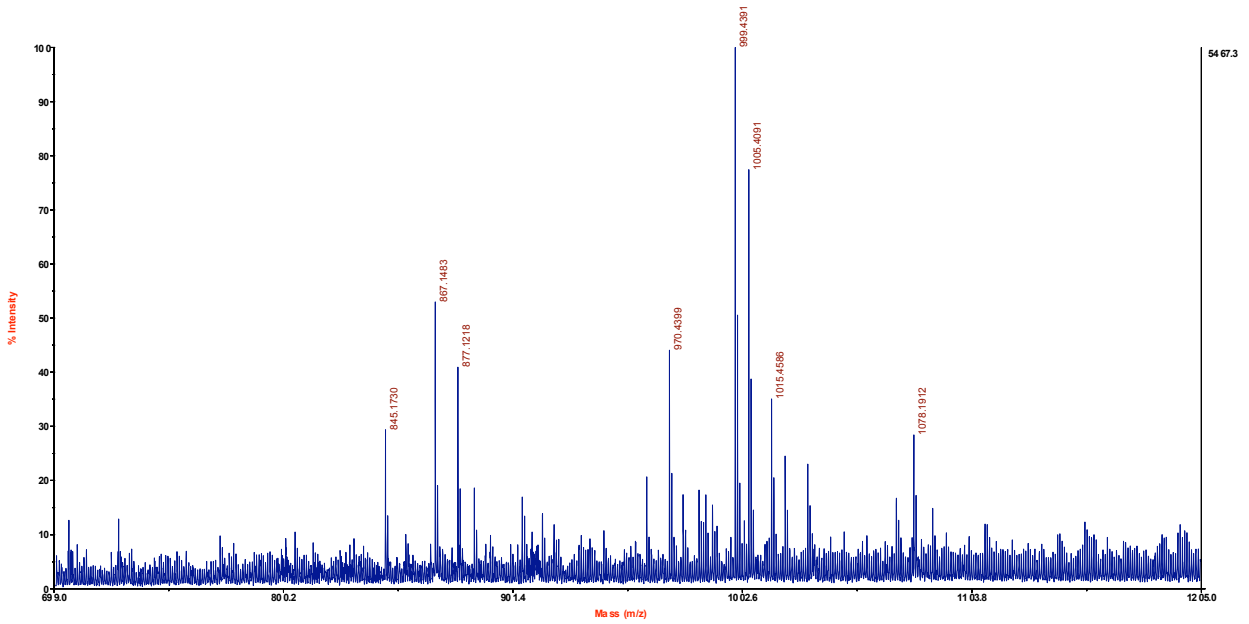


Figure S2c. Mass spectrum for the hits identified in library **L3** upon screening with **RT3** in DCM.

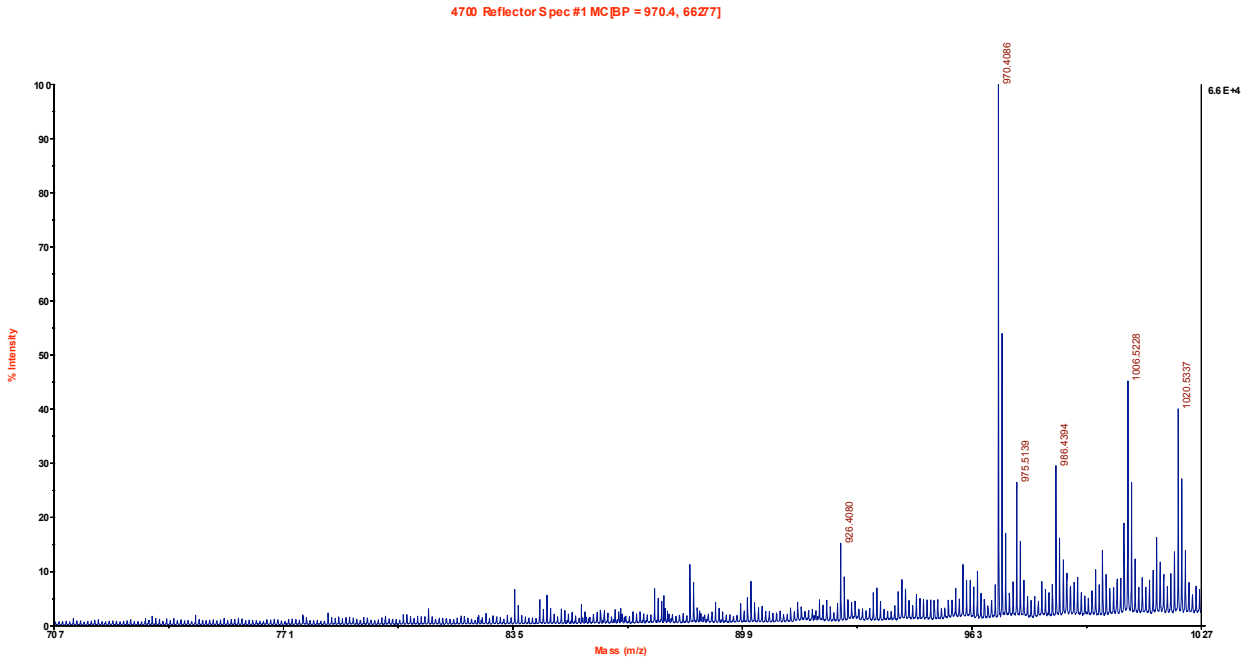


Figure S2d. Mass spectrum for the hits identified in library **L3** upon screening with **RT4** in DCM.

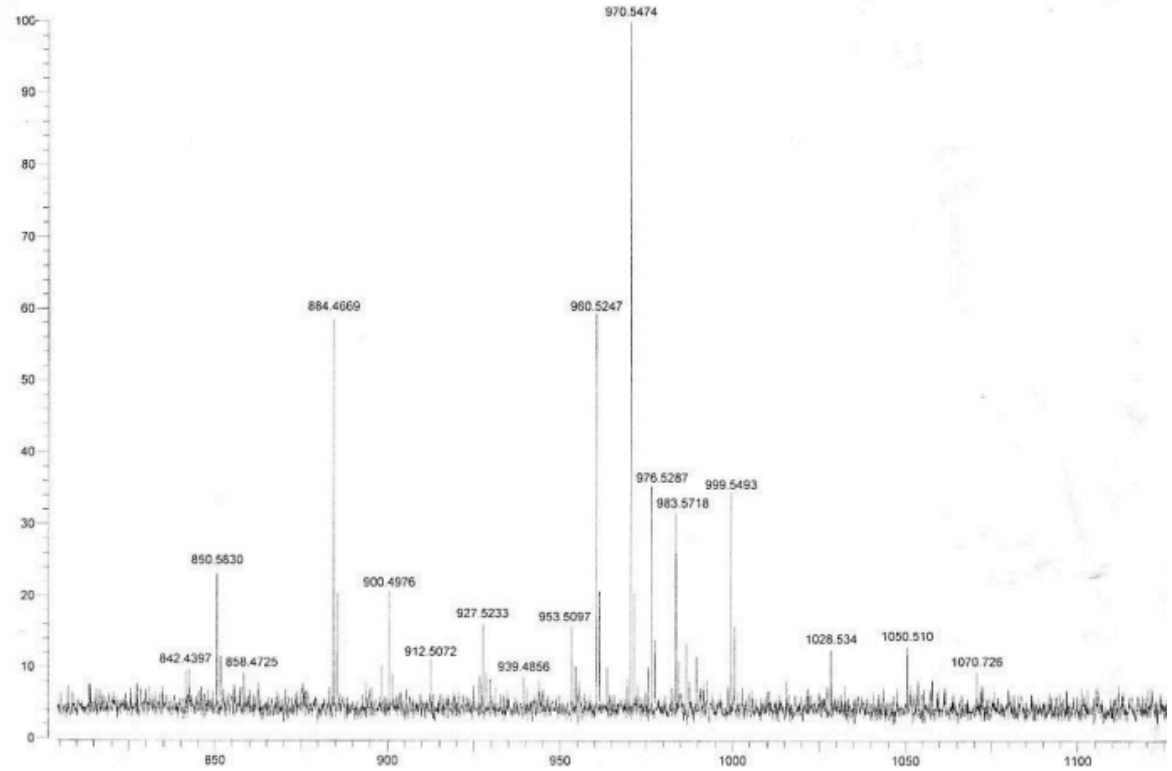


Figure S2e. Mass spectrum for the hits identified in library **L3** upon screening with **RT2** in TFE.

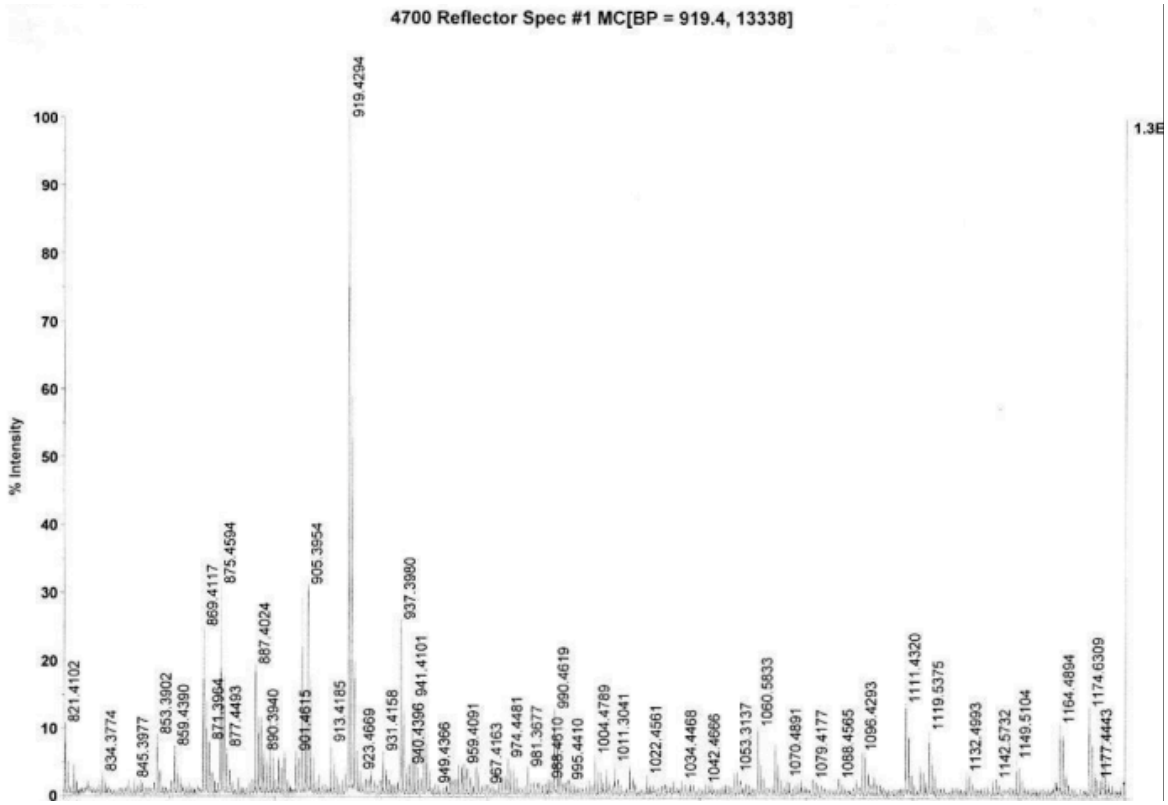


Figure S2f. Mass spectrum for the hits identified in library **L3** upon two-step screening with **RT2** (acylation was run in DCM and deacylation was run in TFE).

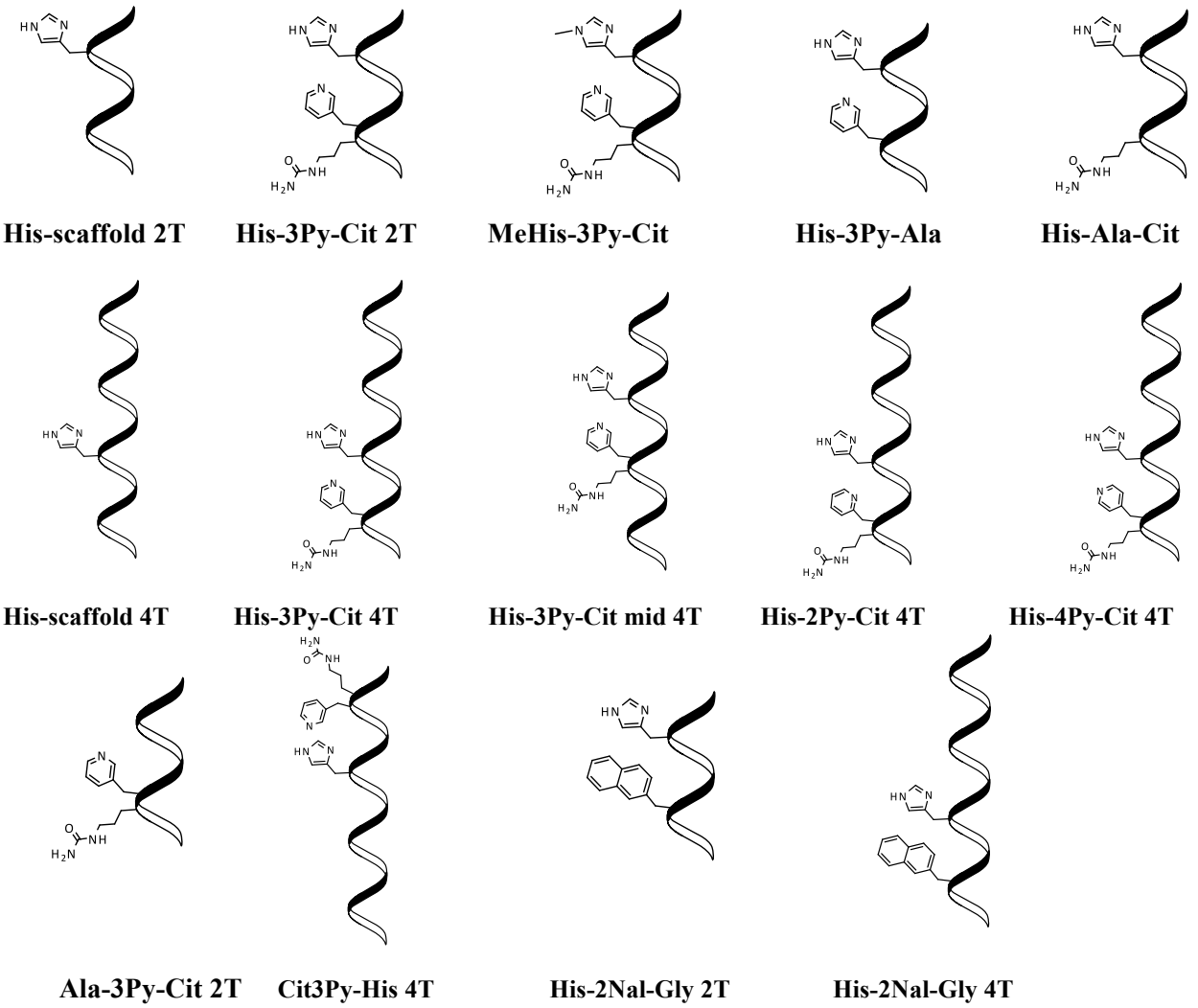
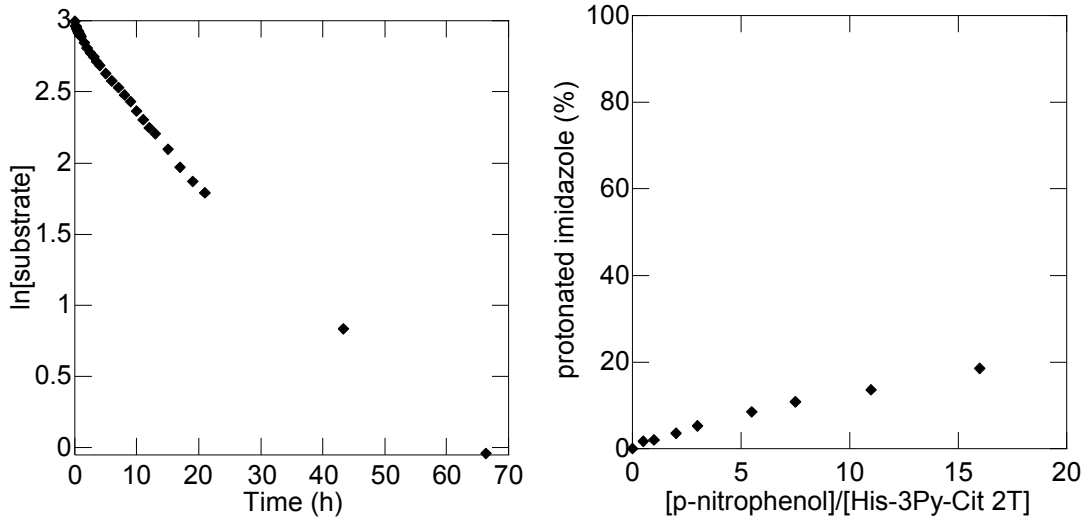


Figure S3. Cartoon representation for the studied peptide catalysts.



(a) (b)

Figure S4. (a) First-order kinetics plot for transesterification reaction of 4-nitrophenyl 2-methoxyacetate (20 mM) in presence of 10 mol% **His-3Py-Cit 4T** in TFE at 25 ºC. (b) Imidazole protonation determined from Δδ of the δCH protons of imidazole for **His-3Py-Cit 2T** upon p-nitrophenol addition.

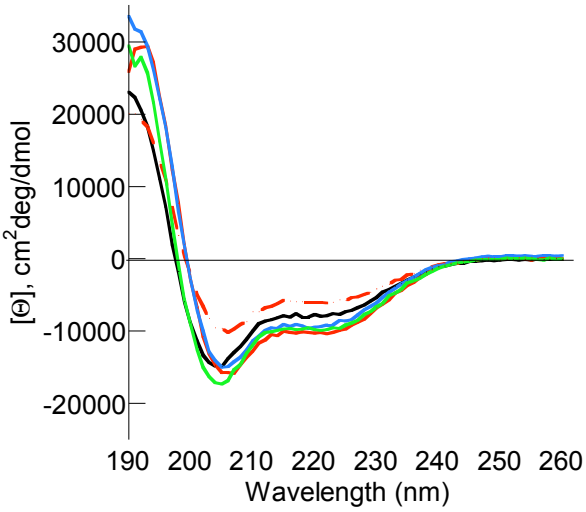
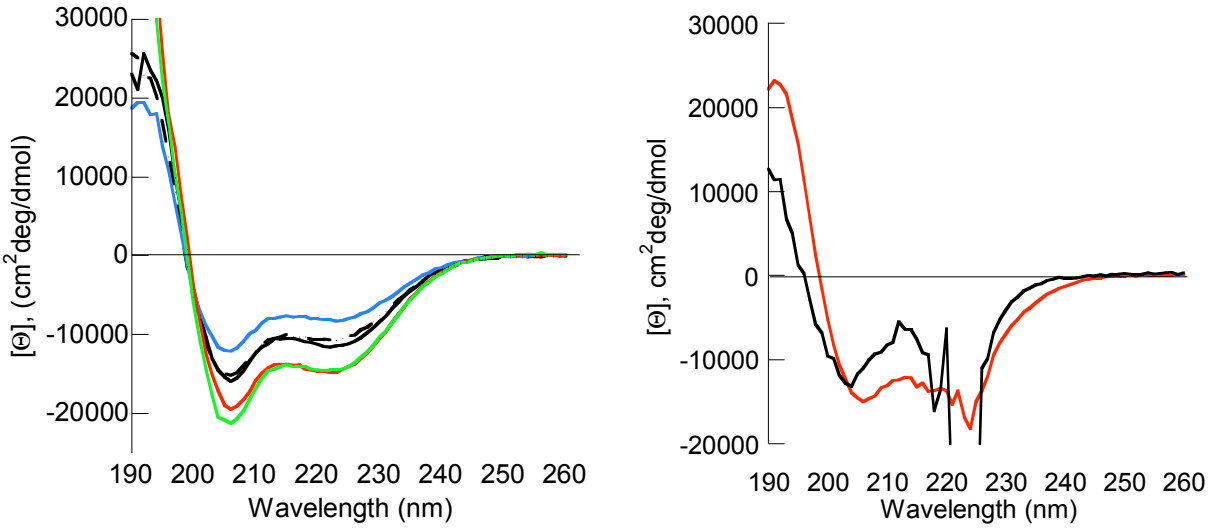


Figure S5. CD spectra of 0.2 peptide solutions in TFE at 25 ºC; **His-scaffold 2T** (black line), **His-3Py-Cit 2T** (red line), **MeHis-3Py-Cit 2T** (red broken line), **His-3Py-Ala** (blue line), **His-Ala-Cit** (green line).



(a) (b)

Figure S6. CD spectra of 200 μM peptide solutions in TFE at 25 ºC; (a) **His-3Py-Cit 4T** (black solid line), **Cit-3Py-His 4T** (black broken line), **His-3Py-Cit in 4T** (red solid line), **His-2Py-Cit 4T** (blue solid line), **His-4Py-Cit 4T** (green solid line); (b) **His-2Nal-Gly 2T** (black line), **His-2Nal-Gly 4T** (red line).

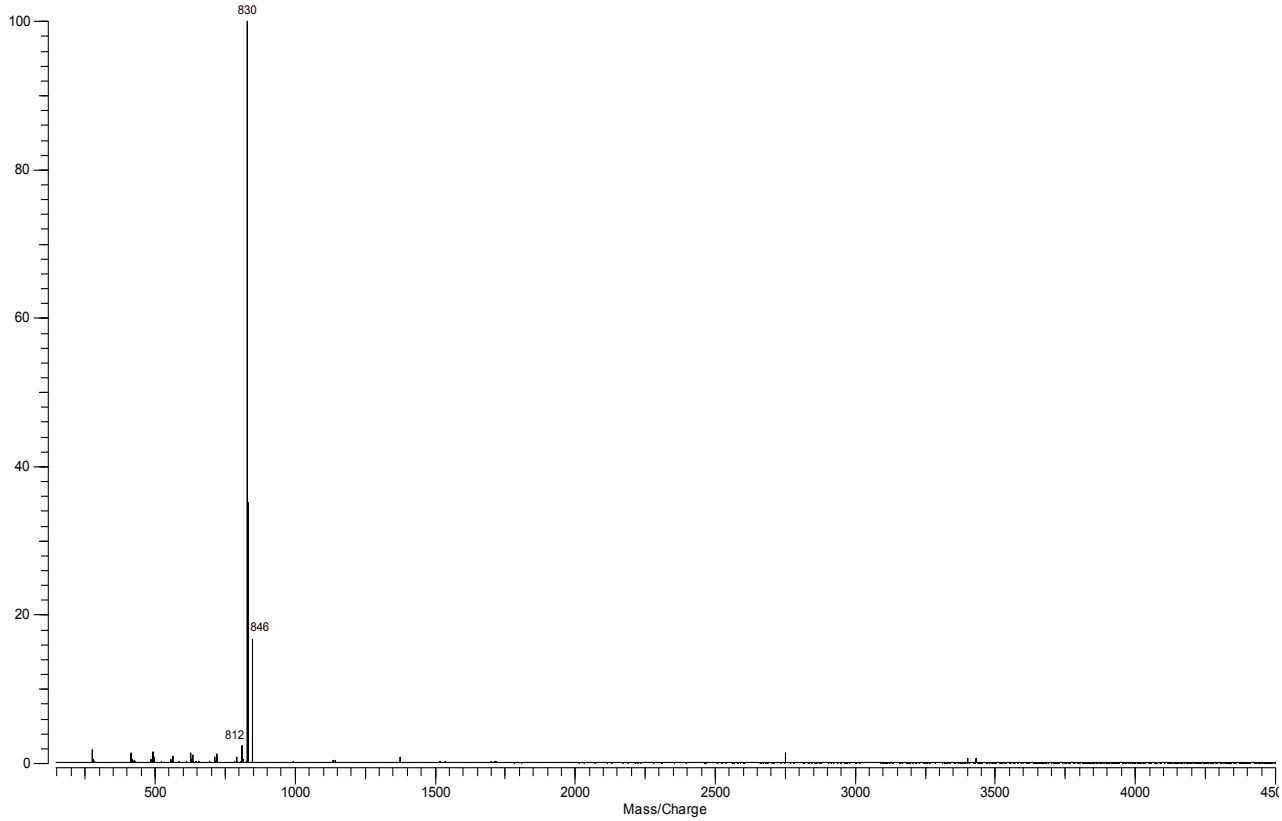


Figure S7a. Mass spectrum recorded for **His-scaffold 2T**.

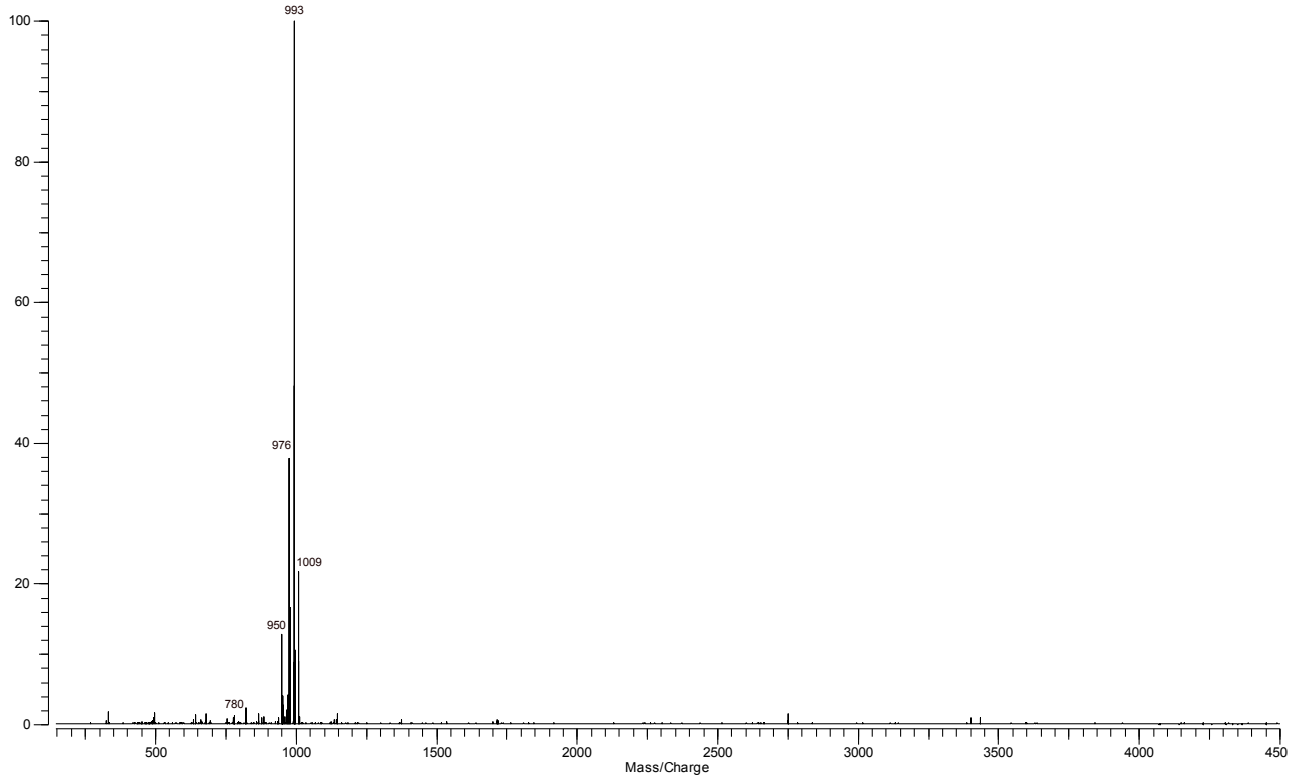


Figure S7b. Mass spectrum recorded for **His-3Py-Cit 2T**.

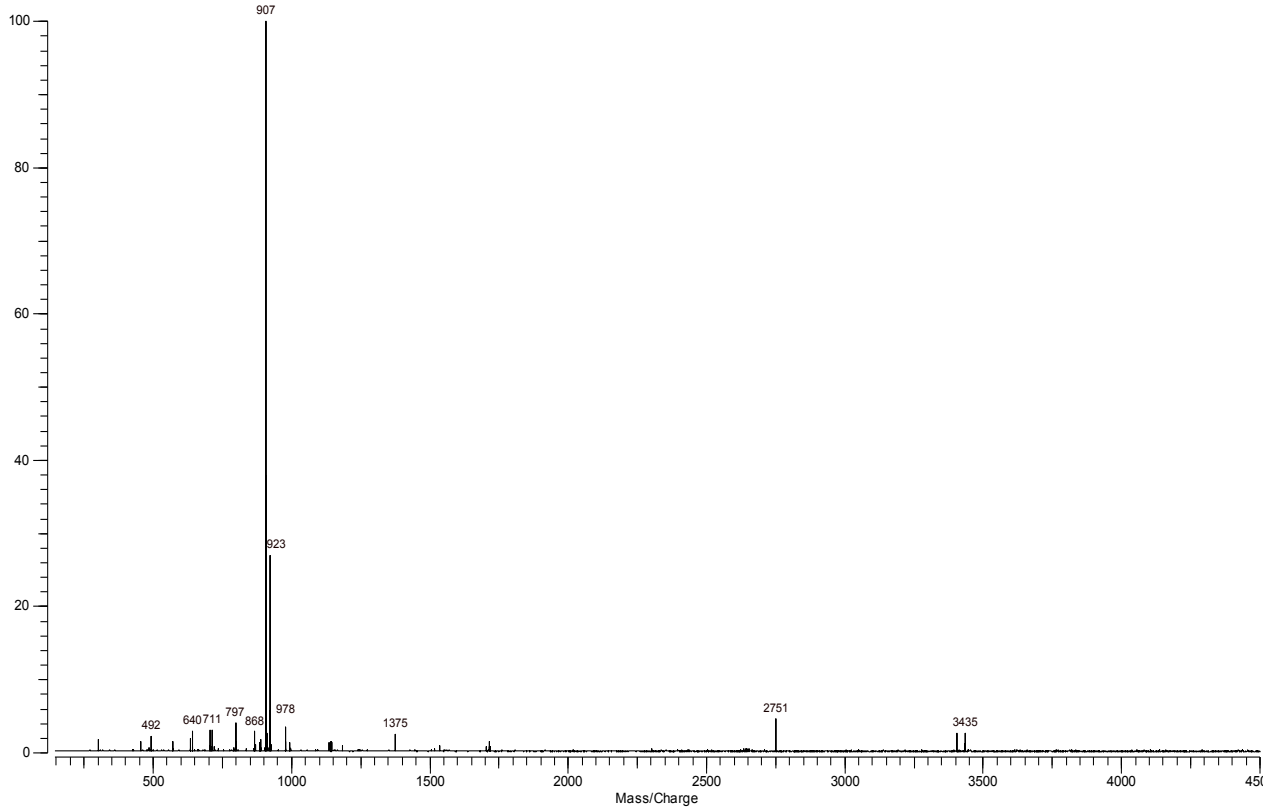


Figure S7c. Mass spectrum recorded for **His-3Py-Ala**.

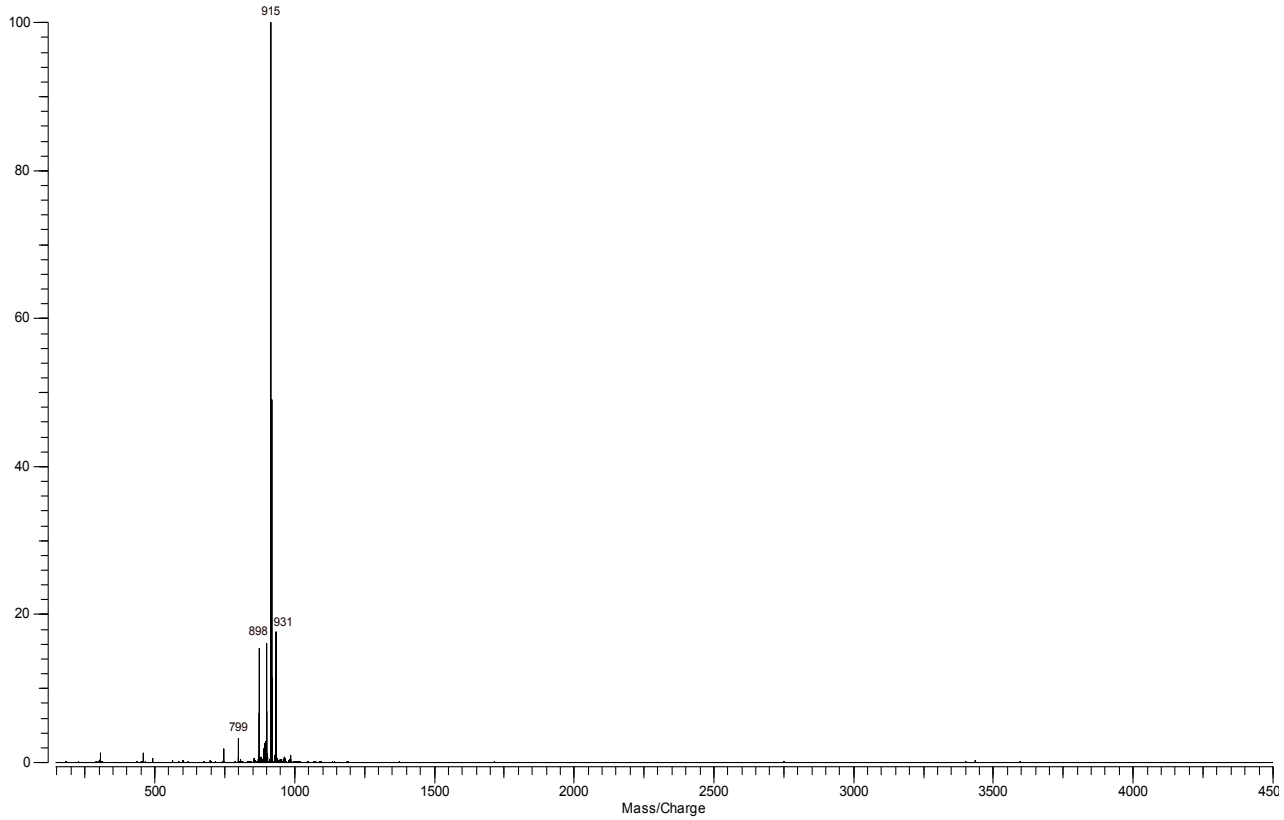


Figure S7d. Mass spectrum recorded for **His-Ala-Cit**.

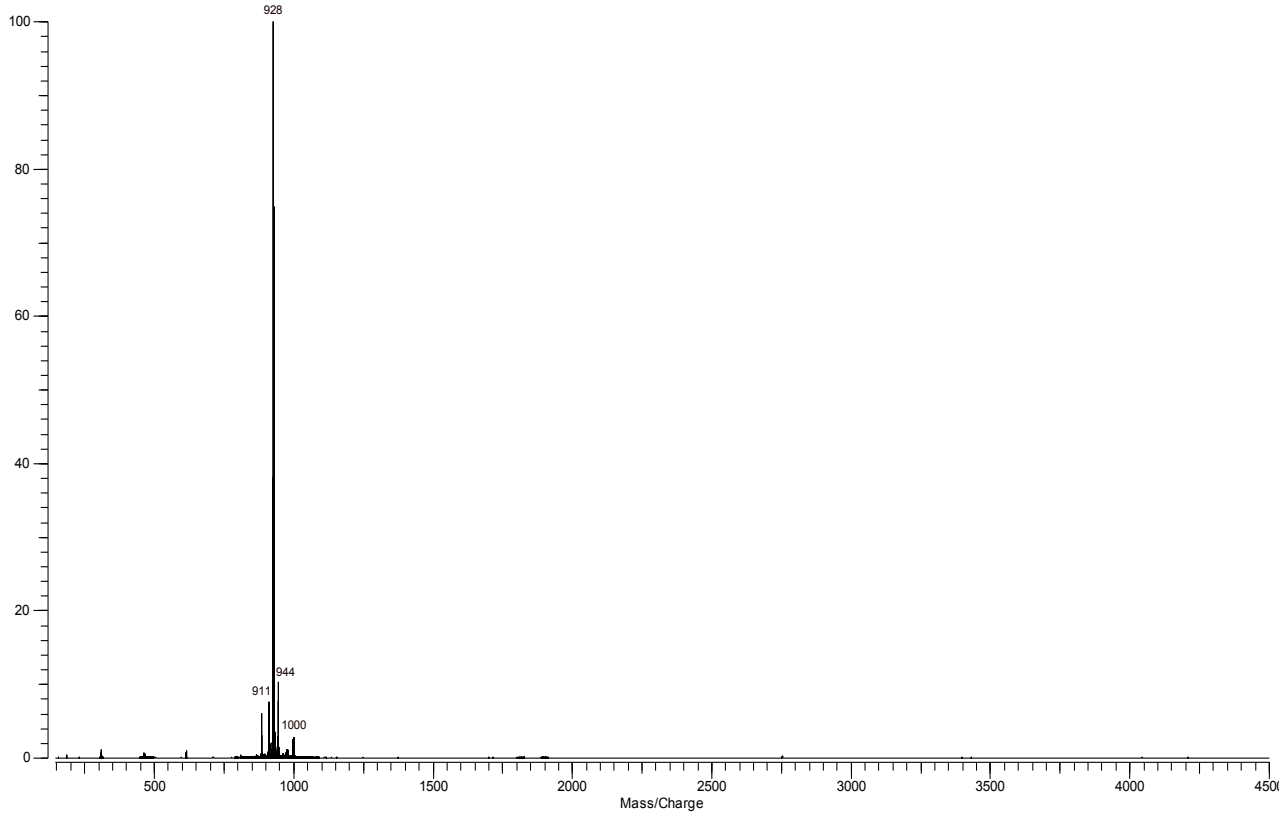


Figure S7e. Mass spectrum recorded for **Ala-3Py-Cit**.

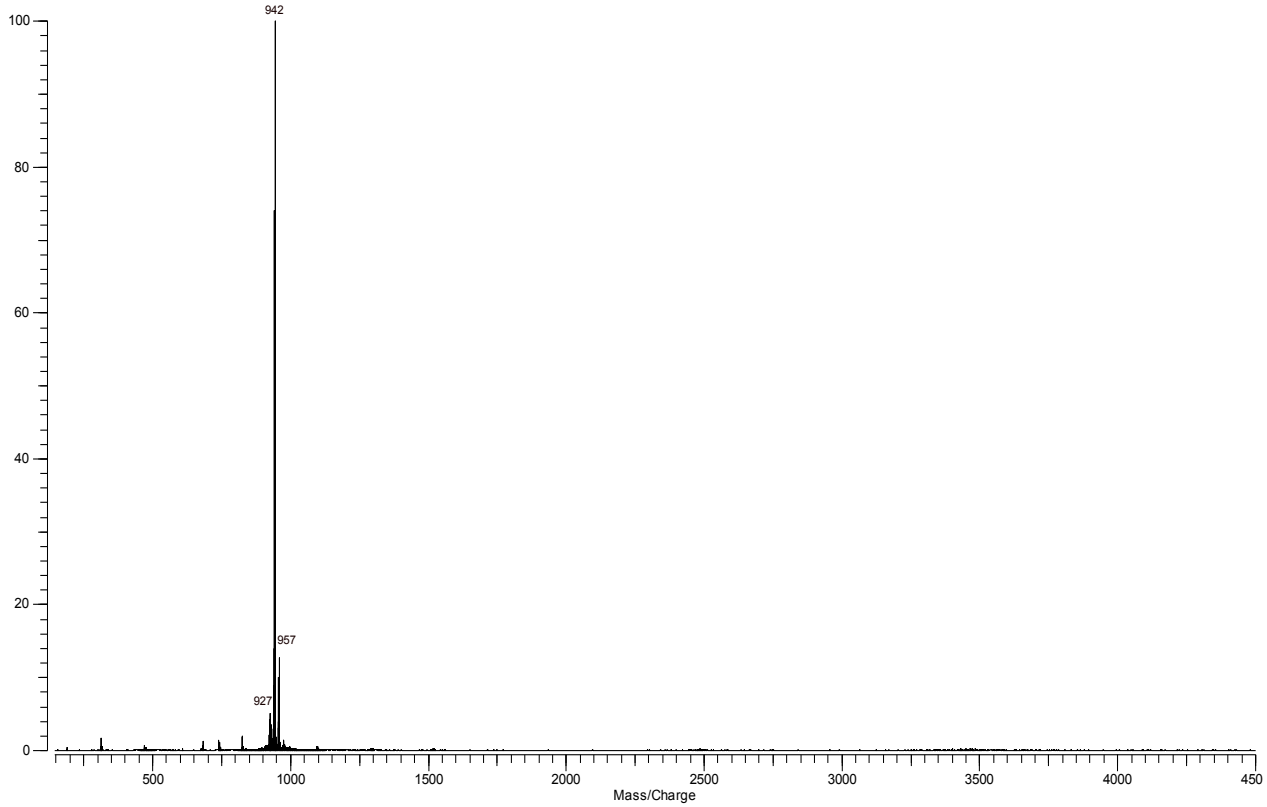


Figure S7f. Mass spectrum recorded for **His-2Nal-Gly 2T**.

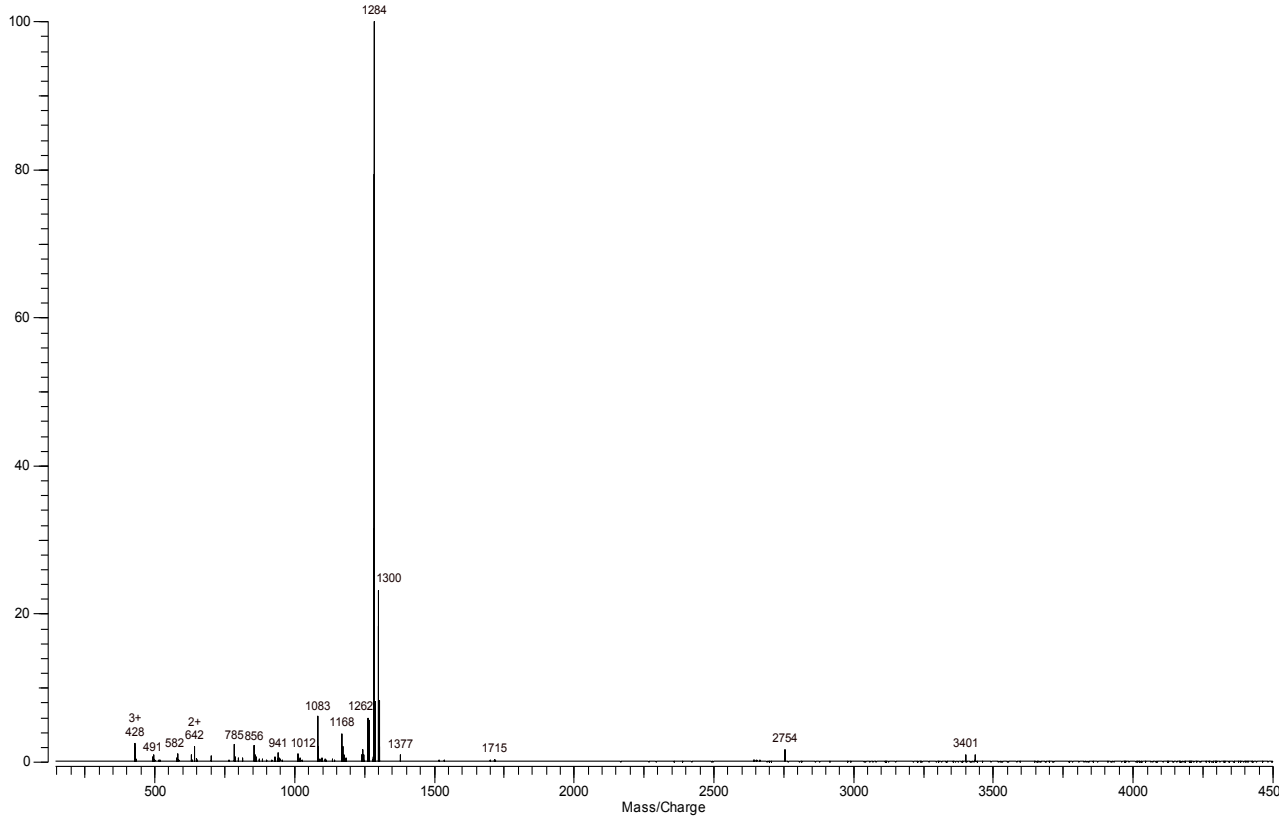


Figure S7g. Mass spectrum recorded for **His-scaffold 4T**.

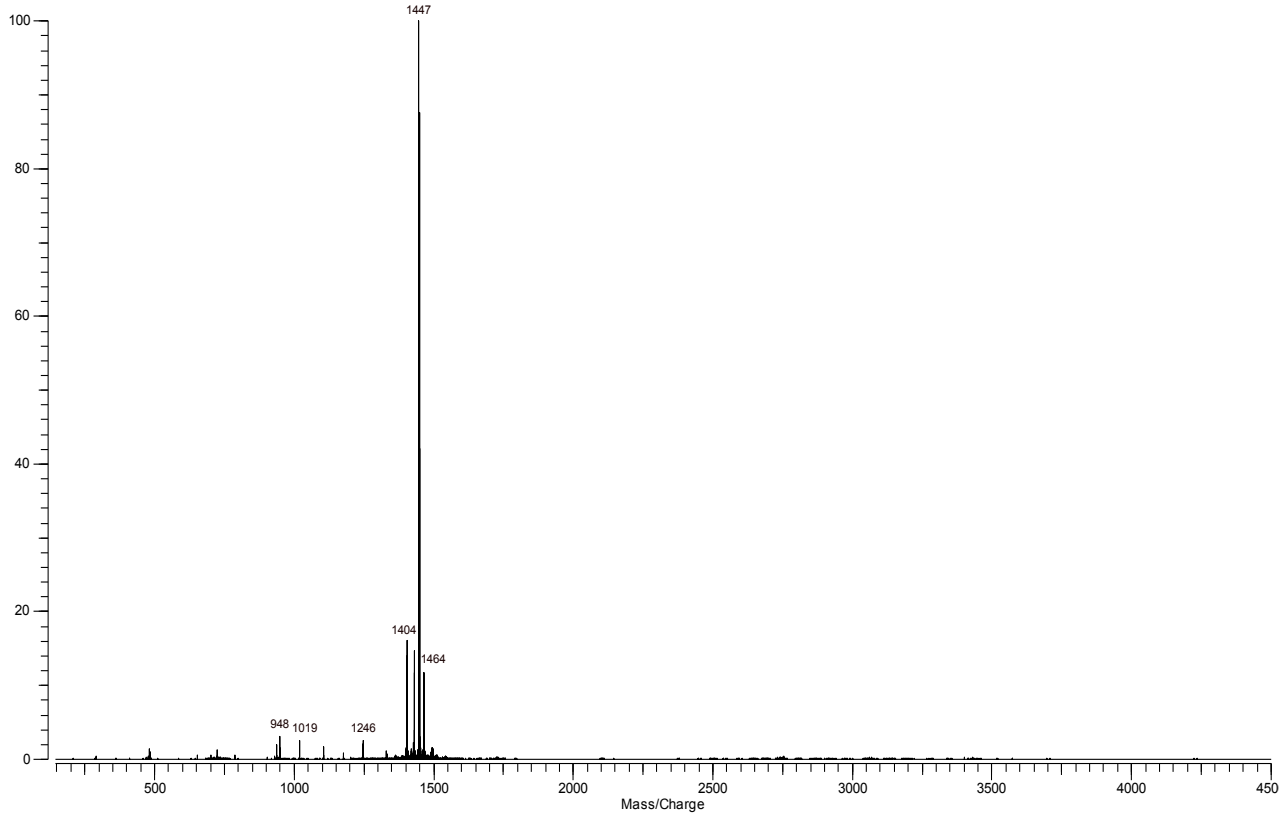


Figure S7h. Mass spectrum recorded for **His-3Py-Cit 4T**.

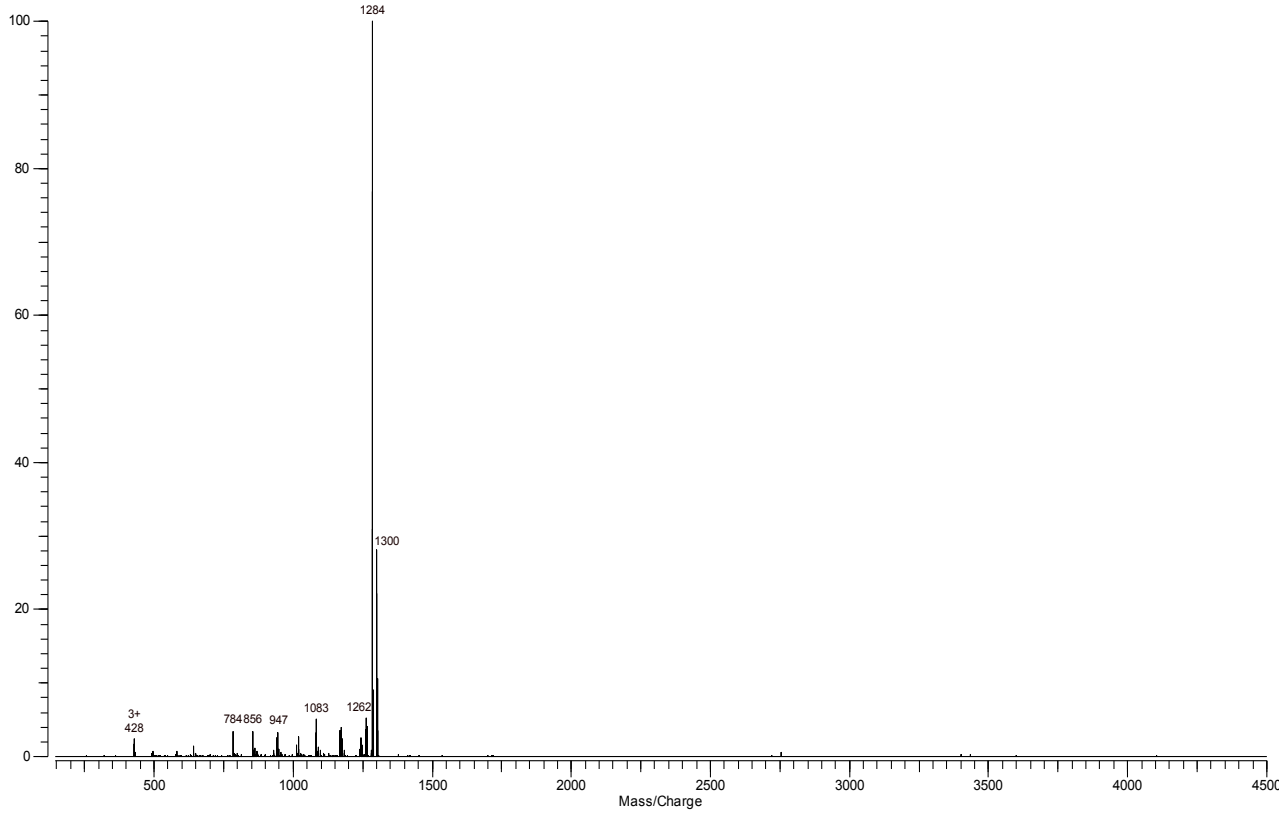


Figure S7j. Mass spectrum recorded for **His-4Py-Cit 4T**.

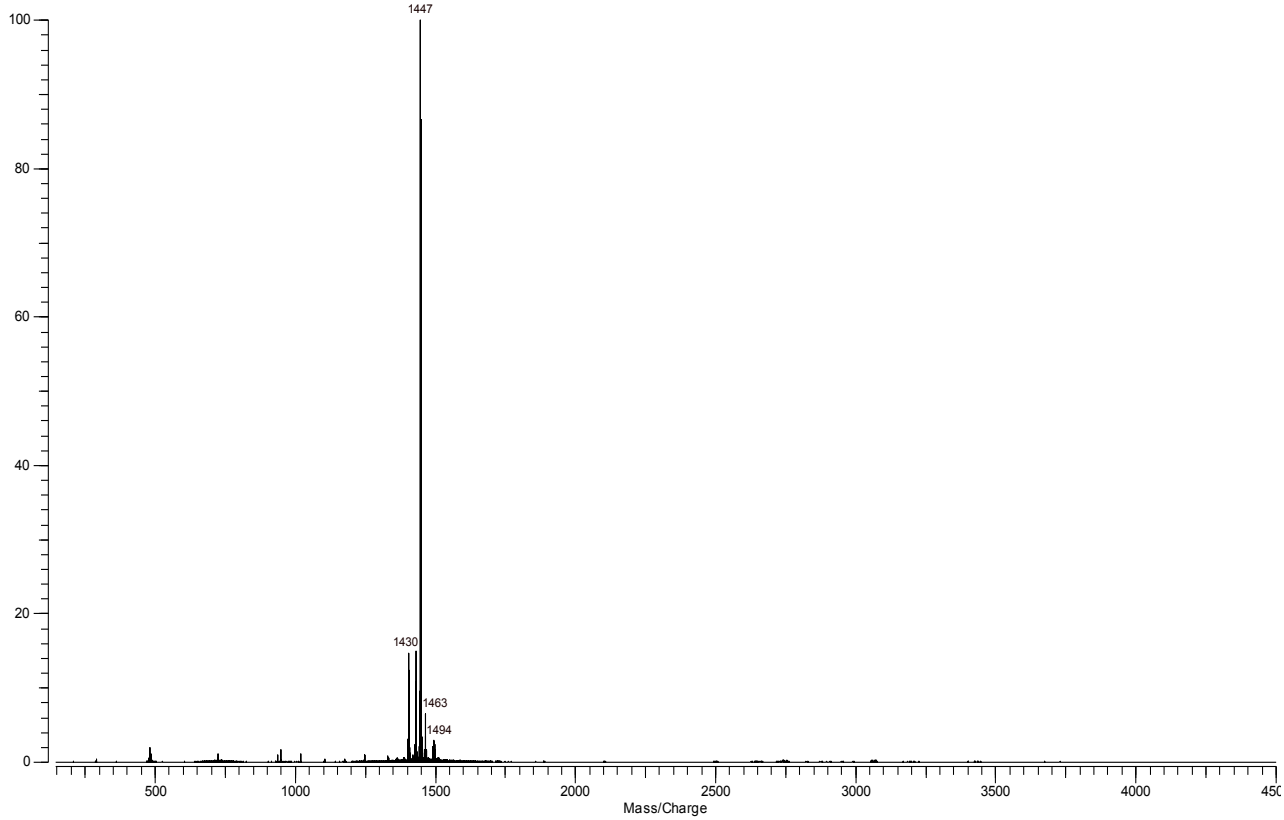


Figure S7k. Mass spectrum recorded for **His-2Py-Cit 4T**.

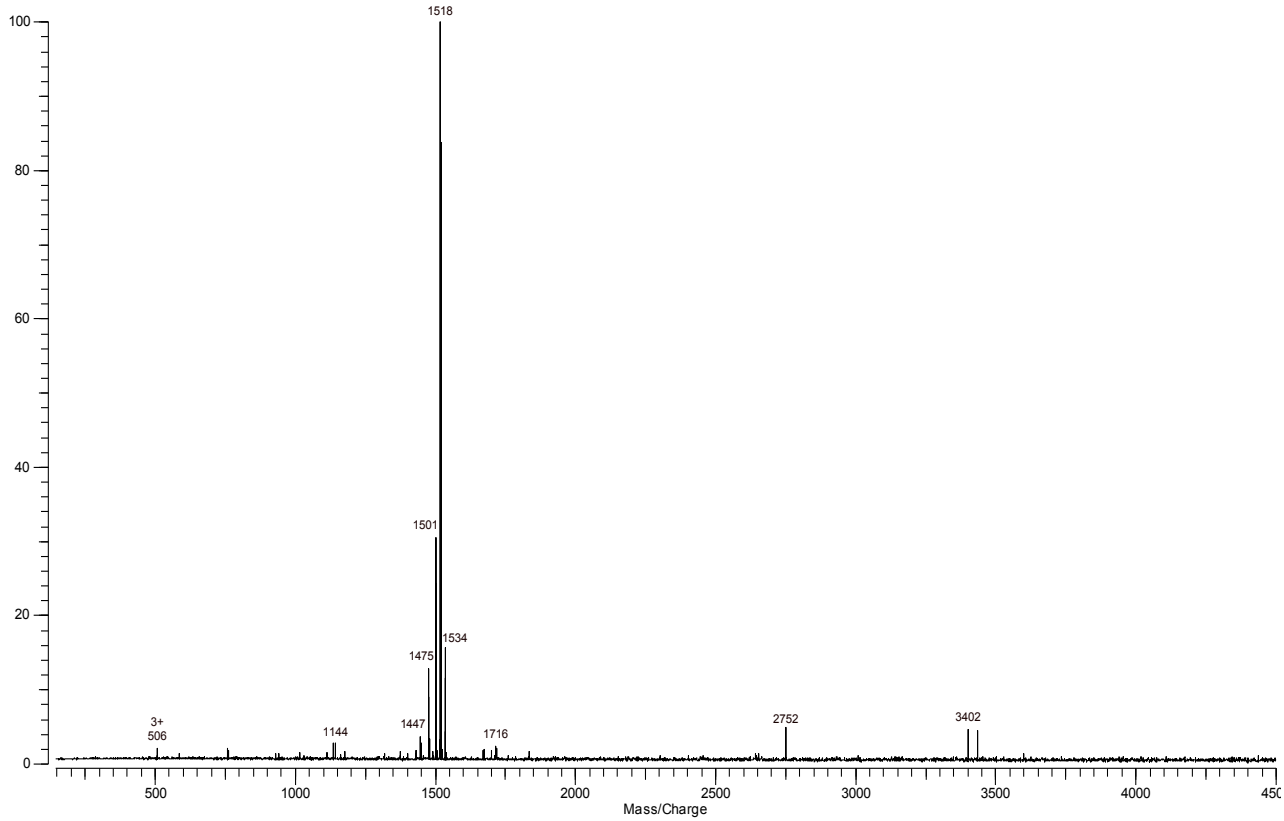


Figure S7l. Mass spectrum recorded for **Cit-3Py-His 4T**.

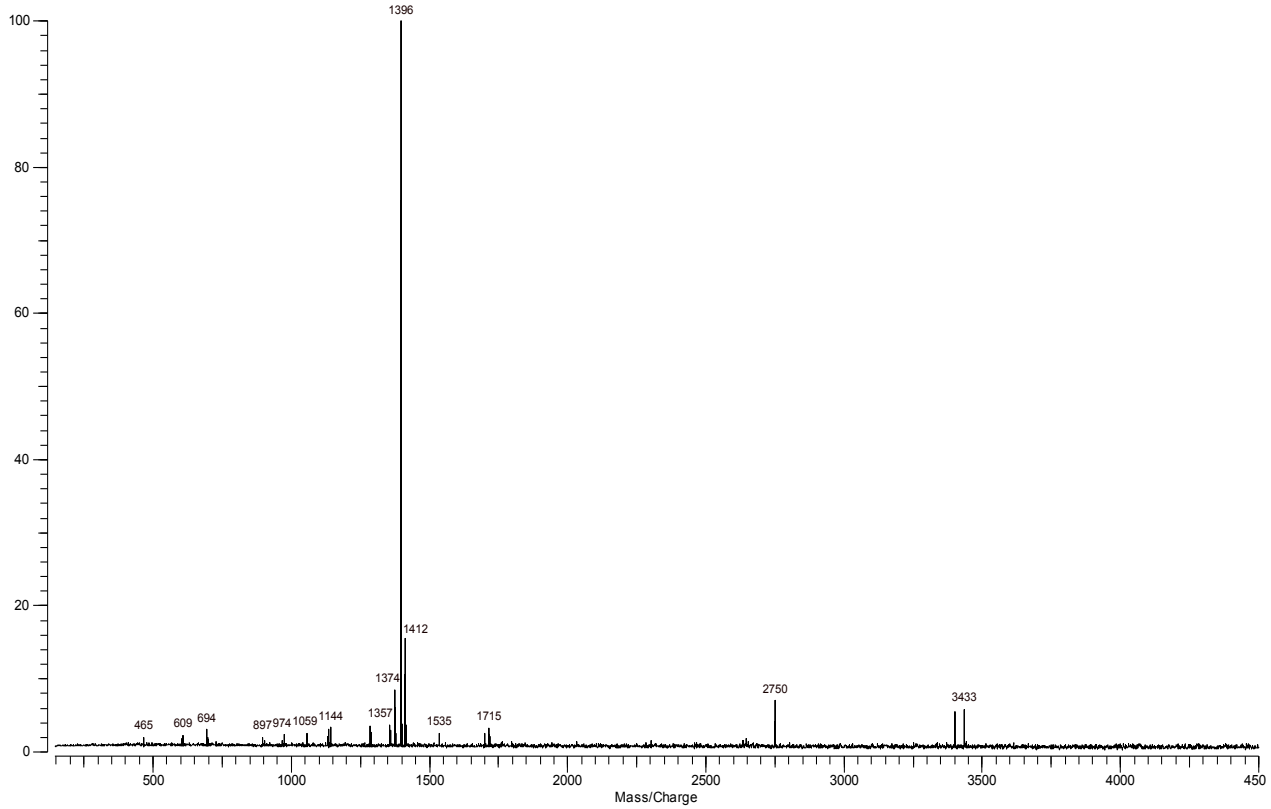


Figure S7m. Mass spectrum recorded for **His-2Nal-Gly 4T**.

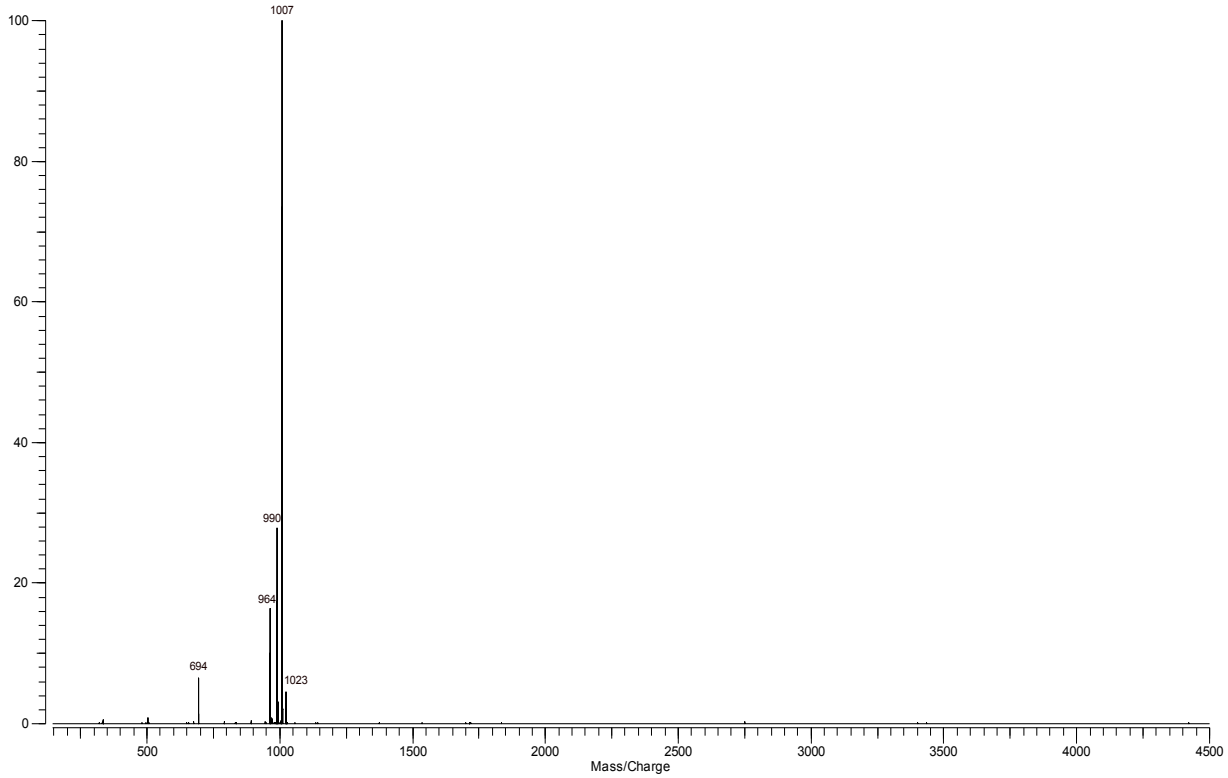


Figure S7n. Mass spectrum recorded for **MeHis-3Py-Cit**.

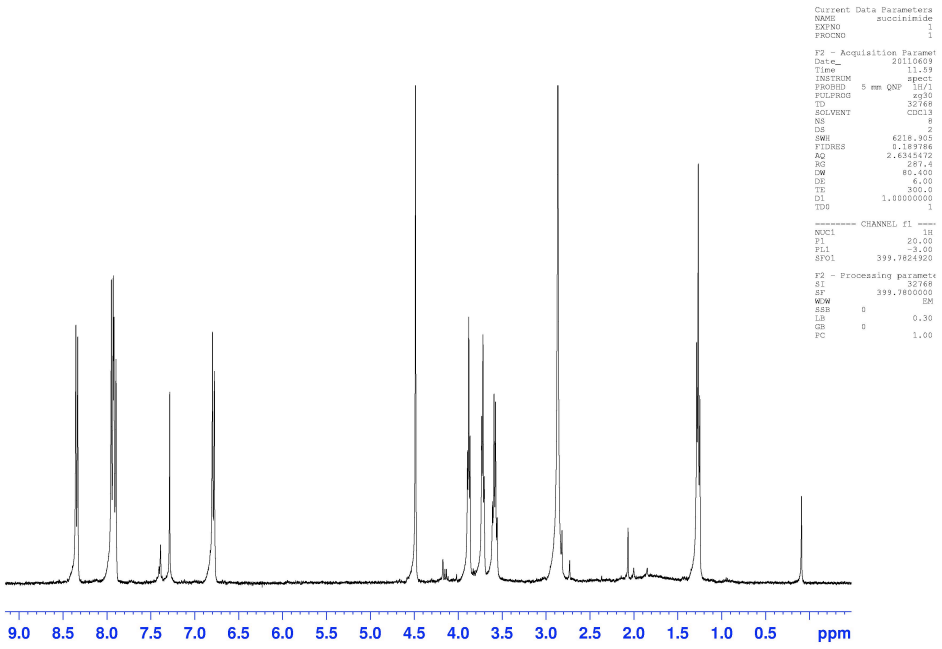


Figure S8a. ^{1}H-NMR spectrum of RT1 (Compound [2])

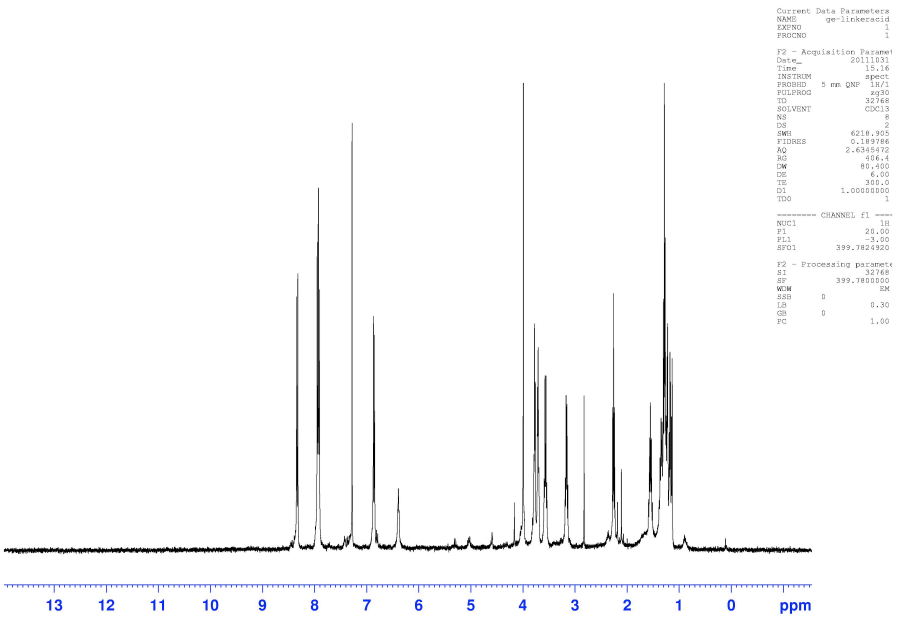


Figure S8b. ^{1}H-NMR spectrum of Compound [4]

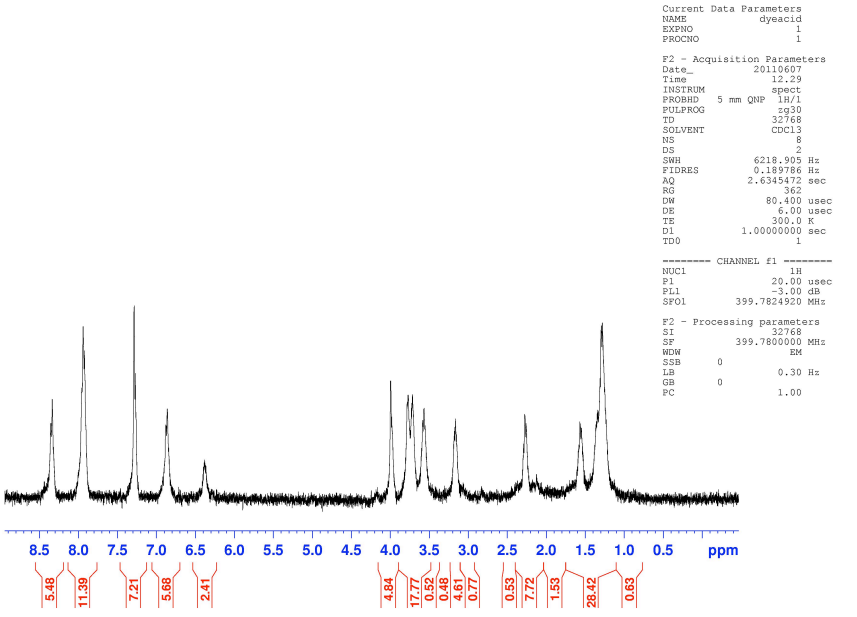


Figure S8c. ^{1}H-NMR spectrum of Compound [5]

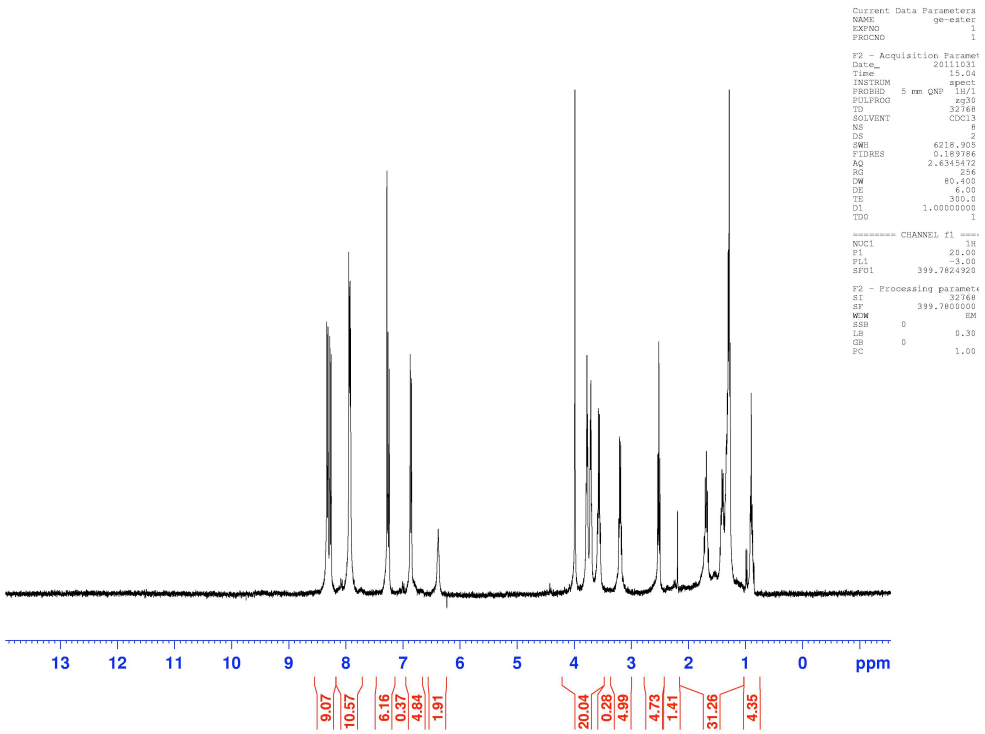


Figure S8d. ^{1}H-NMR spectrum of RT3 (Compound [6])

Table S1. Reactivity trend in library **L3** in presence of reactive tag and 40 mg of library on solid support.

Library	RT2	RT3	RT4
L3	3 min (0.5 mM)	20 min (8 mM)	2 h (3 mM)

Table S2. Peptide masses identified in the screening of **L3** with **Dye 3** run in DCM and TFE. X indicates a hit; - indicates that the peptide was not observed. Red indicates hits found in both solvents.

Mass	DCM	TFE
850	-	x
877	x	-
884	x	x
900	-	x
912	x	x
927	-	x
953	-	x
960	x	x
970	x	x
976	x	x
983	x	x
996	x	-
999	x	x
1005	x	-

Table S3. Experimental and calculated molecular weights of the synthesized peptides.

Catalyst	Aligned Peptide Sequence	MW+Na$^+$ (calc/exp)
His-scaffold 2T	Ac-BA**H**••ABA•••A•••BA-NH_2	829.4/830
His-3Py-Cit 2T	Ac-BA**H**••AB**3Py**•**Cit**•BA-NH_2	993.1/993
His-2Nal-Gly 2T	Ac-BA**H**••AB**2NalG**•••BA-NH_2	941.5/942
His-Ala-Cit 2T	Ac-BA**H**••AB***A***•••**Cit**•BA-NH_2	915.5/916
His-3Py-Ala 2T	Ac-BA**H**••AB**3Py**•***A***•••BA-NH_2	906.5/907
MeHis-3Py-Cit 2T	Ac-BA**MeH**AB**3Py**•**Cit**•BA-NH_2	1006.5/1007
Ala-3Py-Cit	Ac-BA***A***••AB**3Py**•**Cit**•BA-NH_2	926.5/927
His-scaffold 4T	Ac-BAA••B••AABA**H**••A••BA••A••BA-NH_2	1283.7/1283
His-3Py-Cit 4T	Ac-BAA••B••AABA**H**••A••B**3PyCit**BA-NH_2	1446.8/1447
His-2Py-Cit 4T	Ac-BAA••B••AABA**H**••A••B**2PyCit**BA-NH_2	1446.8/1447
His-4Py-Cit 4T	Ac-BAA••B••AABA**H**••A••B**4PyCit**BA-NH_2	1446.8/1447
His-3Py-Cit mid 4T	Ac-BAA••B••A**H**AB**3PyCit**BA•••A•BA-NH_2	1446.8/1447
Cit-3Py-His 4T	Ac-AB**Cit3Py**BA**H**AB••A••AB•••A•BA-NH_2	1517.8/1518
His-2Nal-Gly 4T	Ac-BAA••B••AABA**H**••A••B**2NalG**•BA-NH_2	1395.7/1396

Computational Modeling of A8H.

The model alpha-helical scaffold (Figure 7) was optimized with GAUSSIAN09 [7] at the M06-2X/6-31G(d) level of theory[8, 9] including the effects of TFE solvent with the SMD solvent continuum model. The resulting structure was characterized as a minimum by the absence of imaginary frequencies and was visualized with CYLview. [10] The coordinates are included below.

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	7.579164	-0.435399	-1.268002
2	6	6.279650	-1.130411	-0.972897
3	8	5.183421	-0.637963	-1.283086
4	7	6.350249	-2.298931	-0.307433
5	6	5.150615	-3.061845	-0.019035
6	6	4.166419	-2.262479	0.826031
7	8	2.951215	-2.453336	0.705325
8	7	4.662237	-1.392548	1.719978
9	6	3.758312	-0.584658	2.519778

10	6	2.882943	0.293858	1.625123
11	8	1.702591	0.515838	1.918507
12	7	3.472807	0.847597	0.554929
13	6	2.698360	1.661685	-0.361582
14	6	1.636179	0.823023	-1.066457
15	8	0.499237	1.264593	-1.266262
16	7	2.011594	-0.396784	-1.482242
17	6	1.037561	-1.273066	-2.110452
18	6	-0.131003	-1.538156	-1.158594
19	8	-1.298047	-1.563701	-1.568315
20	7	0.188708	-1.780538	0.119224
21	6	-0.844625	-2.047272	1.101656
22	6	-1.761252	-0.832939	1.258258
23	8	-2.988317	-0.961749	1.353659
24	7	-1.158678	0.362173	1.314811
25	6	-1.942525	1.577205	1.439592
26	6	-2.907051	1.711769	0.260934
27	8	-4.076823	2.075277	0.418544
28	7	-2.397024	1.443054	-0.952006
29	6	-3.237596	1.530651	-2.130892
30	6	-2.406963	1.248146	-3.378123
31	1	8.441228	-1.095337	-1.152713
32	1	4.619449	-3.276654	-0.953295
33	1	7.255484	-2.714674	-0.118573
34	1	5.119133	-0.350401	4.180367
35	1	5.224986	0.947451	2.963881
36	1	3.067550	-1.241703	3.057377
37	1	5.665045	-1.249831	1.787245
38	1	2.163616	2.425528	0.210567
39	1	4.407895	0.557917	0.276353
40	1	0.415791	-3.309544	2.316729
41	1	0.431211	-1.593375	2.790435
42	1	-1.484899	-2.861272	0.745946
43	1	1.165865	-1.772528	0.411512
44	1	-0.403919	2.848196	0.601293
45	1	-1.600668	3.701164	1.603919
46	1	-2.569343	1.522284	2.335778
47	1	-0.143400	0.429784	1.242505
48	1	-1.952690	0.254054	-3.315922
49	1	-3.039712	1.292600	-4.268422
50	1	-3.691330	2.525326	-2.186576
51	1	-1.429228	1.136813	-1.047944
52	1	0.604291	-0.769715	-2.980911
53	1	-0.349779	2.699471	2.374576
54	1	-0.973710	-2.613976	3.181183
55	6	1.692881	-2.587088	-2.520110

56	1	2.504319	-2.398102	-3.228823
57	1	2.097261	-3.101601	-1.642714
58	6	3.605510	2.332293	-1.402599
59	1	4.040066	1.571289	-2.058821
60	1	3.849521	0.888246	4.087898
61	1	6.137900	-4.981936	0.054449
62	1	6.030050	-4.159557	1.631221
63	1	4.587257	-4.916342	0.916492
64	1	7.546954	-0.041467	-2.286172
65	1	7.682524	0.408480	-0.577513
66	6	5.502808	-4.362824	0.693822
67	6	4.541478	0.280565	3.499541
68	6	-1.012943	2.784345	1.508742
69	6	-0.200790	-2.413563	2.434783
70	1	2.957878	-0.732307	-1.303750
71	6	-4.405691	0.549083	-2.025869
72	8	-5.560498	0.880123	-2.321246
73	7	-4.101109	-0.693344	-1.622187
74	6	-5.141368	-1.696656	-1.495797
75	6	-6.214538	-1.267347	-0.492945
76	8	-7.392191	-1.599137	-0.642561
77	7	-5.783511	-0.558757	0.564243
78	6	-6.687199	-0.131424	1.610001
79	6	-7.614427	1.008900	1.184037
80	8	-8.571046	1.303430	1.907371
81	1	-5.663065	-1.807285	-2.452254
82	1	-3.142359	-0.929082	-1.364101
83	1	-5.273532	-0.518753	3.201637
84	1	-5.239988	1.149564	2.580794
85	1	-7.349065	-0.964648	1.870943
86	1	-4.791108	-0.352775	0.663442
87	1	-6.576530	0.616532	3.628610
88	1	-3.801797	-3.364736	-1.810001
89	1	-4.024441	-2.916544	-0.101510
90	1	-5.313854	-3.781376	-0.972934
91	6	-4.529381	-3.026010	-1.066669
92	6	-5.890803	0.306963	2.836652
93	7	-7.314285	1.665857	0.057928
94	1	-6.534155	1.413289	-0.541885
95	1	-7.909577	2.435869	-0.222248
96	1	2.968044	2.976695	-2.018705
97	1	0.953651	-3.234325	-2.998985
98	1	-1.612148	1.993279	-3.475763
99	6	4.705050	3.114878	-0.760743
100	6	6.055080	2.973075	-0.951724
101	7	6.638545	3.900145	-0.123893

102	1	6.631928	2.332230	-1.601371
103	6	5.643548	4.546119	0.527463
104	1	7.630962	4.076269	-0.022807
105	1	5.839195	5.329437	1.246711
106	7	4.457682	4.099584	0.171478

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