

Supporting Information

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1. Experimental details

1.1 Reagents

All reagents and materials required for the solid-phase synthesis of **Rb-SWHEFQ-NH₂**, including the Rhodamine B molecule, side-chain protected amino acids, and dichloromethane resin, were purchased from Shanghai Top-peptide Biotechnology Co., Ltd. AgNO₃, FeCl₃·6H₂O, KCl, NiCl₂·6H₂O, BaCl₂·2H₂O, CuBr₂, AlCl₃, (CH₃COO)₂Co, Pb(CH₃COO)₂·3H₂O, ZnBr₂, CaCl₂·2H₂O, NaBr, C₄N₆HgO₄, CrCl₃·6H₂O, Mg(NO₃)₂, CdCl₂·21/2H₂O, and DMSO were all purchased from the reagent supplier of Lanzhou University (Table S1). The CCK-8 cell counting kit was purchased from GLPBIO.

Table S1. Laboratory-related chemical reagents

Reagents	Grade	Manufacturer (of a product)
Dichlororesin	/	Shanghai Taopu Biological Co.
Rhodamine B molecule	/	Shanghai Taopu Biological Co.
Fmoc-Gln(Trt)-OH	/	Shanghai Taopu Biological Co.
Fmoc-Phe-OH	/	Shanghai Taopu Biological Co.
Fmoc-Glu(OtBU)-OH	/	Shanghai Taopu Biological Co.
Fmoc-His(trt)-OH	/	Shanghai Taopu Biological Co.
Fmoc-Trp(Boc)-OH	/	Shanghai Taopu Biological Co.
Fmoc-Ser(tBu)-OH	/	Shanghai Taopu Biological Co.
CuBr ₂	AR	Tianjin Guangfu Technology Development Co.
C ₄ H ₆ HgO ₄	AR	Shanghai Zhongqin Chemical Reagent Co.
Mg(NO ₃) ₂	AR	Sinopharm Chemical Reagent Co.
Pb(CH ₃ COO) ₂ ·3H ₂ O	AR	Tianjin Kaixin Chemical Industry Co.
NiCl ₂ ·6H ₂ O	AR	Chengdu Kelong Chemical Reagent Factory
AlCl ₃	AR	Sarn Chemical Technology (Shanghai) Co.
AgNO ₃	AR	Sinopharm Chemical Reagent Co.
NaBr	AR	Tianjin Guangfu Technology Development Co.
KCl	AR	Changshu Chemical·Plante
(CH ₃ COO) ₂ Co	AR	Shanghai Fengshun Fine Chemical Co.
ZnBr ₂	CP	Sinopharm Chemical Reagent Co.
CaCl ₂ ·2H ₂ O	AR	Tianjin Kaixin Chemical Industry Co.
FeCl ₃ ·6H ₂ O	AR	Tianjin Komeo Chemical Reagent Co.
BaCl ₂ ·2H ₂ O	AR	Chengdu Kelong Chemical Reagent Factory

$\text{CrCl}_3 \cdot 6\text{H}_2\text{O}$	AR	Tianjin Guangfu Fine Chemical Research Institute
$\text{CdCl}_2 \cdot 2\frac{1}{2}\text{H}_2\text{O}$	AR	Tianjin Guangfu Technology Development Co.
DMSO	AR	Aladdin

62 1.2 Apparatus

63 The apparatus used in the experiment is listed in Table S2.

64 **Table S2.** Experiment Related Instruments

Experimental process	Experimental Instruments
Crude identification	MICROMASS ZQ Mass Spectrometer
Purity analysis	P1300 High Performance Liquid Chromatography
Preparative chromatography	LC3000 high performance liquid chromatograph (10 mM C18 reverse column 30*250mm)
Peptide Probe Dispensing	FA124C Electronic Analytical Balance
Fluorescence measurement	LF-1504007 Fluorescence Spectrophotometer
Cytotoxicity test	M200 Multifunctional Enzyme Labeler
Cellular imaging	LSM 880 Confocal Microscope
DLS	Zetasizer Nano ZS
Field Emission Scanning Electron Microscopy	Apreo S LoVac

65 1.3. Rb-SWHEFQ-NH₂ Solid-phase Synthesis

66 Synthesis of **Rb-SWHEFQ-NH₂** Using Solid-Phase Peptide Synthesis (SPPS)[1, 2]:

67 The peptide reaction vessel was rinsed with dichloromethane (DCM) solution, and the
68 resin was swollen in DCM for approximately 5 min, followed by filtration. Fmoc-
69 Gln(Trt)-OH (3.0 eq) and DIEA (1.0 eq) were added to the DCM solution and
70 allowed to react for 1.5 h. Then, methanol (MeOH) was added, and the reaction
71 continued for 40 min. After the reaction, the resin was washed three times with
72 dimethylformamide (DMF), followed by deprotection with piperidine for 20 min, and
73 filtered. The solid was washed three times each with DMF and MeOH, and upon
74 filtering, the Kaiser test was performed, showing a deep blue color. Coupling the
75 remaining amino acids in the same operational manner. Finally, the deprotected
76 Rhodamine B derivative was added to the DMF solution containing the resin, and the
77 reaction was allowed to proceed under nitrogen at room temperature for 40 min. The

78 resin-bound crude peptide was cleaved using an 87% TFA solution (TFA: EDT: TIS:
79 Thioanisole: H₂O, 87: 4: 3.5: 3.5: 2, v/v/v/v/v) at room temperature for 2 h. After
80 filtration, the filtrate was centrifuged at 4000 rpm for 3 min after adding diethyl ether,
81 and the supernatant was discarded. The centrifugation process with ether was repeated
82 three times. The crude peptide was cleaved from the resin and subsequently
83 lyophilized to obtain the crude peptide.

84 **1.4 Rb-SWHEFQ-NH₂ Characterization**

85 The crude **Rb-SWHEFQ-NH₂** product was purified by preparative chromatography,
86 and ESI-MS characterization confirmed the successful synthesis of the target peptide
87 with a molecular weight of 1244.33 (m/z). Analytical chromatography further
88 determined the purity of **Rb-SWHEFQ-NH₂** to be 96.28%.

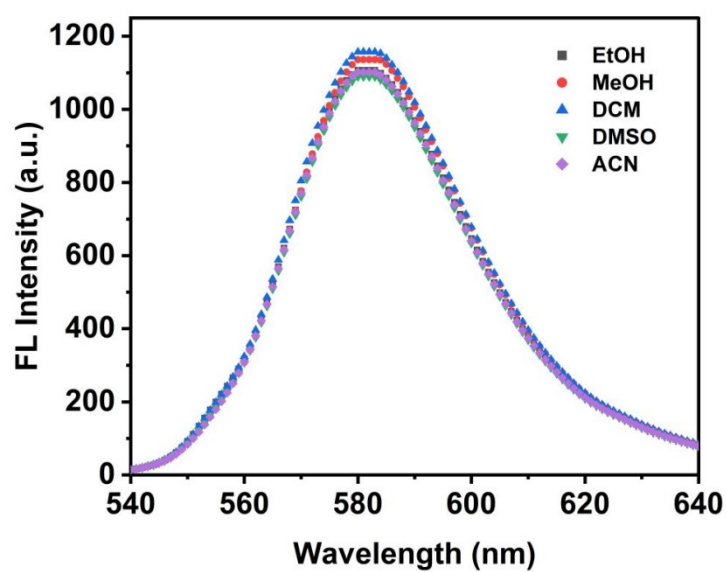
89 **1.5 Cytotoxicity Assay and Cell Imaging Experiments**

90 **CT26 cell** were cultured in DMEM supplemented with 10% heat-inactivated fetal
91 bovine serum (FBS, Pricella) and 1% antibiotics (100 U/mL penicillin and 100 µg/mL
92 streptomycin, Sangon) in a cell incubator (Thermo, 371GPCN) maintained at 37°C
93 with 5% CO₂. The cytotoxicity of **Rb-SWHEFQ-NH₂** was evaluated using the Cell
94 Counting Kit-8 (CCK-8) assay (Adamas-life). **CT26 cell** (10⁴ cells/mL) were seeded
95 into 96-well plates at a total volume of 100 µL per well. After 12 hours of incubation,
96 allowing for cell attachment, the medium was replaced with fresh culture medium
97 containing **Rb-SWHEFQ-NH₂** at final concentrations of 5, 10, 15, 20, 25, 30, 40, and
98 50 µM. After an additional 12-hour incubation, 100 µL of medium containing 10%
99 CCK-8 reagent was added, and the cells were incubated for one more hour.
100 Absorbance was measured at 450 nm using a Thermo Scientific microplate reader.

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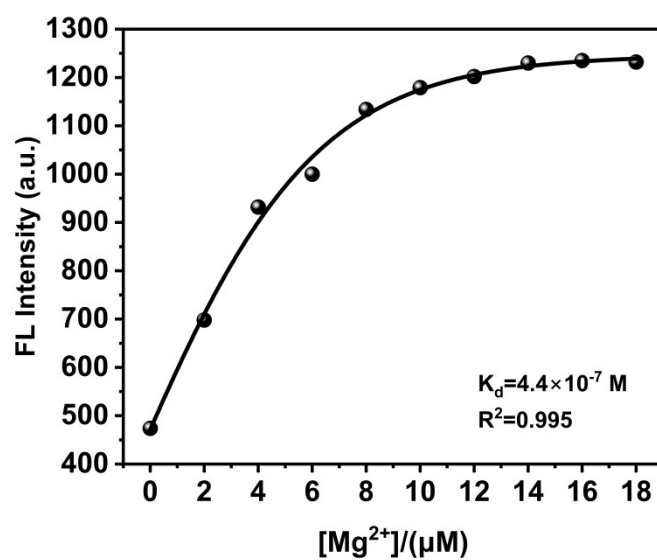
103 2.Experiment results



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105 **Figure S1.** Fluorescence response of the **Rb-SWHEFQ-NH₂** under different systems.

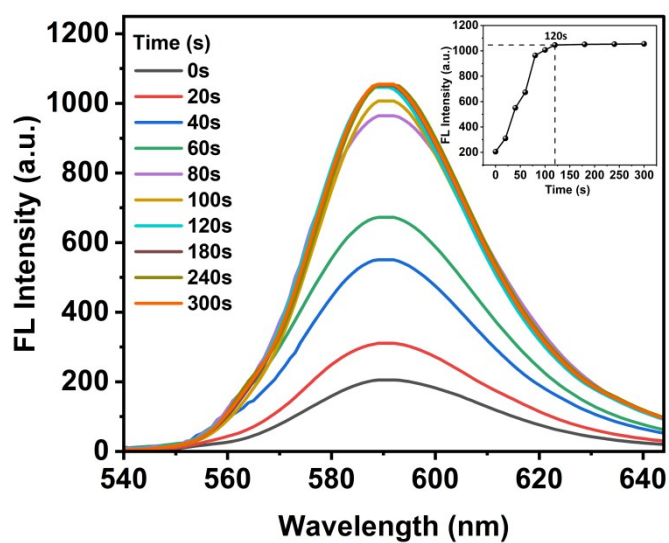
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108 **Figure S2.** Fitting curve of fluorescence titration between **Rb-SWHEFQ-NH₂** and
109 **Mg²⁺** in PBS buffer (pH=7.4).

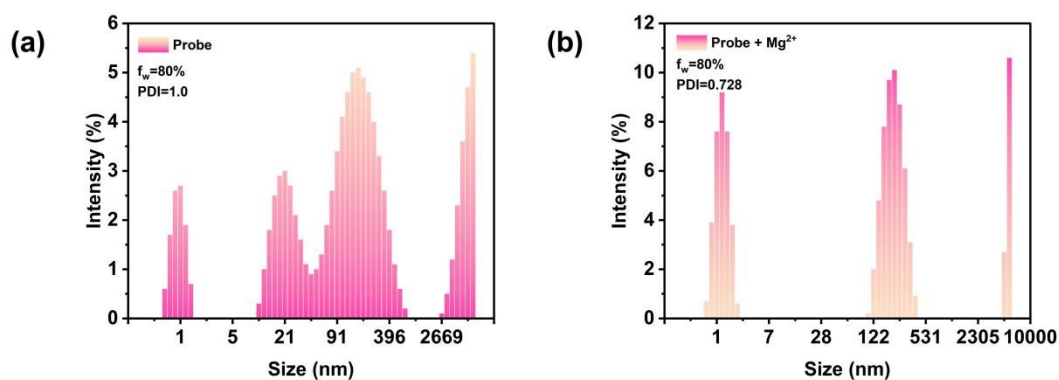
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112 **Figure S3.** Fluorescence of Rb-SWHEFQ-NH₂ and Mg²⁺ over a five-minute period.

113 $\lambda_{ex} = 550 \text{ nm}$, $\lambda_{em} = 590 \text{ nm}$.

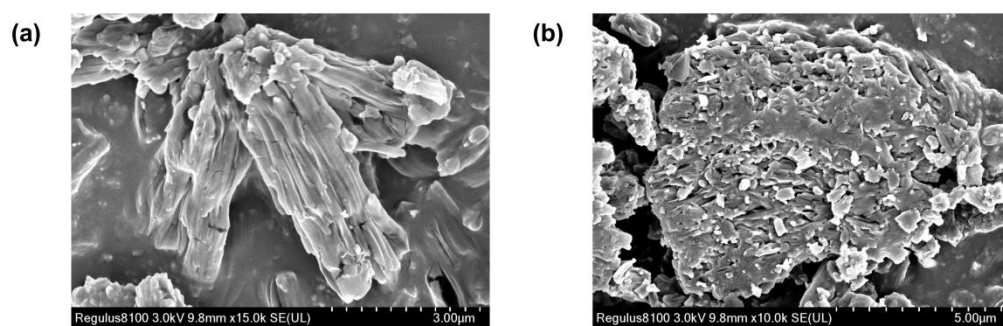


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115 **Figure S4.** DLS detection of the probe Rb-SWHEFQ-NH₂ before and after binding

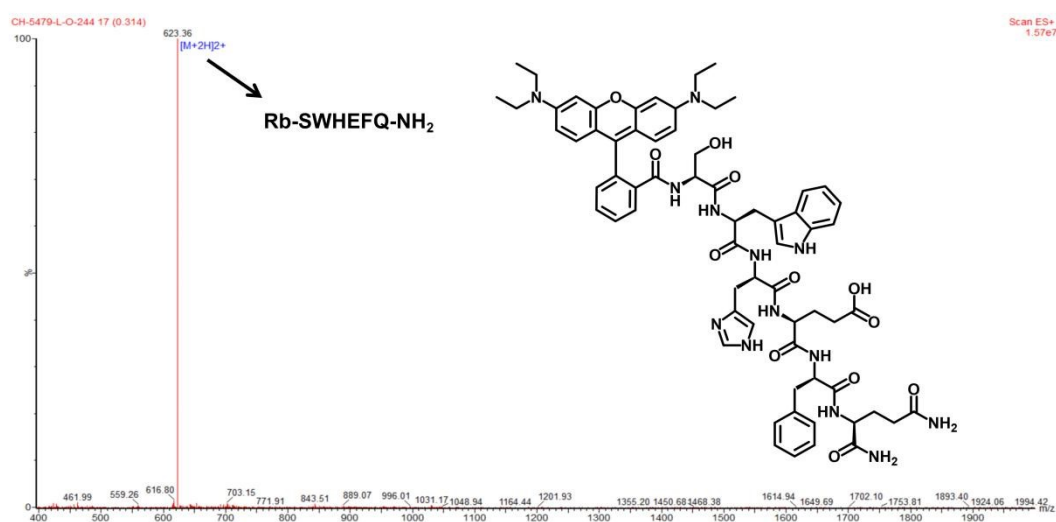
116 to Mg²⁺. (a) Particle size distribution of the probe. (b) Particle size distribution of the

117 probe after binding Mg²⁺.



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119 **Figure S5. SEM detection of the probe Rb-SWHEFQ-NH₂ before and after binding**
 120 **to Mg²⁺ (a) Probe. (b) Probe and Mg²⁺.**



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Figure S6. ESI-MS spectrum of Rb-SWHEFQ-NH₂.

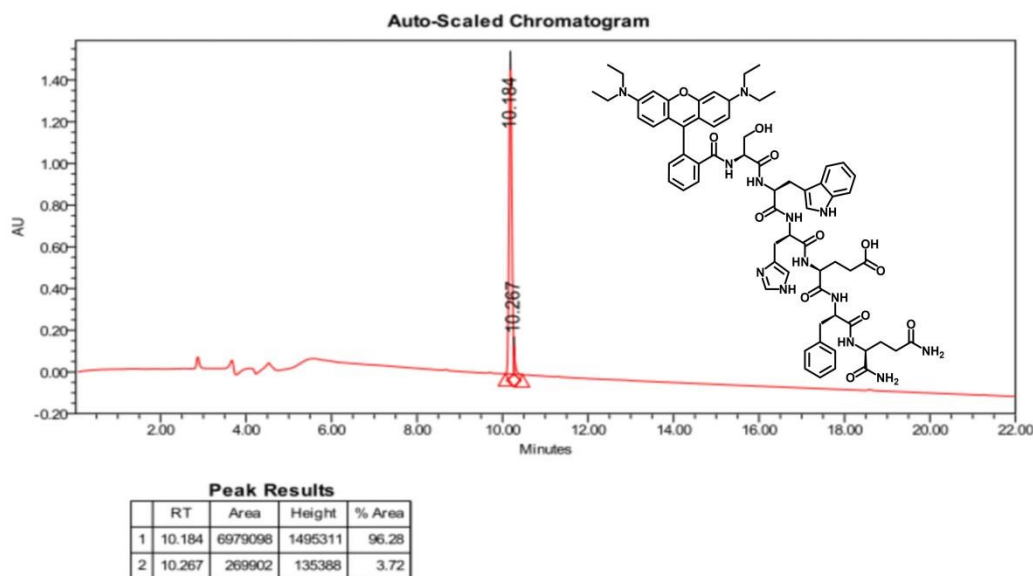


Figure S7. HPLC spectrum of Rb-SWHEFQ-NH₂.

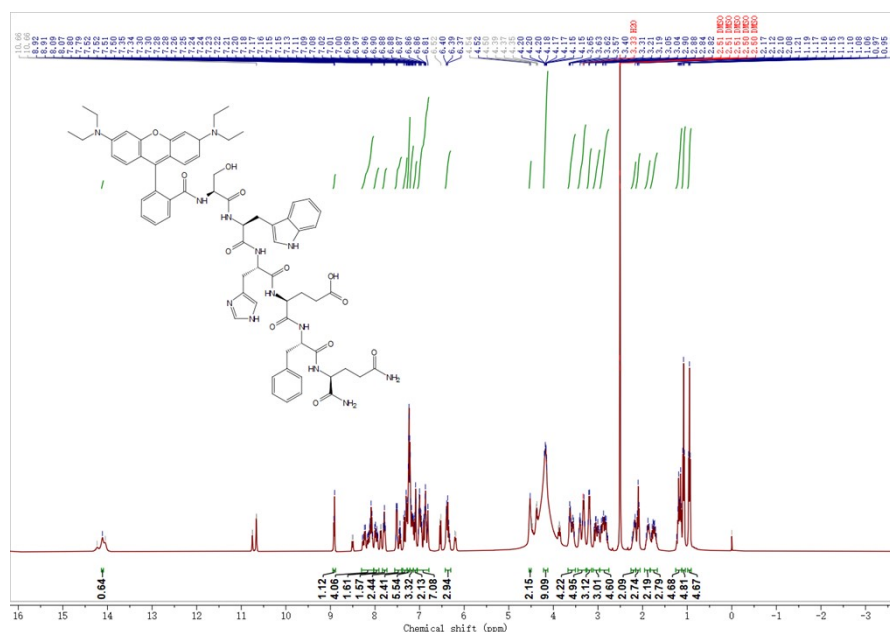


Figure S8. ¹H NMR spectrum of Rb-SWHEFQ-NH₂.

¹H NMR (400 MHz, DMSO) δ 14.11 (s, 1H), 8.91 (d, J = 6.5 Hz, 1H), 8.30 – 8.03 (m, 4H), 8.03 – 7.91 (m, 2H), 7.79 (ddd, J = 9.3, 5.4, 2.8 Hz, 2H), 7.56 – 7.40 (m, 2H), 7.38 – 7.28 (m, 2H), 7.28 – 7.22 (m, 6H), 7.22 – 7.14 (m, 3H), 7.14 – 7.06 (m, 2H), 7.05 – 6.79 (m, 7H), 6.43 – 6.30 (m, 3H), 4.53 (d, J = 7.7 Hz, 2H), 4.22 – 4.13 (m, 9H), 3.59 (dq, J = 30.3, 7.2 Hz, 4H), 3.33 (s, 5H), 3.20 (q, J = 7.1 Hz, 3H), 3.04 (ddd, J = 24.8, 16.9, 7.4 Hz, 3H), 2.96 – 2.76 (m, 5H), 2.19 (dq, J = 13.0, 6.5 Hz, 2H), 2.10

134 (t, J = 8.1 Hz, 3H), 1.89 (dd, J = 16.1, 9.0 Hz, 2H), 1.74 (dq, J = 15.4, 7.7 Hz, 3H),
135 1.17 (dt, J = 18.0, 7.0 Hz, 5H), 1.08 (t, J = 7.0 Hz, 5H), 0.95 (t, J = 7.0 Hz, 5H).

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157 **3.References**

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186 4. Calculation results

187 (1) The optimized coordinates of the ligand/complexes

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189 Rb-SWHEFQ-NH₂

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191	C	5.22940433	-1.76919064	0.73260972
192	C	4.60500869	0.52519957	0.15176082
193	C	5.18450172	-0.76497037	-0.20067143
194	C	4.12868878	0.68274407	1.47394413
195	C	4.66470926	-1.57664063	2.06151529
196	O	4.24336682	-0.30998192	2.41122936
197	C	5.78384891	-3.09707288	0.48885567
198	C	3.53173275	1.83645561	1.94196757
199	C	4.44490767	1.65092990	-0.69549428
200	C	4.52495958	-2.55493399	2.97274760
201	C	5.69336352	-4.09492875	1.38570158
202	C	3.36338013	2.94503039	1.09087591
203	C	3.84650146	2.82305495	-0.22964200
204	C	4.99614605	-3.95519142	2.70789330
205	C	5.61226800	-1.10883936	-1.58976722
206	C	6.88462358	-0.78867163	-2.07343567
207	C	7.31040838	-1.22290174	-3.32474546
208	C	6.47604286	-2.01733009	-4.11856059
209	C	5.22387835	-2.38369493	-3.63961349
210	C	4.78797122	-1.93226863	-2.38391612
211	N	4.89926497	1.58201613	-2.05090596
212	N	2.73860635	4.08640441	1.55446623
213	C	2.73501750	5.26991716	0.69588553
214	C	1.66524900	3.93375713	2.54799694
215	C	3.87679887	1.17479427	-3.02395985
216	C	5.74289615	2.68454905	-2.51056970
217	C	2.91005067	2.26534266	-3.50684991
218	C	6.96410754	2.90704237	-1.62330248
219	C	2.44832080	6.57200169	1.43917851
220	C	2.08928187	4.25728182	3.98119580
221	C	3.45560623	-2.33130944	-1.85451346
222	O	2.68975858	-1.54247093	-1.28828369
223	C	0.70115678	-3.35610546	-1.41792984
224	O	-0.03530773	-3.15301969	-0.44629969
225	N	3.08212237	-3.63753154	-2.04957021
226	C	1.97650910	-4.19466175	-1.26568855
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248	C	-0.85526423	4.15712053	0.00521078
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251	N	0.16026649	4.56185302	-1.97529027
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270	C	-6.77684462	-4.60890404	0.65976015
271	C	-5.52063403	-4.15803707	1.06473108
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277	C	-5.31478752	3.14509010	-1.20162839
278	C	-6.81095163	3.38950027	-1.31214582
279	O	-7.46565380	3.15003577	-2.32381773
280	N	-7.35404793	3.86609829	-0.15354868
281	N	-3.21958572	2.45396848	2.75779263
282	C	-5.45783641	-1.97650937	-1.77054048
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284	H	3.21931065	1.86013867	2.97665523
285	H	4.08219278	-2.32296199	3.93698531
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288	H	5.66750427	-4.29233404	3.51556499
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323	H	-6.98510222	0.35901506	-2.81893997
324	H	-6.07260622	1.86452341	-4.52857103
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331	H	-1.31163490	3.73599742	0.88571773
332	H	-0.92951490	6.22959809	0.50767416
333	H	0.24169360	6.68597489	-1.71747245
334	H	1.13195992	-1.03254545	0.20365170
335	H	0.62654579	-2.04999331	2.13230917
336	H	2.03942743	-0.12494558	2.89737794
337	H	0.57111294	0.72684394	3.38427301
338	H	0.10506869	-0.86868175	5.12189309
339	H	1.22176625	-2.07530026	4.45882342
340	H	2.93682014	1.07028275	6.15656871
341	H	-1.44203710	-2.10650489	0.67127625
342	H	-3.63906235	-2.22100687	0.44714247
343	H	-3.33775911	-3.58082830	2.61982808
344	H	-4.05409442	-2.19829991	3.45773698
345	H	-6.46109509	-2.01045510	3.51006509
346	H	-8.69746979	-2.83692433	2.83209230
347	H	-8.90712929	-4.49156363	0.98605123
348	H	-6.85536071	-5.32690520	-0.15264060
349	H	-4.63363478	-4.50978691	0.54529891
350	H	-2.58486533	0.20736331	0.17499148
351	H	-3.03958359	2.38906684	-0.00238760
352	H	-4.87040506	1.03035125	-1.19325620
353	H	-5.93755781	1.50769394	0.11773219
354	H	-4.85199296	3.97298031	-0.65590097
355	H	-4.89220315	3.11073655	-2.20814350
356	H	-8.36134058	3.85167765	-0.07197893
357	H	-6.79464032	3.82083557	0.69574218
358	H	-2.60845322	1.64224260	2.73332644
359	H	-3.46318139	2.81599581	3.66998022
360	H	-5.63717225	-1.53941661	-0.77943100

361	H	-6.30918534	-2.64202665	-1.96200437
362				
363	Rb-SWHEFQ-NH₂ & Mg²⁺			
364				
365	C	-3.16527782	-0.43699796	-1.70891796
366	C	-5.52687419	0.04535661	-0.91206807
367	C	-4.43198238	-0.92169728	-1.15829072
368	C	-5.16886866	1.48143229	-1.06746017
369	C	-2.87190552	1.02467515	-1.69053129
370	O	-3.81274846	1.92648415	-1.10521825
371	C	-2.16681918	-1.25346171	-2.43141666
372	C	-6.12223792	2.50732065	-1.21149425
373	C	-6.97461165	-0.22775309	-0.59996099
374	C	-1.71067651	1.56879989	-2.21135246
375	C	-1.01941598	-0.73685317	-2.98043416
376	C	-7.56501243	2.23166360	-1.18248238
377	C	-7.89594840	0.86042580	-0.84257432
378	C	-0.62632733	0.74379655	-2.89185173
379	C	-4.68480171	-2.44010972	-1.20321603
380	C	-5.79399461	-2.87939696	-2.02187138
381	C	-6.09613069	-4.25811637	-2.22804749
382	C	-5.26702718	-5.25190458	-1.61599912
383	C	-4.14834794	-4.84109218	-0.83285150
384	C	-3.82543325	-3.45869968	-0.60348151
385	N	-7.54972577	-1.46405758	-0.10142649
386	N	-8.55804926	3.25146341	-1.38815607
387	C	-10.00278242	2.85846042	-1.18837403
388	C	-8.07421779	4.62431989	-1.79062089
389	C	-6.82995481	-2.46507223	0.75878798
390	C	-9.01536657	-1.77749354	-0.20032562
391	C	-7.28536295	-2.34826093	2.24691947
392	C	-9.51751122	-1.95153477	-1.65866341
393	C	-11.10886352	3.94706276	-1.18742942
394	C	-9.07633445	5.65094387	-2.38459239
395	C	-2.55084604	-3.24067059	0.23143013
396	O	-1.61980218	-4.17721972	0.21873150
397	C	-2.87198201	0.24896192	1.99849601
398	O	-3.77876837	1.16969588	1.94168470
399	N	-2.30784242	-2.12589903	1.13837468
400	C	-3.25924334	-1.28663403	1.91077369
401	C	-3.58913364	-1.89476447	3.31512830
402	O	-4.05139257	-3.26071461	3.05252579
403	C	0.02254030	0.27287362	4.13868427
404	O	-0.22604219	-0.35963283	5.23543158

405	N	-1.46307091	0.55649240	2.09428055
406	C	-0.42411051	-0.30495322	2.73449327
407	C	0.72669391	-0.70447065	1.73646830
408	C	1.09096900	-2.19402763	1.84569420
409	C	1.51883561	-5.64156982	0.48649300
410	N	1.46411552	-2.72073397	3.04631039
411	C	1.44902772	-4.46004141	1.28471372
412	C	0.73520082	-3.10143249	-0.68332397
413	C	1.18640954	-5.54274009	-0.90734929
414	C	0.79867519	-4.28509642	-1.48426015
415	C	1.72756064	-4.22105577	2.79096162
416	C	1.05997455	-3.19869307	0.71257476
417	C	2.70985767	2.56015868	3.26877945
418	O	3.23675388	2.41344589	4.43305962
419	N	0.63366702	1.57768239	4.15075429
420	C	1.15362044	2.39316790	3.02565709
421	C	0.48820812	3.81692088	3.03309379
422	C	-0.83130069	3.80237220	2.26233571
423	C	-0.99559811	3.54383532	0.86165249
424	N	-2.42725612	3.63904623	0.62194997
425	C	-3.08151195	3.95494270	1.87695350
426	N	-2.12169756	4.06277580	2.89864288
427	C	3.15402202	1.69725950	-0.01572811
428	O	2.06501189	1.15312161	-0.45167652
429	N	3.53556921	2.93488220	2.13483872
430	C	3.14551534	3.10778977	0.70820101
431	C	4.10205173	4.20008407	0.12101406
432	C	3.87874556	4.55385142	-1.39214766
433	O	5.91623784	5.96433111	-1.89110486
434	C	5.92102409	-0.86238127	0.36213354
435	O	6.02881125	-1.40640823	1.52200356
436	N	4.42742677	1.03915783	-0.05342496
437	C	4.52734908	-0.43326729	-0.26637013
438	C	4.30209433	-0.85370199	-1.78099266
439	C	4.94580335	-2.18722545	-2.21897786
440	C	4.58242790	-3.41234414	-1.56662075
441	C	5.19879535	-4.65040241	-1.92971790
442	C	6.20230688	-4.67899900	-2.95167742
443	C	6.57921089	-3.46289055	-3.60557500
444	C	5.95423896	-2.23069618	-3.24106628
445	C	8.98128988	-2.03129368	0.45853070
446	O	10.13468170	-2.16194173	1.01863126
447	N	7.04204355	-0.56696042	-0.49334428
448	C	8.47978458	-0.62506522	-0.09028021

449	C	8.91123174	0.55071927	0.84495828
450	C	9.17832818	1.91547444	0.13101533
451	C	8.04102605	2.63891650	-0.65888930
452	O	6.97980891	2.05028912	-1.24649343
453	N	8.19677551	4.04242923	-0.68954153
454	N	8.08752888	-3.11545217	0.24040718
455	O	6.27321324	4.20962920	-3.10034484
456	C	5.27314874	4.58755208	-2.24446975
457	Mg	6.73745933	2.30263147	-3.18132260
458	H	-2.32532827	-2.32002500	-2.62074788
459	H	-5.72226120	3.51442945	-1.35098924
460	H	-1.55094143	2.65253551	-2.14524540
461	H	-0.33583424	-1.39894293	-3.52886604
462	H	-8.95301377	0.66976111	-0.70122710
463	H	-0.47912363	1.13435495	-3.92251753
464	H	0.33160317	0.84941580	-2.33122804
465	H	-6.40799786	-2.14413228	-2.55373075
466	H	-6.94152495	-4.55163042	-2.86323070
467	H	-5.47795451	-6.31851203	-1.76402356
468	H	-3.52743623	-5.63046239	-0.38777159
469	H	-10.27809514	2.10882107	-1.95886184
470	H	-10.08610858	2.39276693	-0.18486751
471	H	-7.58144344	5.10084129	-0.91738474
472	H	-7.32520412	4.49226493	-2.59614236
473	H	-7.02368057	-3.49102195	0.39566197
474	H	-5.74455290	-2.32564112	0.79156929
475	H	-9.17519487	-2.76557426	0.27224497
476	H	-9.65149361	-1.11693113	0.42313297
477	H	-6.72957644	-3.06736634	2.86924571
478	H	-7.08829681	-1.33499789	2.63109037
479	H	-8.35732307	-2.55751648	2.38224986
480	H	-10.58439912	-2.22438499	-1.66121396
481	H	-9.40387734	-1.04348405	-2.27049447
482	H	-8.95600574	-2.75667588	-2.15716951
483	H	-12.06427600	3.46860686	-0.91756283
484	H	-10.91551512	4.72904625	-0.43829574
485	H	-11.26376667	4.40296293	-2.17436851
486	H	-8.50712050	6.52316573	-2.74496221
487	H	-9.62251152	5.23929317	-3.24621880
488	H	-9.78643566	6.03899236	-1.64262351
489	H	-1.32493560	-2.16079720	1.47540759
490	H	-4.22428637	-1.26554639	1.37881144
491	H	-2.70048241	-1.92042535	3.99210781
492	H	-4.39513745	-1.30617296	3.81868456

493	H	-4.21958355	-3.66780056	3.98724138
494	H	-1.22426387	1.55468838	1.88892812
495	H	-0.91826353	-1.24993361	3.01224905
496	H	0.37680500	-0.48987107	0.71211761
497	H	1.64931849	-0.12710536	1.91064272
498	H	1.81673409	-6.60015033	0.93050640
499	H	0.44427015	-2.14278329	-1.12937881
500	H	1.23212389	-6.43787378	-1.54141511
501	H	0.55345547	-4.23138671	-2.55252252
502	H	1.03213609	-4.80859806	3.42196125
503	H	2.78327003	-4.44153061	3.04386903
504	H	0.87702112	1.93625345	5.10191696
505	H	0.96434882	1.90129530	2.05799011
506	H	0.32830933	4.16879928	4.06505984
507	H	1.16140449	4.55957755	2.56320180
508	H	-0.27747974	3.30680766	0.07610947
509	H	-2.89666016	3.47873558	-0.29631960
510	H	-4.16690536	4.07399058	1.96971883
511	H	4.55032418	3.02645475	2.36558986
512	H	2.12042980	3.51693860	0.62456340
513	H	3.98376767	5.11357290	0.73321937
514	H	5.14762336	3.87353976	0.26705053
515	H	3.33584864	3.66362409	-1.80678969
516	H	3.14214770	5.35036083	-1.60752777
517	H	5.41112366	6.61820289	-1.27585882
518	H	5.31501623	1.57042519	0.07926668
519	H	3.76163446	-0.94151668	0.35424136
520	H	3.21421230	-0.92737636	-1.96038331
521	H	4.68595123	-0.04313838	-2.42632731
522	H	3.83621888	-3.40038423	-0.76562965
523	H	4.91015875	-5.57468049	-1.41318206
524	H	6.68525573	-5.62551781	-3.22630848
525	H	7.35354283	-3.47629400	-4.38317372
526	H	6.26299266	-1.30650882	-3.74664344
527	H	6.83896606	-0.16042292	-1.42503225
528	H	9.04243076	-0.50320622	-1.04291723
529	H	8.17069813	0.68787029	1.65307894
530	H	9.85457834	0.26126913	1.34497688
531	H	10.01245298	1.76008862	-0.58518555
532	H	9.54191613	2.63382203	0.88733806
533	H	7.50279410	4.64738189	-1.19968899
534	H	9.01604556	4.49904065	-0.22949012
535	H	7.16135772	-2.99032184	-0.19970806
536	H	8.37305260	-4.06701712	0.54741960

537

538 **(2)The HOMO-LUMO energy gaps**

539

540 **Rb-SWHEFQ-NH₂**

541

542 Orbital HOMO, energy: -0.17471 a.u. -4.75410 eV

543 Orbital LUMO, energy: -0.06996 a.u. -1.90371 eV

544 HOMO-LUMO gap: 0.10475 a.u. 2.85039 eV 275.0211 kJ/mol

545

546 **Rb-SWHEFQ-NH₂ & Mg²⁺**

547 Orbital HOMO, energy: -0.23570 a.u. -6.41373 eV

548 Orbital LUMO, energy: -0.22531 a.u. -6.13100 eV

549 HOMO-LUMO gap: 0.01039 a.u. 0.28273 eV 27.27894 kJ/mol