

Supporting information

New Journal of Chemistry

LC-MS/MS identification and cytotoxic assessment of jaspamide and its congeners from the sponge *jaspis diastra*

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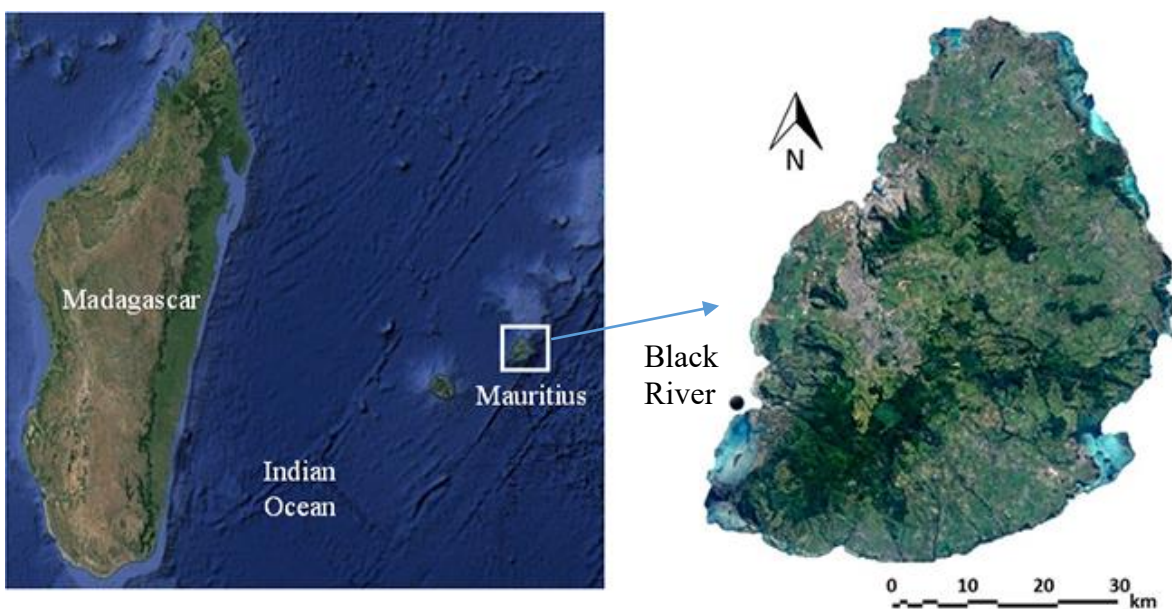


Fig. 1S. Map showing collection site of *Jaspis diastra* in Mauritius waters

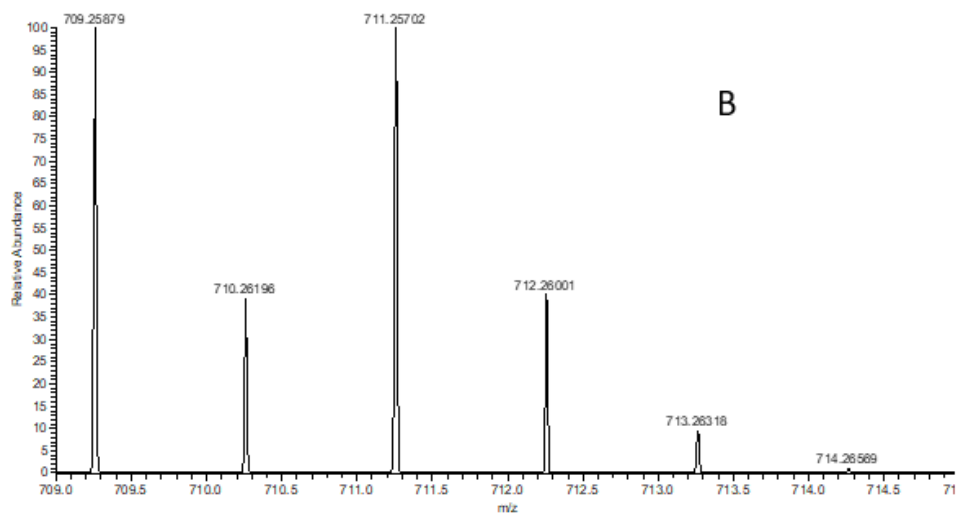
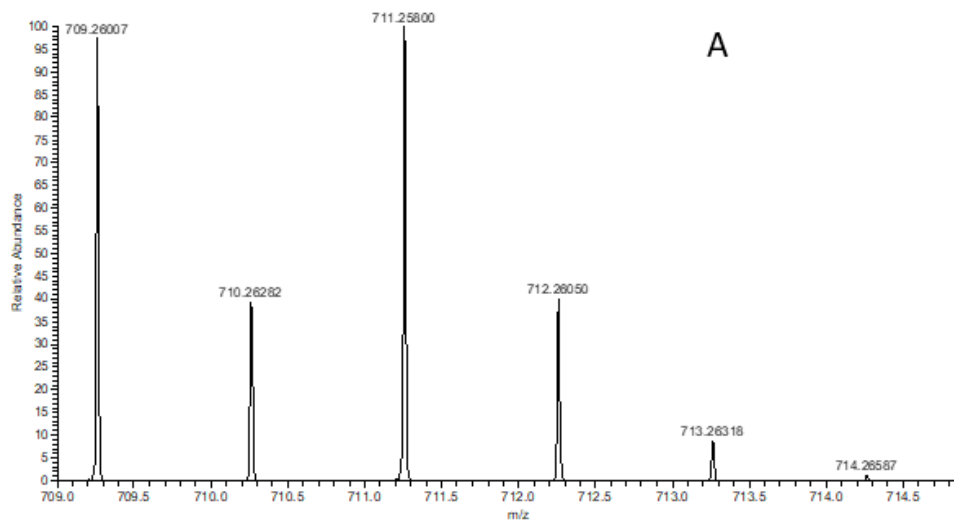


Fig 2S. Comparison of the isotope pattern of reference Jaspamide (1) (A) with its measured pattern (B) in JDH-1.

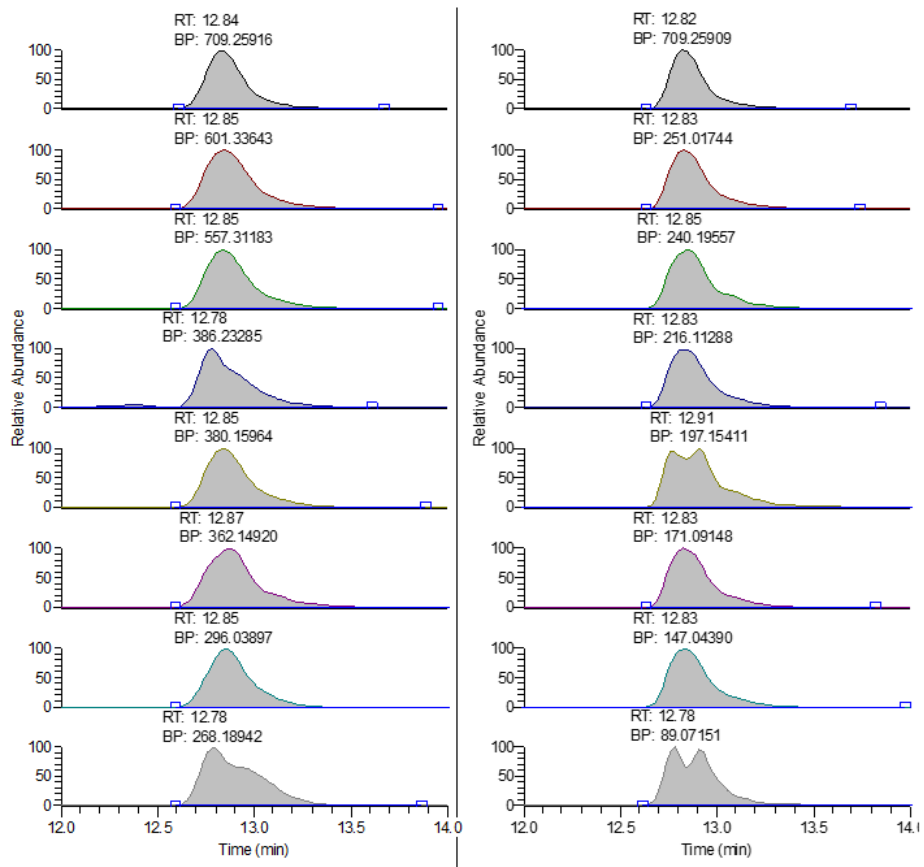


Fig 3S. EICs of fragments of reference Jaspamide (1)

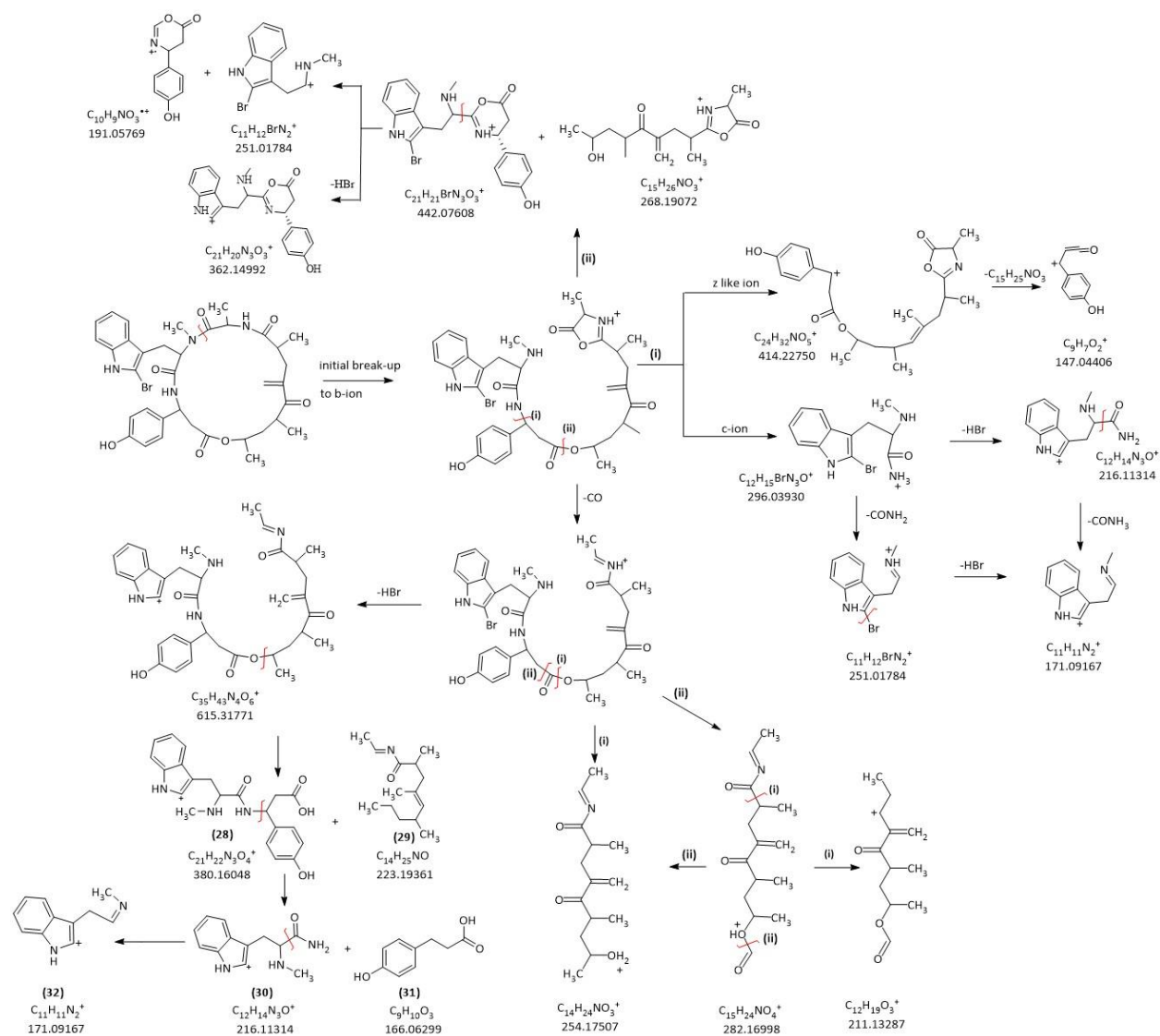


Fig 4S. Proposed fragmented pathways of Jaspamide B

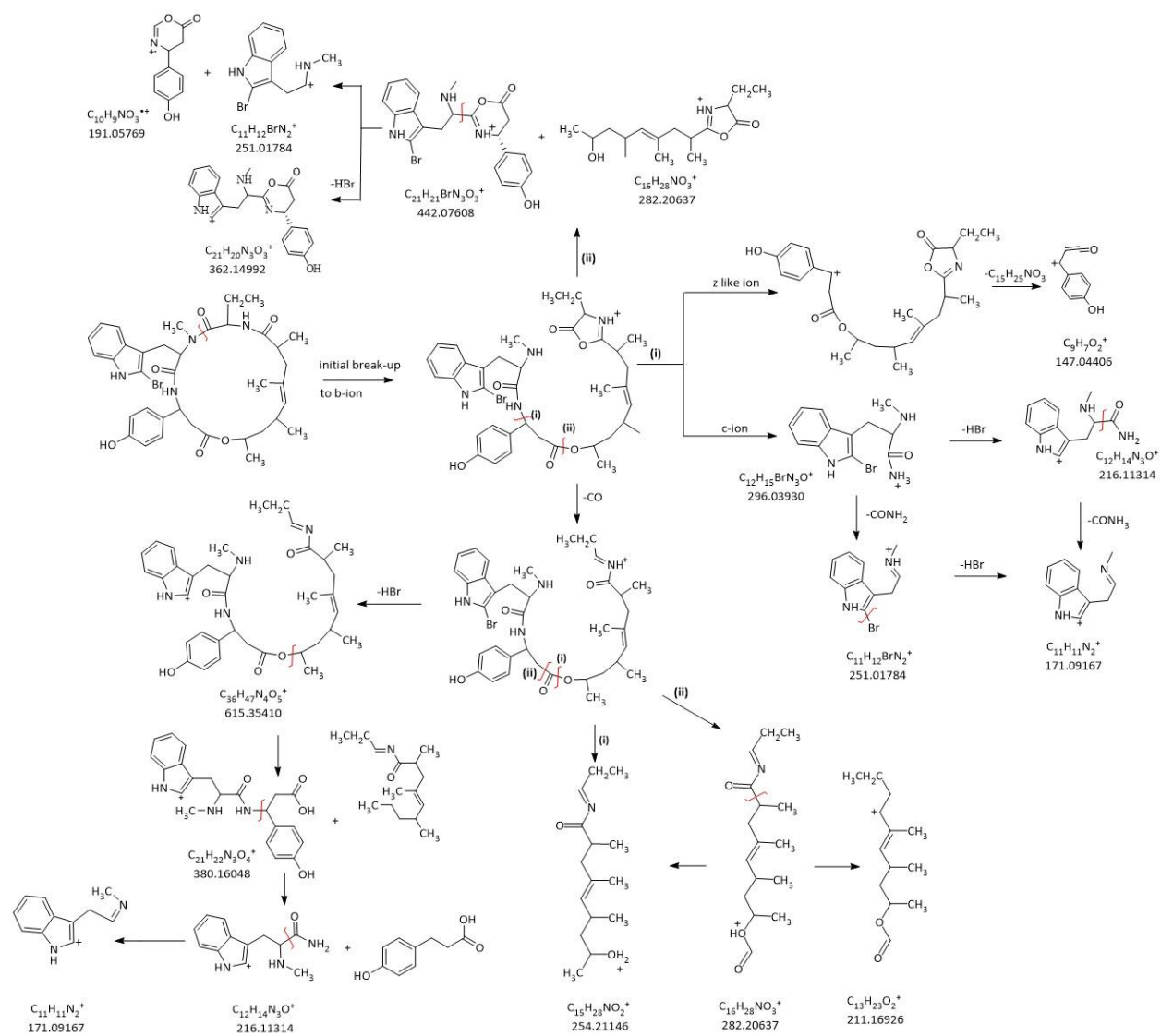


Fig 6S. Proposed fragmented pathways of Jaspamide D

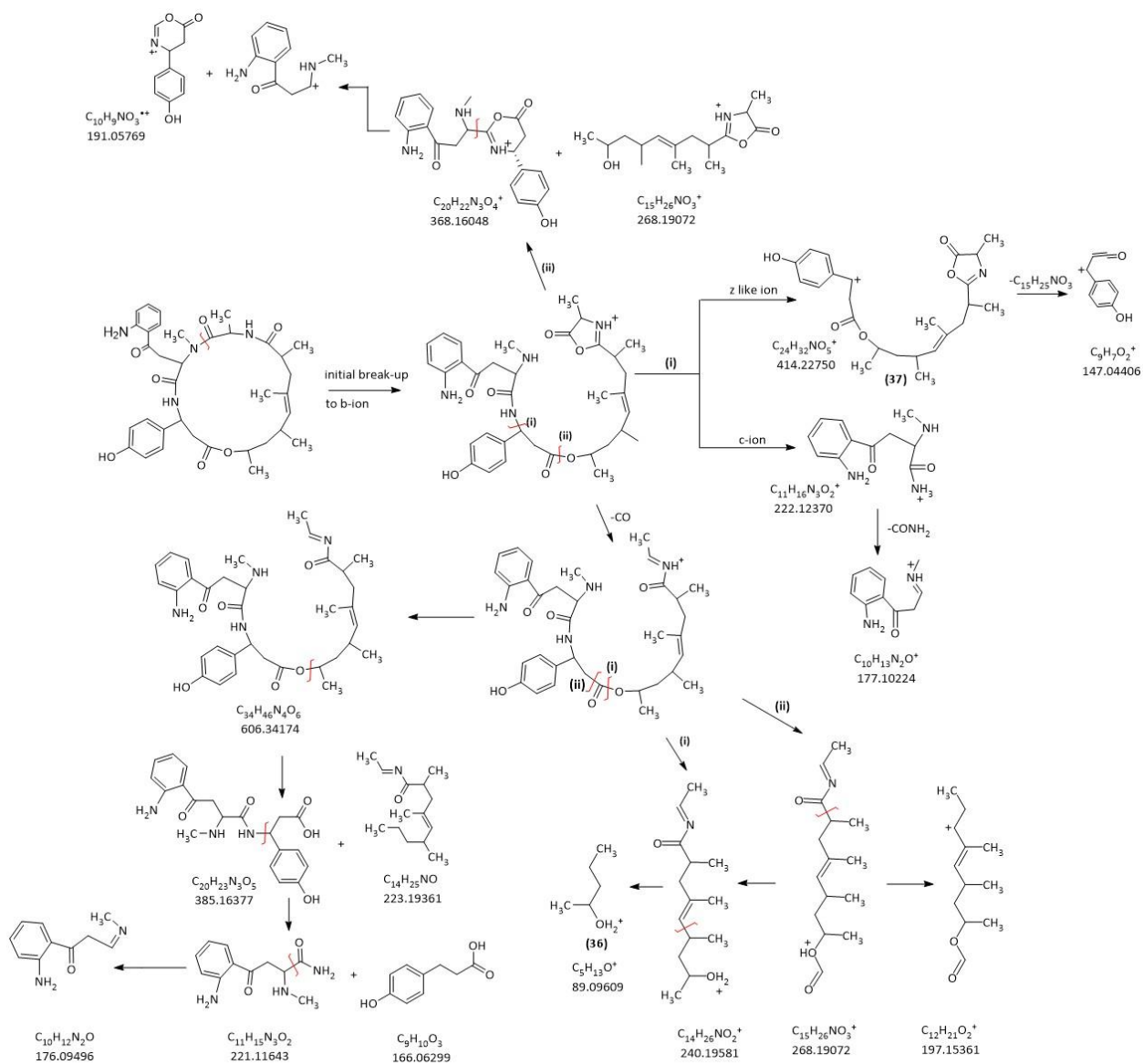


Fig 9S. Proposed fragmented pathways of Jaspamide O

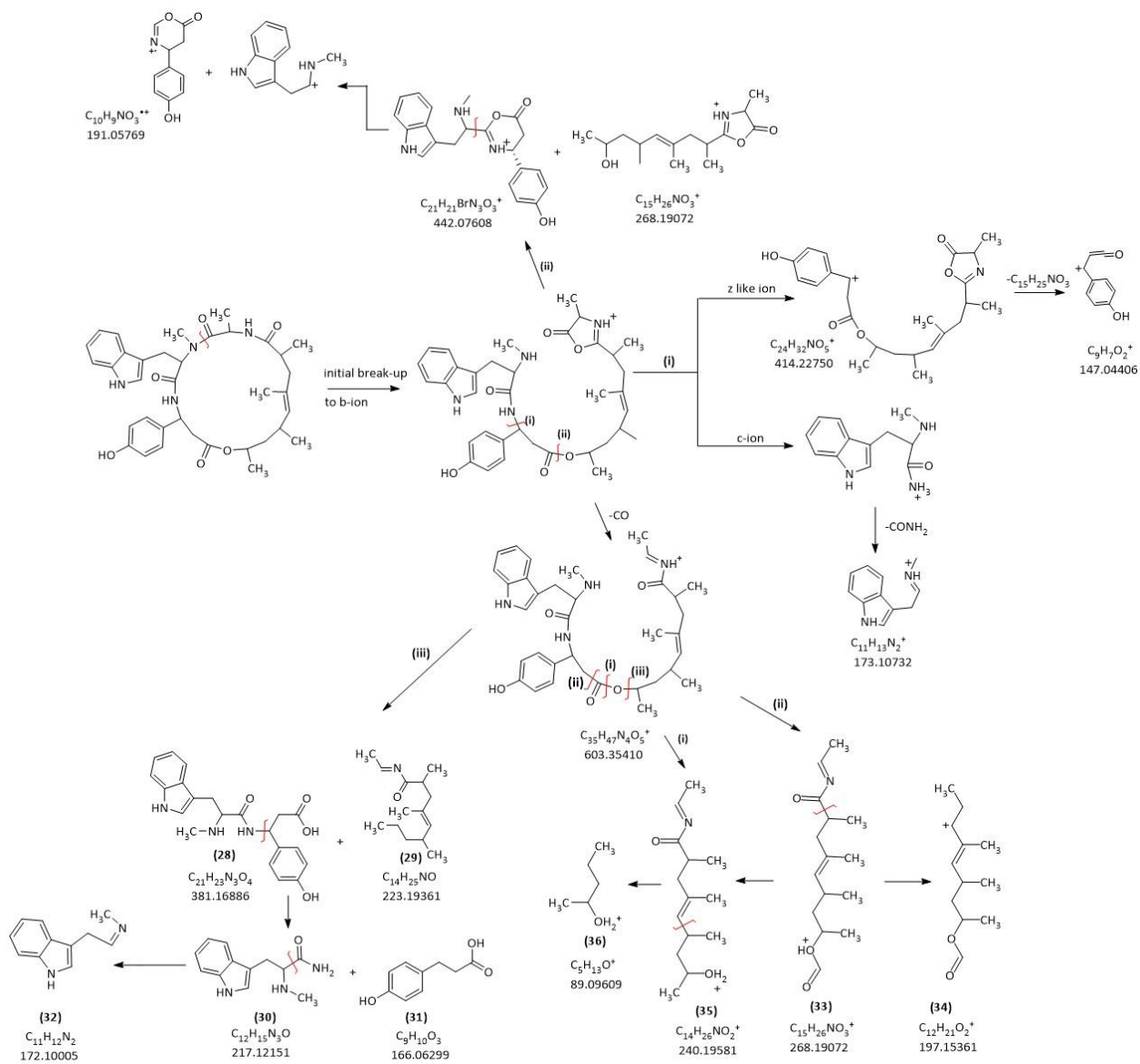


Fig 10S. Proposed fragmented pathways of Jaspamide Q

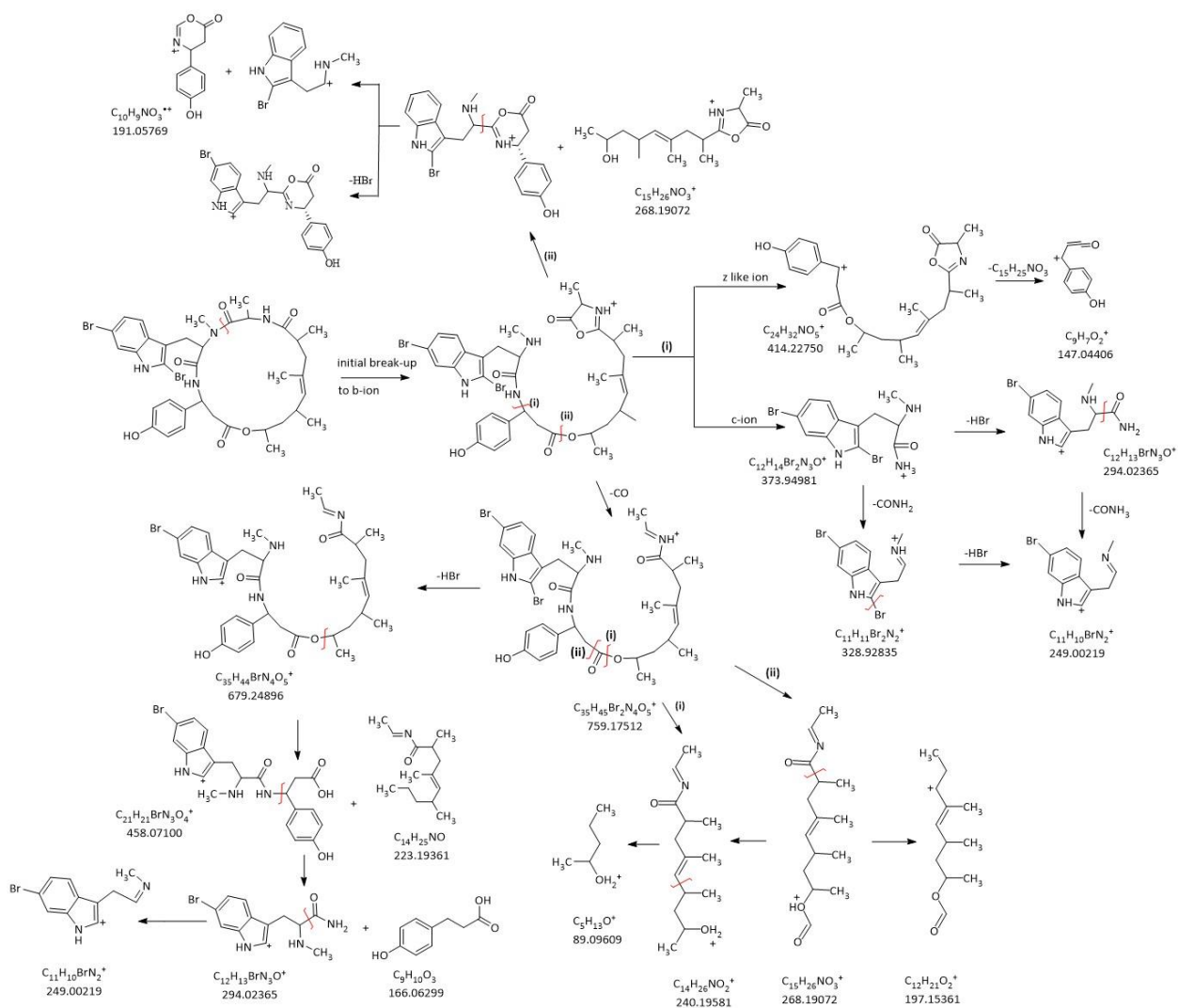


Fig 11S. Proposed fragmented pathways of Jaspamide R

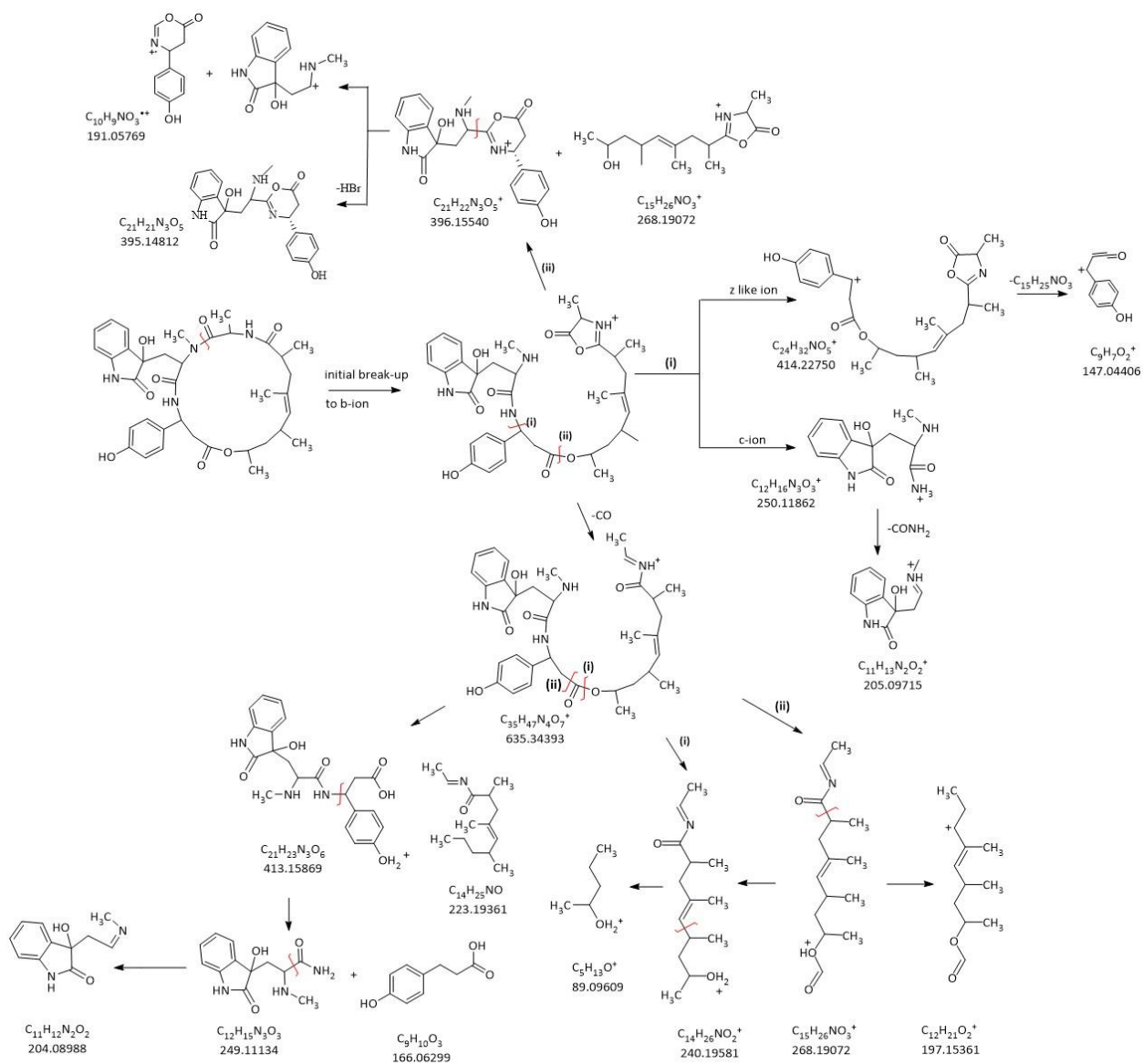


Fig 12S. Proposed fragmented pathways of Jaspamide S

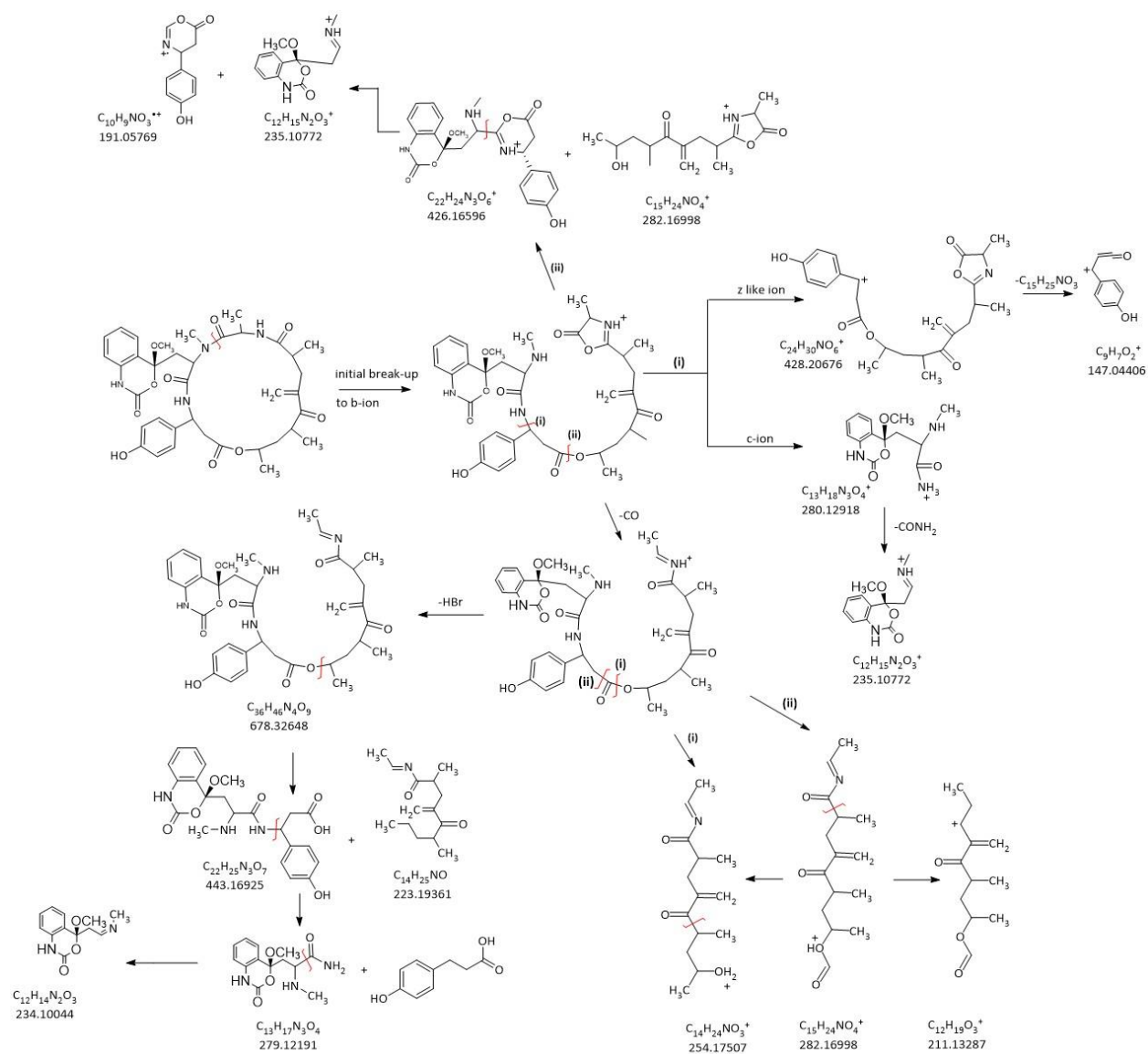


Fig 13S. Proposed fragmented pathways of Jaspamide U

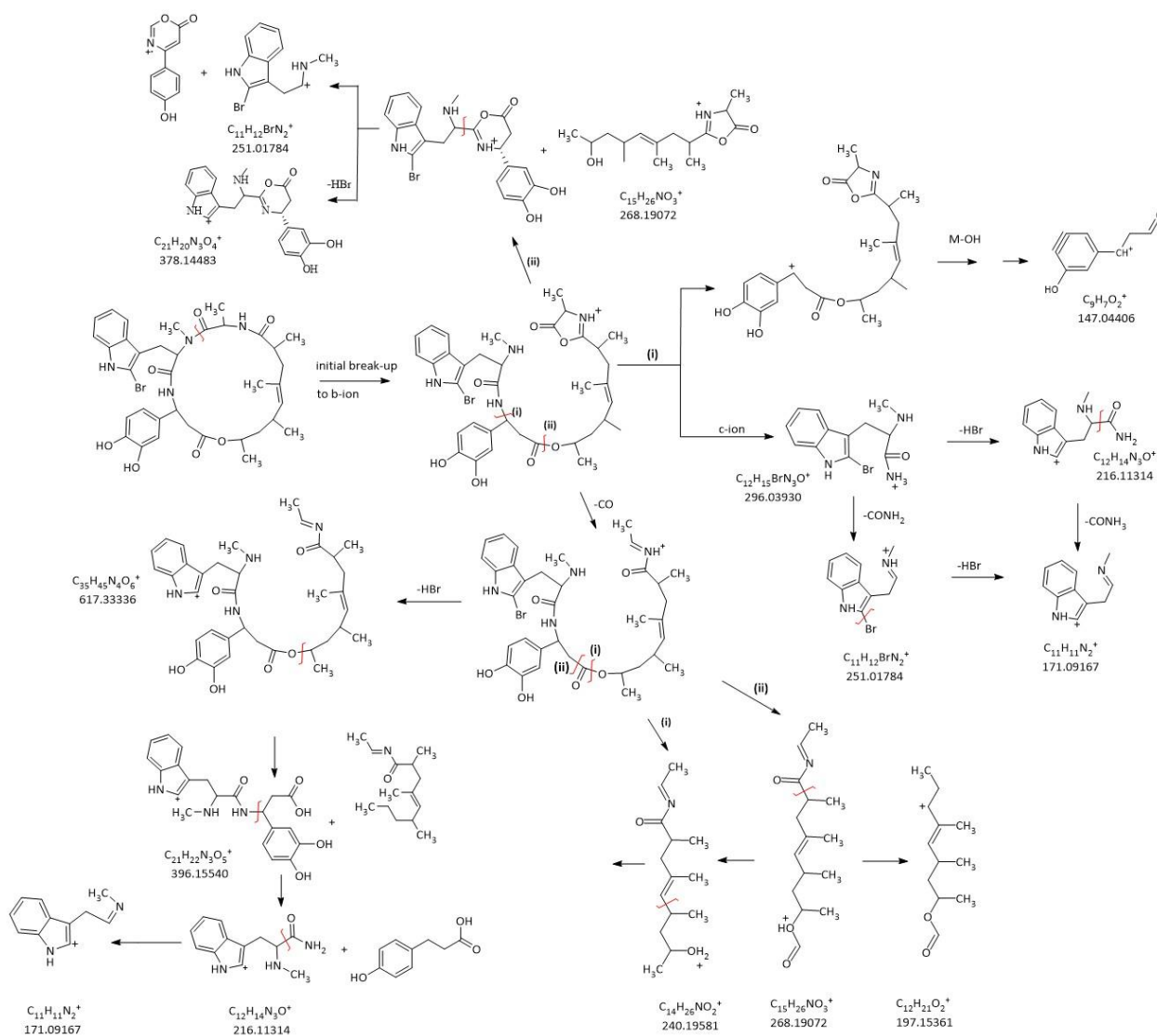


Fig 14S. Proposed fragmented pathways of Jaspamide V

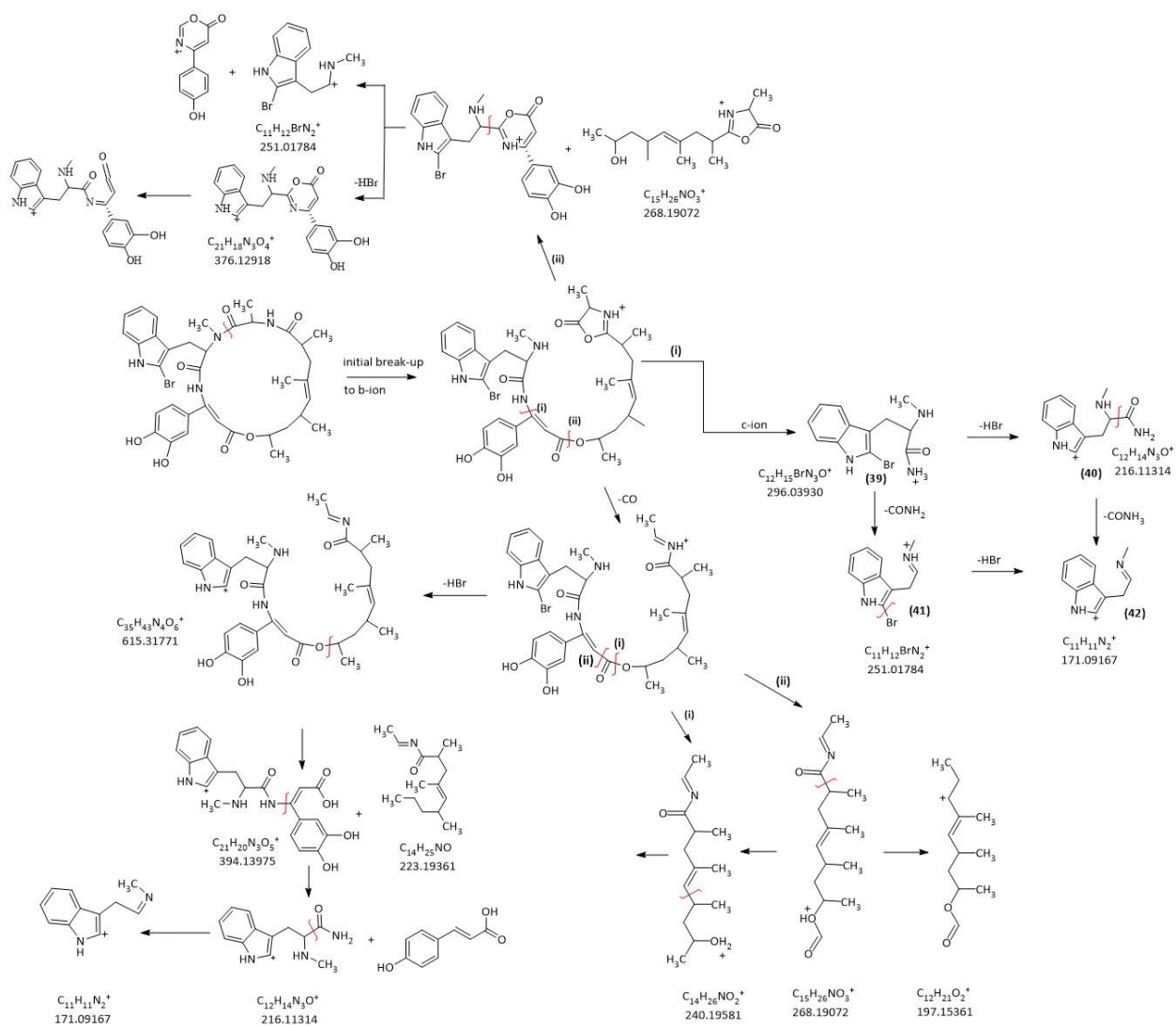


Fig 15S. Proposed fragmented pathways of Jaspamide W

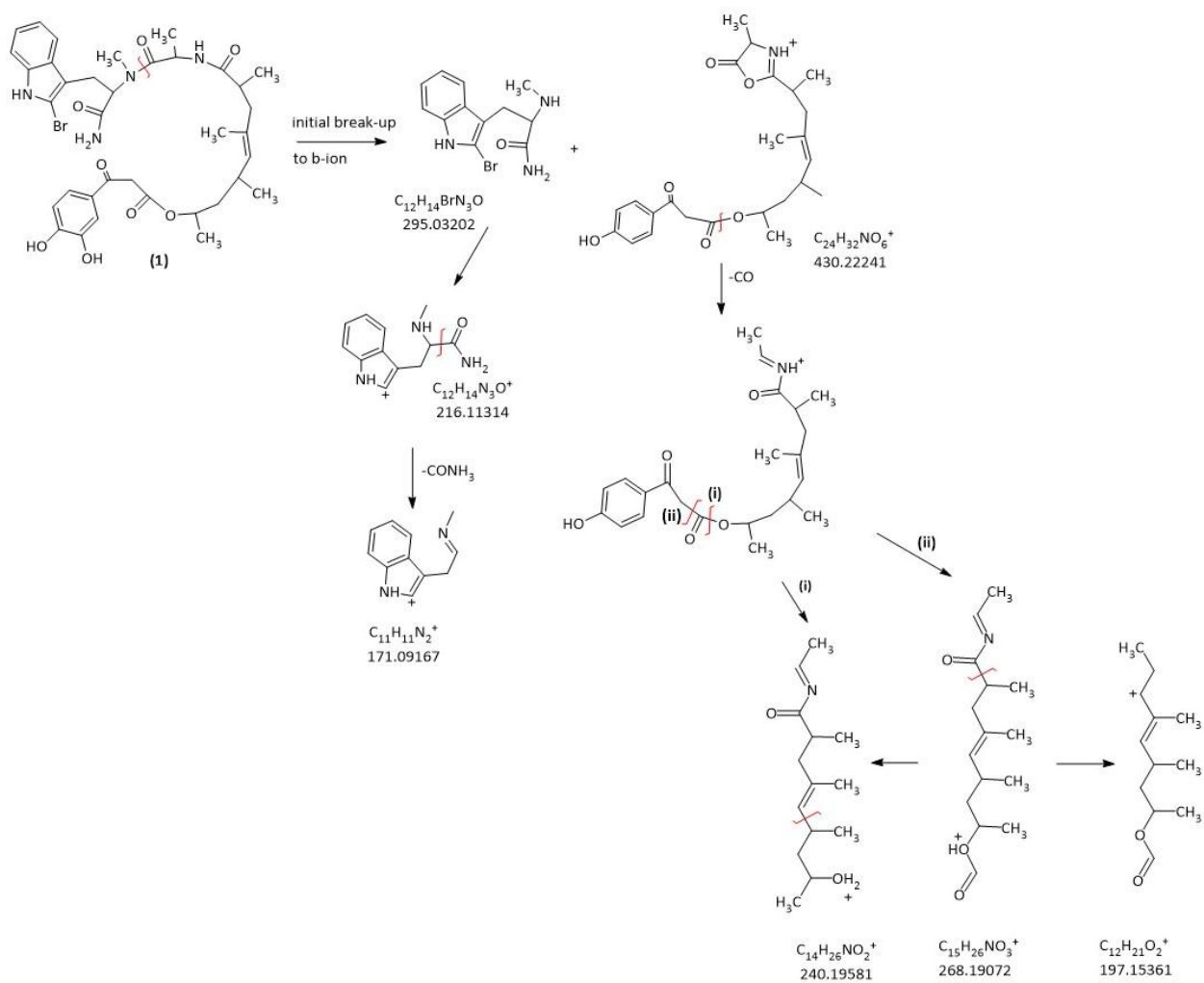


Fig 18S. Proposed fragmented pathways of Jaspamide Z5

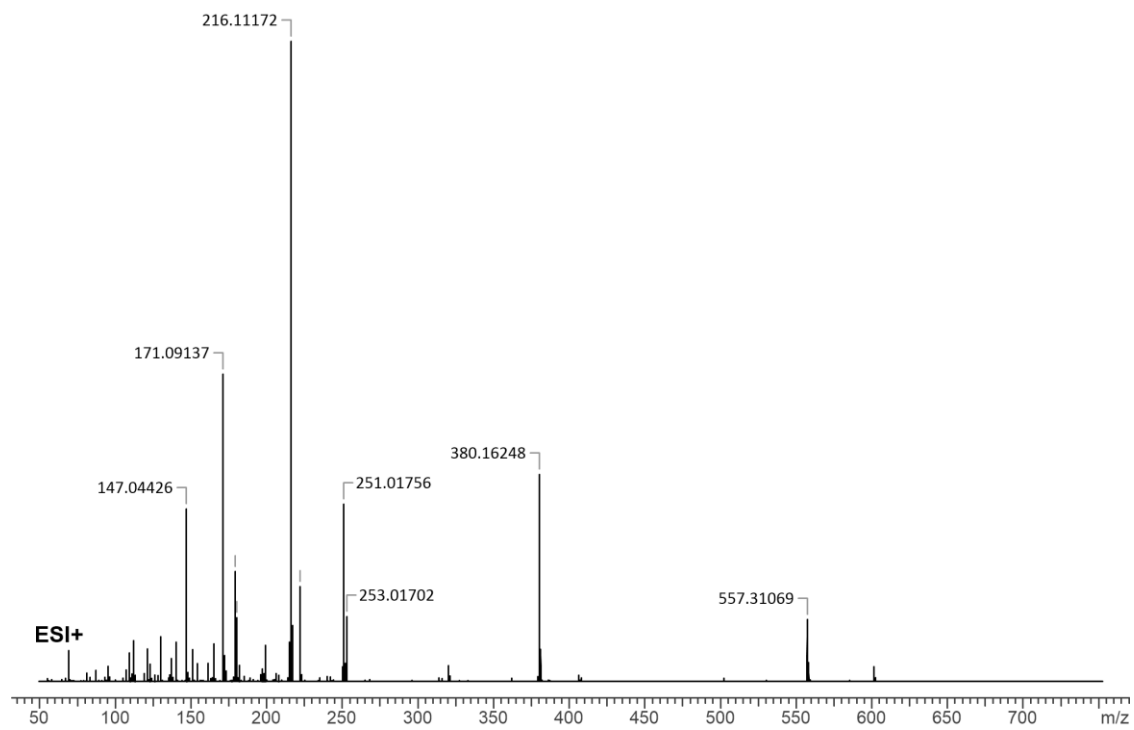


Fig 19S. MS/MS spectrum of Jaspamide (1) in JDH-1

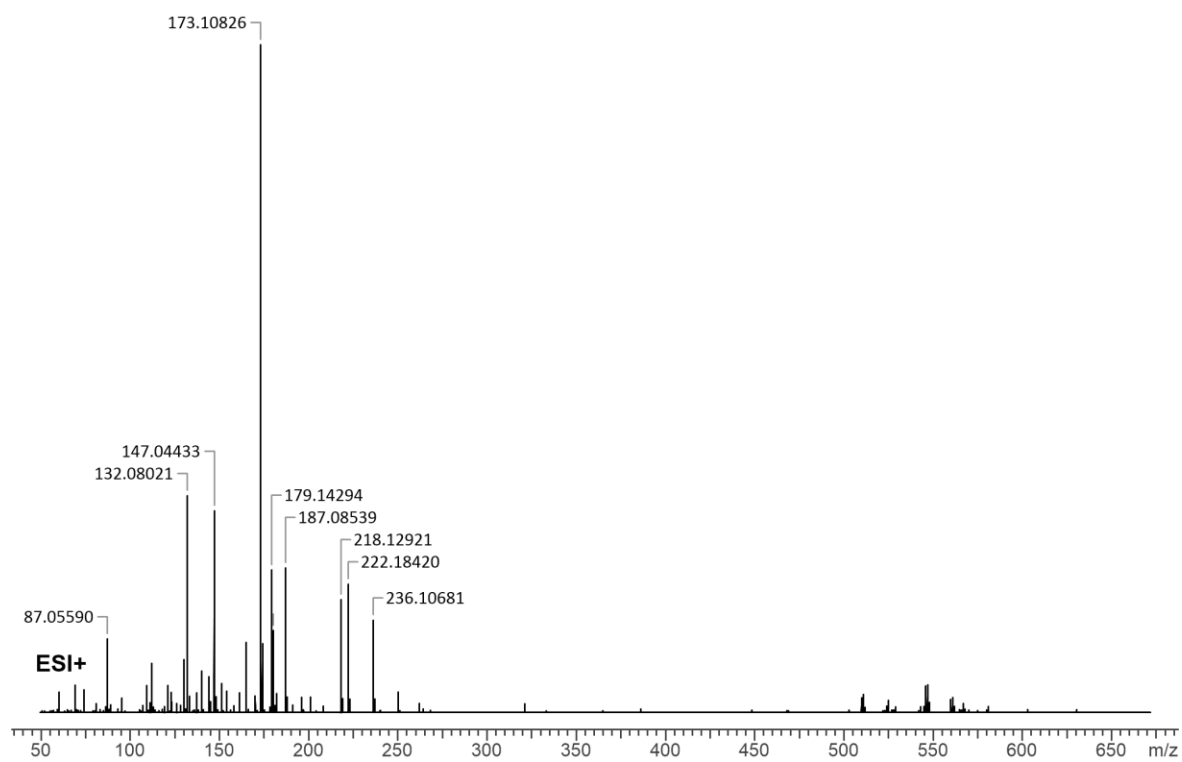


Fig 20S. MS/MS spectrum of Jaspamide Q in JDH-1

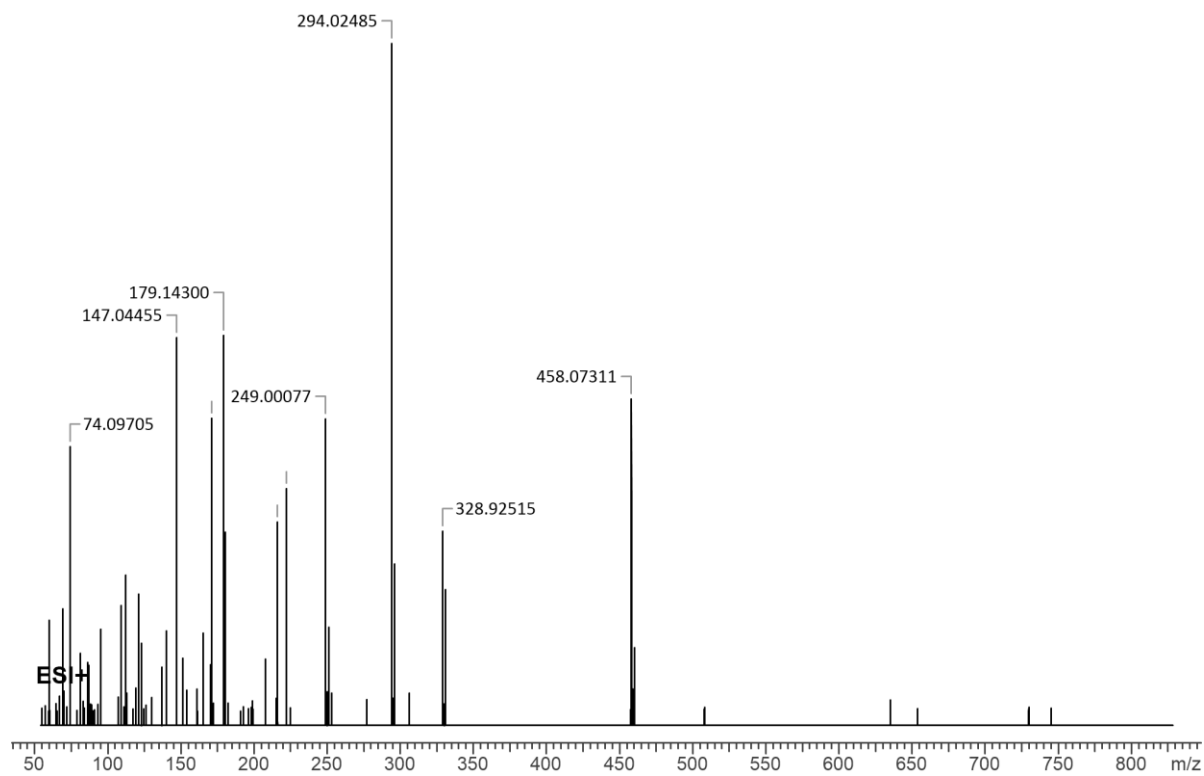


Fig 21S. MS/MS spectrum of Jaspamide R in JDH-1

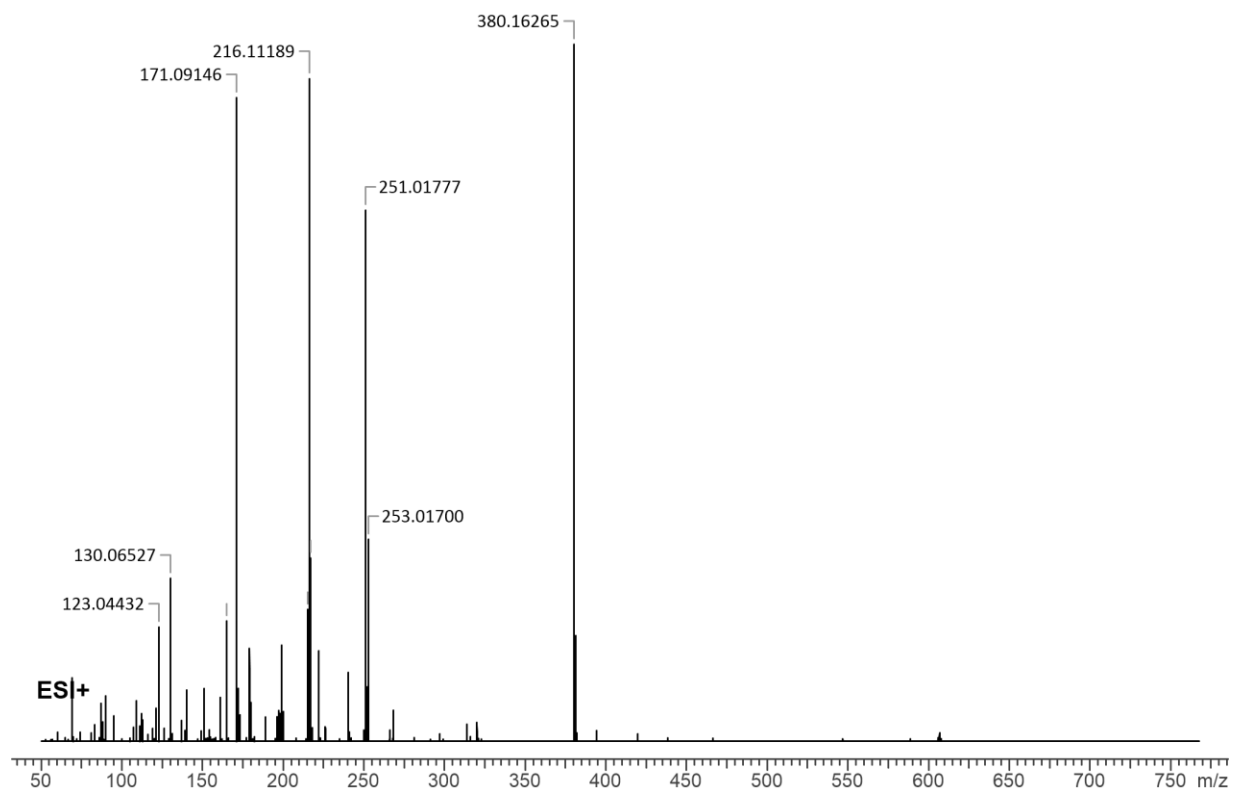


Fig 22S. MS/MS spectrum of Jaspamide Z1 in JDH-1

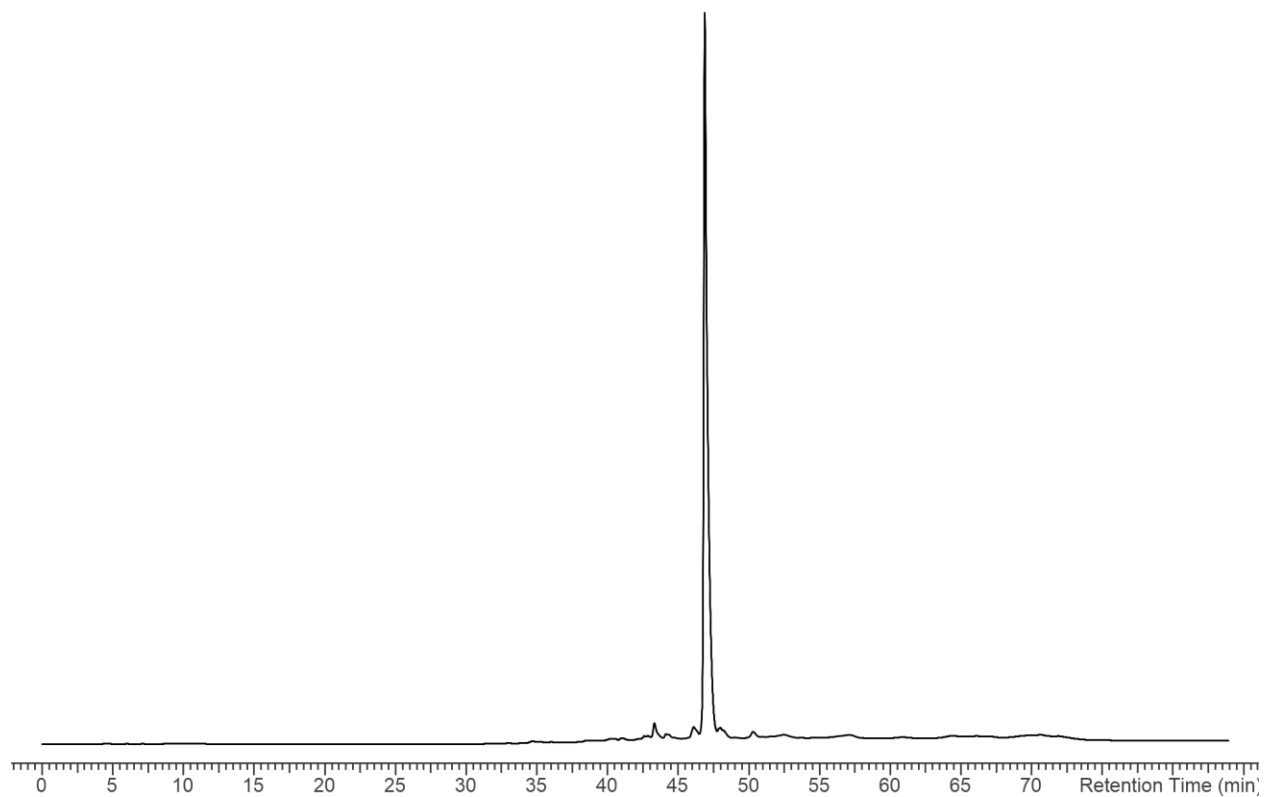


Figure 25S. HPLC chromatogram of JC-1

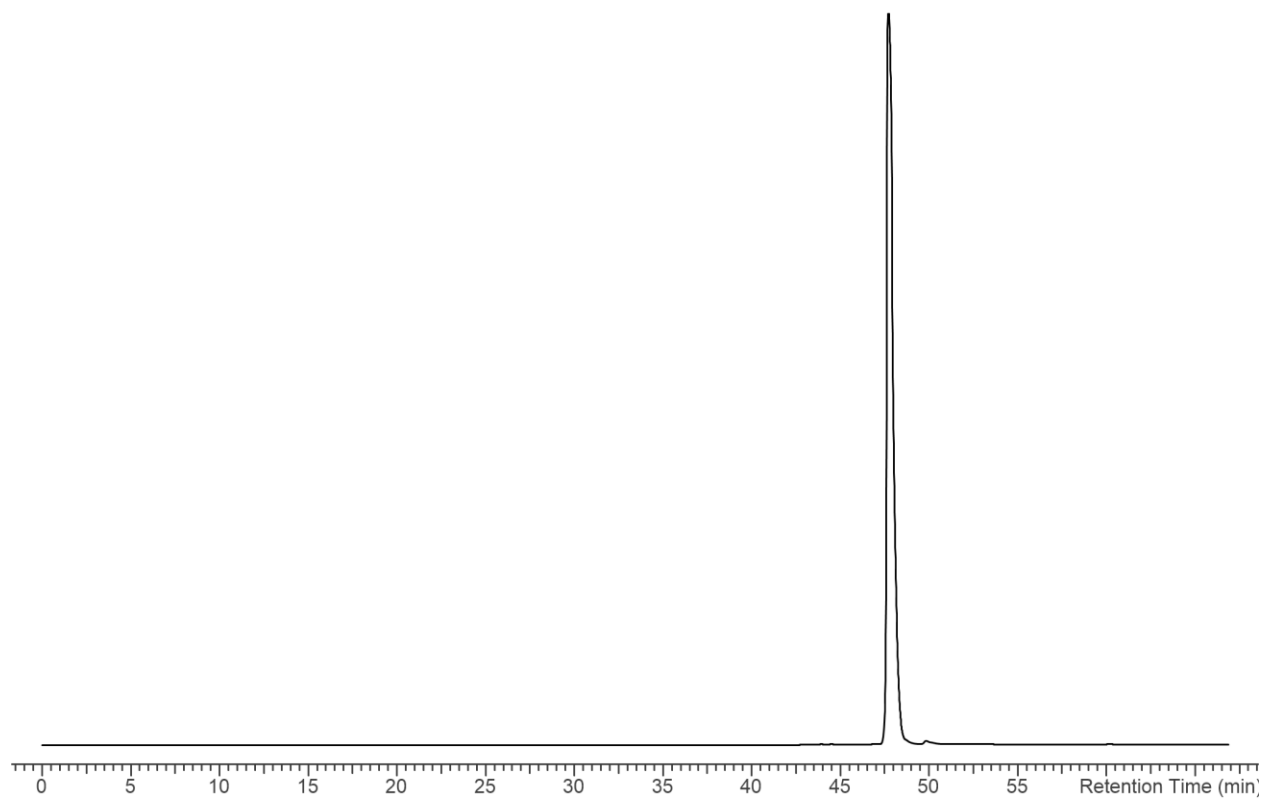


Figure 26S. HPLC chromatogram of JC-1P (purified Jaspamide)

Table 1S. Theoretical and measured isotope pattern of Jaspamide (1) and its congeners

Jaspamide (1) and its congeners	Theoretical isotope pattern	Measured isotope pattern
Jaspamide (1)	709.25506, 710.24965, 711.25301, 712.25636, 713.25972, 714.26061, 715.26396, 716.26732, 717.27067, 718.27156	709.25934, 710.26257, 711.25745, 712.26062, 713.26251, 714.26575, 715.46820
B/G/W	723.23432, 724.22892, 725.23227, 726.23563, 727.23898, 728.23987, 729.24323, 730.24658, 731.24994, 732.25083	723.23846, 724.53748, 725.23227, 726.28741, 729.19141, 730.36780, 732.07013
C/E/K/L/N/V	725.25444, 726.25779, 727.25239, 728.25575, 729.25910, 730.26246, 731.26335, 732.26670, 733.27006, 734.27314, 735.27430	725.25470, 727.25226, 728.70313, 729.65717
D	723.27517, 724.27853, 725.27313, 726.27648, 727.27984, 728.28319, 729.28408, 730.28744, 731.29079, 732.29415, 733.29504	723.27557, 724.27789, 725.27252, 726.28613, 728.28412, 729.28687
F/H/J/M	695.24387, 696.24723, 697.24183, 698.24518, 699.24854, 700.25189, 701.25278, 702.25614, 703.25949, 704.26285, 705.26374	695.24353, 696.24670, 697.55695
O	635.34393, 636.34728, 637.35064, 638.35399, 639.35488, 640.35824, 641.36159, 642.36248, 643.36584	635.34430, 639.91980, 642.40503
P	693.34941, 694.35276, 695.35612, 696.35947, 697.36036, 698.36372, 699.36707, 700.36796, 701.37132, 702.37467	693.44653, 697.45563, 698.45447, 700.43042, 701.38837, 702.94000
Q	631.34901, 632.35237, 633.35572, 634.35908, 635.35997, 636.36332, 637.36668, 638.37003, 639.37092	631.34778, 632.35297
R	787.17004, 788.17339, 789.16799, 790.17134, 791.16594, 792.16930, 793.17265, 794.17601, 795.17690, 796.18025, 797.18361, 798.18696, 799.18785	787.17010, 789.16827, 790.17120, 791.16663, 792.17151, 793.41370, 794.81537, 798.58917
S	663.33884, 664.34220, 665.34555, 666.34891, 667.34980, 668.35315, 669.35651, 670.35740, 671.36075, 672.36411	663.33856, 664.34021, 671.46448, 672.52258
U	707.32867, 708.33202, 709.33538, 710.33873, 711.33963, 712.34298, 713.34634, 714.34723, 715.35058, 716.35394	707.33136, 708.33240, 709.91211, 711.28094, 712.87341, 714.26752, 716.89777

Z ₁	727.27009, 728.27344, 729.26804, 730.27140, 731.27475, 732.27811, 733.27900, 734.28235, 735.28571, 736.28906, 737.28995	727.27020, 728.27319, 729.26819, 730.27179, 731.27466
Z ₄	563.22274, 564.22610, 565.22070, 566.22405, 567.22741, 568.23076, 569.23165, 570.23501, 571.23836, 572.24172	563.22766, 564.39600, 565.36981, 566.44757, 567.43848, 568.45844, 569.38263, 570.43817, 571.41840, 572.42426
Z ₅ /Z ₆	741.24935, 724.25271, 743.24731, 744.25066, 745.25402, 746.25737, 747.25826, 748.26162, 749.26497, 750.26586, 751.26922	741.25061, 742.94446

Table 2S. Standard Jaspamide (1) and their corresponding peak area calculated by HPLC

Standard Jaspamide, µg/mL	Retention Time, R _t / min Jaspamide UV_VIS_280 nm	Peak Area/ mAU Jaspamide UV_VIS_280 nm
25	30.367	5.1120
50	30.363	10.2764
75	30.363	13.0962
100	30.363	18.6352

Table 3S. Percentage of Jaspamide (1) in JDH-2, JDE-3 and JDM-1

Description	Retention Time, R _t / min	Peak area/mAU	Concentration of Jaspamide, µg/mL	Dilution factor	Mass of Jaspamide, µg	Mass of Jaspamide, mg	Mass of sample used/mg	% Jaspamide
JDH-2	30.3270	4.4538	23.9452	1	23.9452	0.0239	3.2	0.75
JDH-2	30.3230	3.6718	19.7409	1	19.7409	0.0197	3.2	0.62
JDH-2	30.3200	2.5510	13.7151	1	13.7151	0.0137	3.2	0.43
JDE-3	30.4130	13.3652	71.8560	20	1437.1194	1.4371	3.9	36.85
JDE-3	30.4130	13.1368	70.6280	20	1412.5591	1.4126	3.9	36.22
JDE-3	30.4130	12.8374	69.0181	20	1380.3624	1.3804	3.9	35.39
JDM-1	30.4230	0.6075	3.2661	1	3.2661	0.0033	5.6	0.06
JDM-1	30.4270	0.4028	2.1656	1	2.1656	0.0022	5.6	0.04
JDM-1	30.4330	0.2584	1.3892	1	1.3892	0.0014	5.6	0.02

Table 4S. Inter-day HPLC-analysis (sample solution analyzed (JC-1P) 6 times inter-day to determine the repeatability)

Description	Retention Time, Rt / min	Peak area/mAU	Concentration of Jaspamide, µg/mL	Dilution factor	Mass of Jaspamide, µg	Mass of Jaspamide, mg	Mass of sample used/mg	% Purity	% Mean purity	SD	%RSD
Pure JP	30.4200	4.9685	26.7125	10	267.1247	0.2671	0.3	89.04	87.54	1.61	1.84
Pure JP	30.4200	4.9441	26.5811	10	265.8108	0.2658	0.3	88.60			
Pure JP	30.4200	4.9014	26.3517	10	263.5167	0.2635	0.3	87.84			
Pure JP	30.4230	4.9401	26.5597	10	265.5968	0.2656	0.3	88.53			
Pure JP	30.4200	4.8217	25.9231	10	259.2312	0.2592	0.3	86.41			
Pure JP	30.4230	4.7341	25.4520	10	254.5204	0.2545	0.3	84.84			

Table 5S. Intra-day HPLC-analysis (sample solution was analysed for 3 consecutive days to determine the reproducibility).

Description	Retention Time, Rt / min	Peak area/mAU	Concentration of Jaspamide, µg/mL	Dilution factor	Mass of Jaspamide, µg	Concentration of Jaspamide, mg	Mass of sample used/mg	% Purity	% Mean purity	SD	%RSD
Pure JP	30.4200	4.9449	26.5853	10	265.8532	0.2659	0.3	88.62	87.80	0.71	0.81
Pure JP	30.4200	4.8785	26.2286	10	262.2860	0.2623	0.3	87.43			
Pure JP	30.4230	4.8741	26.2047	10	262.0473	0.2620	0.3	87.35			