

Supplementary Material

S1 Details of MS spectra of *Arachnocampa* spp. adhesives

S1.1 *Arachnocampa luminosa* (New Zealand)

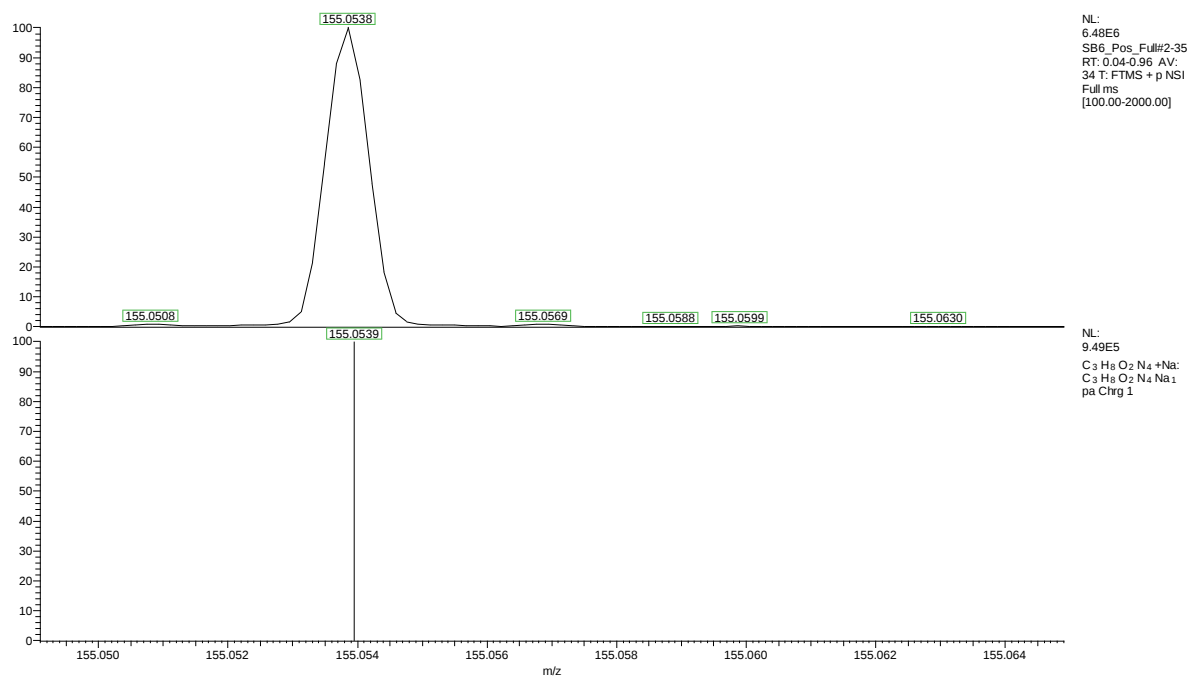


Figure S1.1.1. Detail of MS spectrum of *A. luminosa*, indicating the presence of a molecule with the formula $C_3H_8O_2N_4$, most likely methylenediurea or another isomer.

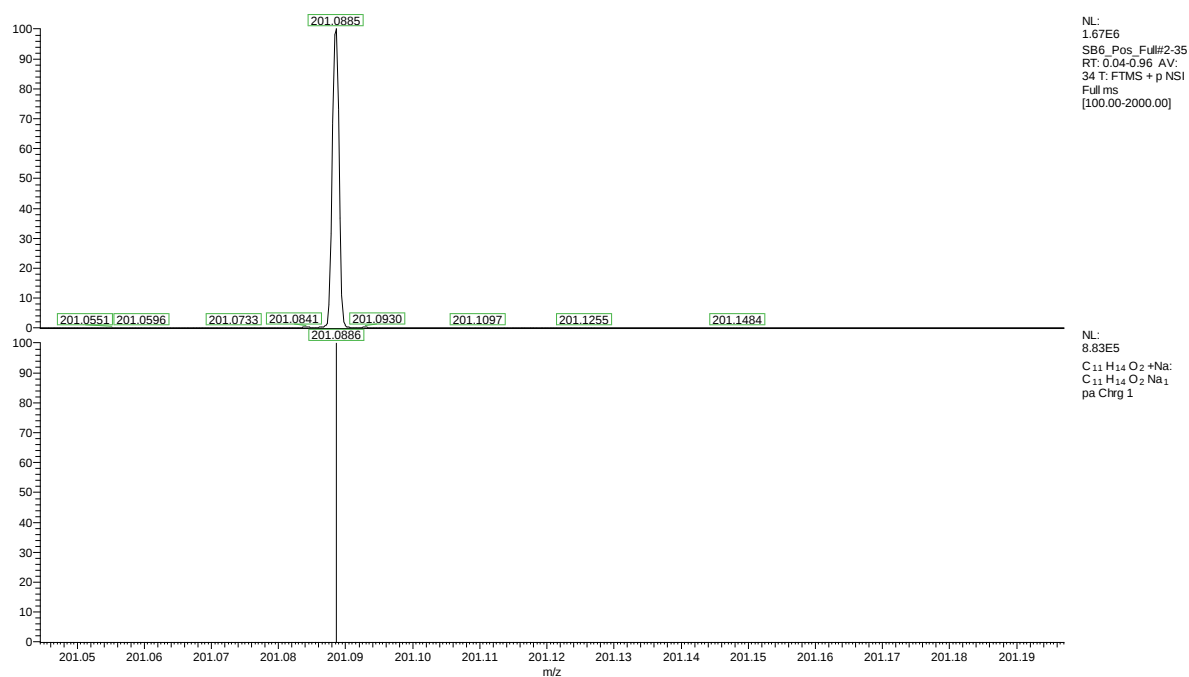


Figure S1.1.2. Detail of MS spectrum of *A. luminosa*, indicating the presence of a molecule with the formula C₁₁H₄N₁O₂.

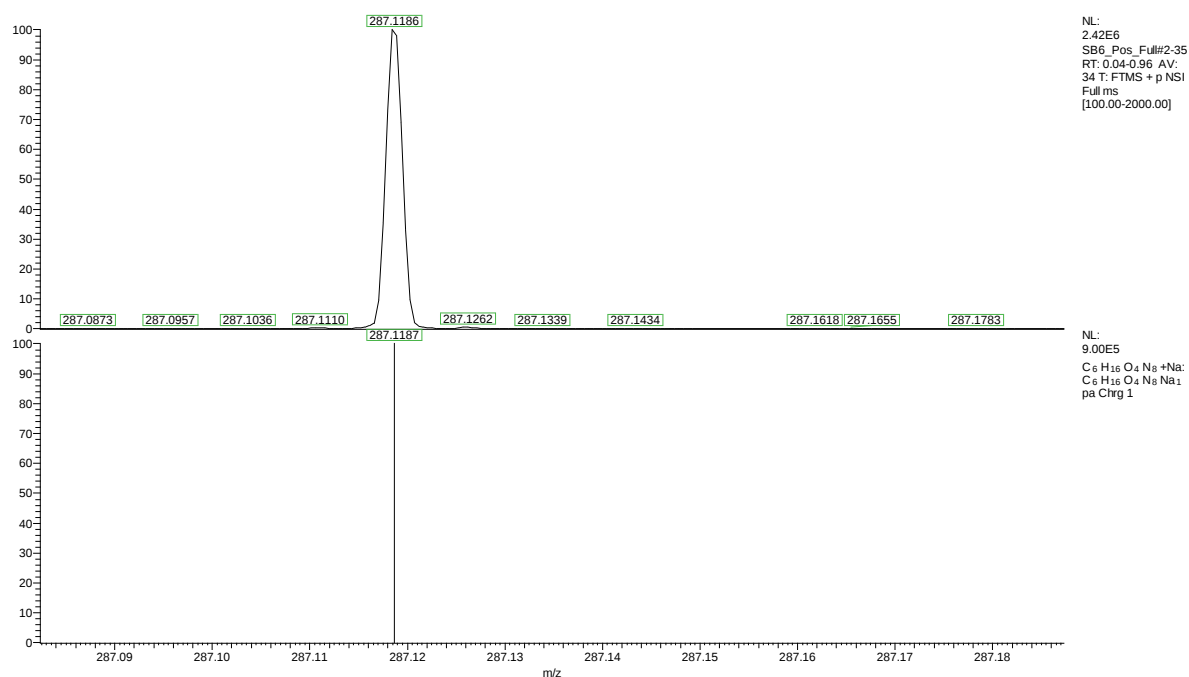


Figure S1.1.3. Detail of MS spectrum of *A. luminosa*, indicating the presence of a molecule with the formula C₆H₁₆O₄N₈, potentially N'-{2-[2-(2,2-Dihydroxyhydrazino)-4,5-dihydro-1H-imidazol-1-yl]ethyl}-2,2-dihydroxyhydrazinecarboximidamide.

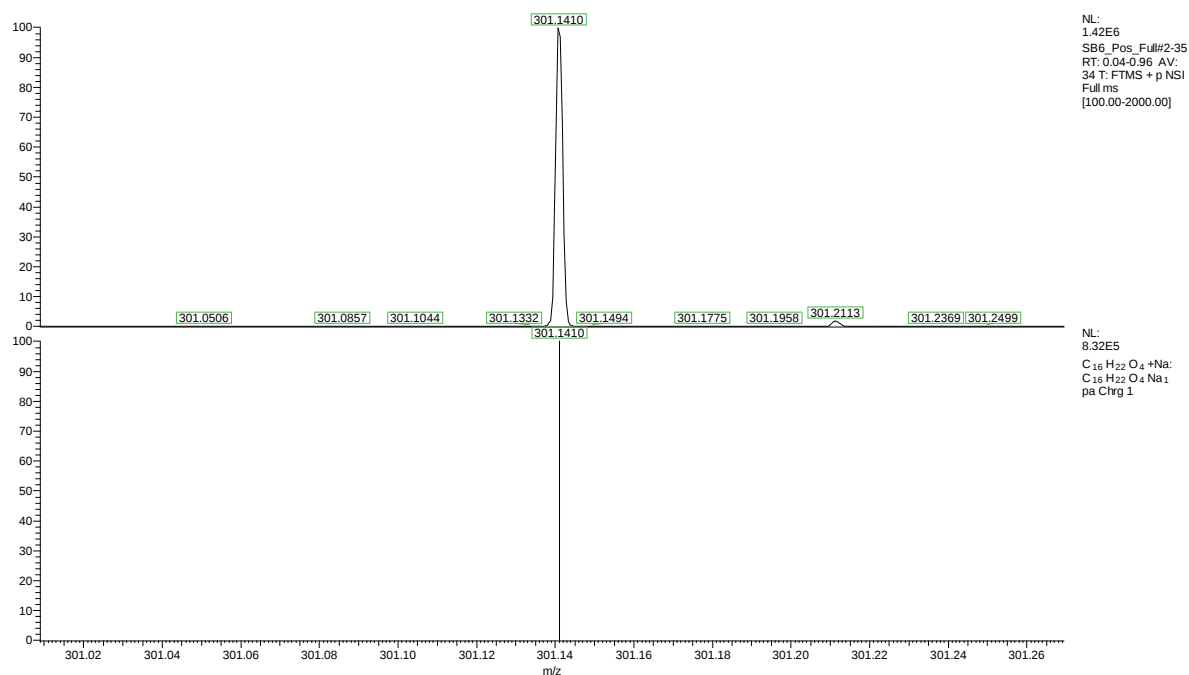


Figure S1.1.4. Detail of MS spectrum of *A. luminosa*, indicating the presence of a molecule with the formula C₁₆H₂₂O₄, most likely di-butyl phalate, an abundant environmental contaminant.

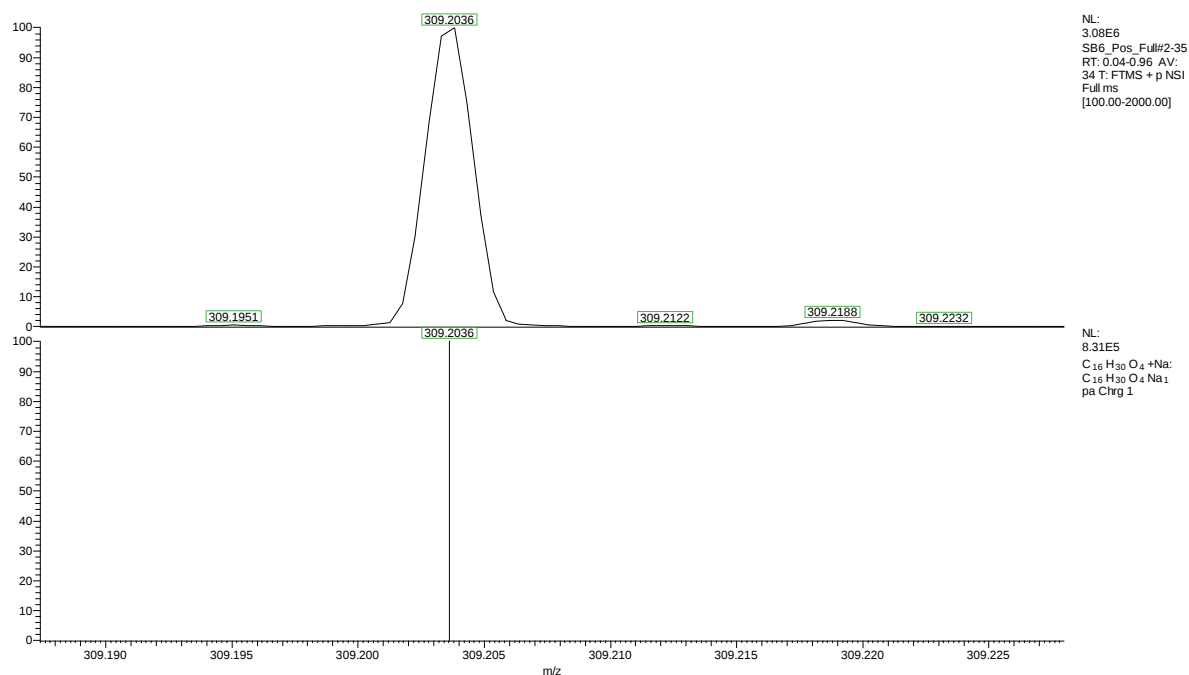


Figure S1.1.5. Detail of MS spectrum of *A. luminosa*, indicating the presence of a molecule with the formula $C_{16}H_{30}O_4$, most likely hexadecandioic acid or a similar isomer.

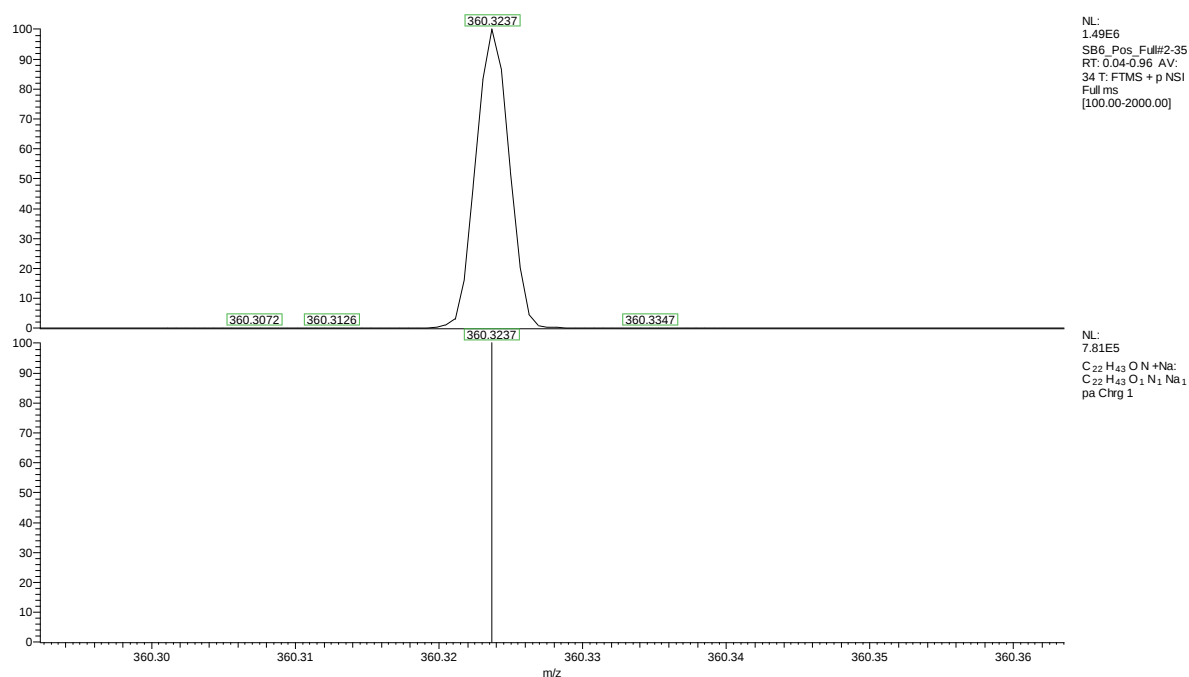


Figure S1.1.6. Detail of MS spectrum of *A. luminosa*, indicating the presence of a molecule with the formula $C_{22}H_{43}O_1N_1$, which could be Erucamide, (13E)-13-Docosenamide or an isomer thereof.

S 1.2 *Arachnocampa tasmaniensis* (Tasmania)

SB2_Pos_Full_60-400 #1-18 RT: 0.01-0.96 AV: 18 NL: 4.11E5
T: FTMS + p NSI Full ms [60.00-400.00]

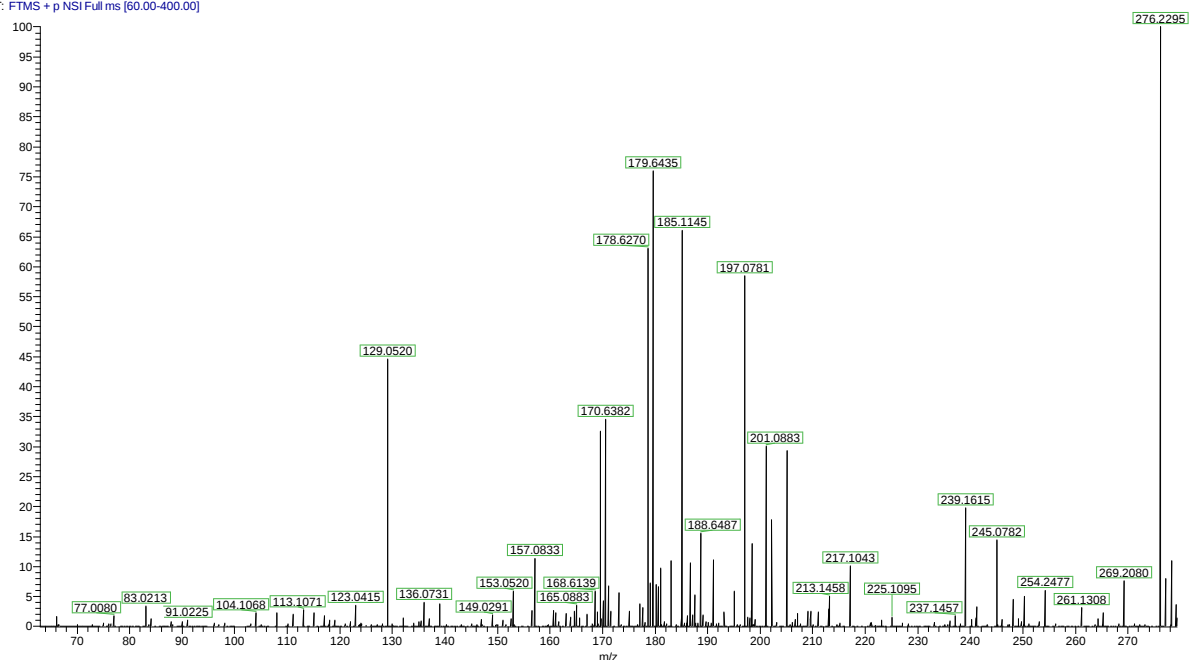


Figure S1.2.1. Detail of MS spectrum of *A. tasmaniensis*.

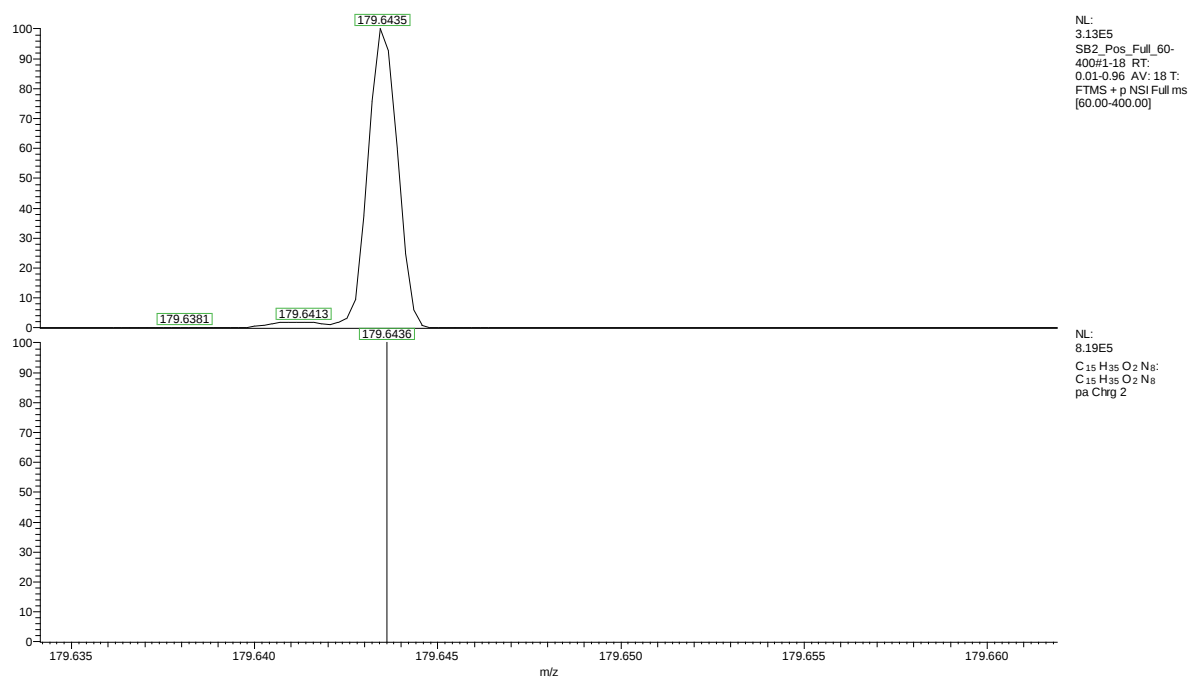


Figure S1.2.2. Detail of MS spectrum of *A. tasmaniensis*, indicating the presence of a molecule with the likely formula C₁₅H₃₅O₂N₈ (2+)

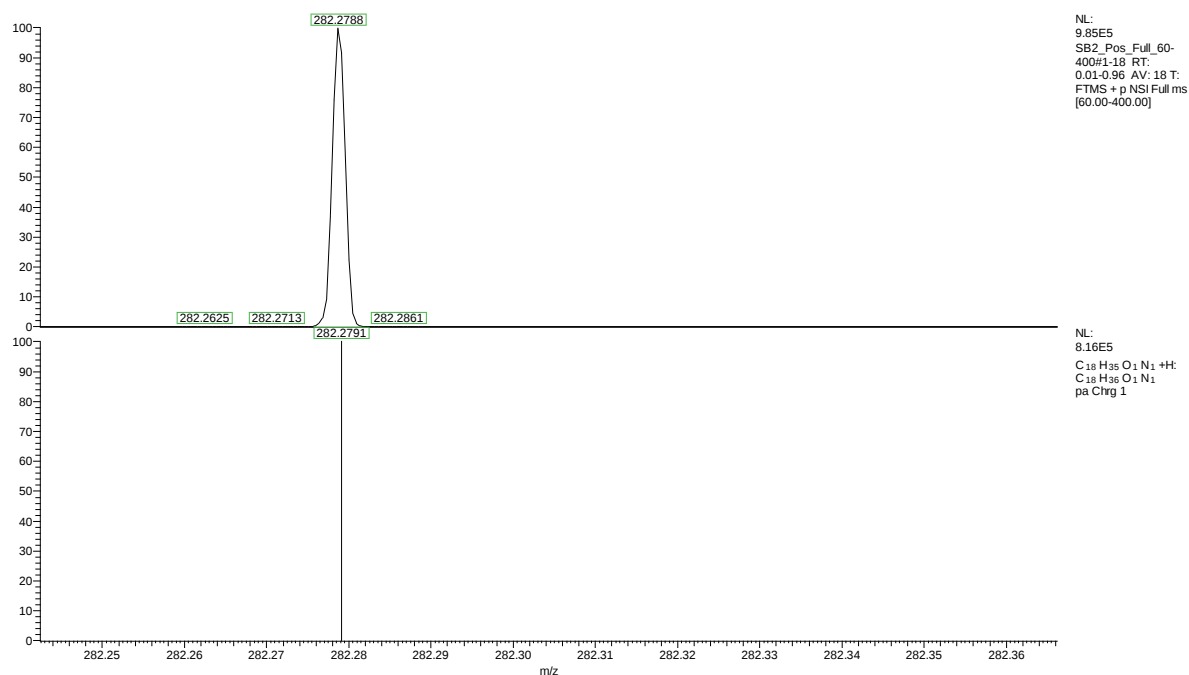


Figure S1.2.3. Detail of MS spectrum of *A. tasmaniensis*, indicating the presence of a molecule with the formula C18 H35 O1 N1, most likely 9Z)-9-Octadecenamide, 1-Dodecyl-2-azepanone or an isomer.

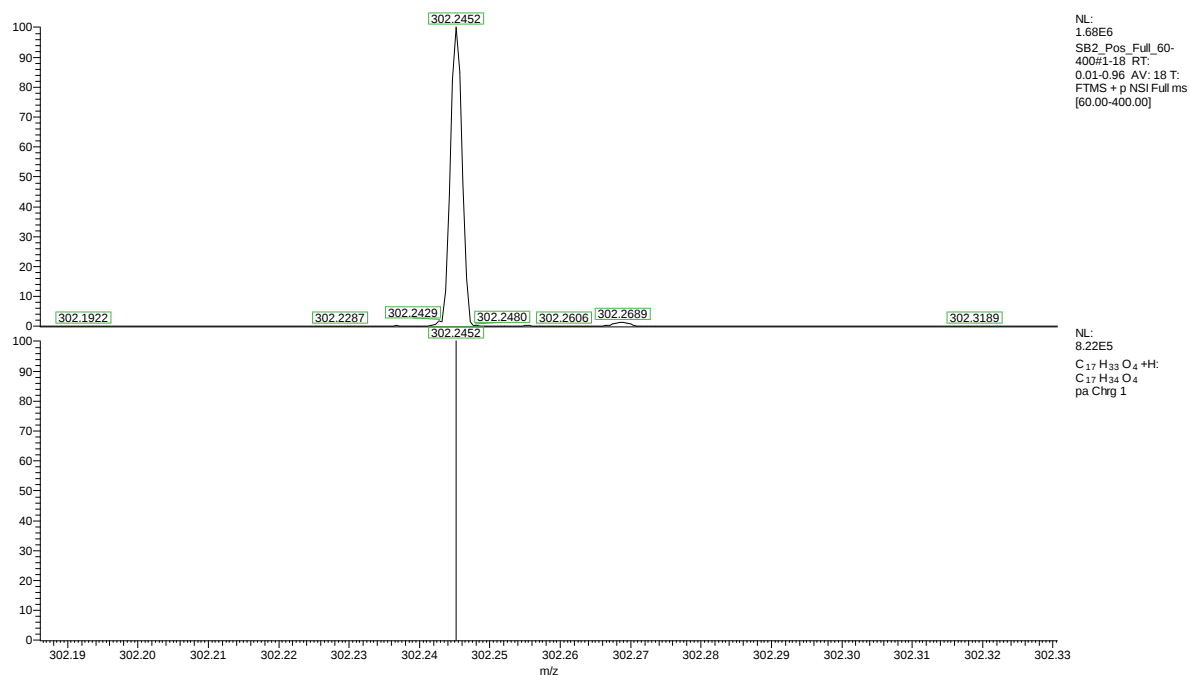


Figure S1.2.4. Detail of MS spectrum of *A. tasmaniensis*, indicating the presence of a molecule with the formula C17H33O4, i.e. [2-(Tridecyloxy)ethoxy]acetate.

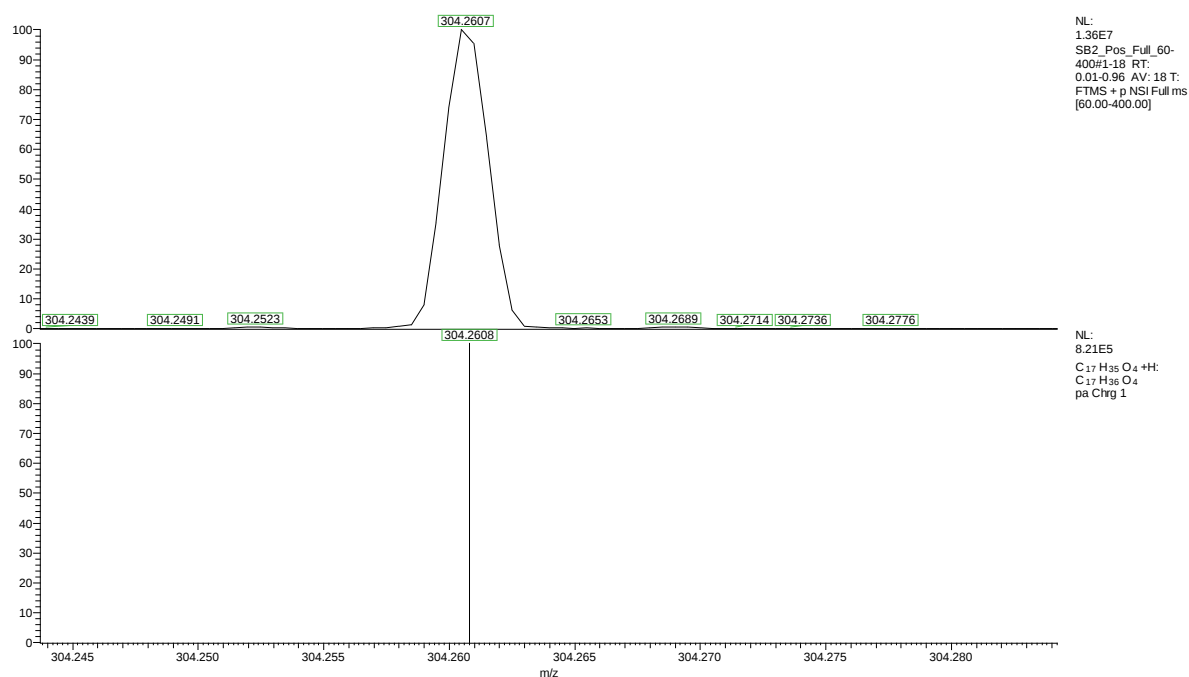


Figure S1.2.5. Detail of MS spectrum of *A. tasmaniensis*, indicating the presence of a molecule with the likely formula C₁₇H₃₅O₄.

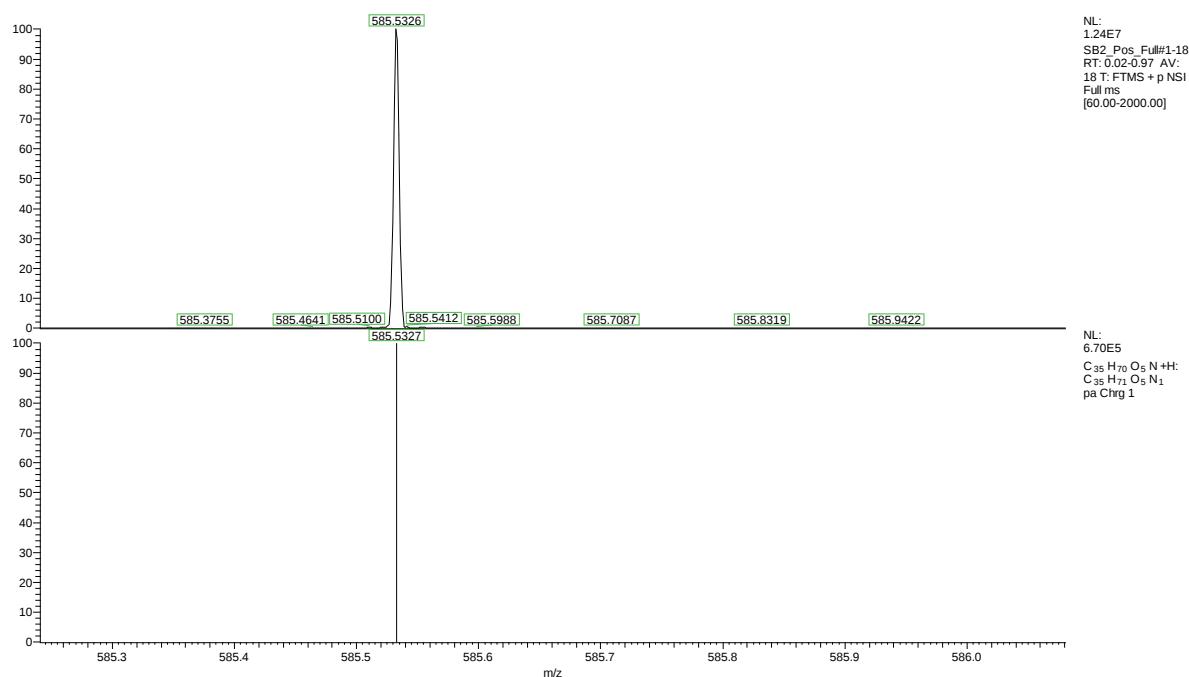


Figure S1.2.6. Detail of MS spectrum of *A. tasmaniensis*, indicating the presence of a molecule with the most likely formula C₃₅H₇₀O₅N₁, which could be N-(2-Hydroxyethyl)-N,N-dimethyl-1,2-bis(tetradecanoyloxy)-1-propanaminium or a similar isomer.

S1.3 *Arachnocampa richardsae* (New South Wales)

SB1_Pos_Full#1-18 RT: 0.02-0.97 AV: 18 NL: 2.79E7
T: FTMS + p NSI Full ms [100.00-2000.00]

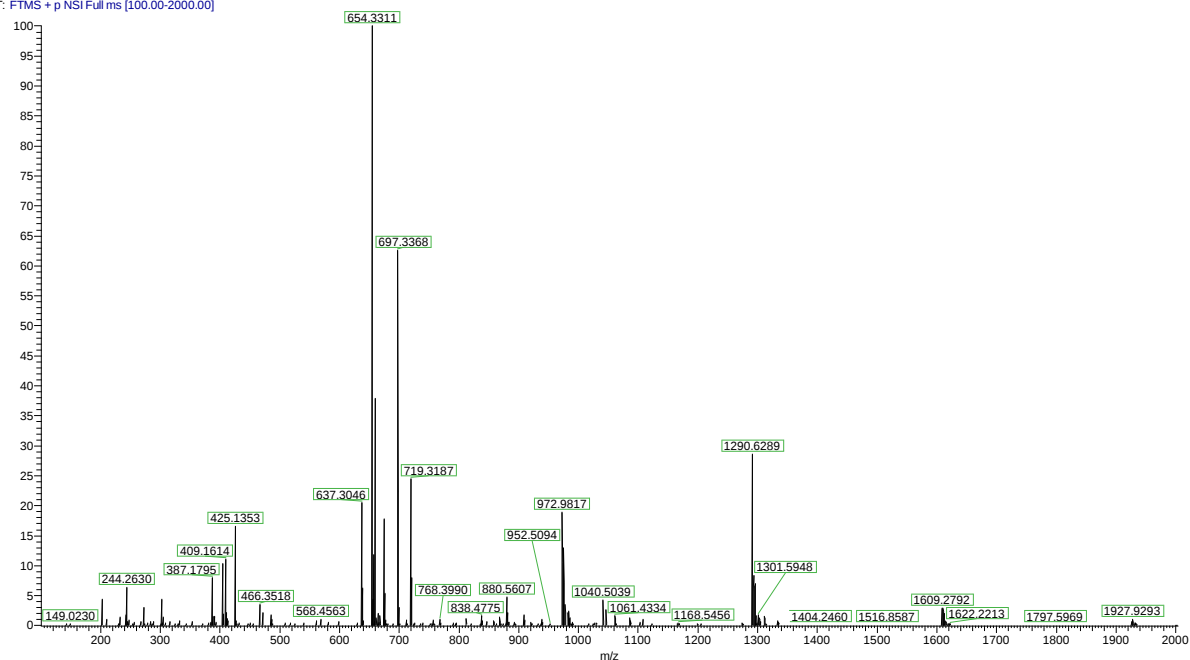


Figure S1.3.1. MS spectrum of *A. richardsae*.

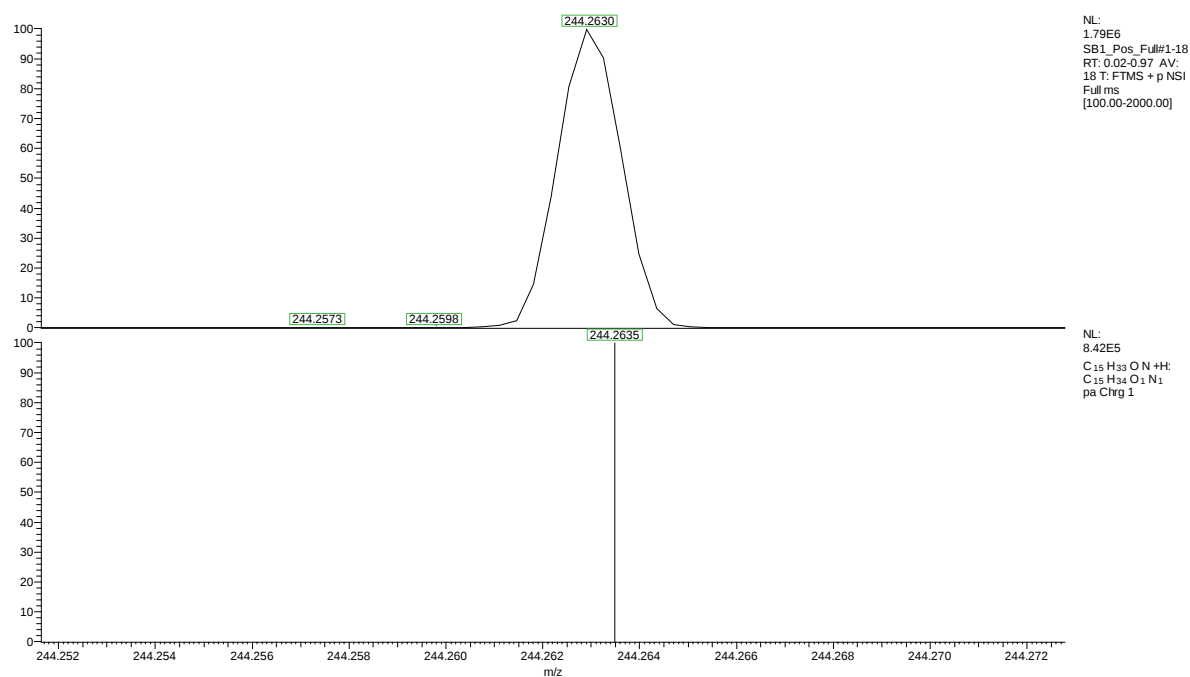


Figure S1.3.2. Detail of MS spectrum of *A. richardsae*, indicating the presence of a molecule with the most likely formula C₁₅H₃₃O₁N₁, which could be 3-(Dodecyloxy)-1-propanamine (Laurixamine) or an isomer.

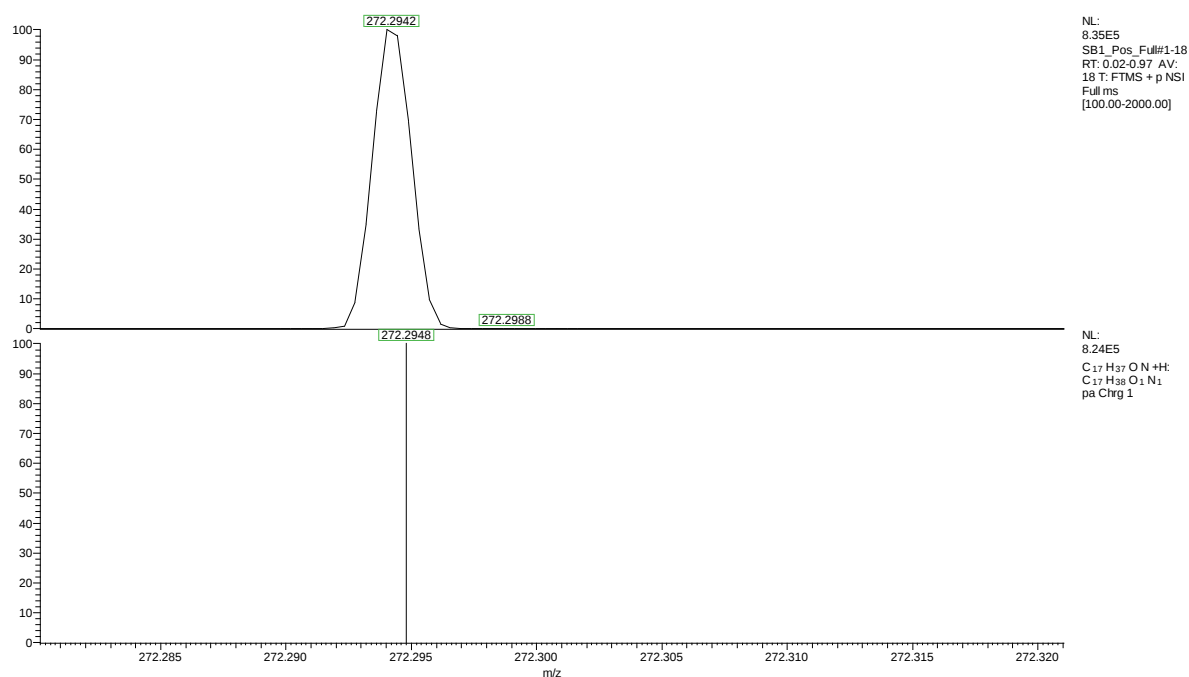


Figure S1.3.3. Detail of MS spectrum of *A. richardsae*, indicating the presence of a molecule with the most likely formula C₁₇H₃₇O₁N₁.

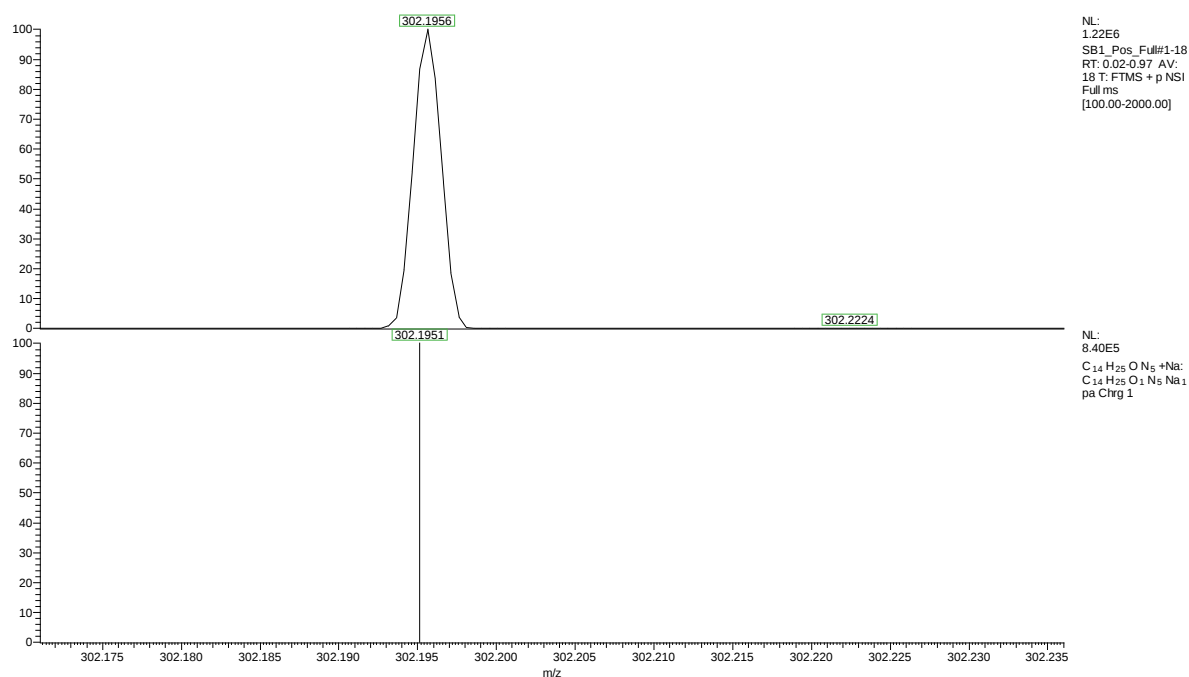


Figure S1.3.4. Detail of MS spectrum of *A. richardsae*, indicating the presence of a molecule with the most likely formula C₁₄H₂₅O₁N₅.

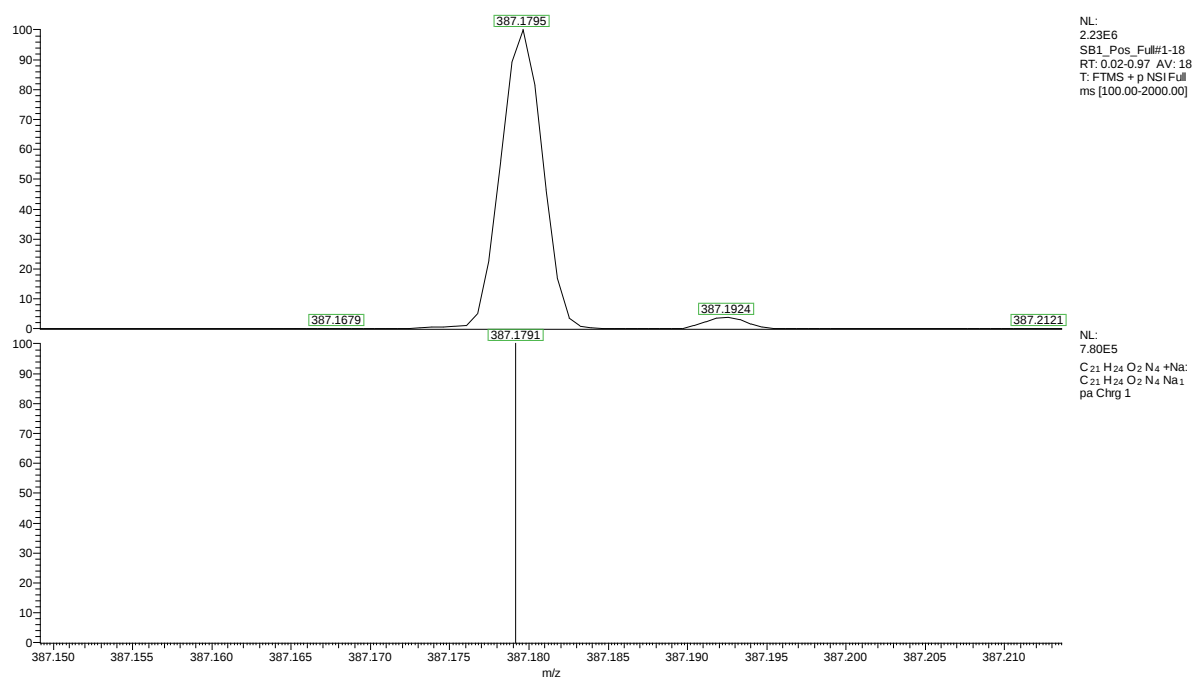


Figure S1.3.5. Detail of MS spectrum of *A. richardsae*, indicating the presence of a molecule with the most likely formula C₂₁H₂₄O₂N₄.

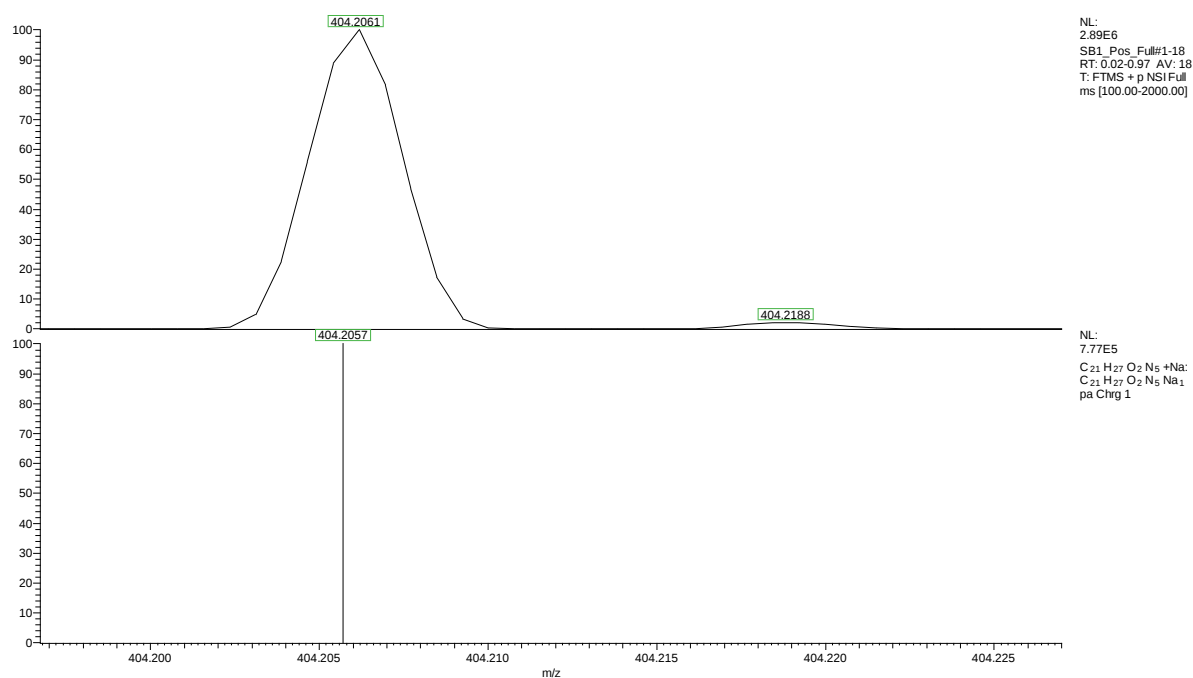


Figure S1.3.6. Detail of MS spectrum of *A. richardsae*, indicating the presence of a molecule with the most likely formula C₂₁H₂₇O₂N₅.

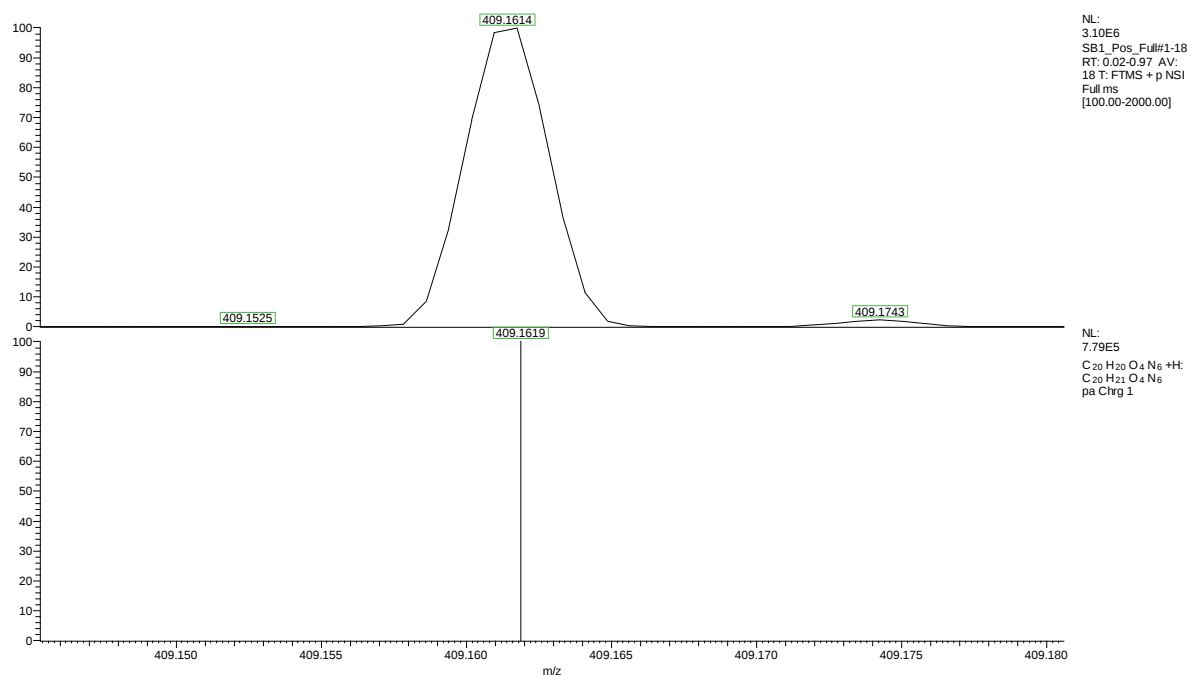


Figure S1.3.7. Detail of MS spectrum of *A. richardsae*, indicating the presence of a molecule with the most likely formula $C_{20}H_{20}O_4N_6$, which could be 1-{2-[(6-Amino-1-benzyl-2,4-dioxo-1,2,3,4-tetrahydro-5-pyrimidinyl)(methyl)amino]-2-oxoethyl}-3-carbamoylpyridinium or a similar isomer.

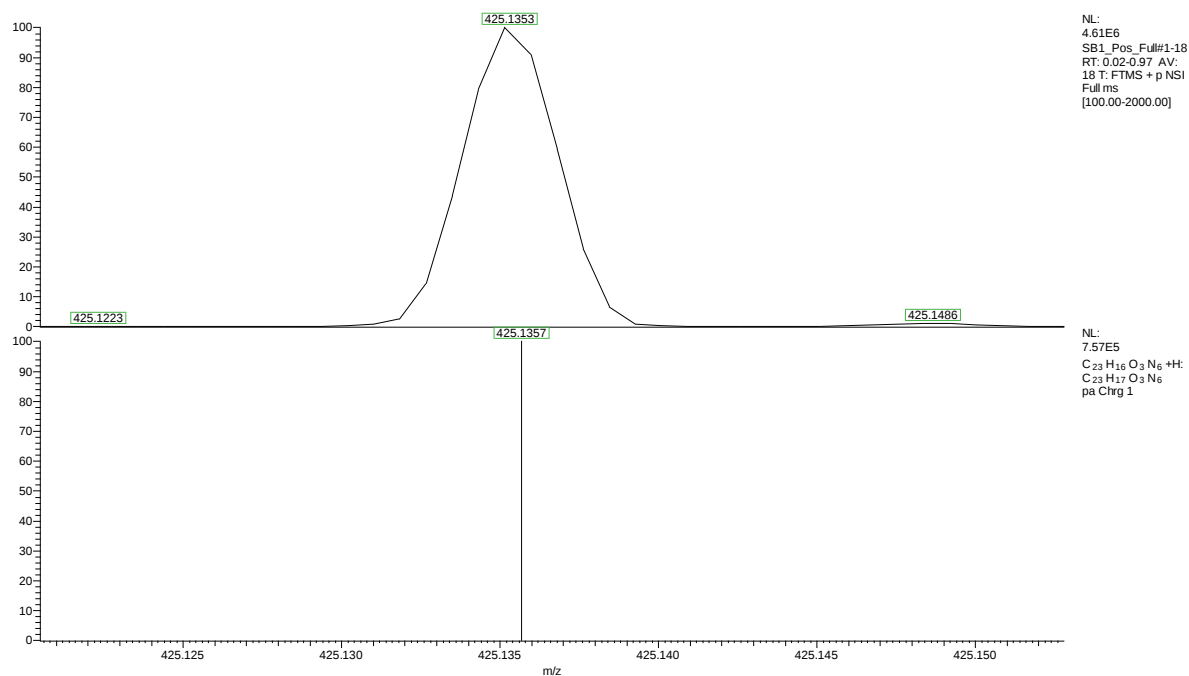


Figure S1.3.8. Detail of MS spectrum of *A. richardsae*, indicating the presence of a molecule with the most likely formula $C_{23}H_{16}O_3N_6$.

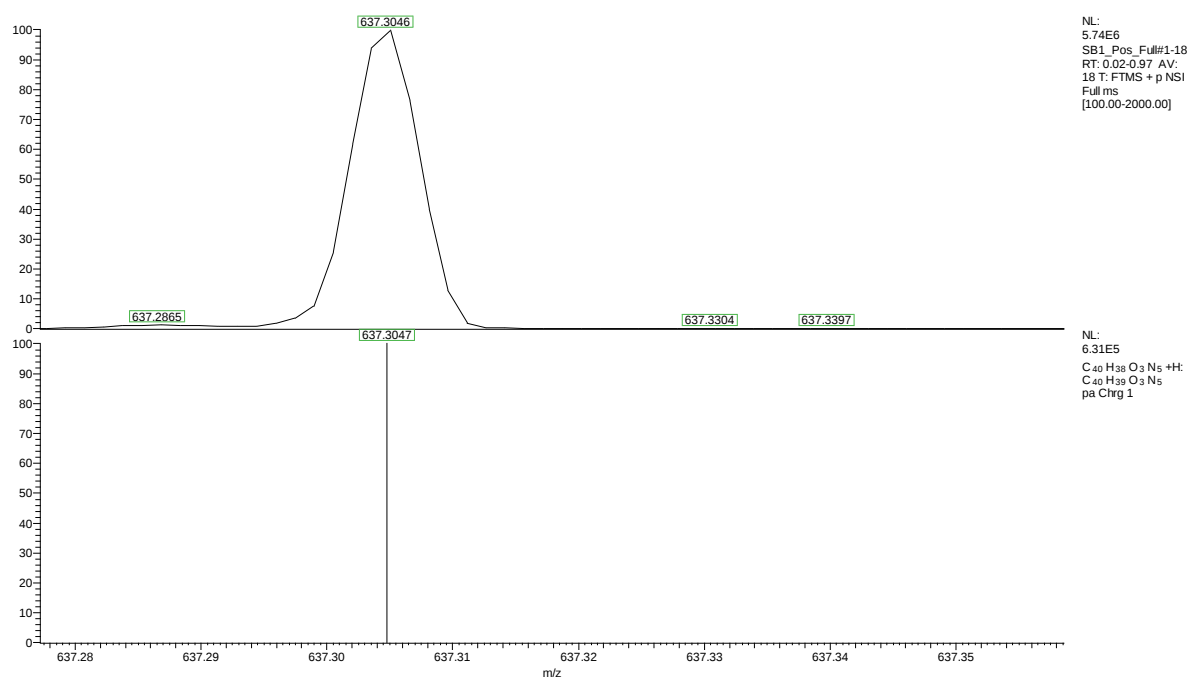


Figure S1.3.9. Detail of MS spectrum of *A. richardsae*, indicating the presence of a molecule with the most likely formula C₄₀H₃₈O₃N₅.

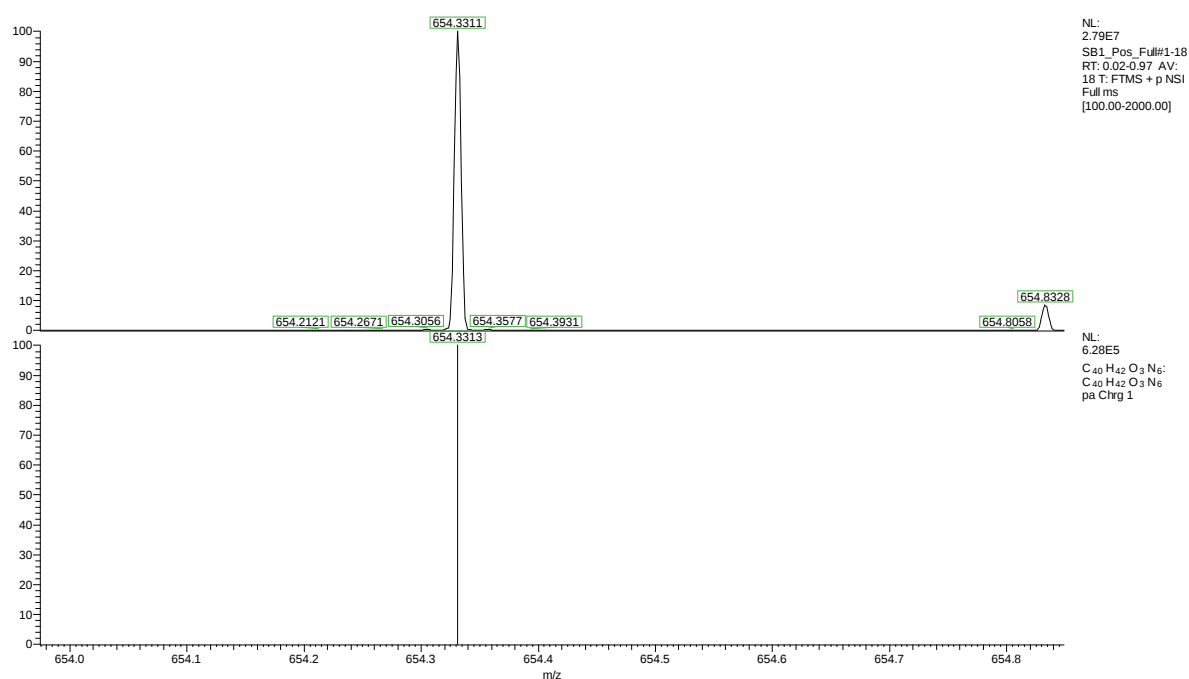


Figure S1.3.10. Detail of MS spectrum of *A. richardsae*, indicating the presence of a molecule with the most likely formula C₄₀H₄₂O₃N₆, which could be 2-Cyano-N-[2-(3,4-diethoxyphenyl)ethyl]-2-{3-[4-(diphenylmethyl)-1-piperazinyl]-2-quinoxaliny]acetamide or a similar isomer.

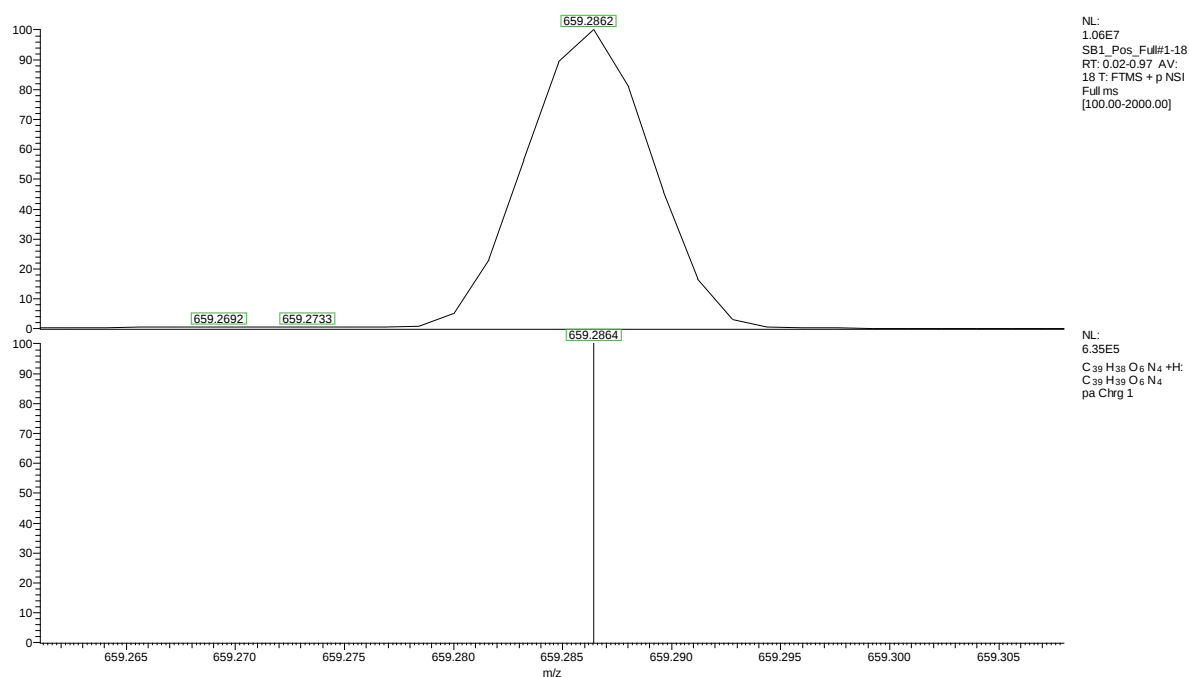


Figure S1.3.11. Detail of MS spectrum of *A. richardsae*, indicating the presence of a molecule with the most likely formula C₃₉H₃₈O₆N₄.

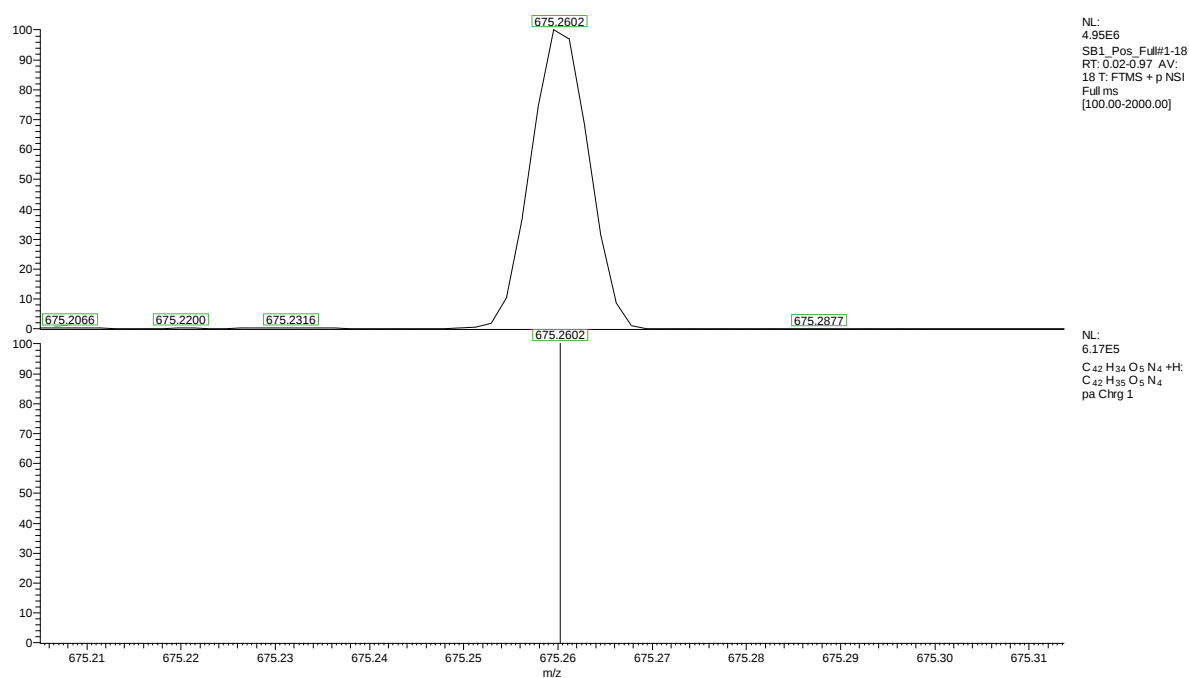


Figure S1.3.12. Detail of MS spectrum of *A. richardsae*, indicating the presence of a molecule with the most likely formula C₄₂H₃₄O₅N₄, which matches 5-(4-Methoxyphenyl)-2,3-bis(4-nitrophenyl)-1,4,7-triphenyl-2,3,4,5-tetrahydro-1H-1,4-diazepine.

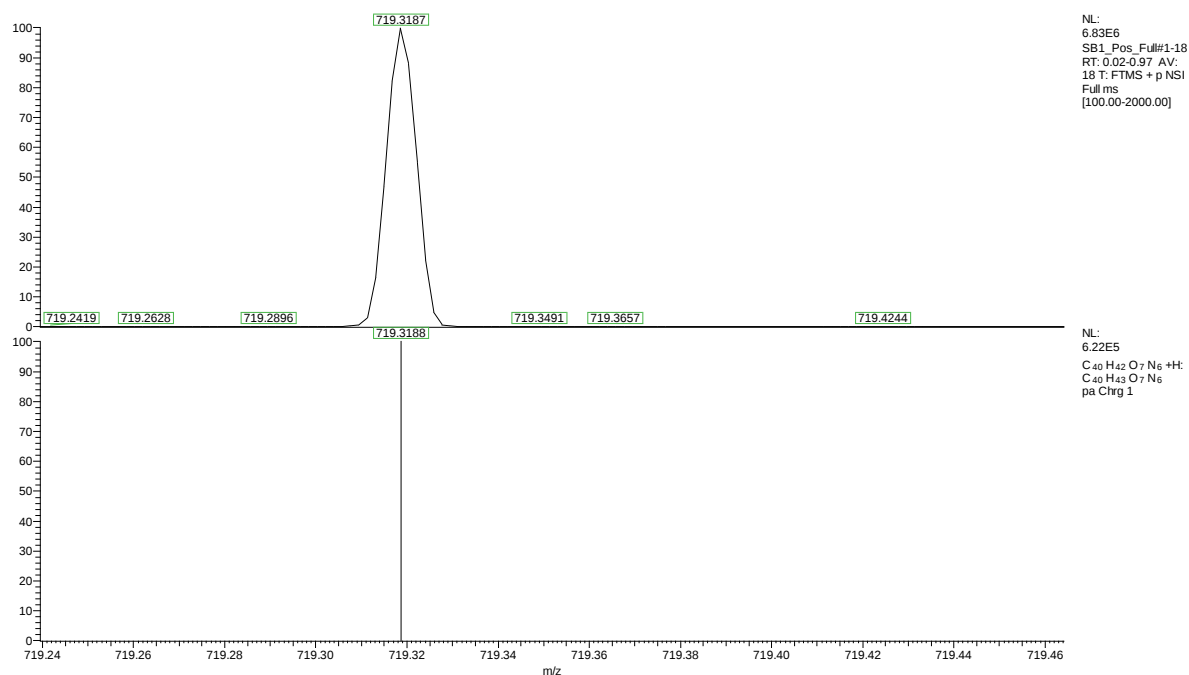


Figure S1.3.13. Detail of MS spectrum of *A. richardsae*, indicating the presence of a molecule with the most likely formula C₄₀H₄₂O₇N₆, which could be Glycylphenylalanyltyrosyltryptophylphenylalanine or a similar isomer (note that 10 isomers are very similar).

S2 Full list of compounds identified from *Arachnocampa* glue with solution state NMR

S1.1 *Arachnocampa luminosa* (New Zealand, North Island)

Table S1.1.1. Results of Bayesil analysis for adhesives of North Island *A. luminosa*.

HMDB ID	Compound Name	Concentration (~μM)	Threshold	Confidence Score
HMDB00042	Acetic acid	0	1.1	10
HMDB00043	Betaine	0	1.6	10
HMDB00087	Dimethylamine	0.7	1.6	10
HMDB00094	Citric acid	5.4	1.6	10
HMDB00097	Choline	0	0.5	10
HMDB00122	D-Glucose	9.2	7.8	10
HMDB00123	Glycine	1.3	1.6	10
HMDB00148	L-Glutamic acid	0	1.6	10
HMDB00157	Hypoxanthine	0	1.6	10
HMDB00158	Tyrosine	9.9	1.6	10
HMDB00159	L-Phenylalanine	5	1.6	10
HMDB00161	L-Alanine	0.5	3.1	10
HMDB00162	L-Proline	2.3	1.6	10
HMDB00190	L-Lactic acid	6.7	3.1	10
HMDB00267	Pyroglutamic acid	1.4	1.6	10
HMDB00357	3-Hydroxybutyric acid	5.5	1.6	10
HMDB00407	2-Hydroxyisovalerate	0.3	1.6	10
HMDB00562	Creatinine	0.1	1.6	10
HMDB00641	L-Glutamine	9.3	1.6	10
HMDB00687	L-Leucine	2	1.6	10
HMDB00696	Methionine	1.1	1.6	10
HMDB00863	Isopropyl alcohol	1.2	1.6	10
HMDB00883	Valine	0.9	3.1	10
HMDB01659	Acetone	0.8	1.6	10
HMDB01873	Isobutyric acid	0.6	1.2	10
HMDB01875	Methanol	7.8	3.1	10
HMDB01881	Propylene glycol	0.3	1.6	10
HMDB04983	Dimethyl sulfone	5.3	1.6	10
HMDB15109	EDTAmg	0.1	1.6	10
HMDB00008	2-Hydroxybutyric acid	3.5	1.6	9
HMDB00023	3-Hydroxyisobutyrate	1.7	1.6	9
HMDB00062	Carnitine	0	1.6	9
HMDB00108	Ethanol	2	1.6	9
HMDB00131	Glycerol	3.1	1.6	9
HMDB00142	Formate	1.4	1.2	9
HMDB00167	L-Threonine	6.5	1.6	9
HMDB00182	L-Lysine	2.6	1.6	9
HMDB00191	Aspartate	5.1	3.9	9
HMDB00211	Myo-inositol	0	1.6	9
HMDB00060	Acetoacetate	0.3	1.6	8
HMDB00243	Pyruvic acid	1	1.6	8
HMDB00254	Succinate	6.7	1.6	8
HMDB00294	Urea	21.5	77.8	8
HMDB00064	Creatine	1.1	1.6	7
HMDB00172	Isoleucine	2.7	1.6	7
HMDB00177	L-Histidine	4.1	1.6	7
HMDB00292	Xanthine	0.6	1.6	7
HMDB00660	Fructose	0	1.6	7
HMDB00691	Malonate	0	3.1	7
HMDB00214	L-Ornithine	3.3	4.7	6
HMDB00517	L-Arginine	0	1.6	6
HMDB00754	3-Hydroxyisovaleric acid	86	1.6	6
HMDB00001	1-Methylhistidine	26.1	1.6	5
HMDB00929	Tryptophan	2.3	4.7	5
HMDB00187	L-Serine	14.5	1.6	4
HMDB00168	L-Asparagine	3.8	4.7	3
HMDB00169	Mannose	0	3.1	3
HMDB00192	L-Cystine	1.5	3.1	3
HMDB00574	L-Cysteine	0	3.1	3
-	DSS	500	0.2	
HMDB00019	Alpha-ketoisovaleric acid	7	1.6	

HMDB00020	p-Hydroxyphenylacetic acid	0.3	1.6
HMDB00039	Butyrate	2.9	1.6
HMDB00044	Ascorbic acid	0	1.6
HMDB00092	Dimethylglycine	3.7	1.6
HMDB00115	Glycolate	13.1	1.6
HMDB00128	Guanidoacetate	0	1.6
HMDB00134	Fumaric acid	0.7	1.6
HMDB00143	D-Galactose	2.7	1.6
HMDB00149	Ethanolamine	1.7	1.6
HMDB00164	Methylamine	22.3	1.6
HMDB00174	L-Fucose	5.5	1.6
HMDB00186	Alpha-Lactose	0	1.6
HMDB00202	Methylmalonic acid	15.5	1.6
HMDB00208	2-Oxopentanedioate	1.2	1.6
HMDB00209	Phenylacetate	0	1.6
HMDB00223	Oxalacetic acid	1	1.6
HMDB00247	Sorbitol	0	1.6
HMDB00251	Taurine	2.1	1.6
HMDB00271	Sarcosine	3.1	1.6
HMDB00300	Uracil	1.2	1.6
HMDB00479	3-Methylhistidine	38.6	1.6
HMDB00625	Gluconic acid	0	1.6
HMDB00714	Hippuric acid	0.7	1.6
HMDB00718	Isovaleric acid	7.6	1.6
HMDB00755	Hydroxyphenyllactic acid	2.5	1.6
HMDB00906	Trimethylamine	0.2	1.6
HMDB01565	Phosphorylcholine	0	1.6
HMDB01847	Caffeine	0.2	1.6
HMDB03355	5-Aminopentanoate	1.1	1.6
HMDB11635	p-Cresol sulfate	3.9	1.6

S1.2 *Arachnocampa luminosa* (New Zealand, South Island)

Table S1.2.1. Results of Bayesil analysis for adhesives of South Island *A. luminosa*.

HMDB ID	Compound Name	Concentration	Confidence	
		(~µM)	Threshold	Score
HMDB00042	Acetic acid	39.9	1.8	10
HMDB00043	Betaine	20.7	2.6	10
HMDB00087	Dimethylamine	0.5	2.6	10
HMDB00094	Citric acid	1.3	2.6	10
HMDB00097	Choline	0	0.8	10
HMDB00122	D-Glucose	25.5	12.8	10
HMDB00123	Glycine	0	2.6	10
HMDB00148	L-Glutamic acid	16.3	2.6	10
HMDB00157	Hypoxanthine	0.1	2.6	10
HMDB00158	Tyrosine	42.3	2.6	10
HMDB00159	L-Phenylalanine	5.1	2.6	10
HMDB00161	L-Alanine	1.1	5.1	10
HMDB00162	L-Proline	7.9	2.6	10
HMDB00190	L-Lactic acid	4	5.1	10
HMDB00267	Pyroglutamic acid	2.3	2.6	10
HMDB00357	3-Hydroxybutyric acid	5.6	2.6	10
HMDB00407	2-Hydroxyisovalerate	2.7	2.6	10
HMDB00562	Creatinine	0	2.6	10
HMDB00641	L-Glutamine	6.8	2.6	10
HMDB00687	L-Leucine	6.2	2.6	10
HMDB00696	Methionine	3.7	2.6	10
HMDB00863	Isopropyl alcohol	4	2.6	10
HMDB00883	Valine	4.7	5.1	10
HMDB01659	Acetone	6.9	2.6	10
HMDB01873	Isobutyric acid	3.4	2	10
HMDB01875	Methanol	12.3	5.1	10
HMDB01881	Propylene glycol	1.8	2.6	10
HMDB04983	Dimethyl sulfone	12.7	2.6	10
HMDB15109	EDTA mg	0.3	2.6	10
HMDB00008	2-Hydroxybutyric acid	7.8	2.6	9
HMDB00023	3-Hydroxyisobutyrate	0.3	2.6	9

HMDB00062	Carnitine	0	2.6	9
HMDB00108	Ethanol	148.4	2.6	9
HMDB00131	Glycerol	69.7	2.6	9
HMDB00142	Formate	36.1	2	9
HMDB00167	L-Threonine	10.7	2.6	9
HMDB00182	L-Lysine	2.9	2.6	9
HMDB00191	Aspartate	3.2	6.4	9
HMDB00211	Myo-inositol	4.5	2.6	9
HMDB00060	Acetoacetate	4.5	2.6	8
HMDB00243	Pyruvic acid	9.7	2.6	8
HMDB00254	Succinate	0.1	2.6	8
HMDB00294	Urea	124.9	128	8
HMDB00064	Creatine	0.3	2.6	7
HMDB00172	Isoleucine	4.5	2.6	7
HMDB00177	L-Histidine	6.5	2.6	7
HMDB00292	Xanthine	0.6	2.6	7
HMDB00660	Fructose	0	2.6	7
HMDB00691	Malonate	20.6	5.1	7
HMDB00214	L-Ornithine	0	7.7	6
HMDB00517	L-Arginine	0	2.6	6
HMDB00754	3-Hydroxyisovaleric acid	0.5	2.6	6
HMDB00001	1-Methylhistidine	97.7	2.6	5
HMDB00929	Tryptophan	2.1	7.7	5
HMDB00187	L-Serine	0	2.6	4
HMDB00168	L-Asparagine	5.2	7.7	3
HMDB00169	Mannose	0	5.1	3
HMDB00192	L-Cystine	0.1	5.1	3
HMDB00574	L-Cysteine	0	5.1	3
-	TSP	500	0.3	
HMDB00019	Alpha-ketoisovaleric acid	27.2	2.6	
HMDB00020	p-Hydroxyphenylacetic acid	8.2	2.6	
HMDB00039	Butyrate	5.4	2.6	
HMDB00044	Ascorbic acid	15.8	2.6	
HMDB00092	Dimethylglycine	0.3	2.6	
HMDB00115	Glycolate	29	2.6	
HMDB00128	Guanidoacetate	0	2.6	
HMDB00134	Fumaric acid	0.7	2.6	
HMDB00143	D-Galactose	5.2	2.6	
HMDB00149	Ethanolamine	1.4	2.6	
HMDB00164	Methylamine	0.6	2.6	
HMDB00174	L-Fucose	16.1	2.6	
HMDB00186	Alpha-Lactose	0	2.6	
HMDB00202	Methylmalonic acid	148.8	2.6	
HMDB00208	2-Oxopentanedioate	1.8	2.6	
HMDB00209	Phenylacetate	0.5	2.6	
HMDB00223	Oxalacetic acid	22.4	2.6	
HMDB00247	Sorbitol	37.5	2.6	
HMDB00251	Taurine	0	2.6	
HMDB00271	Sarcosine	1.4	2.6	
HMDB00300	Uracil	0	2.6	
HMDB00479	3-Methylhistidine	5.9	2.6	
HMDB00625	Gluconic acid	0	2.6	
HMDB00714	Hippuric acid	0.4	2.6	
HMDB00718	Isovaleric acid	1.5	2.6	
HMDB00755	Hydroxyphenyllactic acid	1.5	2.6	
HMDB00906	Trimethylamine	0.1	2.6	
HMDB01565	Phosphorylcholine	0	2.6	
HMDB01847	Caffeine	0.6	2.6	
HMDB03355	5-Aminopentanoate	11.4	2.6	
HMDB11635	p-Cresol sulfate	1.6	2.6	

S1.3 *Arachnocampa tasmaniensis* (Tasmania)

Table S1.3.1. Results of Bayesil analysis for adhesives of *A. tasmaniensis*.

HMDB ID	Compound Name	Concentration (~μM)	Threshold	Confidence Score
HMDB00042	Acetic acid	6.1	2.1	10
HMDB00043	Betaine	0.3	3	10
HMDB00094	Citric acid	4.7	3	10
HMDB00097	Choline	0	0.9	10
HMDB00122	D-Glucose	21.7	15.1	10
HMDB00123	Glycine	7.5	3	10
HMDB00148	L-Glutamic acid	5.1	3	10
HMDB00157	Hypoxanthine	0.3	3	10
HMDB00158	Tyrosine	45	3	10
HMDB00159	L-Phenylalanine	4.8	3	10
HMDB00161	L-Alanine	15	6	10
HMDB00162	L-Proline	11.8	3	10
HMDB00190	L-Lactic acid	24.2	6	10
HMDB00267	Pyroglutamic acid	0	3	10
HMDB00357	3-Hydroxybutyric acid	9.1	3	10
HMDB00407	2-Hydroxyisovalerate	0.7	3	10
HMDB00562	Creatinine	1.3	3	10
HMDB00641	L-Glutamine	19.7	3	10
HMDB00687	L-Leucine	14.6	3	10
HMDB00696	Methionine	3.4	3	10
HMDB00863	Isopropyl alcohol	0	3	10
HMDB00883	Valine	14.3	6	10
HMDB01659	Acetone	2.2	3	10
HMDB01873	Isobutyric acid	1.8	2.4	10
HMDB01875	Methanol	2.9	6	10
HMDB01881	Propylene glycol	0.9	3	10
HMDB15109	EDTAmg	0.2	3	10
HMDB00008	2-Hydroxybutyric acid	4.1	3	9
HMDB00023	3-Hydroxyisobutyrate	0	3	9
HMDB00062	Carnitine	0.2	3	9
HMDB00108	Ethanol	83.9	3	9
HMDB00131	Glycerol	30.2	3	9
HMDB00142	Formate	31.4	2.4	9
HMDB00167	L-Threonine	15.2	3	9
HMDB00182	L-Lysine	5.3	3	9
HMDB00191	Aspartate	4.6	7.5	9
HMDB00211	Myo-inositol	4.3	3	9
HMDB00060	Acetoacetate	0	3	8
HMDB00254	Succinate	1.6	3	8
HMDB00294	Urea	260.4	150.9	8
HMDB00064	Creatine	1	3	7
HMDB00172	Isoleucine	11.6	3	7
HMDB00177	L-Histidine	0	3	7
HMDB00292	Xanthine	9	3	7
HMDB00660	Fructose	0.8	3	7
HMDB00691	Malonate	2	6	7
HMDB00214	L-Ornithine	9.8	9.1	6
HMDB00517	L-Arginine	0.3	3	6
HMDB00754	3-Hydroxyisovaleric acid	1.1	3	6
HMDB00001	1-Methylhistidine	73.1	3	5
HMDB00929	Tryptophan	9.4	9.1	5
HMDB00187	L-Serine	0	3	4
HMDB00168	L-Asparagine	22.9	9.1	3
HMDB00169	Mannose	1.1	6	3
HMDB00192	L-Cystine	0	6	3
HMDB00574	L-Cysteine	3.1	6	3
-	TSP	5000	0.3	
HMDB00019	Alpha-ketoisovaleric acid	9.1	3	
HMDB00020	p-Hydroxyphenylacetic acid	3.8	3	
HMDB00039	Butyrate	10.2	3	
HMDB00044	Ascorbic acid	0	3	
HMDB00092	Dimethylglycine	0	3	
HMDB00115	Glycolate	1.3	3	
HMDB00128	Guanidoacetate	1.6	3	

HMDB00134	Fumaric acid	2.2	3
HMDB00143	D-Galactose	3.8	3
HMDB00149	Ethanolamine	0.4	3
HMDB00174	L-Fucose	9.2	3
HMDB00186	Alpha-Lactose	0	3
HMDB00202	Methylmalonic acid	38.1	3
HMDB00208	2-Oxopentanedioate	7.2	3
HMDB00209	Phenylacetate	0.8	3
HMDB00247	Sorbitol	6.2	3
HMDB00251	Taurine	2	3
HMDB00271	Sarcosine	0.8	3
HMDB00300	Uracil	6.6	3
HMDB00479	3-Methylhistidine	7.5	3
HMDB00625	Gluconic acid	2.2	3
HMDB00714	Hippuric acid	2.2	3
HMDB00718	Isovaleric acid	0	3
HMDB00755	Hydroxyphenyllactic acid	5.2	3
HMDB00906	Trimethylamine	0.6	3
HMDB01565	Phosphorylcholine	0	3
HMDB01847	Caffeine	3.6	3
HMDB03355	5-Aminopentanoate	5.6	3
HMDB11635	p-Cresol sulfate	1.2	3

S1.4 *Arachnocampa richardsae* (New South Wales)

Table S1.4.1. Results of Bayesil analysis for adhesives of *A. richardsae*.

HMDB ID	Compound Name	Concentration (~μM)	Threshold	Confidence Score
HMDB00042	Acetic acid	0.2	0.7	10
HMDB00043	Betaine	0	1	10
HMDB00087	Dimethylamine	0.7	1	10
HMDB00094	Citric acid	1.3	1	10
HMDB00097	Choline	1.4	0.3	10
HMDB00122	D-Glucose	3.2	4.8	10
HMDB00123	Glycine	0.6	1	10
HMDB00148	L-Glutamic acid	8.5	1	10
HMDB00157	Hypoxanthine	0.1	1	10
HMDB00158	Tyrosine	0.1	1	10
HMDB00159	L-Phenylalanine	0.6	1	10
HMDB00161	L-Alanine	0	1.9	10
HMDB00162	L-Proline	0	1	10
HMDB00190	L-Lactic acid	2.9	1.9	10
HMDB00267	Pyroglutamic acid	1.5	1	10
HMDB00357	3-Hydroxybutyric acid	1	1	10
HMDB00407	2-Hydroxyisovalerate	2	1	10
HMDB00562	Creatinine	0.2	1	10
HMDB00641	L-Glutamine	1.8	1	10
HMDB00687	L-Leucine	3.1	1	10
HMDB00696	Methionine	0.7	1	10
HMDB00863	Isopropyl alcohol	1.3	1	10
HMDB00883	Valine	5.8	1.9	10
HMDB01659	Acetone	0.1	1	10
HMDB01873	Isobutyric acid	3.5	0.8	10
HMDB01875	Methanol	76.8	1.9	10
HMDB01881	Propylene glycol	0.1	1	10
HMDB04983	Dimethyl sulfone	0	1	10
HMDB15109	EDTAmg	0	1	10
HMDB00008	2-Hydroxybutyric acid	0	1	9
HMDB00023	3-Hydroxyisobutyrate	1.6	1	9
HMDB00062	Carnitine	0.9	1	9
HMDB00108	Ethanol	3.1	1	9
HMDB00131	Glycerol	0.1	1	9
HMDB00142	Formate	0.6	0.8	9
HMDB00167	L-Threonine	1.7	1	9
HMDB00182	L-Lysine	1.6	1	9
HMDB00191	Aspartate	2.9	2.4	9
HMDB00211	Myo-inositol	0.5	1	9

HMDB00060	Acetoacetate	0	1	8
HMDB00243	Pyruvic acid	0.1	1	8
HMDB00254	Succinate	0.5	1	8
HMDB00294	Urea	7.2	47.6	8
HMDB00064	Creatine	0.2	1	7
HMDB00172	Isoleucine	66.3	1	7
HMDB00177	L-Histidine	0	1	7
HMDB00292	Xanthine	0.3	1	7
HMDB00660	Fructose	0.5	1	7
HMDB00691	Malonate	0	1.9	7
HMDB00214	L-Ornithine	1.5	2.9	6
HMDB00517	L-Arginine	2.4	1	6
HMDB00754	3-Hydroxyisovaleric acid	0.1	1	6
HMDB00001	1-Methylhistidine	0	1	5
HMDB00929	Tryptophan	0.3	2.9	5
HMDB00187	L-Serine	0.3	1	4
HMDB00168	L-Asparagine	2.4	2.9	3
HMDB00169	Mannose	0.7	1.9	3
HMDB00192	L-Cystine	0	1.9	3
HMDB00574	L-Cysteine	0	1.9	3
-	TSP	500	0.1	
HMDB00019	Alpha-ketoisovaleric acid	3.5	1	
HMDB00020	p-Hydroxyphenylacetic acid	0.2	1	
HMDB00039	Butyrate	1.9	1	
HMDB00044	Ascorbic acid	0.1	1	
HMDB00092	Dimethylglycine	0.1	1	
HMDB00115	Glycolate	0	1	
HMDB00128	Guanidoacetate	0.7	1	
HMDB00134	Fumaric acid	0.6	1	
HMDB00143	D-Galactose	0	1	
HMDB00149	Ethanolamine	0	1	
HMDB00164	Methylamine	1.2	1	
HMDB00174	L-Fucose	0.4	1	
HMDB00186	Alpha-Lactose	0.1	1	
HMDB00202	Methylmalonic acid	2.5	1	
HMDB00208	2-Oxopentanedioate	4	1	
HMDB00209	Phenylacetate	0	1	
HMDB00223	Oxalacetic acid	0.2	1	
HMDB00247	Sorbitol	0	1	
HMDB00251	Taurine	0.2	1	
HMDB00271	Sarcosine	6.9	1	
HMDB00300	Uracil	0.3	1	
HMDB00479	3-Methylhistidine	0	1	
HMDB00625	Gluconic acid	0	1	
HMDB00714	Hippuric acid	0.2	1	
HMDB00718	Isovaleric acid	3.5	1	
HMDB00755	Hydroxyphenyllactic acid	0.2	1	
HMDB00906	Trimethylamine	0.1	1	
HMDB01565	Phosphorylcholine	0.4	1	
HMDB01847	Caffeine	0.2	1	
HMDB03355	5-Aminopentanoate	0	1	
HMDB11635	p-Cresol sulfate	0.3	1	