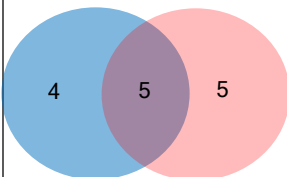




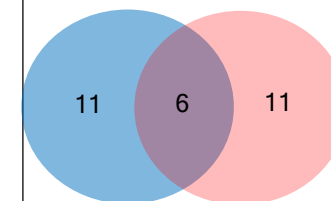
Modified endogenous sequence	Formula	RT (RP)	RT (HILIC)	Molecular Weight	Adduct	Experimental m/z	Calculated m/z	Δmass (ppm)	Mean Area (RP)	Mean Area (HILIC)	Major Fragments
Lac-Xle	C <sub>9</sub> H <sub>17</sub> NO <sub>4</sub>	9.13	-	203.1159	[M+H] <sup>+</sup>	204.1231	204.1230	0.45	2.64E+07	-	158.1175; 132.1018; 86.0963; 73.0284
Pyr-Pro	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>	3.82	5.11	226.0954	[M+H] <sup>+</sup>	227.1027	227.1026	0.10	1.13E+08	1.40E+08	116.0706; 84.0444; 70.0652
Pro-Hyp	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>	0.94	8.55	228.1111	[M+H] <sup>+</sup>	229.1184	229.1183	0.40	1.79E+07	3.22E+07	132.0656; 115.0865; 86.0601; 70.0652
Cit-Gly	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub>	-	9.94	232.1172	[M+H] <sup>+</sup>	233.1245	233.1244	0.19	-	7.21E+06	233.1245; 159.0764; 116.0708; 76.03936; 70.0652
Pyr-Xle	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>	7.89	-	242.1267	[M+H] <sup>+</sup>	243.1340	243.1339	0.30	1.76E+07	-	132.1021; 86.0965; 84.0444
Lac-Arg	C <sub>9</sub> H <sub>16</sub> N <sub>4</sub> O <sub>4</sub>	1.14	7.82	245.1255	[M+H] <sup>+</sup>	246.1328	246.1328	-0.23	9.68E+06	4.63E+07	175.1190; 158.0924; 116.0708; 112.0869; 73.0285; 70.0652
Hyp-His	C <sub>11</sub> H <sub>18</sub> N <sub>4</sub> O <sub>4</sub>	0.97	10.68	268.1170	[M+H] <sup>+</sup>	269.1243	269.1244	-0.43	2.39E+08	8.80E+07	156.0769; 114.0550; 110.0714; 86.0600
Cit-Pro	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub>	-	8.41	272.1484	[M+H] <sup>+</sup>	273.1557	273.1557	-0.10	-	1.05E+07	158.0962; 140.0821; 116.0707; 70.0653
Phe-Hyp	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>	-	4.38	278.1264	[M+H] <sup>+</sup>	279.1337	279.1339	-0.92	-	1.30E+08	132.0656; 120.0808; 86.0600
Cit-Asp	C <sub>10</sub> H <sub>18</sub> N <sub>4</sub> O <sub>6</sub>	-	9.77	290.1226	[M+H] <sup>+</sup>	291.1299	291.1299	0.01	-	2.30E+08	291.1301; 159.0764; 158.0925; 116.0708; 113.0710; 112.0870; 88.0393; 70.0652; 70.0287
Asp-MeArg	C <sub>11</sub> H <sub>21</sub> N <sub>5</sub> O <sub>5</sub>	1.32	-	303.1543	[M+H] <sup>+</sup>	304.1616	304.1615	0.16	1.59E+07	-	189.1347; 172.1081; 126.0914; 88.0393; 70.0561; 70.0287
Cit-Lys	C <sub>12</sub> H <sub>23</sub> N <sub>5</sub> O <sub>4</sub>	-	11.58	303.1913	[M+H] <sup>+</sup>	304.1985	304.1979	2.02	-	7.45E+05	158.0924; 147.1128; 140.0821; 130.0865; 113.0710; 84.0808
Hyp-Glu-Gly	C <sub>12</sub> H <sub>19</sub> N <sub>3</sub> O <sub>7</sub>	0.89	5.29	317.1223	[M+H] <sup>+</sup>	318.1296	318.1296	0.12	7.35E+06	4.86E+07	225.0870; 197.0922; 114.0550; 102.0550; 86.0601; 84.0444; 76.0394
Pyr-Xle-Ser	C <sub>14</sub> H <sub>23</sub> N <sub>3</sub> O <sub>6</sub>	5.96	-	329.1588	[M+H] <sup>+</sup>	330.1661	330.1660	0.46	1.58E+07	-	219.1343; 197.1287; 106.0499; 86.0965; 84.0444; 60.0447

Only RP 4  
Both columns 5  
Only HILIC 5  
14



Modified endogenous sequence	Molecular Weight	Adduct	Experimental m/z	Major Fragments
Hyp-Ala-Pro	299.1480	[M+H] <sup>+</sup>	300.1553	142.050; 124.038; 116.071; 86.061; 70.064; 68.050
Pyr-Gly-Gly-Gly	300.1065	[M+H] <sup>+</sup>	301.1138	209.055; 186.087; 181.061; 173.055; 169.061; 123.055; 84.044; 76.039
Hyp-Gly-Hyp	301.1275	[M+H] <sup>+</sup>	302.1348	189.087; 171.077; 153.066; 143.081; 132.067; 96.044; 86.060; 68.050
Asp-MeArg	303.1540	[M+H] <sup>+</sup>	304.1613	215.116; 198.096; 189.134; 172.108; 133.061; 88.039; 70.065; 70.029
Glu-Cit	304.1380	[M+H] <sup>+</sup>	305.1453	185.055; 176.103; 159.077; 147.077; 130.050; 112.039; 102.055; 84.044; 70.065
Cit-Glu	304.1380	[M+H] <sup>+</sup>	305.1453	175.119; 158.093; 148.060; 130.050; 113.021; 102.055; 84.044; 70.066
Pyr-Gly-Ala-Gly	314.1220	[M+H] <sup>+</sup>	315.1293	223.071; 212.102; 195.076; 187.071; 169.060; 147.076; 141.066; 129.066; 84.044; 76.039
Hyp-Glu-Gly	317.1223	[M+H] <sup>+</sup>	318.1296	187.071; 143.081; 130.050; 114.055; 102.055; 86.060; 68.050
Pyr-Pro-Pro	323.1482	[M+H] <sup>+</sup>	324.1555	213.123; 209.094; 181.099; 116.070; 84.044; 70.065
Pyr-Xle-Ser	329.1587	[M+H] <sup>+</sup>	330.1660	197.126; 129.066; 106.051; 88.040; 86.097; 84.045; 60.044
Hyp-Glu-Ala	331.1379	[M+H] <sup>+</sup>	332.1452	225.087; 215.103; 197.095; 102.056; 90.056; 86.060; 84.044; 68.050
AcLys-Phe	335.1844	[M+H] <sup>+</sup>	336.1917	174.055; 151.075; 120.080
Asp-Gly-Mes	337.0944	[M+H] <sup>+</sup>	338.1017	223.075; 173.056; 166.054; 149.027; 145.061; 127.055; 102.055 88.039; 70.029; 56.050
Hyp-Xle-Pro	341.1950	[M+H] <sup>+</sup>	342.2023	131.087; 125.022; 116.071; 101.059; 99.044; 86.096; 70.065
Cit-Gly-Asn	346.1599	[M+H] <sup>+</sup>	347.1672	232.140; 215.112; 198.185; 190.181; 175.118; 173.093; 158.095; 140.181; 133.060; 130.097; 116.073; 112.085; 87.054; 70.065; 70.028
sTyr-Pro	358.0837	[M+H] <sup>+</sup>	359.0910	216.033; 136.076; 116.071; 70.065
Hyp-Gly-Gly-Hyp	358.1489	[M+H] <sup>+</sup>	359.1562	245.021; 189.087; 171.077; 153.066; 143.081; 132.067; 96.044; 86.060; 68.051
Suclys-Xle	359.2055	[M+H] <sup>+</sup>	360.2128	201.126; 183.112; 132.101; 86.096
Cit-Ala-Asn	360.1758	[M+H] <sup>+</sup>	361.1831	344.156; 246.156; 229.130; 212.113; 175.119; 158.092; 140.082; 133.061; 112.087; 70.065
Asp-sTyr	376.0572	[M+H] <sup>+</sup>	377.0645	262.037; 182.045; 165.064; 136.076; 133.062; 88.039; 70.029
Hyp-Pro-Gly-Pro	382.1851	[M+H] <sup>+</sup>	383.1924	211.107; 183.112; 173.072; 166.086; 142.049; 116.070; 114.054; 98.060; 86.061; 70.064
Hyp-Asp-His	384.1507	[M+H] <sup>+</sup>	385.1580	253.092; 156.077; 139.050; 110.071; 86.060
Pyr-Gln-Gln	385.1593	[M+H] <sup>+</sup>	386.1666	258.108; 212.103; 147.077; 130.050; 129.066; 101.071; 84.044
Cit-Gly-Gly-Asn	403.1818	[M+H] <sup>+</sup>	404.1891	289.162; 272.135; 255.109; 227.114; 215.114; 175.119; 173.056; 158.093; 140.082; 133.101; 130.098; 112.087; 87.055; 84.081; 70.065; 70.028
Pyr-Pro-Pro-Pro	420.2010	[M+H] <sup>+</sup>	421.2083	213.123; 209.094; 181.099; 129.066; 116.070; 84.044; 70.065
Hyp-His-Ala-His	476.2134	[M+H] <sup>+</sup>	477.2207	251.114; 227.114; 223.119; 156.077; 110.071; 86.060
Glu-Mes-Ser-Cys	484.1290	[M+H] <sup>+</sup>	485.1363	130.050; 122.027; 112.039; 84.044; 76.021
Asp-Asp-sTyr	491.0847	[M+H] <sup>+</sup>	492.0913	262.037; 203.067; 185.056; 182.081; 165.055; 136.076; 88.039; 70.029

Only RP 11  
Both columns 6  
Only HILIC 11  
28



Modified endogenous sequence	Molecular Weight
Pyr-Gly	186.0641
Lac-Val	189.1003
Lac-Xle	203.1159
Lac-Glu	219.0744
Pyr-Pro	226.0954
Lac-His	227.0907
Pro-Hyp	228.1111
Cit-Gly	232.1172
Hyp-Cys	234.0674
Lac-Phe	237.1002
Pyr-Xle	242.1267
Pyr-Asn	243.0856
Xle-Hyp	244.1423
Lac-Arg	246.1328
Ala-Cit	246.1328
Lac-Tyr	253.0950
Pyr-Lys	257.1376
Pyr-Glu	258.0851
Gln-Hyp	259.1169
Glu-Hyp	260.1006
Pyr-His	266.1015
Hyp-His	268.1170
Cit-Pro	272.1484
Lac-Trp	276.1110
Phe-Hyp	278.1265
Phe-Hyp	278.1265
Pro-Hyp-Gly	285.1325
Pyr-Arg	285.1437
Hyp-Arg	287.1593
Pyr-Gly-Cys	289.0733
Cit-Asp	290.1226
Pyr-Tyr	292.1056
Tyr-Hyp	294.1217
Hyp-Ala-Pro	299.1480
Pyr-Gly-Gly-Gly	300.1065
Hyp-Gly-Hyp	301.1275
Asp-MeArg	303.1543
Cit-Lys	303.1913
Glu-Cit	304.1383
Cit-Glu	304.1384
Pyr-Gly-Ala-Gly	314.1220
Pyr-Trp	315.1222
Hyp-Glu-Gly	317.1223
SucLys-Ala	317.1588
Pyr-Pro-Pro	323.1482
Lac-Ala-Tyr	324.1320
Pyr-Xle-Ser	329.1584
Pyr-Xle-Ser	329.1588
Hyp-Glu-Ala	331.1381
Lac-Xle-Glu	332.1584
AcLys-Phe	335.1844
Asp-Gly-Mes	337.0944
Hyp-Xle-Pro	341.1950
Lac-Asp-His	342.1171
Cit-Gly-Asn	346.1601
Hyp-Ser-His	355.1491
Pro-Hyp-Gln	356.1696
sTyr-Pro	358.0837
Hyp-Gly-Gly-Hyp	358.1489
SucLys-Xle	359.2055
Cit-Ala-Asn	360.1757
SucLys-Gln	374.1801
SucLys-Lys	374.2166
Asp-sTyr	376.0572
Pyr-Asp-His	381.1286
Hyp-Pro-Gly-Pro	382.1851
Hyp-Asp-His	384.1507
Pyr-Gln-Gln	385.1597
Pyr-Glu-Lys	386.1801
SucLys-Phe	393.1901
Cit-Gly-Gly-Asn	403.1818
Pyr-Pro-Pro-Pro	420.2010
sTyr-Tyr	424.0938
Hyp-Tyr-Phe	441.1898
Hyp-His-Ala-His	476.2134
Glu-Mes-Ser-Cys	484.1290
Asp-Asp-sTyr	491.0847

Only CD 49  
Both methods 13  
Only pNovo 15

