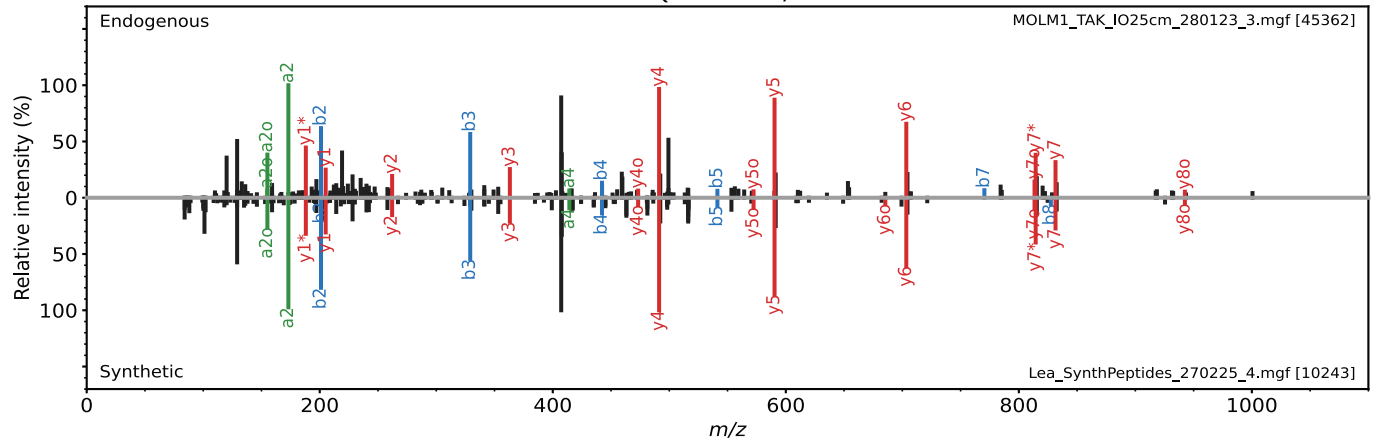


Supplementary File 1:

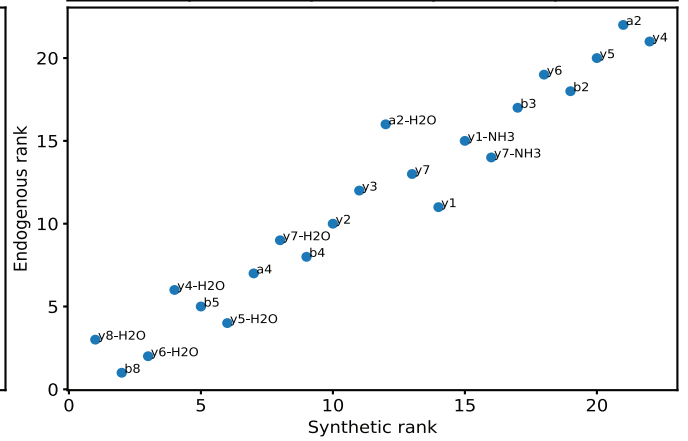
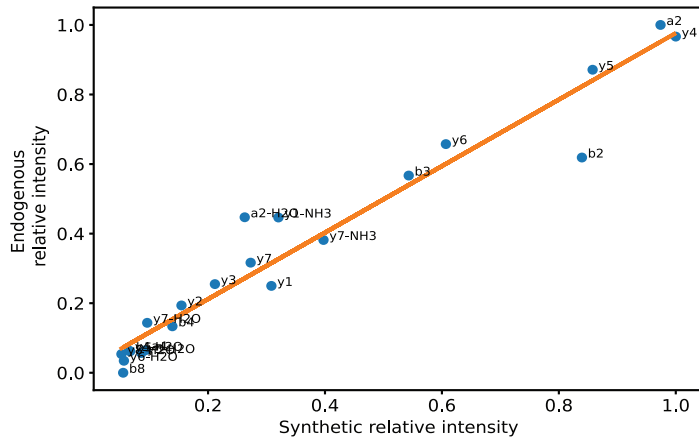
Mirror plots comparing the MS/MS spectra for endogenous peptide (top) with their synthetic standard (bottom). Peptide sequences and charge stage are displayed at the top of each panel. b, y and a ions are respectively displayed in blue, red, and green. The raw file name followed by scan number (in square brackets) of each spectrum are displayed on the top and bottom right of each plot. The tables under the plot report the endogenous, and synthetic m/z with mass errors, the Pearson and Spearman correlation coefficient (r/θ), p-value, and 95% confidence intervals (95% CI) for the correlation as well as the spectral angle.

AEQLVKTGW / 2+

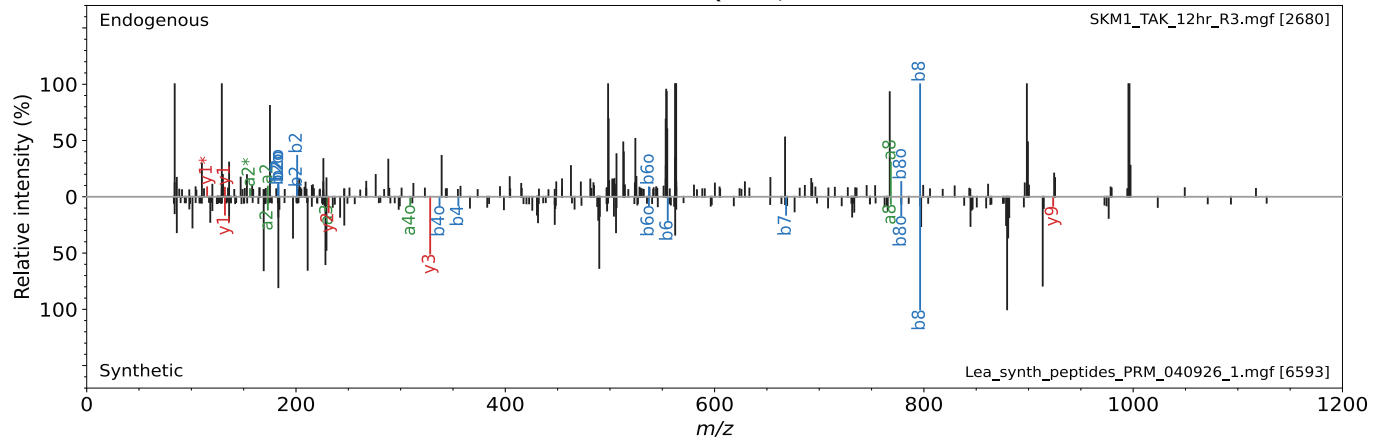


Spectrum	m/z	error (ppm)
Endogenous	516.2794	-0.4
Synthetic	516.2802	1.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.93	0.99	4.8e-14
Spearman	0.97	0.93	0.99	5.2e-14
Spectral angle	0.90	-	-	-

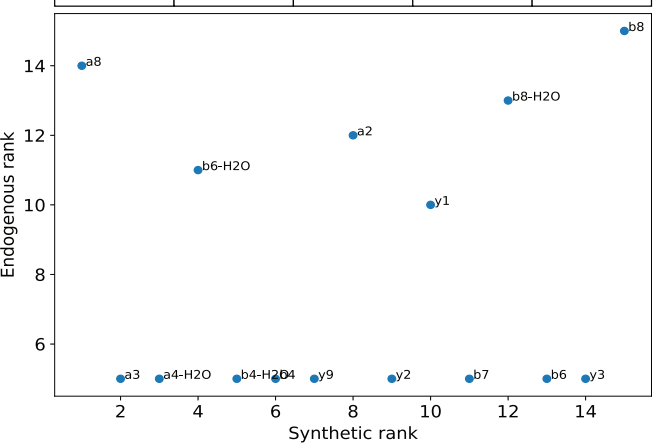
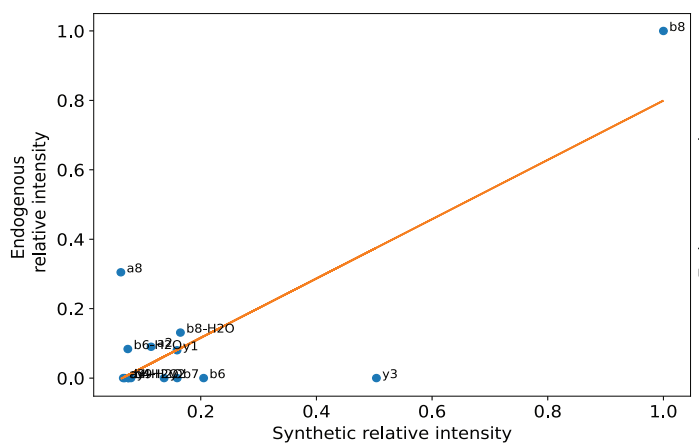


AEGPAEIQPVL / 2+

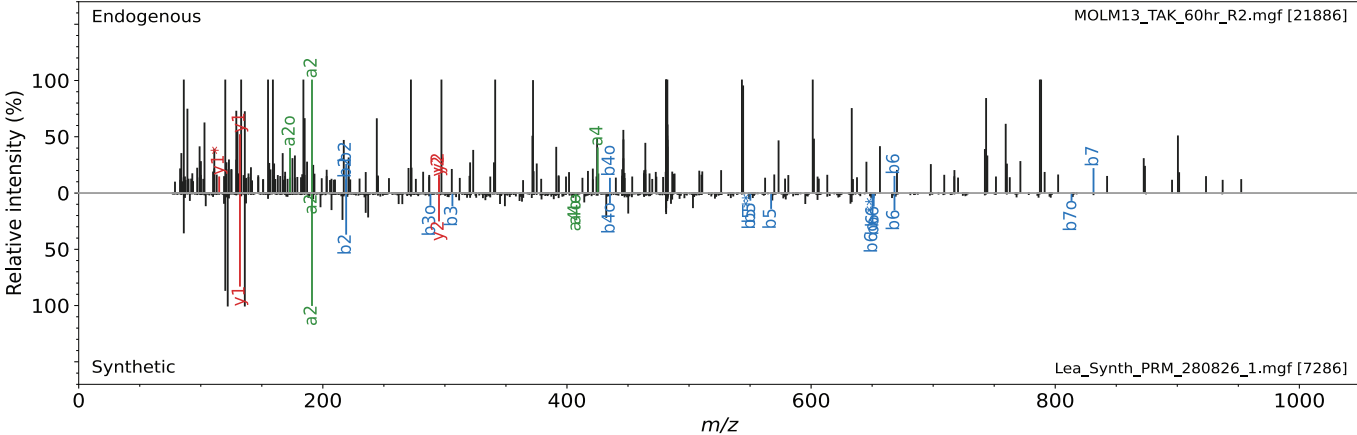


Spectrum	m/z	error (ppm)
Endogenous	562.3011	-3.9
Synthetic	562.3056	4.1

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.82	0.53	0.94	1.9e-04
Spearman	0.10	-0.43	0.58	7.2e-01
Spectral angle	0.63	-	-	-

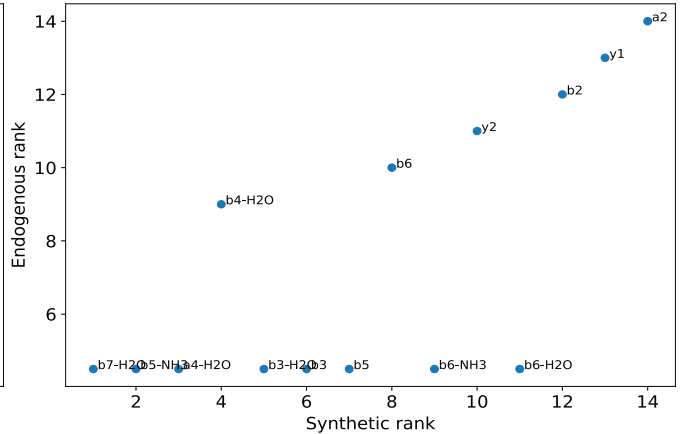
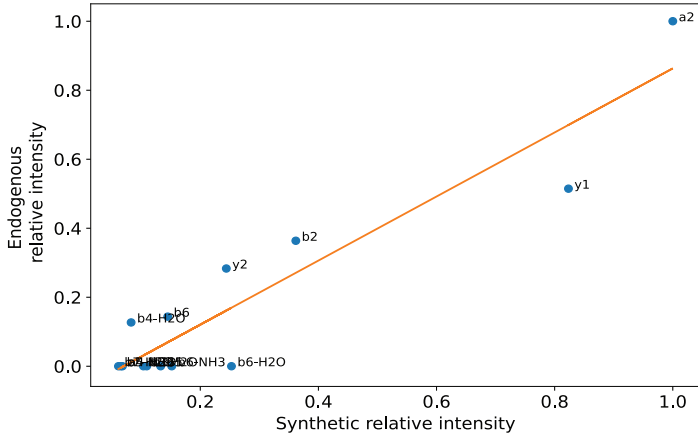


AFSFNTYL / 2+

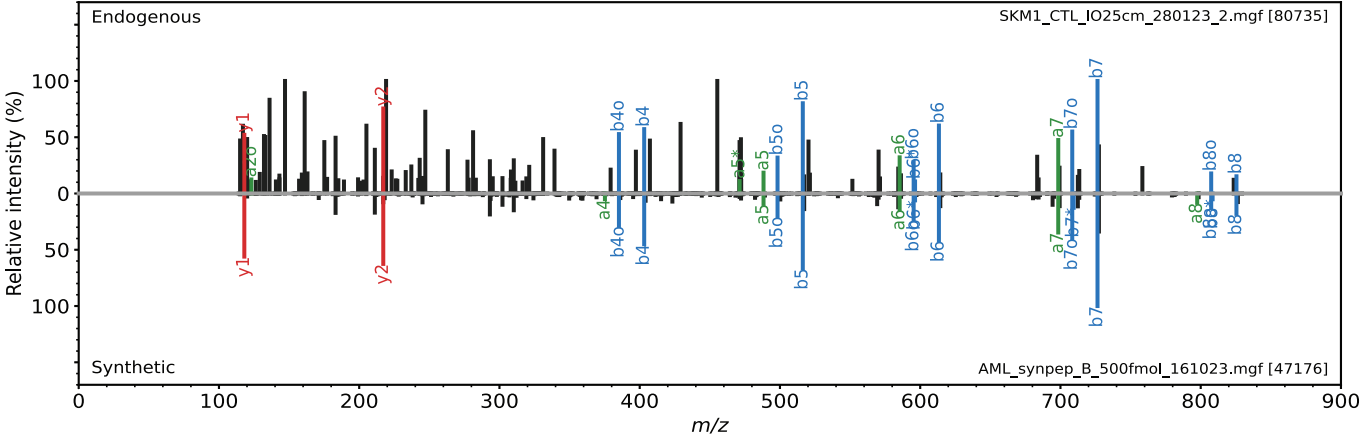


Spectrum	m/z	error (ppm)
Endogenous	481.7327	-3.7
Synthetic	481.7357	2.5

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.94	0.81	0.98	8.6e-07
Spearman	0.71	0.28	0.90	4.6e-03
Spectral angle	0.78	-	-	-

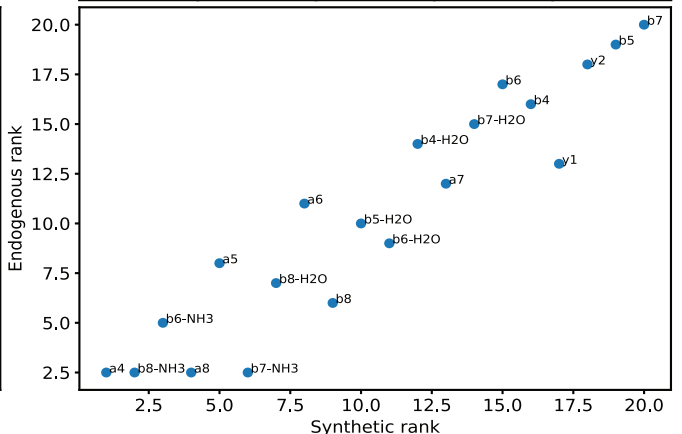
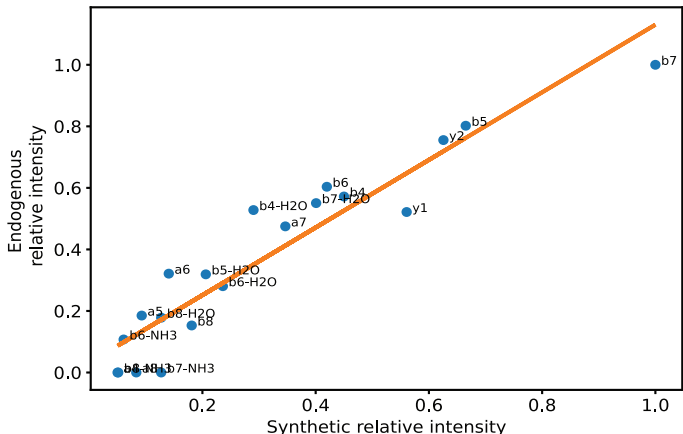


APFSLPLVV / 2+

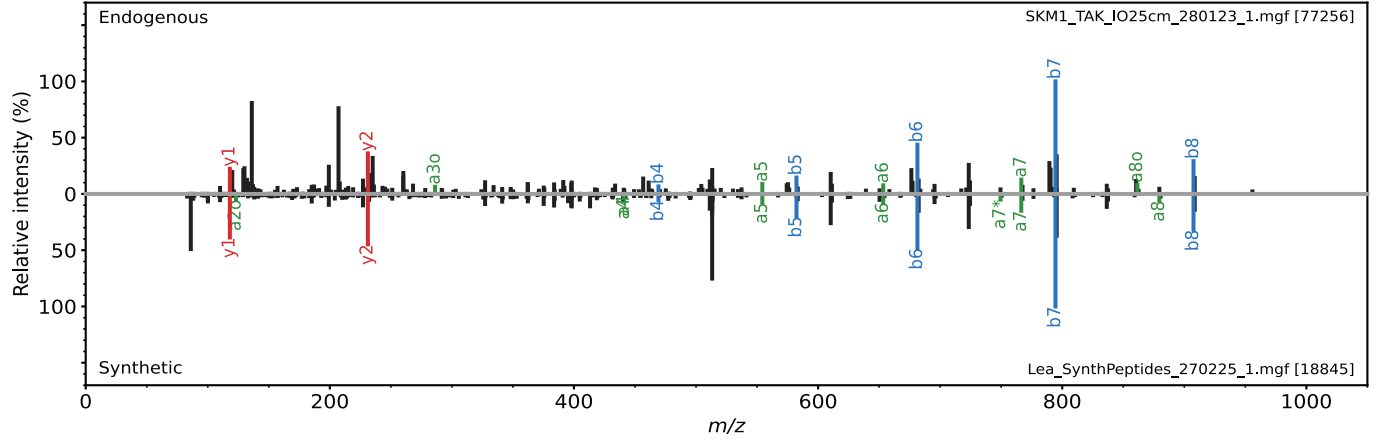


Spectrum	m/z	error (ppm)
Endogenous	471.7863	-0.6
Synthetic	471.7871	0.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.94	0.86	0.98	4.4e-10
Spearman	0.94	0.85	0.98	6.5e-10
Spectral angle	0.87	-	-	-

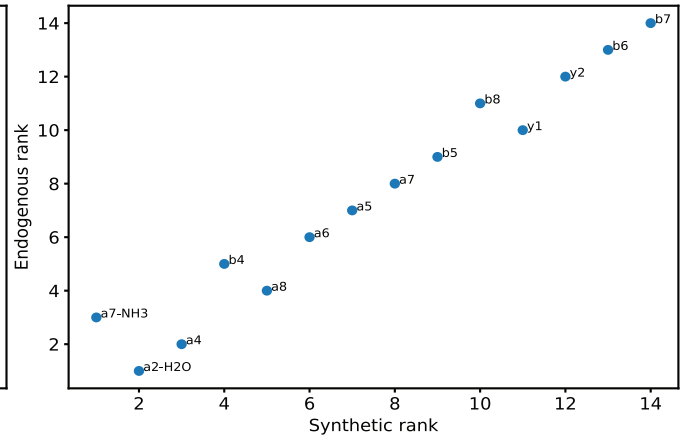
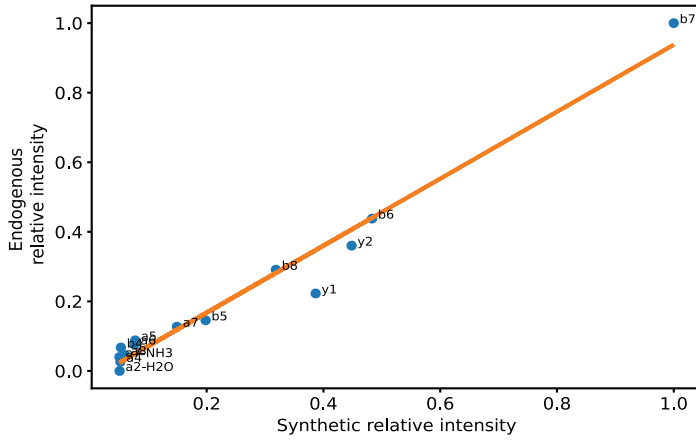


APYHLVLLV / 2+

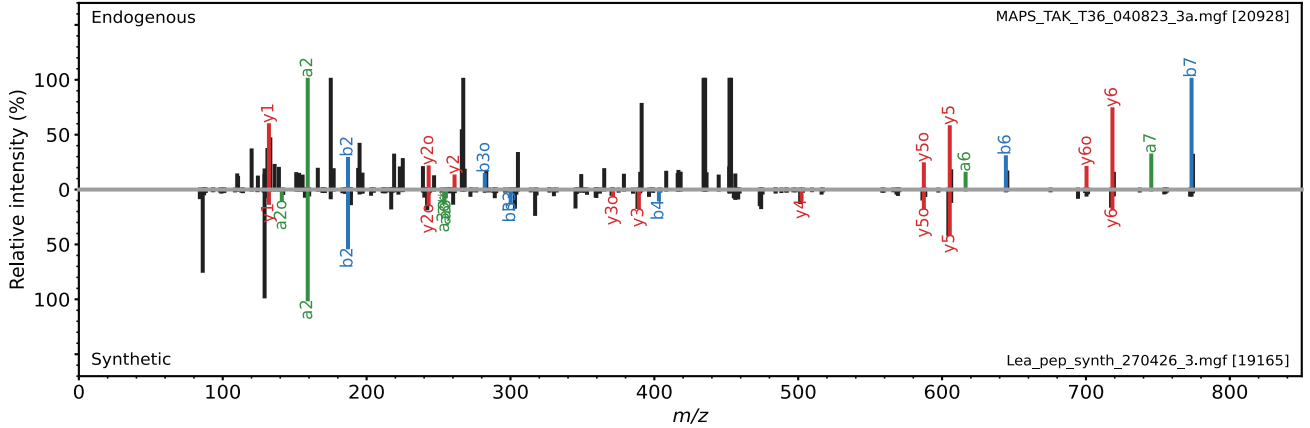


Spectrum	m/z	error (ppm)
Endogenous	512.8126	-1.0
Synthetic	512.8137	1.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.98	0.95	1.00	1.6e-10
Spearman	0.98	0.93	0.99	1.6e-09
Spectral angle	0.91	-	-	-

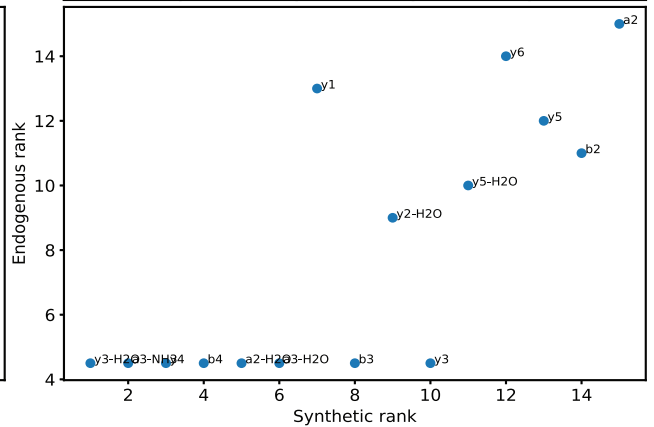
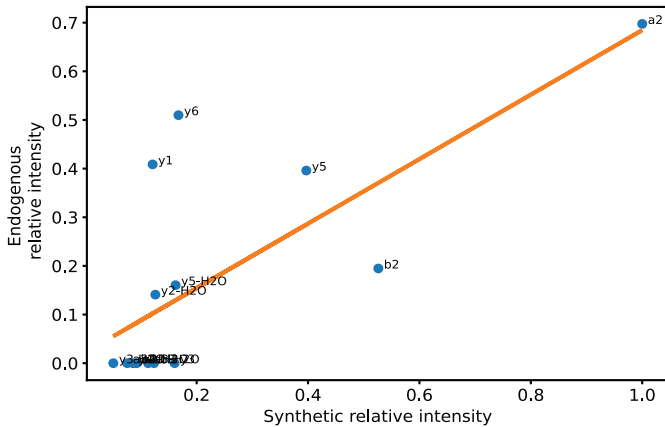


DAICLKQ[+0.98]L / 2+

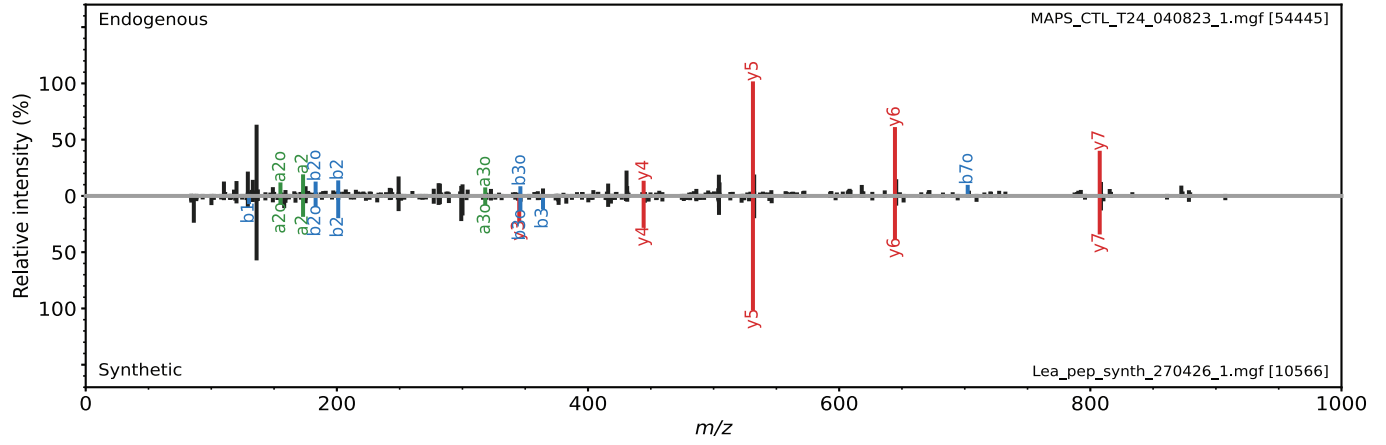


Spectrum	m/z	error (ppm)
Endogenous	452.7458	4.0
Synthetic	452.7452	2.7

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.73	0.34	0.90	2.1e-03
Spearman	0.78	0.44	0.92	6.6e-04
Spectral angle	0.63	-	-	-

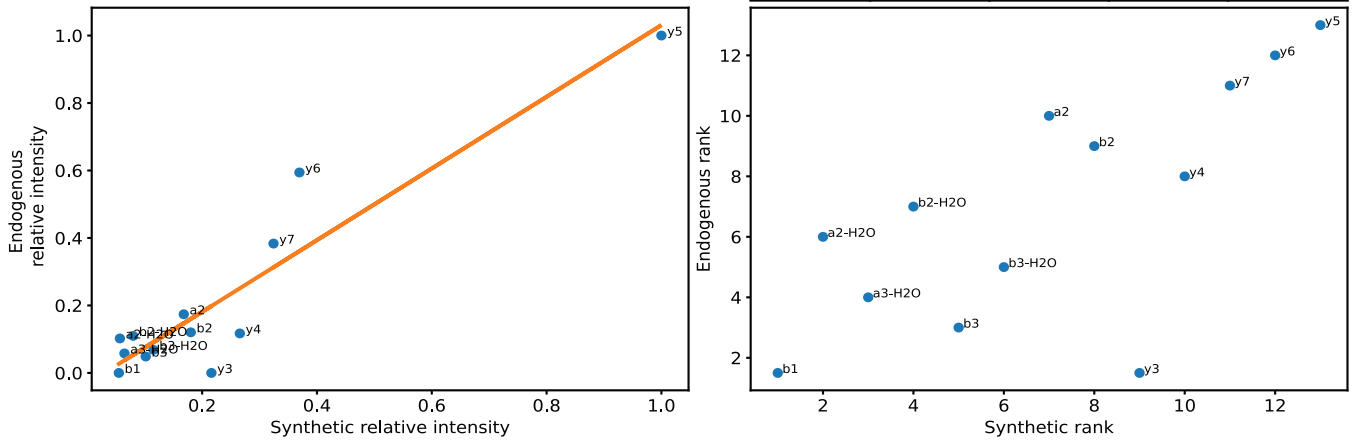


EAYLSVGRL / 2+

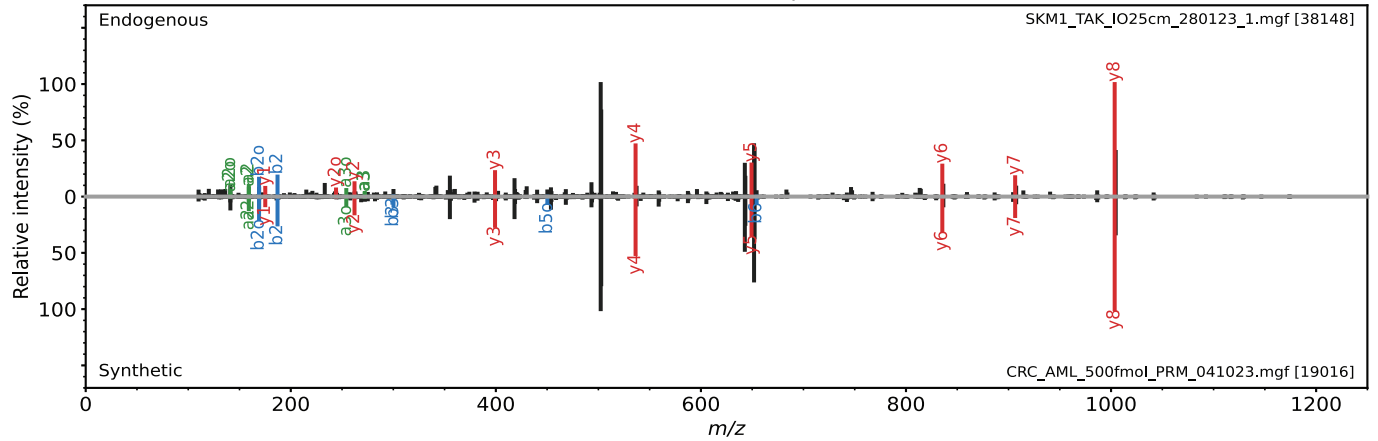


Spectrum	m/z	error (ppm)
Endogenous	504.2851	10.9
Synthetic	504.2791	-1.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.93	0.78	0.98	3.5e-06
Spearman	0.72	0.28	0.91	5.4e-03
Spectral angle	0.81	-	-	-

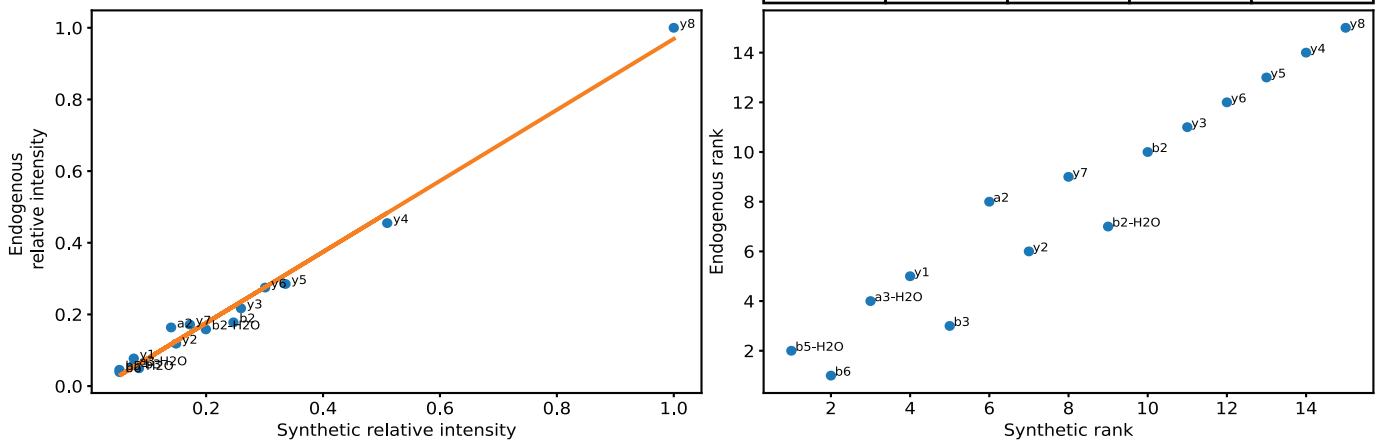


EGIPAWIHHSR / 2+

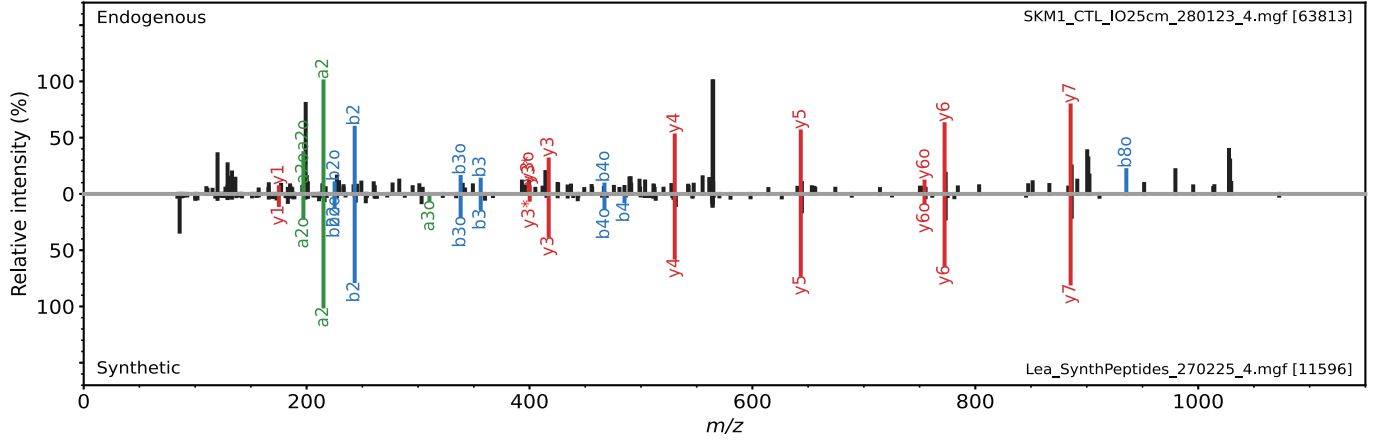


Spectrum	m/z	error (ppm)
Endogenous	651.8382	-0.8
Synthetic	651.8402	2.3

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.99	0.98	1.00	3.5e-14
Spearman	0.97	0.90	0.99	3.6e-09
Spectral angle	0.94	-	-	-

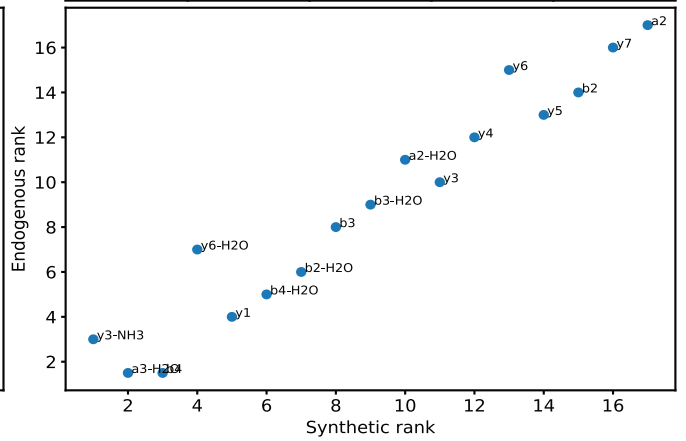
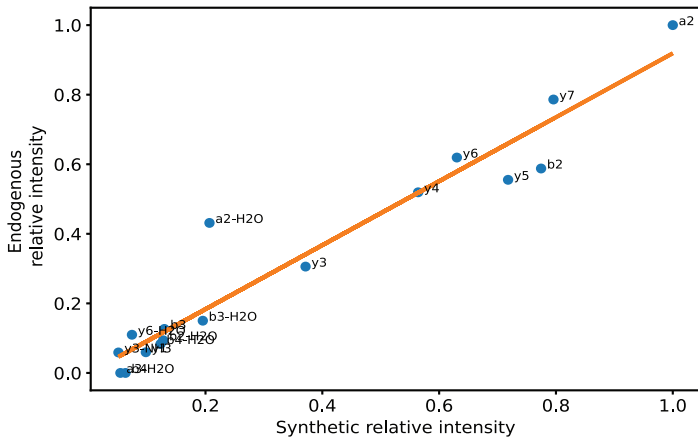


EILEILQNR / 2+

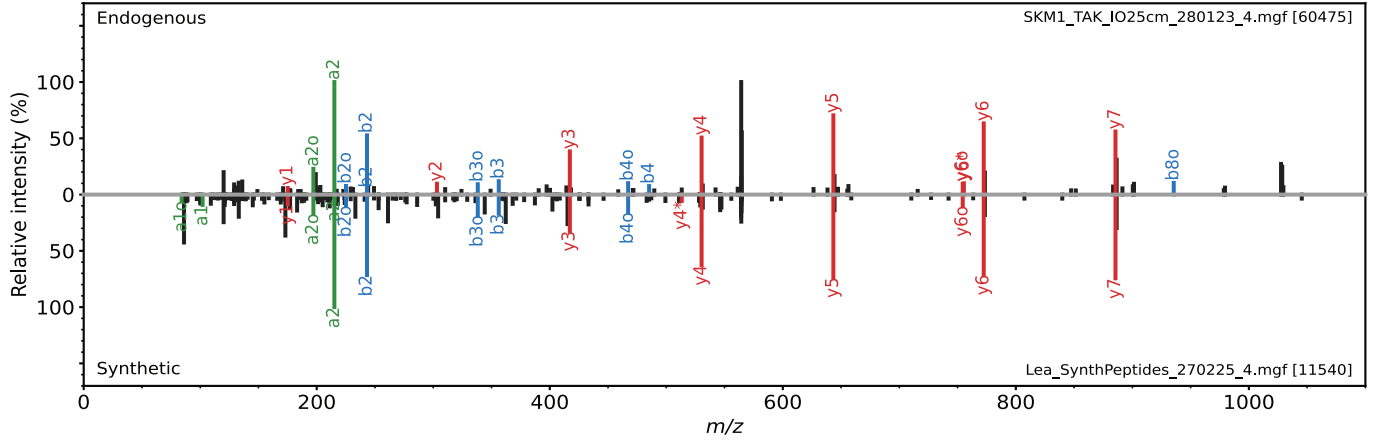


Spectrum	m/z	error (ppm)
Endogenous	564.3245	-0.2
Synthetic	564.3257	1.9

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.96	0.90	0.99	5.4e-10
Spearman	0.97	0.91	0.99	2.3e-10
Spectral angle	0.88	-	-	-

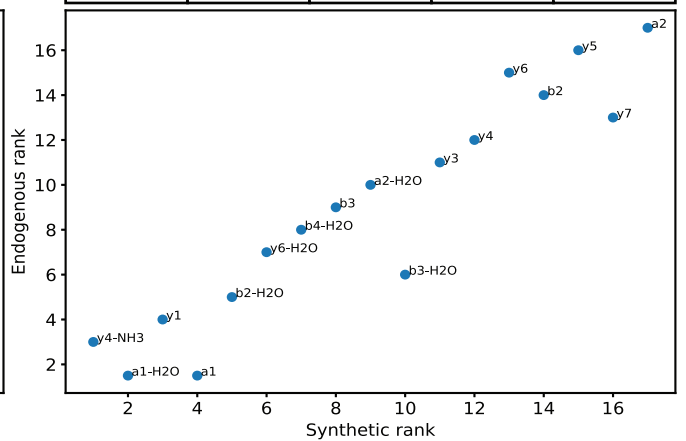
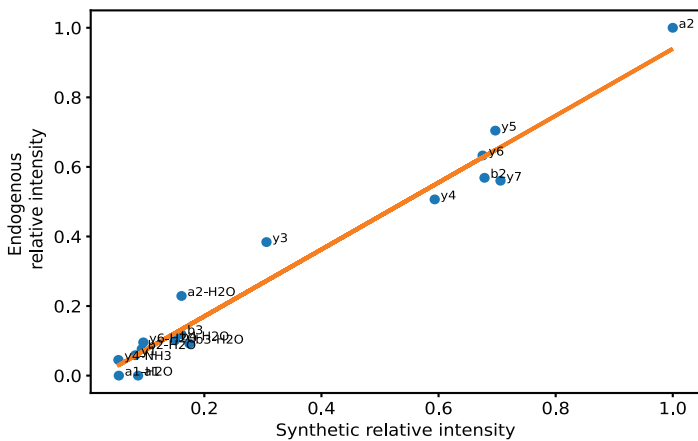


EILELNQR / 2+

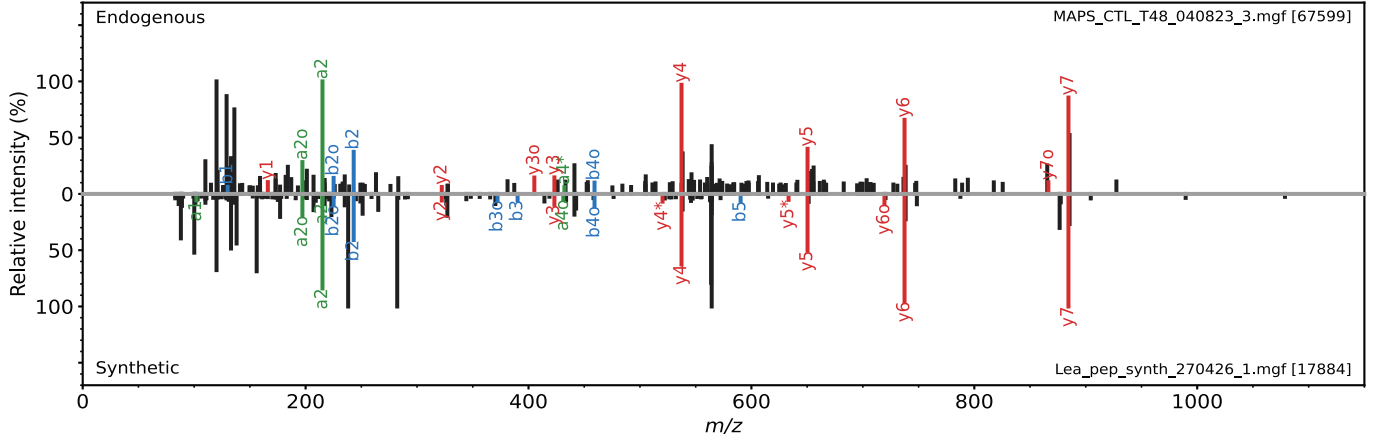


Spectrum	m/z	error (ppm)
Endogenous	564.3243	-0.5
Synthetic	564.3257	1.9

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.98	0.95	0.99	2.9e-12
Spearman	0.94	0.85	0.98	1.2e-08
Spectral angle	0.91	-	-	-

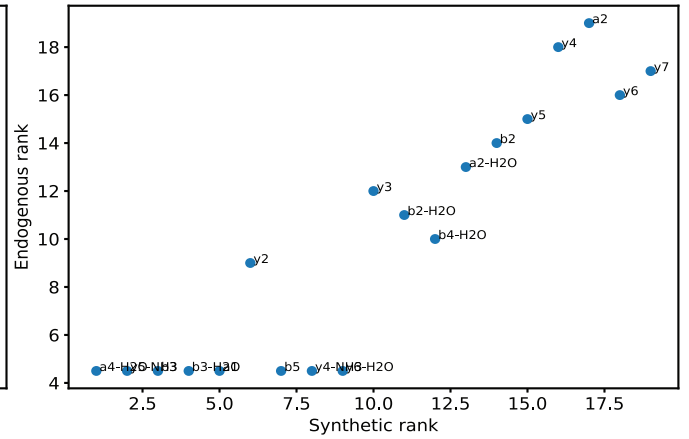
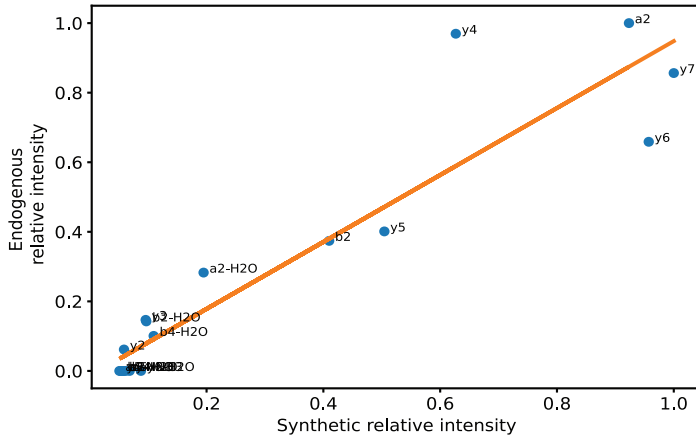


ELFSLNTRF / 2+

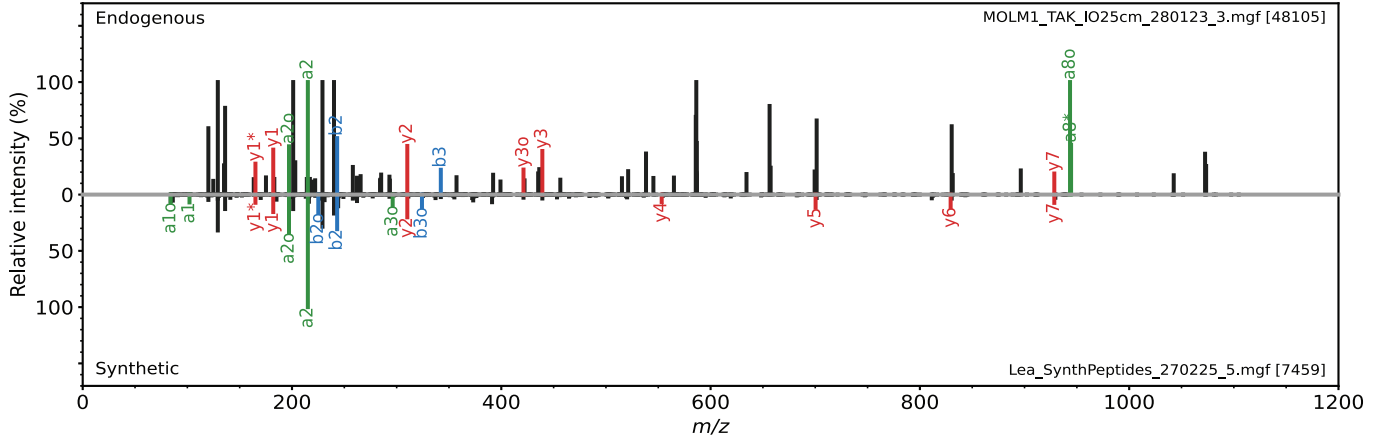


Spectrum	m/z	error (ppm)
Endogenous	563.8038	9.9
Synthetic	563.7971	-2.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.94	0.84	0.98	3.6e-09
Spearman	0.92	0.79	0.97	3.7e-08
Spectral angle	0.82	-	-	-

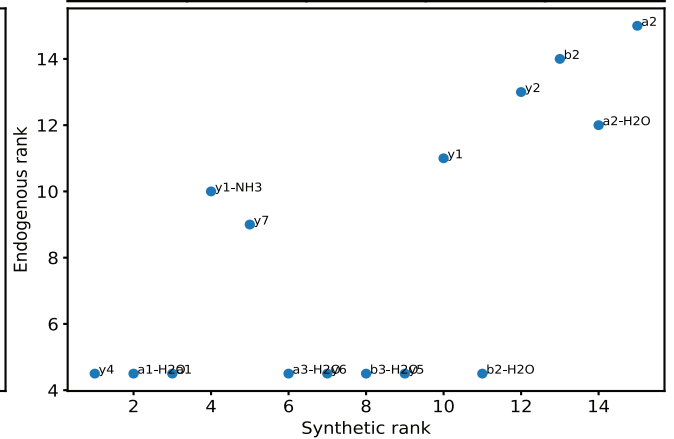
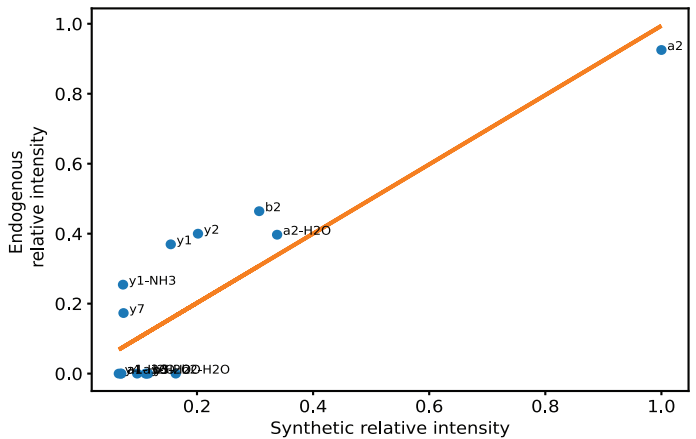


ELVEFNEKY / 2+

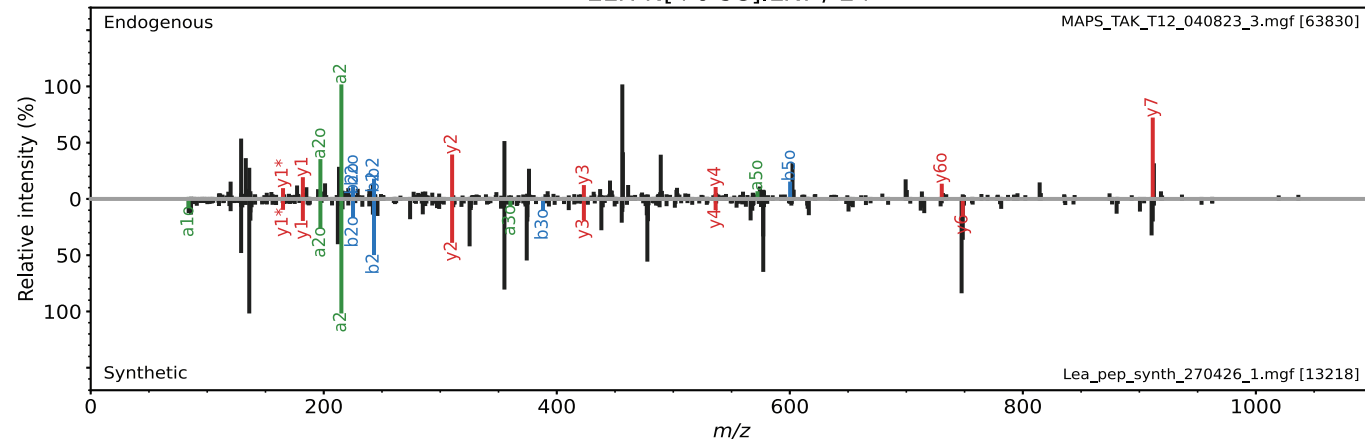


Spectrum	m/z	error (ppm)
Endogenous	585.7875	0.0
Synthetic	585.7885	1.7

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.87	0.64	0.96	2.6e-05
Spearman	0.69	0.27	0.89	4.6e-03
Spectral angle	0.74	-	-	-

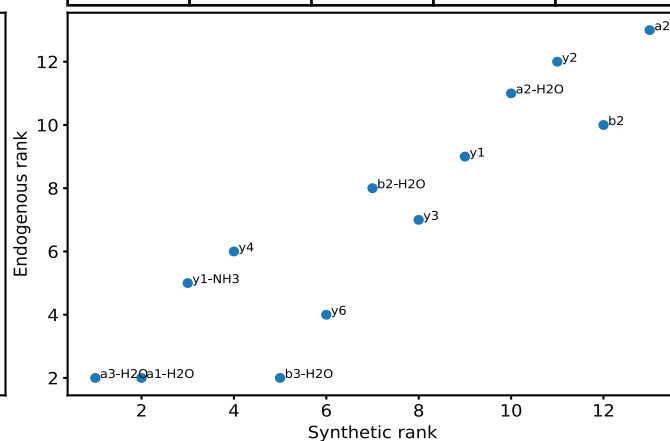
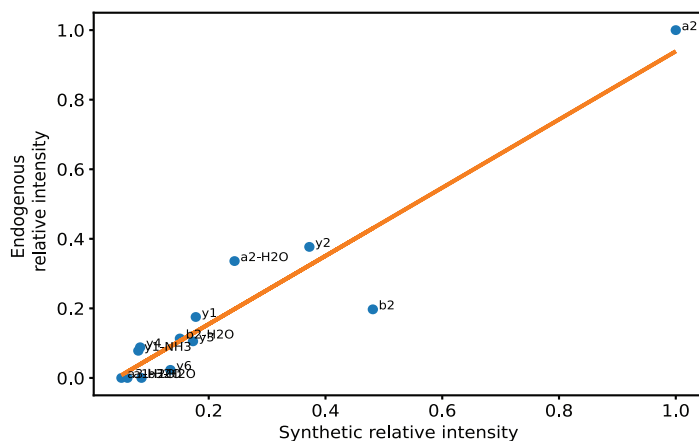


ELYPN[+0.98]ILKY / 2+

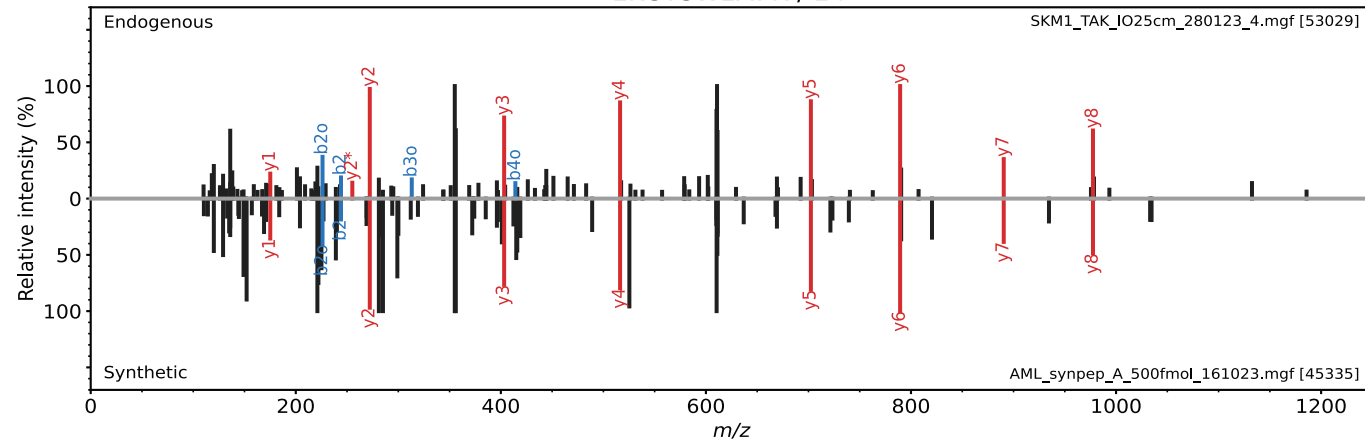


Spectrum	m/z	error (ppm)
Endogenous	577.3160	9.4
Synthetic	577.3091	-2.6

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.95	0.82	0.98	1.0e-06
Spearman	0.92	0.74	0.98	1.0e-05
Spectral angle	0.82	-	-	-

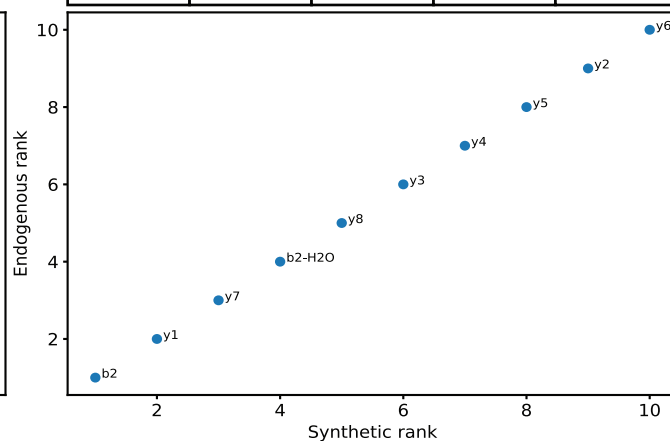
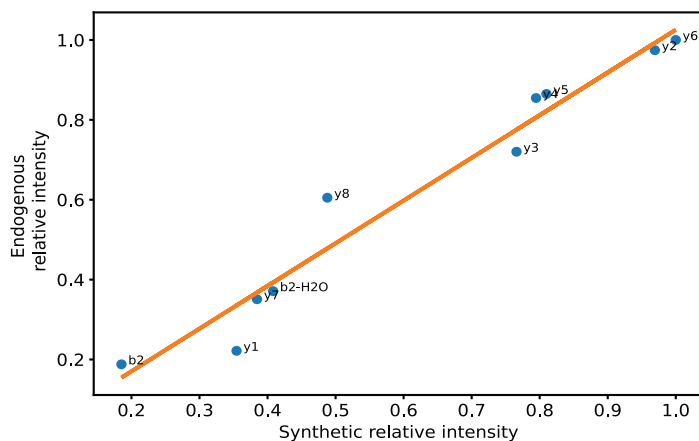


ENSTSWLMPR / 2+

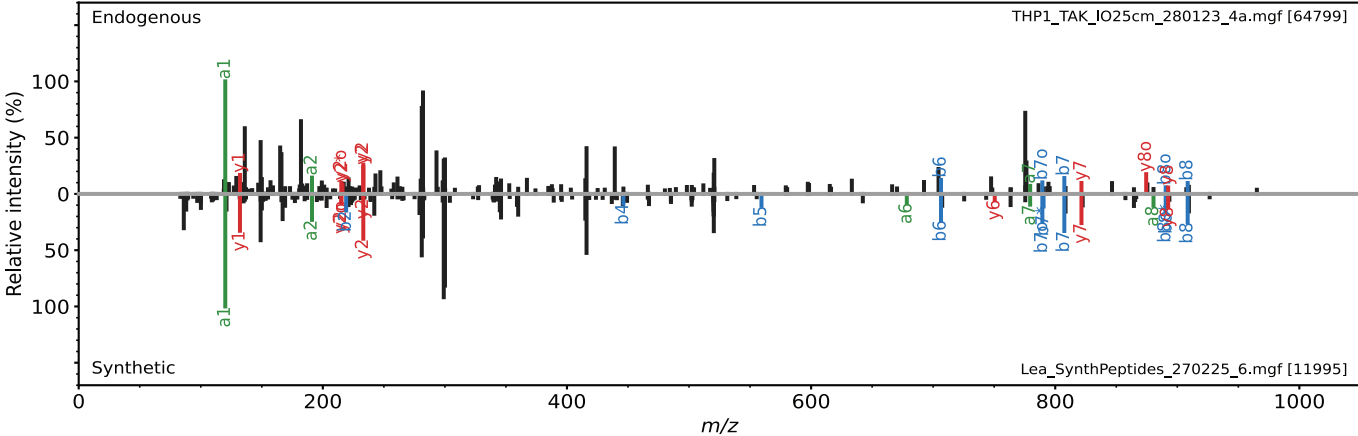


Spectrum	m/z	error (ppm)
Endogenous	610.7898	-0.4
Synthetic	610.7907	0.1

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.98	0.90	0.99	1.1e-06
Spearman	1.00	1.00	1.00	6.6e-64
Spectral angle	0.94	-	-	-

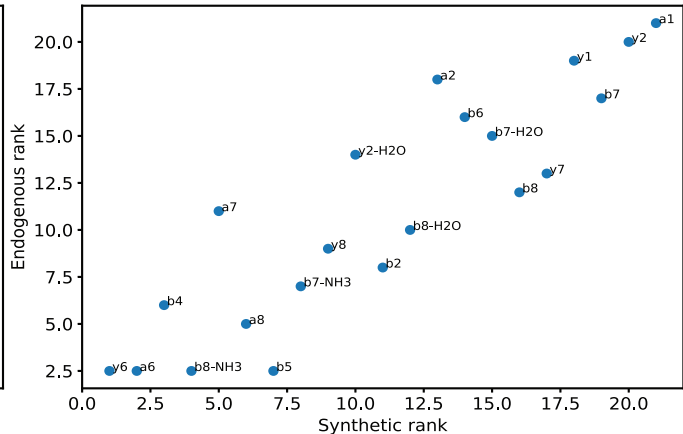
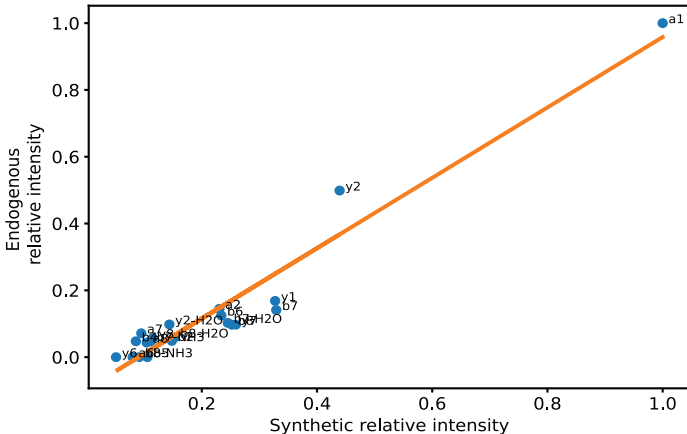


FAARIFTTL / 2+

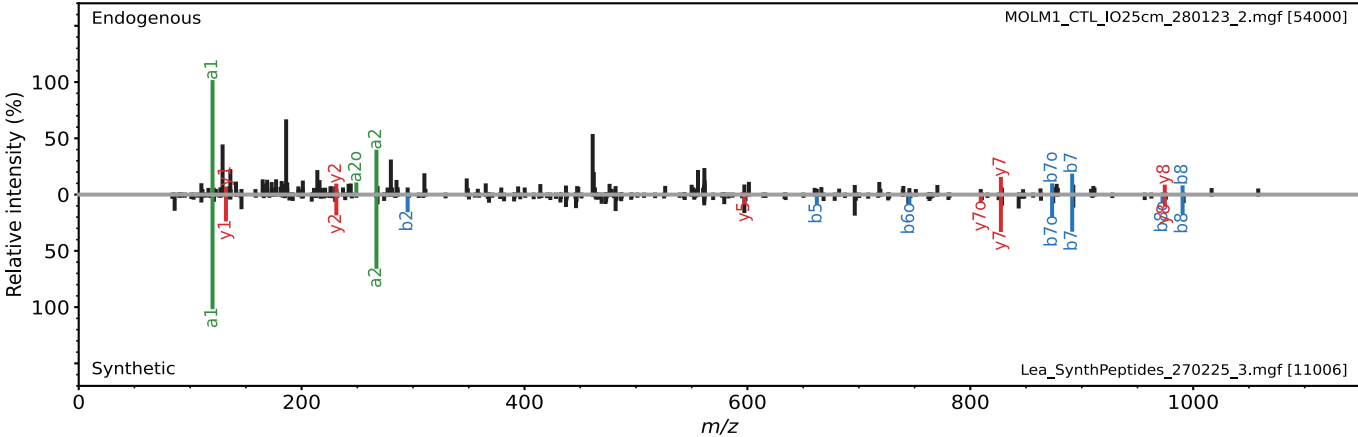


Spectrum	m/z	error (ppm)
Endogenous	520.3007	0.7
Synthetic	520.3014	1.9

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.92	0.99	1.4e-12
Spearman	0.89	0.75	0.96	6.0e-08
Spectral angle	0.78	-	-	-

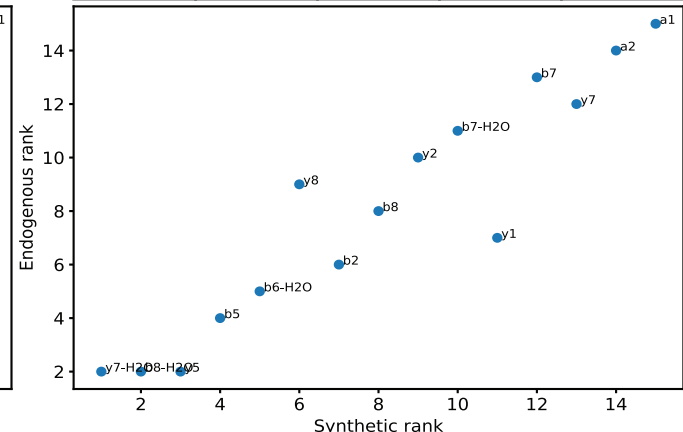
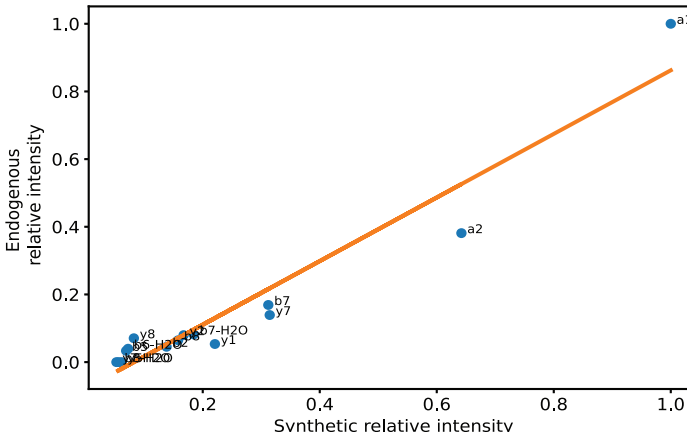


FFTEHTQVL / 2+

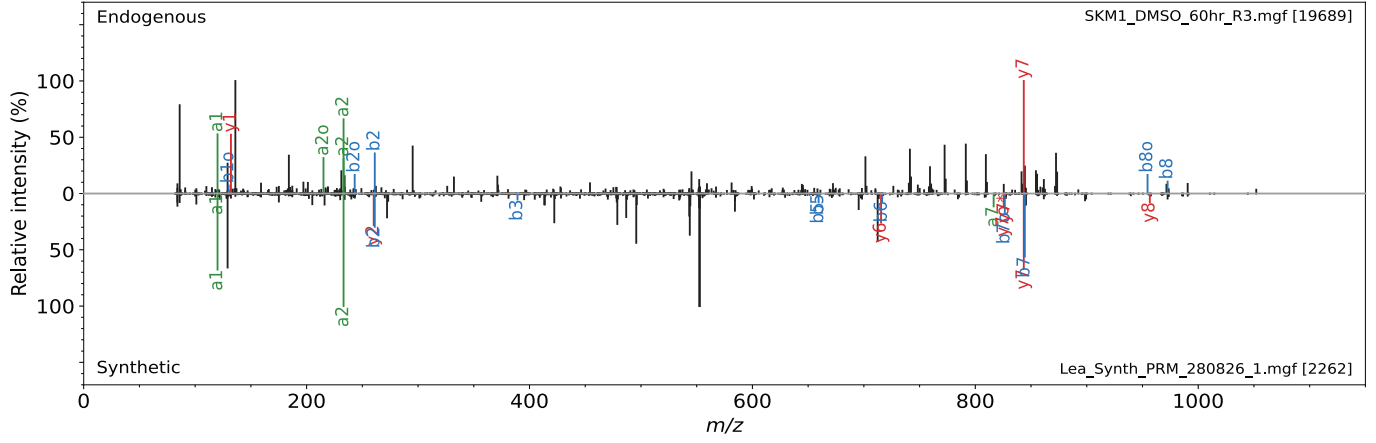


Spectrum	m/z	error (ppm)
Endogenous	561.2857	1.4
Synthetic	561.2854	0.9

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.96	0.89	0.99	8.5e-09
Spearman	0.94	0.83	0.98	1.5e-07
Spectral angle	0.80	-	-	-

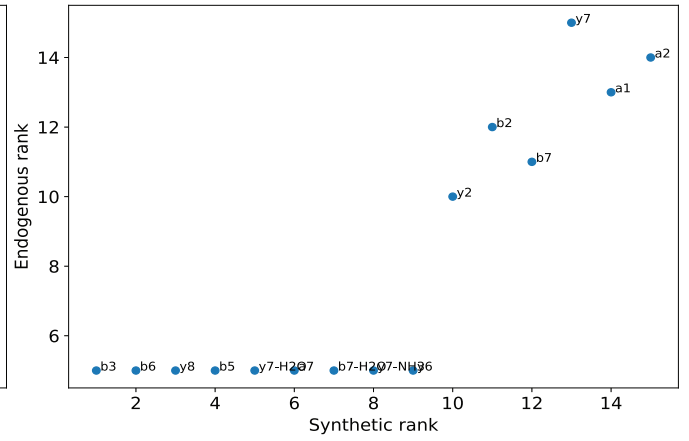
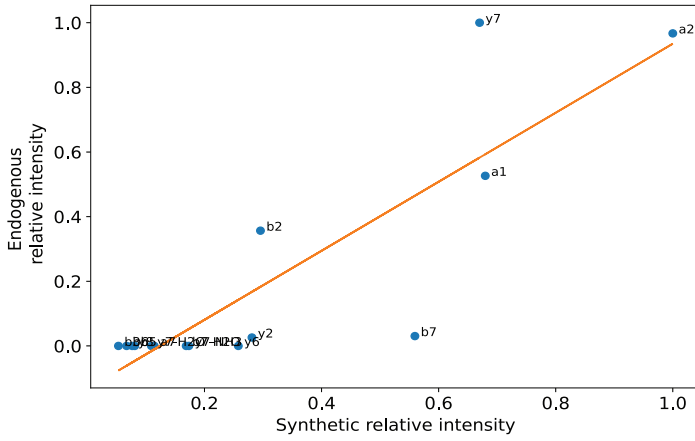


FLQNRGQKL / 2+

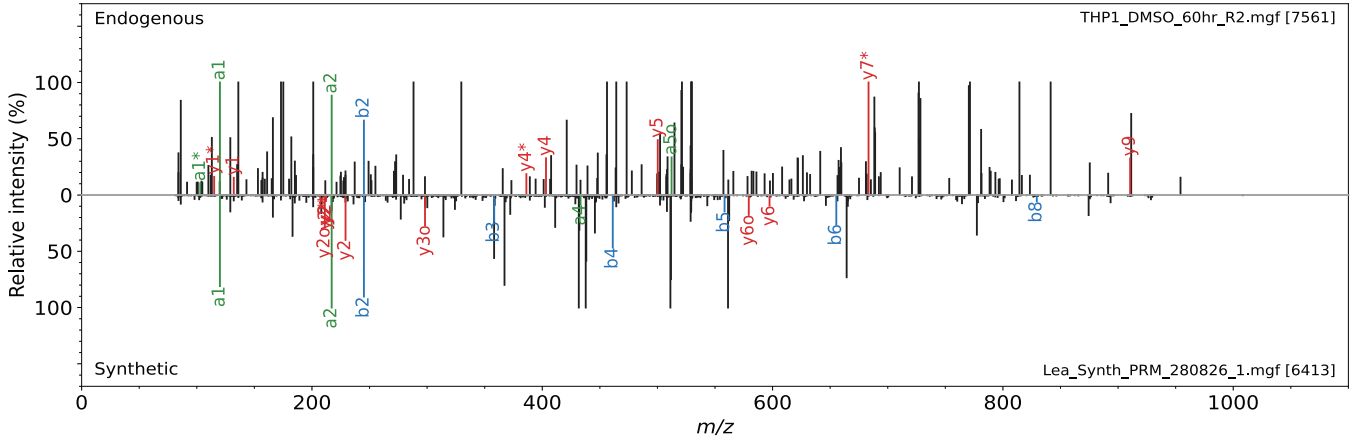


Spectrum	m/z	error (ppm)
Endogenous	552.3203	1.3
Synthetic	552.3195	-0.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.86	0.63	0.95	3.7e-05
Spearman	0.87	0.65	0.96	2.5e-05
Spectral angle	0.67	-	-	-

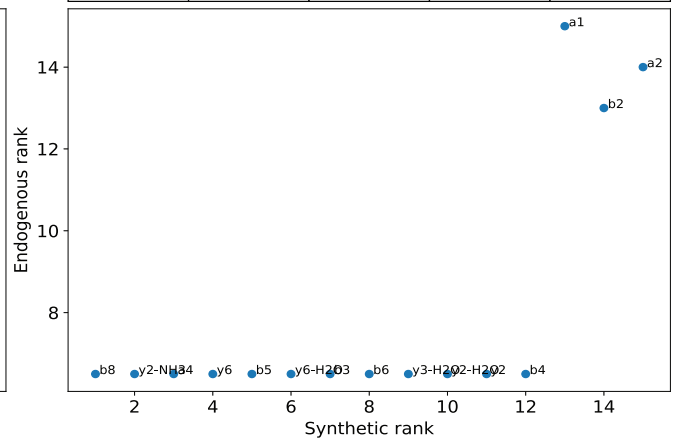
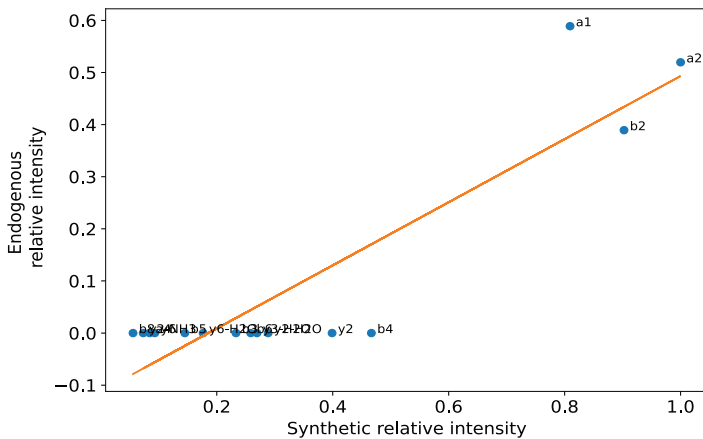


FPLCPPSSPL / 2+

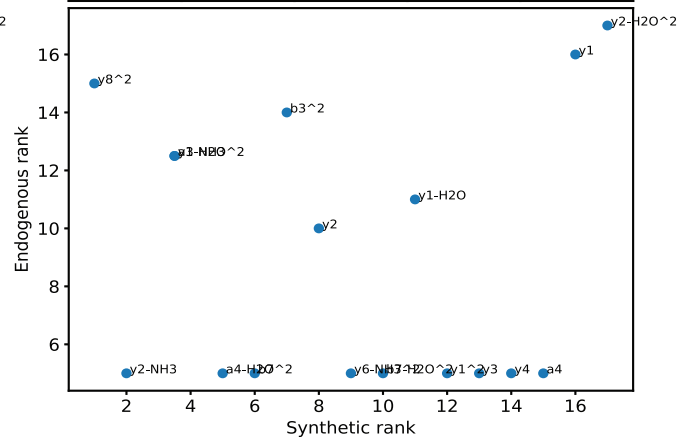


Spectrum	m/z	error (ppm)
Endogenous	529.2766	6.8
Synthetic	529.2726	-0.8

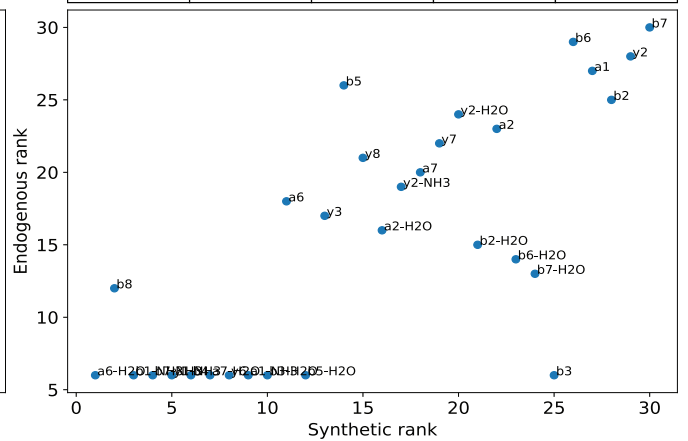
Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.90	0.71	0.97	5.8e-06
Spearman	0.68	0.26	0.89	4.9e-03
Spectral angle	0.66	-	-	-



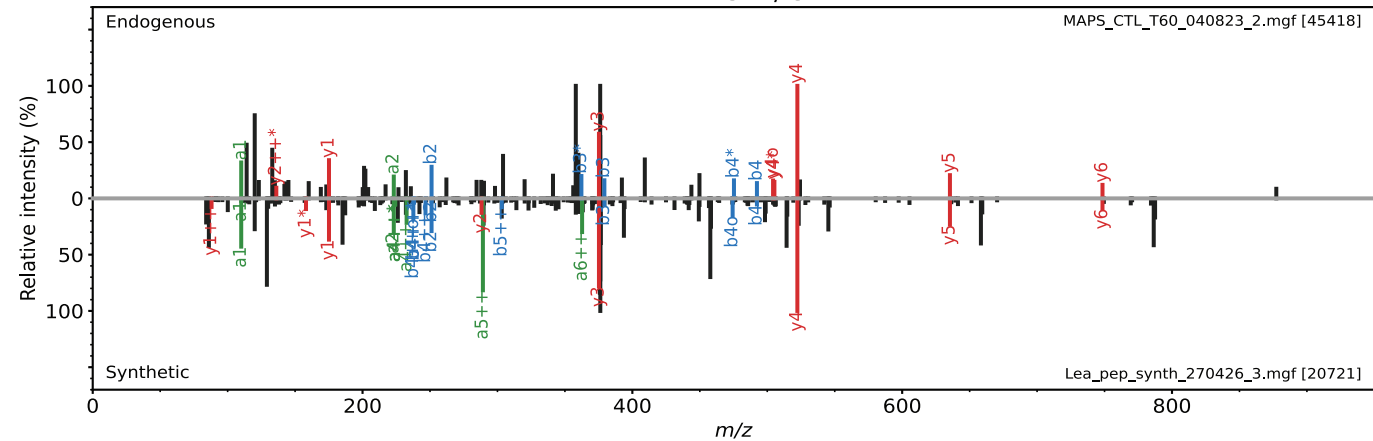
Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.80	0.52	0.93	1.0e-04
Spearman	-0.00	-0.48	0.48	1.0e+00
Spectral angle	0.65	-	-	-



Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.85	0.70	0.93	2.9e-09
Spearman	0.75	0.53	0.87	1.9e-06
Spectral angle	0.70	-	-	-

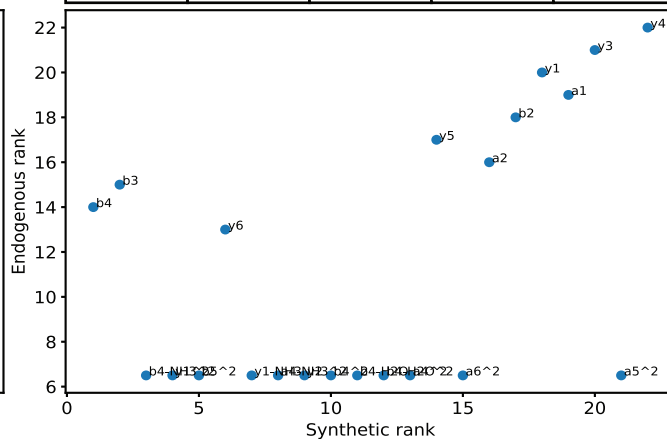
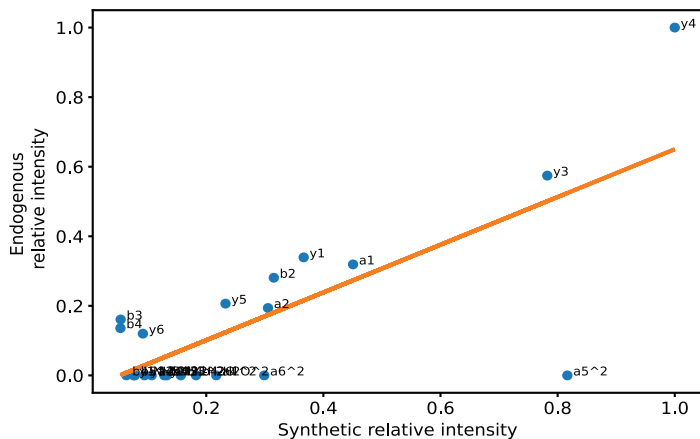


HIKLLFSIR / 3+

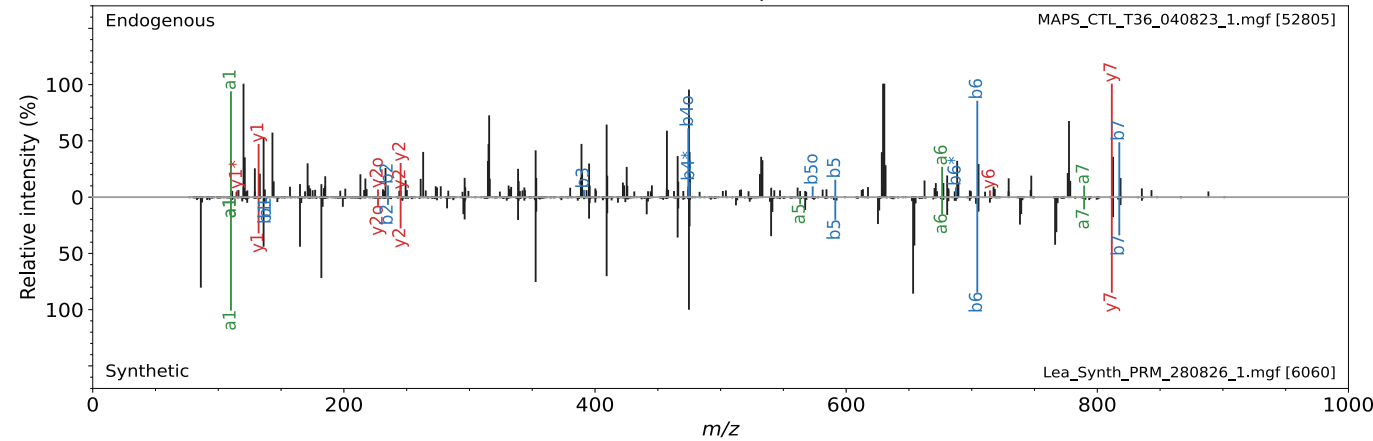


Spectrum	m/z	error (ppm)
Endogenous	376.2450	9.8
Synthetic	376.2401	-3.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.75	0.48	0.89	6.0e-05
Spearman	0.50	0.10	0.76	1.8e-02
Spectral angle	0.62	-	-	-

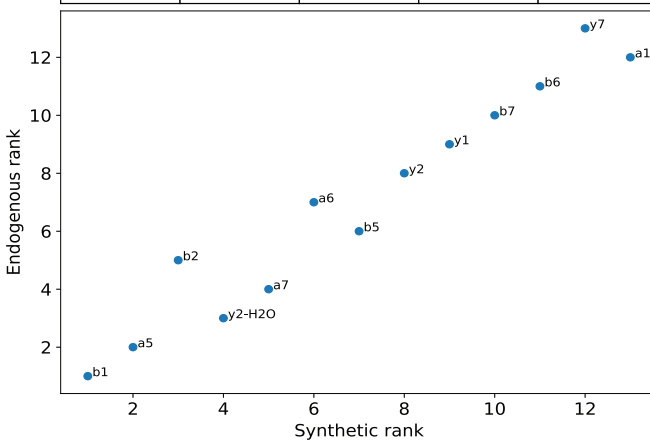
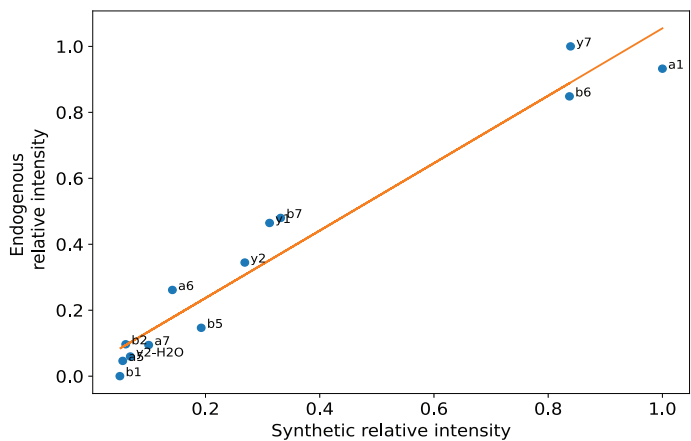


HPRTVLLL / 2+

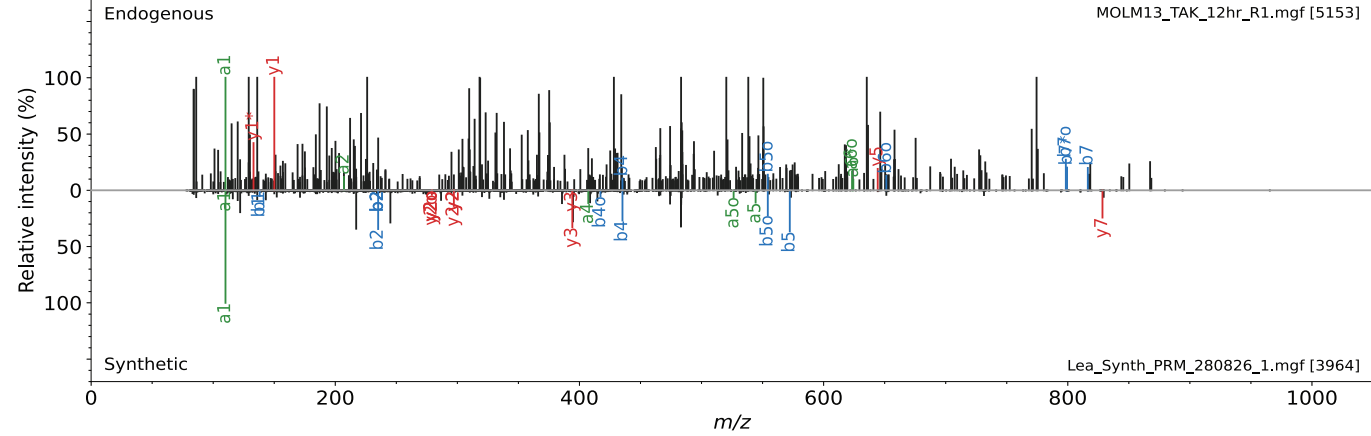


Spectrum	m/z	error (ppm)
Endogenous	474.8076	9.5
Synthetic	474.8024	-1.5

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.91	0.99	2.4e-08
Spearman	0.97	0.91	0.99	2.6e-08
Spectral angle	0.90	-	-	-

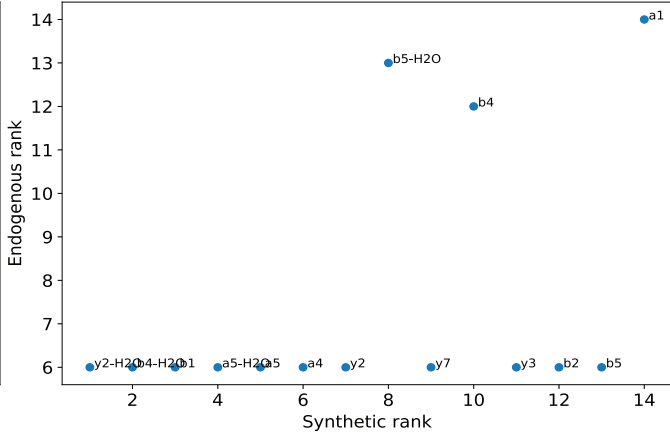
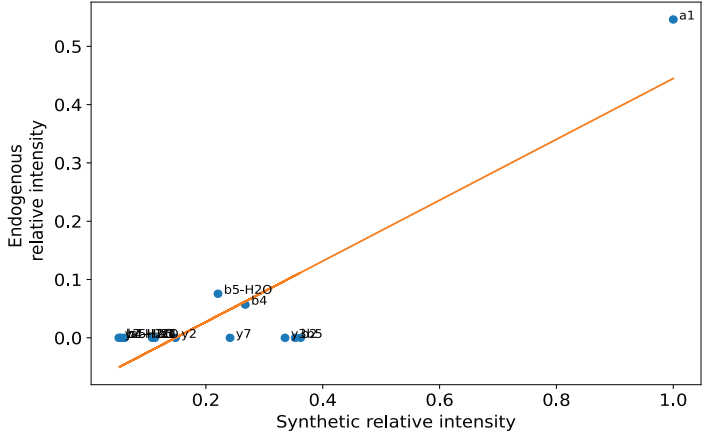


HPSIHPFM / 2+

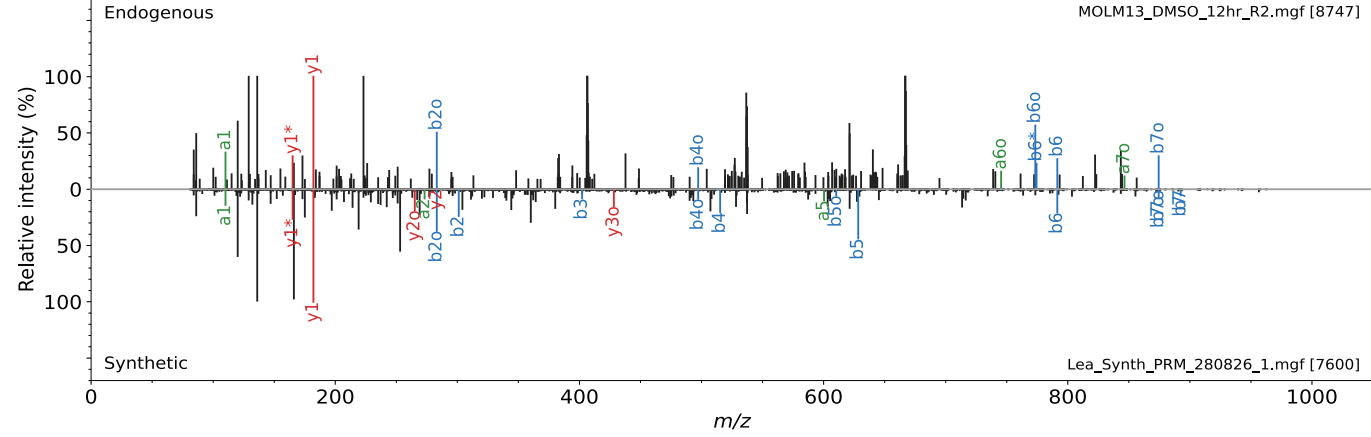


Spectrum	m/z	error (ppm)
Endogenous	483.2335	-6.6
Synthetic	483.2367	0.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.89	0.68	0.96	2.2e-05
Spearman	0.43	-0.13	0.78	1.2e-01
Spectral angle	0.62	-	-	-

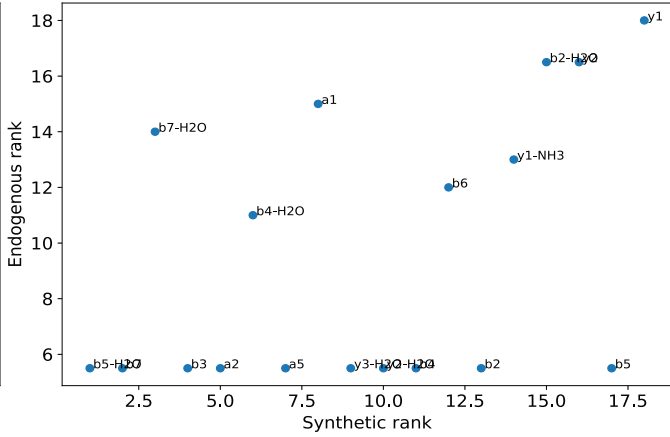
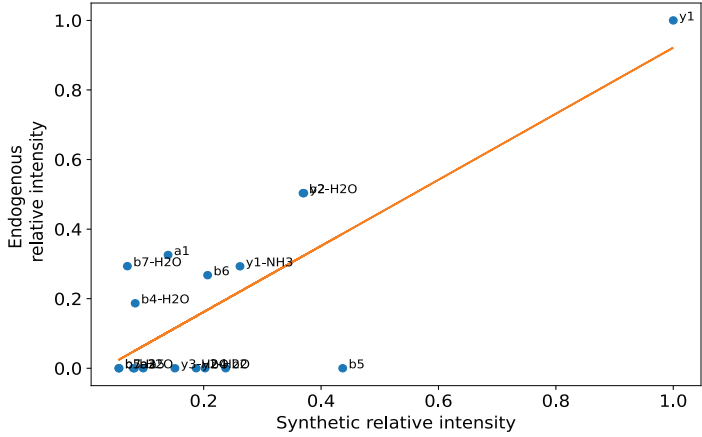


HYTLIYTY / 2+

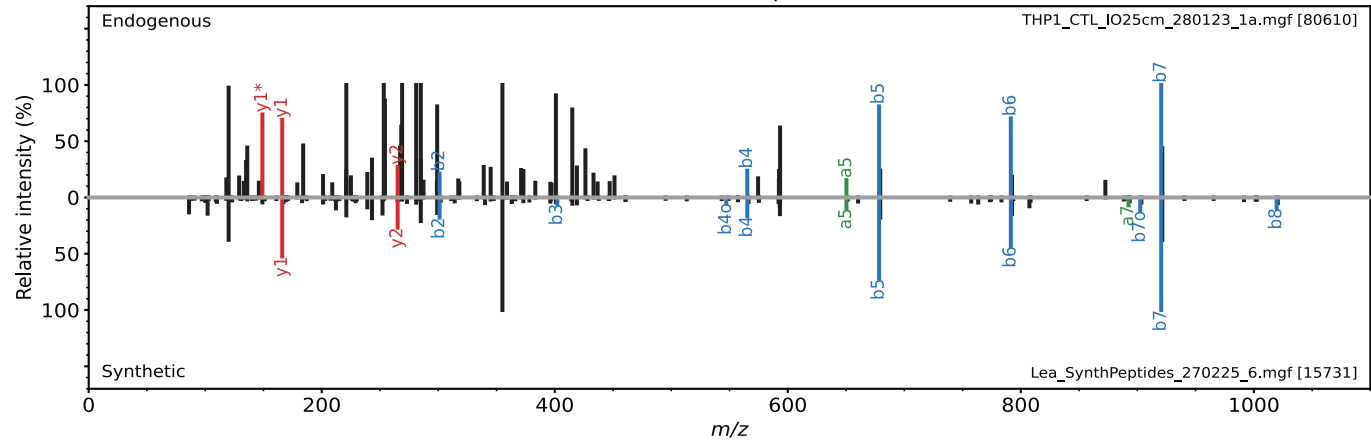


Spectrum	m/z	error (ppm)
Endogenous	537.2662	-4.7
Synthetic	537.2687	0.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.79	0.51	0.92	1.1e-04
Spearman	0.45	-0.02	0.76	5.9e-02
Spectral angle	0.66	-	-	-

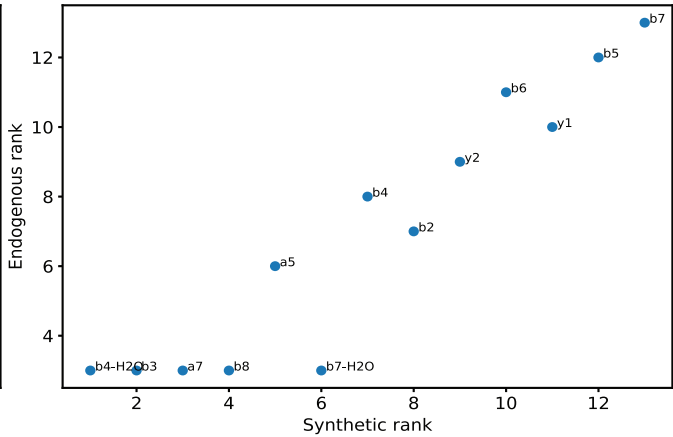
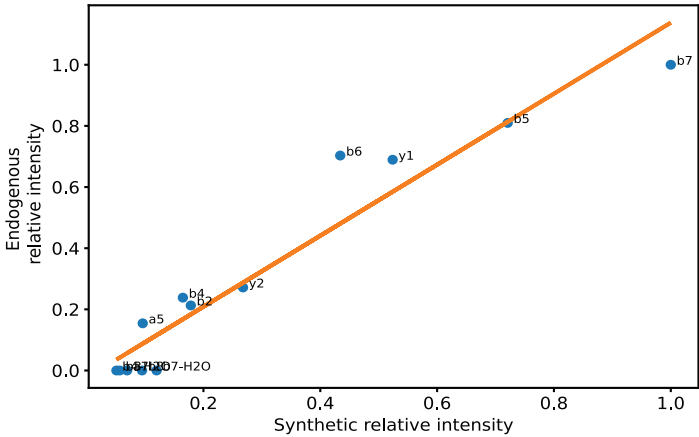


HYTYILEVF / 2+

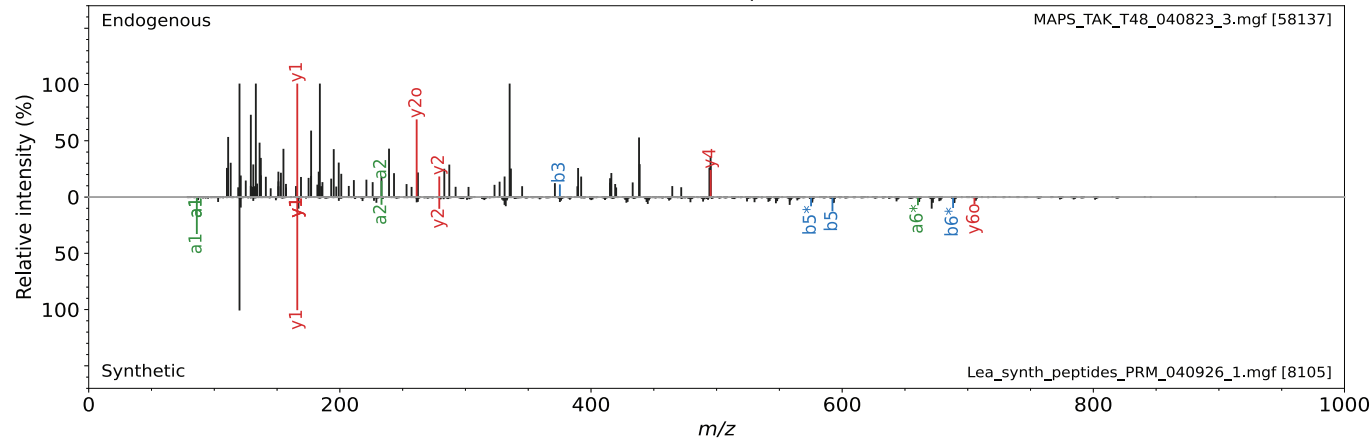


Spectrum	m/z	error (ppm)
Endogenous	592.8030	0.2
Synthetic	592.8043	2.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.96	0.87	0.99	1.7e-07
Spearman	0.94	0.82	0.98	1.3e-06
Spectral angle	0.87	-	-	-

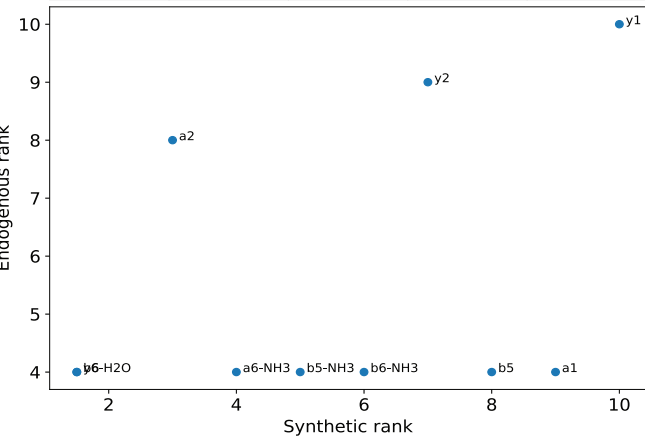
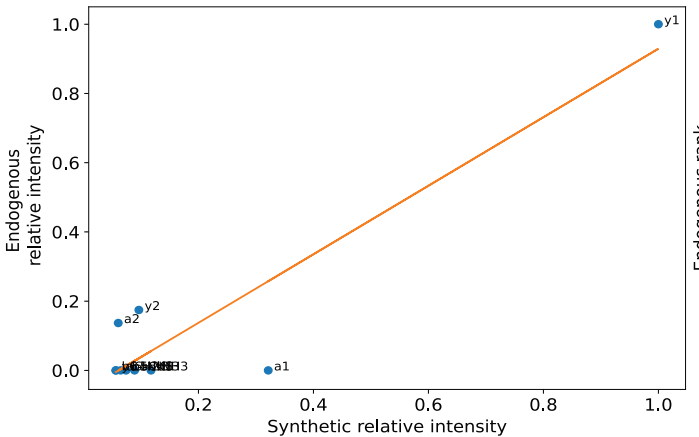


IFNNCLIF / 2+

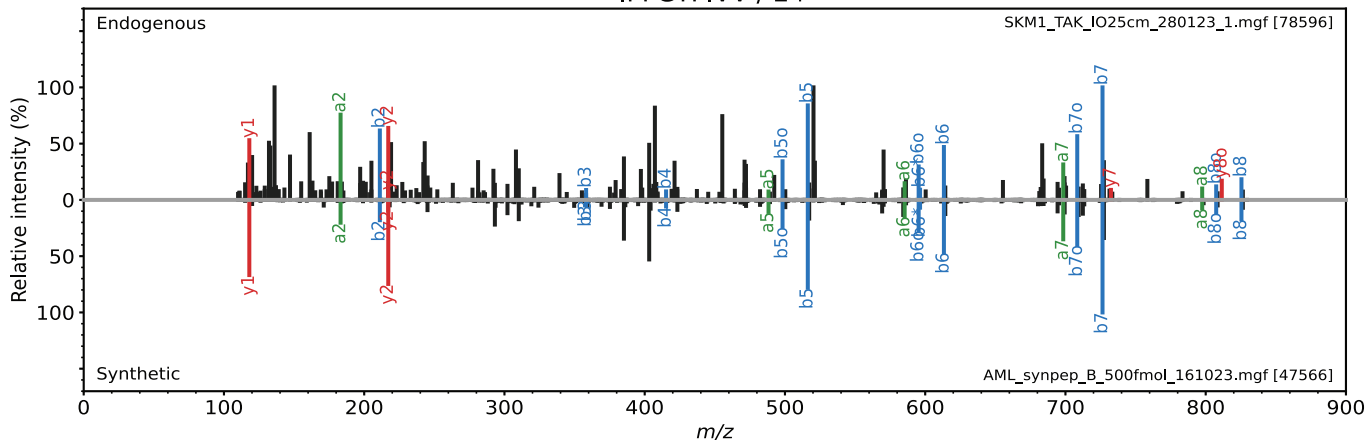


Spectrum	m/z	error (ppm)
Endogenous	492.2599	10.8
Synthetic	492.2567	4.3

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.93	0.73	0.98	8.2e-05
Spearman	0.37	-0.34	0.81	3.0e-01
Spectral angle	0.76	-	-	-

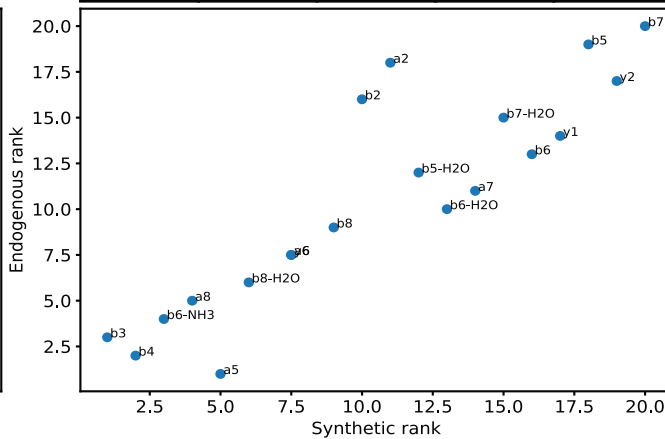
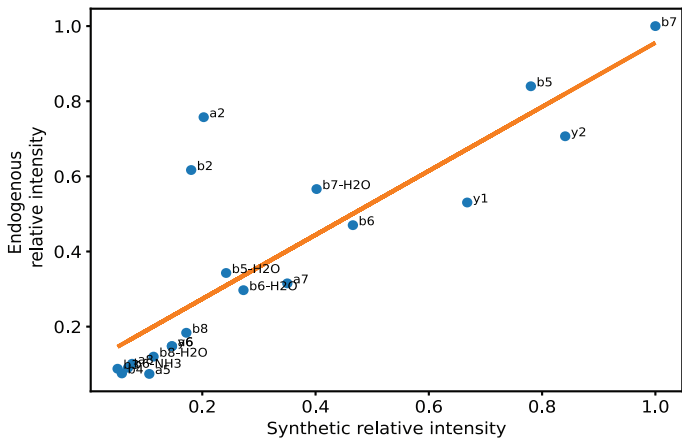


IPFGTPIVV / 2+

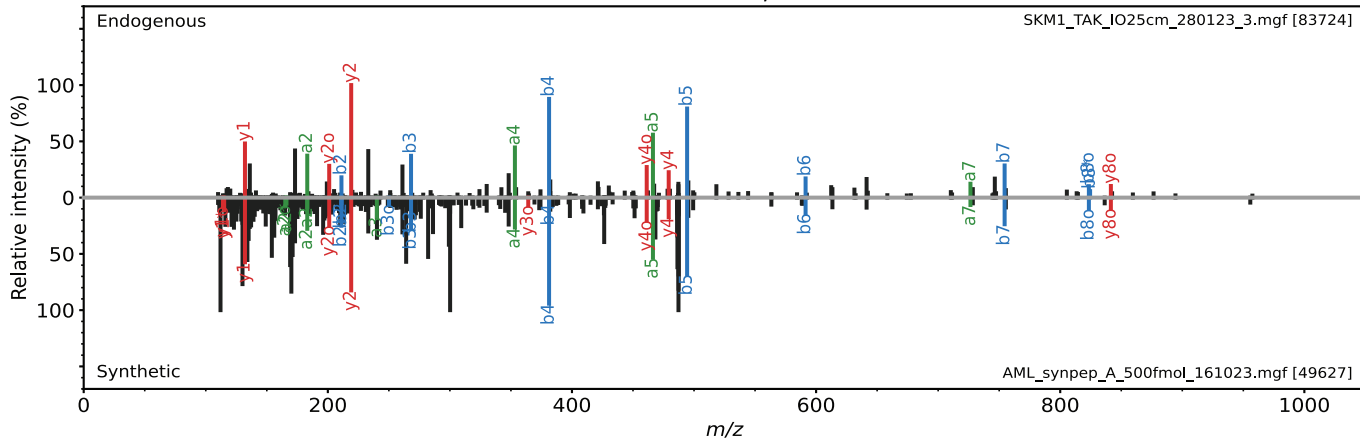


Spectrum	m/z	error (ppm)
Endogenous	471.7866	0.1
Synthetic	471.7871	0.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.84	0.63	0.93	4.0e-06
Spearman	0.89	0.74	0.96	1.7e-07
Spectral angle	0.76	-	-	-

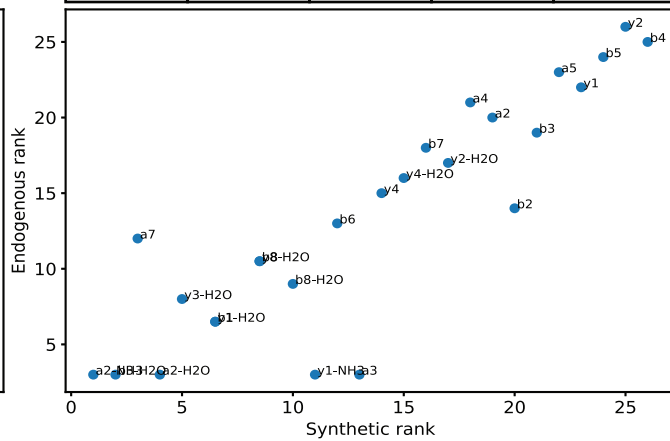
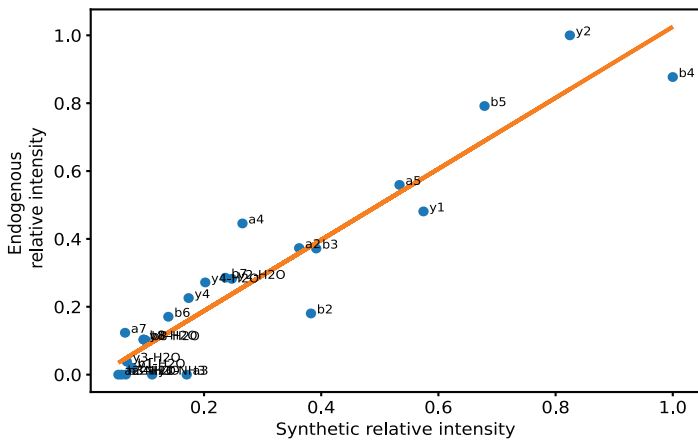


IPGILPYSL / 2+

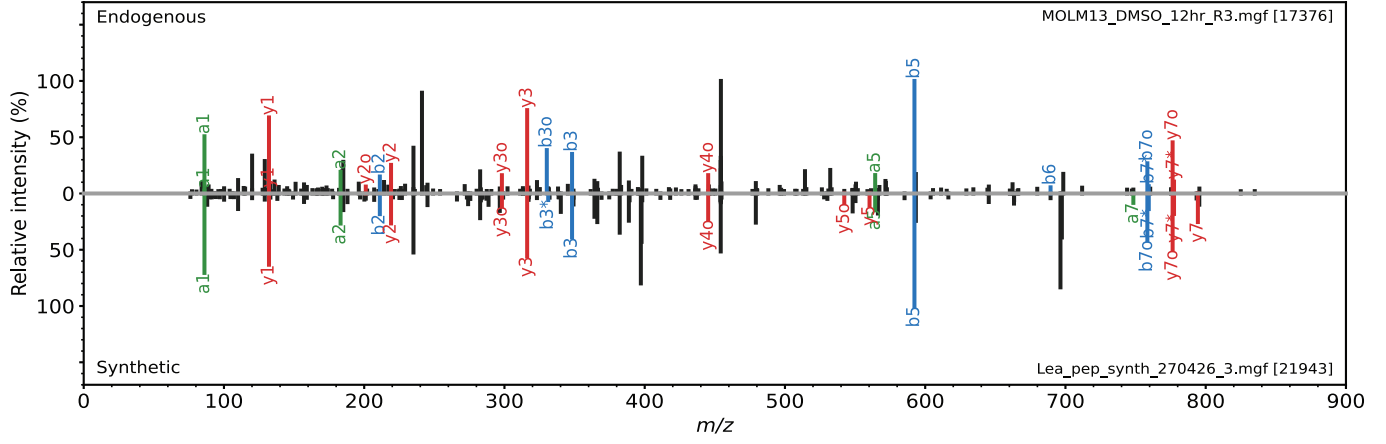


Spectrum	m/z	error (ppm)
Endogenous	486.7920	0.3
Synthetic	486.7924	0.1

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.95	0.88	0.98	2.9e-13
Spearman	0.89	0.76	0.95	1.6e-09
Spectral angle	0.85	-	-	-

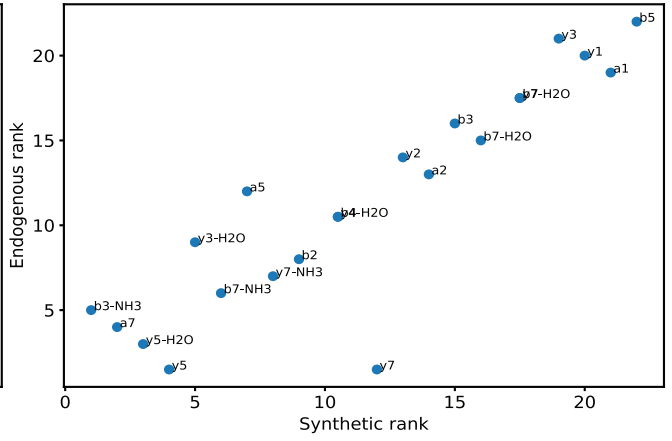
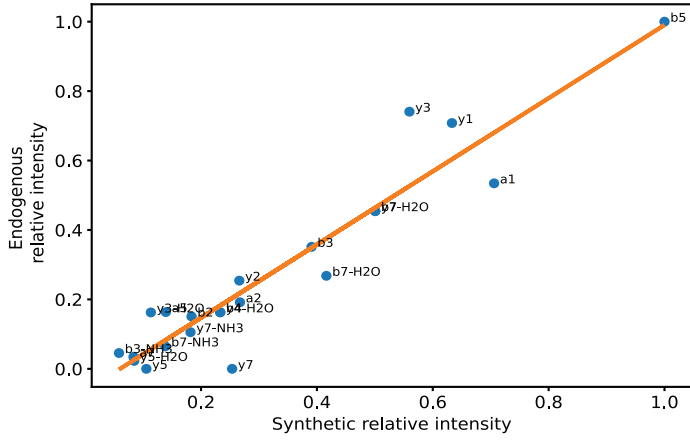


IPHPFPSL / 2+

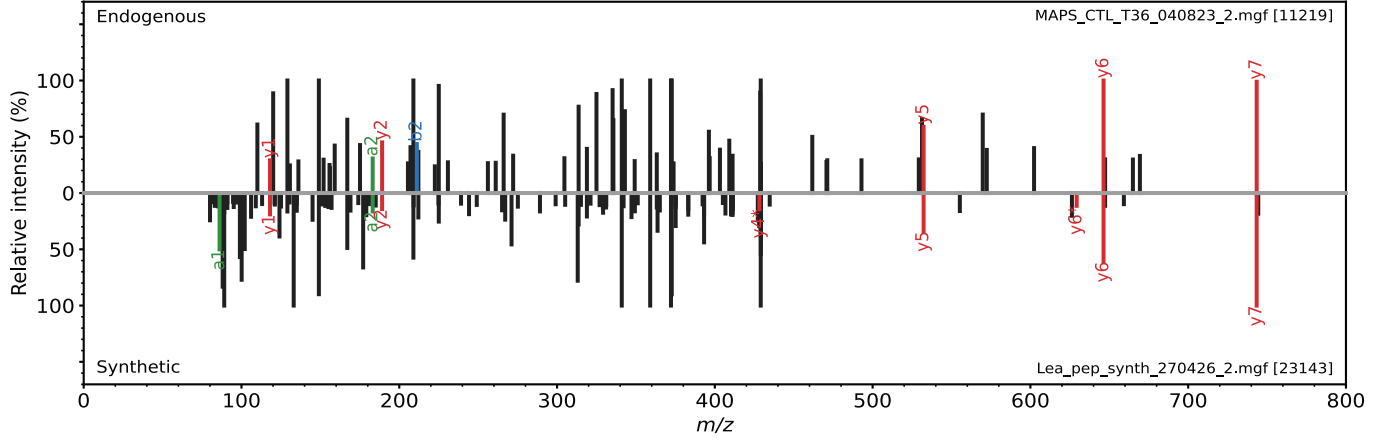


Spectrum	m/z	error (ppm)
Endogenous	454.2555	0.2
Synthetic	454.2551	-0.7

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.95	0.88	0.98	2.4e-11
Spearman	0.89	0.75	0.95	2.5e-08
Spectral angle	0.84	-	-	-

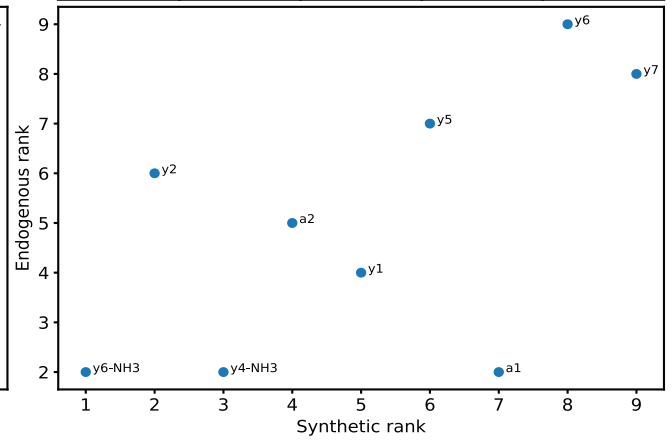
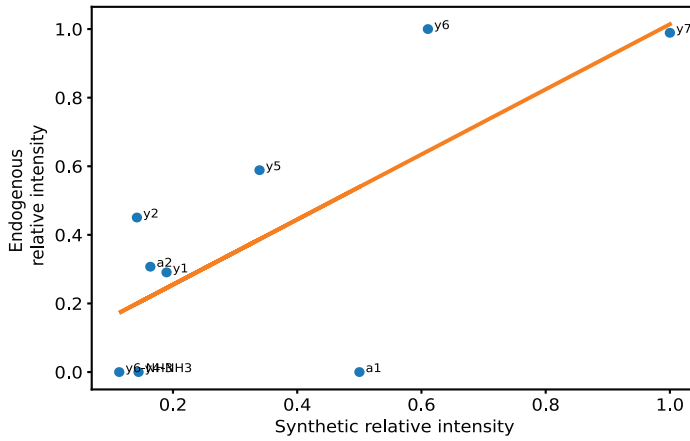


IPNSKQAV / 2+

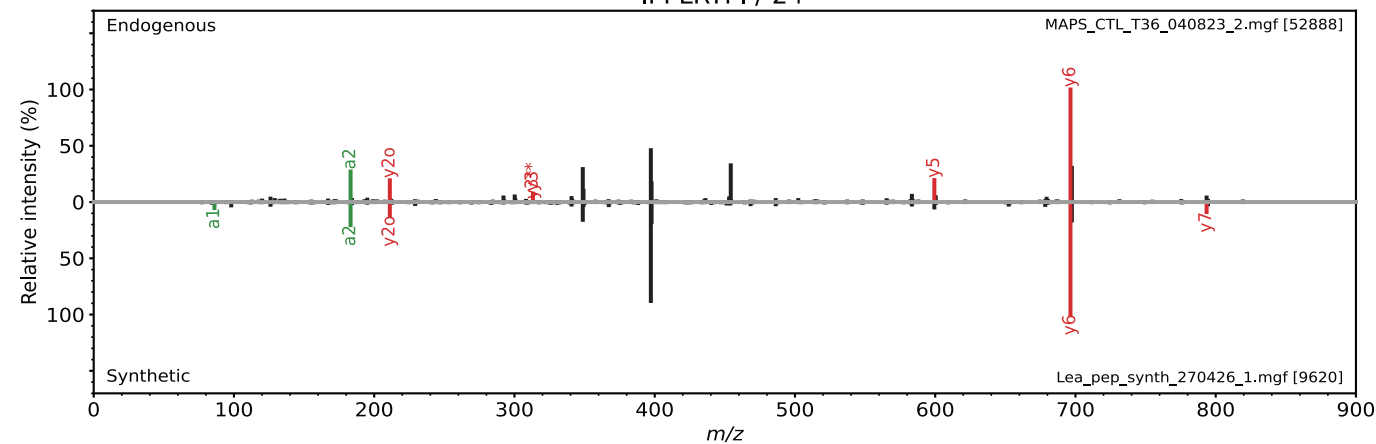


Spectrum	m/z	error (ppm)
Endogenous	428.7524	10.3
Synthetic	428.7478	-0.5

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.72	0.10	0.94	2.9e-02
Spearman	0.59	-0.12	0.90	9.2e-02
Spectral angle	0.68	-	-	-

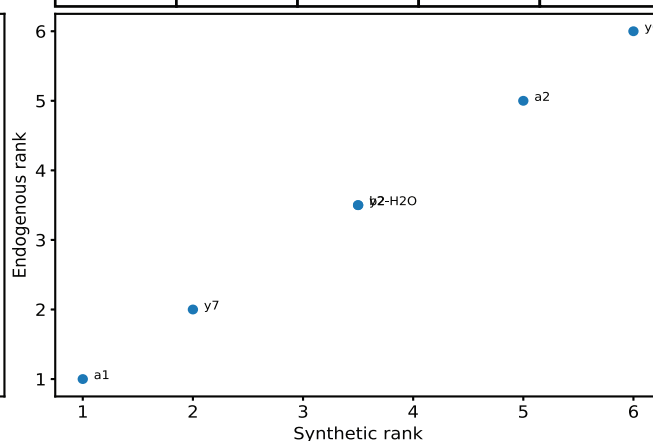
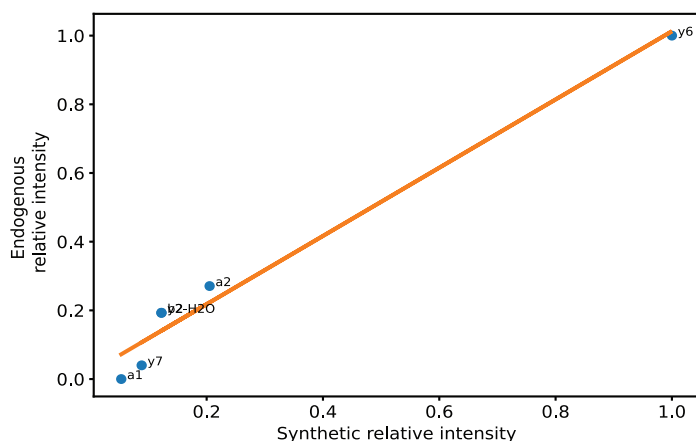


IPPLRTPI / 2+

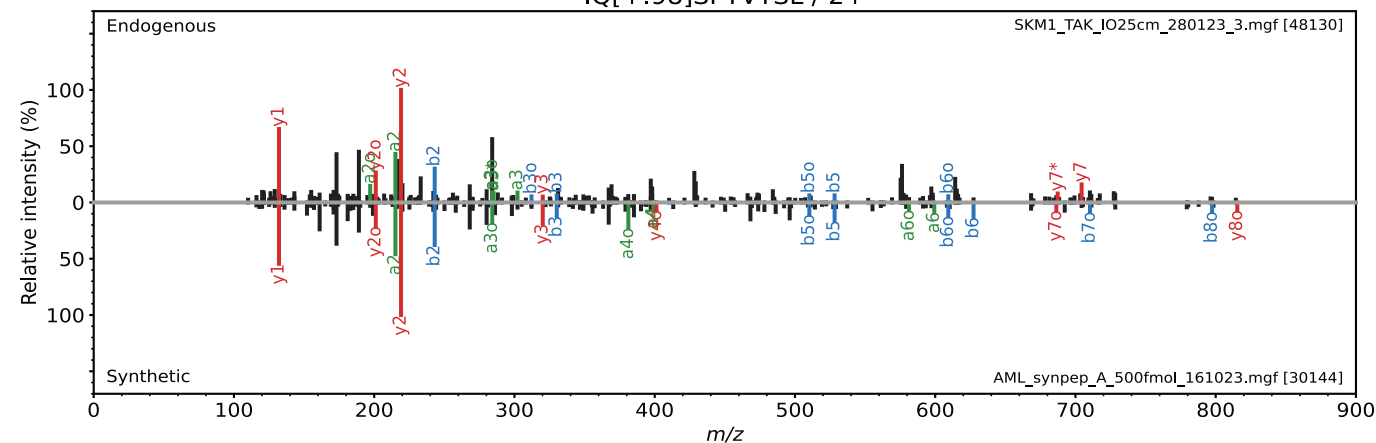


Spectrum	m/z	error (ppm)
Endogenous	453.7967	9.9
Synthetic	453.7921	-0.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.99	0.88	1.00	2.6e-04
Spearman	1.00	1.00	1.00	0.0e+00
Spectral angle	0.92	-	-	-

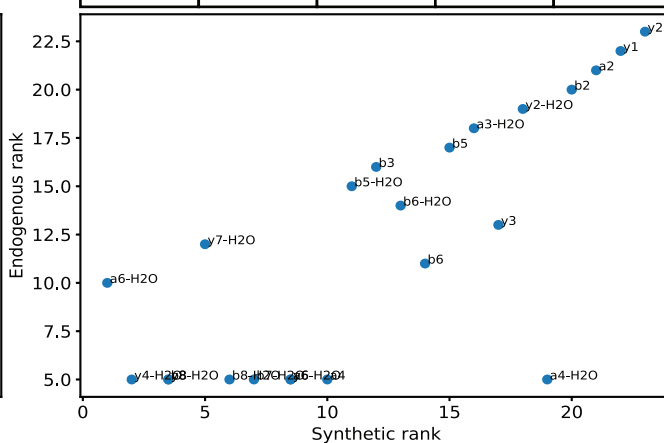
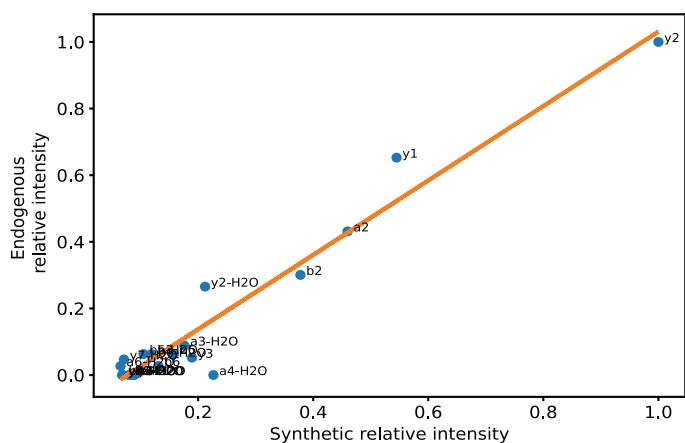


IQ[+.98]SPTVTSL / 2+

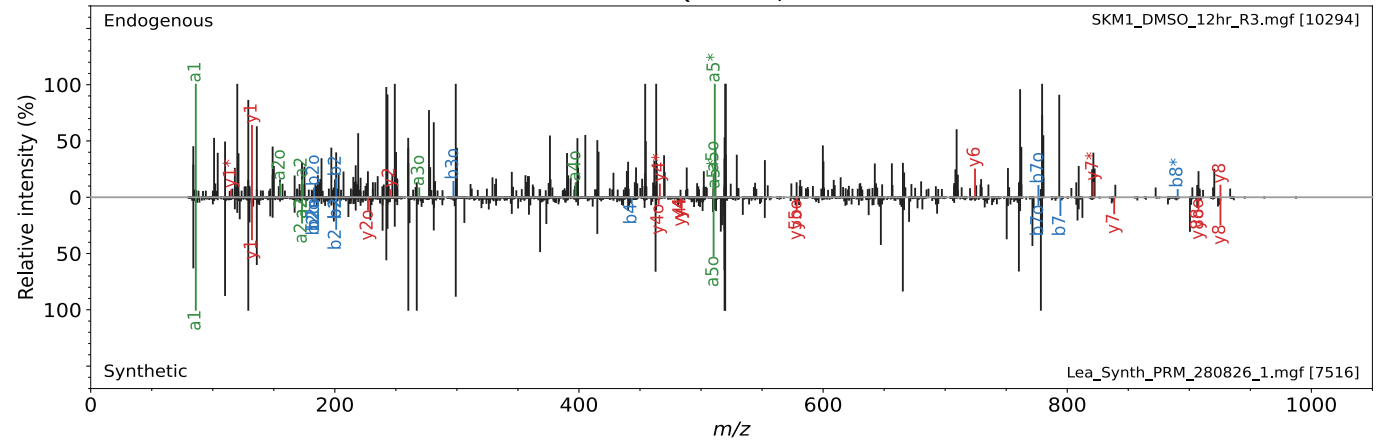


Spectrum	m/z	error (ppm)
Endogenous	473.7585	0.6
Synthetic	473.7588	0.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.94	0.99	8.7e-15
Spearman	0.77	0.52	0.90	2.1e-05
Spectral angle	0.80	-	-	-

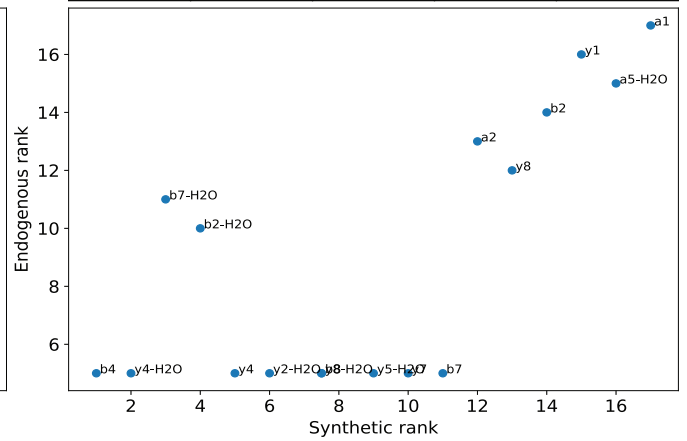
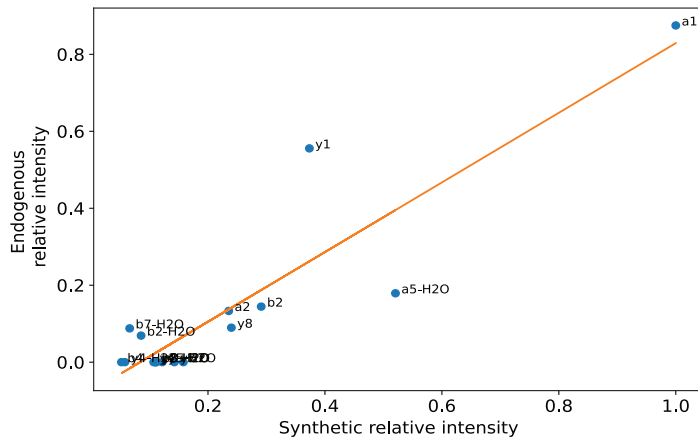


ISNQLHTLL / 2+

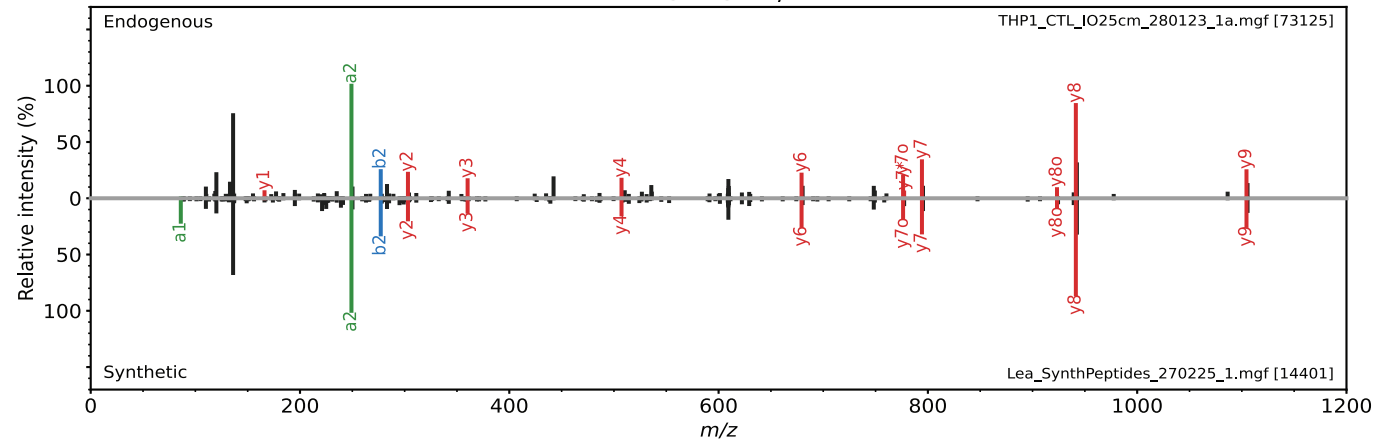


Spectrum	m/z	error (ppm)
Endogenous	519.7968	-7.5
Synthetic	519.8021	2.7

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.90	0.74	0.96	7.4e-07
Spearman	0.71	0.35	0.89	1.4e-03
Spectral angle	0.72	-	-	-

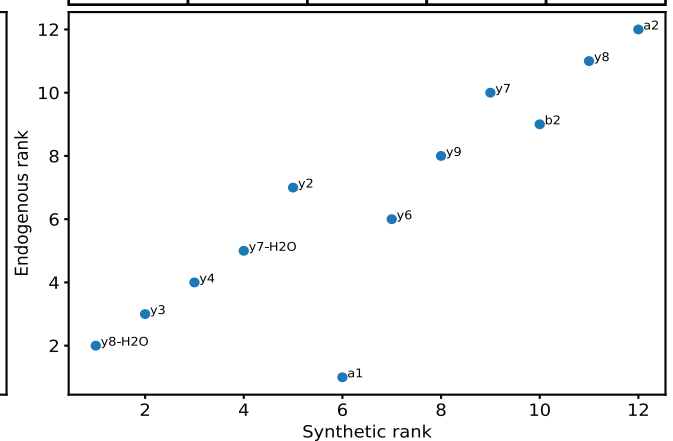
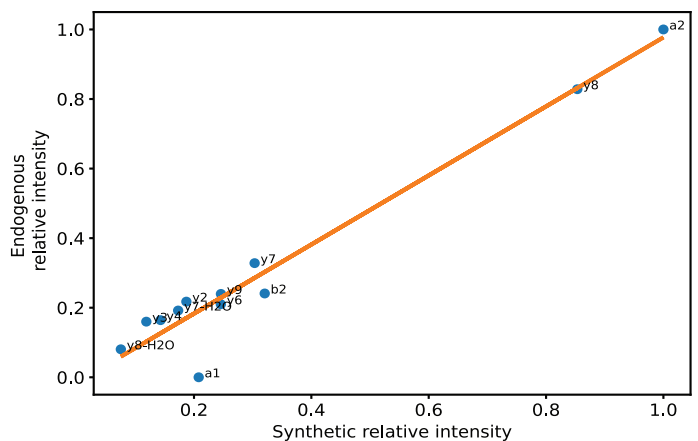


IYFDGDFGHF / 2+

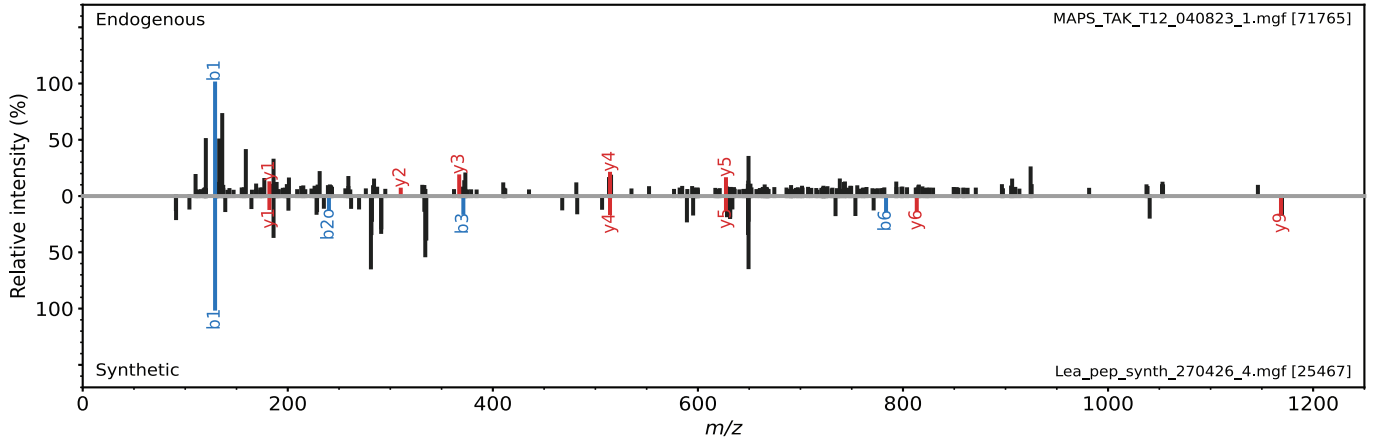


Spectrum	m/z	error (ppm)
Endogenous	609.2664	-0.5
Synthetic	609.2669	0.3

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.90	0.99	1.0e-07
Spearman	0.87	0.60	0.96	2.0e-04
Spectral angle	0.90	-	-	-

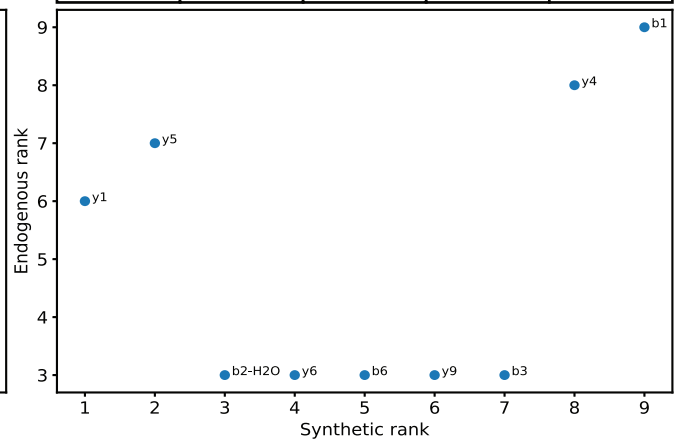
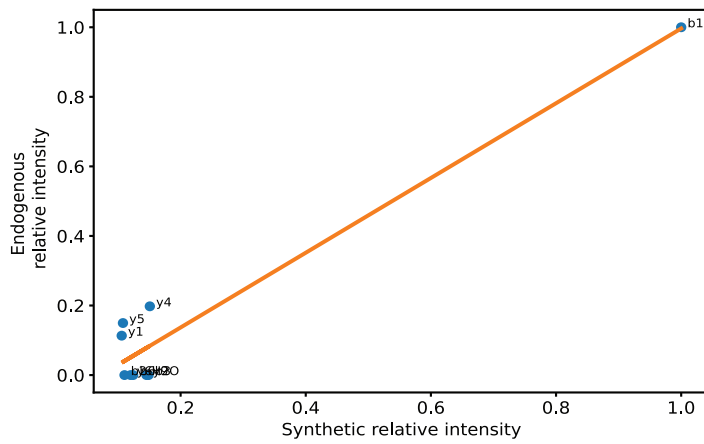


KEILWLFGKY / 2+

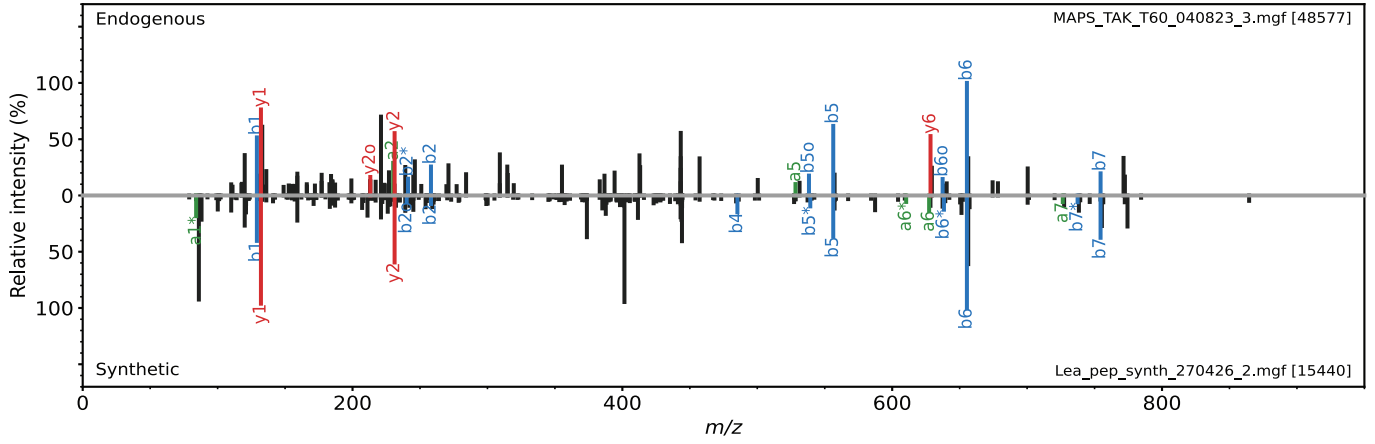


Spectrum	m/z	error (ppm)
Endogenous	648.8772	9.2
Synthetic	648.8721	1.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.85	0.99	1.7e-05
Spearman	0.27	-0.48	0.79	4.8e-01
Spectral angle	0.82	-	-	-

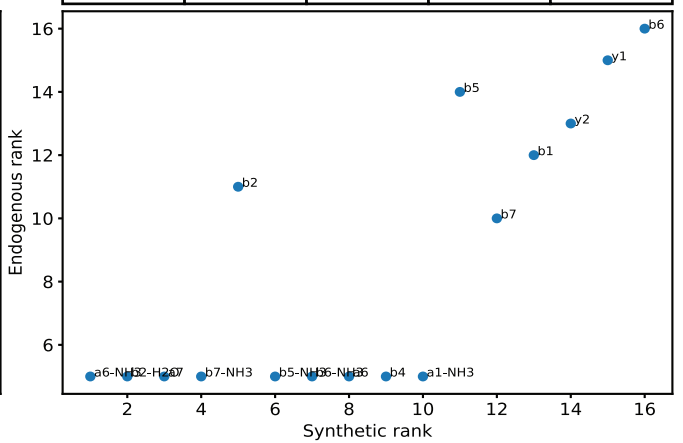
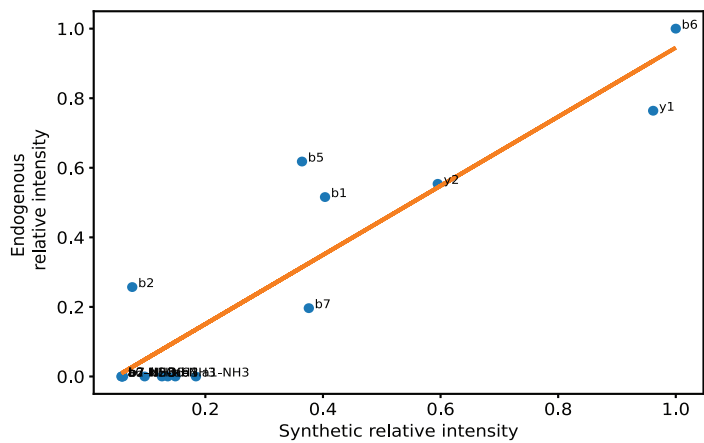


KENLAVVI / 2+

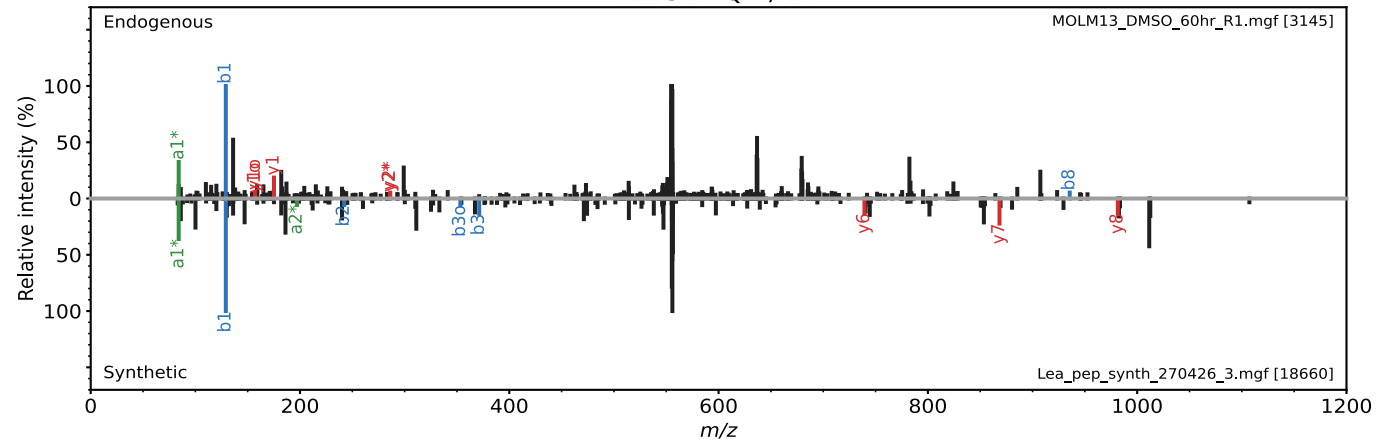


Spectrum	m/z	error (ppm)
Endogenous	443.2786	10.8
Synthetic	443.2734	-0.9

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.92	0.78	0.97	4.2e-07
Spearman	0.78	0.47	0.92	3.2e-04
Spectral angle	0.79	-	-	-

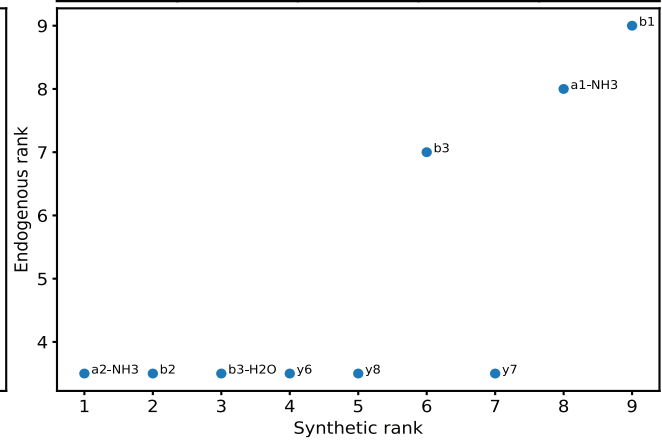
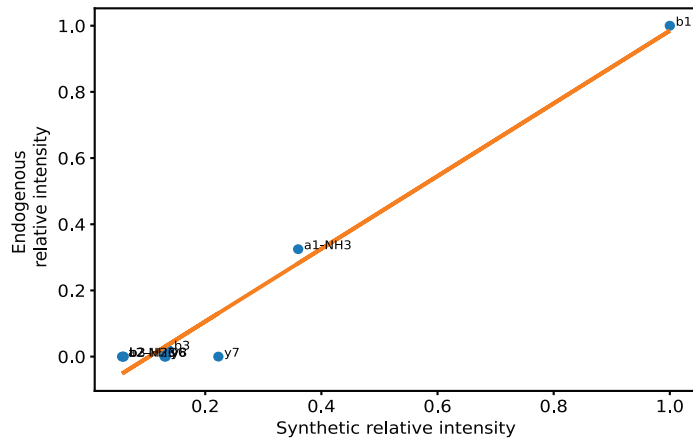


KLEGEIHQR / 2+

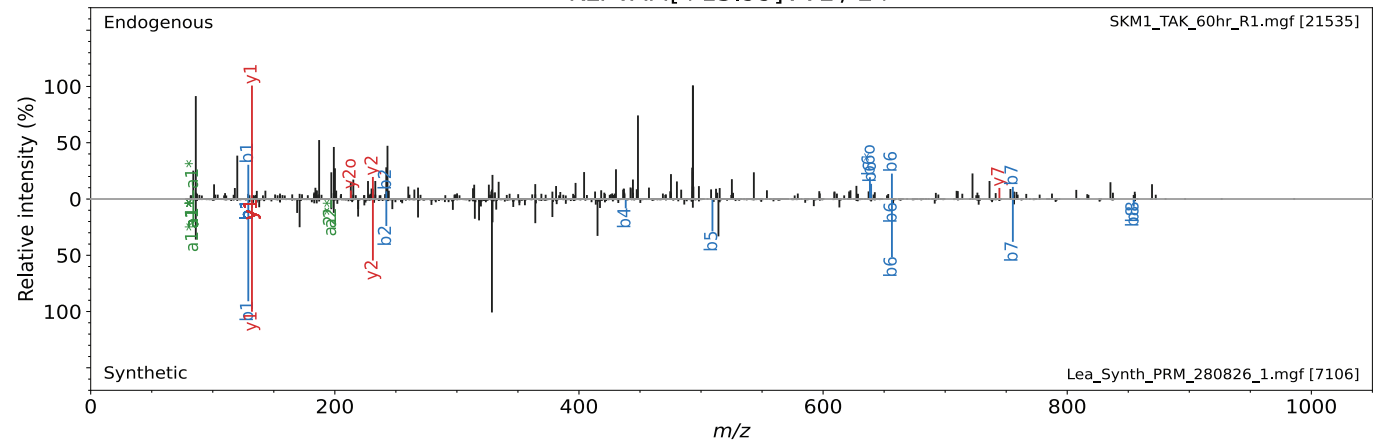


Spectrum	m/z	error (ppm)
Endogenous	555.3106	7.0
Synthetic	555.3061	-1.1

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.98	0.92	1.00	1.7e-06
Spearman	0.77	0.22	0.95	1.5e-02
Spectral angle	0.81	-	-	-

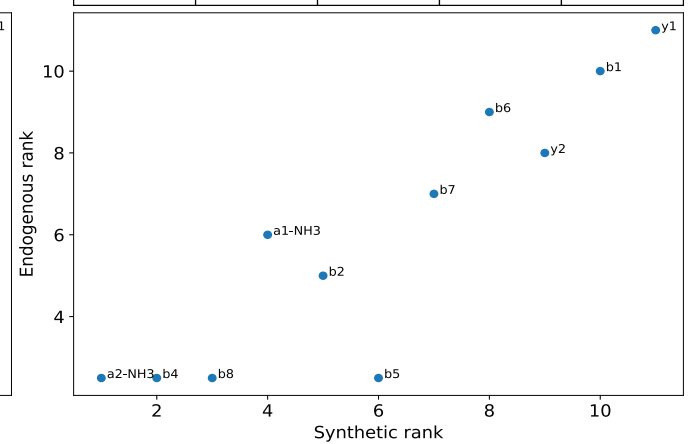
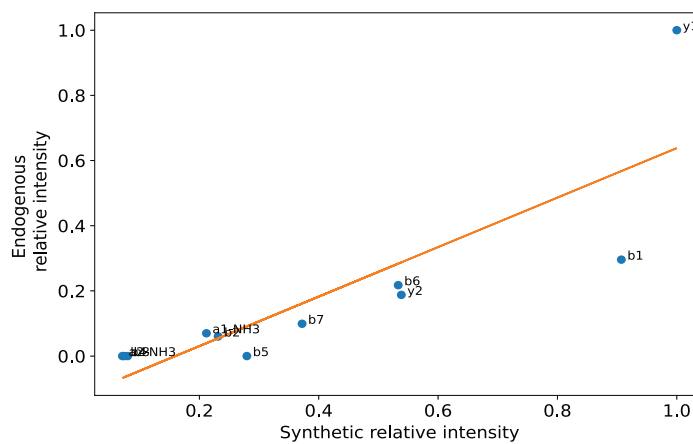


KLPVAM[+15.99]VVL / 2+

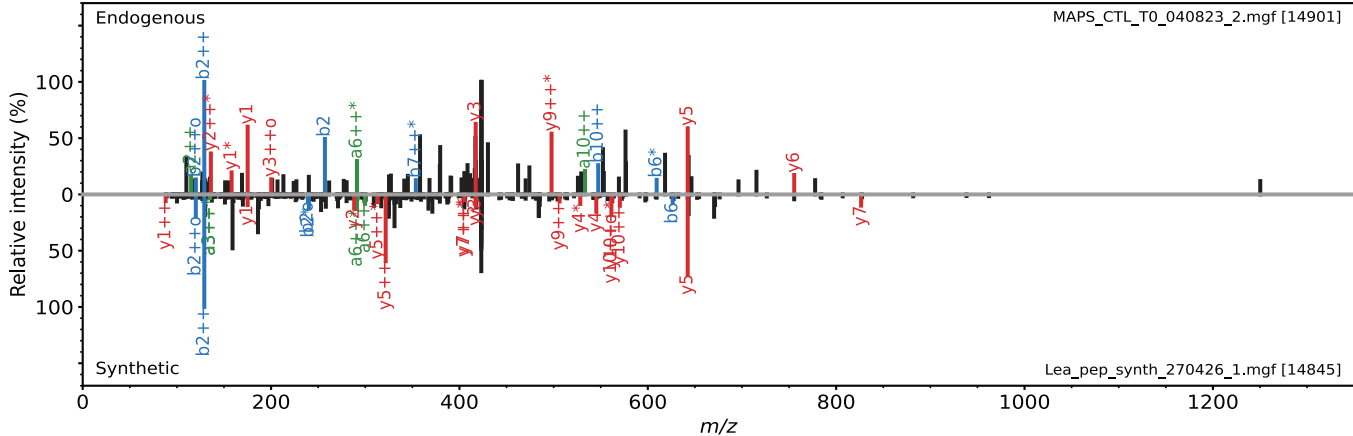


Spectrum	m/z	error (ppm)
Endogenous	493.3083	-2.0
Synthetic	493.3090	-0.6

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.84	0.49	0.96	1.1e-03
Spearman	0.90	0.66	0.97	1.4e-04
Spectral angle	0.66	-	-	-

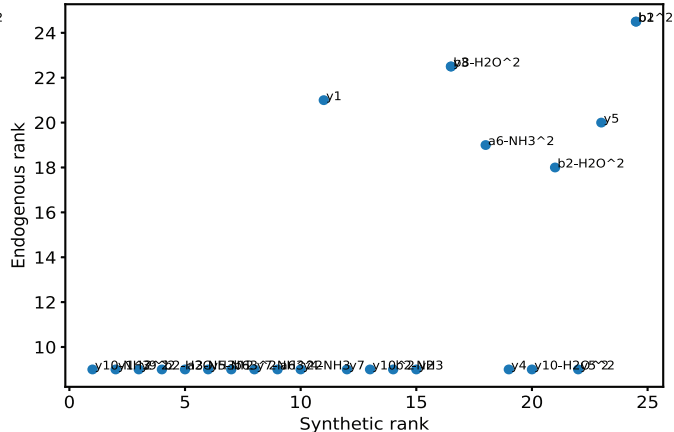
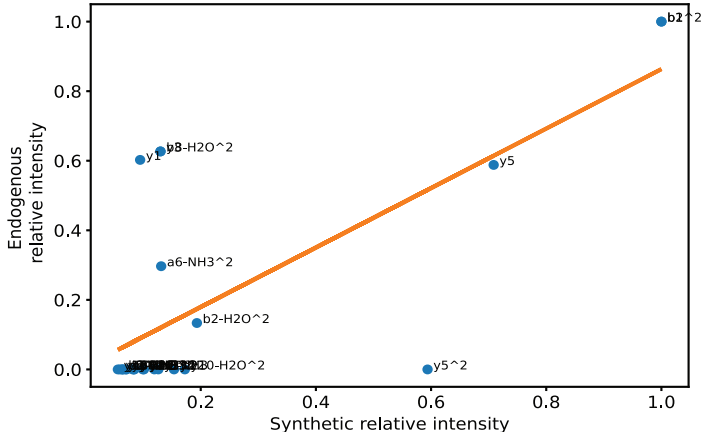


KQGKALPQELR / 3+

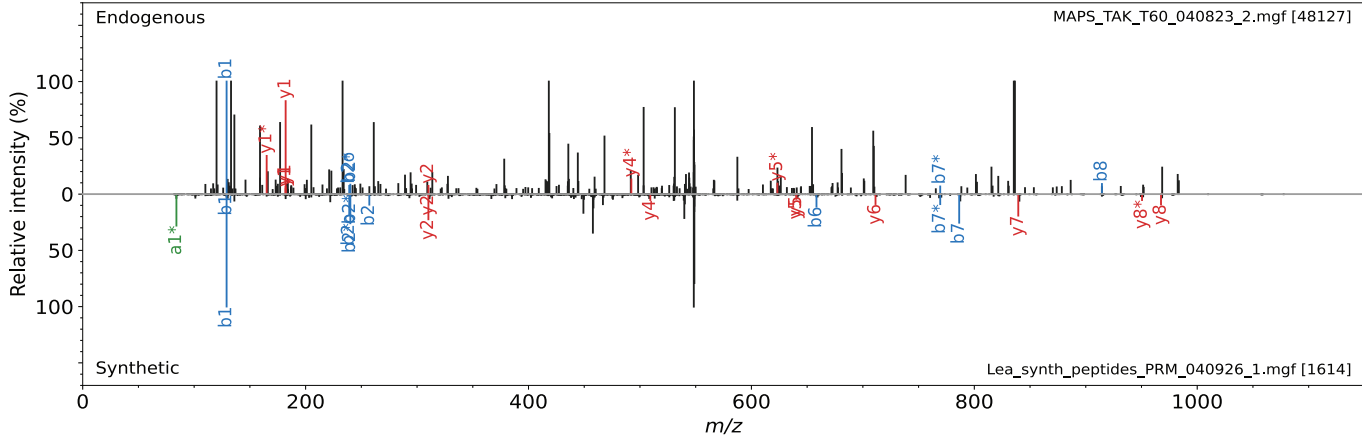


Spectrum	m/z	error (ppm)
Endogenous	423.2617	17.7
Synthetic	423.2539	-0.7

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.73	0.47	0.87	3.8e-05
Spearman	0.61	0.29	0.81	1.1e-03
Spectral angle	0.60	-	-	-

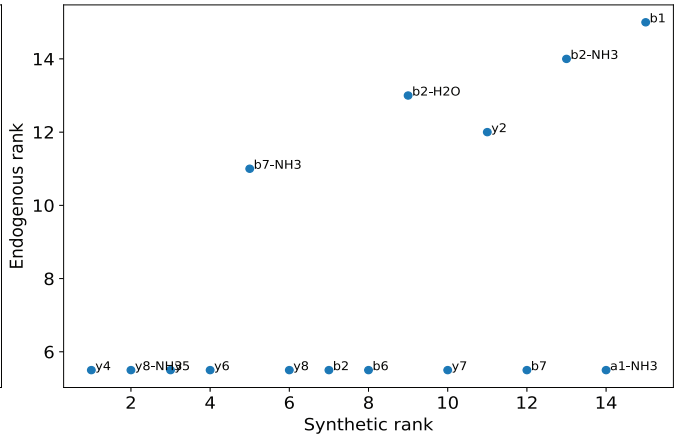
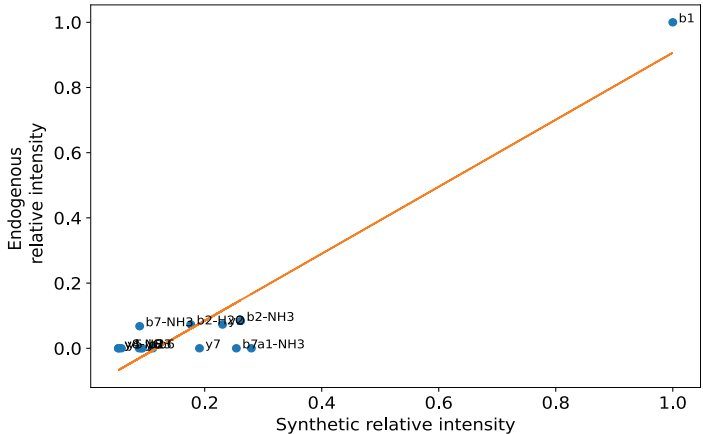


KQKAMAQKY / 2+

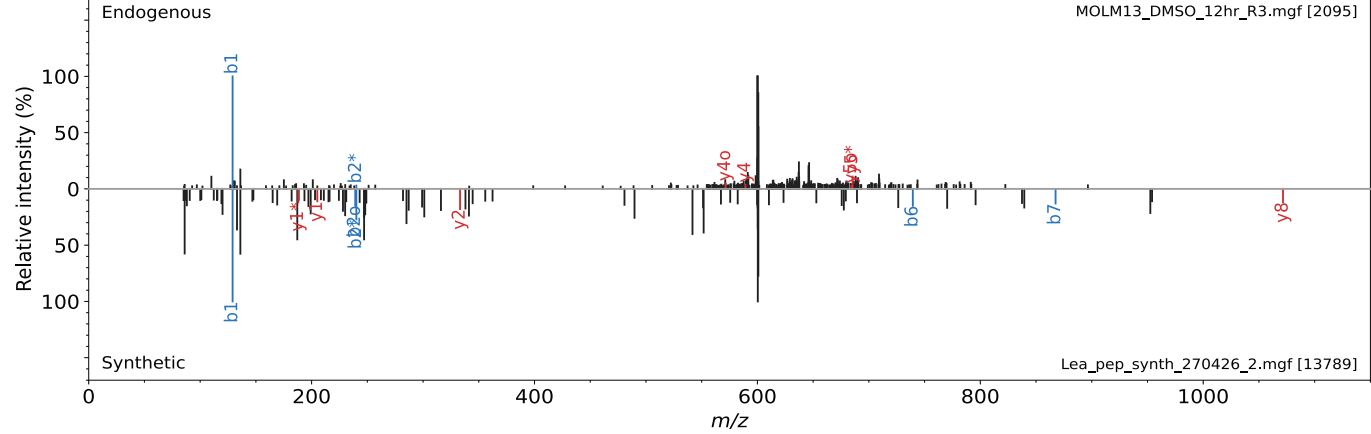


Spectrum	m/z	error (ppm)
Endogenous	548.3011	-3.8
Synthetic	548.3055	5.3

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.95	0.85	0.98	8.0e-08
Spearman	0.51	-0.01	0.81	5.3e-02
Spectral angle	0.70	-	-	-

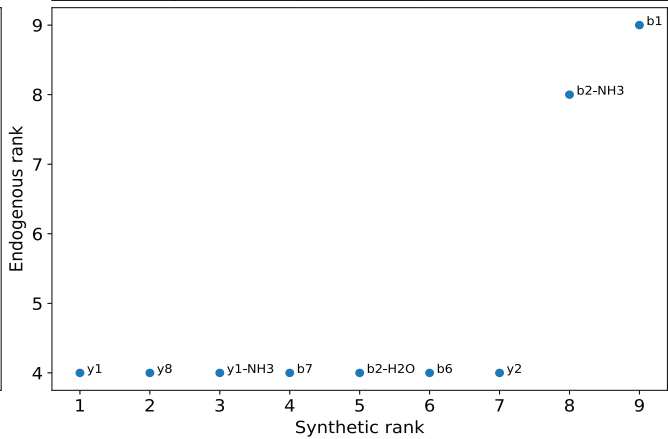
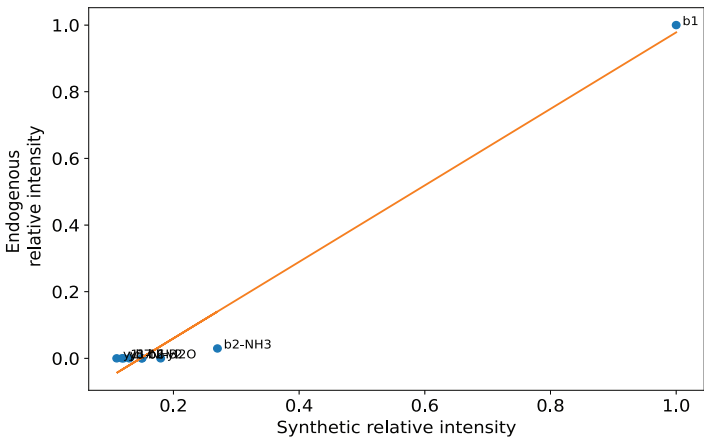


KQLQLQQKW / 2+

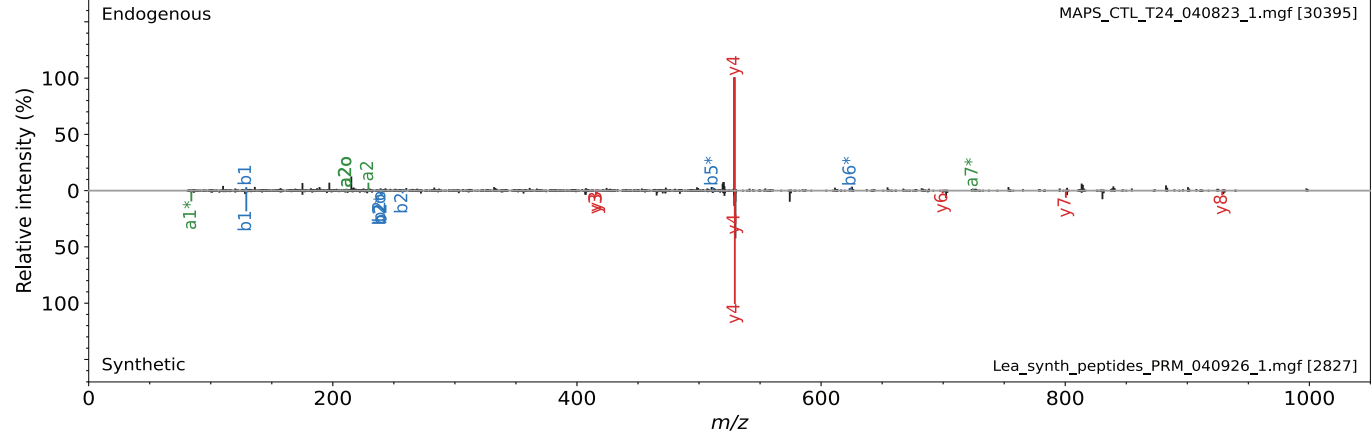


Spectrum	m/z	error (ppm)
Endogenous	600.3514	5.0
Synthetic	600.3474	-1.7

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.99	0.95	1.00	4.0e-07
Spearman	0.73	0.13	0.94	2.5e-02
Spectral angle	0.74	-	-	-

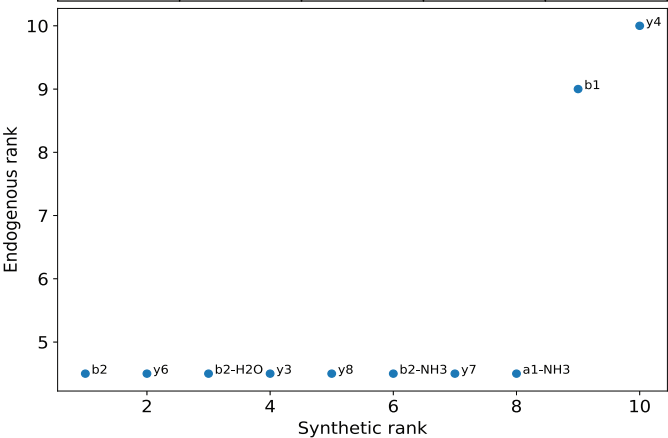
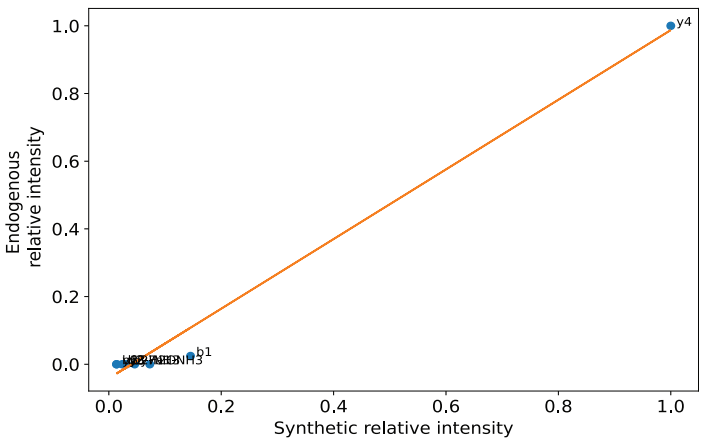


KQTGLIQR / 2+

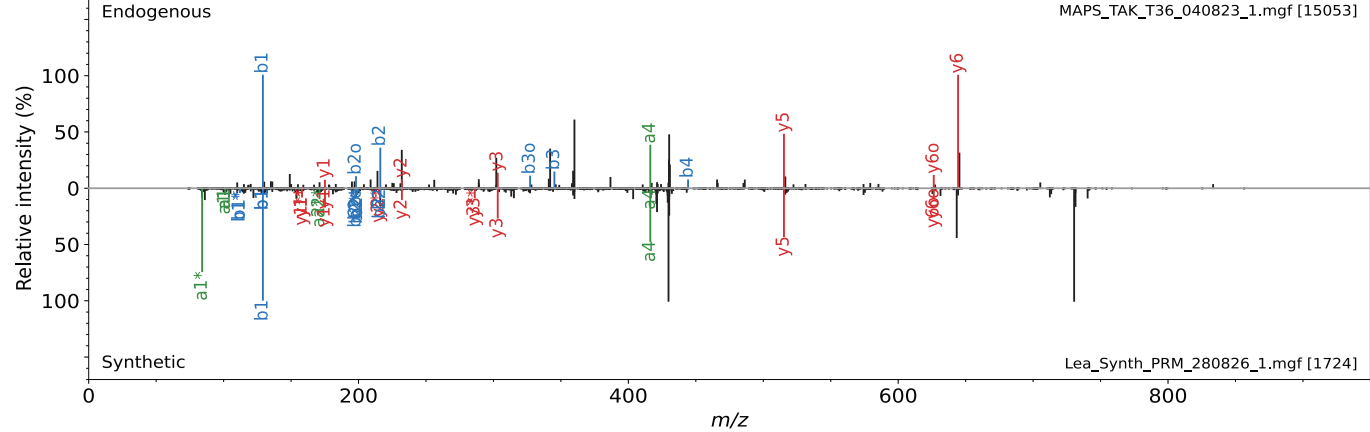


Spectrum	m/z	error (ppm)
Endogenous	528.8353	9.2
Synthetic	528.8320	4.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.99	0.97	1.00	5.4e-09
Spearman	0.70	0.13	0.92	2.4e-02
Spectral angle	0.90	-	-	-

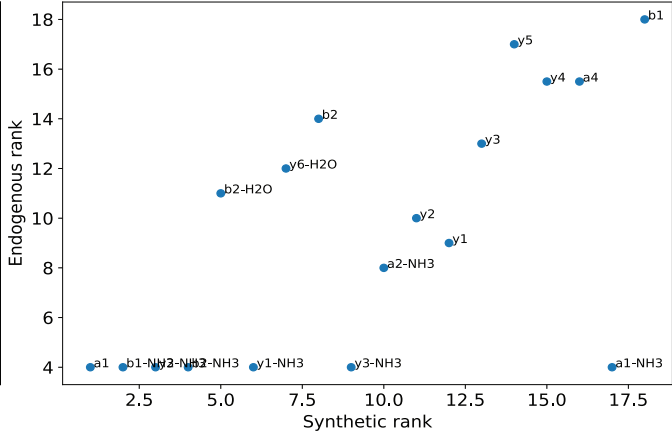
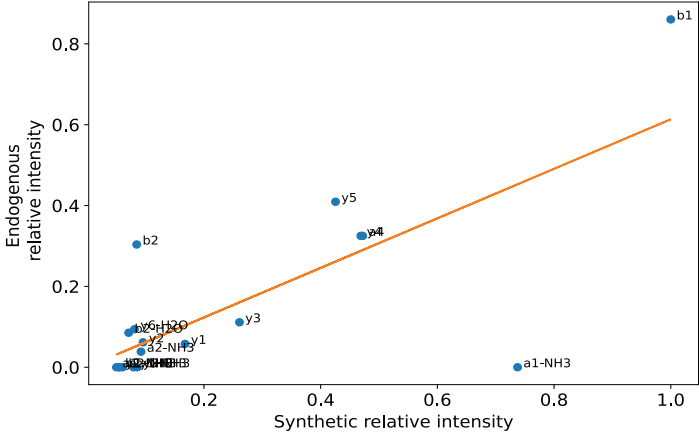


KSQ[+0.98]VIAGR / 2+

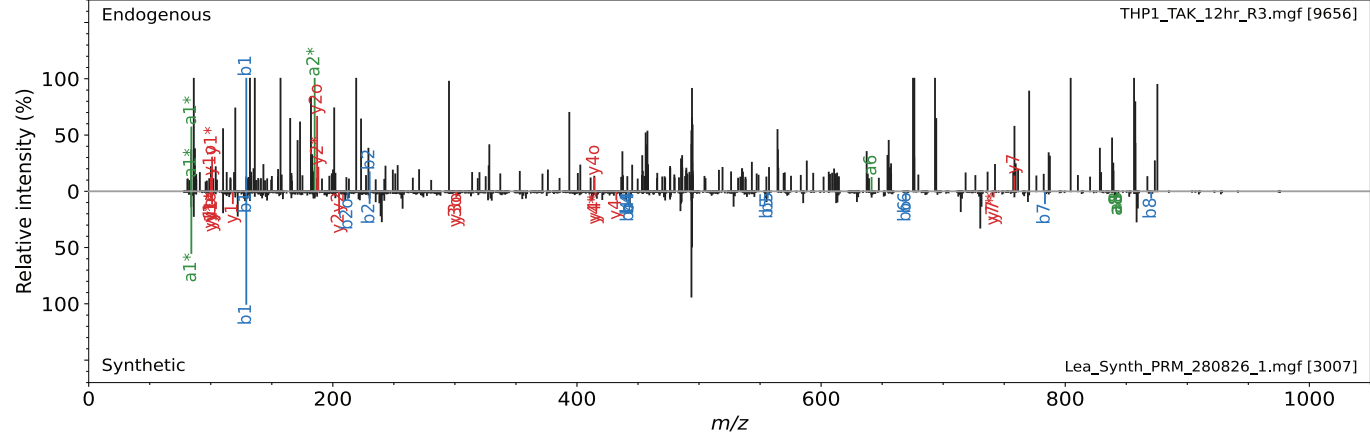


Spectrum	m/z	error (ppm)
Endogenous	430.2572	8.8
Synthetic	430.2536	0.5

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.75	0.44	0.90	3.3e-04
Spearman	0.65	0.26	0.86	3.7e-03
Spectral angle	0.63	-	-	-

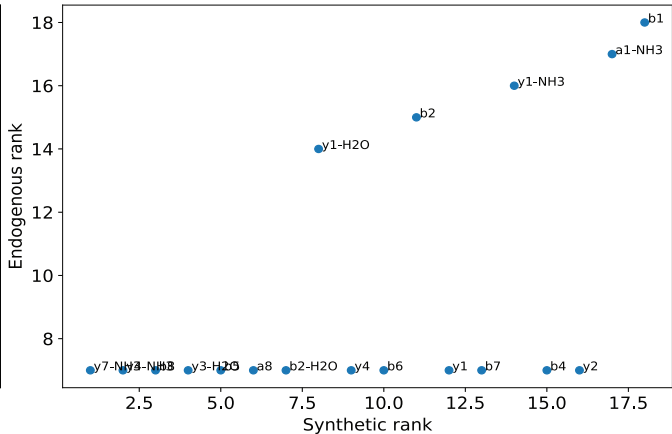
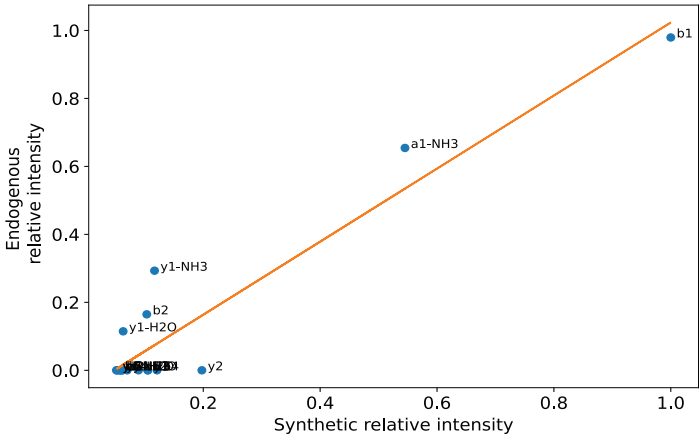


KTPDNINSV / 2+

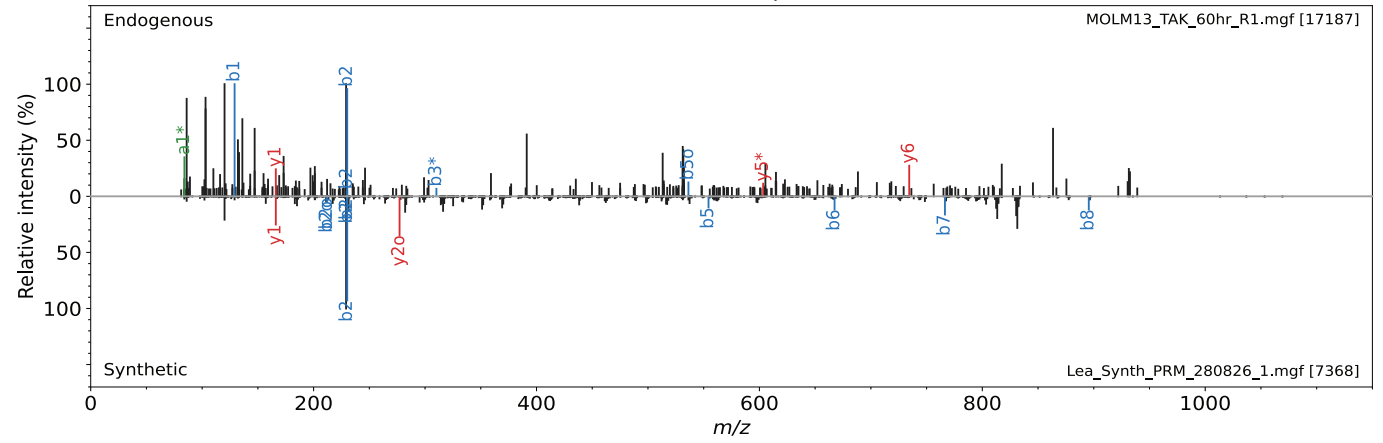


Spectrum	m/z	error (ppm)
Endogenous	494.2625	7.3
Synthetic	494.2590	0.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.95	0.86	0.98	2.6e-09
Spearman	0.55	0.11	0.81	1.8e-02
Spectral angle	0.79	-	-	-

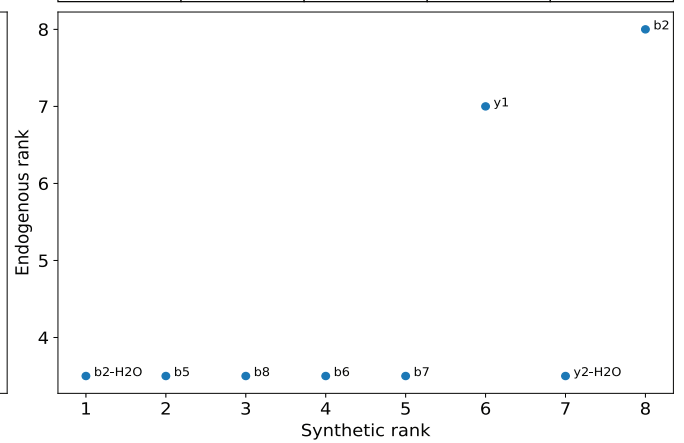
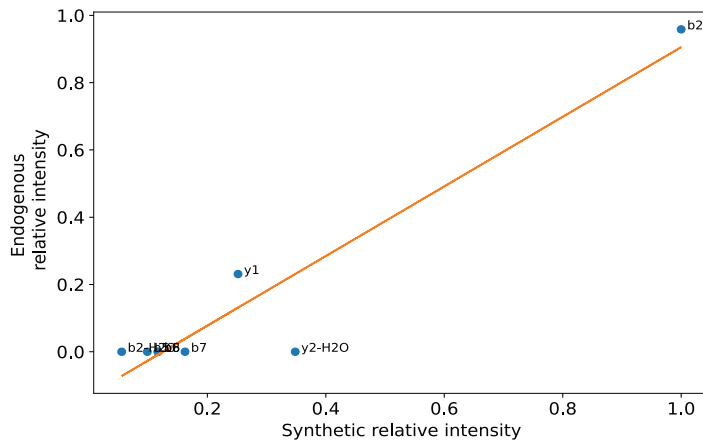


KTPNILVEF / 2+

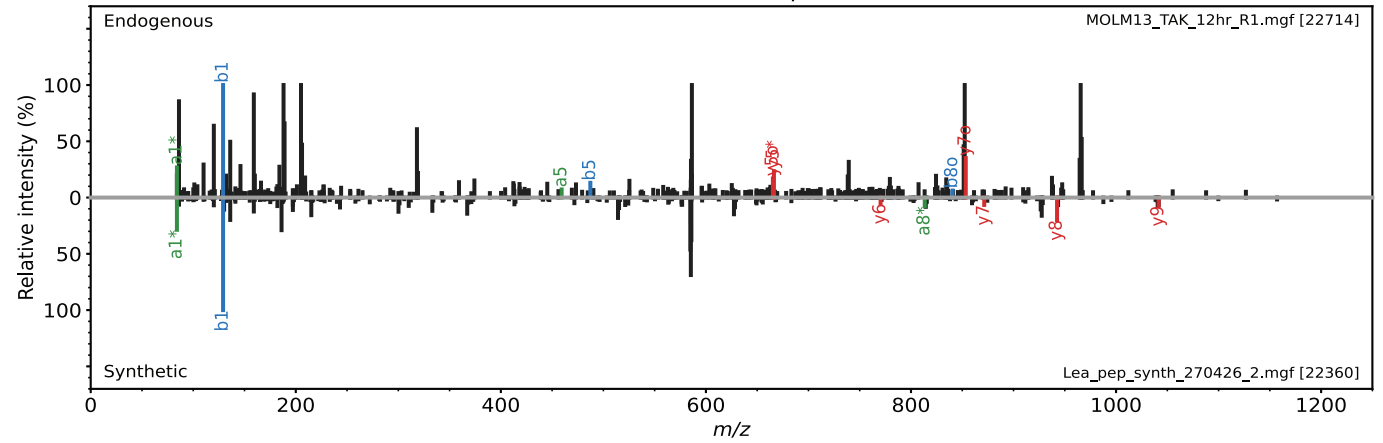


Spectrum	m/z	error (ppm)
Endogenous	530.8015	-7.5
Synthetic	530.8052	-0.6

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.95	0.75	0.99	2.6e-04
Spearman	0.65	-0.09	0.93	7.8e-02
Spectral angle	0.75	-	-	-

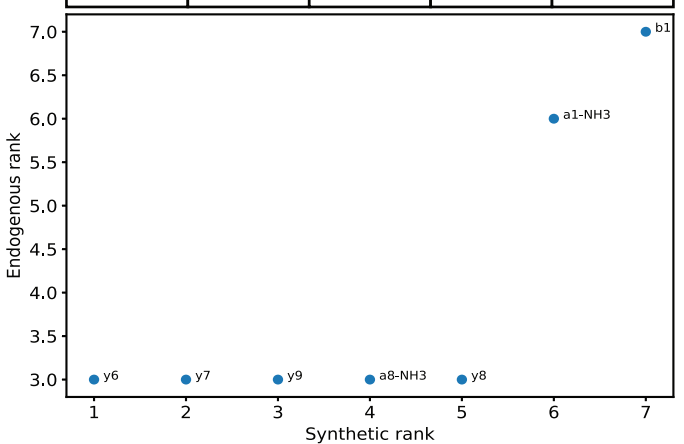
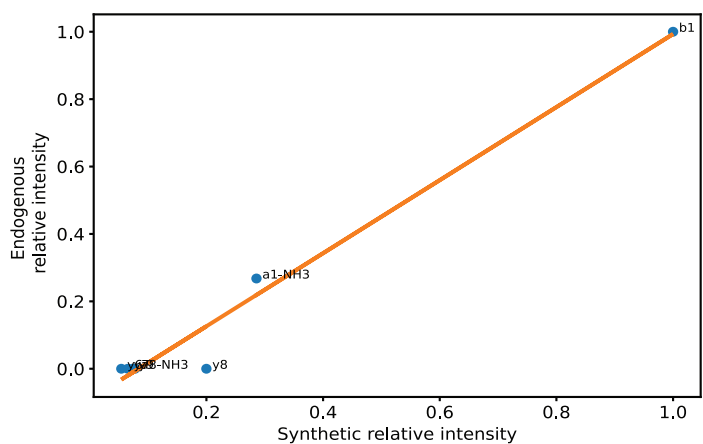


KVATSSFHHR / 2+

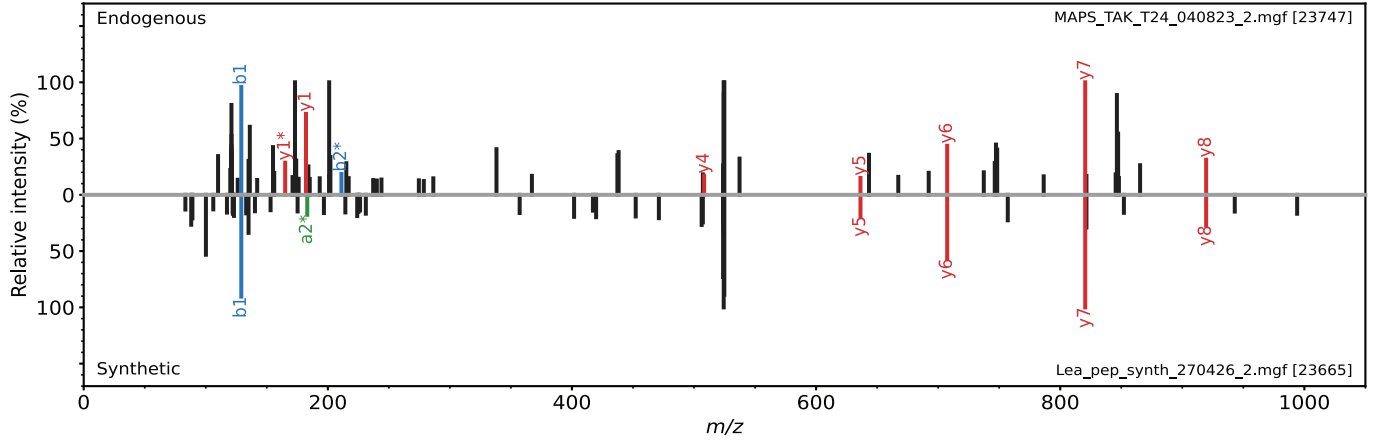


Spectrum	m/z	error (ppm)
Endogenous	585.3089	-5.8
Synthetic	585.3110	-2.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.99	0.92	1.00	2.9e-05
Spearman	0.80	0.12	0.97	3.0e-02
Spectral angle	0.85	-	-	-

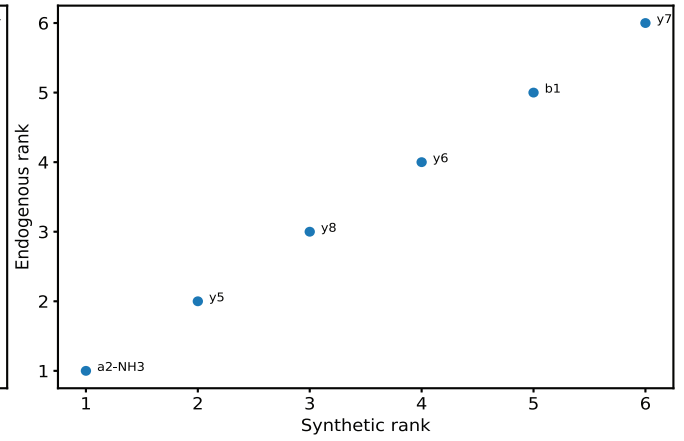
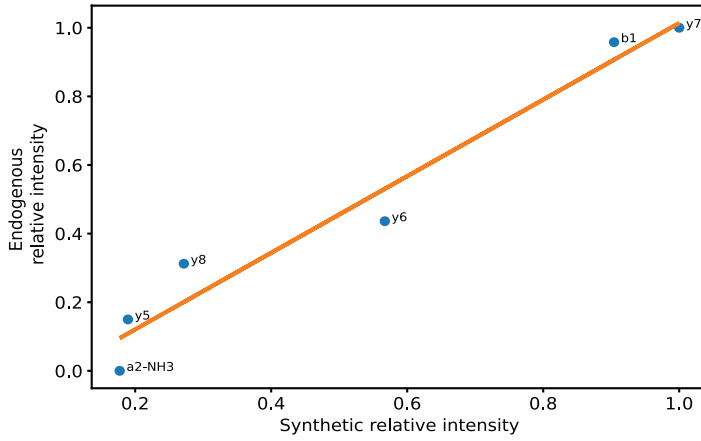


KVIAQRGIY / 2+

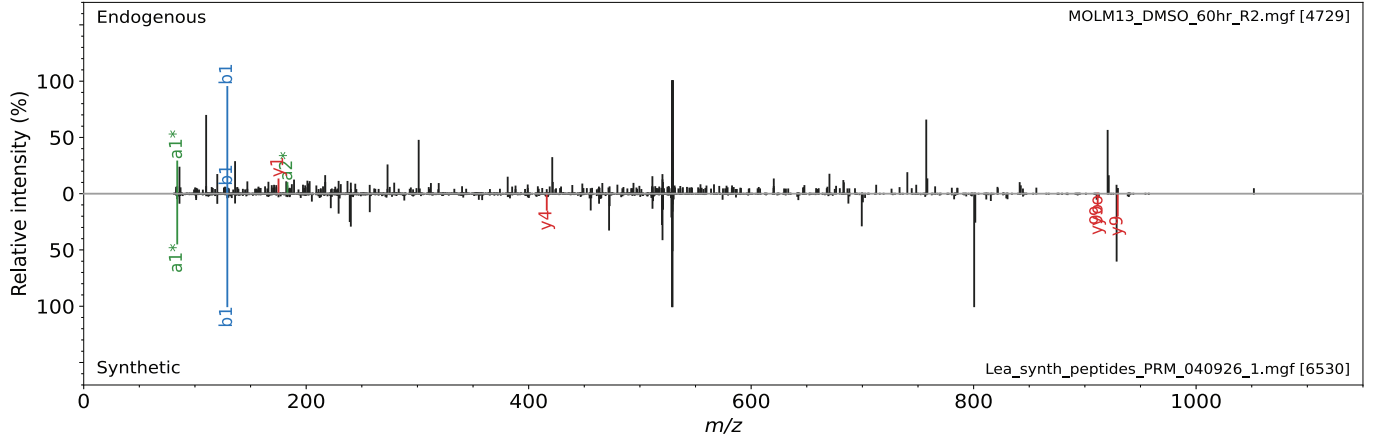


Spectrum	m/z	error (ppm)
Endogenous	524.3241	9.5
Synthetic	524.3190	-0.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.98	0.82	1.00	6.1e-04
Spearman	1.00	1.00	1.00	0.0e+00
Spectral angle	0.90	-	-	-

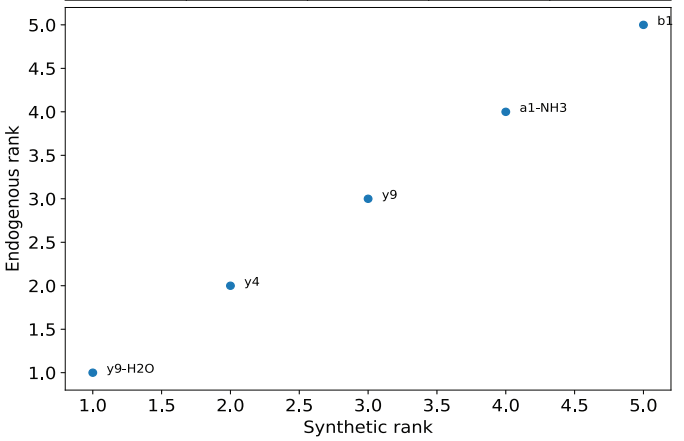
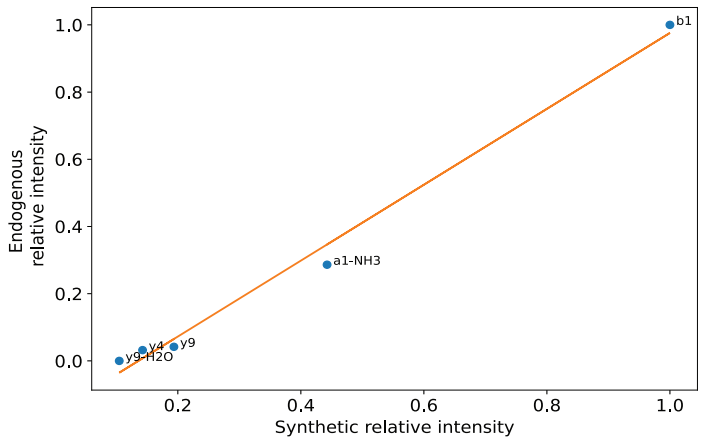


KVQKGTIAGR / 2+

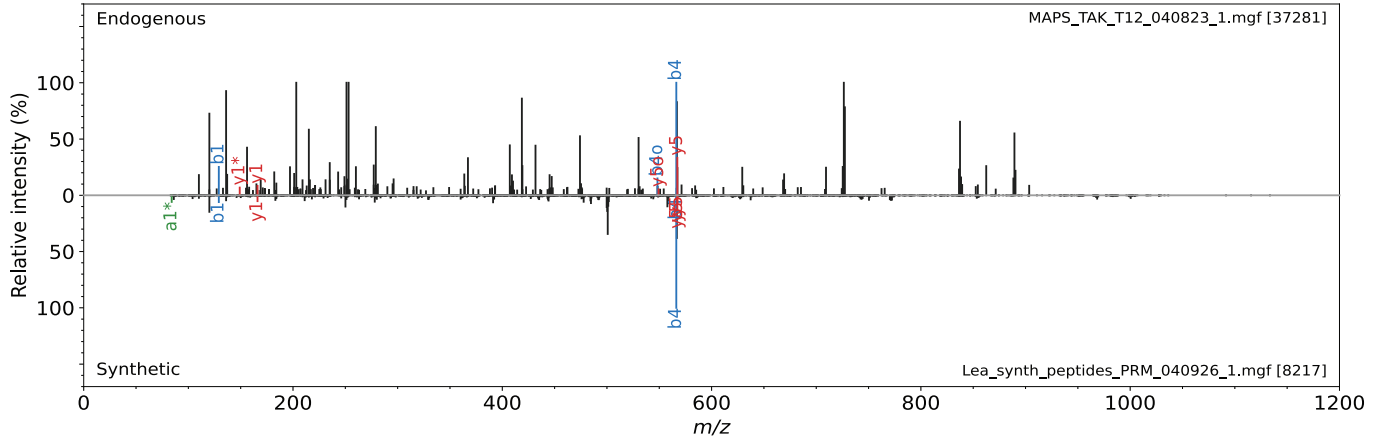


Spectrum	m/z	error (ppm)
Endogenous	529.3264	-2.1
Synthetic	529.3334	11.1

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	1.00	0.93	1.00	3.8e-04
Spearman	1.00	1.00	1.00	1.4e-24
Spectral angle	0.85	-	-	-

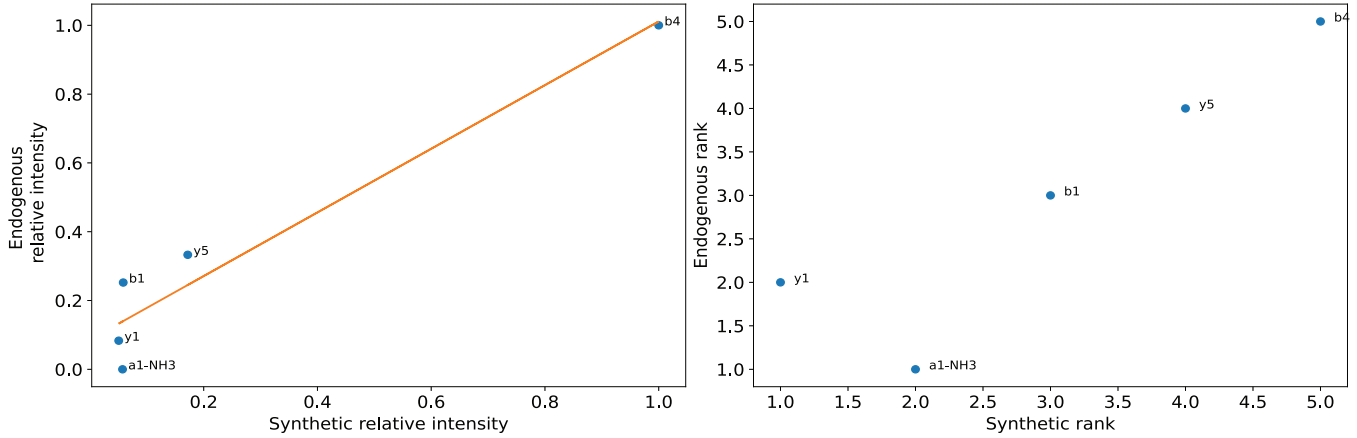


KWNHAICNF / 2+

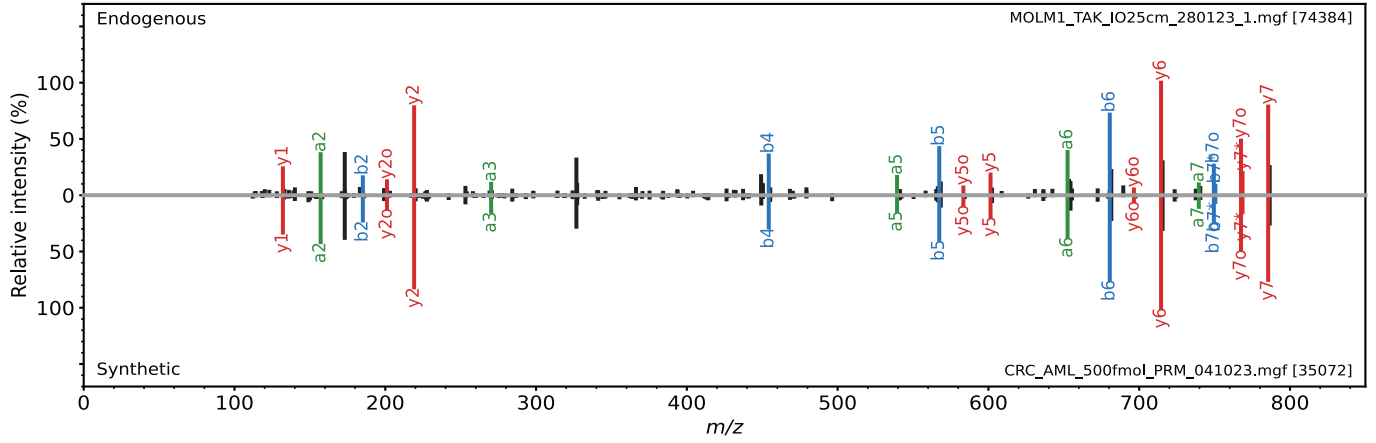


Spectrum	m/z	error (ppm)
Endogenous	566.7706	-2.5
Synthetic	566.7736	3.7

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.56	1.00	7.6e-03
Spearman	0.90	0.09	0.99	3.7e-02
Spectral angle	0.85	-	-	-

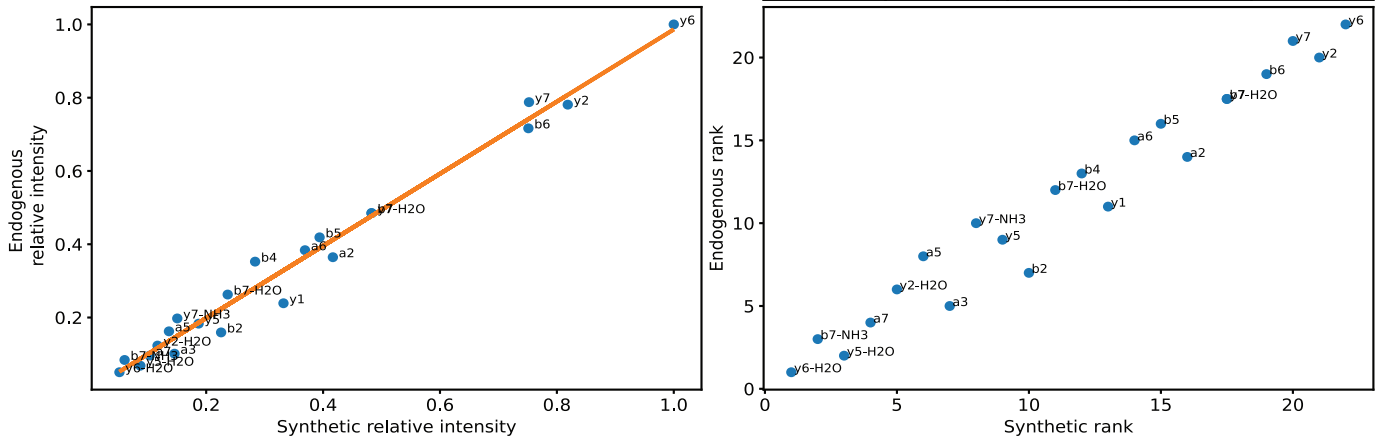


LALRIISI / 2+

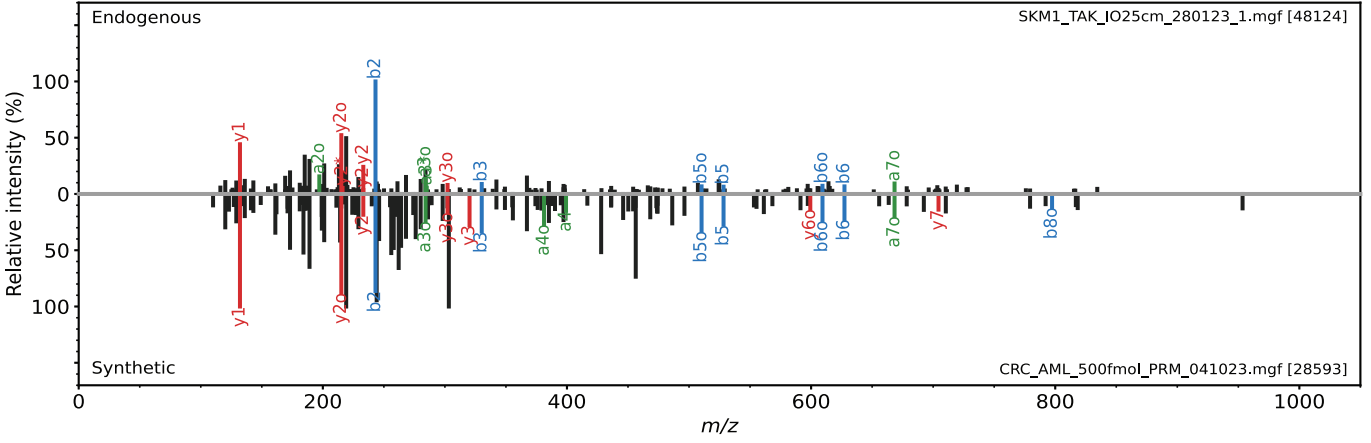


Spectrum	m/z	error (ppm)
Endogenous	449.8079	0.2
Synthetic	449.8095	3.8

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.99	0.98	1.00	2.1e-18
Spearman	0.98	0.95	0.99	3.4e-15
Spectral angle	0.94	-	-	-

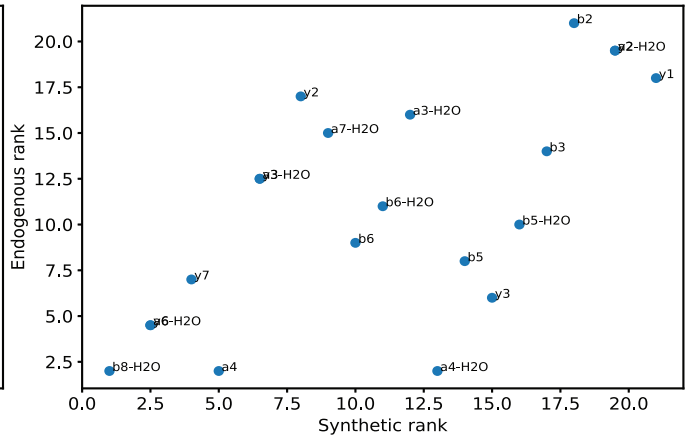
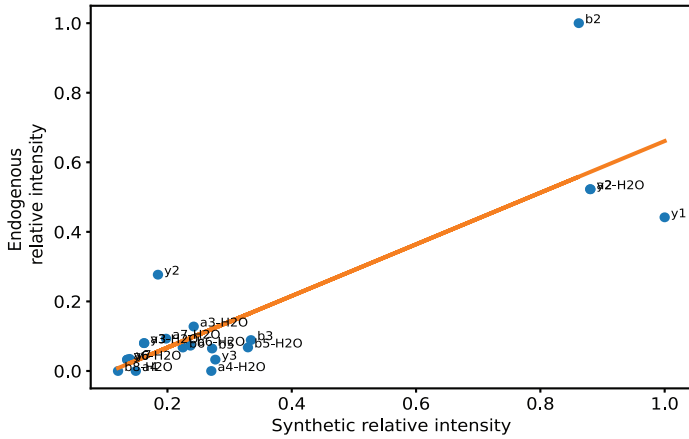


LESPTVSTL / 2+

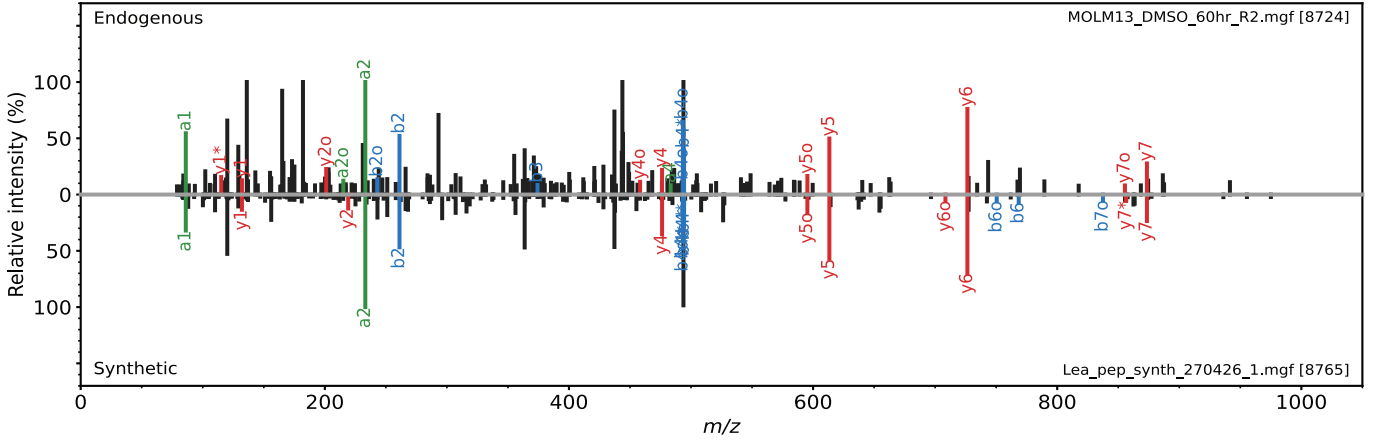


Spectrum	m/z	error (ppm)
Endogenous	473.7585	0.7
Synthetic	473.7584	0.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.85	0.66	0.94	9.7e-07
Spearman	0.65	0.31	0.85	1.4e-03
Spectral angle	0.70	-	-	-

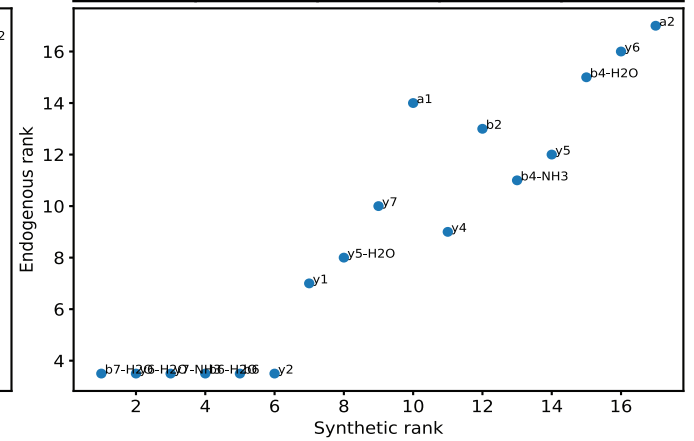
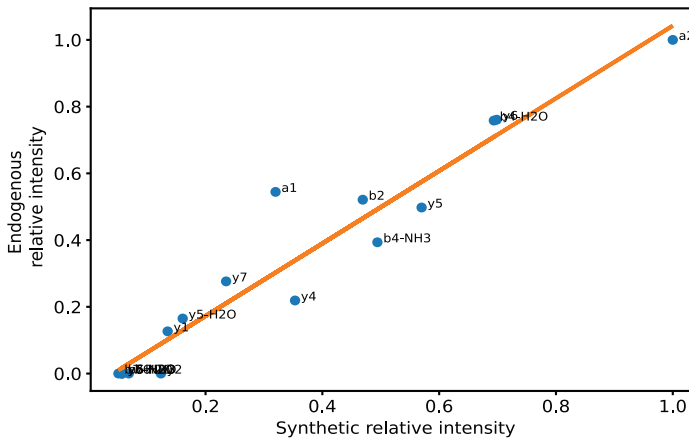


LFLHKESL / 2+

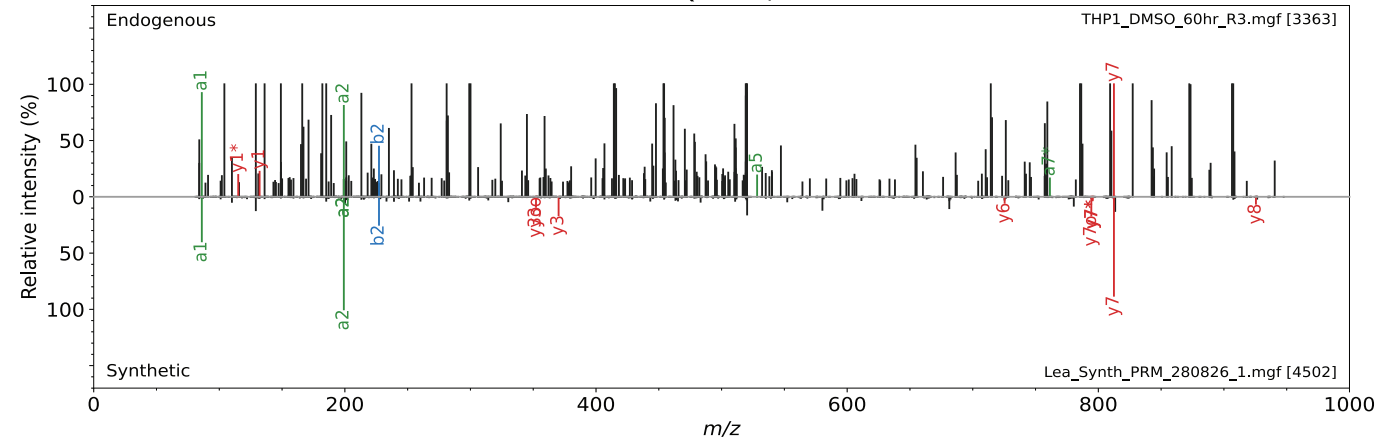


Spectrum	m/z	error (ppm)
Endogenous	493.7867	-0.8
Synthetic	493.7881	2.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.90	0.99	3.9e-10
Spearman	0.94	0.84	0.98	1.9e-08
Spectral angle	0.87	-	-	-

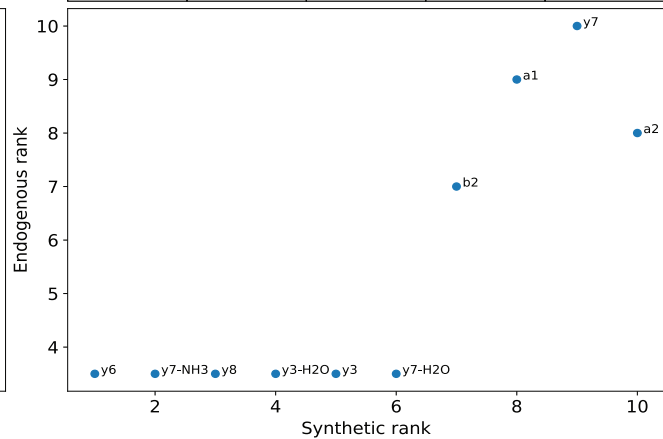
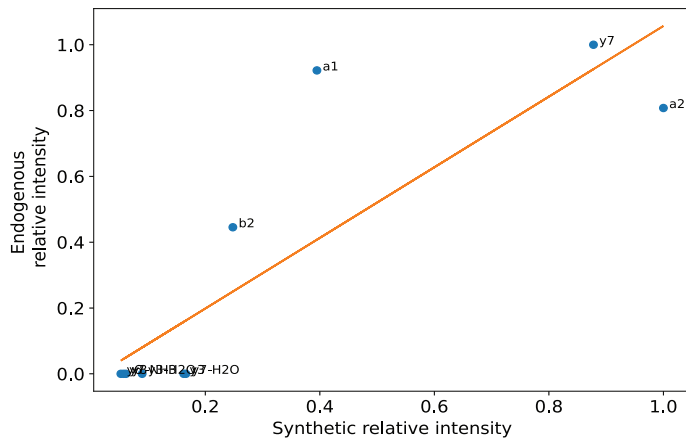


LISNQLHTL / 2+

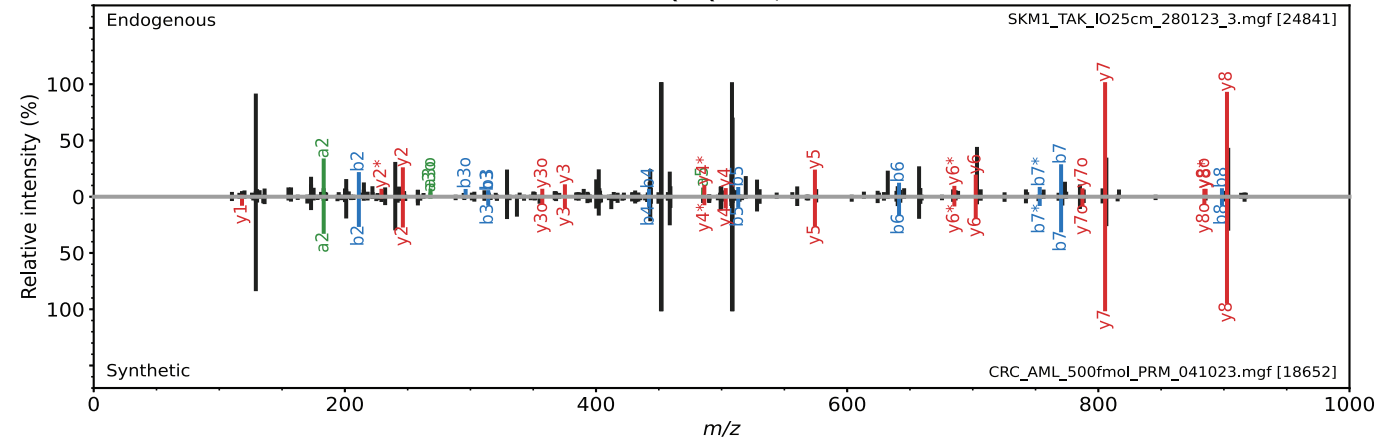


Spectrum	m/z	error (ppm)
Endogenous	519.7994	-2.5
Synthetic	519.8002	-1.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.86	0.51	0.97	1.3e-03
Spearman	0.85	0.46	0.96	2.0e-03
Spectral angle	0.74	-	-	-

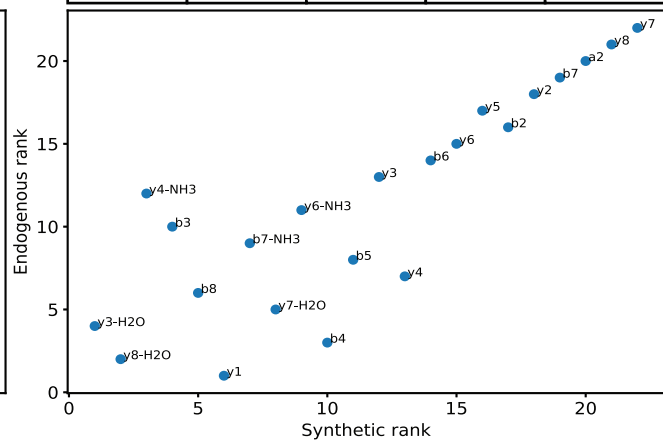
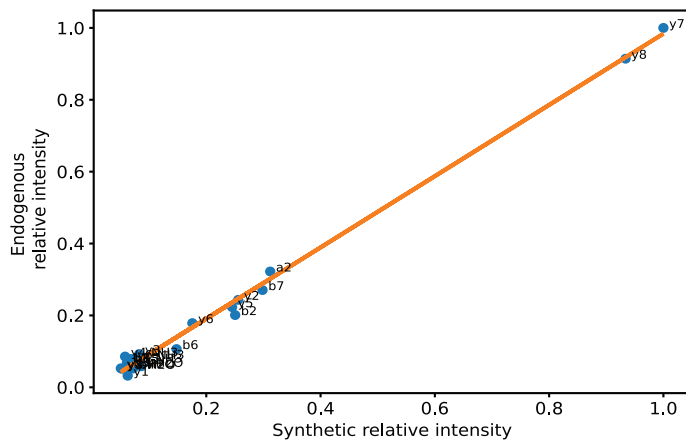


LPCQAQEKV / 2+

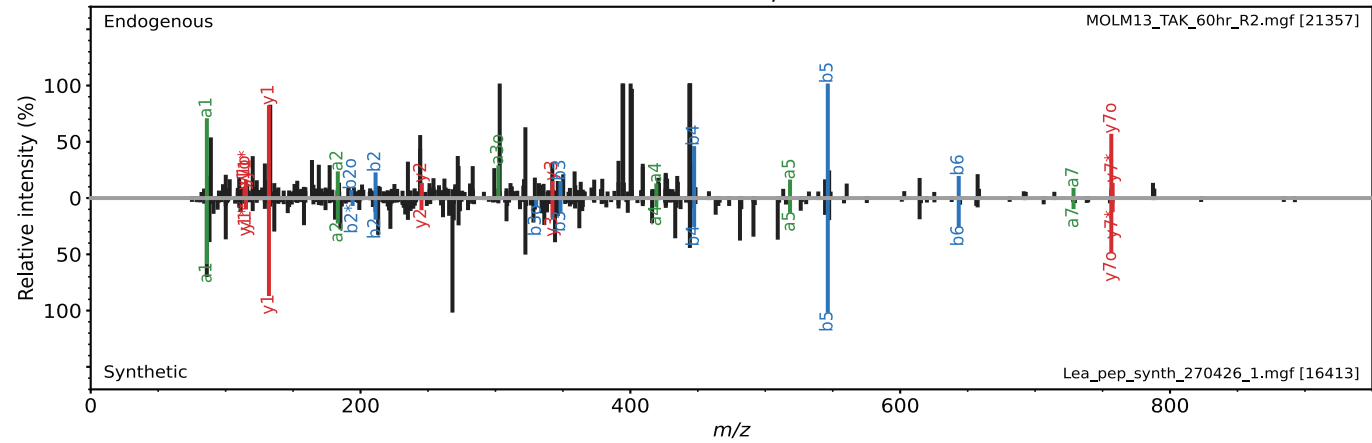


Spectrum	m/z	error (ppm)
Endogenous	508.2649	-1.5
Synthetic	508.2657	0.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	1.00	0.99	1.00	3.0e-24
Spearman	0.85	0.67	0.94	5.6e-07
Spectral angle	0.96	-	-	-

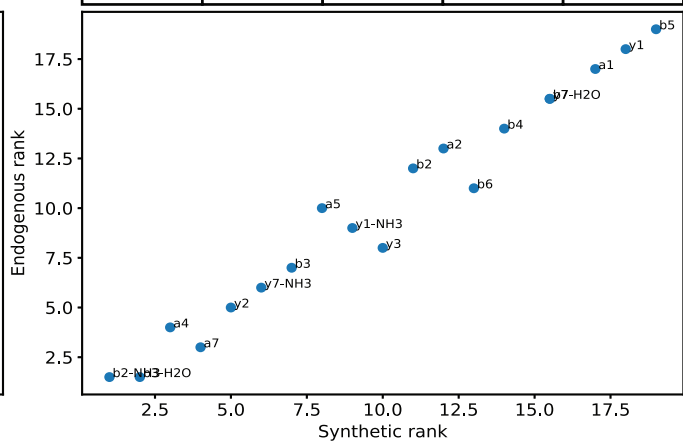
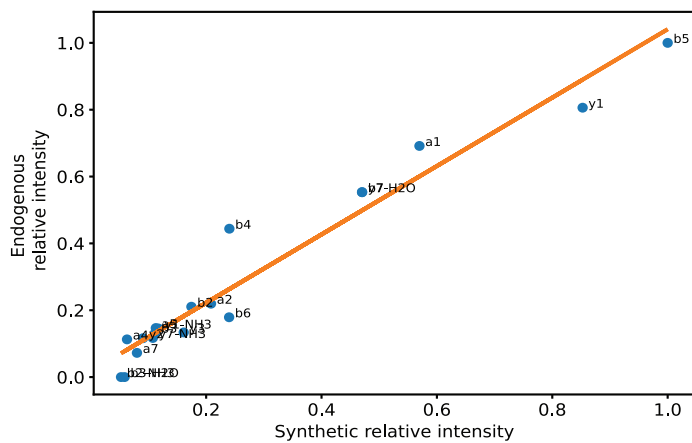


LPHVVPLL / 2+

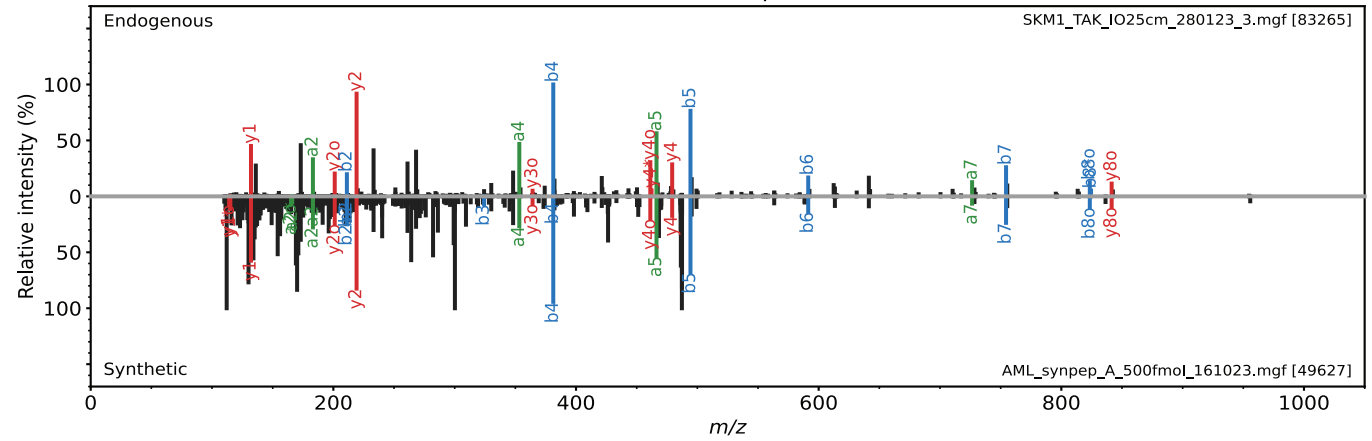


Spectrum	m/z	error (ppm)
Endogenous	444.2893	0.0
Synthetic	444.2885	-1.8

Metric	r / θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.93	0.99	2.3e-12
Spearman	0.99	0.96	0.99	1.5e-14
Spectral angle	0.90	-	-	-

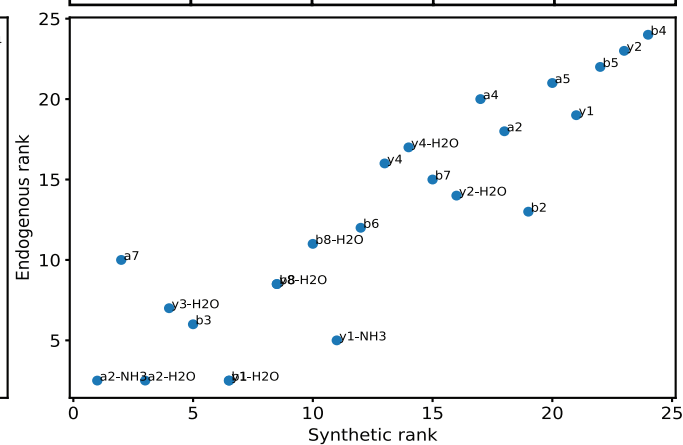
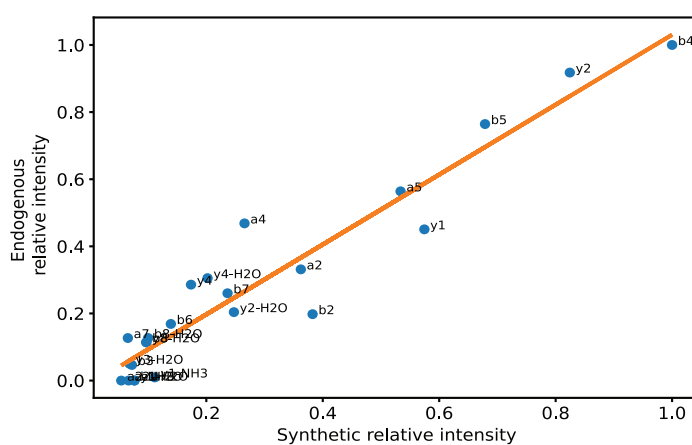


LPIGIPYSI / 2+

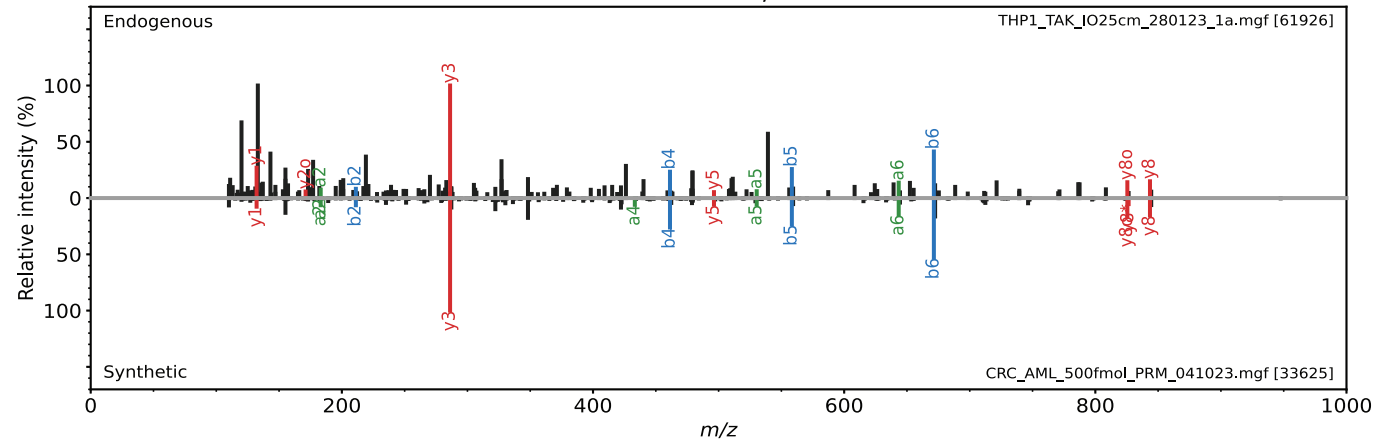


Spectrum	m/z	error (ppm)
Endogenous	486.7920	0.3
Synthetic	486.7924	0.1

Metric	r / θ	95% CI min	95% CI max	p-value
Pearson	0.96	0.90	0.98	3.8e-13
Spearman	0.91	0.79	0.96	1.2e-09
Spectral angle	0.86	-	-	-

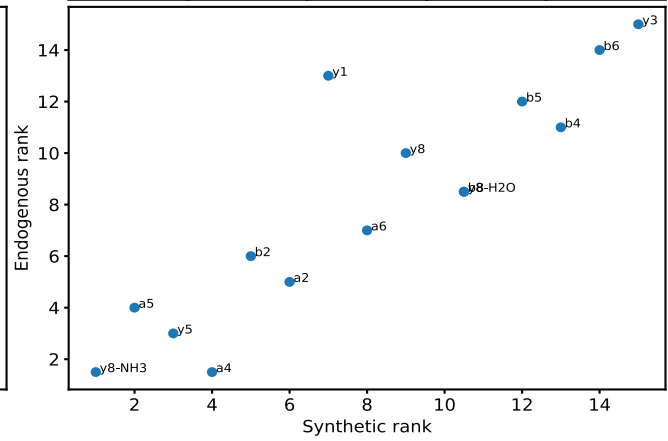
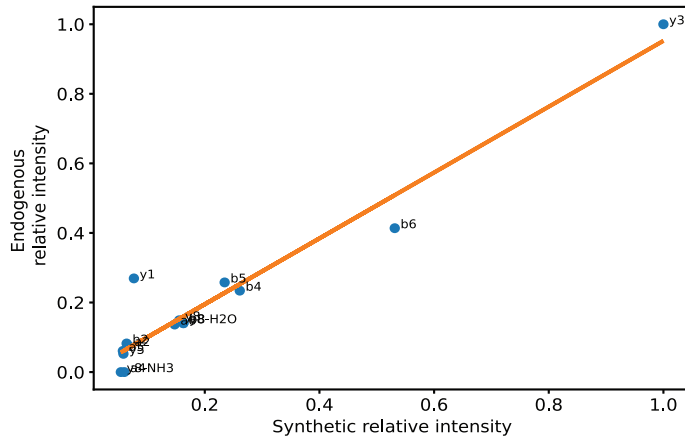


LPIHPLPGL / 2+

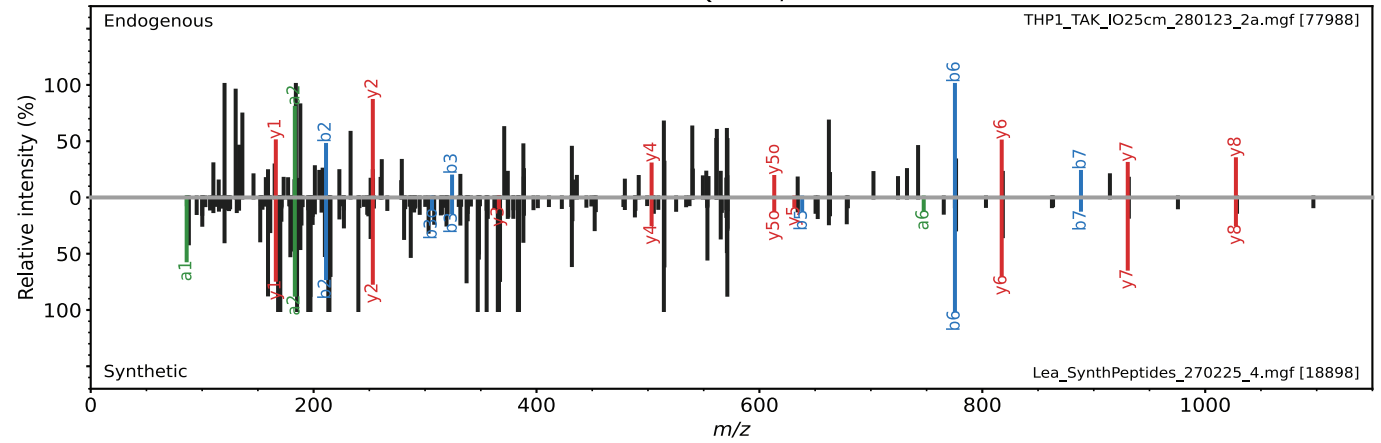


Spectrum	m/z	error (ppm)
Endogenous	478.8001	0.2
Synthetic	478.8011	2.3

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.90	0.99	5.1e-09
Spearman	0.89	0.69	0.96	9.8e-06
Spectral angle	0.87	-	-	-

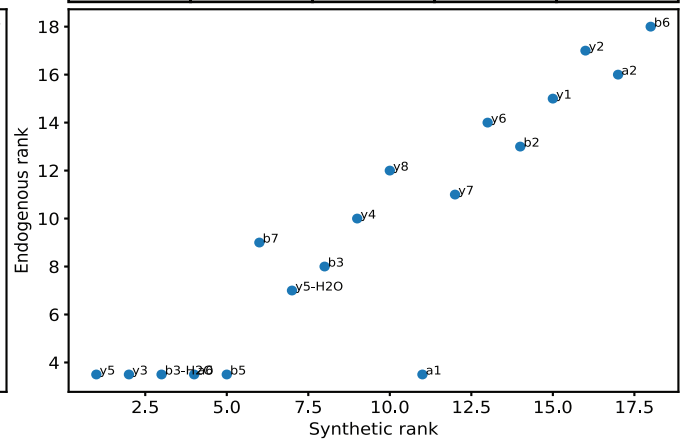
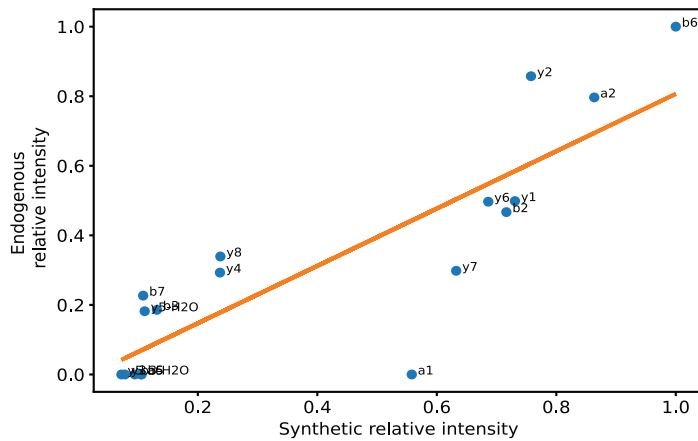


LPLWQHISF / 2+

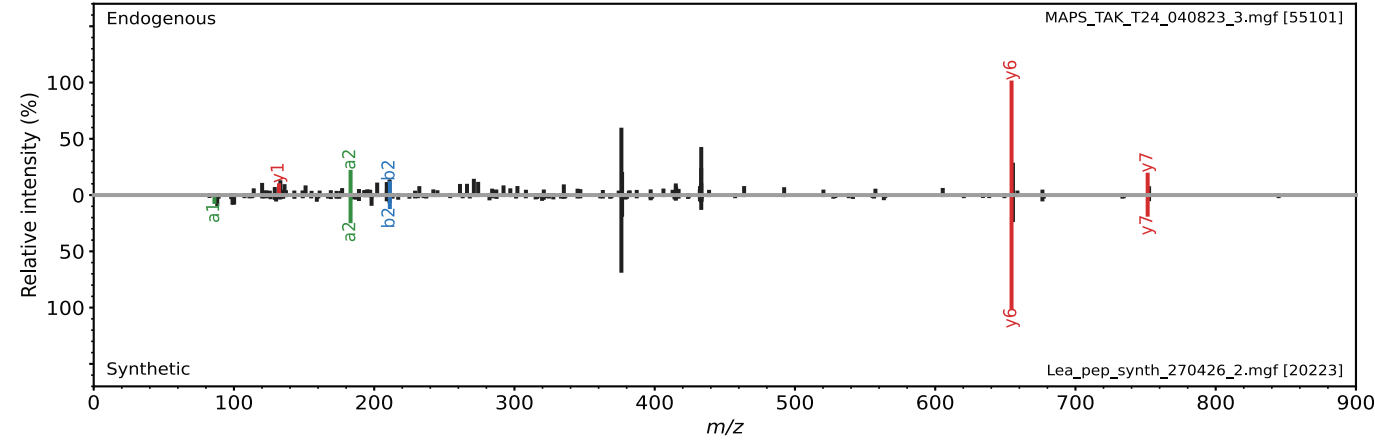


Spectrum	m/z	error (ppm)
Endogenous	570.8143	1.1
Synthetic	570.8146	1.8

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.85	0.64	0.94	7.0e-06
Spearman	0.91	0.77	0.97	1.7e-07
Spectral angle	0.76	-	-	-

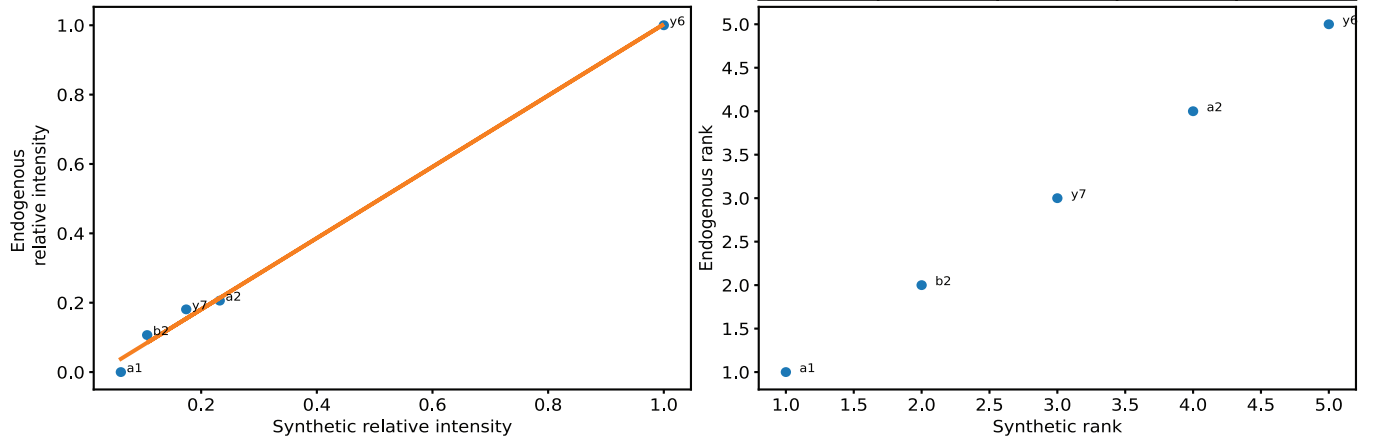


LPPRVIGL / 2+

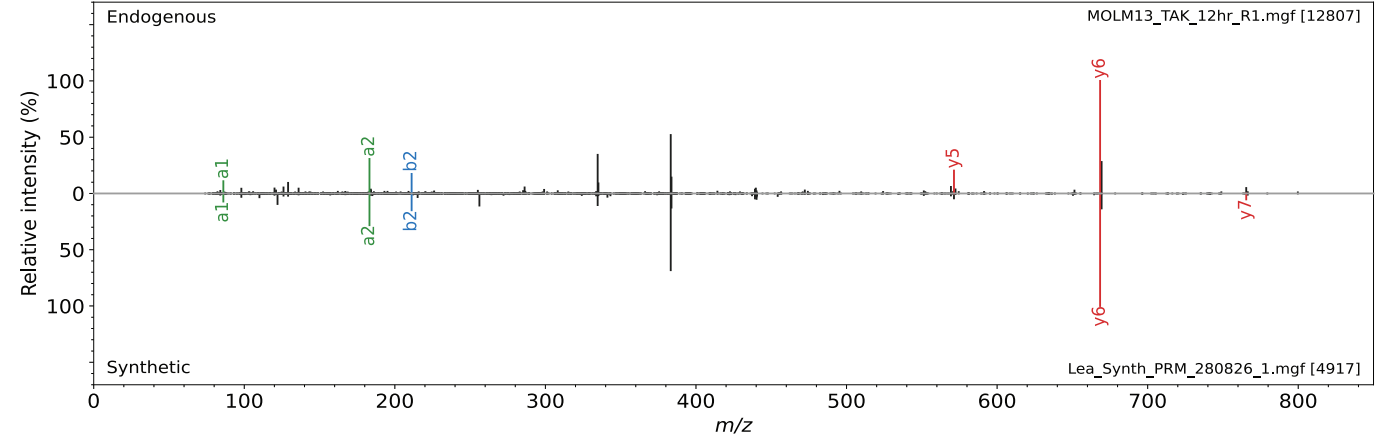


Spectrum	m/z	error (ppm)
Endogenous	432.7908	9.0
Synthetic	432.7863	-1.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	1.00	0.97	1.00	1.2e-04
Spearman	1.00	1.00	1.00	1.4e-24
Spectral angle	0.96	-	-	-

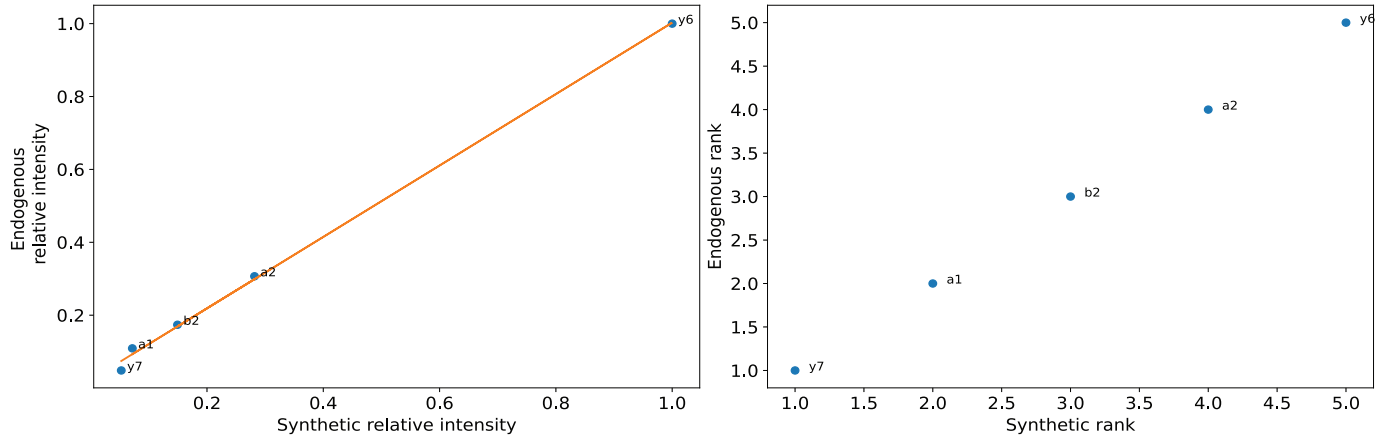


LPPSRLPV / 2+

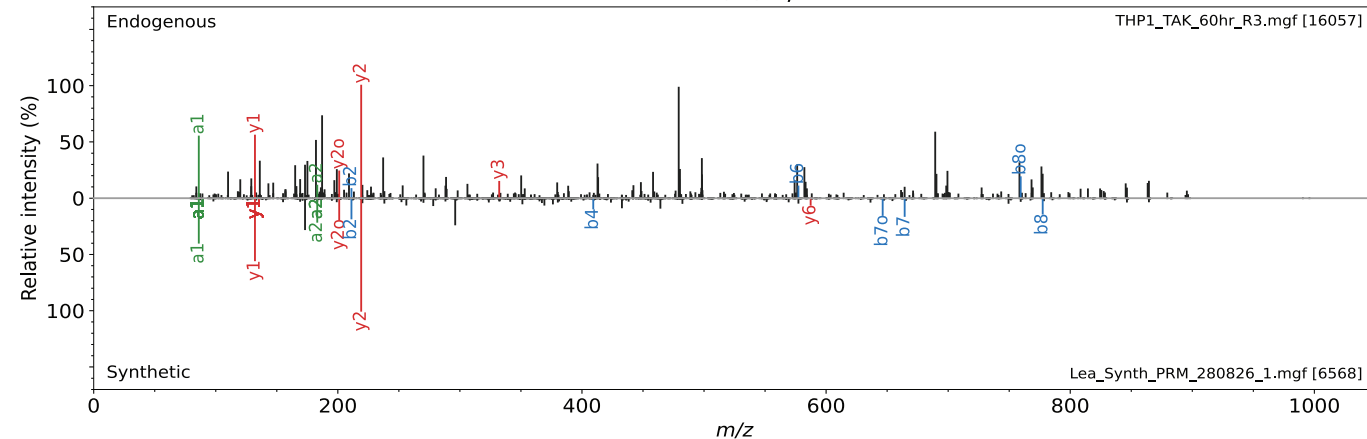


Spectrum	m/z	error (ppm)
Endogenous	439.7762	-0.7
Synthetic	439.7764	-0.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	1.00	0.99	1.00	3.0e-05
Spearman	1.00	1.00	1.00	1.4e-24
Spectral angle	0.97	-	-	-

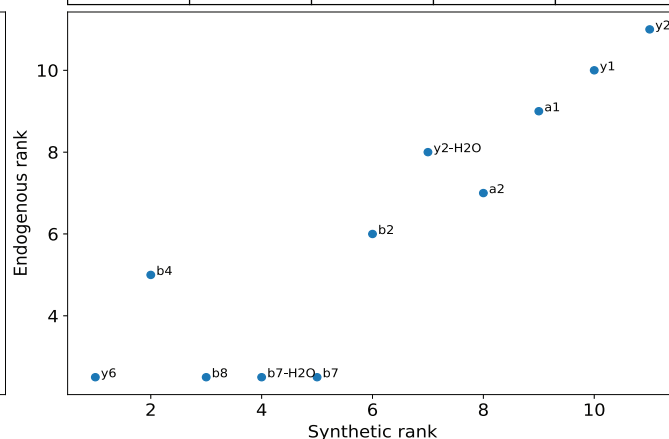
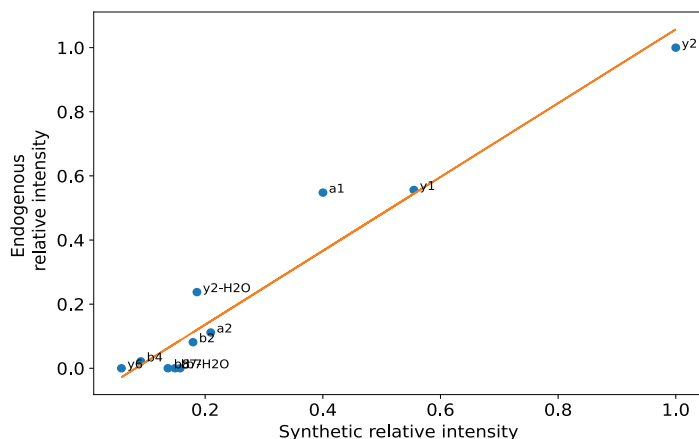


LPPTPASLSL / 2+

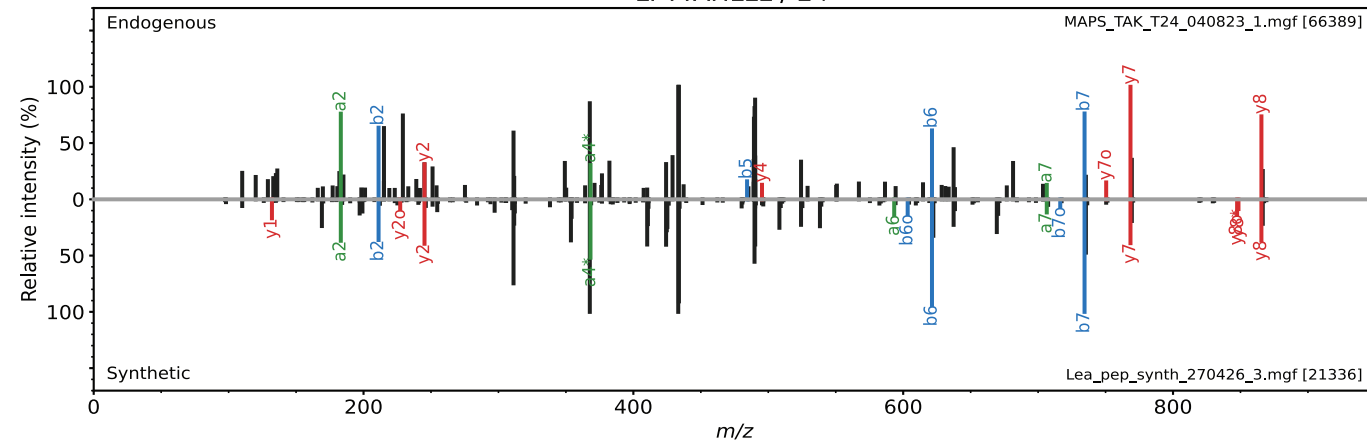


Spectrum	m/z	error (ppm)
Endogenous	498.2918	-0.8
Synthetic	498.2919	-0.6

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.87	0.99	1.2e-06
Spearman	0.90	0.65	0.97	1.7e-04
Spectral angle	0.83	-	-	-

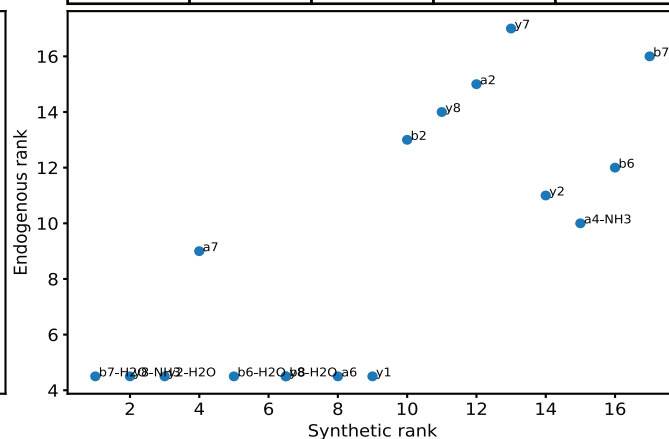
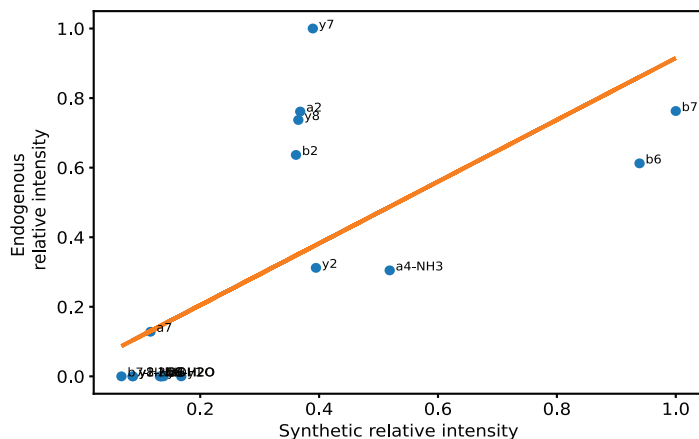


LPTTAHLLL / 2+

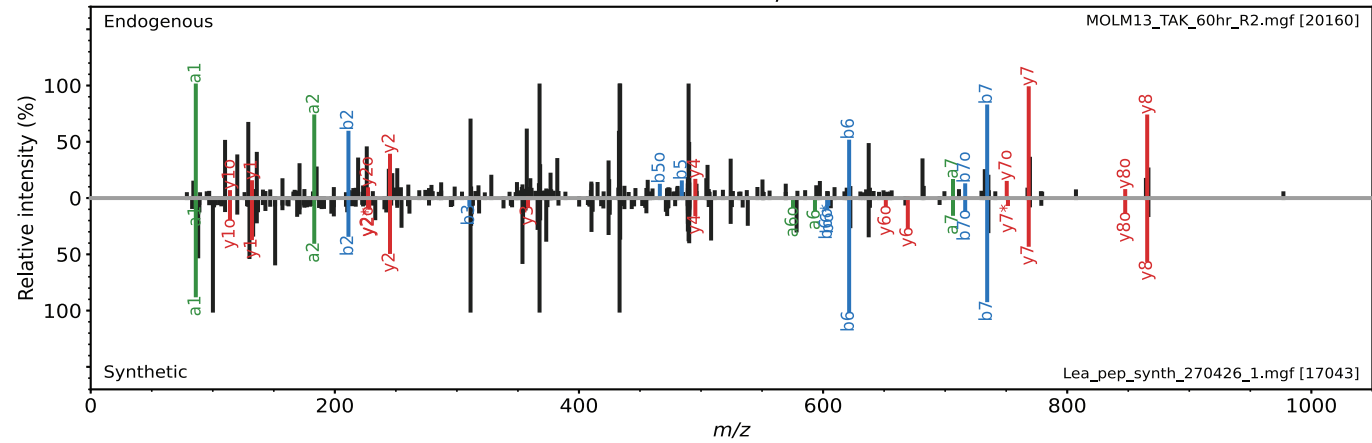


Spectrum	m/z	error (ppm)
Endogenous	489.8078	10.4
Synthetic	489.8049	4.5

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.70	0.33	0.88	1.8e-03
Spearman	0.77	0.46	0.91	3.2e-04
Spectral angle	0.64	-	-	-

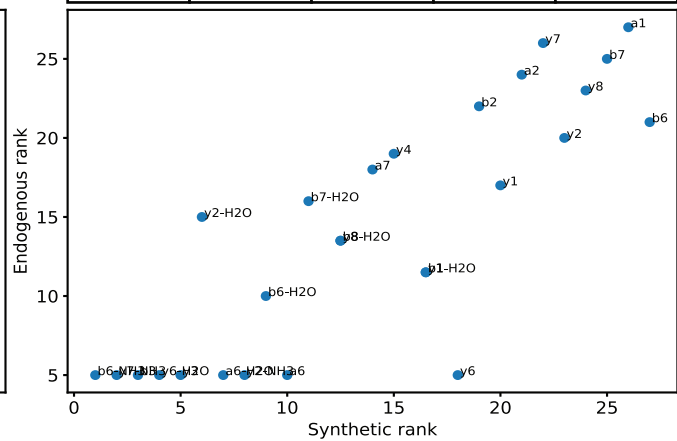
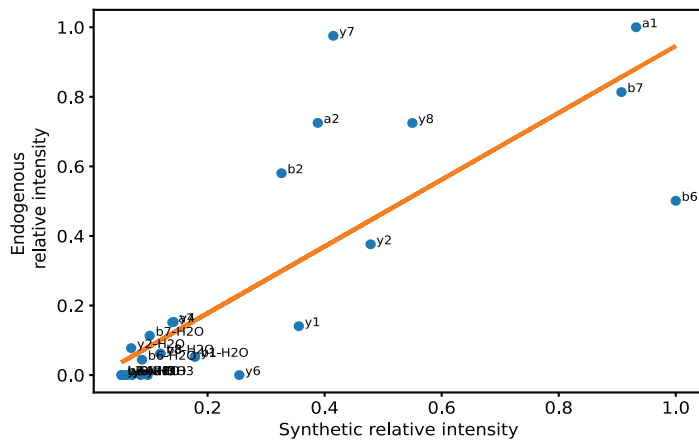


LPVSSHLIL / 2+

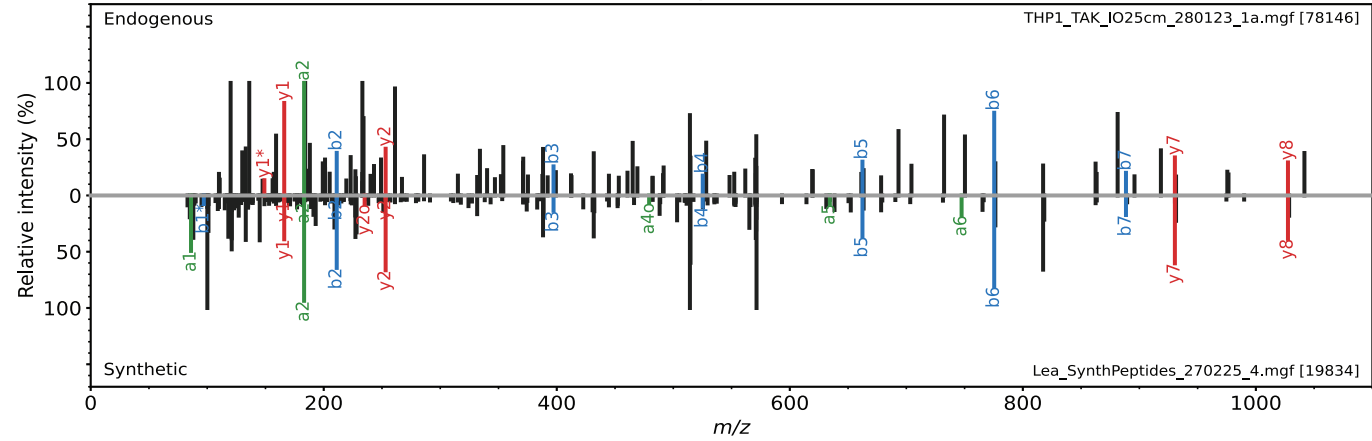


Spectrum	m/z	error (ppm)
Endogenous	489.8036	1.8
Synthetic	489.8030	0.6

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.82	0.63	0.91	2.2e-07
Spearman	0.84	0.67	0.92	4.6e-08
Spectral angle	0.69	-	-	-

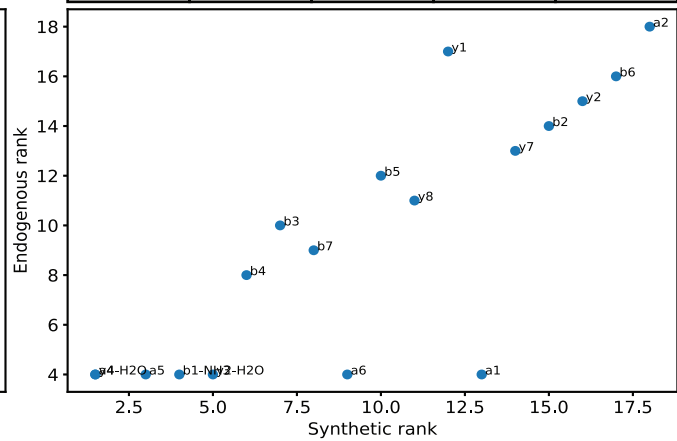
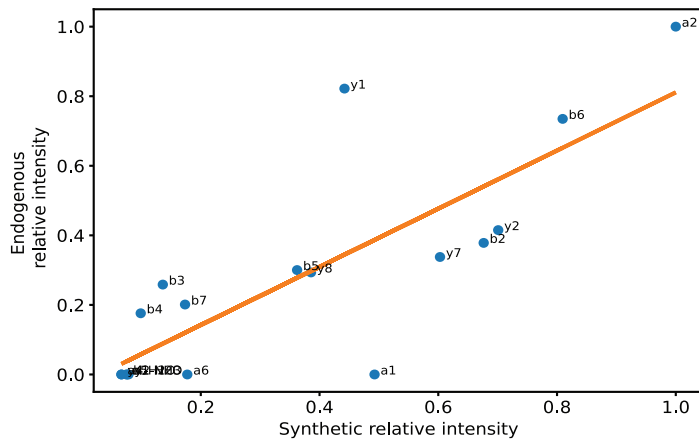


LPWQHIIISF / 2+

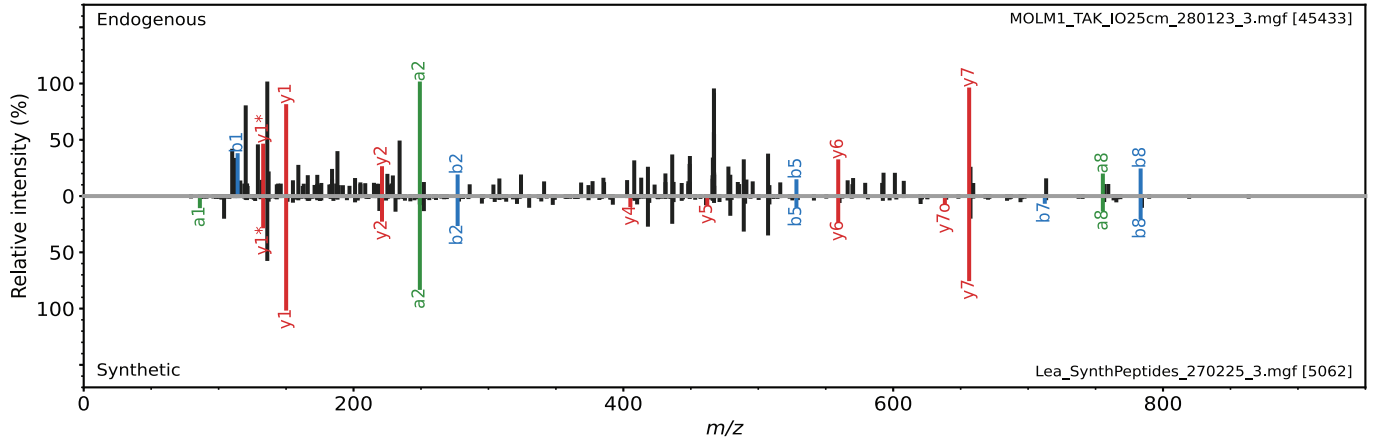


Spectrum	m/z	error (ppm)
Endogenous	570.8138	0.2
Synthetic	570.8145	1.6

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.81	0.55	0.93	4.8e-05
Spearman	0.82	0.58	0.93	2.8e-05
Spectral angle	0.71	-	-	-

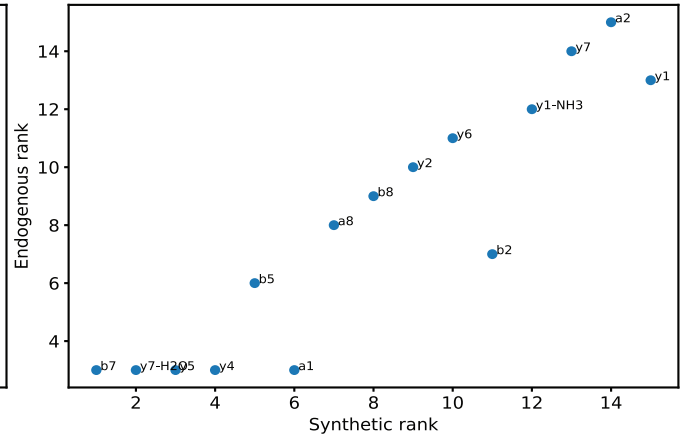
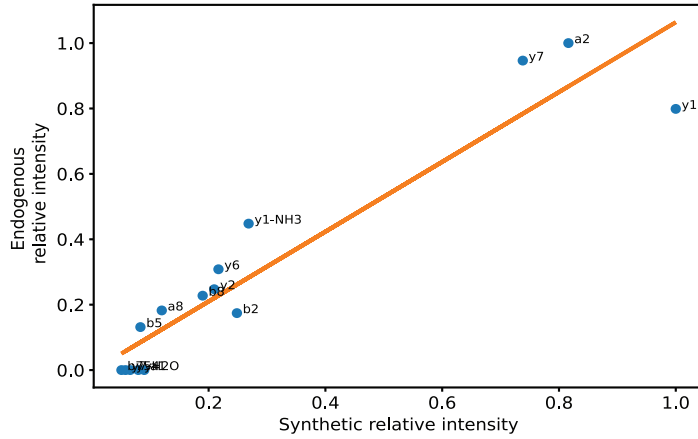


LYPPGPSAM / 2+

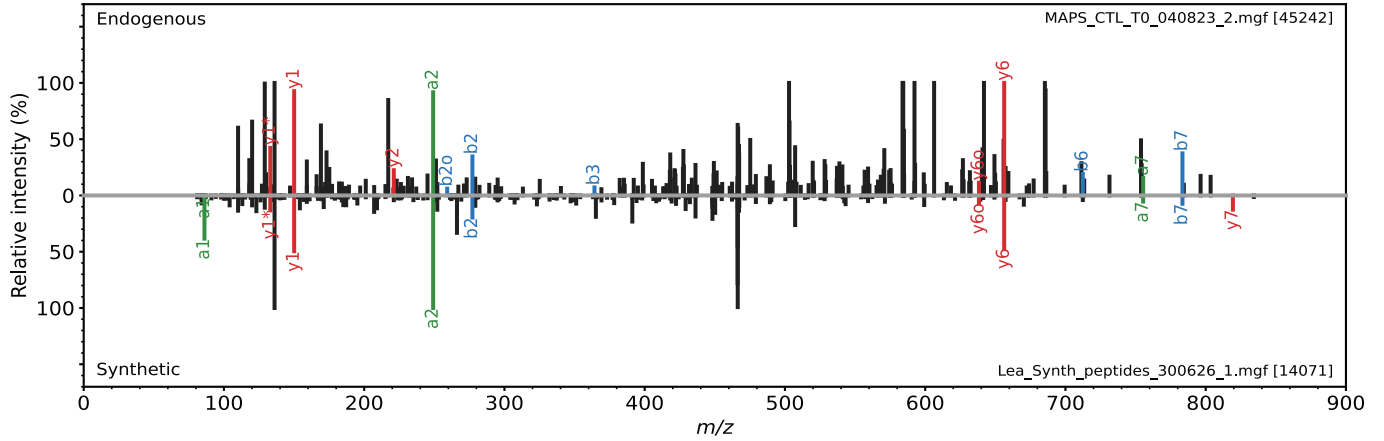


Spectrum	m/z	error (ppm)
Endogenous	466.7309	-0.1
Synthetic	466.7313	0.9

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.94	0.83	0.98	1.4e-07
Spearman	0.92	0.78	0.97	8.8e-07
Spectral angle	0.84	-	-	-

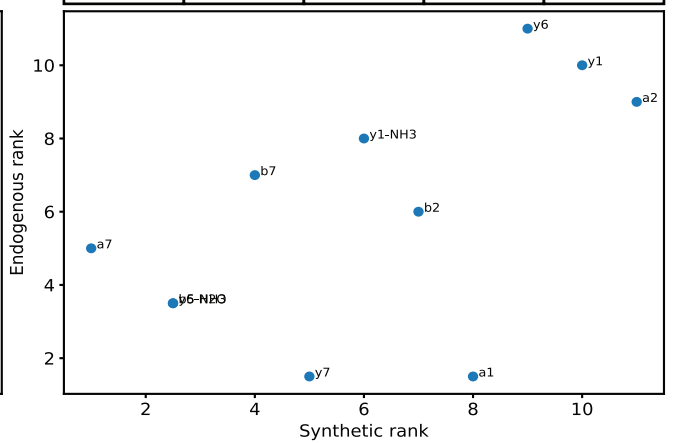
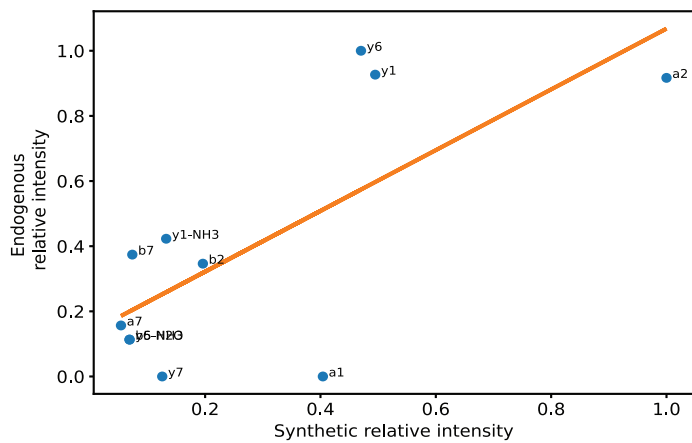


LYSYKGAM / 2+

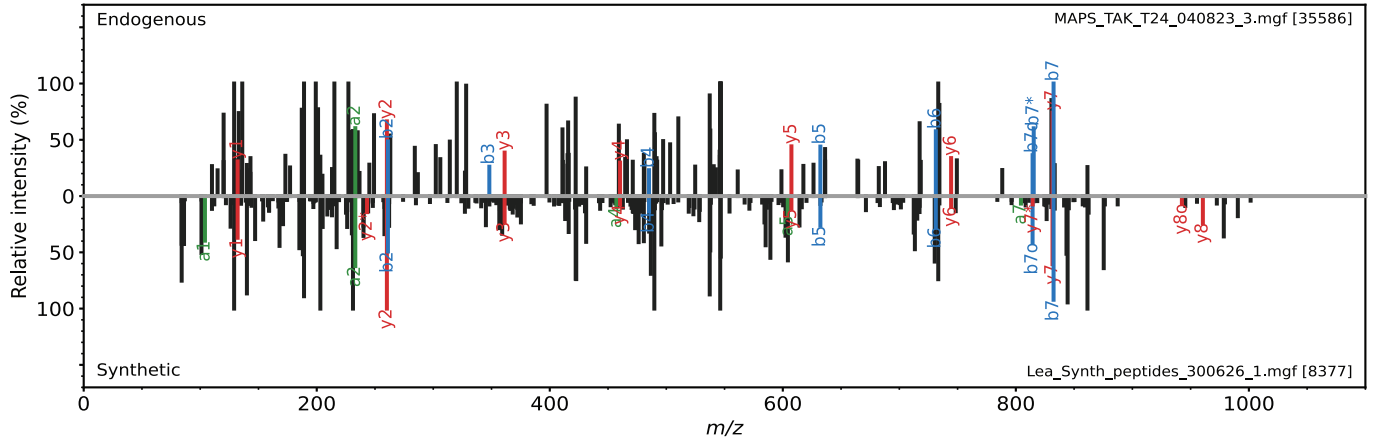


Spectrum	m/z	error (ppm)
Endogenous	466.7355	9.9
Synthetic	466.7307	-0.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.71	0.20	0.92	1.4e-02
Spearman	0.57	-0.05	0.87	6.9e-02
Spectral angle	0.66	-	-	-

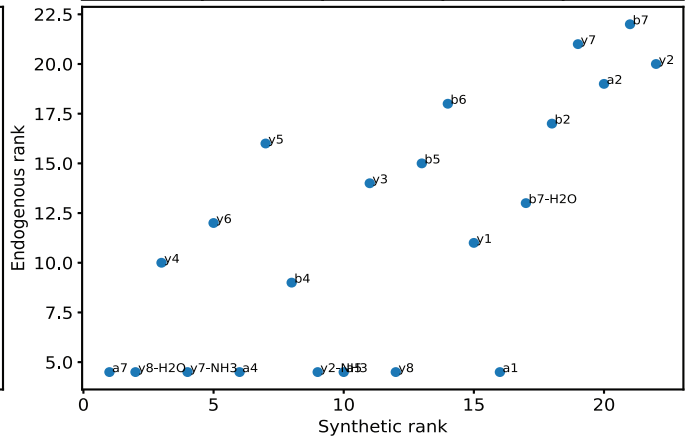
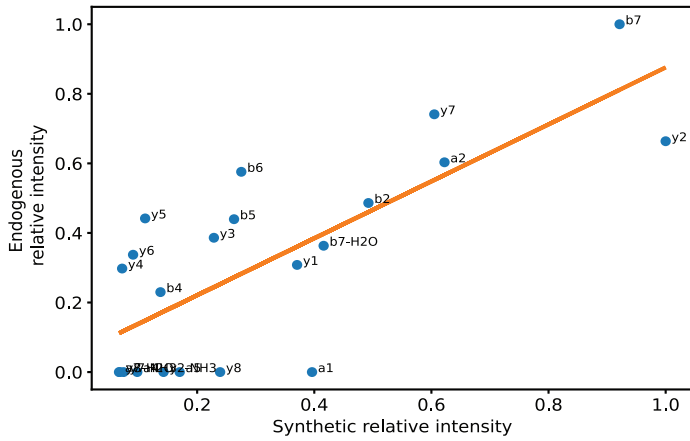


MESHFVTKL / 2+

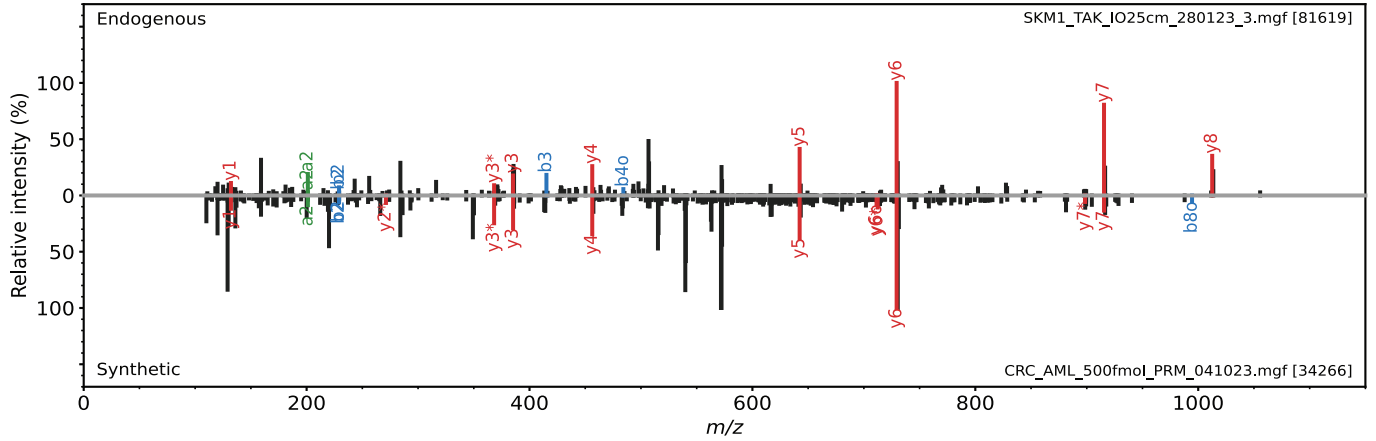


Spectrum	m/z	error (ppm)
Endogenous	546.2853	7.3
Synthetic	546.2824	2.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.76	0.50	0.89	4.1e-05
Spearman	0.70	0.40	0.87	2.6e-04
Spectral angle	0.70	-	-	-

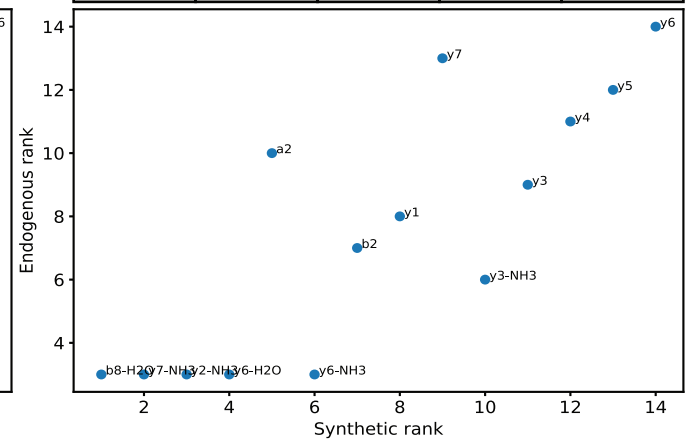
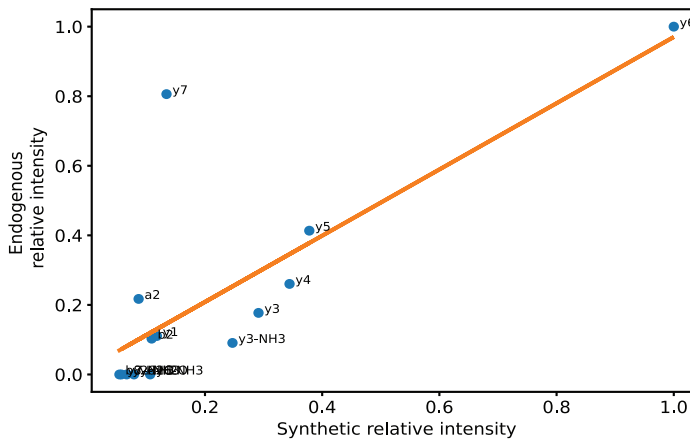


MPWSWAPRL / 2+

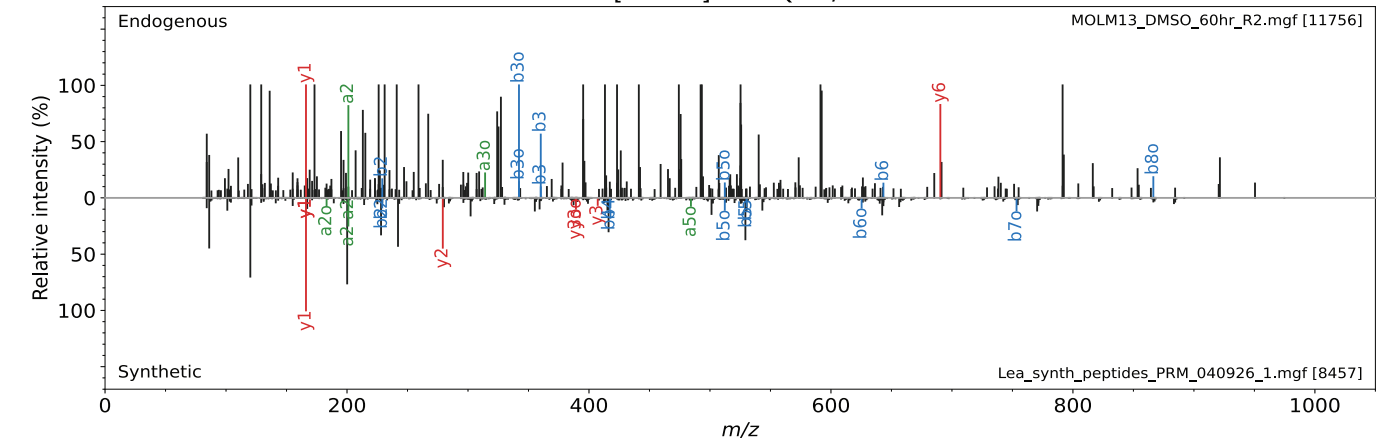


Spectrum	m/z	error (ppm)
Endogenous	572.2921	0.2
Synthetic	572.2920	0.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.76	0.38	0.92	1.6e-03
Spearman	0.82	0.52	0.94	2.8e-04
Spectral angle	0.65	-	-	-

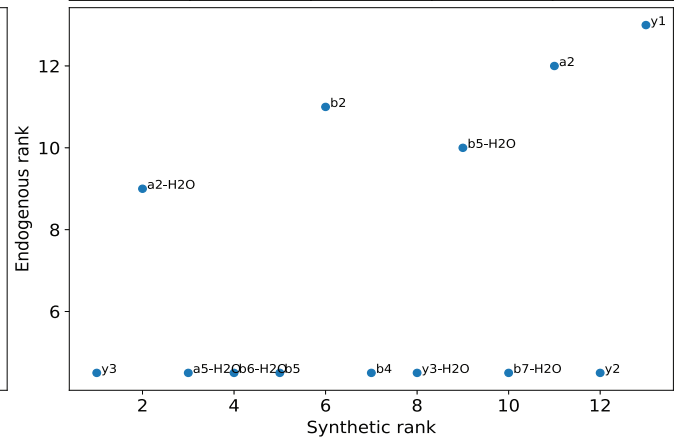
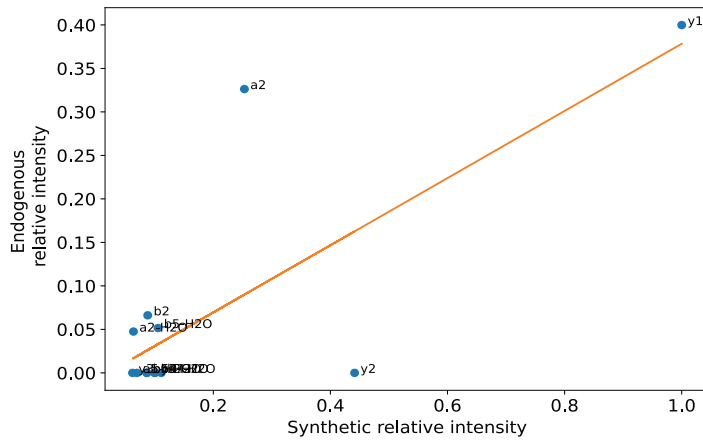


N[+0.98]IMGIIQLF / 2+

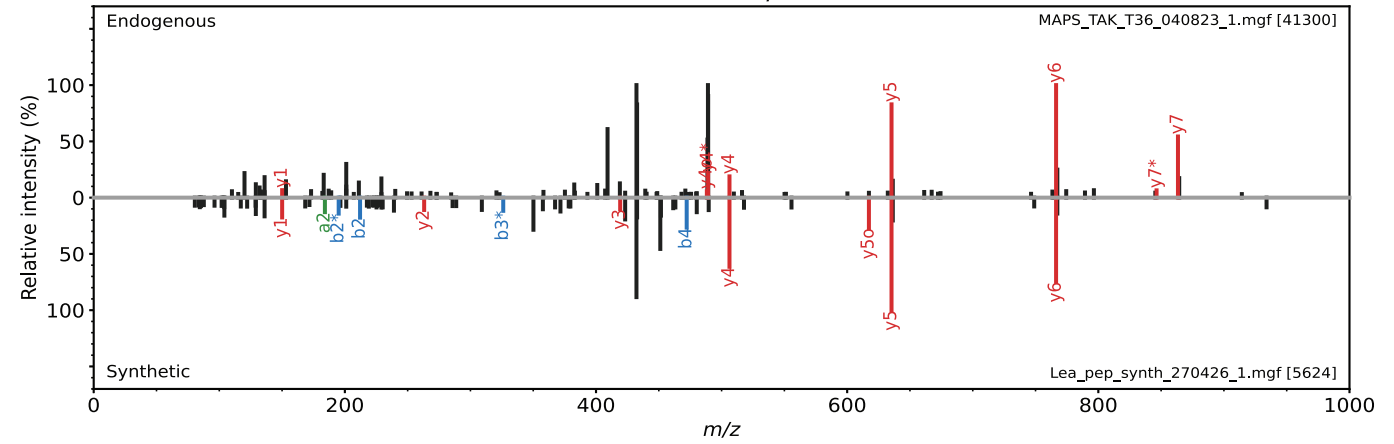


Spectrum	m/z	error (ppm)
Endogenous	525.2895	1.7
Synthetic	525.2908	4.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.76	0.36	0.92	2.6e-03
Spearman	0.39	-0.20	0.78	1.8e-01
Spectral angle	0.61	-	-	-

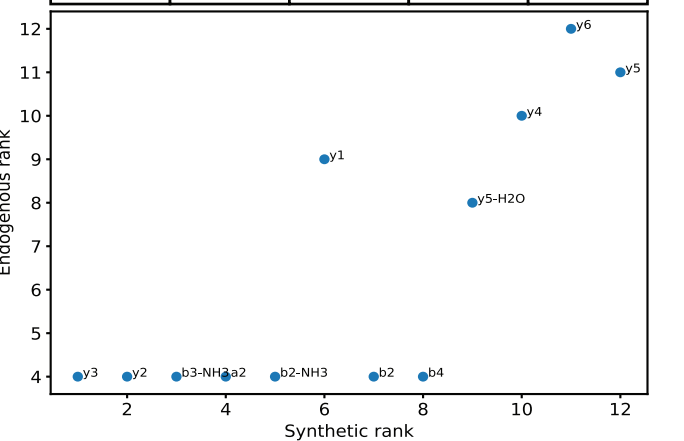
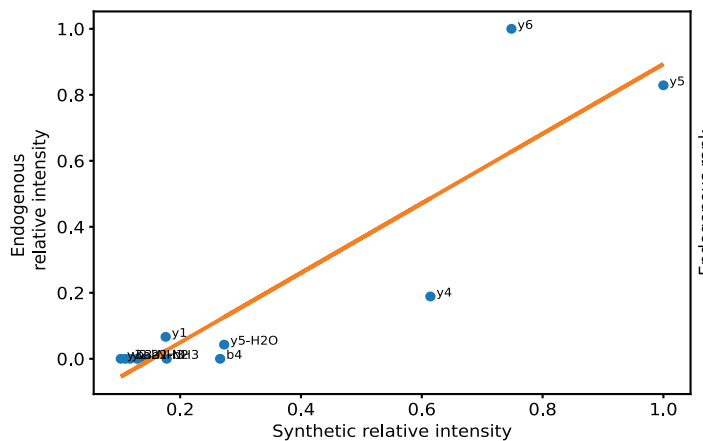


NPMSRIM / 2+

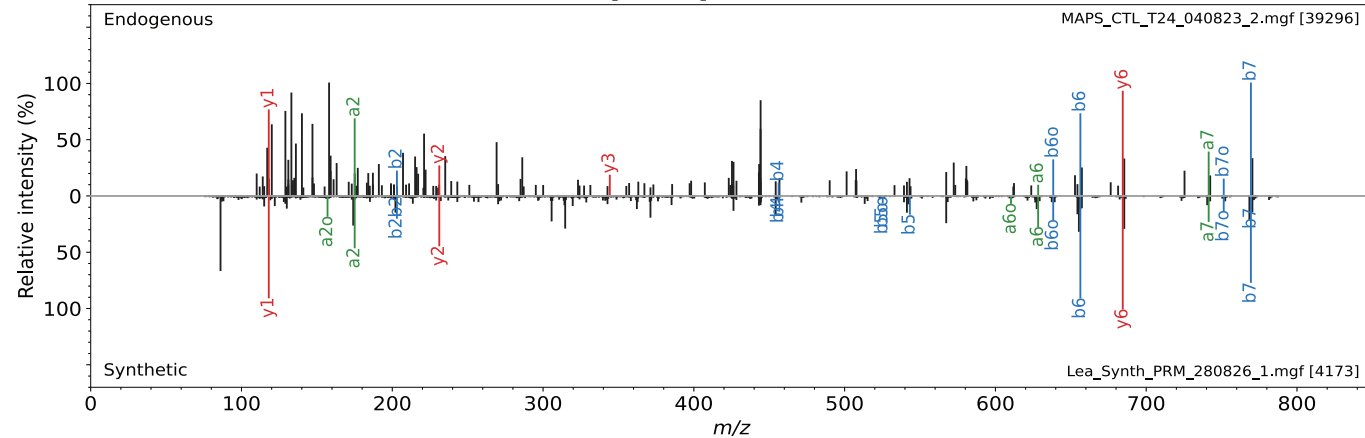


Spectrum	m/z	error (ppm)
Endogenous	489.2387	16.1
Synthetic	489.2305	-0.6

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.90	0.67	0.97	7.4e-05
Spearman	0.80	0.43	0.94	1.7e-03
Spectral angle	0.68	-	-	-

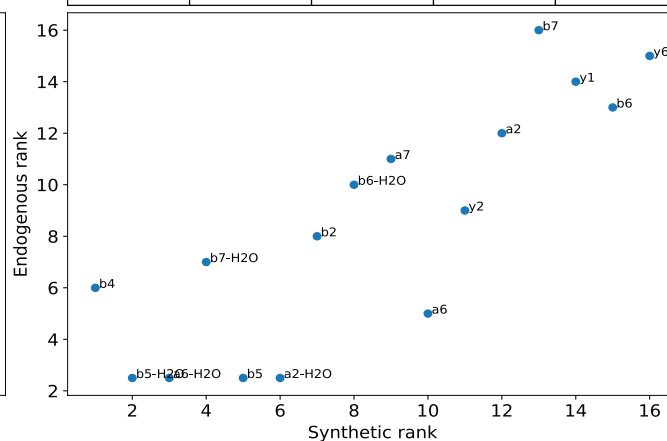
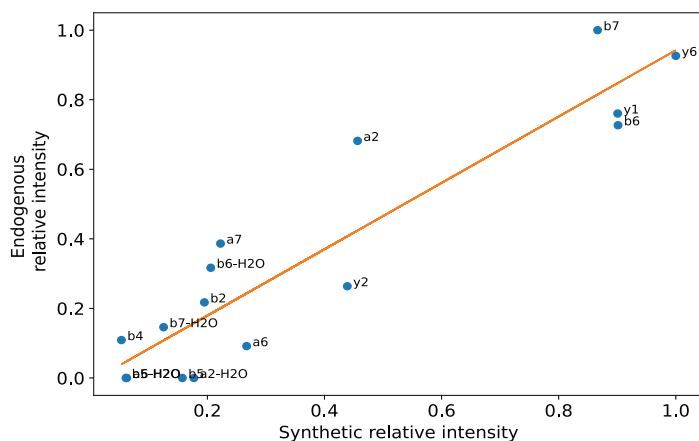


N[+0.98]SPRSILV / 2+

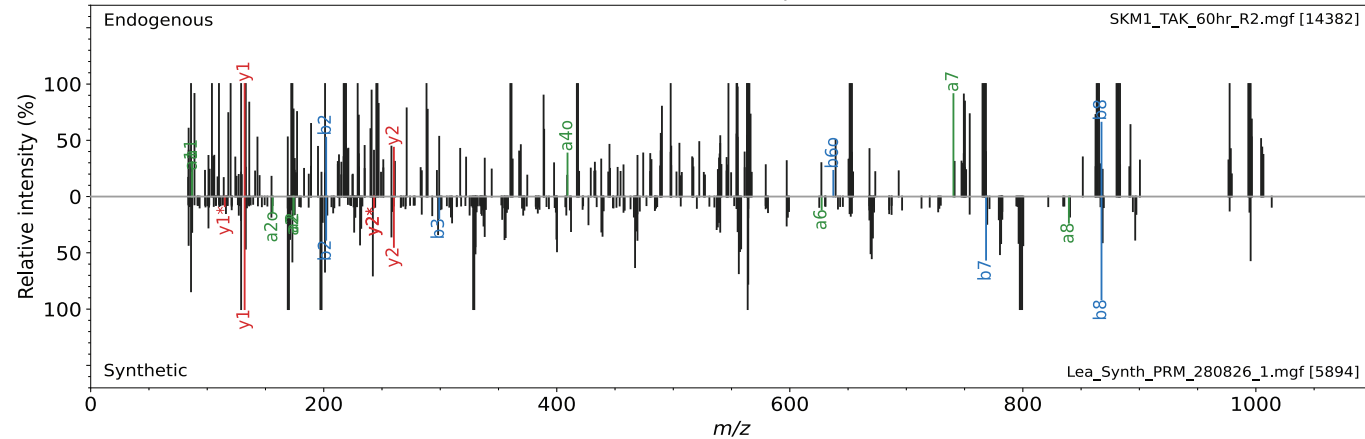


Spectrum	m/z	error (ppm)
Endogenous	443.7574	9.2
Synthetic	443.7531	-0.5

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.92	0.79	0.97	3.5e-07
Spearman	0.84	0.60	0.94	3.9e-05
Spectral angle	0.83	-	-	-

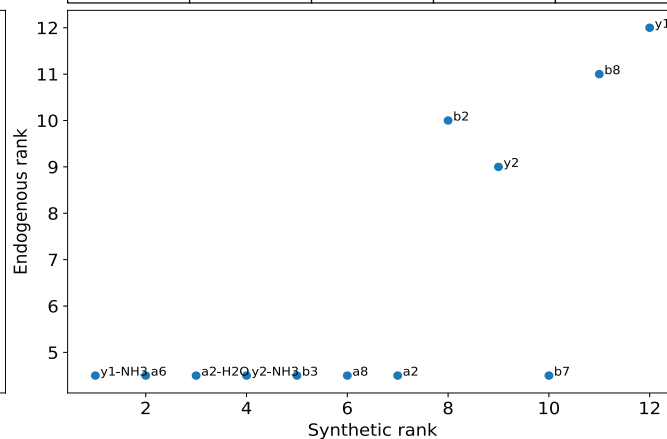
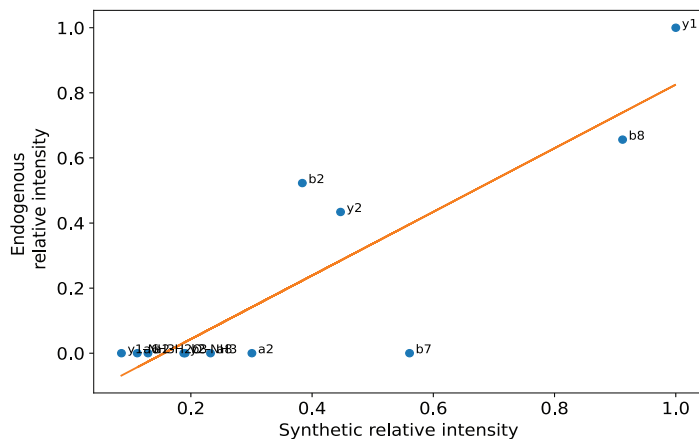


NSPRSILVKL / 2+

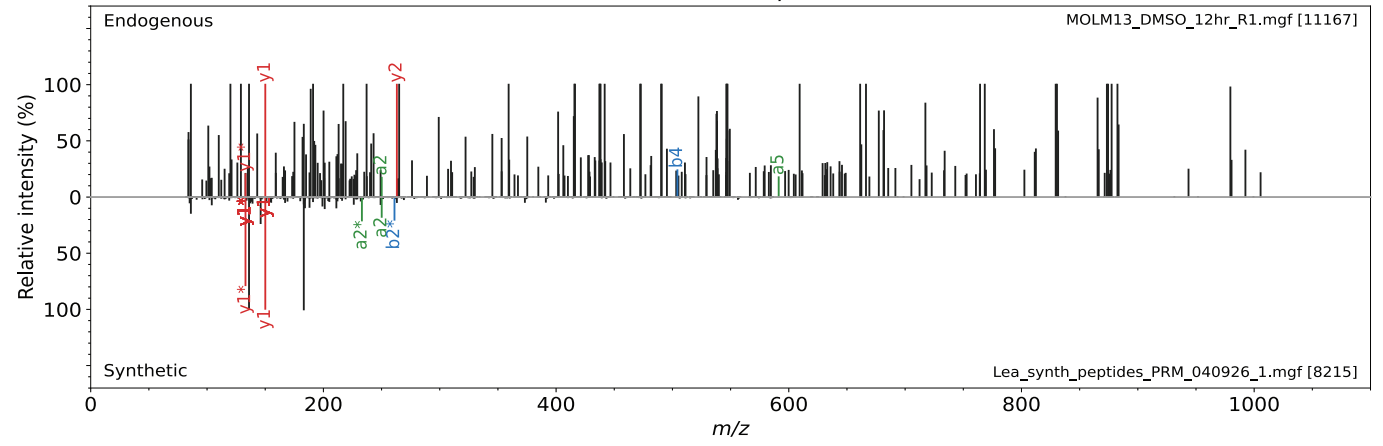


Spectrum	m/z	error (ppm)
Endogenous	563.8492	-2.8
Synthetic	563.8494	-2.5

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.86	0.57	0.96	3.2e-04
Spearman	0.75	0.31	0.93	5.1e-03
Spectral angle	0.68	-	-	-

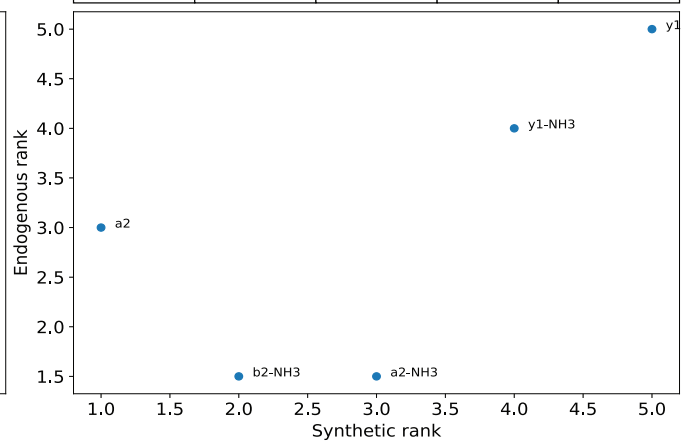
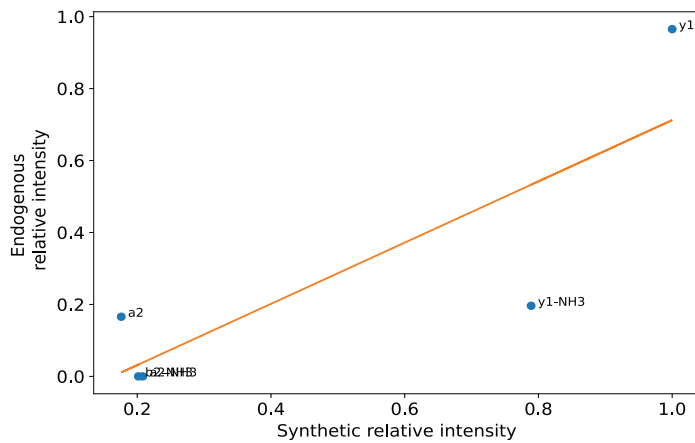


NYLIDLPLM / 2+

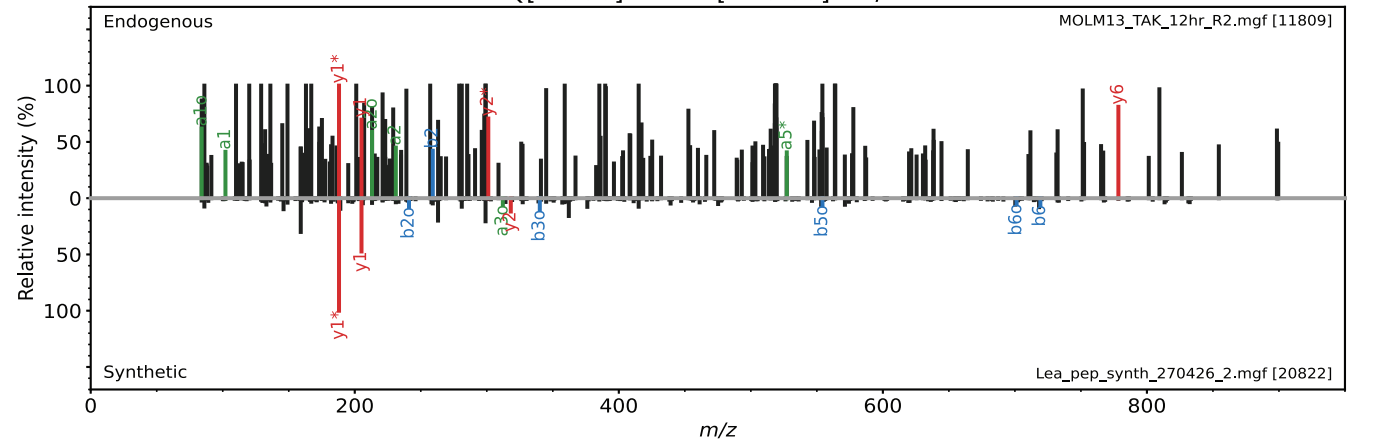


Spectrum	m/z	error (ppm)
Endogenous	546.2904	-6.4
Synthetic	546.2963	4.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.83	-0.20	0.99	8.4e-02
Spearman	0.67	-0.52	0.98	2.2e-01
Spectral angle	0.68	-	-	-

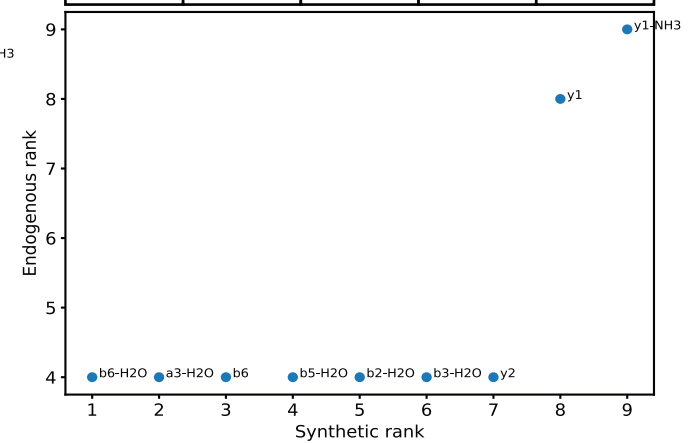
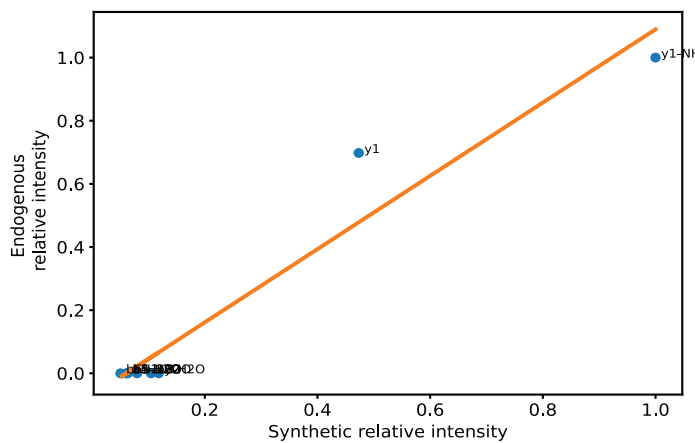


Q[+0.98]EVVDM[+15.99]LW / 2+

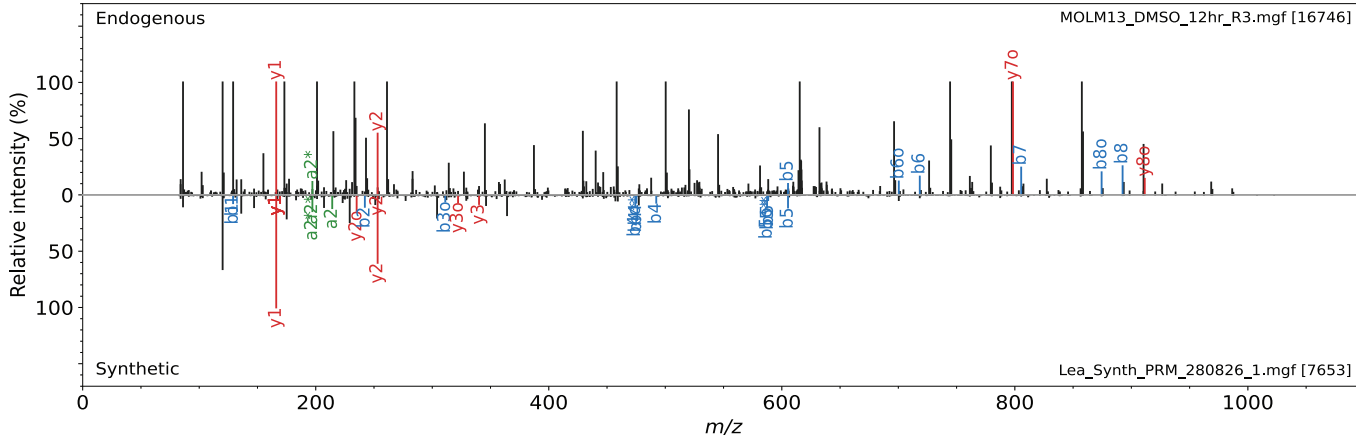


Spectrum	m/z	error (ppm)
Endogenous	518.7399	6.7
Synthetic	518.7354	-1.9

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.87	0.99	1.1e-05
Spearman	0.73	0.13	0.94	2.5e-02
Spectral angle	0.84	-	-	-

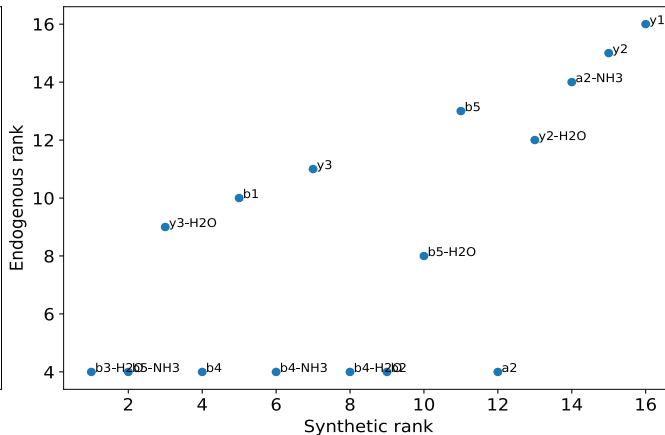
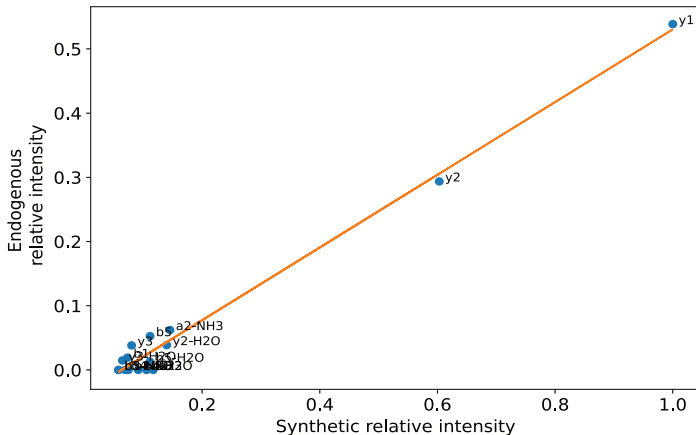


QISYLLSSF / 2+

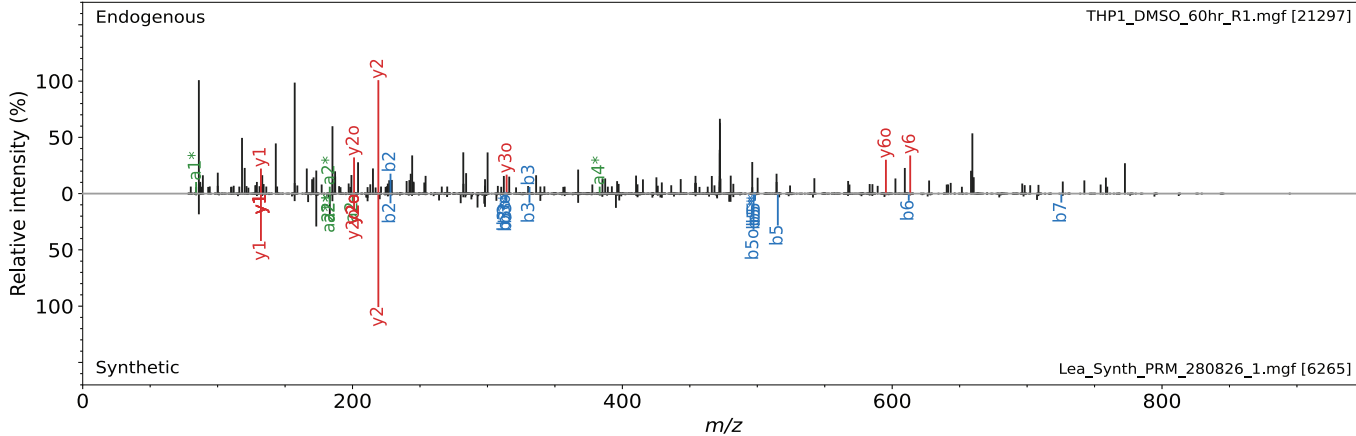


Spectrum	m/z	error (ppm)
Endogenous	529.2816	-0.6
Synthetic	529.2812	-1.3

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.99	0.98	1.00	2.0e-14
Spearman	0.68	0.28	0.88	3.6e-03
Spectral angle	0.86	-	-	-

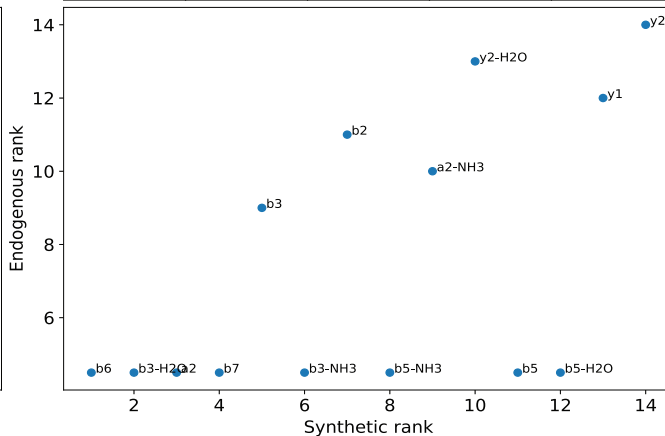
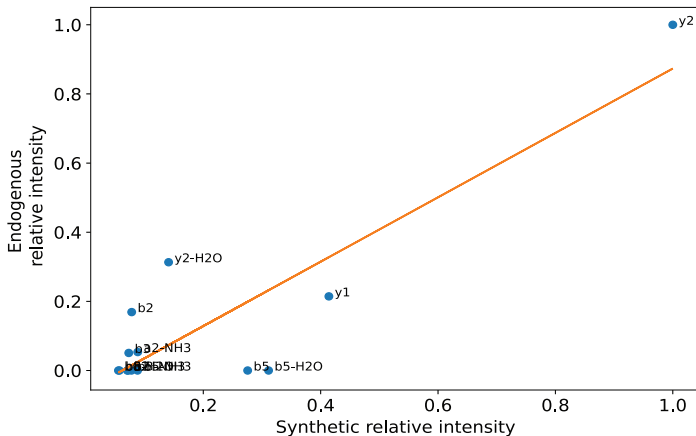


QVCPSISL / 2+

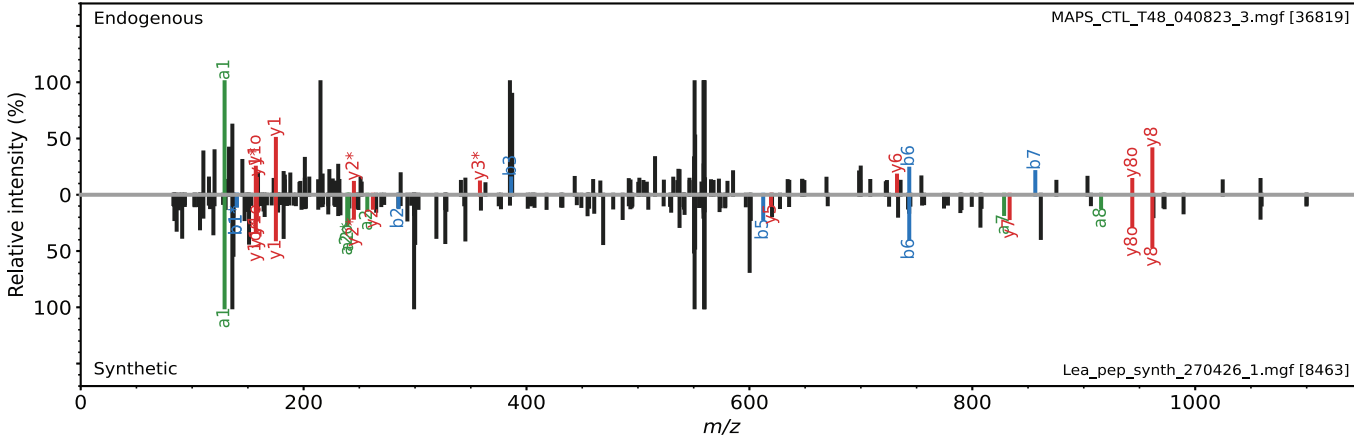


Spectrum	m/z	error (ppm)
Endogenous	472.2532	7.8
Synthetic	472.2486	-1.9

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.88	0.67	0.96	2.7e-05
Spearman	0.57	0.06	0.85	3.2e-02
Spectral angle	0.71	-	-	-

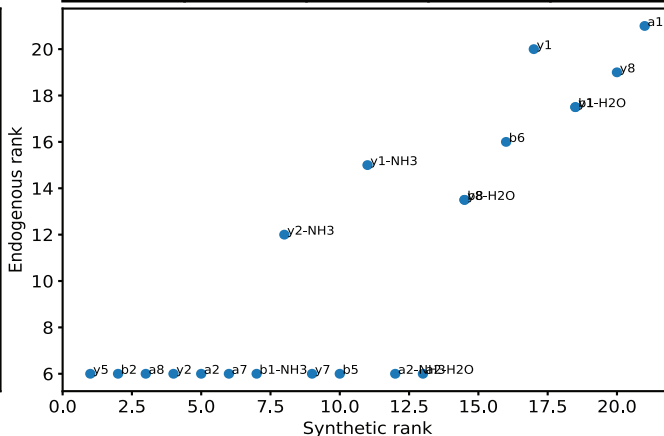
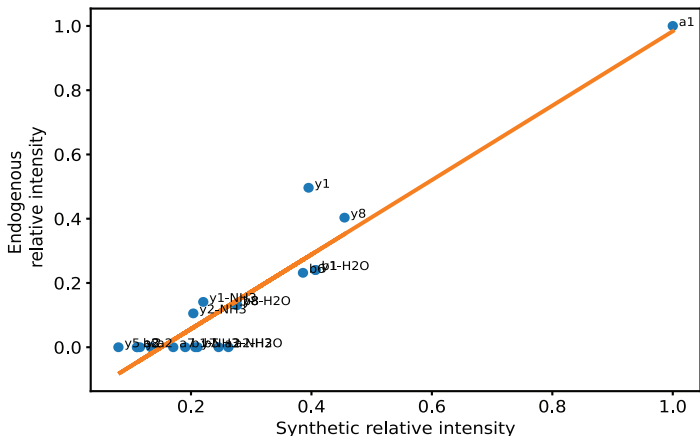


RQTLIMLSR / 2+

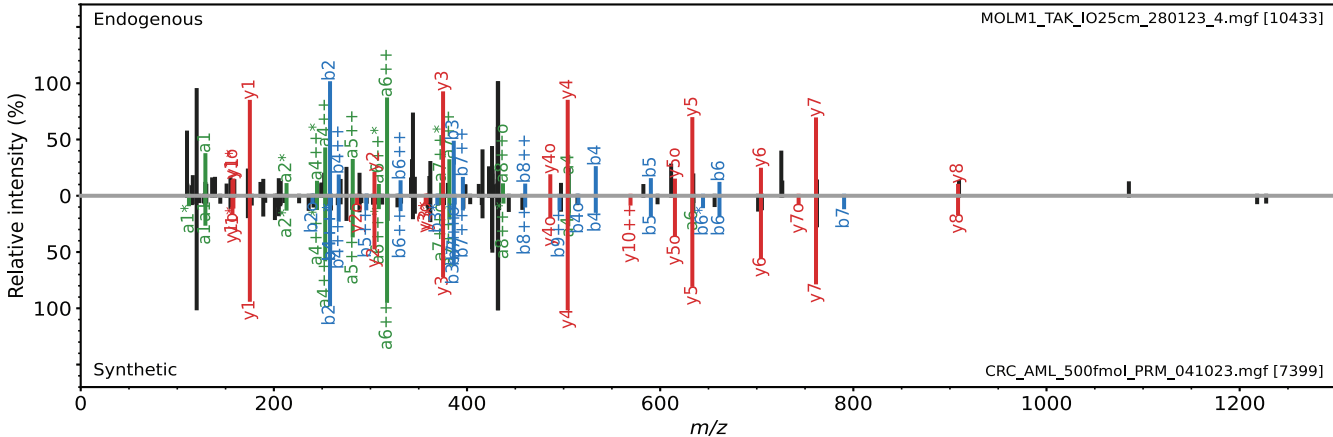


Spectrum	m/z	error (ppm)
Endogenous	559.3322	5.5
Synthetic	559.3295	0.7

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.95	0.88	0.98	5.1e-11
Spearman	0.85	0.67	0.94	8.4e-07
Spectral angle	0.71	-	-	-

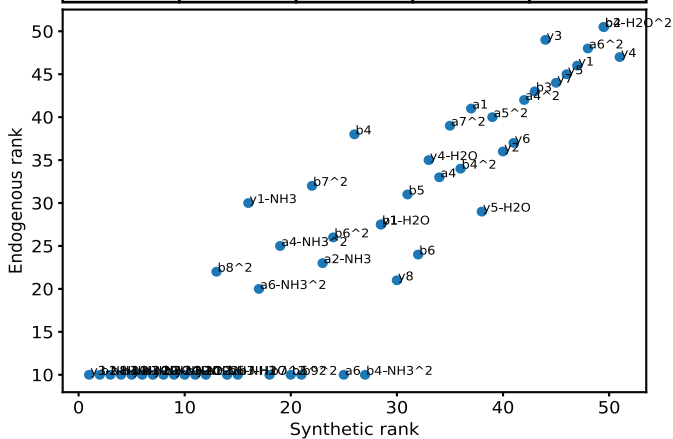
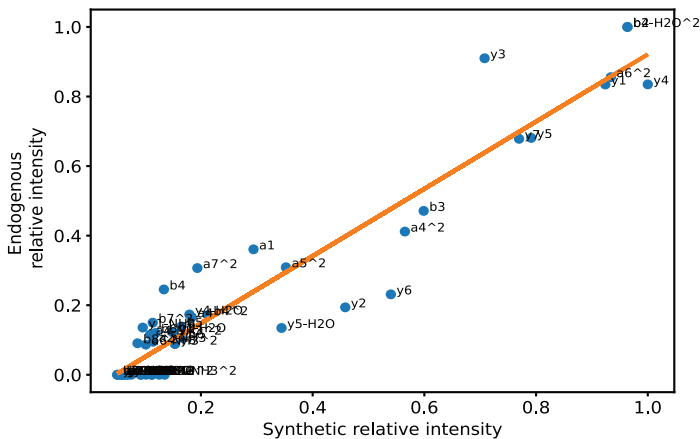


RTKFGAEEAER / 3+

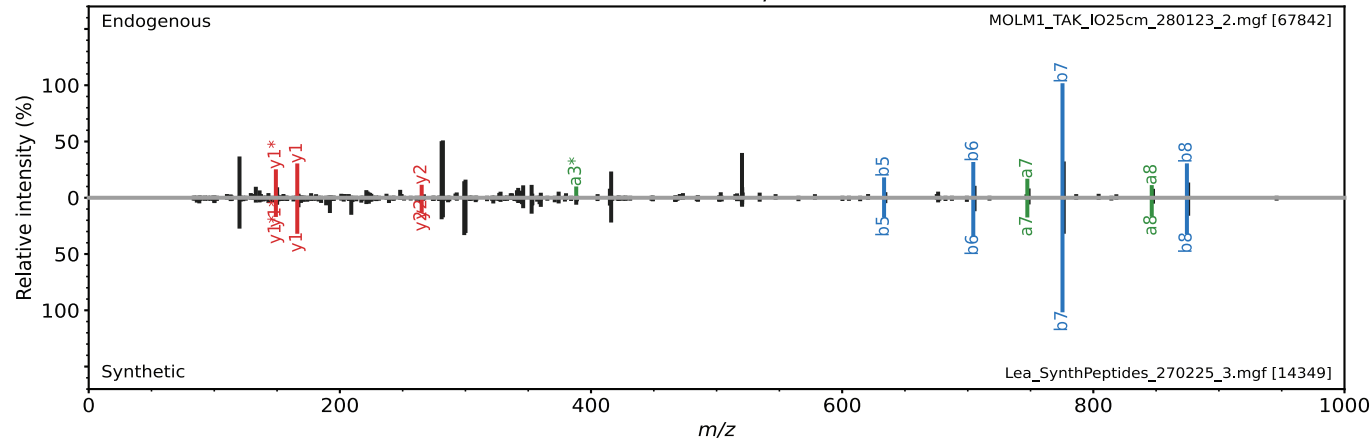


Spectrum	m/z	error (ppm)
Endogenous	431.8894	-0.6
Synthetic	431.8900	0.7

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.96	0.93	0.98	4.8e-28
Spearman	0.91	0.84	0.95	7.7e-20
Spectral angle	0.84	-	-	-

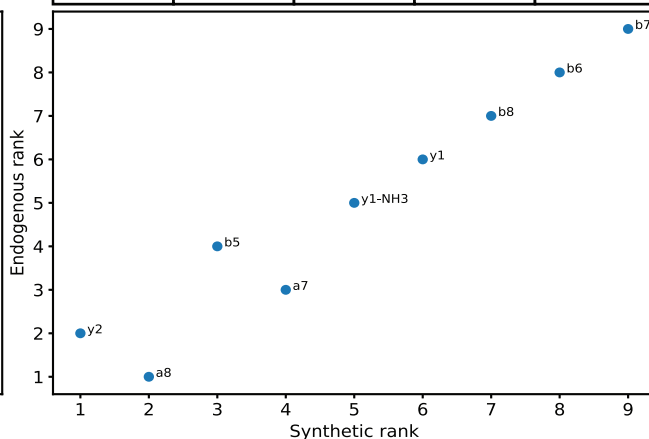
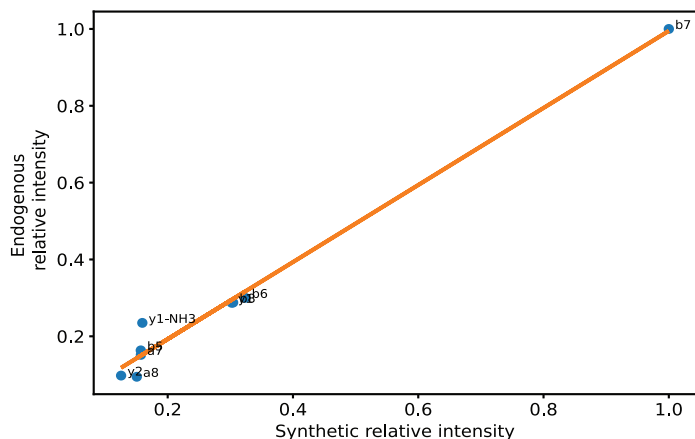


RYLTVAAVF / 2+

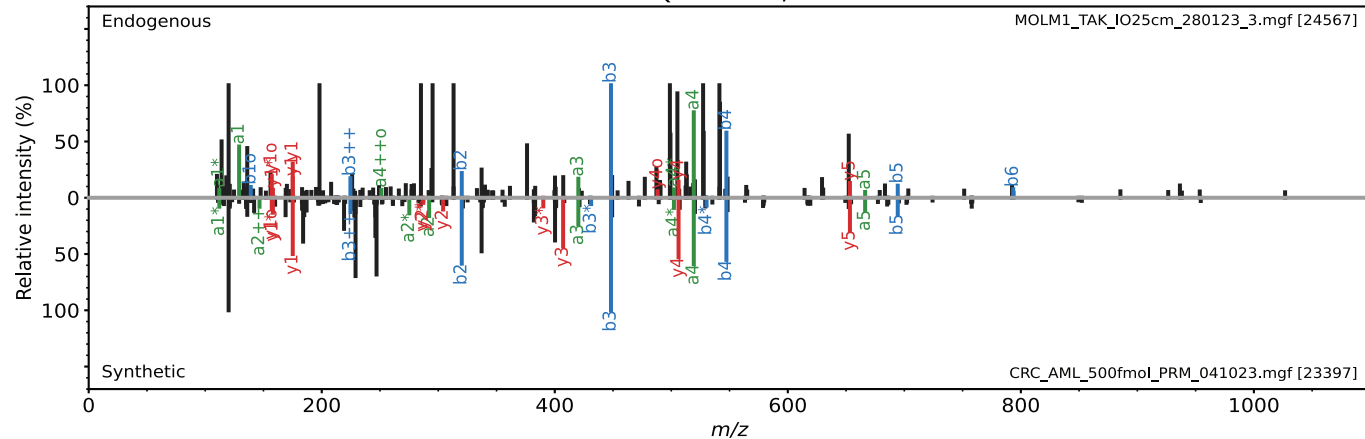


Spectrum	m/z	error (ppm)
Endogenous	520.3001	-0.5
Synthetic	520.3010	1.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.99	0.96	1.00	1.8e-07
Spearman	0.97	0.85	0.99	2.2e-05
Spectral angle	0.94	-	-	-

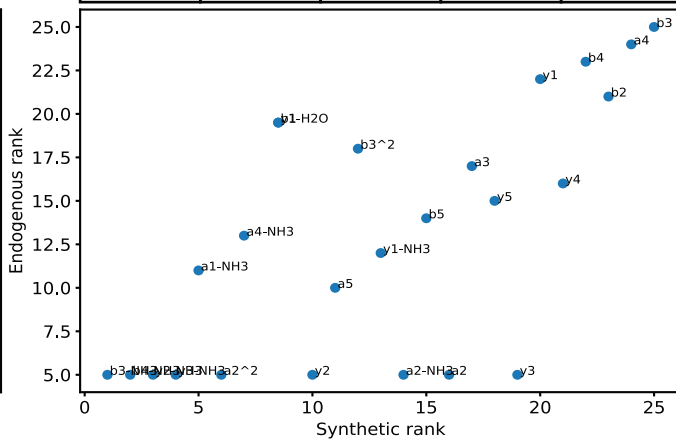
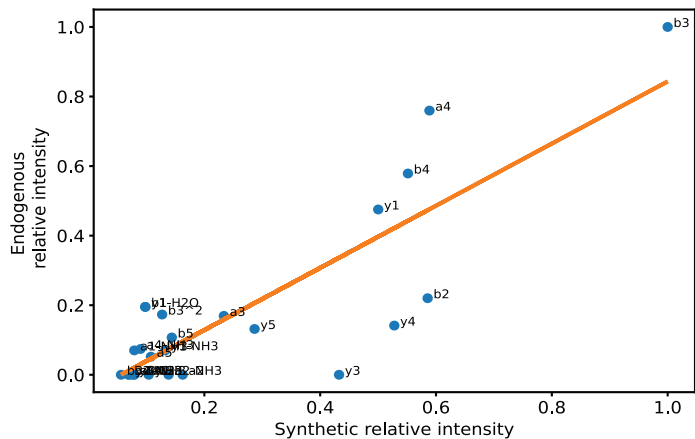


RYQVFVCFER / 3+

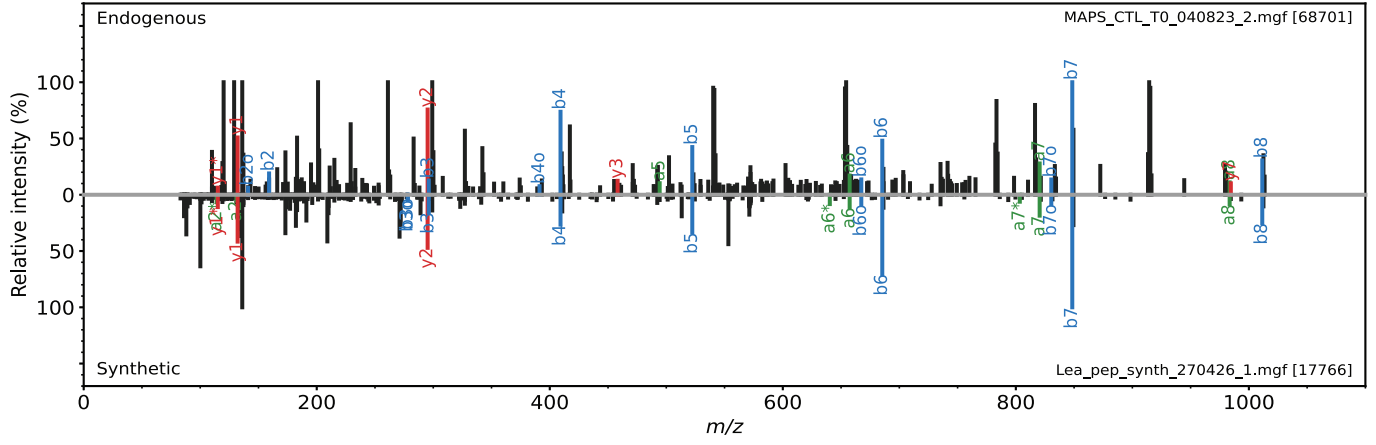


Spectrum	m/z	error (ppm)
Endogenous	400.5383	1.1
Synthetic	400.5395	4.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.84	0.66	0.93	1.6e-07
Spearman	0.67	0.37	0.84	2.8e-04
Spectral angle	0.70	-	-	-

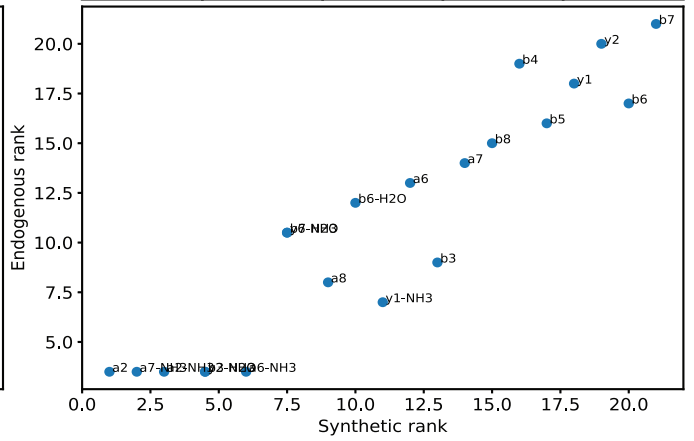
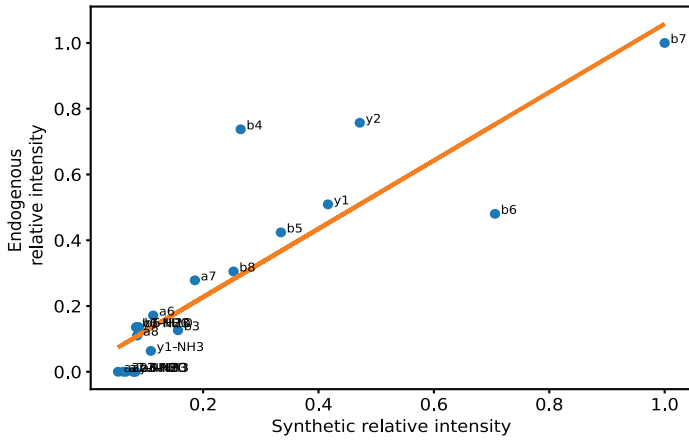


SAHLLYYL / 2+

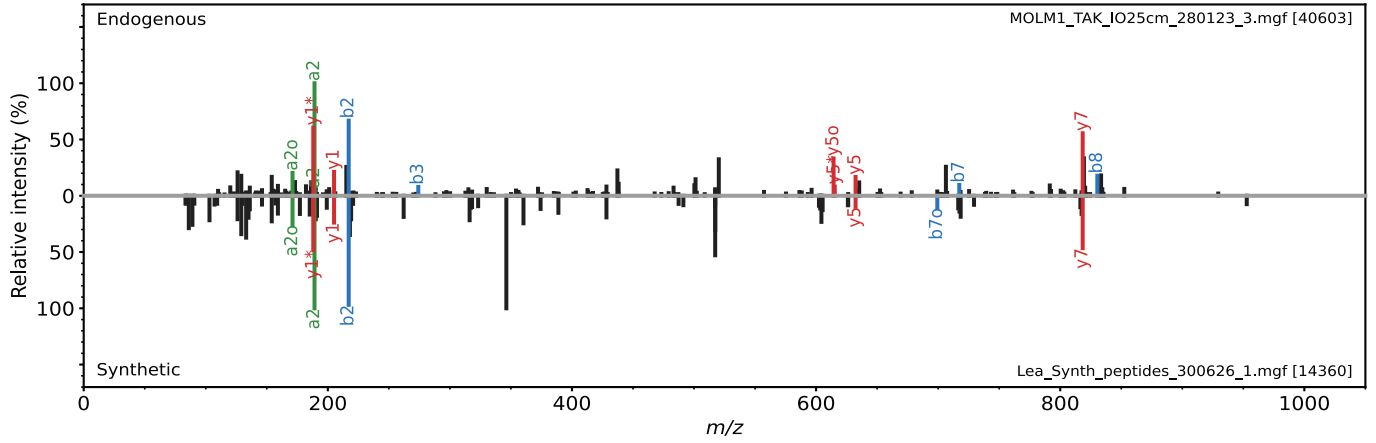


Spectrum	m/z	error (ppm)
Endogenous	571.8033	9.8
Synthetic	571.7969	-1.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.87	0.70	0.95	2.7e-07
Spearman	0.94	0.85	0.98	3.0e-10
Spectral angle	0.76	-	-	-

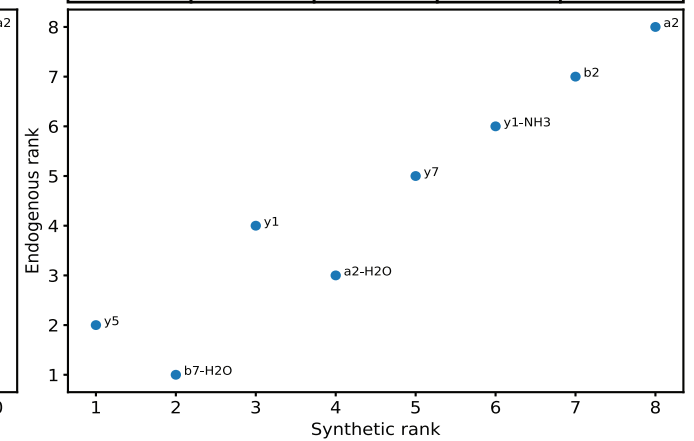
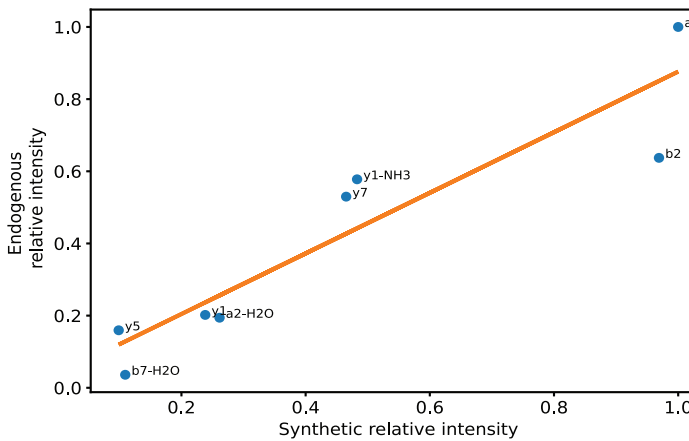


SEGEKELW / 2+

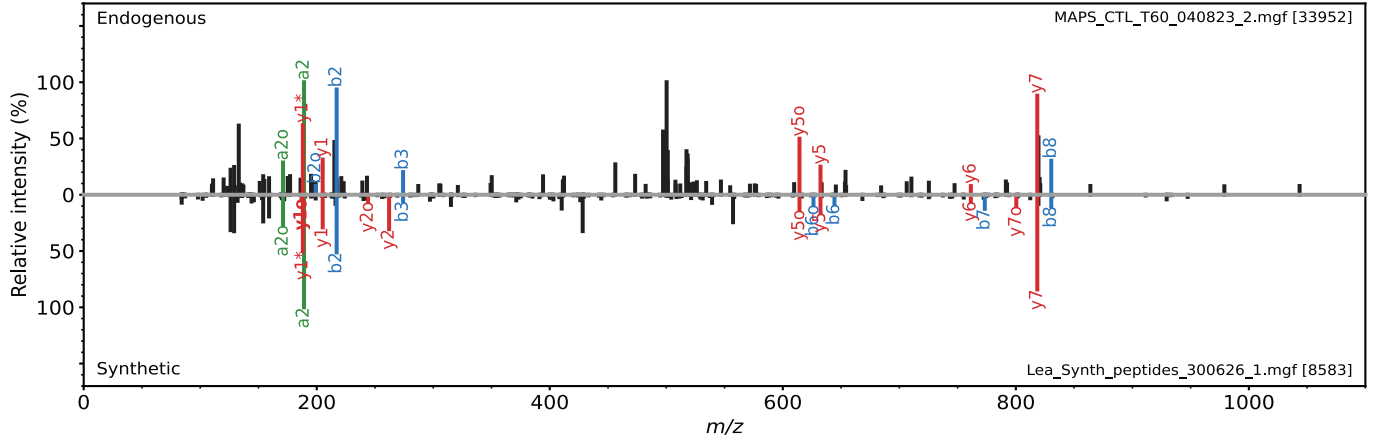


Spectrum	m/z	error (ppm)
Endogenous	517.7427	-0.7
Synthetic	517.7432	0.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.93	0.64	0.99	9.6e-04
Spearman	0.95	0.75	0.99	2.6e-04
Spectral angle	0.85	-	-	-

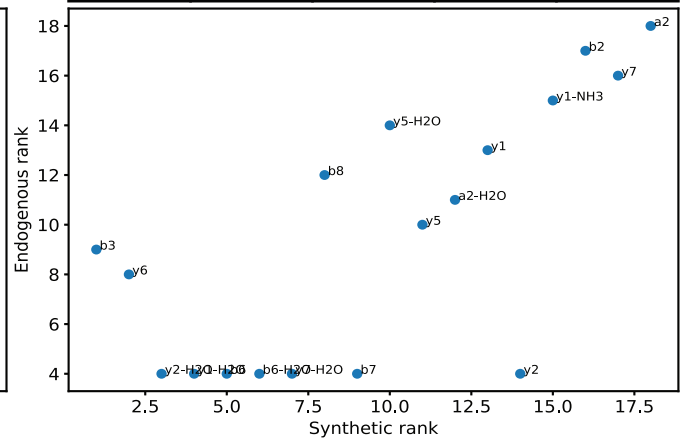
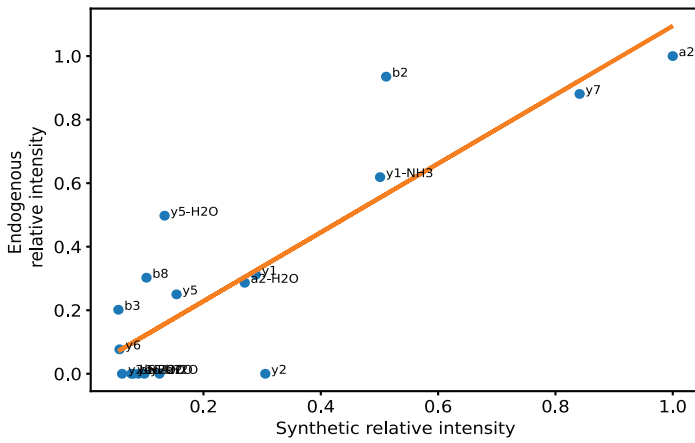


SEGEKIEGW / 2+

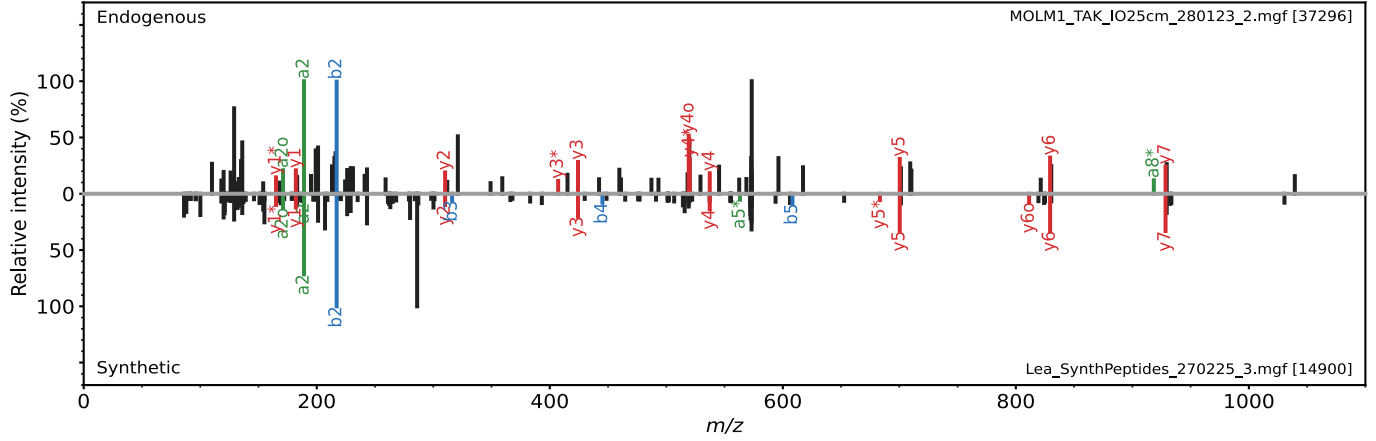


Spectrum	m/z	error (ppm)
Endogenous	517.7479	9.3
Synthetic	517.7433	0.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.87	0.67	0.95	3.2e-06
Spearman	0.71	0.36	0.88	1.0e-03
Spectral angle	0.76	-	-	-

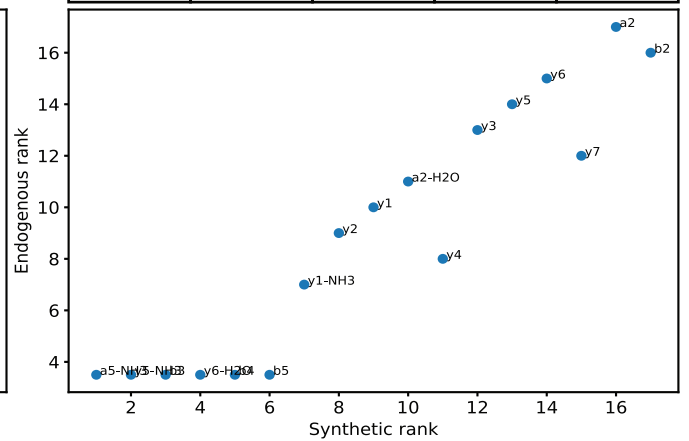
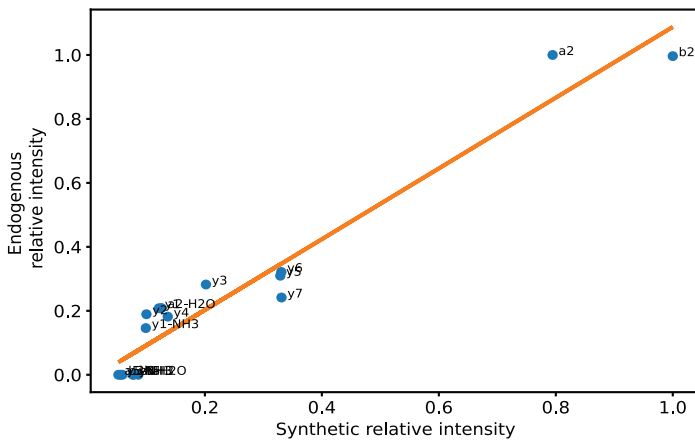


SEVEYINKY / 2+

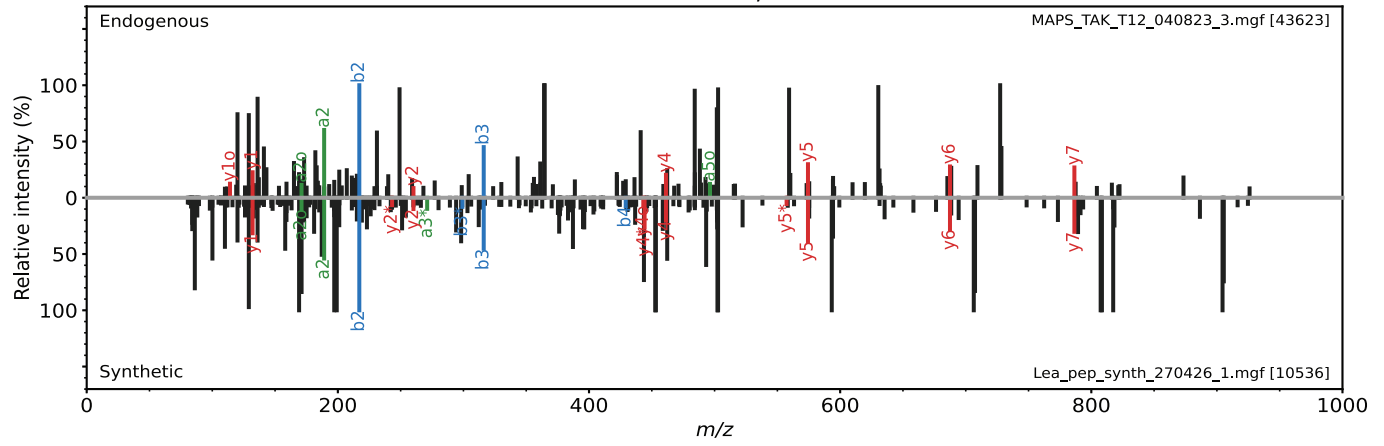


Spectrum	m/z	error (ppm)
Endogenous	572.7795	-0.3
Synthetic	572.7800	0.5

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.91	0.99	2.5e-10
Spearman	0.95	0.85	0.98	1.0e-08
Spectral angle	0.87	-	-	-

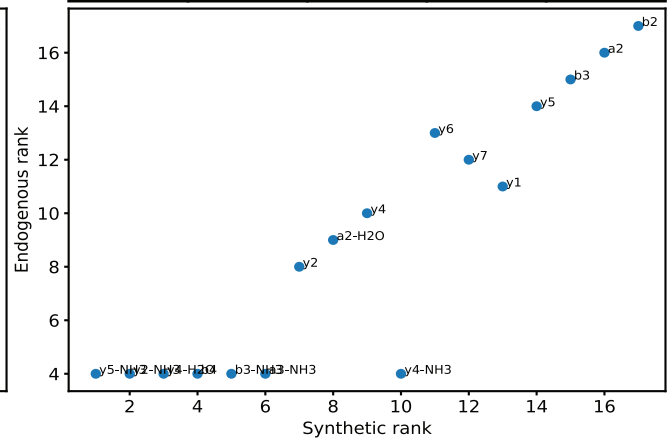
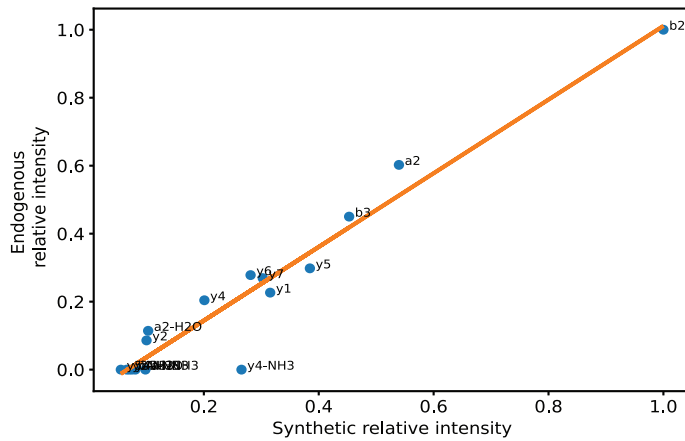


SEVILSNKI / 2+

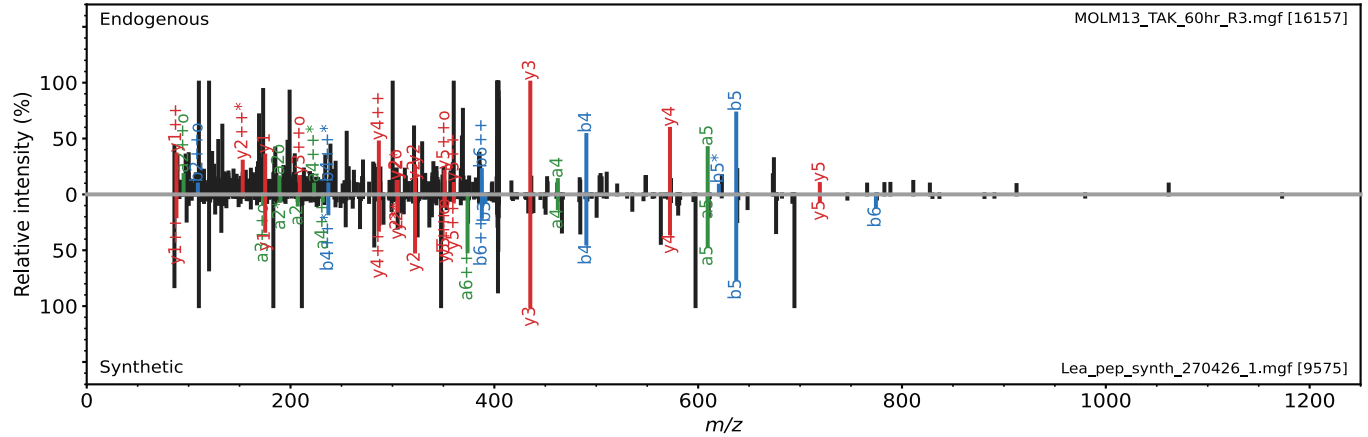


Spectrum	m/z	error (ppm)
Endogenous	501.7990	7.8
Synthetic	501.7938	-2.6

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.91	0.99	2.1e-10
Spearman	0.92	0.78	0.97	2.3e-07
Spectral angle	0.84	-	-	-

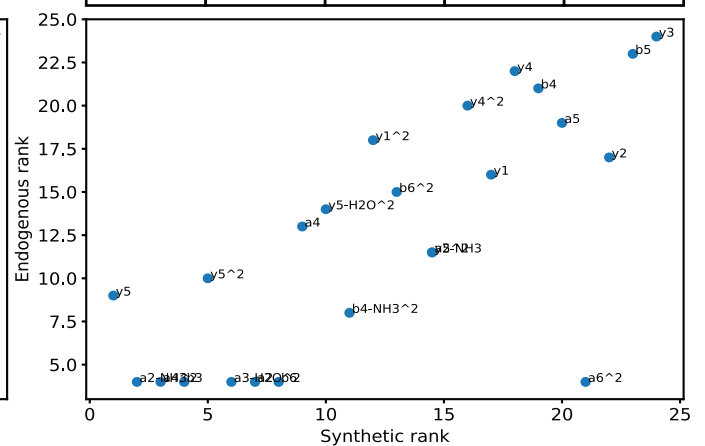
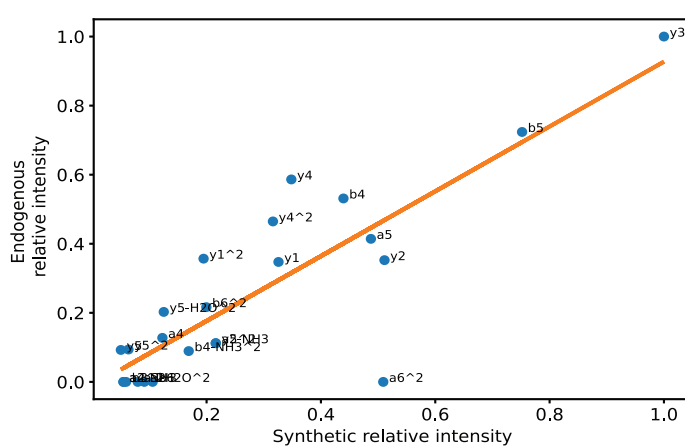


SFRVFHIFR / 3+

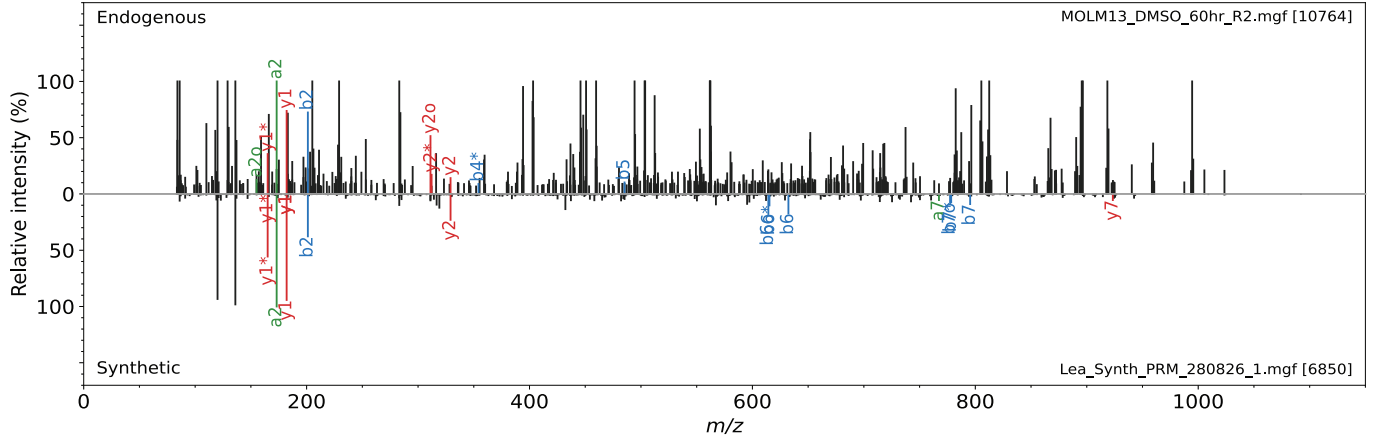


Spectrum	m/z	error (ppm)
Endogenous	403.5609	-0.5
Synthetic	403.5612	0.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.85	0.68	0.93	1.3e-07
Spearman	0.75	0.49	0.88	2.7e-05
Spectral angle	0.75	-	-	-

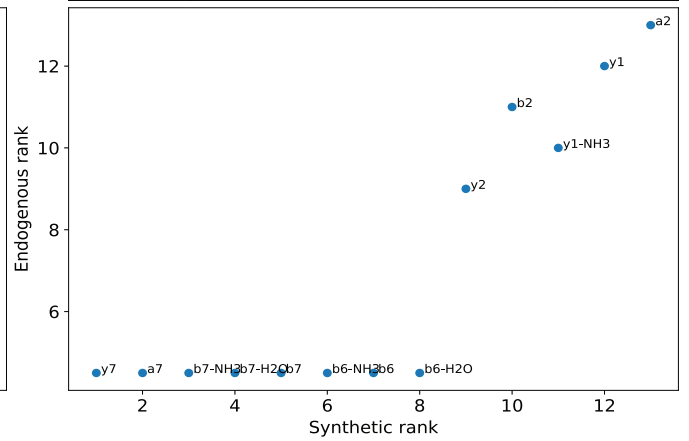
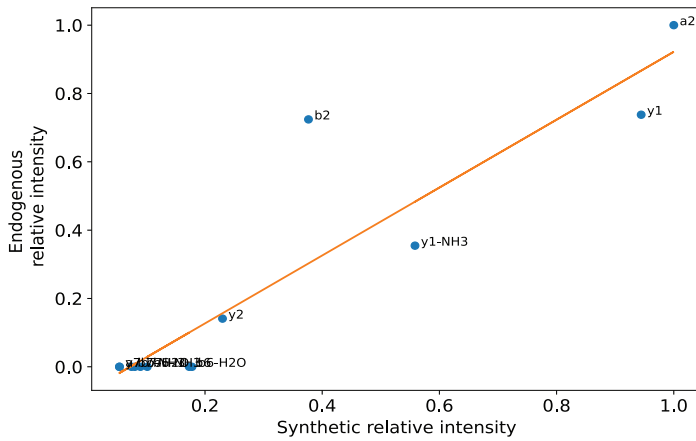


SILGNM[+15.99]YFY / 2+

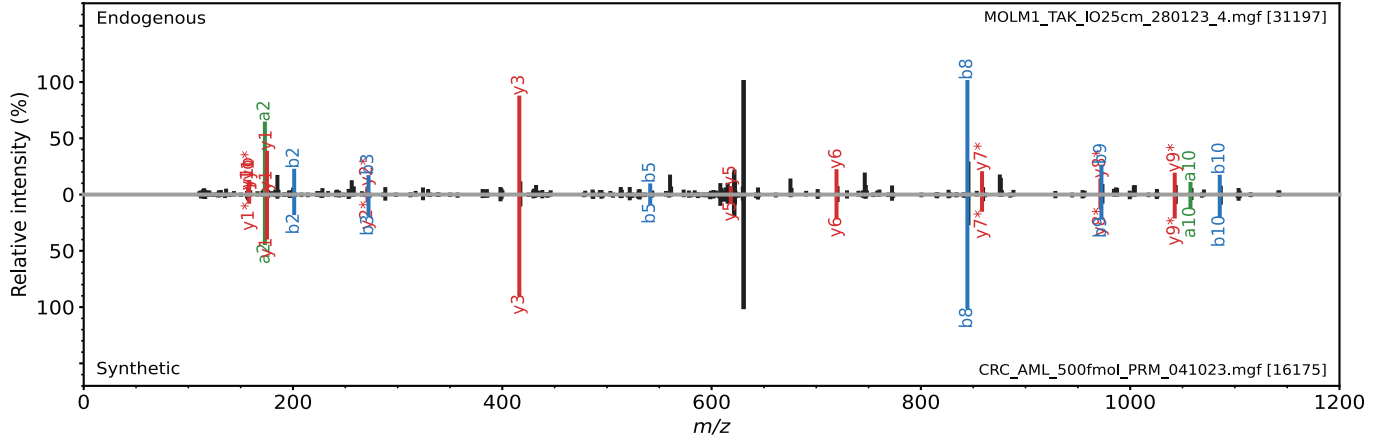


Spectrum	m/z	error (ppm)
Endogenous	562.2554	-8.4
Synthetic	562.2593	-1.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.92	0.74	0.98	9.2e-06
Spearman	0.87	0.61	0.96	1.1e-04
Spectral angle	0.77	-	-	-

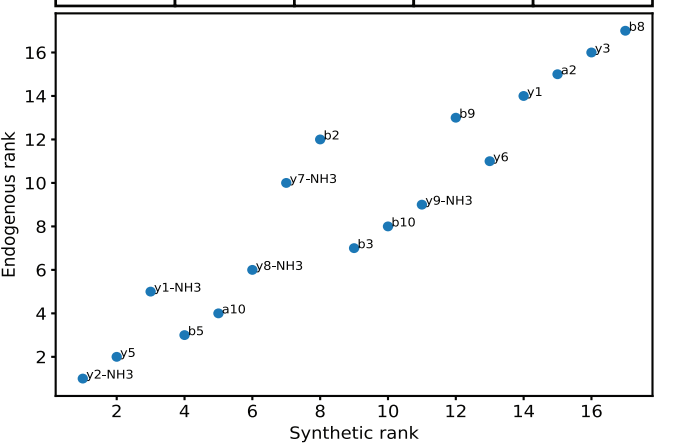
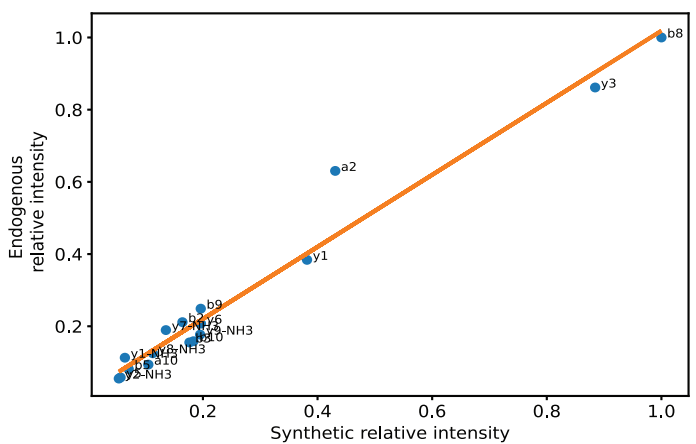


SLALRTSDQLR / 2+

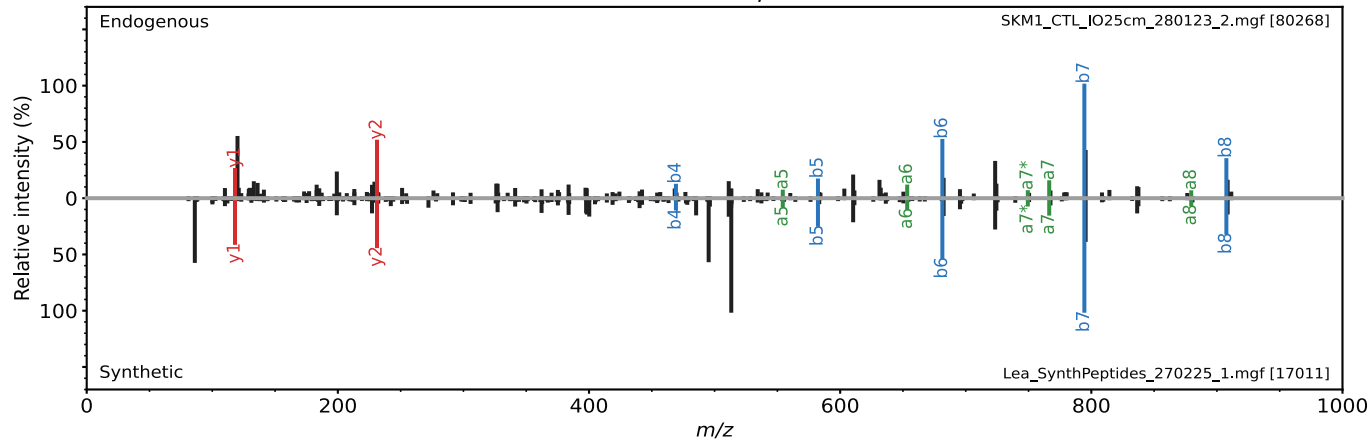


Spectrum	m/z	error (ppm)
Endogenous	630.3569	-0.0
Synthetic	630.3578	1.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.98	0.95	0.99	2.9e-12
Spearman	0.94	0.84	0.98	1.8e-08
Spectral angle	0.91	-	-	-

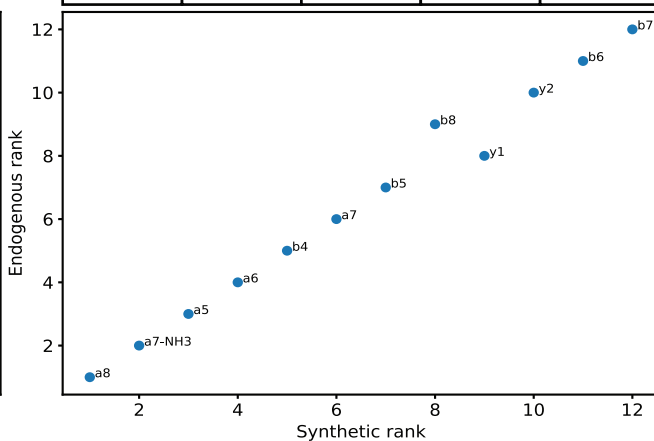
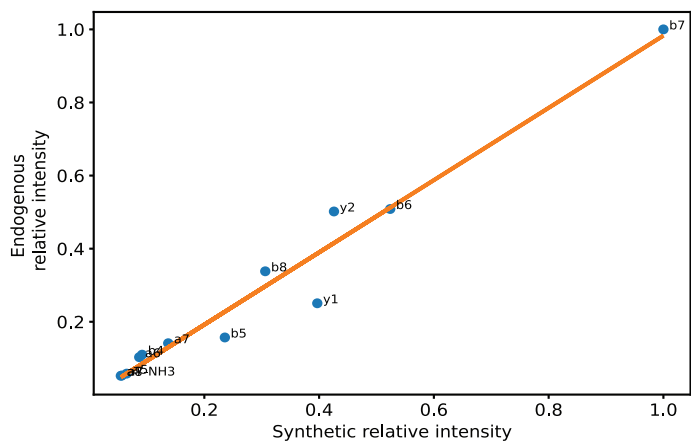


SPFHLVLIV / 2+

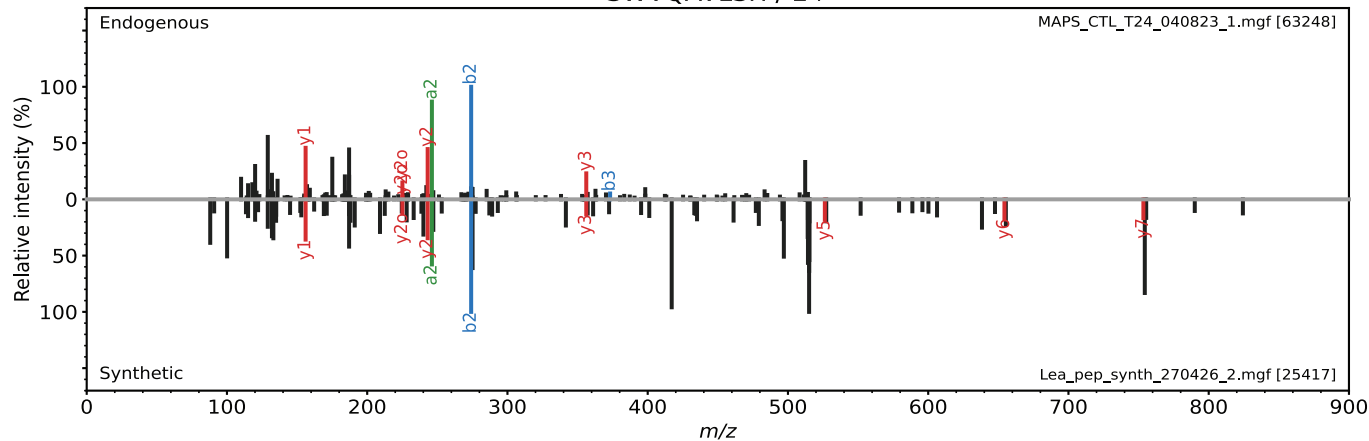


Spectrum	m/z	error (ppm)
Endogenous	512.8126	-1.0
Synthetic	512.8133	0.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.98	0.93	0.99	2.4e-08
Spearman	0.99	0.97	1.00	1.3e-10
Spectral angle	0.91	-	-	-

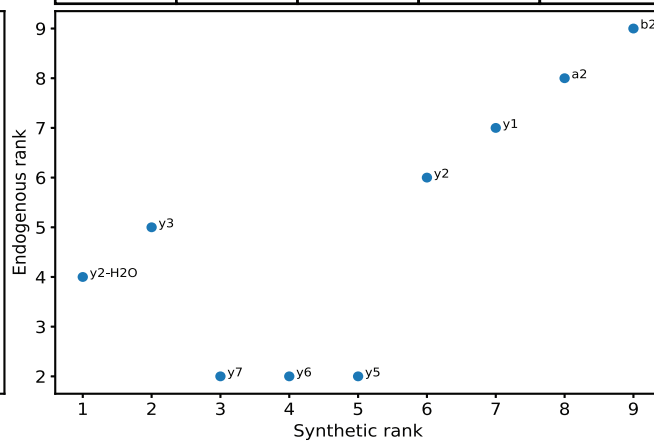
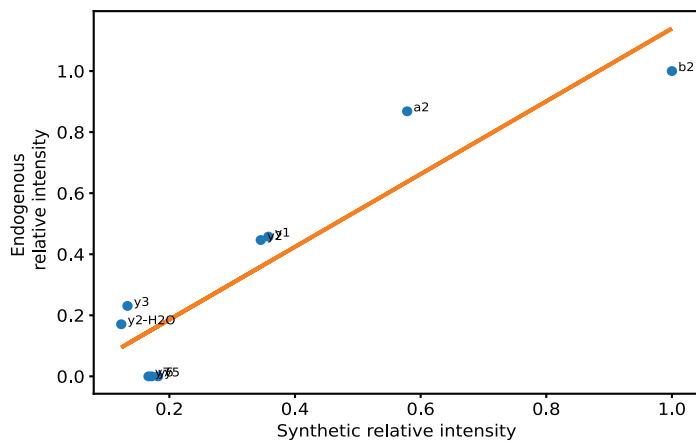


SWVQAVLSH / 2+

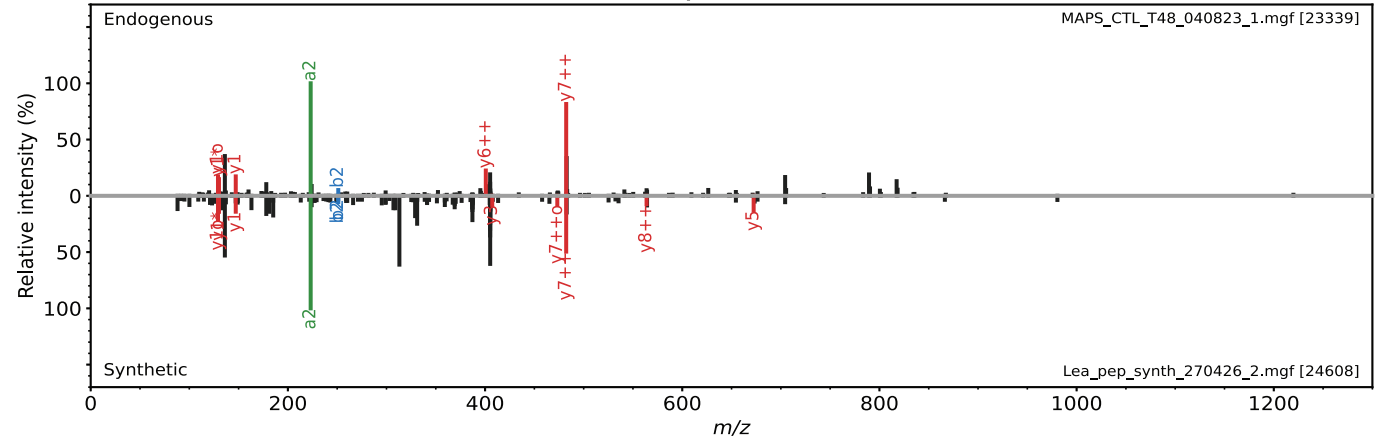


Spectrum	m/z	error (ppm)
Endogenous	513.7762	8.2
Synthetic	513.7718	-0.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.92	0.64	0.98	5.1e-04
Spearman	0.73	0.13	0.94	2.6e-02
Spectral angle	0.81	-	-	-

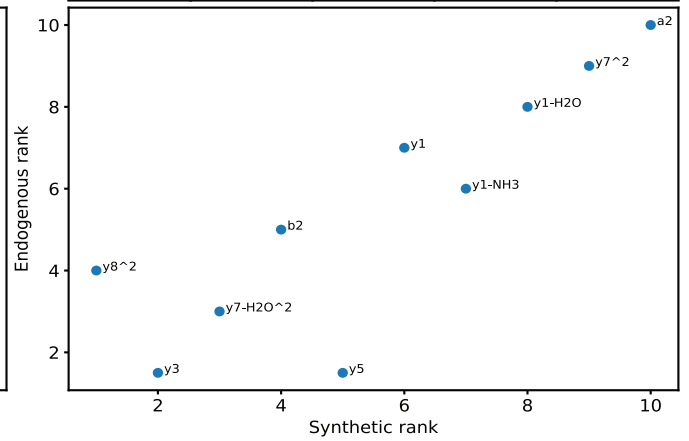
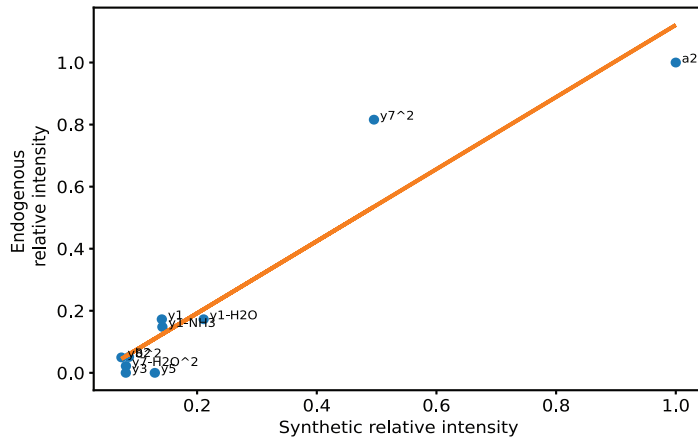


SYIQHKFLK / 3+

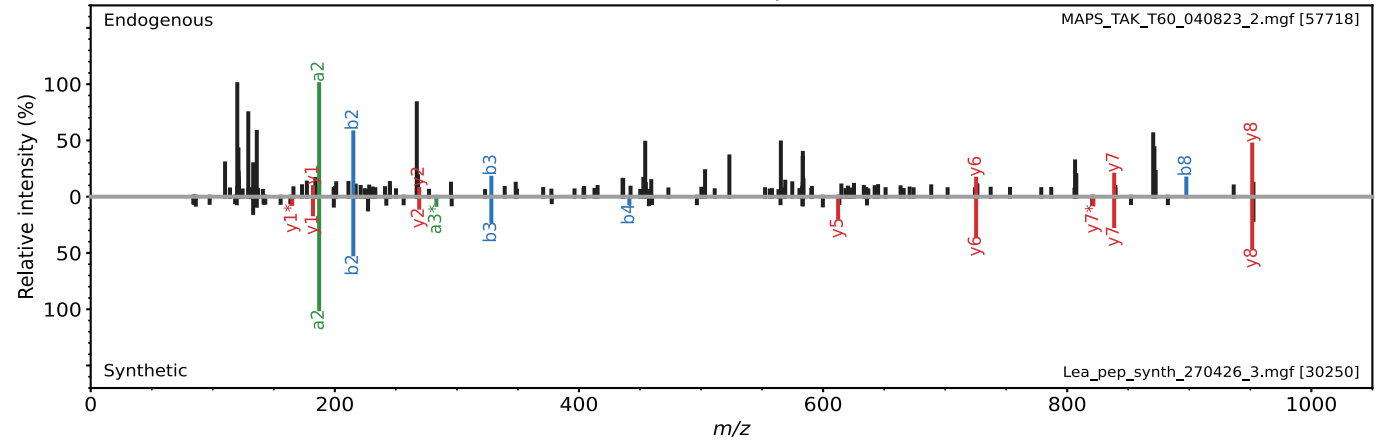


Spectrum	m/z	error (ppm)
Endogenous	405.2194	5.9
Synthetic	405.2159	-2.7

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.95	0.80	0.99	2.6e-05
Spearman	0.85	0.48	0.96	1.8e-03
Spectral angle	0.83	-	-	-

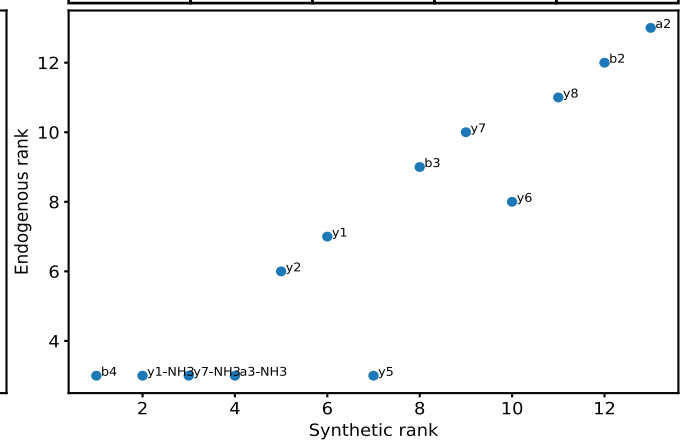
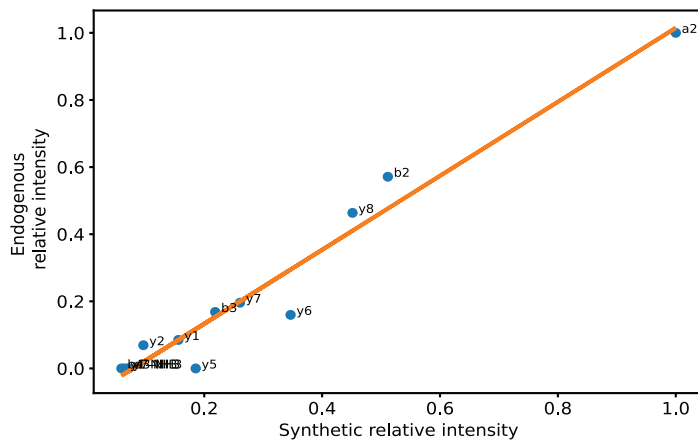


TIILIKNTSY / 2+

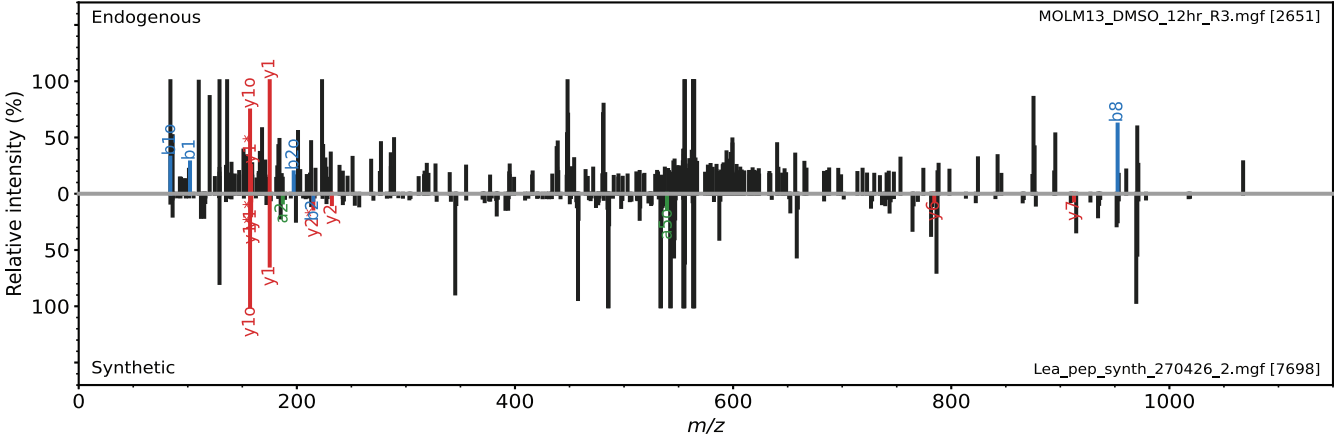


Spectrum	m/z	error (ppm)
Endogenous	583.3506	9.6
Synthetic	583.3433	-2.9

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.98	0.92	0.99	8.5e-09
Spearman	0.92	0.74	0.97	1.1e-05
Spectral angle	0.85	-	-	-

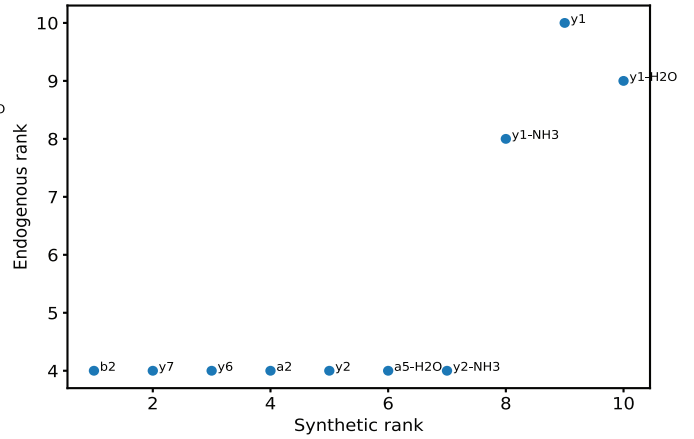
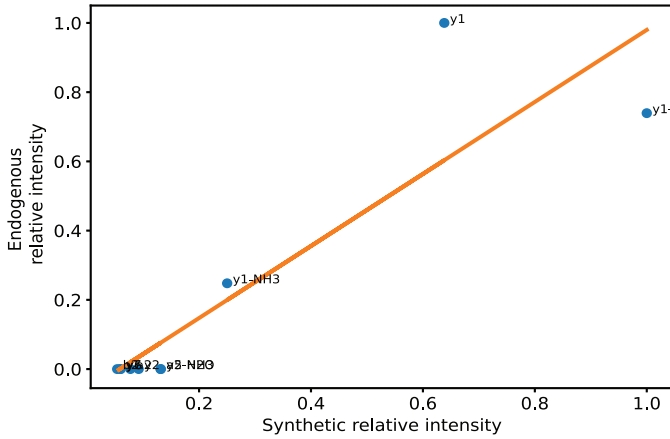


TIKNKYFGR / 2+

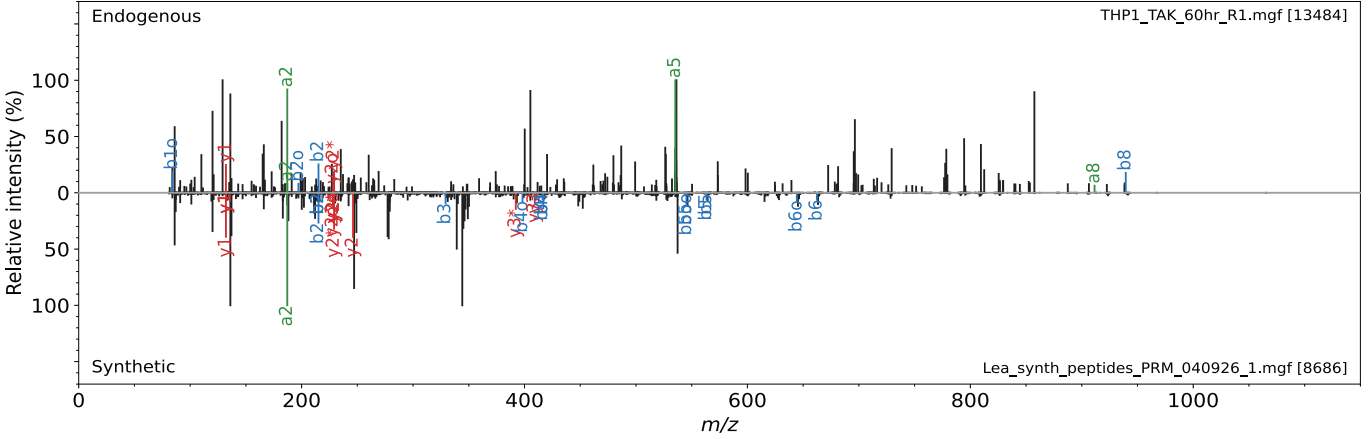


Spectrum	m/z	error (ppm)
Endogenous	563.8251	5.5
Synthetic	563.8215	-0.9

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.90	0.62	0.98	3.9e-04
Spearman	0.80	0.34	0.95	5.7e-03
Spectral angle	0.74	-	-	-

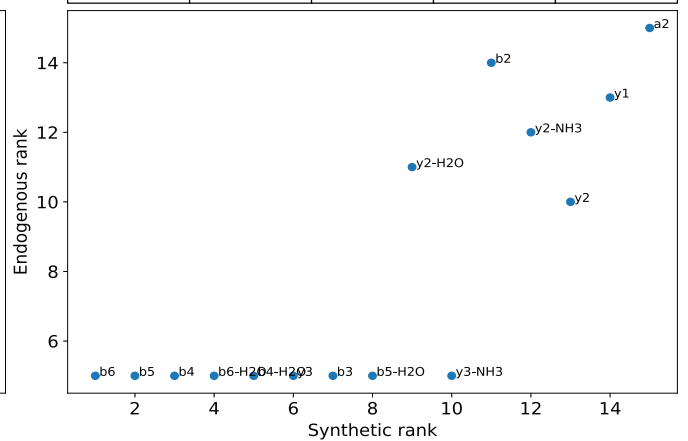
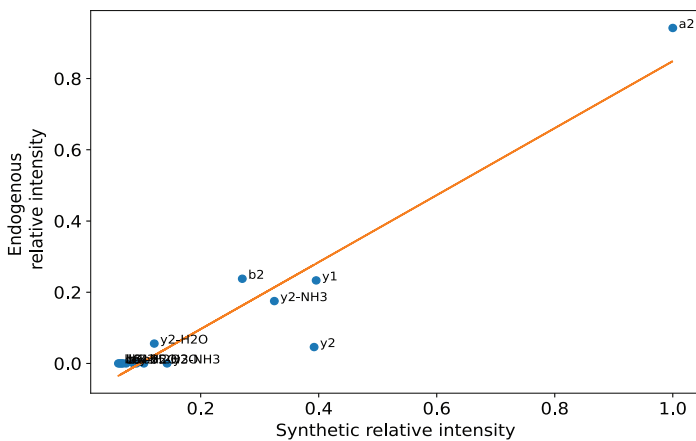


TLNSFVYNL / 2+

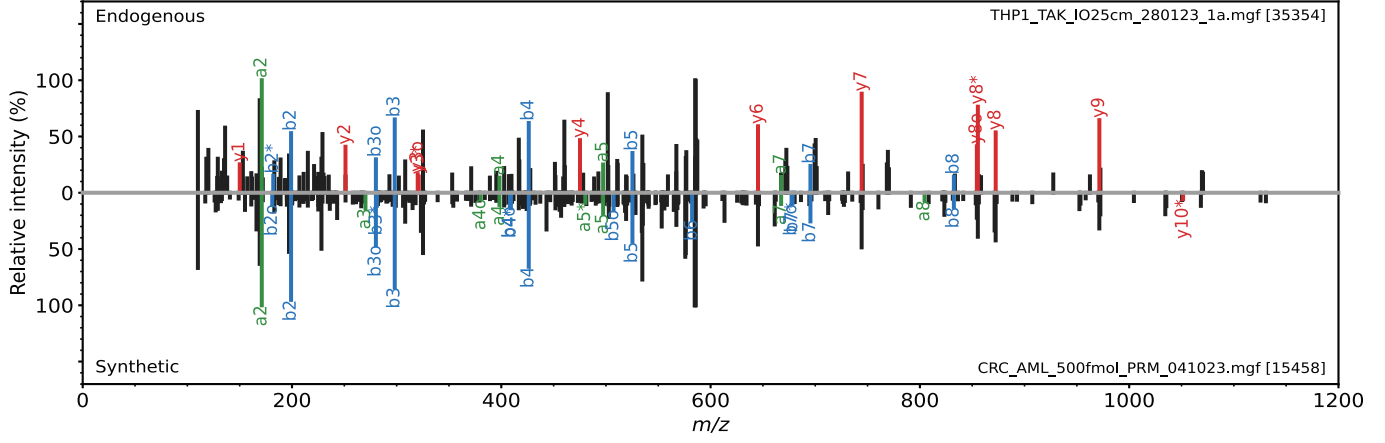


Spectrum	m/z	error (ppm)
Endogenous	535.7842	8.8
Synthetic	535.7830	6.5

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.95	0.86	0.98	4.7e-08
Spearman	0.82	0.53	0.94	1.7e-04
Spectral angle	0.75	-	-	-

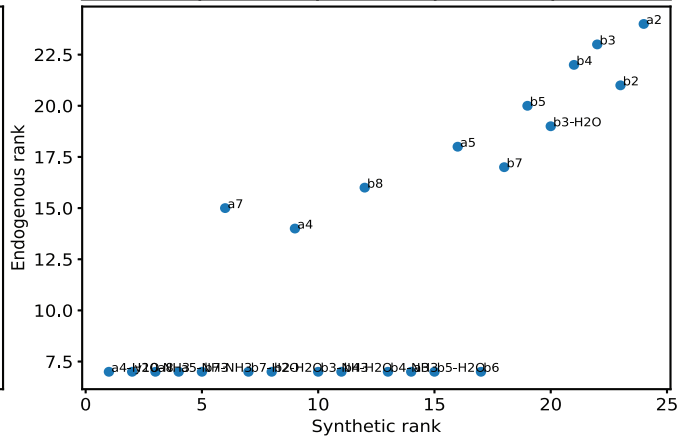
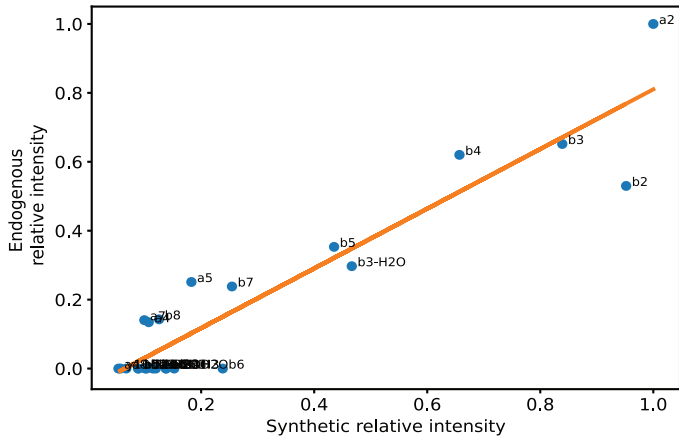


TPVQVGLHSTM / 2+

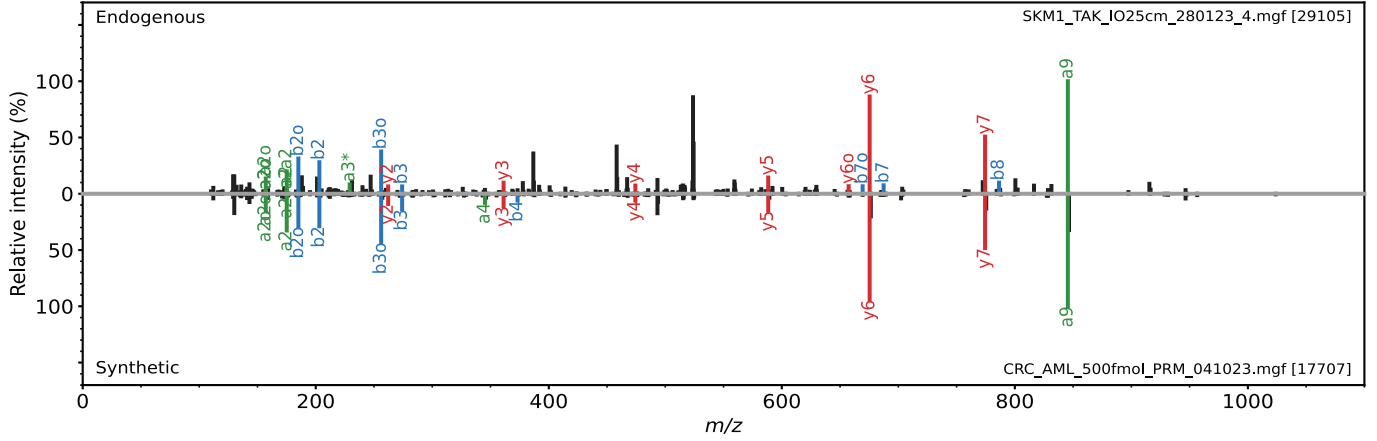


Spectrum	m/z	error (ppm)
Endogenous	585.3027	-0.2
Synthetic	585.3084	9.6

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.94	0.86	0.97	1.9e-11
Spearman	0.77	0.53	0.89	1.2e-05
Spectral angle	0.79	-	-	-

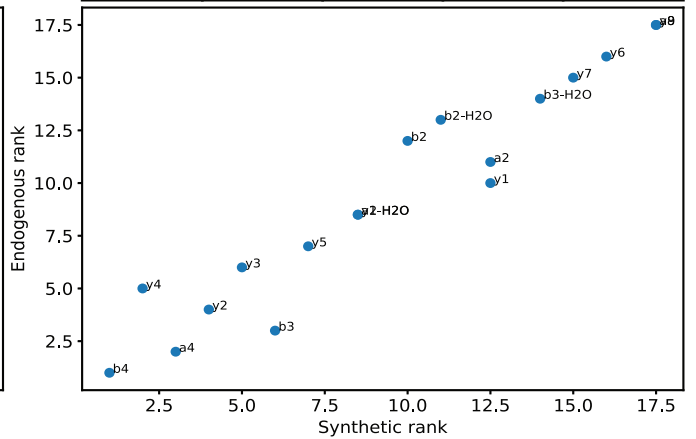
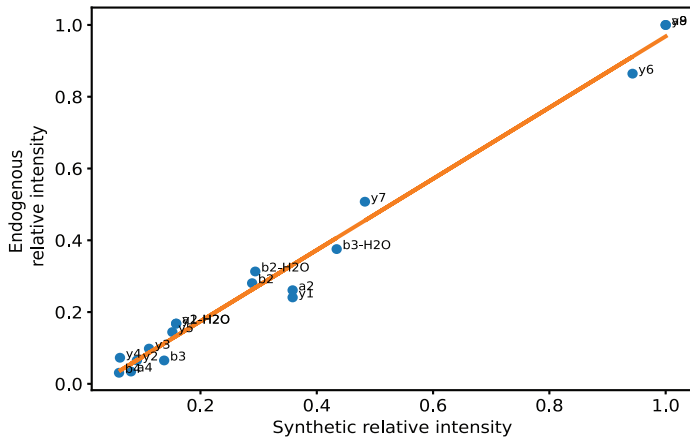


TTAVSNLVSRL / 2+

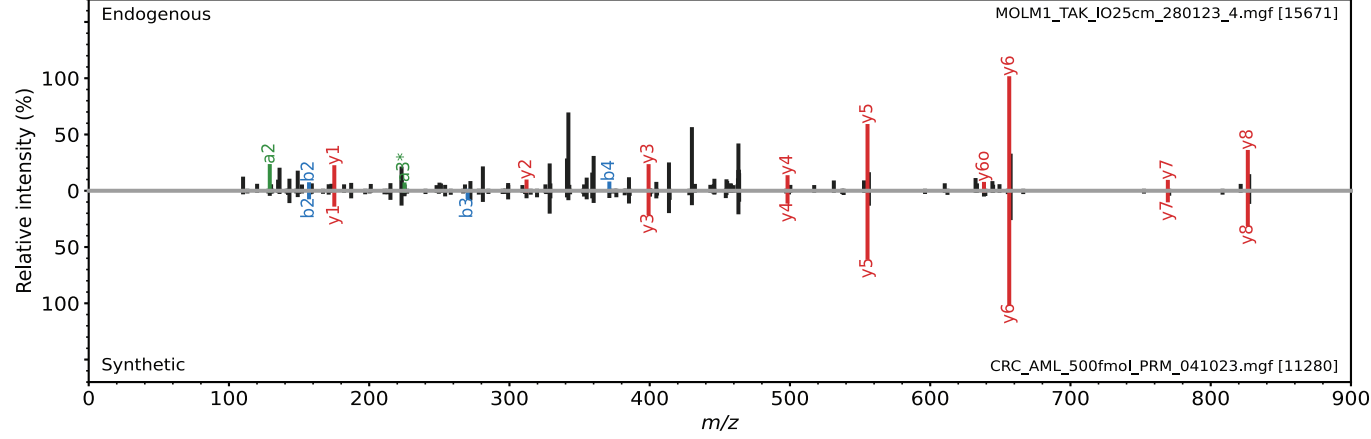


Spectrum	m/z	error (ppm)
Endogenous	524.2932	-0.2
Synthetic	524.2952	3.6

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.99	0.98	1.00	1.7e-15
Spearman	0.96	0.90	0.99	1.8e-10
Spectral angle	0.94	-	-	-

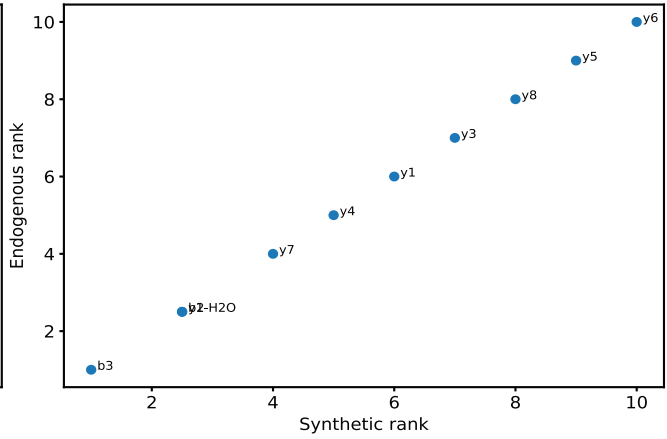
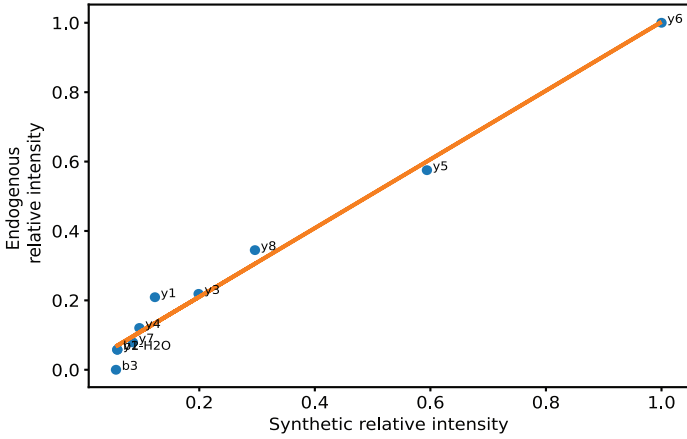


VGITGVSHR / 2+

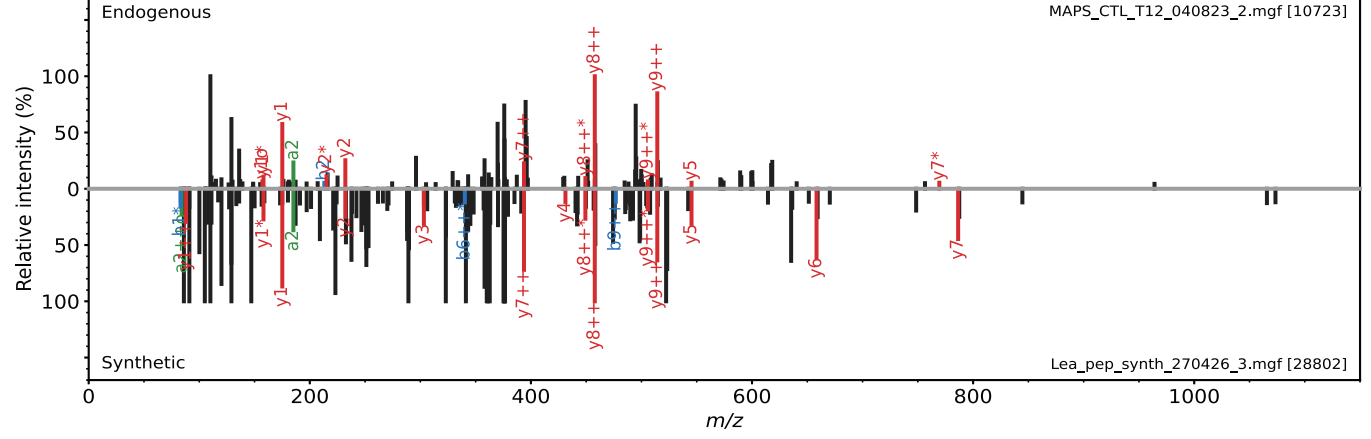


Spectrum	m/z	error (ppm)
Endogenous	463.2644	0.2
Synthetic	463.2652	1.9

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.99	0.97	1.00	1.5e-08
Spearman	1.00	1.00	1.00	0.0e+00
Spectral angle	0.94	-	-	-

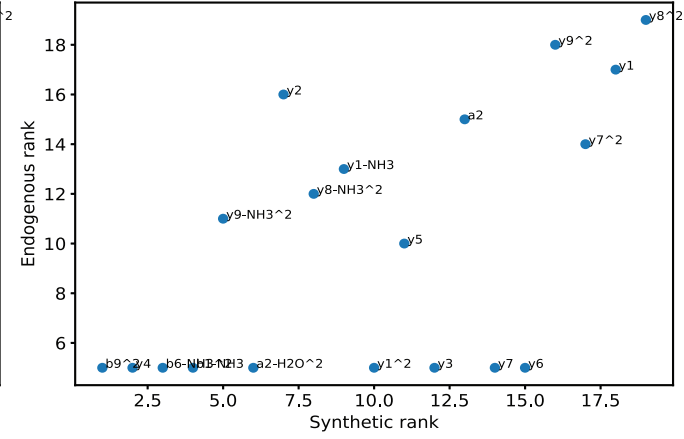
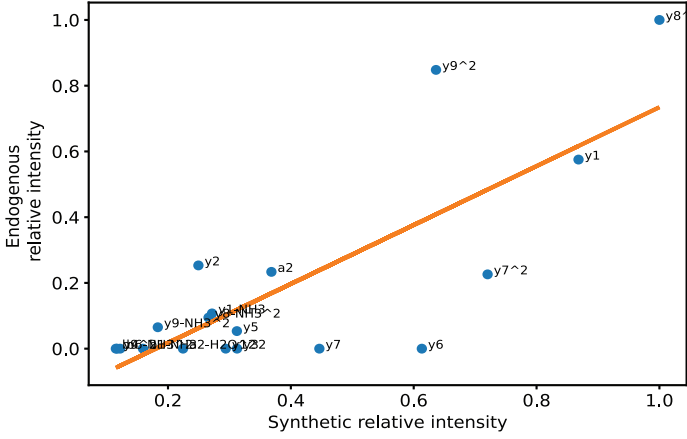


VLKKNQAGR / 3+

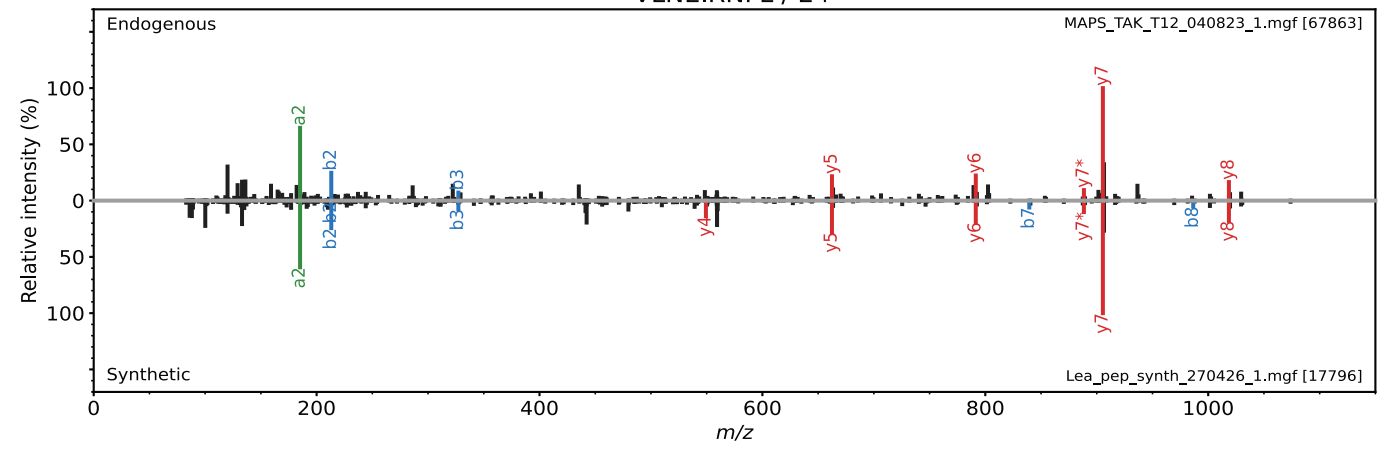


Spectrum	m/z	error (ppm)
Endogenous	376.2435	9.3
Synthetic	376.2403	0.8

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.78	0.51	0.91	7.2e-05
Spearman	0.58	0.17	0.82	9.2e-03
Spectral angle	0.60	-	-	-

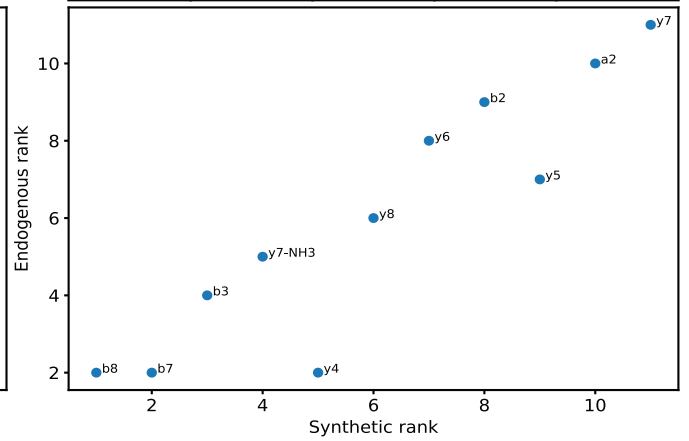
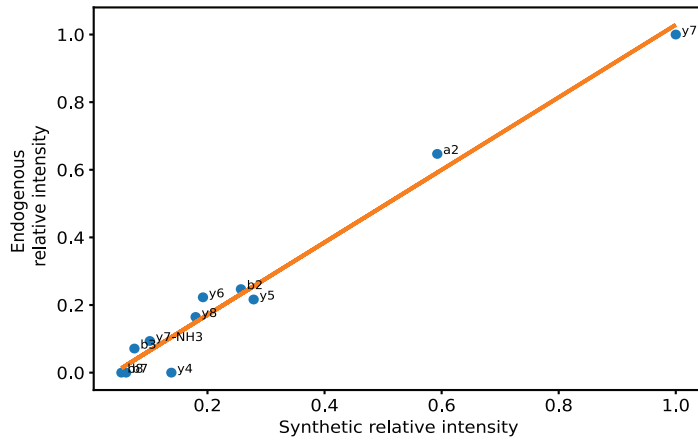


VLNEIRNFL / 2+

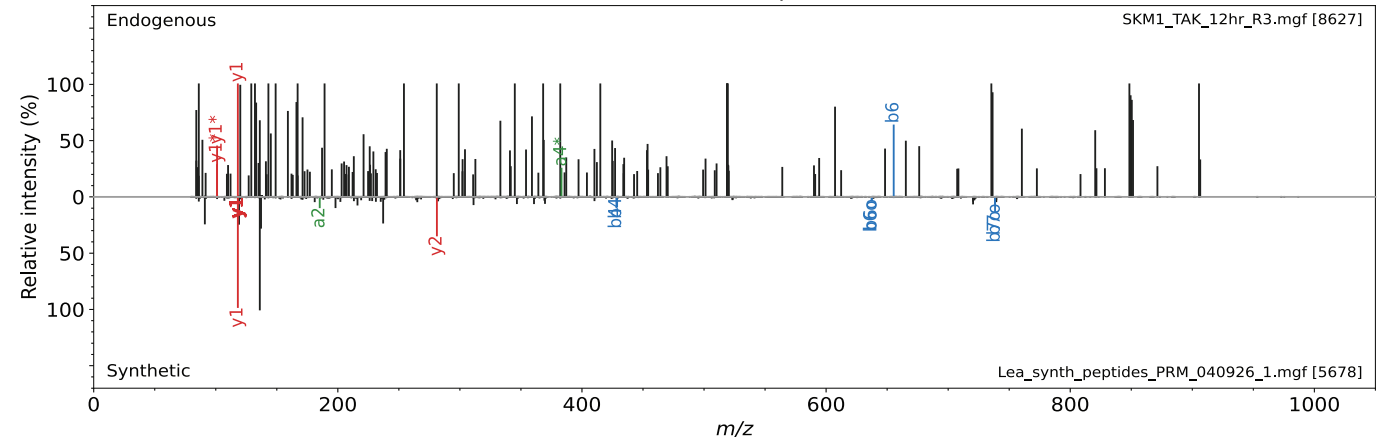


Spectrum	m/z	error (ppm)
Endogenous	559.3274	10.0
Synthetic	559.3216	-0.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.99	0.95	1.00	1.3e-08
Spearman	0.92	0.71	0.98	6.9e-05
Spectral angle	0.91	-	-	-

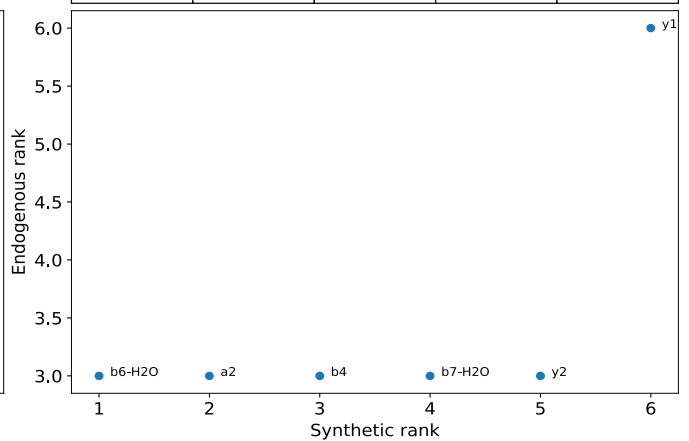
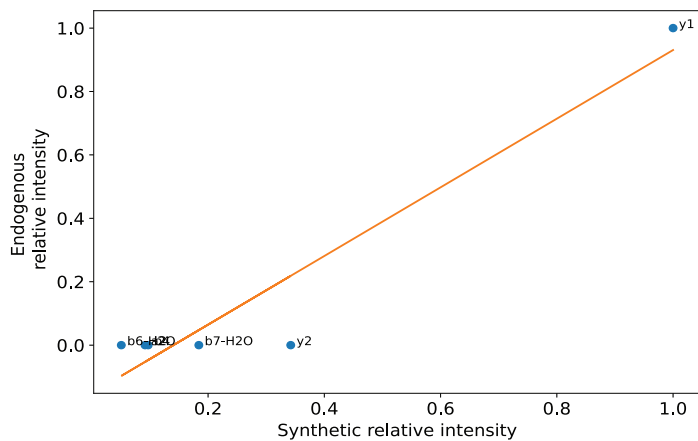


VLTNINTYV / 2+

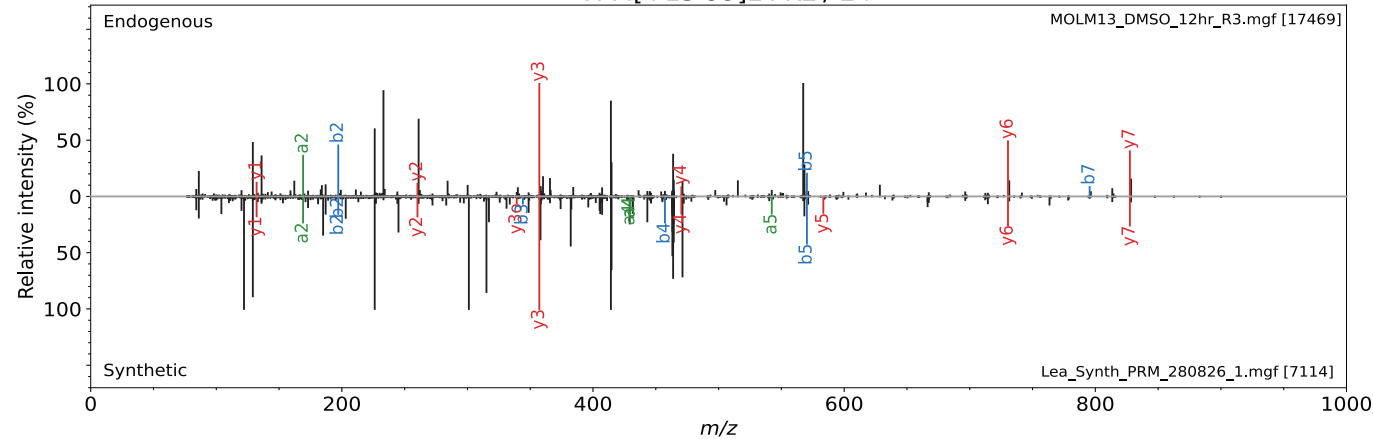


Spectrum	m/z	error (ppm)
Endogenous	518.7841	-6.2
Synthetic	518.7897	4.6

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.96	0.66	1.00	2.7e-03
Spearman	0.65	-0.33	0.96	1.6e-01
Spectral angle	0.75	-	-	-

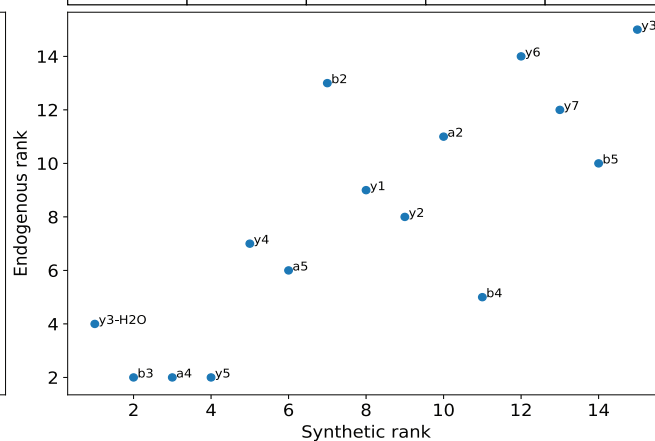
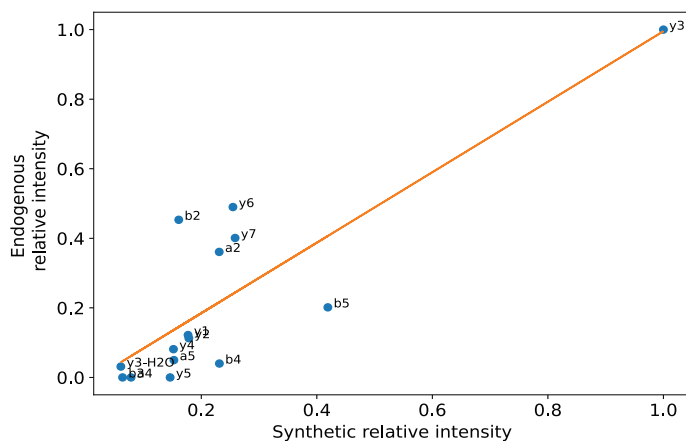


VPM[+15.99]LIPKL / 2+

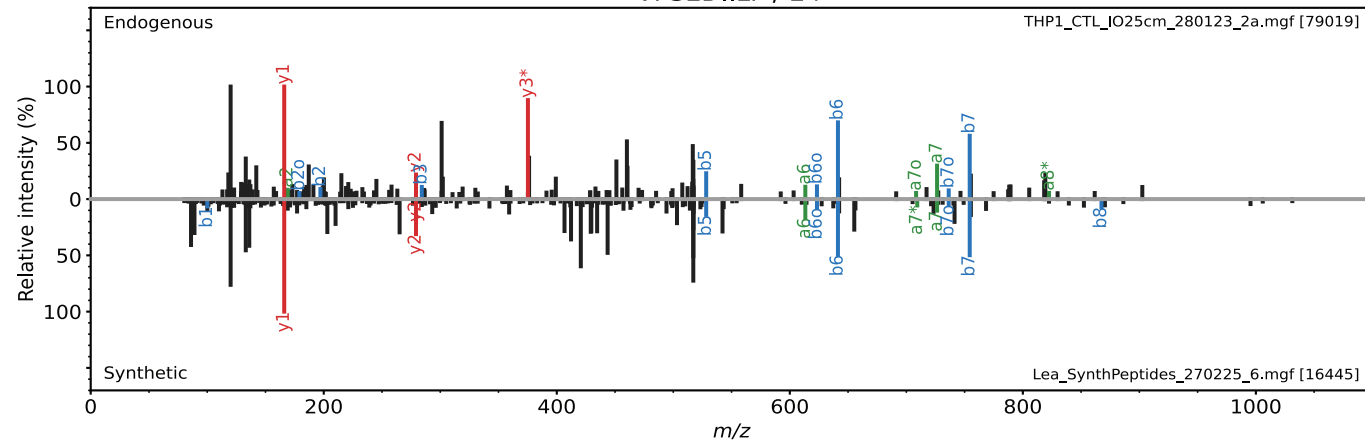


Spectrum	m/z	error (ppm)
Endogenous	463.7886	-4.7
Synthetic	463.7905	-0.6

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.84	0.58	0.95	8.6e-05
Spearman	0.80	0.48	0.93	3.9e-04
Spectral angle	0.73	-	-	-

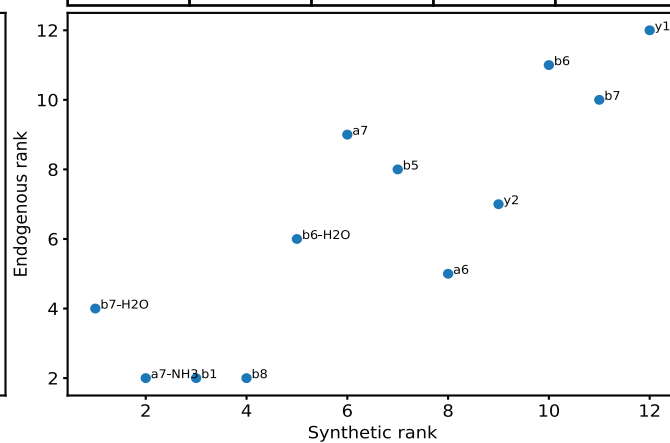
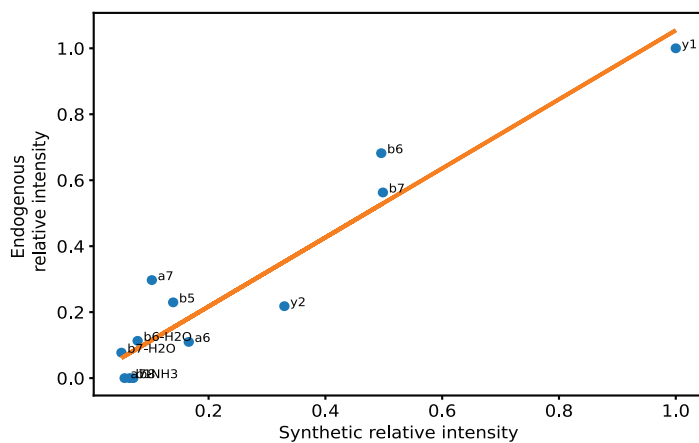


VPSEDIILF / 2+

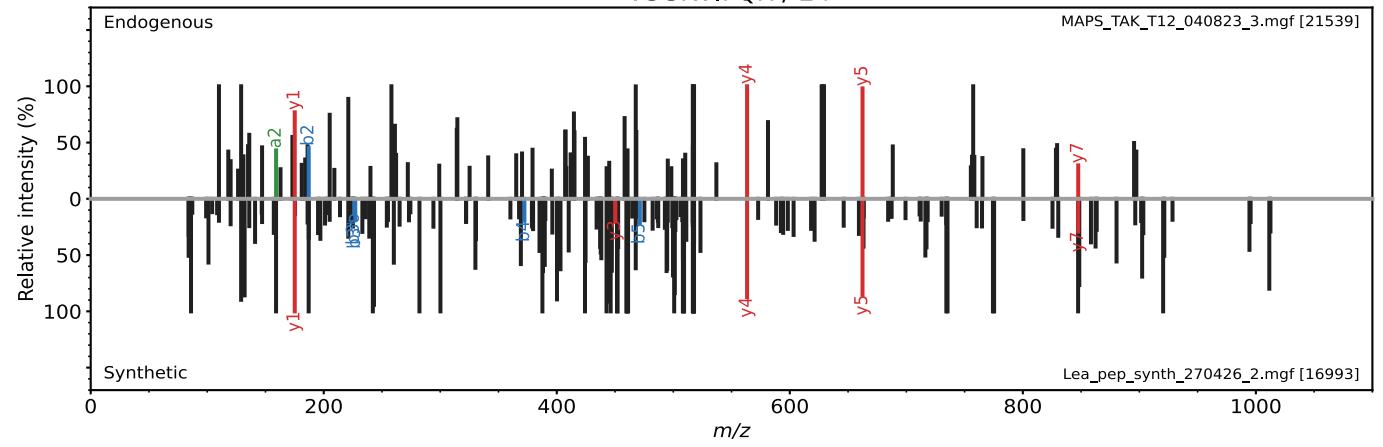


Spectrum	m/z	error (ppm)
Endogenous	516.7848	1.2
Synthetic	516.7853	2.1

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.95	0.83	0.99	2.4e-06
Spearman	0.86	0.56	0.96	3.4e-04
Spectral angle	0.85	-	-	-

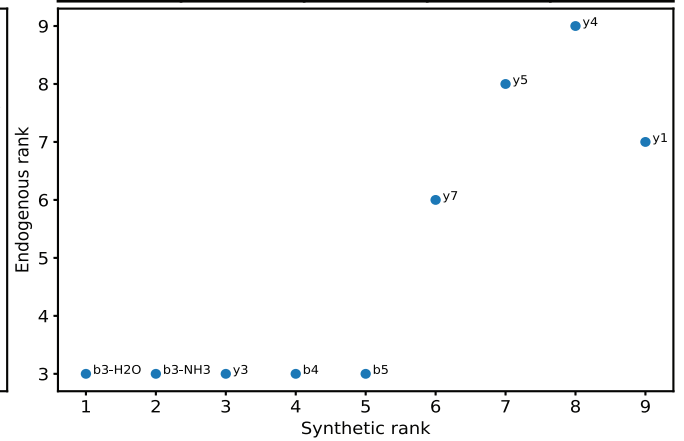
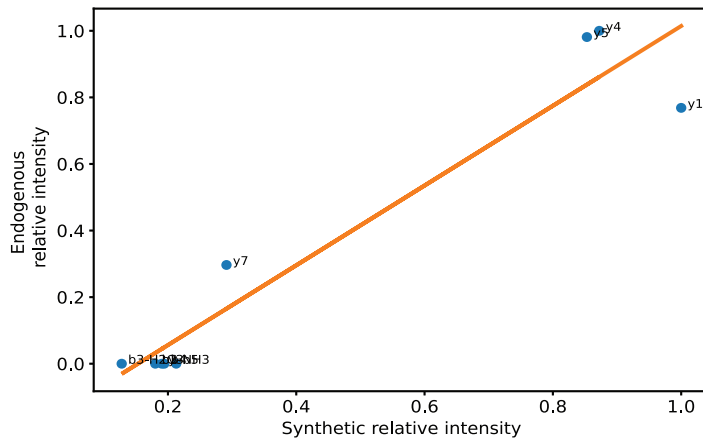


VSGKVFQR / 2+

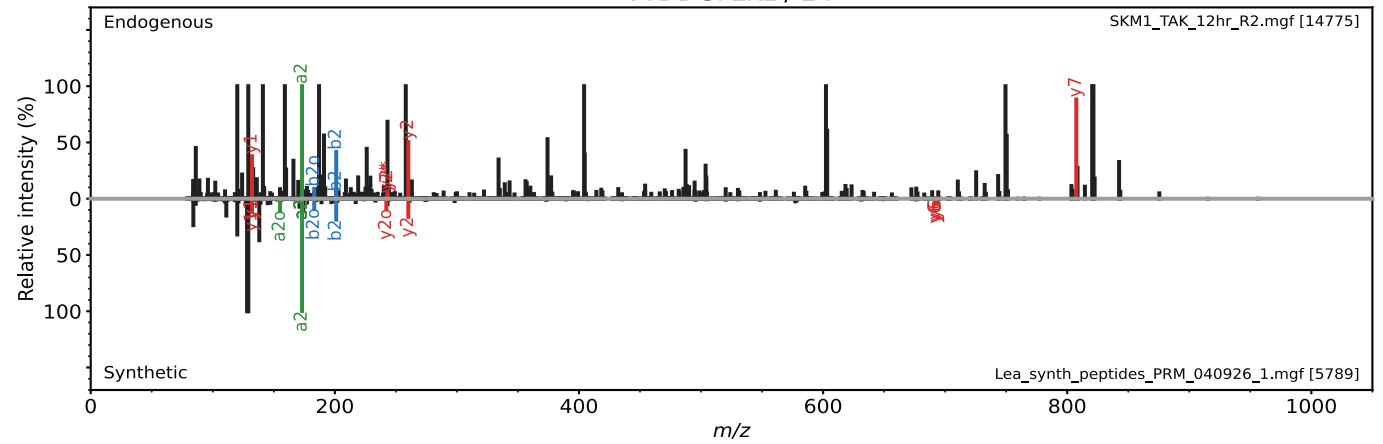


Spectrum	m/z	error (ppm)
Endogenous	517.3154	7.9
Synthetic	517.3107	-1.2

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.96	0.81	0.99	4.3e-05
Spearman	0.86	0.45	0.97	3.1e-03
Spectral angle	0.80	-	-	-

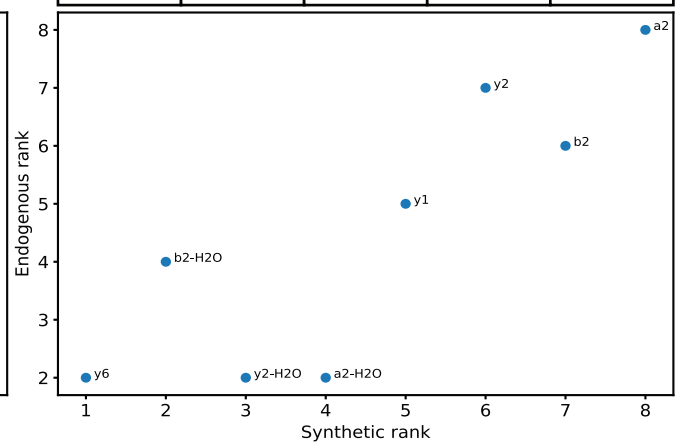
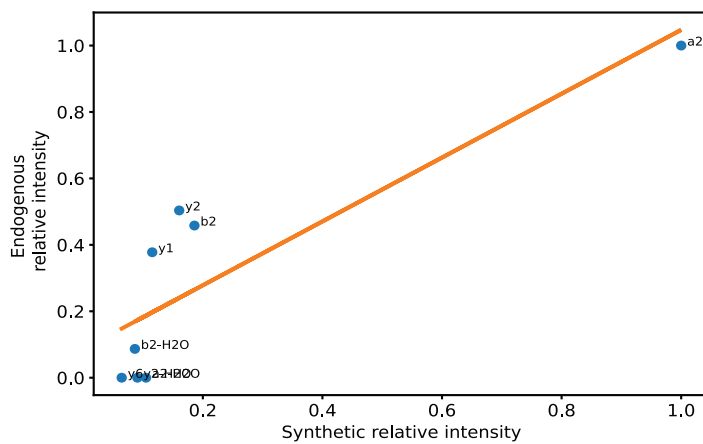


VTDDGFLKL / 2+

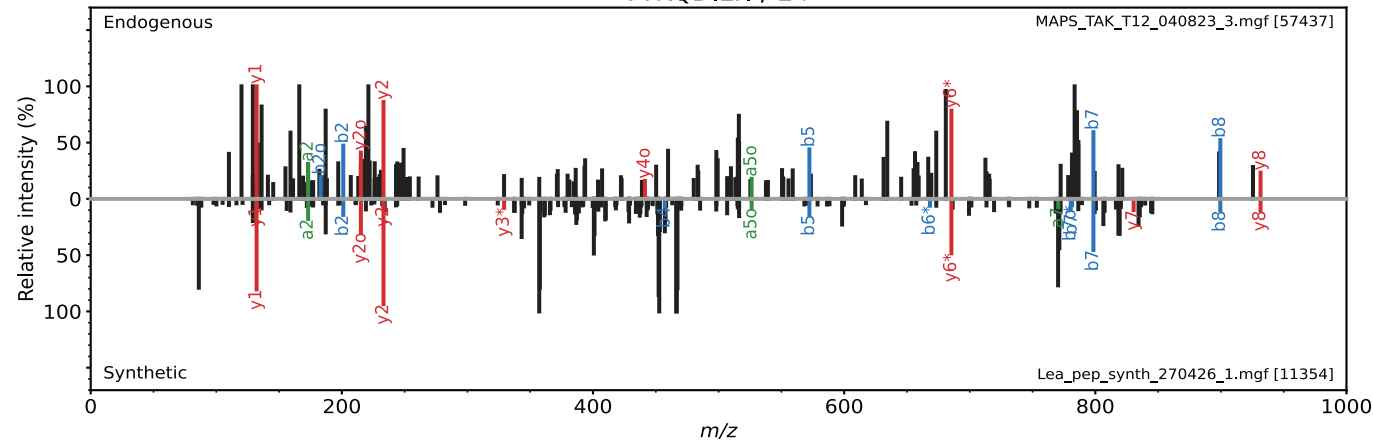


Spectrum	m/z	error (ppm)
Endogenous	504.2737	-0.6
Synthetic	504.2764	4.8

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.86	0.38	0.97	6.7e-03
Spearman	0.85	0.37	0.97	7.0e-03
Spectral angle	0.73	-	-	-

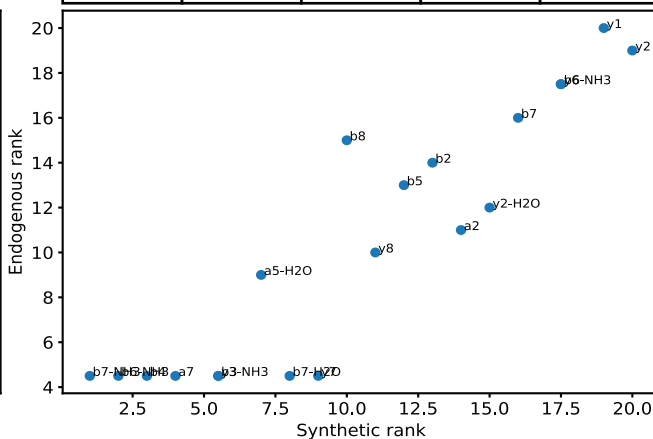
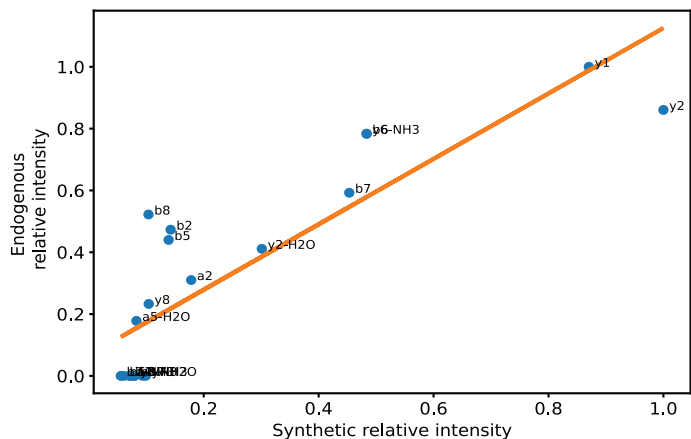


VTKQDILTI / 2+

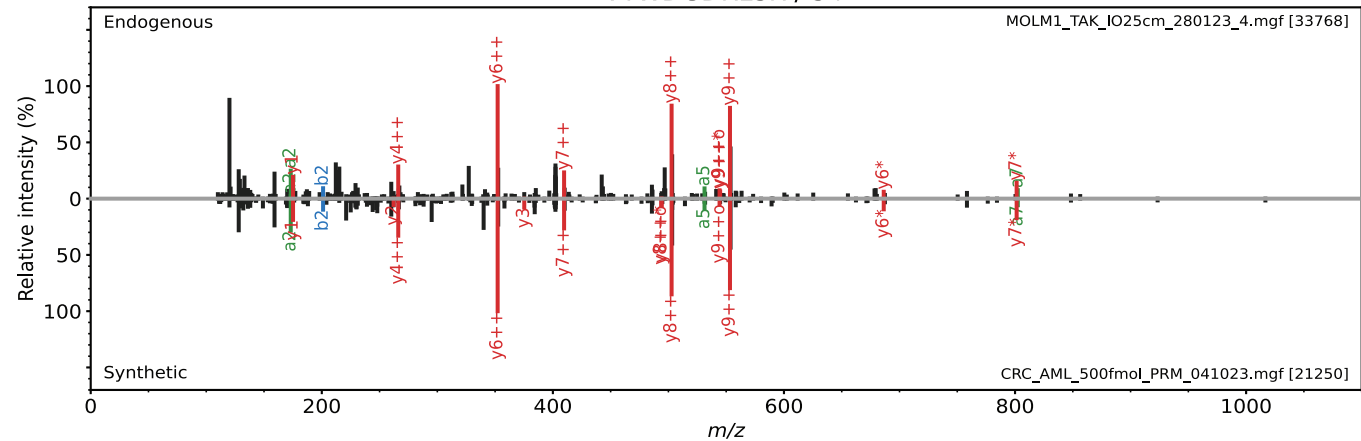


Spectrum	m/z	error (ppm)
Endogenous	515.8154	8.9
Synthetic	515.8110	0.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.86	0.67	0.94	1.3e-06
Spearman	0.92	0.80	0.97	1.3e-08
Spectral angle	0.75	-	-	-

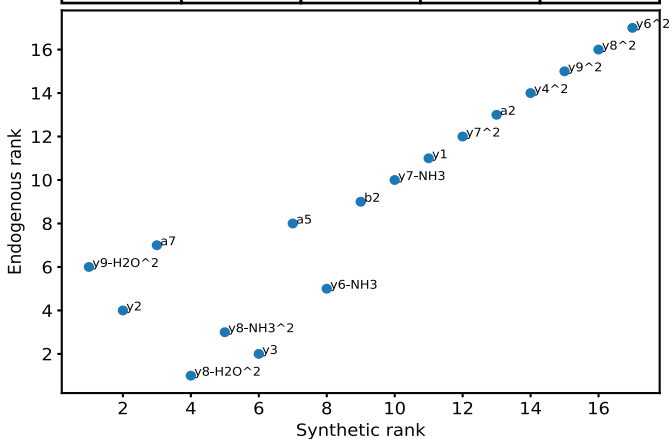
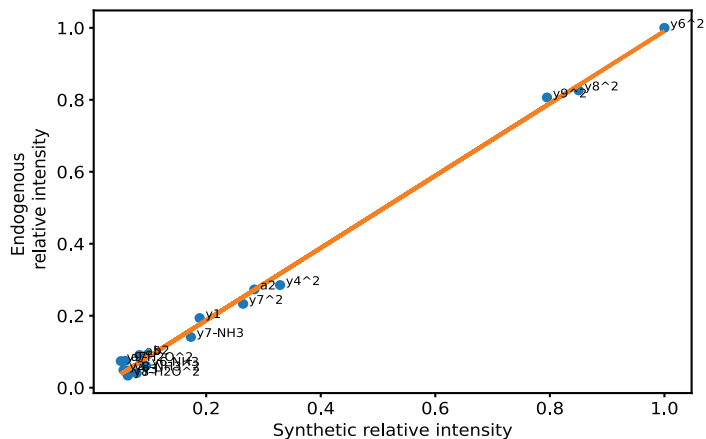


VTWDGDRLSR / 3+

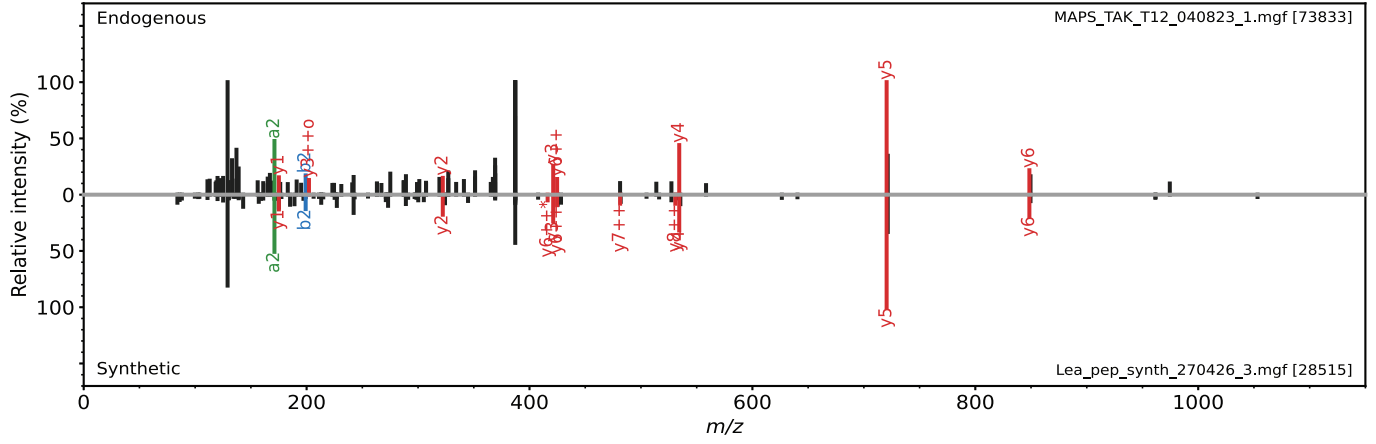


Spectrum	m/z	error (ppm)
Endogenous	402.2071	-0.1
Synthetic	402.2079	2.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	1.00	0.99	1.00	4.7e-19
Spearman	0.90	0.73	0.96	1.1e-06
Spectral angle	0.96	-	-	-

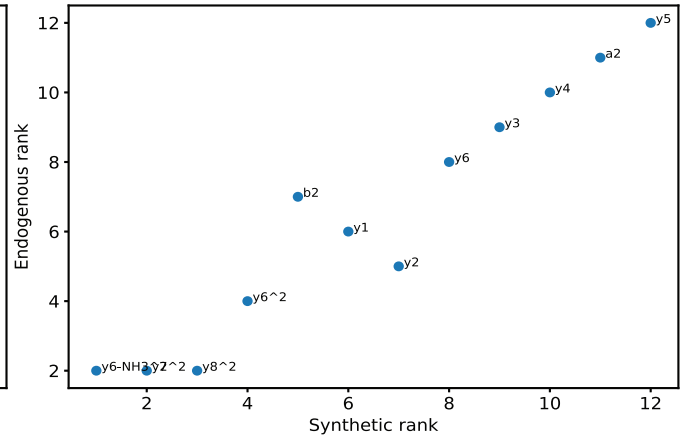
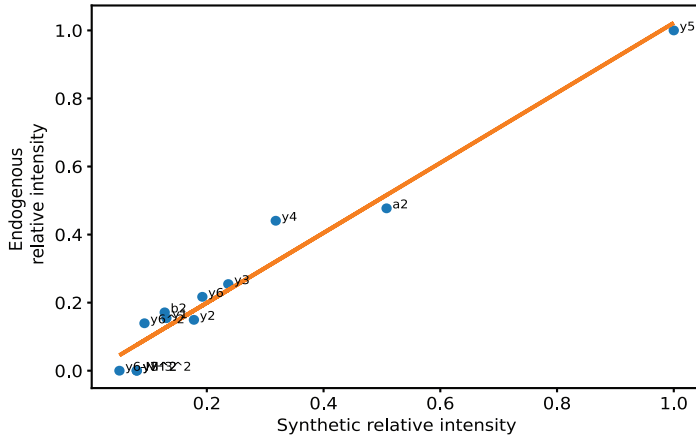


VVLKWLVR / 3+

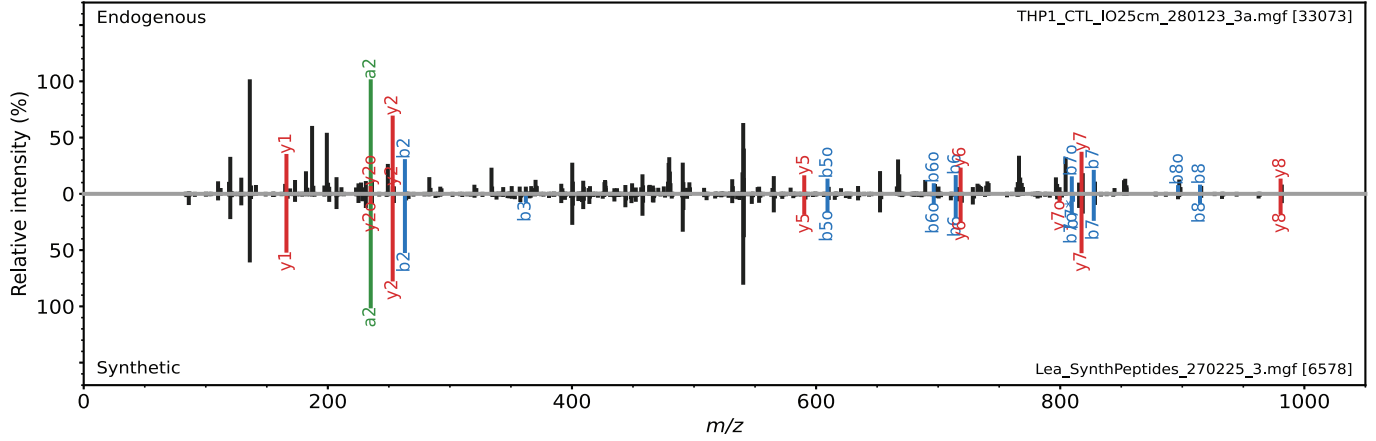


Spectrum	m/z	error (ppm)
Endogenous	387.2530	8.3
Synthetic	387.2492	-1.5

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.98	0.92	0.99	3.3e-08
Spearman	0.96	0.88	0.99	4.0e-07
Spectral angle	0.90	-	-	-

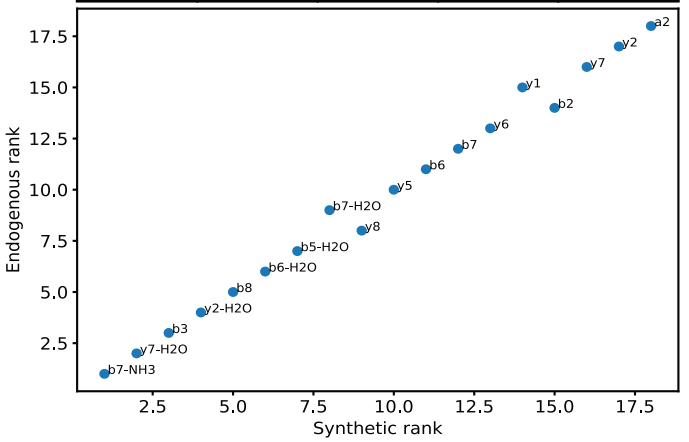
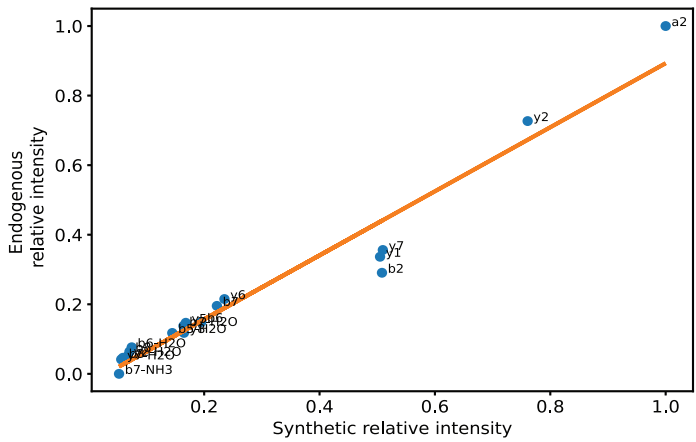


VYVKHSISF / 2+

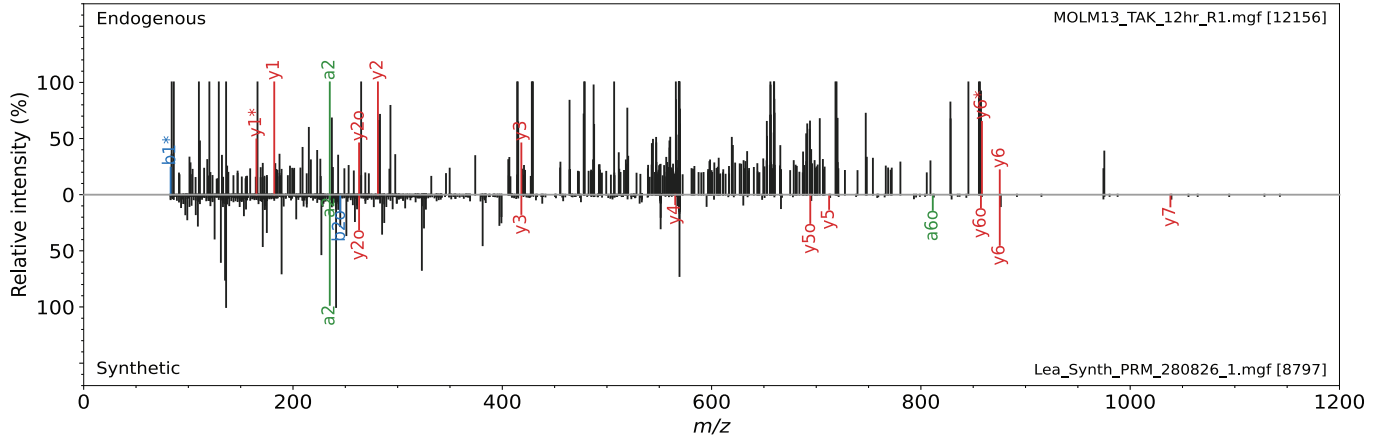


Spectrum	m/z	error (ppm)
Endogenous	540.2976	-0.4
Synthetic	540.2989	2.0

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.93	0.99	1.2e-11
Spearman	1.00	0.99	1.00	4.2e-18
Spectral angle	0.89	-	-	-

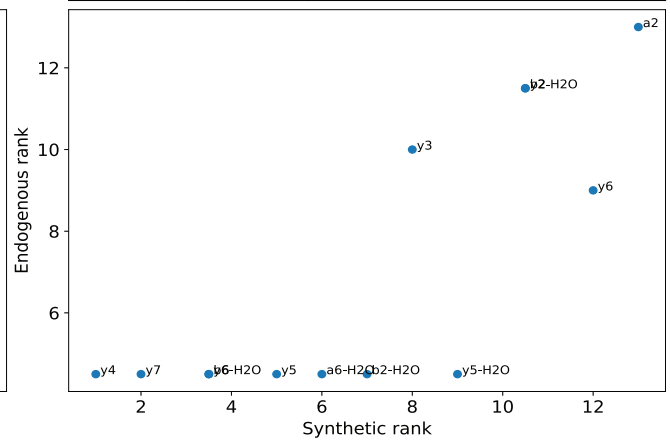
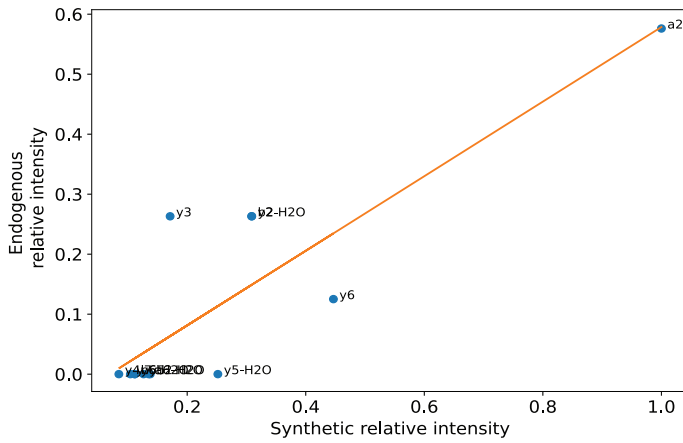


VYYFM[+15.99]HVY / 2+

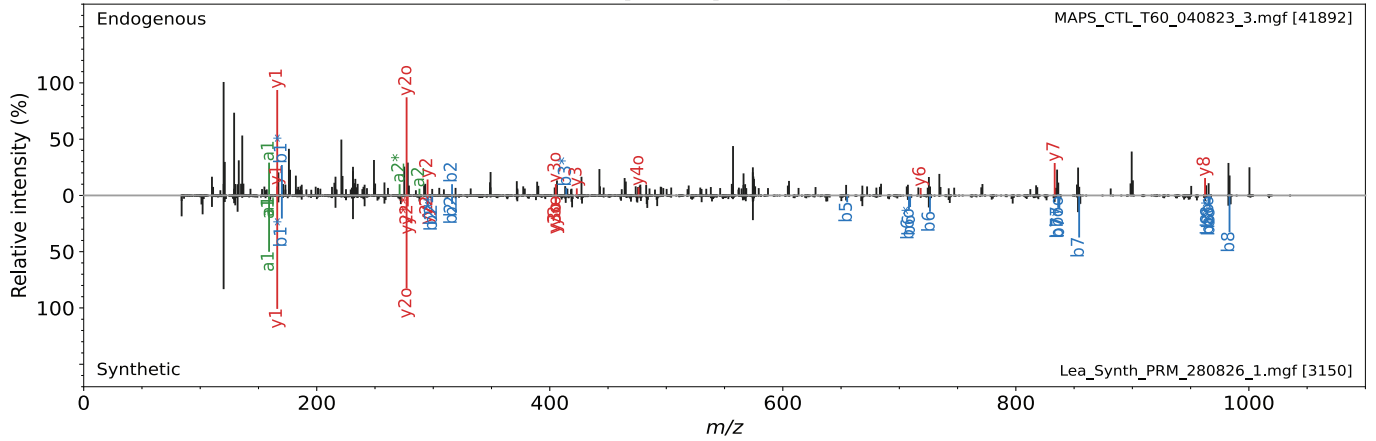


Spectrum	m/z	error (ppm)
Endogenous	569.2555	-3.2
Synthetic	569.2579	1.1

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.86	0.60	0.96	1.4e-04
Spearman	0.81	0.46	0.94	8.9e-04
Spectral angle	0.71	-	-	-

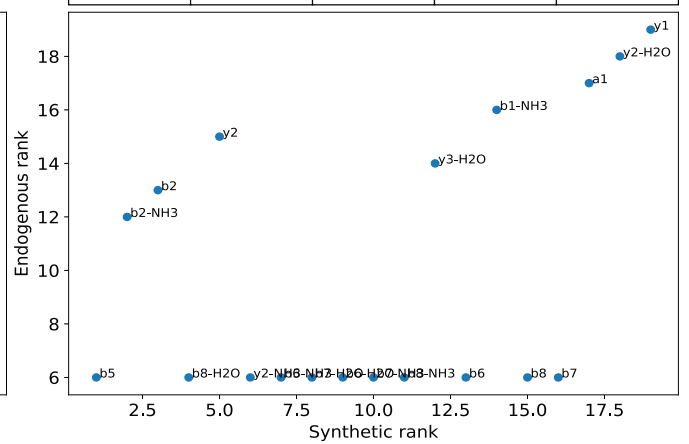
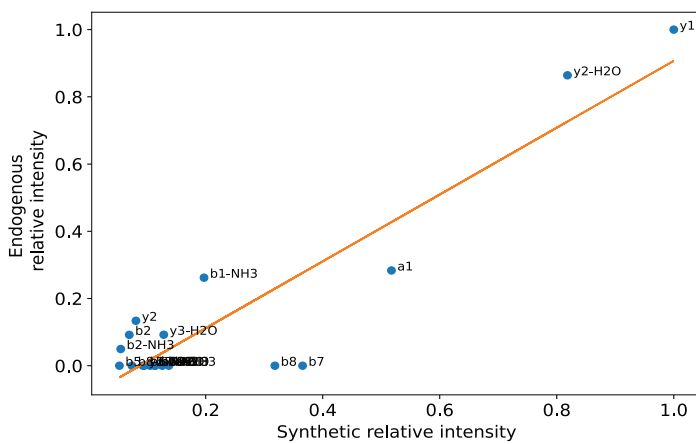


WEN[+0.98]HSAQEF / 2+

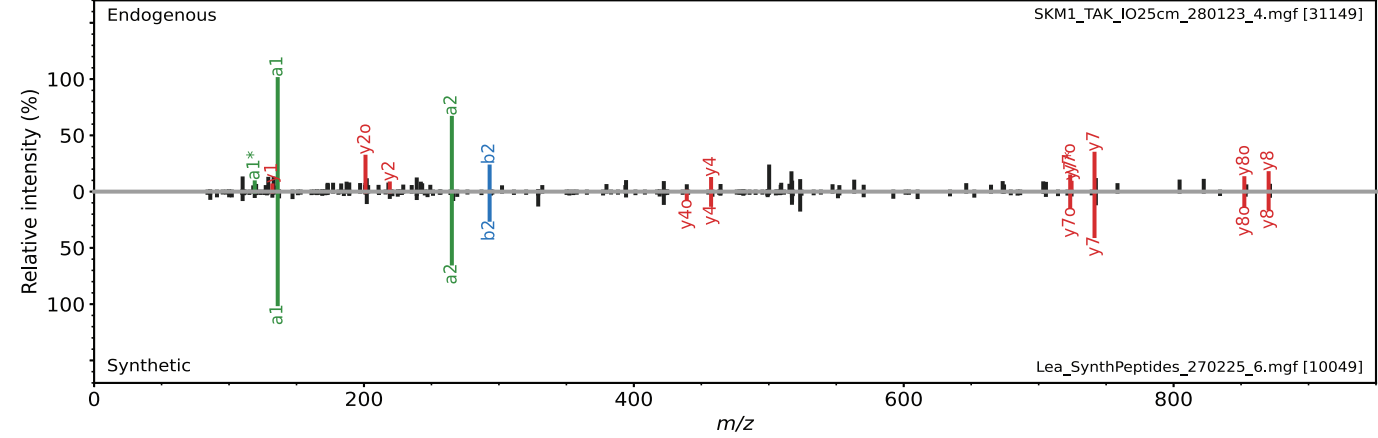


Spectrum	m/z	error (ppm)
Endogenous	574.7406	8.4
Synthetic	574.7347	-1.9

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.91	0.79	0.97	4.2e-08
Spearman	0.40	-0.07	0.72	9.1e-02
Spectral angle	0.73	-	-	-

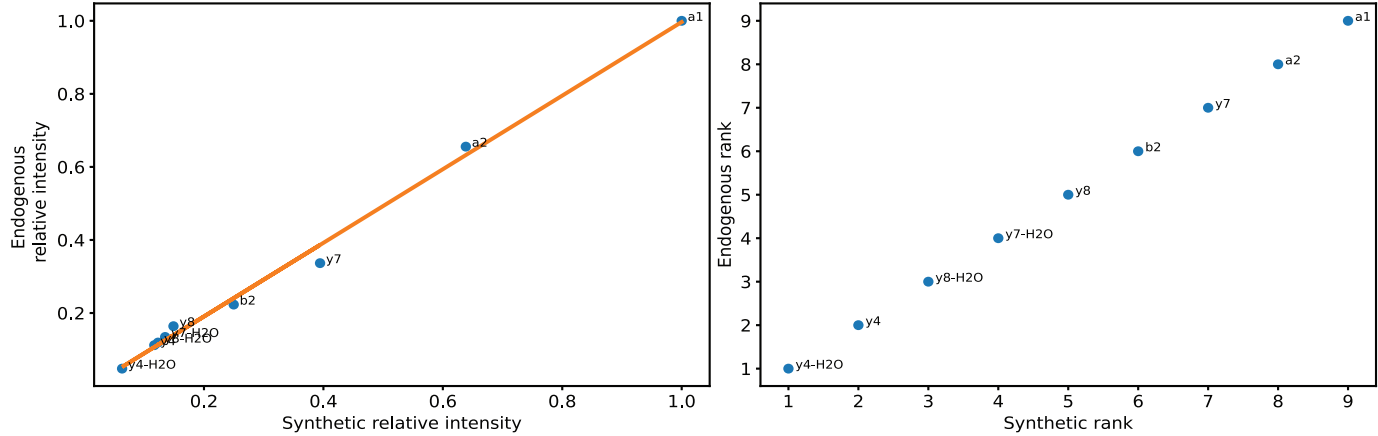


YEGNIHTSL / 2+

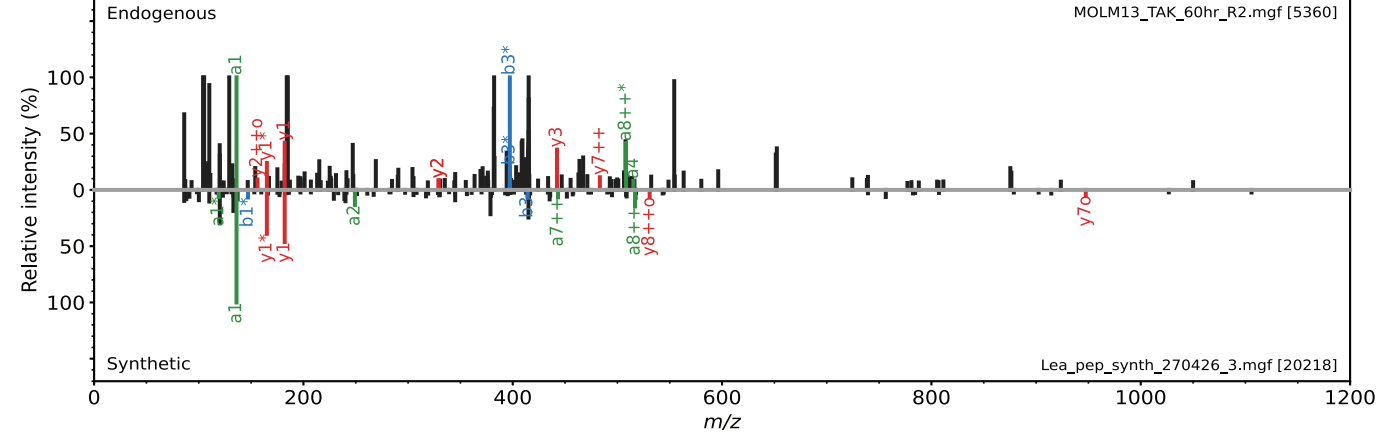


Spectrum	m/z	error (ppm)
Endogenous	517.2510	-0.1
Synthetic	517.2529	3.5

Metric	r / θ	95% CI min	95% CI max	p-value
Pearson	1.00	0.99	1.00	2.9e-09
Spearman	1.00	1.00	1.00	0.0e+00
Spectral angle	0.97	-	-	-

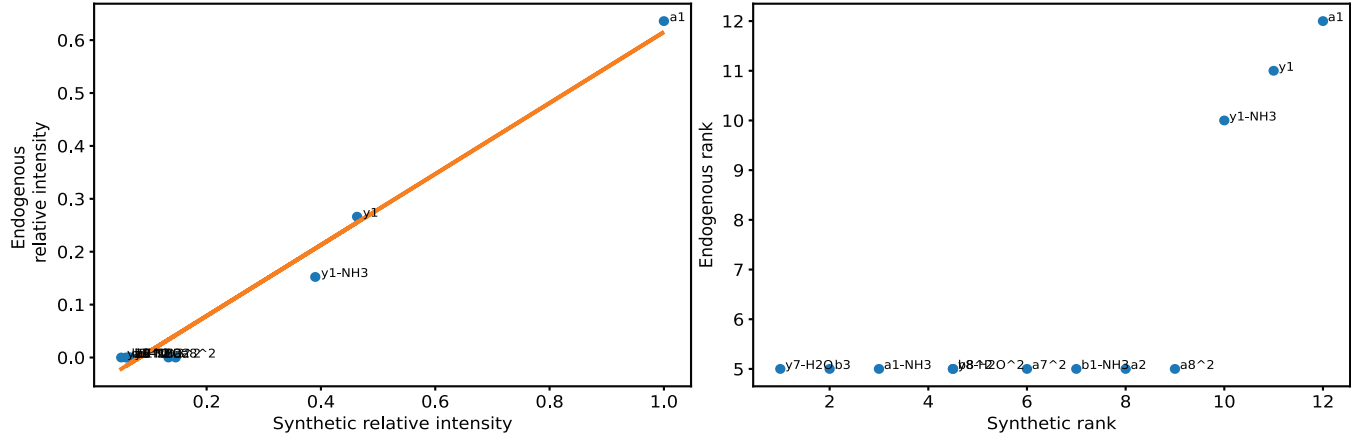


YLHEKELFY / 3+

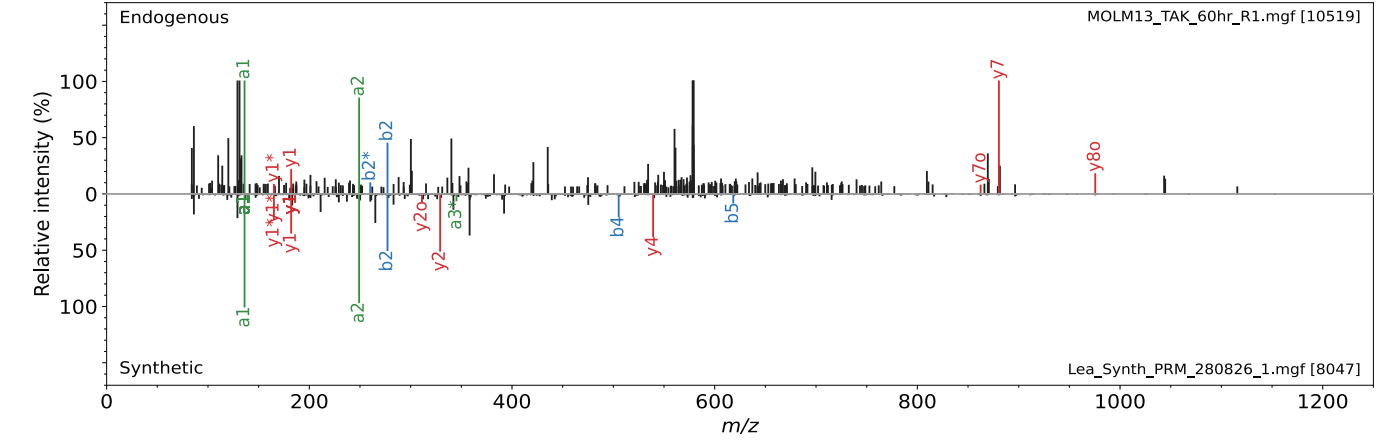


Spectrum	m/z	error (ppm)
Endogenous	414.5446	-0.7
Synthetic	414.5447	-0.5

Metric	r / θ	95% CI min	95% CI max	p-value
Pearson	0.99	0.96	1.00	6.8e-10
Spearman	0.76	0.34	0.93	3.9e-03
Spectral angle	0.84	-	-	-

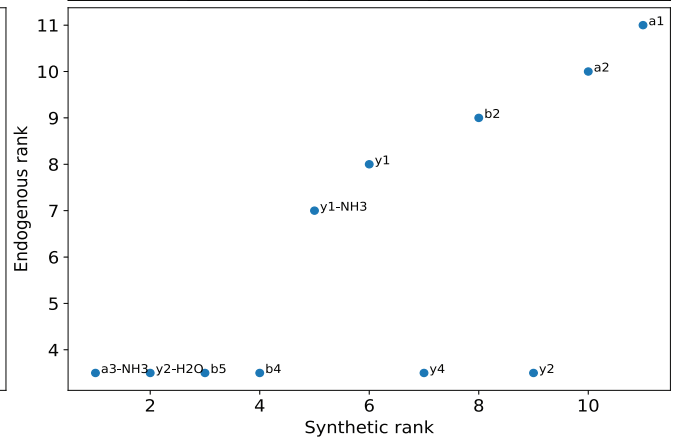
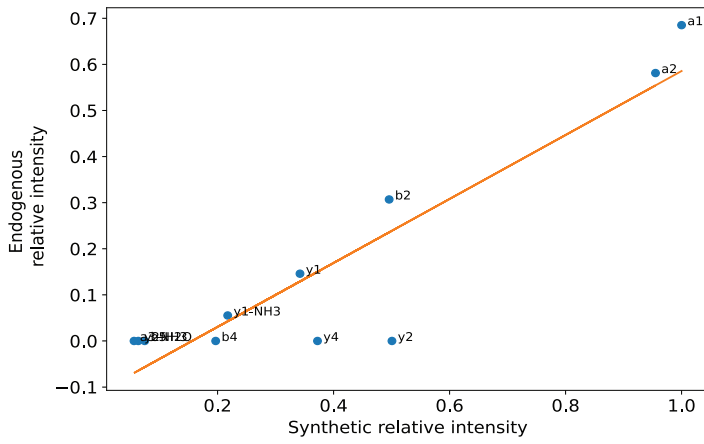


YLIDLPLM[+15.99]Y / 2+

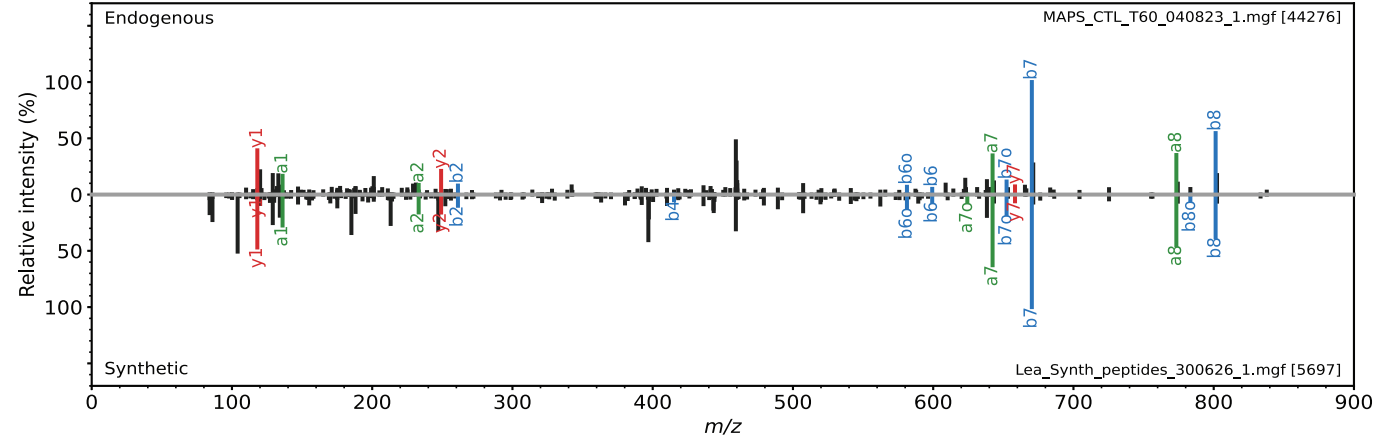


Spectrum	m/z	error (ppm)
Endogenous	578.8032	2.8
Synthetic	578.8011	-0.9

Metric	r / θ	95% CI min	95% CI max	p-value
Pearson	0.91	0.69	0.98	9.6e-05
Spearman	0.70	0.18	0.92	1.6e-02
Spectral angle	0.73	-	-	-

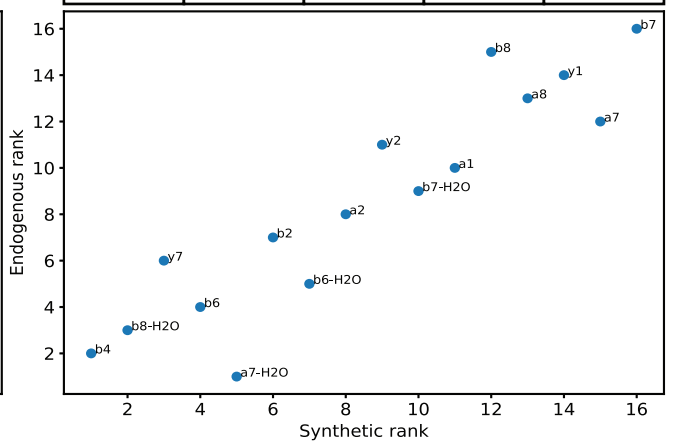
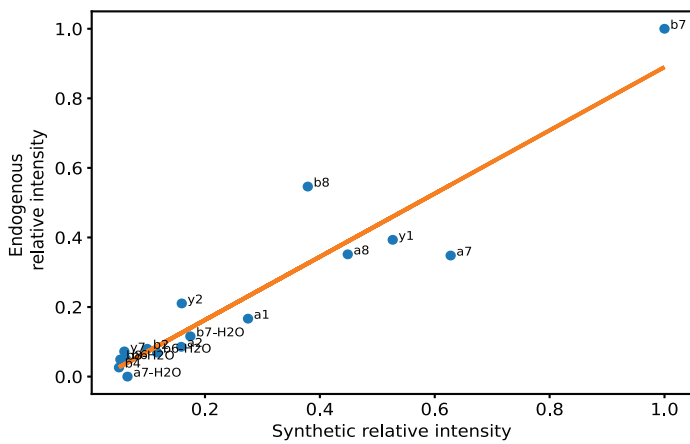


YPPGPSAMV / 2+

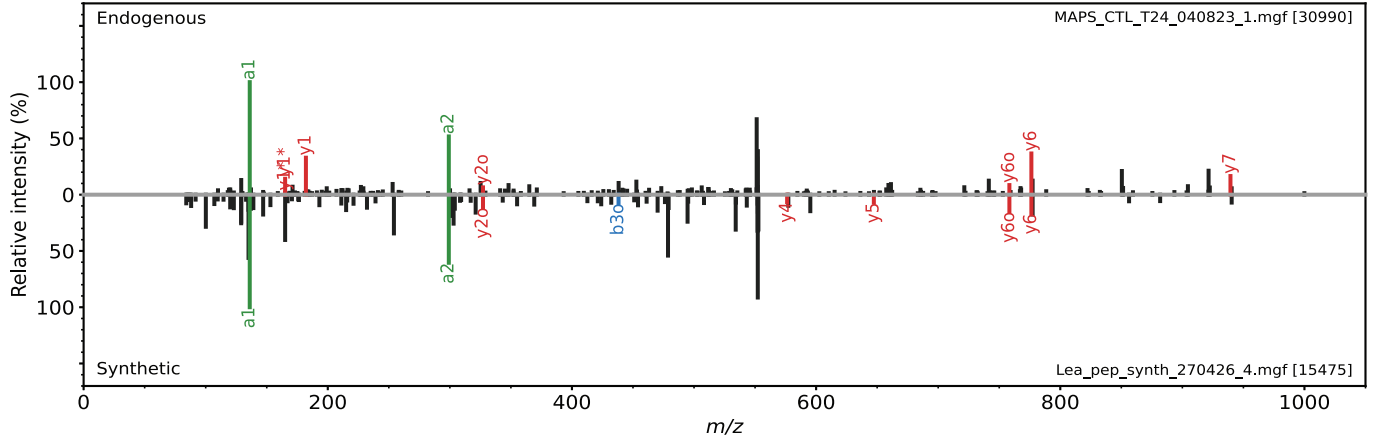


Spectrum	m/z	error (ppm)
Endogenous	459.7272	8.9
Synthetic	459.7234	0.7

Metric	r / θ	95% CI min	95% CI max	p-value
Pearson	0.94	0.82	0.98	9.6e-08
Spearman	0.92	0.77	0.97	5.5e-07
Spectral angle	0.83	-	-	-

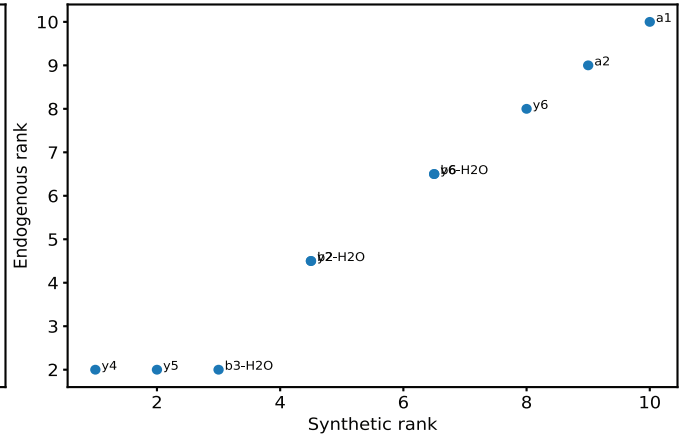
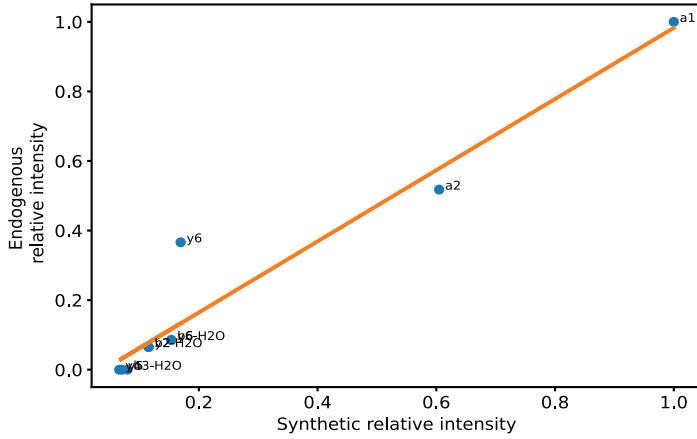


YYEACKYY / 2+



Spectrum	m/z	error (ppm)
Endogenous	551.7333	4.0
Synthetic	551.7303	-1.4

Metric	r/θ	95% CI min	95% CI max	p-value
Pearson	0.97	0.86	0.99	5.9e-06
Spearman	0.99	0.95	1.00	1.0e-07
Spectral angle	0.85	-	-	-



YYEVLGVQR / 2+

