Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Traceless solid-phase synthesis and *β*-turn propensity of thiazole-based peptidomimetics

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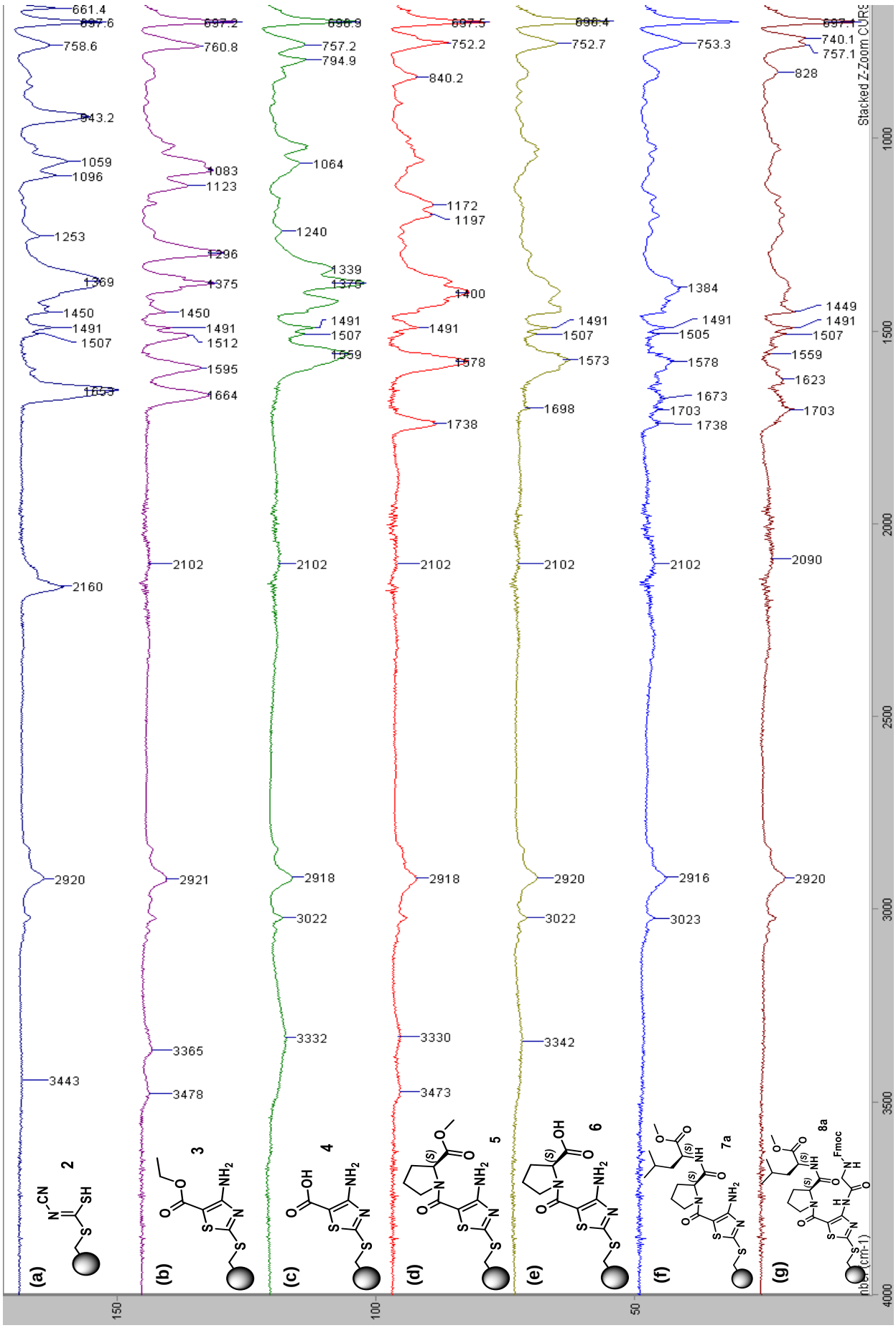
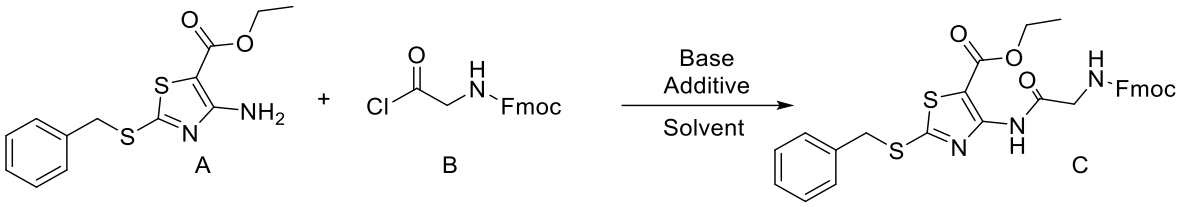
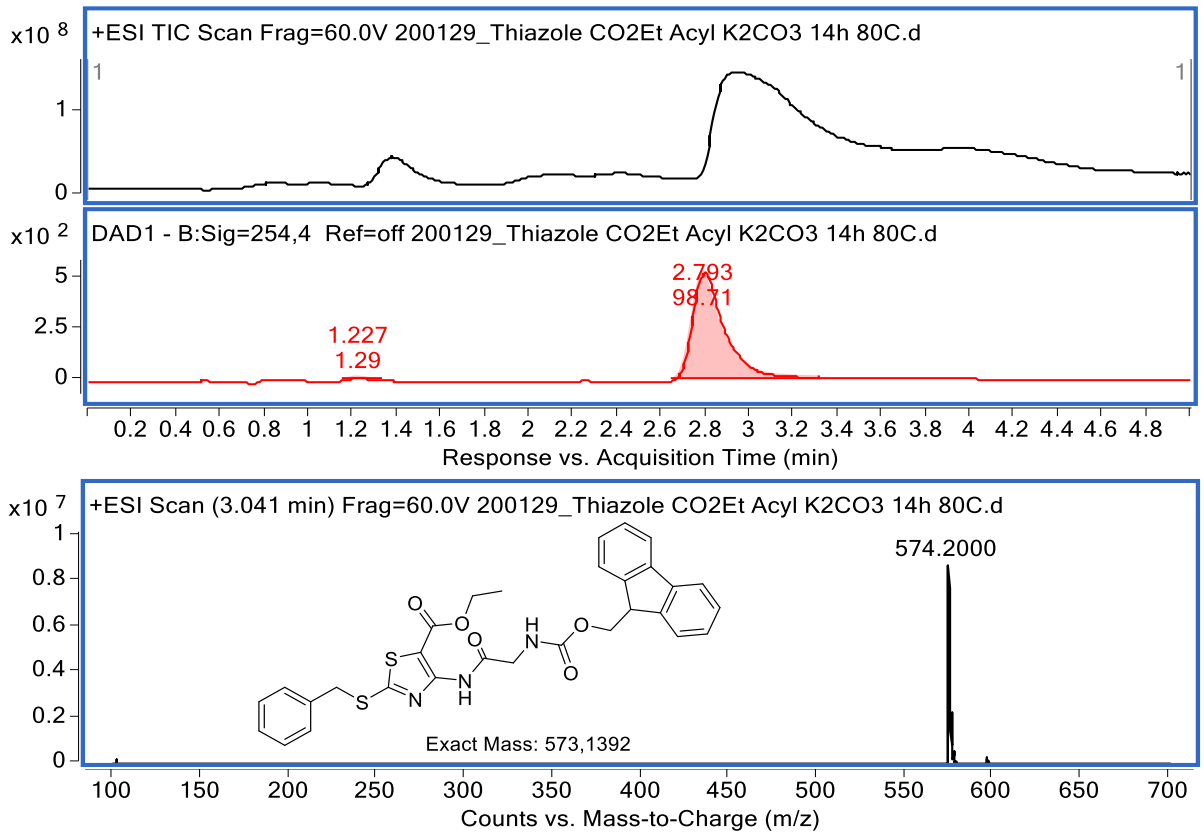


Fig. S1. Representative ATR-FTIR spectrum of the corresponding resins

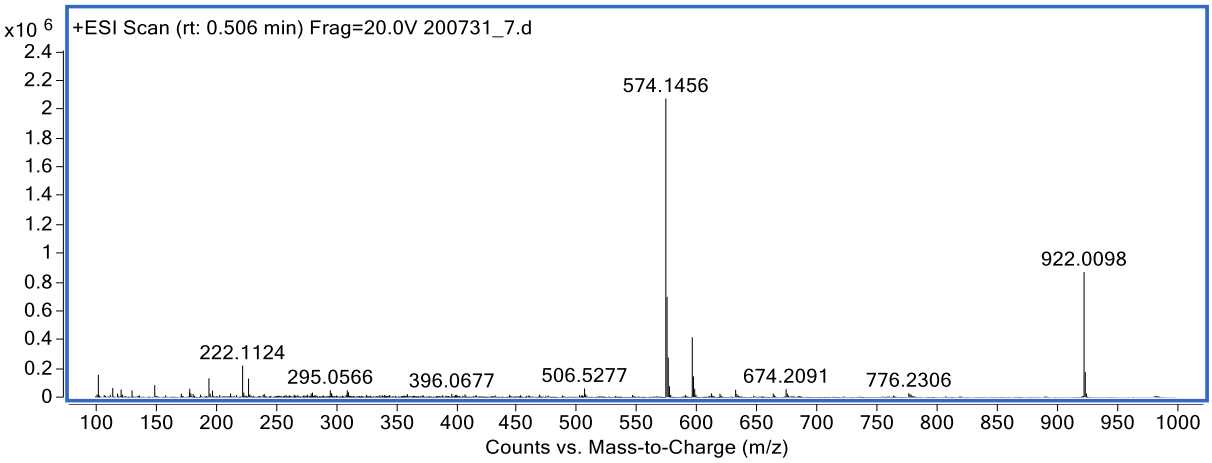
Table S1. Acylation Reaction Conditions Optimization in Solution Phase



No	Base	Additive	Solvent	Temp	Time	Yield	Remark
1	NaH 2.0 eq	-	DMF	RT	17 h	-	No Product
2	**K_2CO_3 2.0 eq**	**-**	**1,4-Dioxane**	**RT → 50 ℃**	**28 h**	**36%**	**LC/MS Checked**
3	*t*-BuOK 2.0 eq	-	DMF	RT	24 h	-	No Product
4	TEA 2.0 eq	-	DCM	RT	24 h	No Reaction	-
5	DIPEA 2.0 eq	-	DCM	RT	24 h	No Reaction	-
6	Pyridine 2.0 eq	-	DCM	RT → 50 ℃	24 h	Traces	LC/MS Crude
7	K_2CO_3 4.0 eq	-	1,4 - Dioxane	60 ℃ → 100 ℃	29 h	-	Decomposition at 100 ℃
8	K_2CO_3 2.0 eq	DMAP Cat. Amount	1,4-Dioxane	60 ℃	23 h	No Reaction	-
9	K_2CO_3 2.0 eq	-	DMF	RT	1 h	-	No Product
10	**K_2CO_3 2.0 eq**	**-**	**1,4-Dioxane**	**80 ℃**	**14 h**	**78%**	**LC/MS Purity 98.7%**


+ESI TIC Scan Frag=60.0V 200129_Thiazole CO2Et Acyl K2CO3 14h 80C.d
DAD1 - B:Sig=254,4 Ref=off 200129_Thiazole CO2Et Acyl K2CO3 14h 80C.d
2.793
98.71
1.227
1.29
Response vs. Acquisition Time (min)
+ESI Scan (3.041 min) Frag=60.0V 200129_Thiazole CO2Et Acyl K2CO3 14h 80C.d
574.2000
Exact Mass: 573,1392
Counts vs. Mass-to-Charge (m/z)

LC/MS – C


+ESI Scan (rt: 0.506 min) Frag=20.0V 200731_7.d
574.1456
922.0098
222.1124
295.0566
396.0677
506.5277
674.2091
776.2306
Counts vs. Mass-to-Charge (m/z)

HR/MS – C

Table S2. Calculated dihedral angles for *β*-turn mimetics **12**

No	*φ(i+1)*	*ψ(i+1)*	*φ(i+2)*	*ψ(i+2)*
12a	-62,85	95,89	-73	116,65
12b	-63,87	84,93	-84,21	103,72
12c	-75,54	41,79	-73,74	-9,69
12d	-53,09	-138,81	36,67	114,21
12e	-74,47	-123,06	-100,22	124,89

Table S3. Calculated physicochemical properties of **12**.

No	Molecular Weight	AlogP	pKa	Number of HBA	Number of HBD	Number of Rotatable Bonds	Molecular Polar Surface Area	Molecular Surface Area
12a	701,833	2,257	4.28 8.91	10	6	17	236,39	740,7
12b	774,886	2,874	4.28 8.91	10	7	17	252,18	786,17
12c	785,865	2,663	4.28 8.91 9.83	11	7	17	256,62	782,9
12d	769,866	2,905	4.28 9.83	10	6	17	236,39	771,57
12e	808,902	3,203	1.65 4.28 9.83	10	7	17	252,18	801

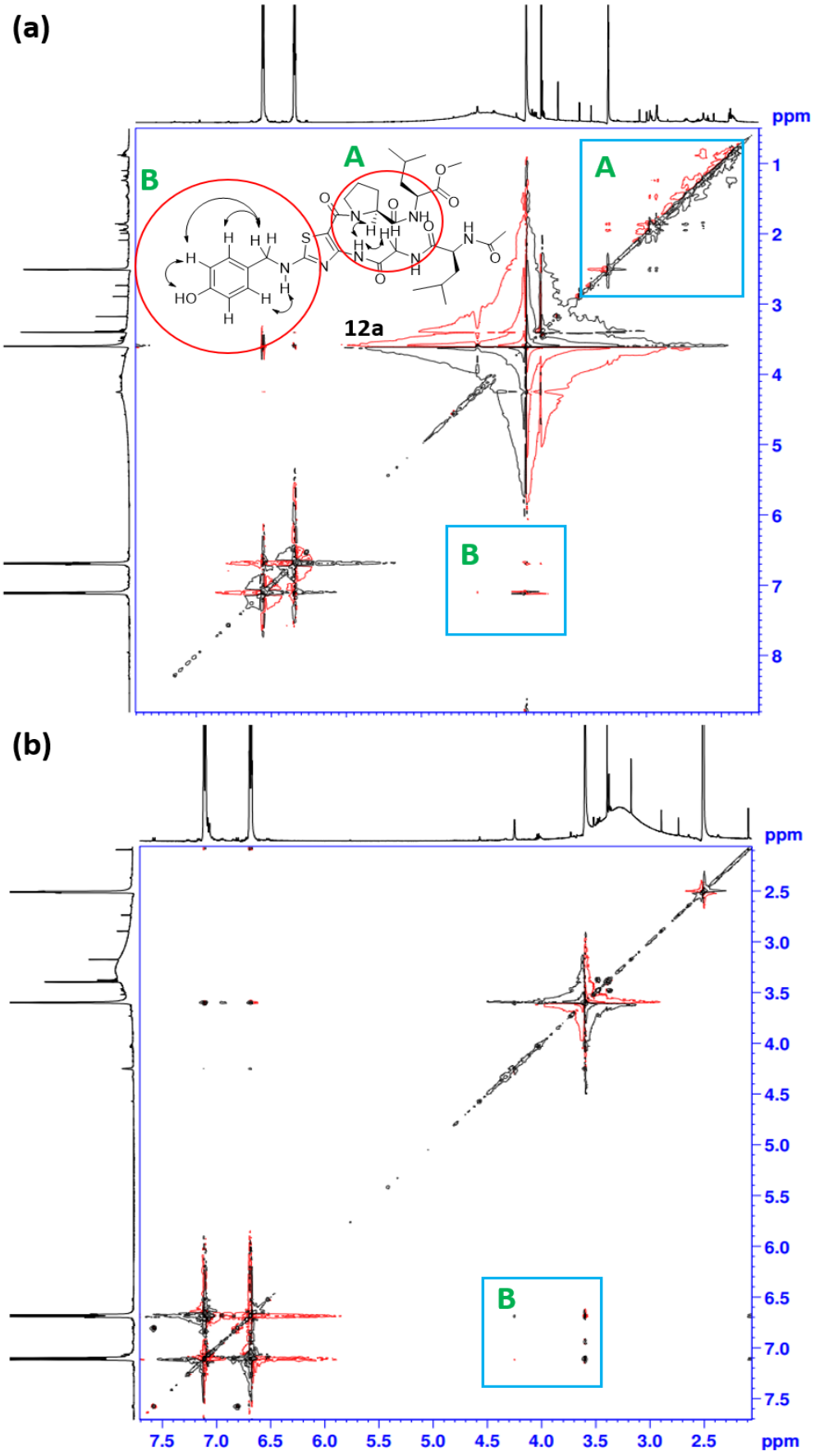
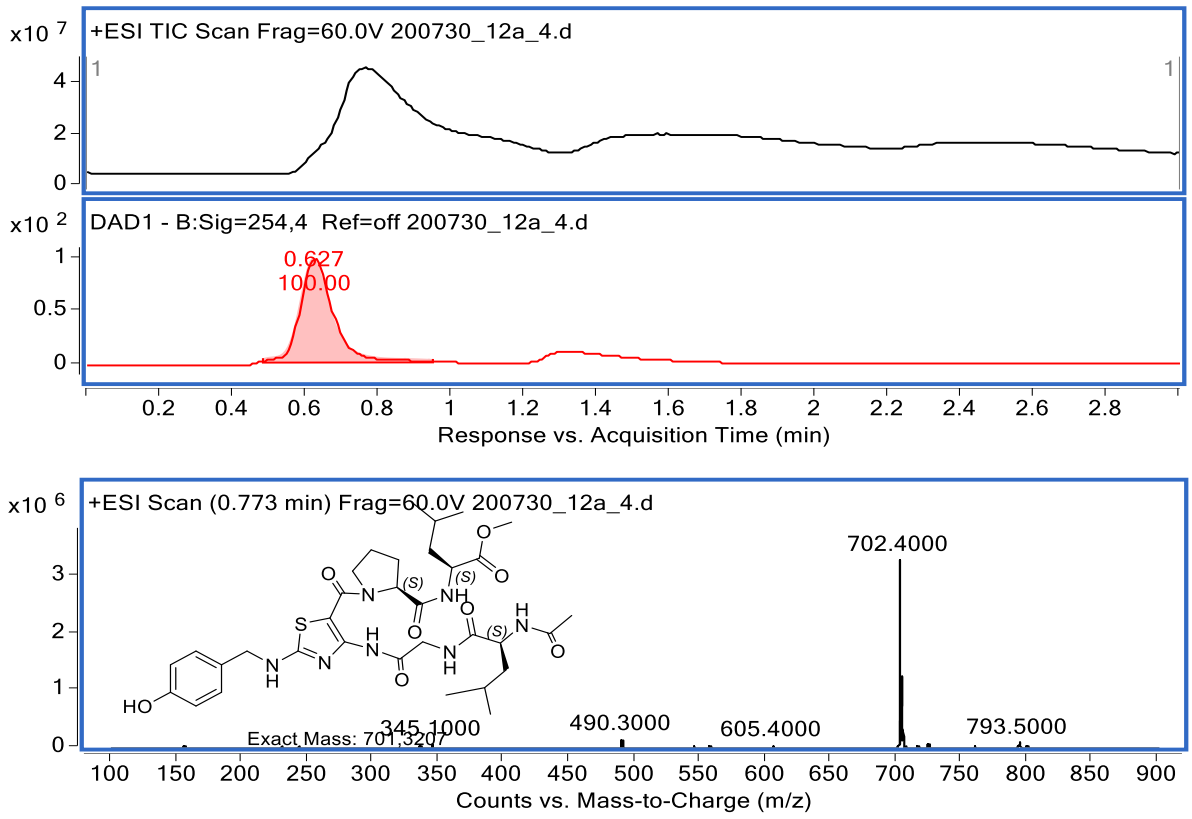
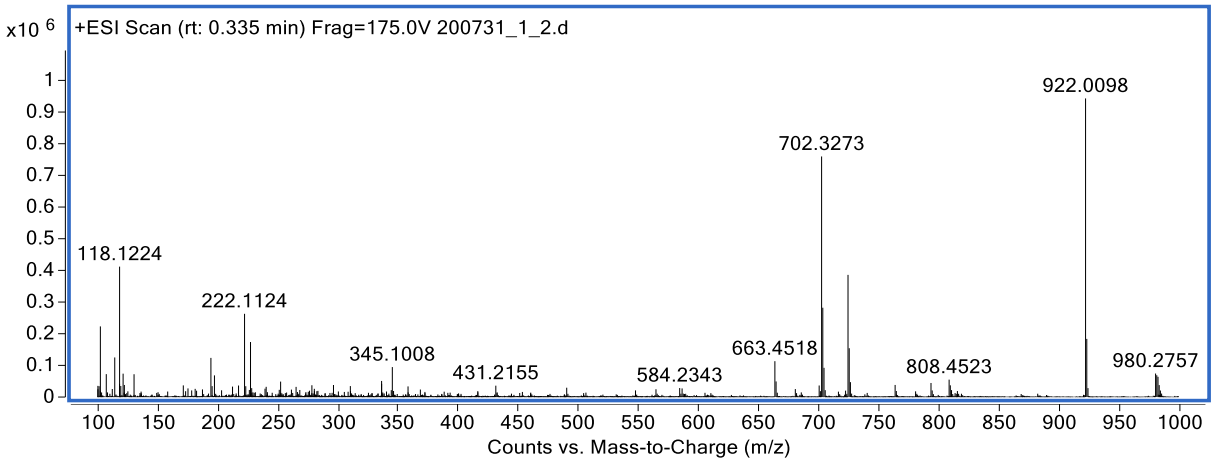


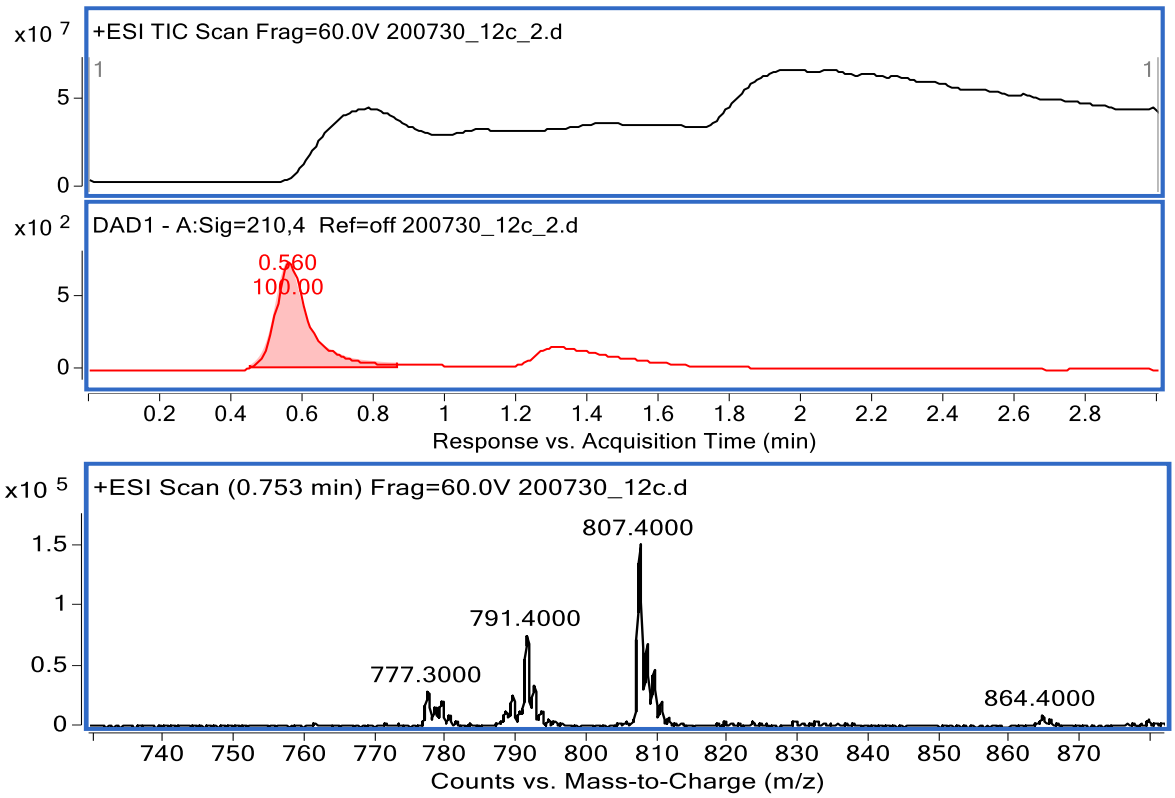
Fig. S2. 2D NMR studies of compound **12a** in DMSO-d6: (a) ^{1}H-^{1}H ROESY with NOE cross peaks at sections **A** (for Gly-Pro) and **B** (for 4-OH-Bn-NH); (b) ^{1}H-^{1}H TOCSY cross peaks for 4-OH-Bn-NH (section **B**).



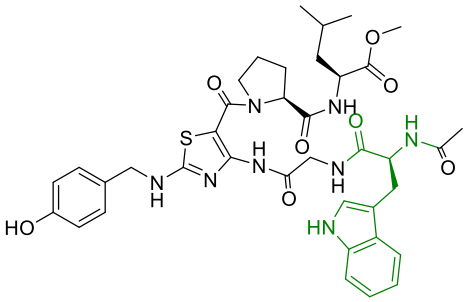
LC/MS – 12a



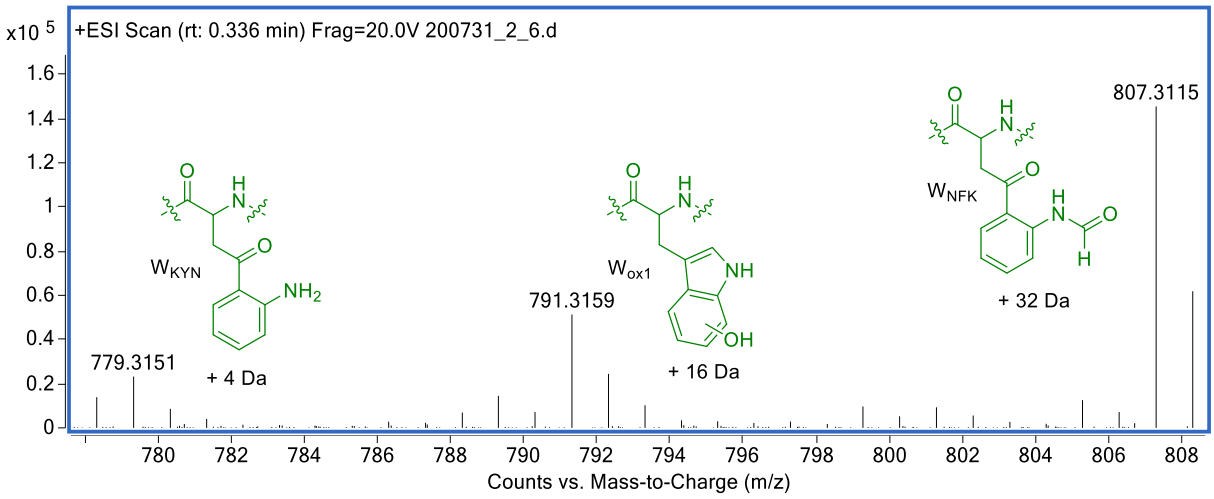
HR/MS – 12a



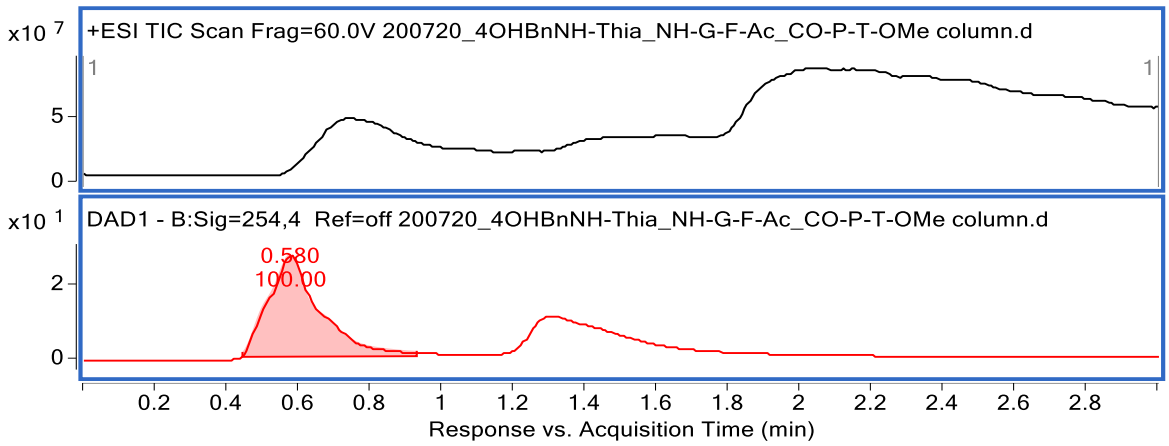
LC/MS – 12b

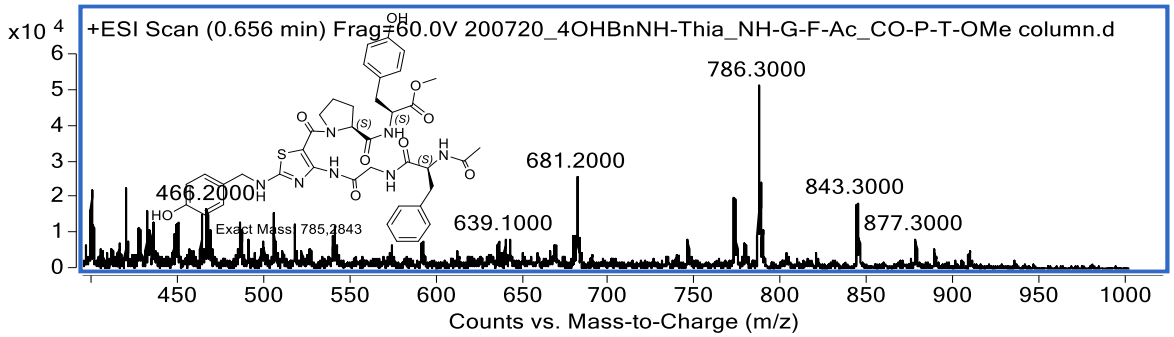


Exact Mass: 774,3159
m/z: [M+H]+ = 775,3232

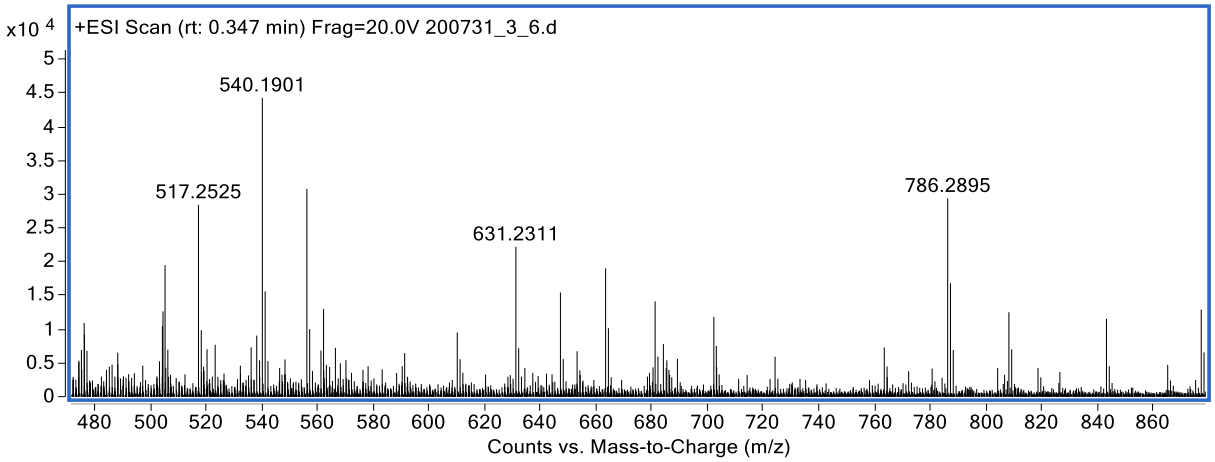


HR/MS – 12b

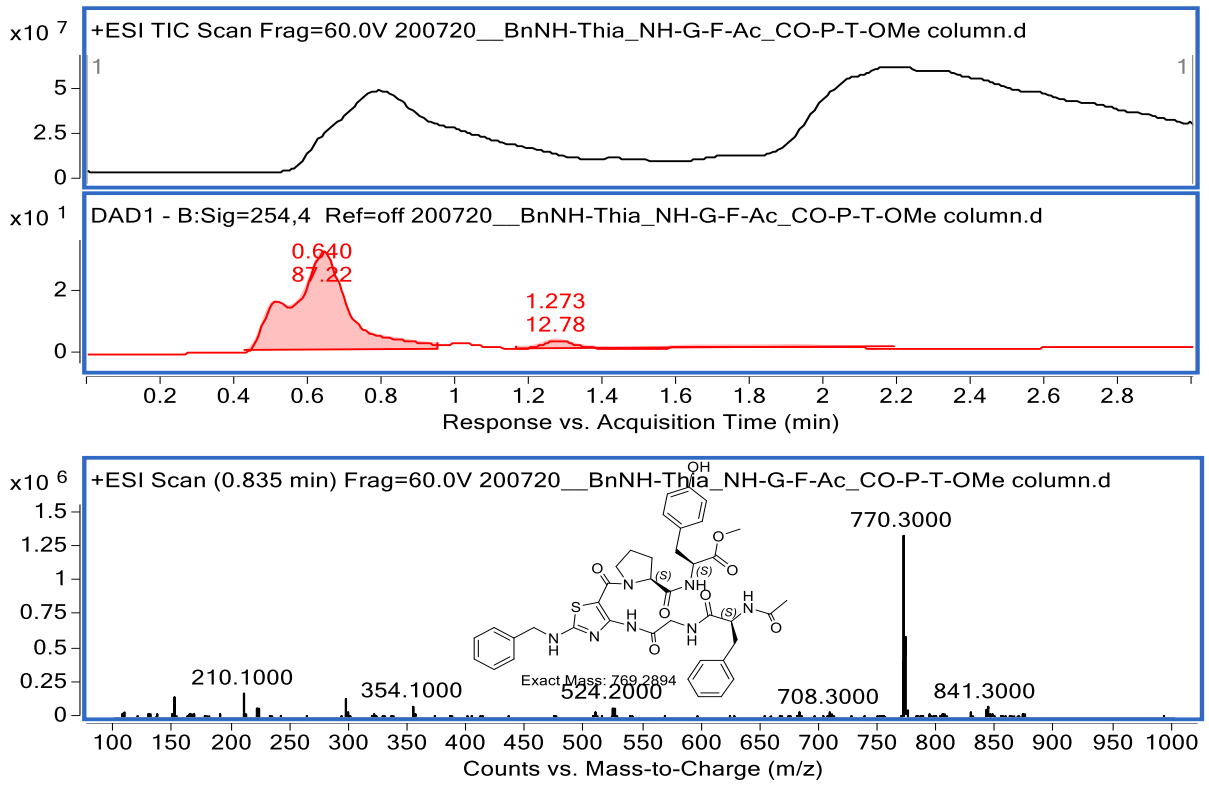




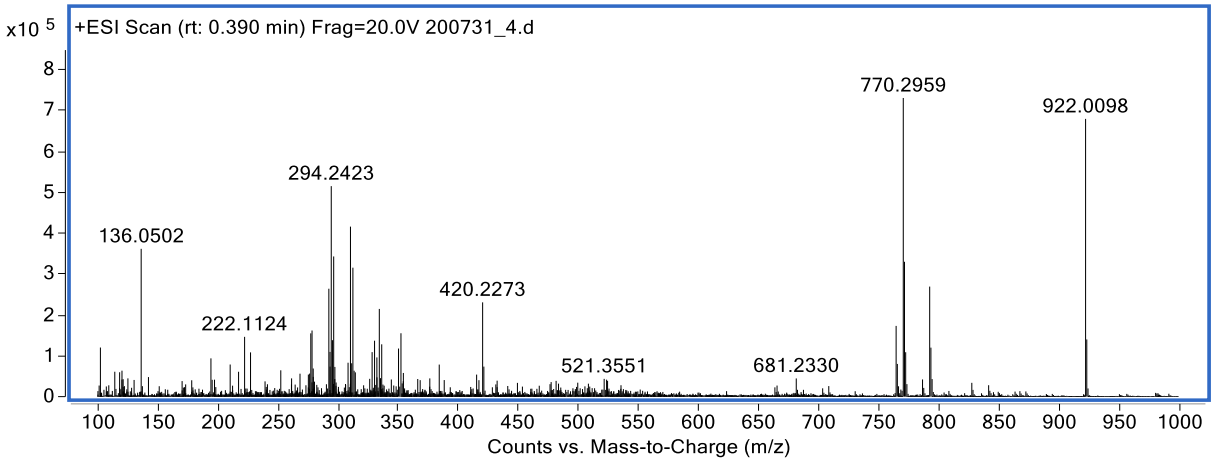
LC/MS – 12c



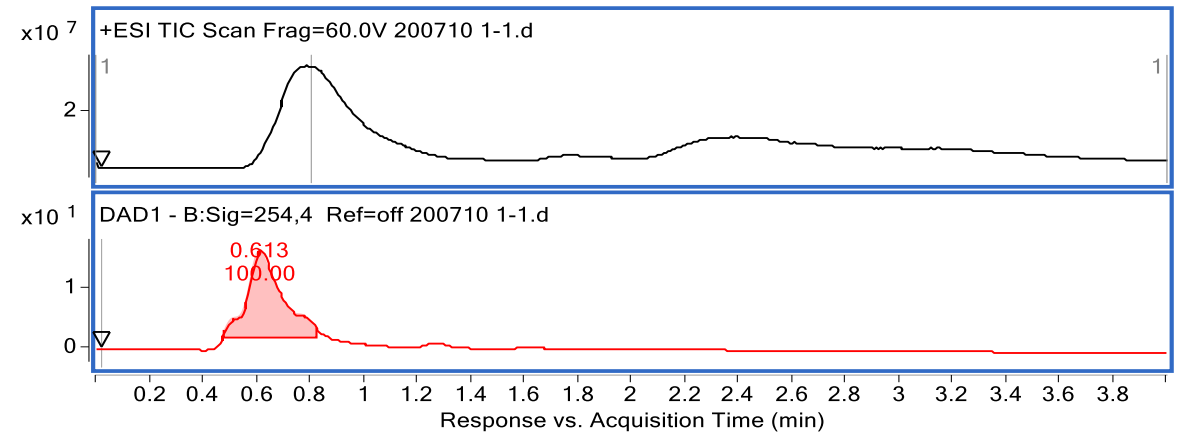
HR/MS – 12c

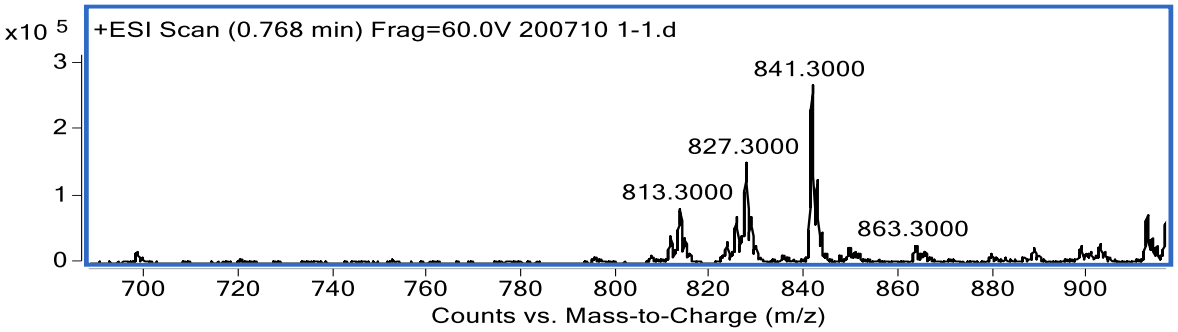


LC/MS – 12d

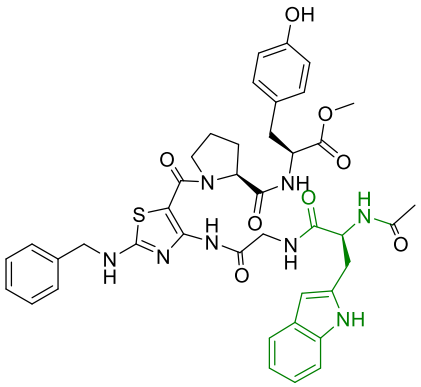


HR/MS – 12d

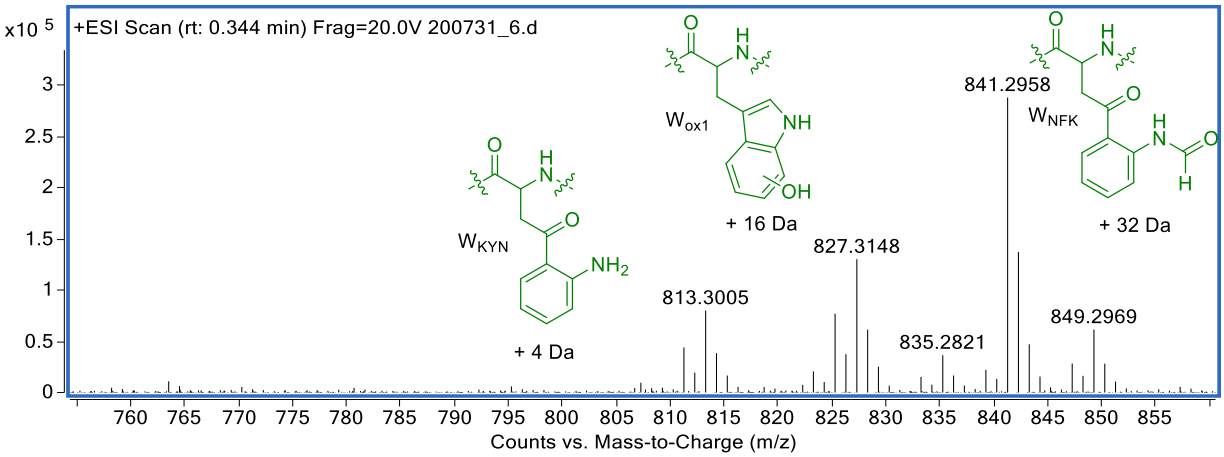




LC/MS – 12e



Exact Mass: 808,3003
m/z: [M+H]+ = 809,3075



HR/MS – 12e