

Supporting Information

Design, Synthesis and Biological Evaluation of Neocryptolepine Derivatives as Potential Anti-gastric Cancer Agents

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Table S1 The molecular docking scoring of compound **C5** and proteins

Number	Target	PDB ID	Resolution	Organisms	Docking score
1	AKT	6hhf	2.90	<i>Homo sapiens</i>	-8.529
2	Cyclin E1	5l2w	2.80	<i>Homo sapiens</i>	-8.171
3	PI3K	6gvf	2.50	<i>Homo sapiens</i>	-8.077
4	CDK2	5nev	2.97	<i>Homo sapiens</i>	-7.744
5	Cyclin A	6gue	1.99	<i>Homo sapiens</i>	-7.535
6	CDK6	3nux	2.70	<i>Homo sapiens</i>	-7.497
7	BCI-xl	7lh7	1.41	<i>Homo sapiens</i>	-7.377
8	MEK	5eym	2.70	<i>Homo sapiens</i>	-7.357
9	Raf	5fd2	2.89	<i>Homo sapiens</i>	-7.322
10	JNK	4y5h	2.06	<i>Homo sapiens</i>	-7.254
11	JAK	5tq6	2.06	<i>Homo sapiens</i>	-7.129
12	PARP	6bhv	2.30	<i>Homo sapiens</i>	-7.011
13	mTOR	4jt6	3.60	<i>Homo sapiens</i>	-6.81
14	GSK-3 β	1pyx	2.40	<i>Homo sapiens</i>	-6.392
15	Cyclin D1	5vzu	2.70	<i>Homo sapiens</i>	-6.138
16	CDK7	1ua2	3.02	<i>Homo sapiens</i>	-5.656
17	Bax	4zie	1.80	<i>Homo sapiens</i>	-5.403
18	MAPK	6tca	3.70	<i>Homo sapiens</i>	-5.279
19	Bad	4ieh	2.10	<i>Homo sapiens</i>	-5.101
20	Bcl-2	6qgg	1.50	<i>Homo sapiens</i>	-5.035
21	Caspase-3	3kjf	2.00	<i>Homo sapiens</i>	-4.634
22	Ras	7jhp	2.77	<i>Homo sapiens</i>	-4.323
23	Casepase-9	1nw9	2.40	<i>Homo sapiens</i>	-4.076
24	STAT3	6nuq	3.15	<i>Homo sapiens</i>	-3.788
25	Wnt	6gbi	1.25	<i>Homo sapiens</i>	-2.6

Table S2 The molecular docking scoring of compound **C8** and proteins

Number	Target	PDB ID	Resolution	Organisms	Docking score
1	AKT	6hhf	2.90	<i>Homo sapiens</i>	-8.359
2	Cyclin E1	5l2w	2.80	<i>Homo sapiens</i>	-8.033
3	Cyclin A	6gue	1.99	<i>Homo sapiens</i>	-7.643
4	CDK6	3nux	2.70	<i>Homo sapiens</i>	-7.536
5	MEK	5eym	2.70	<i>Homo sapiens</i>	-7.518
6	Raf	5fd2	2.89	<i>Homo sapiens</i>	-7.494
7	JNK	4y5h	2.06	<i>Homo sapiens</i>	-7.316
8	CDK2	5nev	2.97	<i>Homo sapiens</i>	-7.256
9	BCI-xl	7lh7	1.41	<i>Homo sapiens</i>	-7.255
10	PARP	6bhv	2.30	<i>Homo sapiens</i>	-7.239
11	PI3K	6gvf	2.50	<i>Homo sapiens</i>	-7.123
12	mTOR	4jt6	3.60	<i>Homo sapiens</i>	-6.931
13	JAK	5tq6	2.06	<i>Homo sapiens</i>	-6.84
14	Cyclin D1	5vzu	2.70	<i>Homo sapiens</i>	-6.639
15	GSK-3 β	1pyx	2.40	<i>Homo sapiens</i>	-6.185
16	Caspase-3	3kjf	2.00	<i>Homo sapiens</i>	-5.887
17	CDK7	1ua2	3.02	<i>Homo sapiens</i>	-5.501
18	Bad	4ieh	2.10	<i>Homo sapiens</i>	-5.211
19	MAPK	6tca	3.70	<i>Homo sapiens</i>	-5.107
20	Bcl-2	6qgg	1.50	<i>Homo sapiens</i>	-4.911
21	Ras	7jhp	2.77	<i>Homo sapiens</i>	-4.281
22	Casepase-9	1nw9	2.40	<i>Homo sapiens</i>	-3.995
23	NF- κ B	5e6a	2.20	<i>Homo sapiens</i>	-3.878
24	STAT3	6nuq	3.15	<i>Homo sapiens</i>	-3.648
25	ERK	6hkn	2.33	<i>Homo sapiens</i>	-3.131

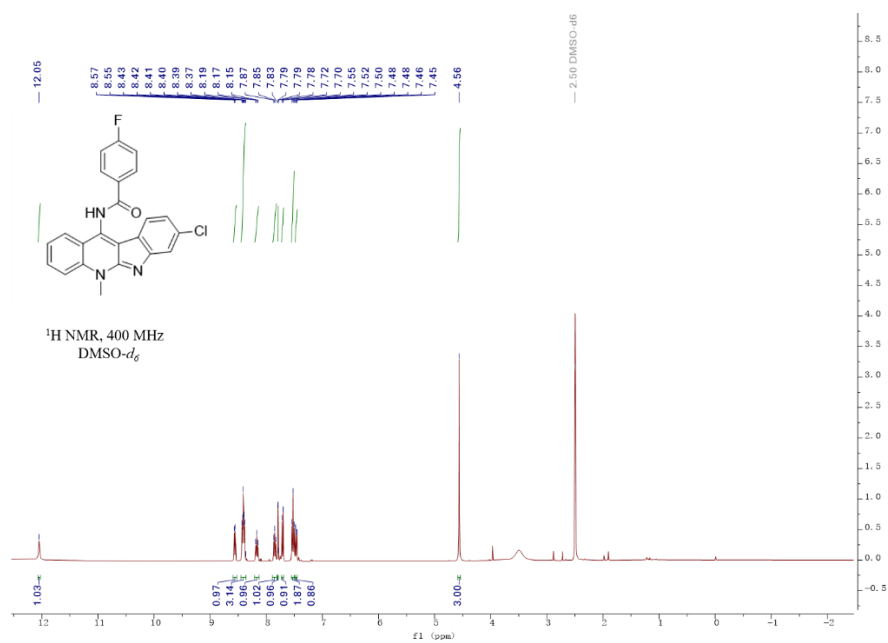


Figure S1. ¹H NMR spectra of compound **C5**

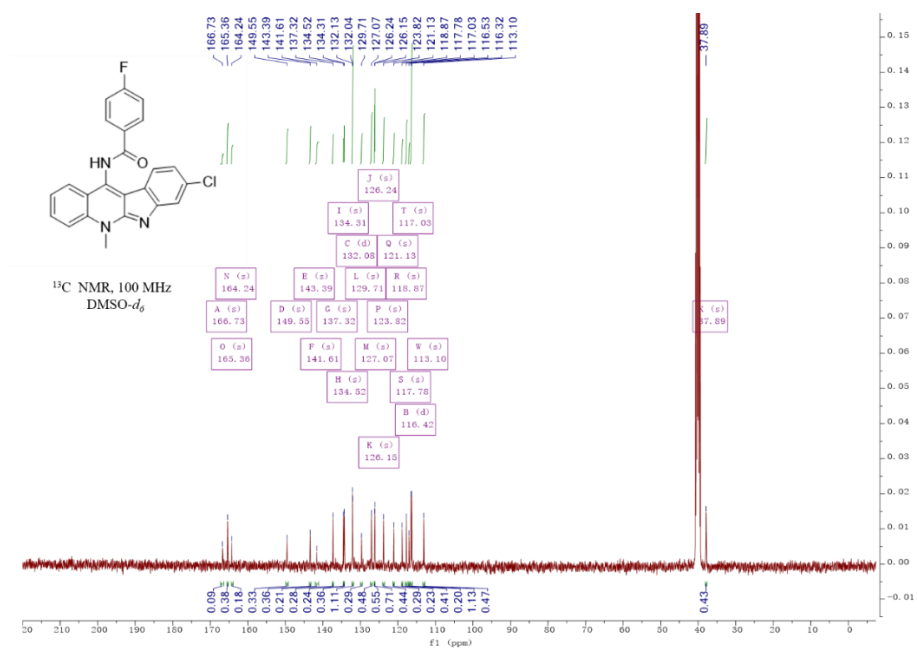


Figure S2. ¹³C NMR spectra of compound C5

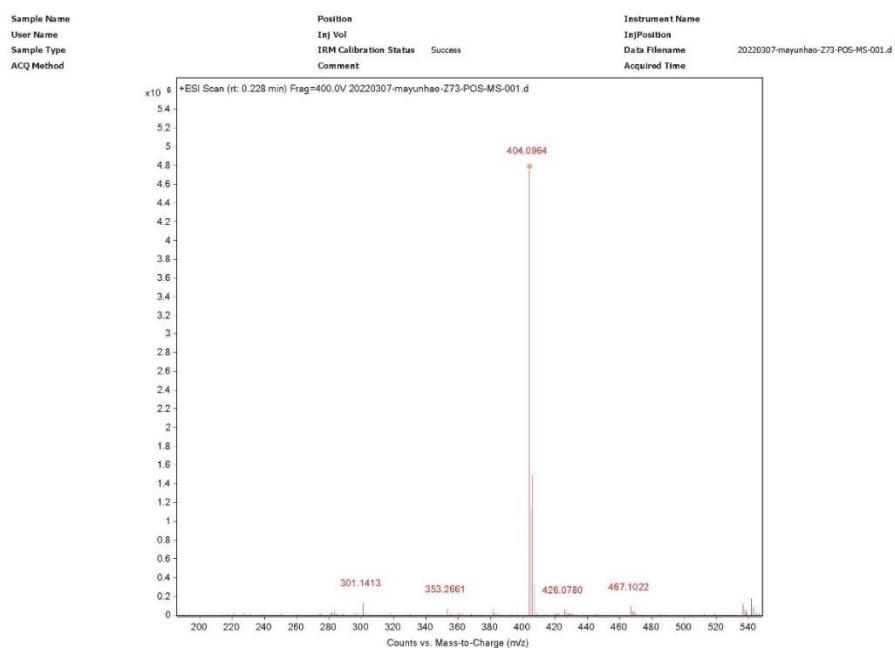


Figure S3. Mass spectrometry of compound **C5**

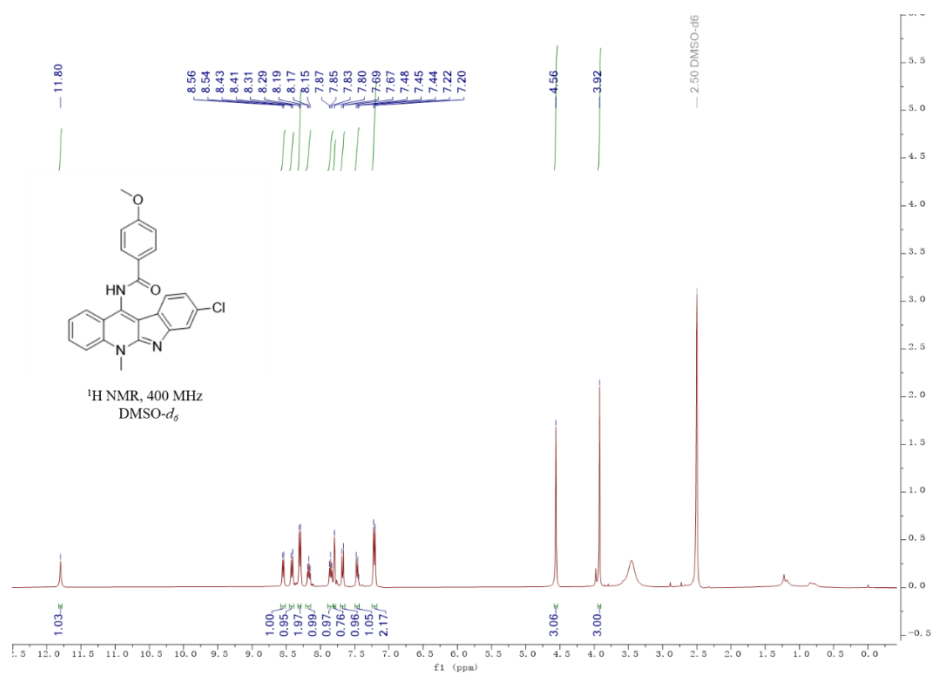


Figure S4. ¹H NMR spectra of compound **C8**

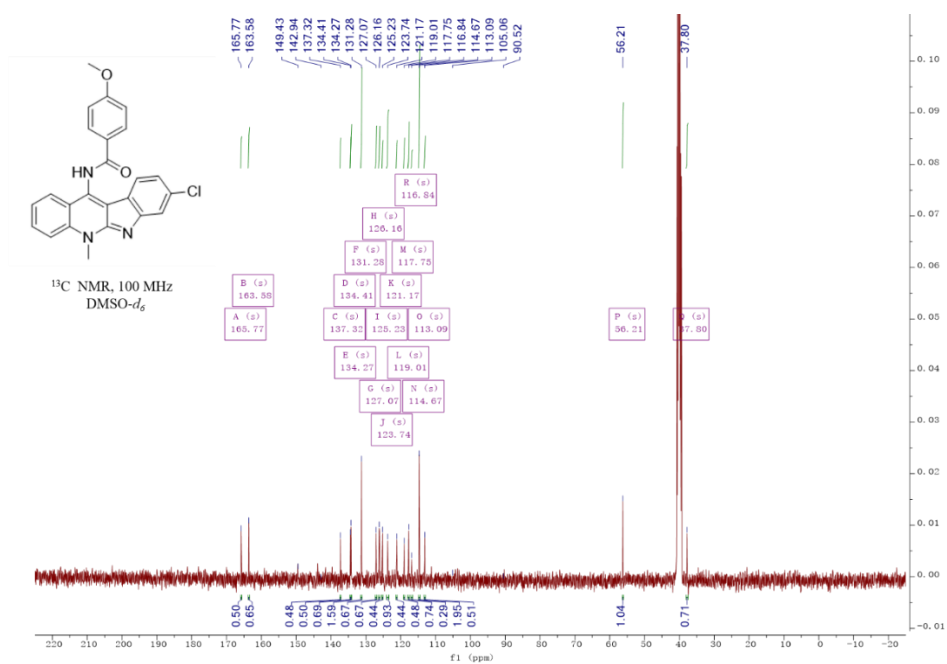


Figure S5. ¹³C NMR spectra of compound C8

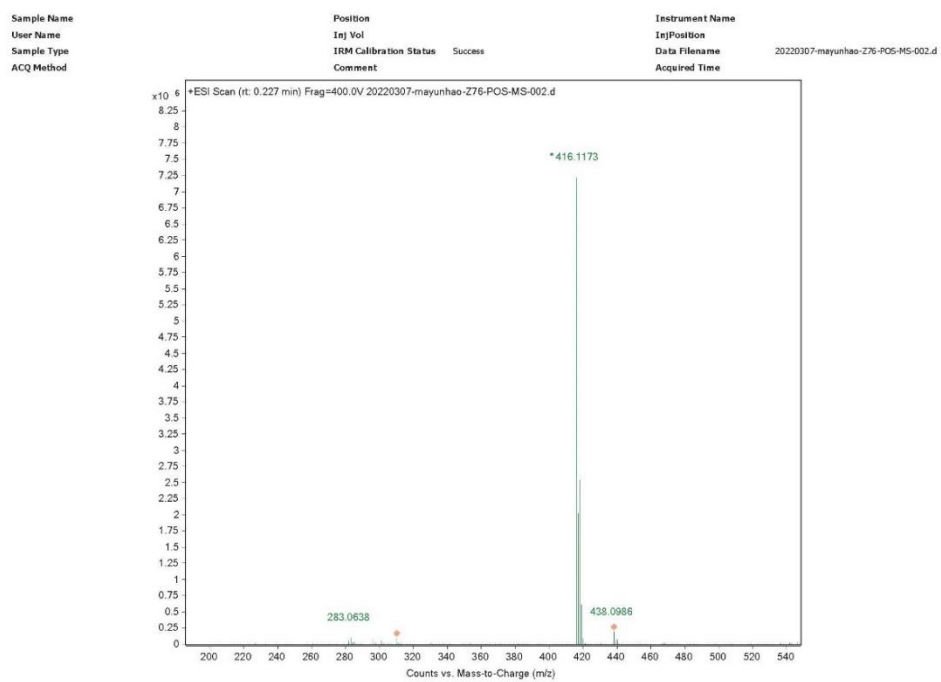


Figure S6. Mass spectrometry of compound **C8**

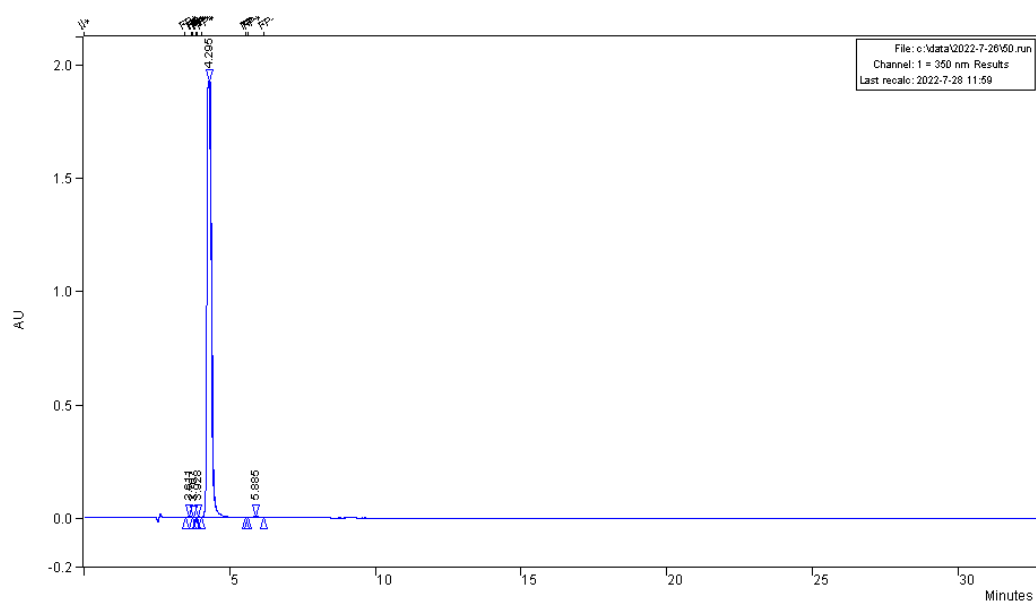


Figure S7. Purity test of compound **A1** by HPLC

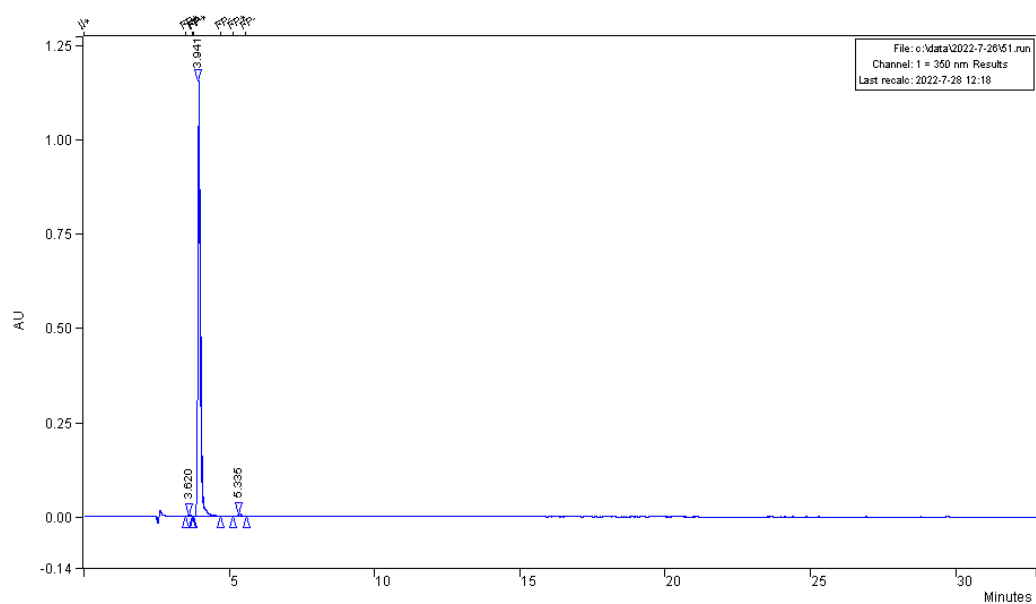


Figure S8. Purity test of compound **A2** by HPLC

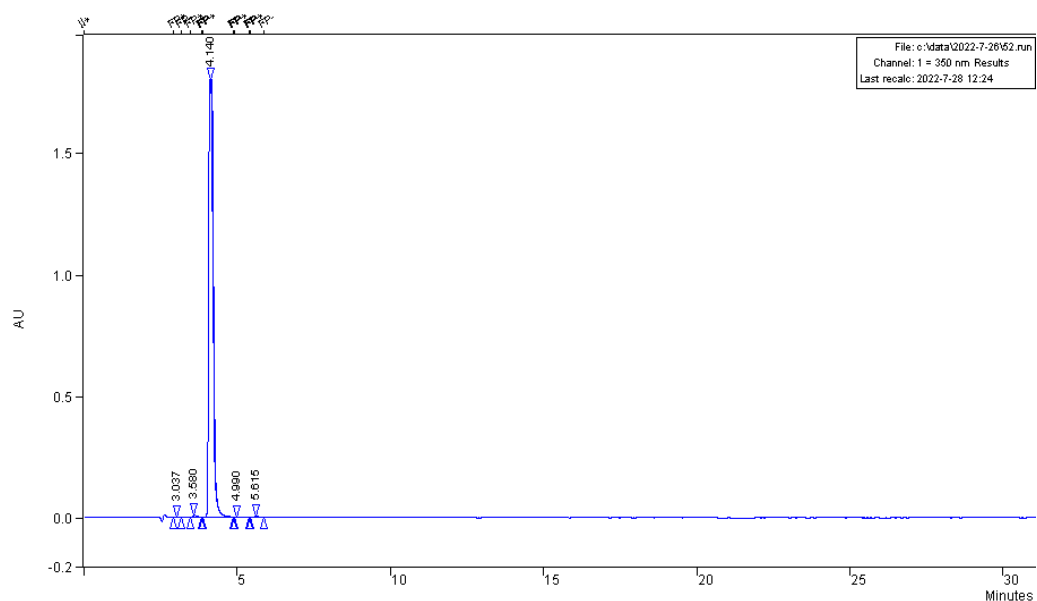


Figure S9. Purity test of compound **A3** by HPLC

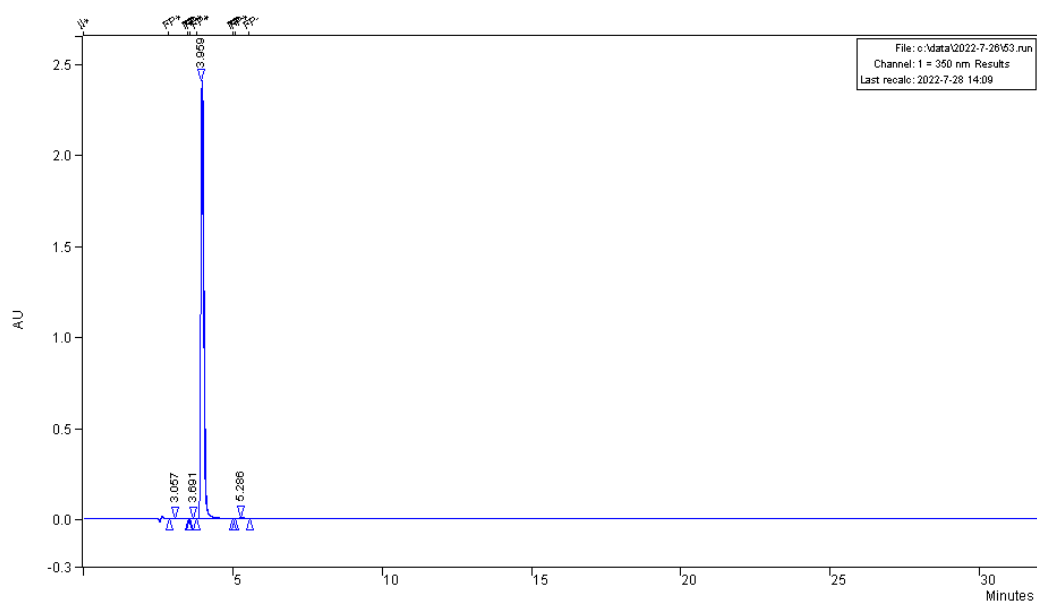


Figure S10. Purity test of compound **A4** by HPLC

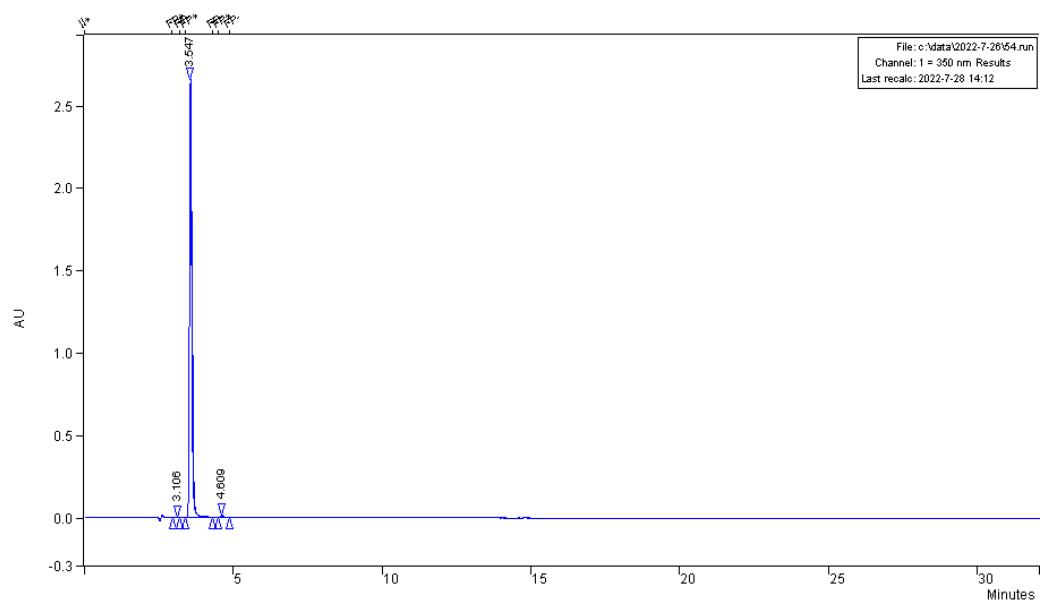


Figure S11. Purity test of compound **A5** by HPLC

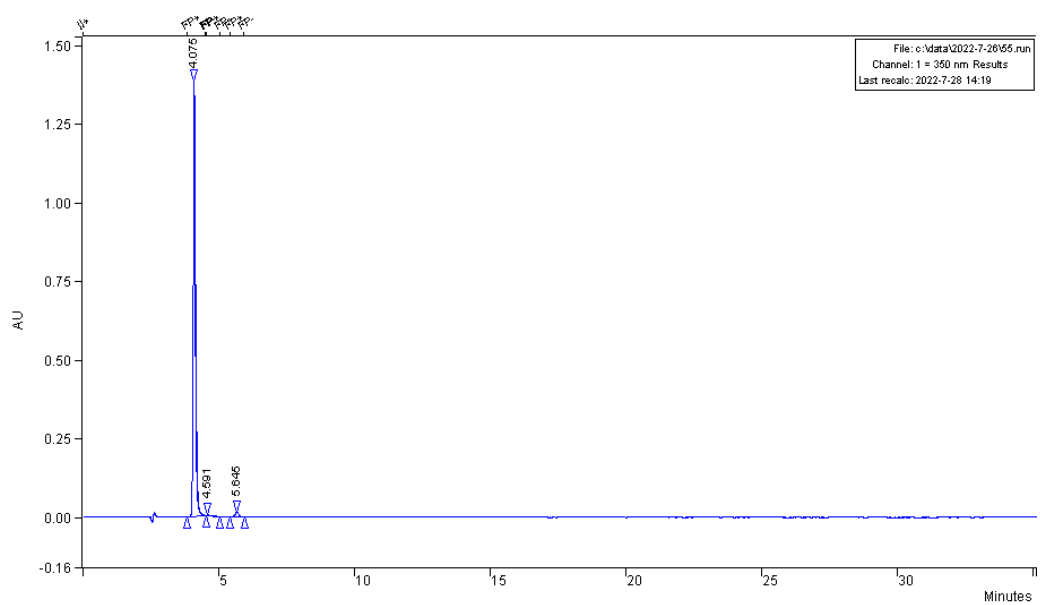


Figure S12. Purity test of compound **A6** by HPLC

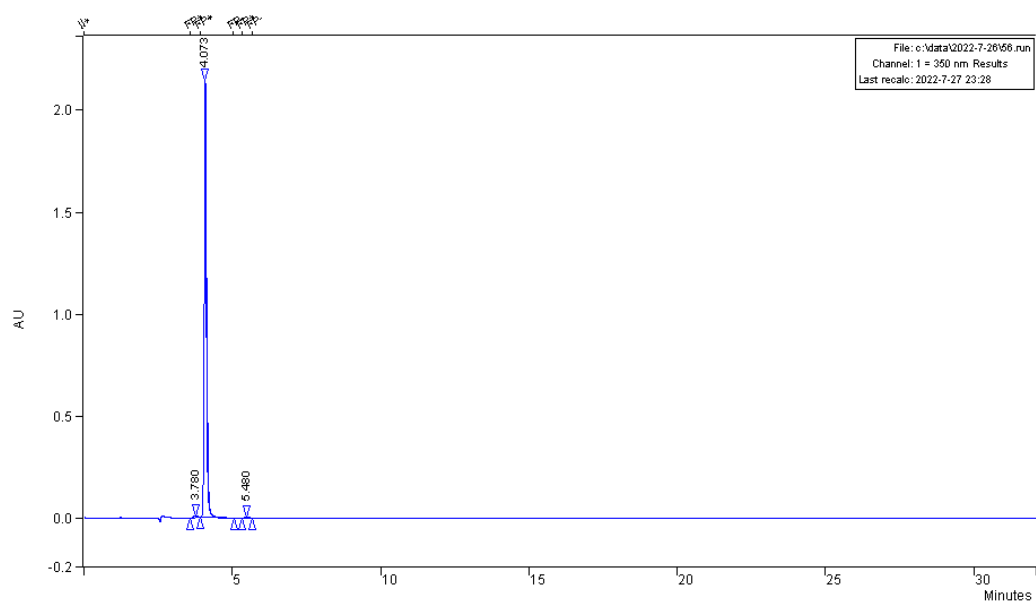


Figure S13. Purity test of compound **A7** by HPLC

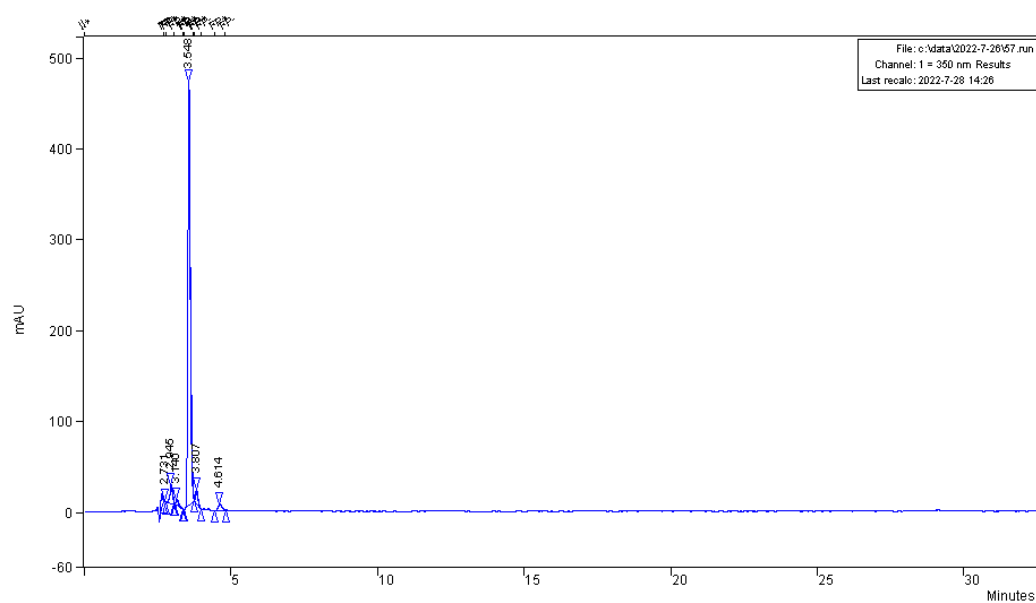


Figure S14. Purity test of compound **A8** by HPLC

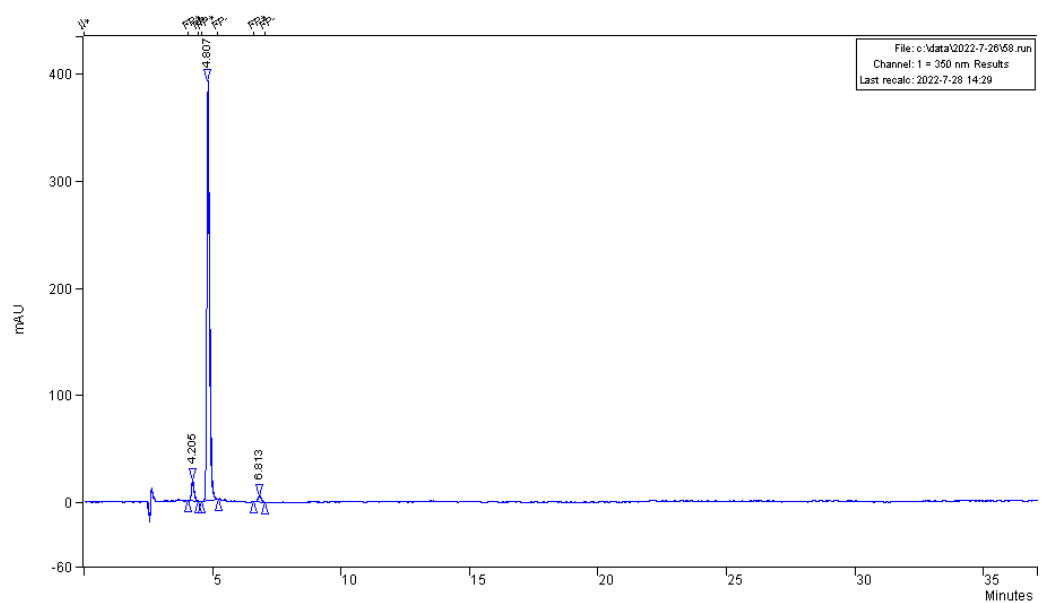


Figure S15. Purity test of compound **A9** by HPLC

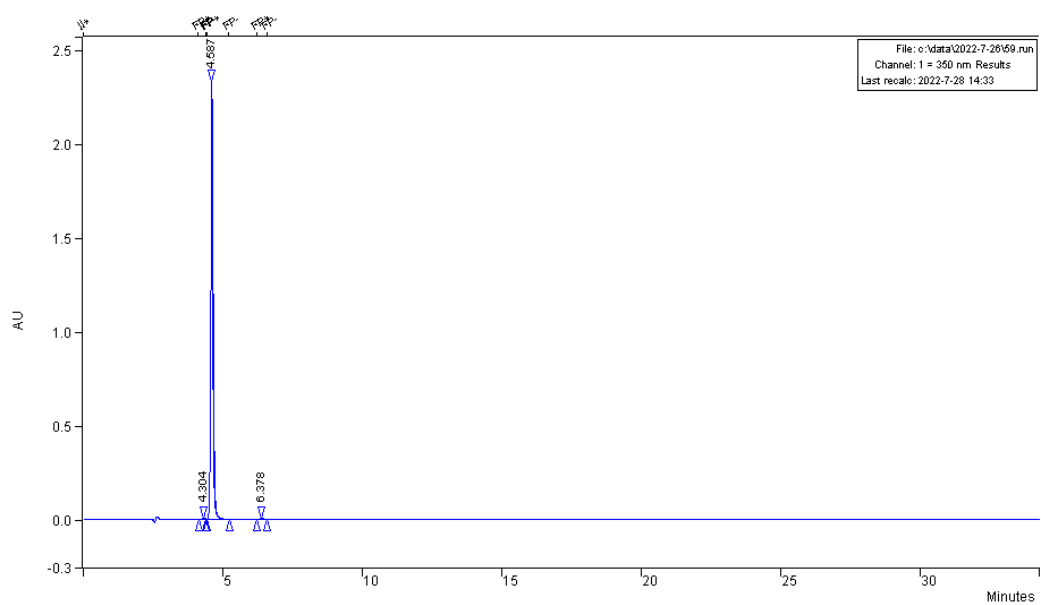


Figure S16. Purity test of compound **A10** by HPLC

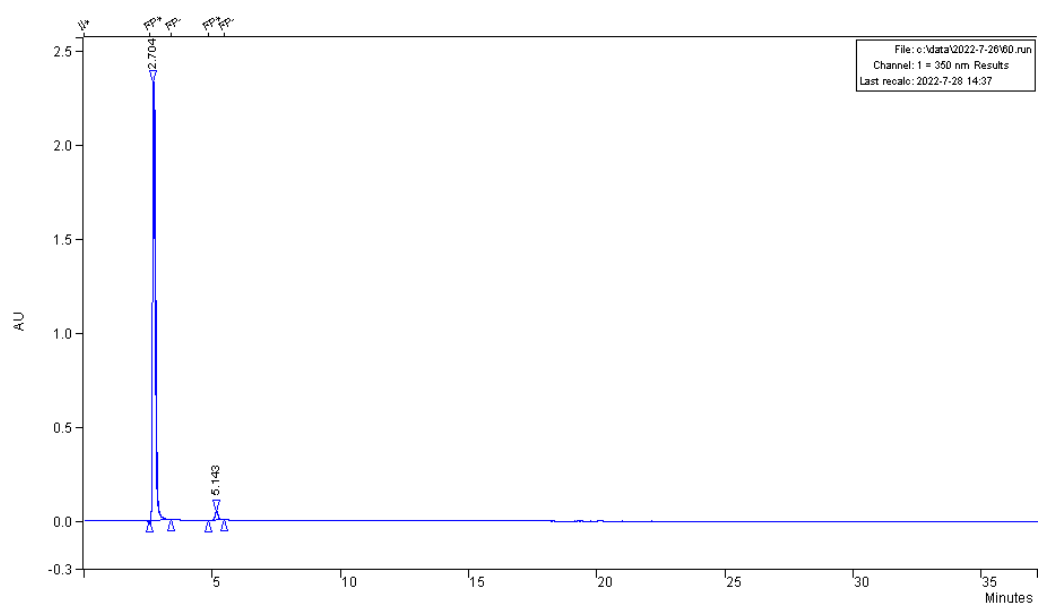


Figure S17. Purity test of compound **B1** by HPLC

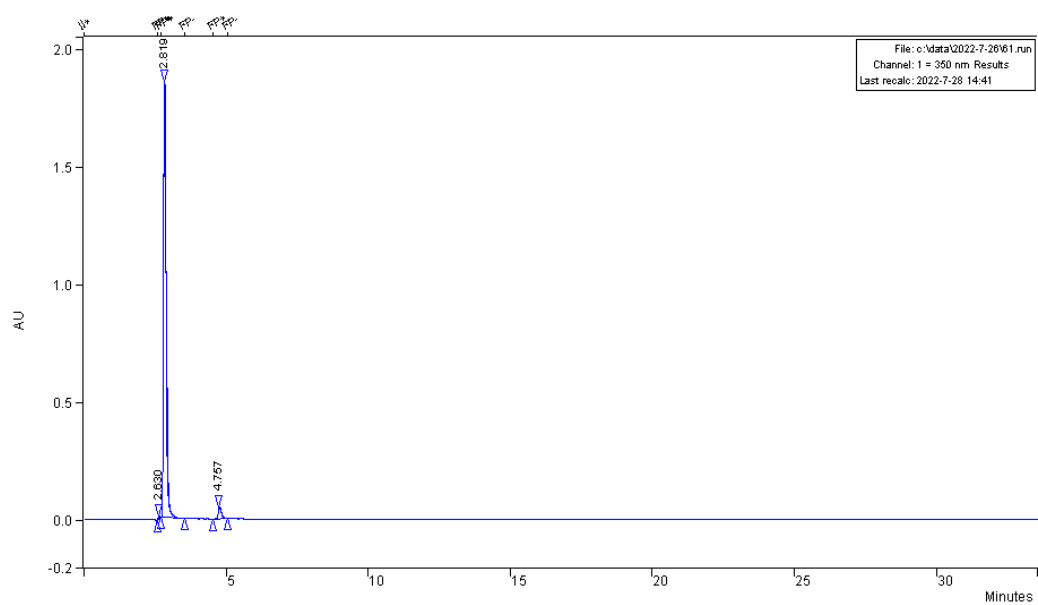


Figure S18. Purity test of compound **B2** by HPLC

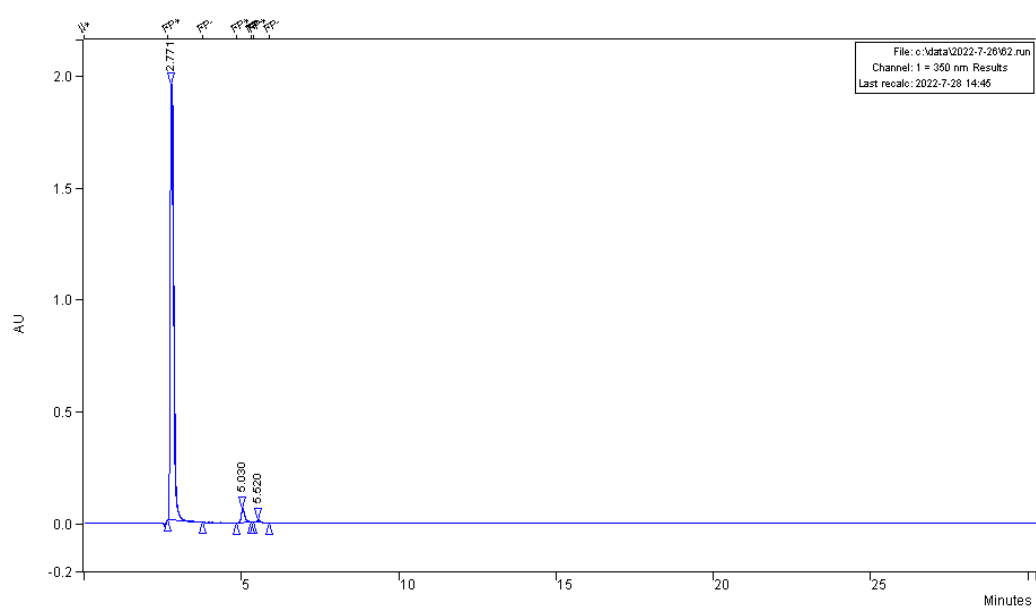


Figure S19. Purity test of compound **B3** by HPLC

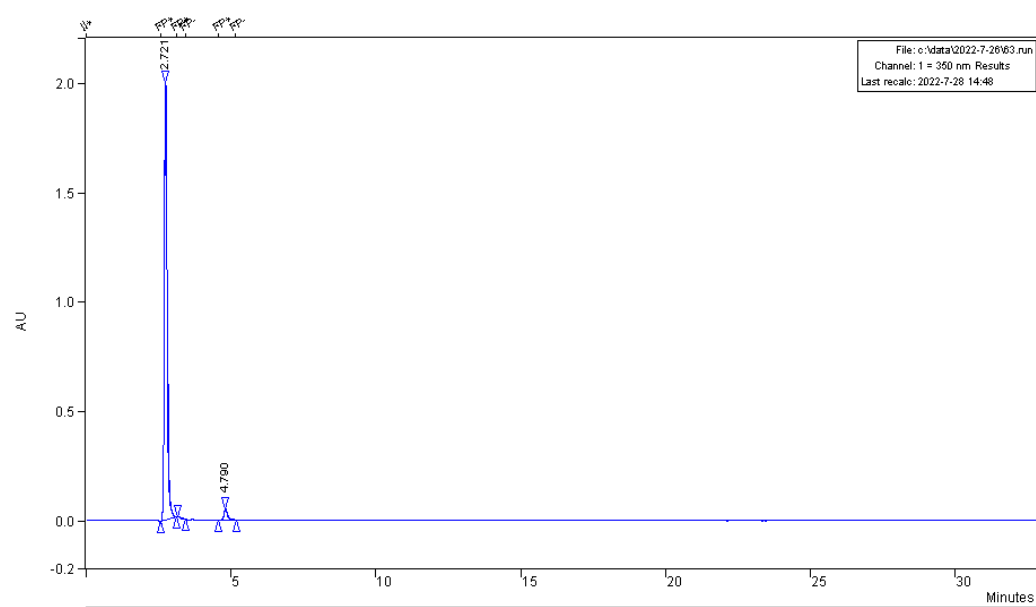


Figure S20. Purity test of compound **B4** by HPLC

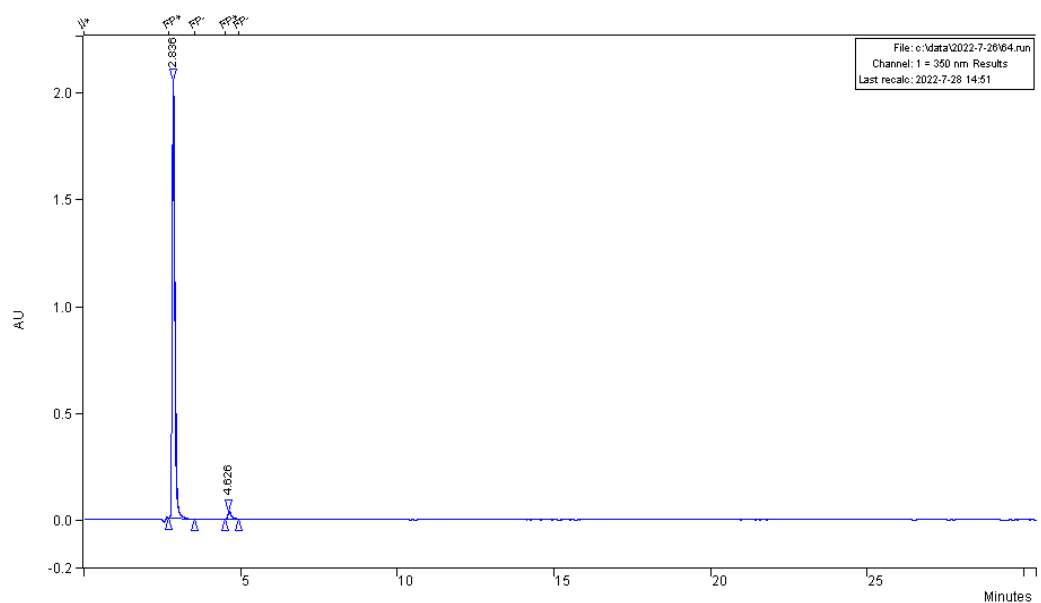


Figure S21. Purity test of compound **B5** by HPLC

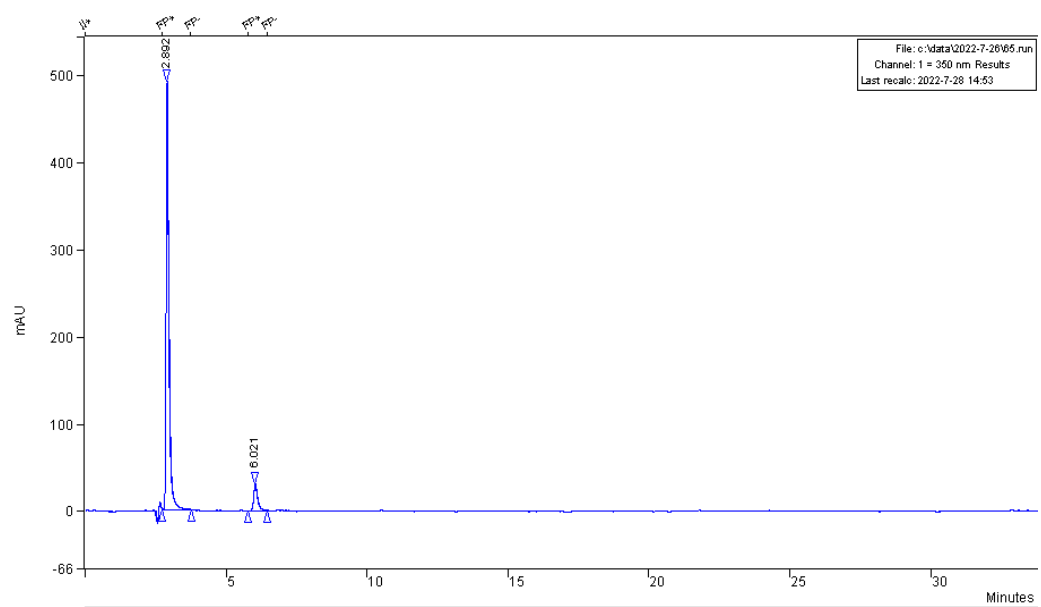


Figure S22. Purity test of compound **B6** by HPLC

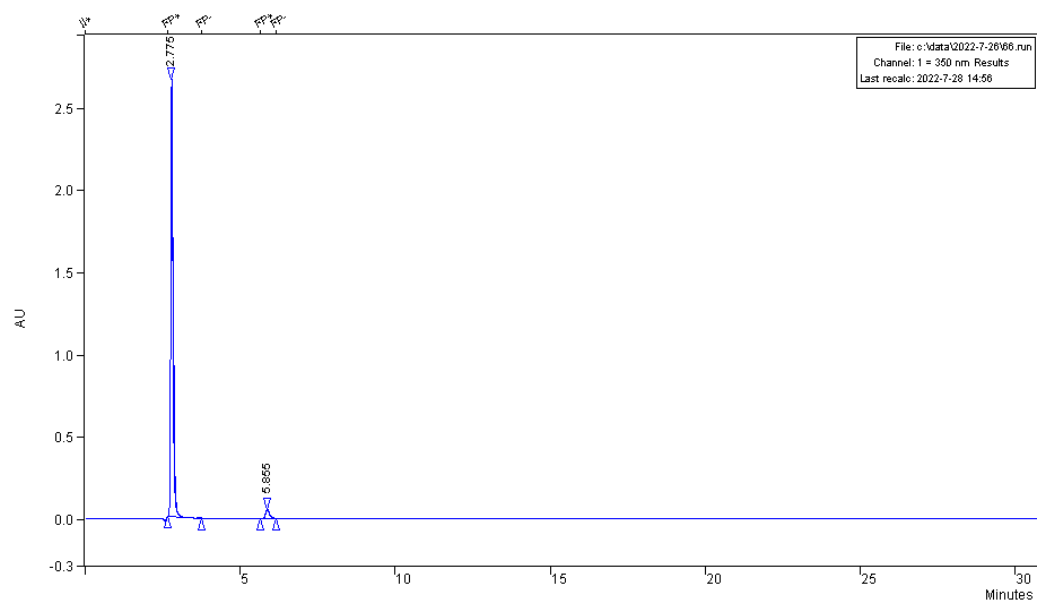


Figure S23. Purity test of compound **B7** by HPLC

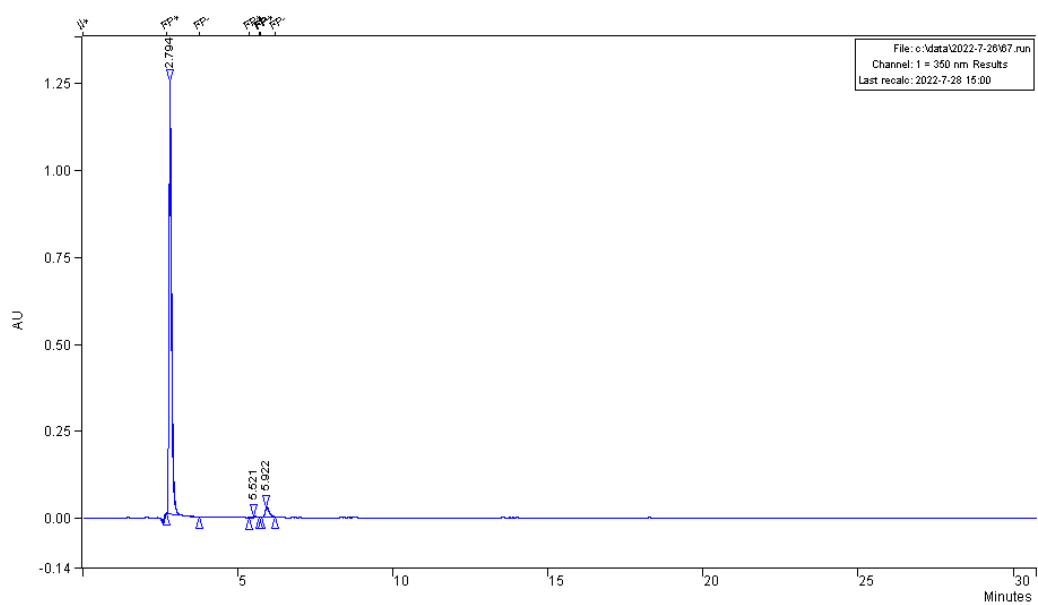


Figure S24. Purity test of compound **B8** by HPLC

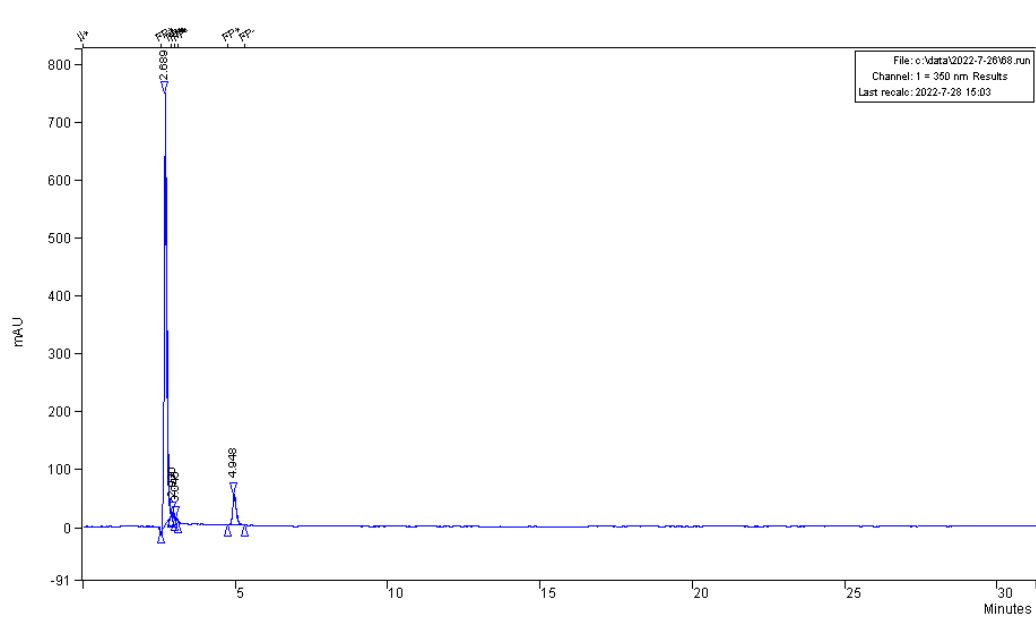


Figure S25. Purity test of compound **B9** by HPLC

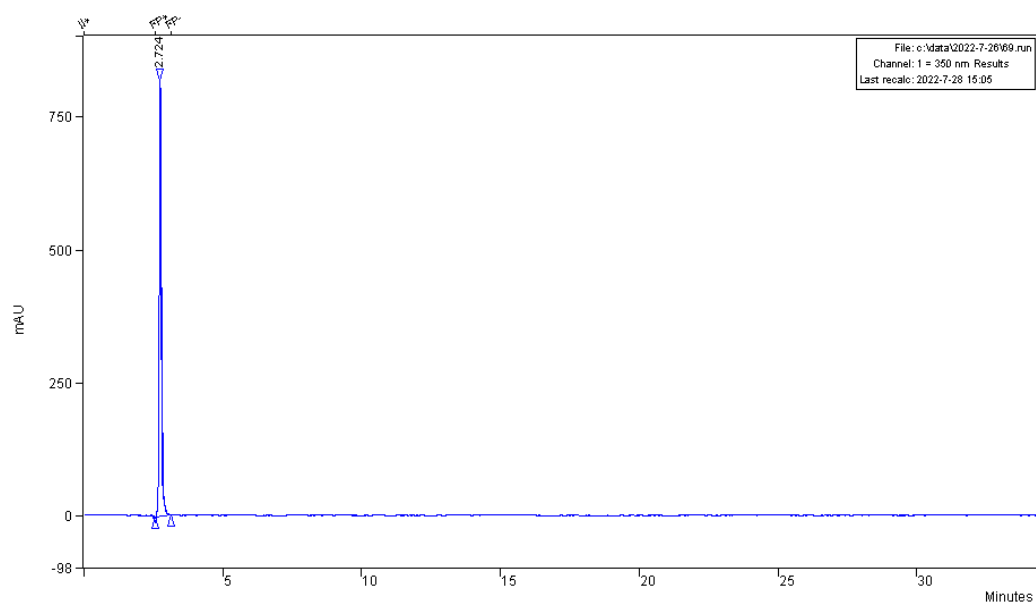


Figure S26. Purity test of compound **C1** by HPLC

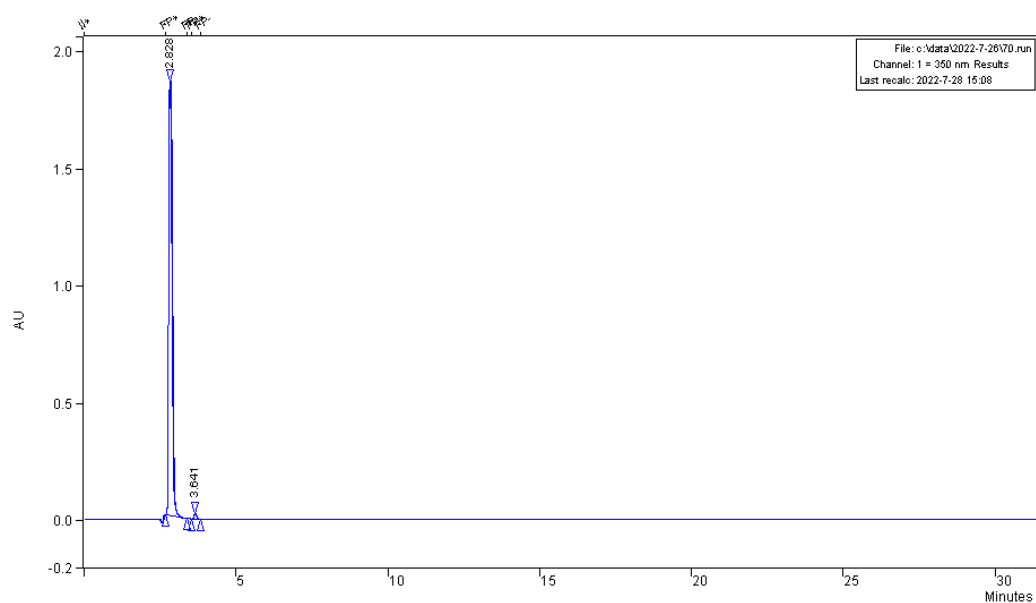


Figure S27. Purity test of compound **C2** by HPLC

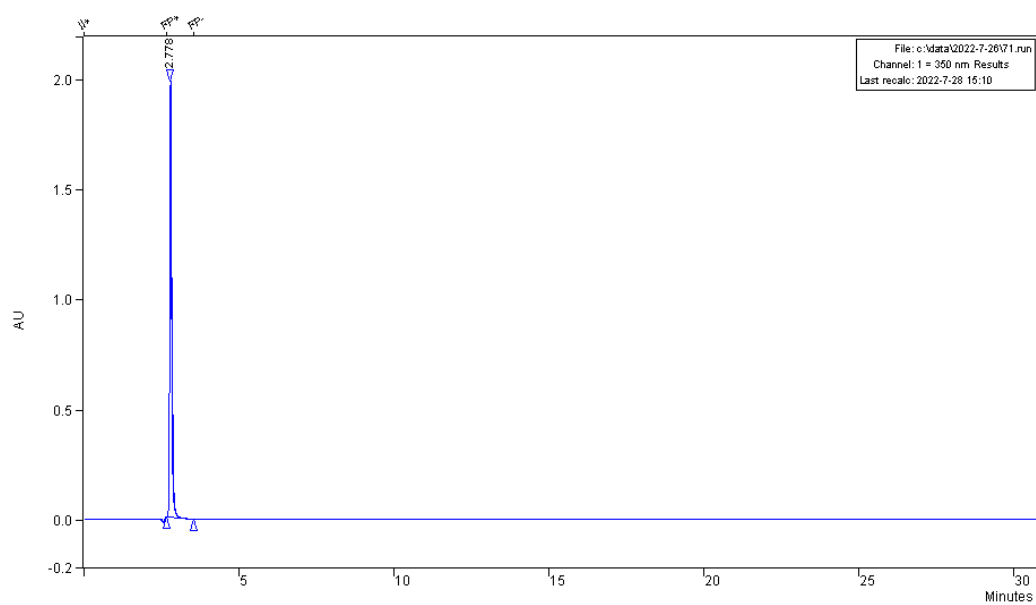


Figure S28. Purity test of compound **C3** by HPLC

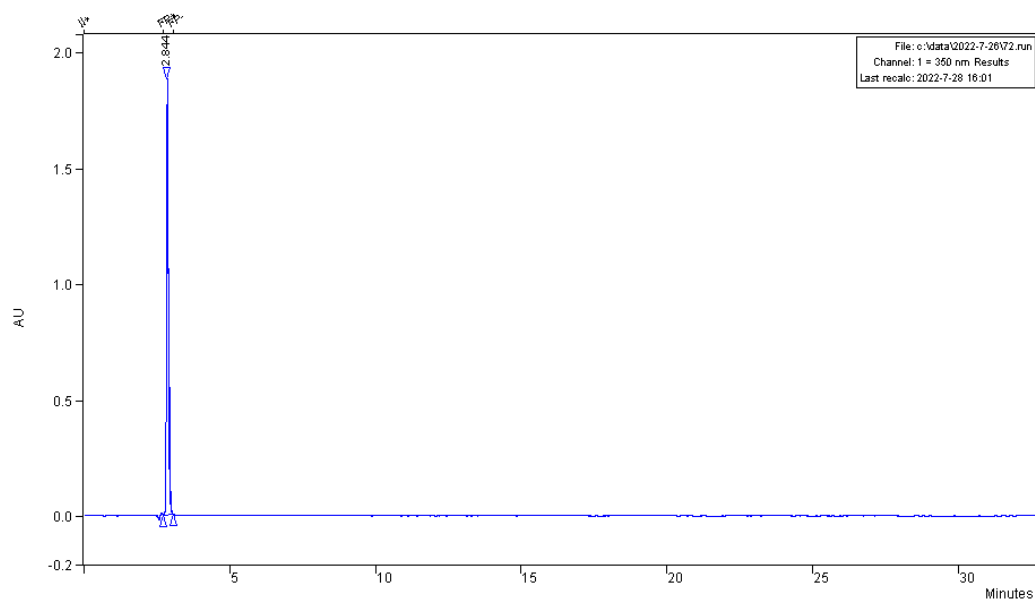


Figure S29. Purity test of compound **C4** by HPLC

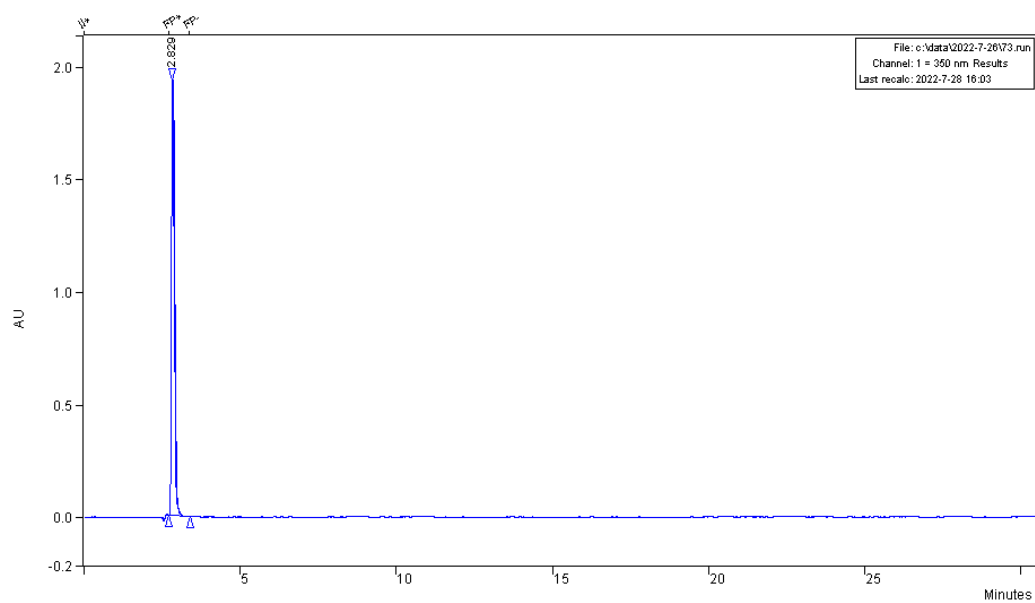


Figure S30. Purity test of compound **C5** by HPLC

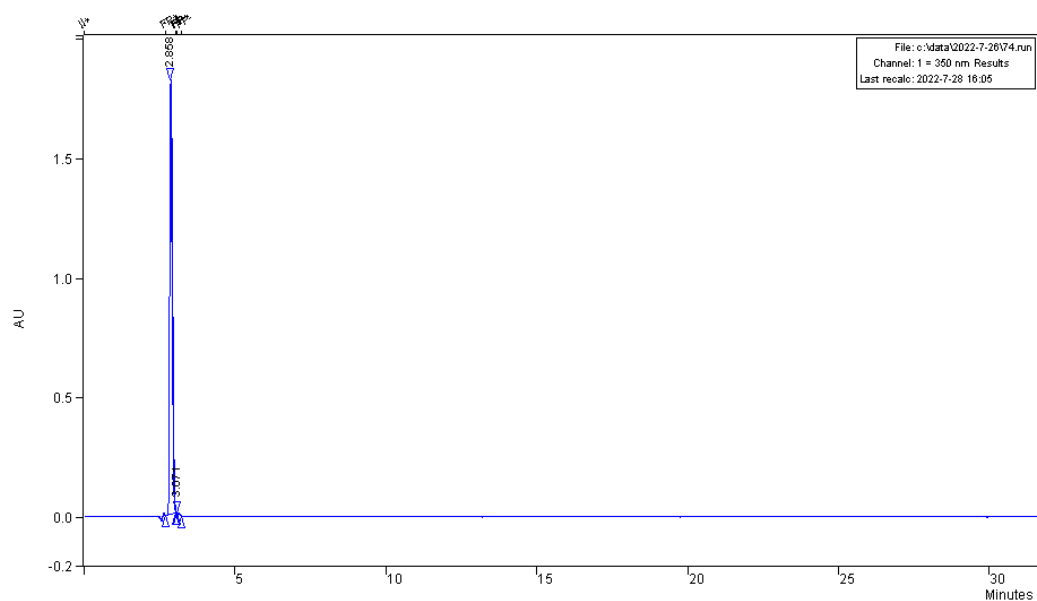


Figure S31. Purity test of compound **C6** by HPLC

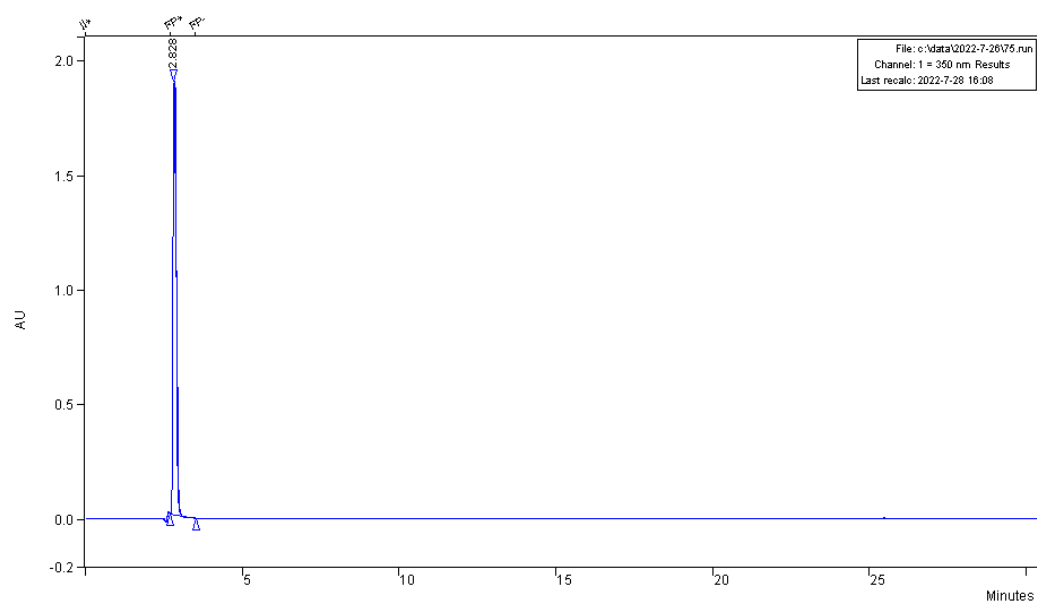


Figure S32. Purity test of compound **C7** by HPLC

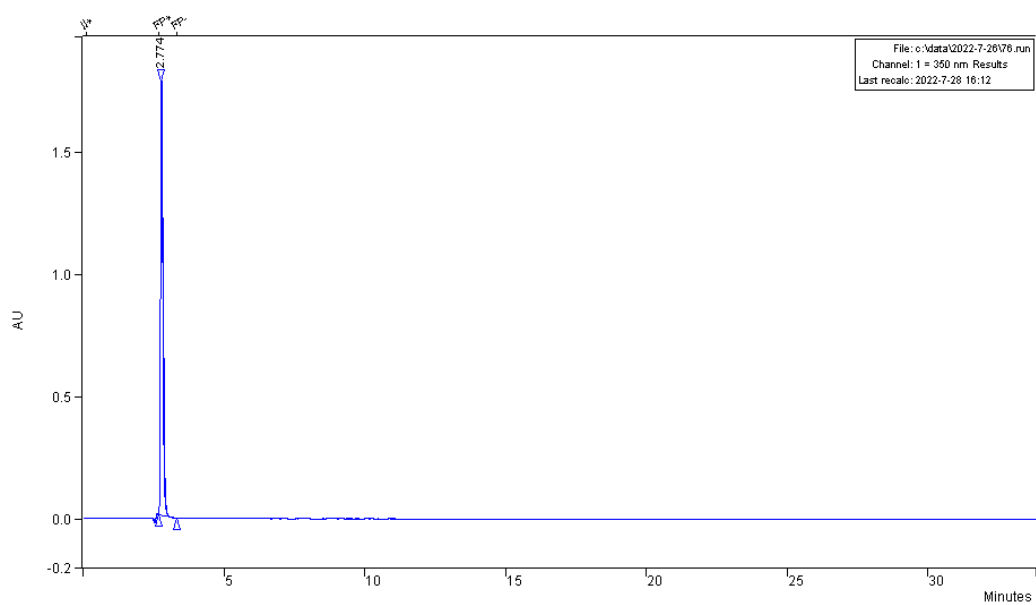


Figure S33. Purity test of compound **C8** by HPLC

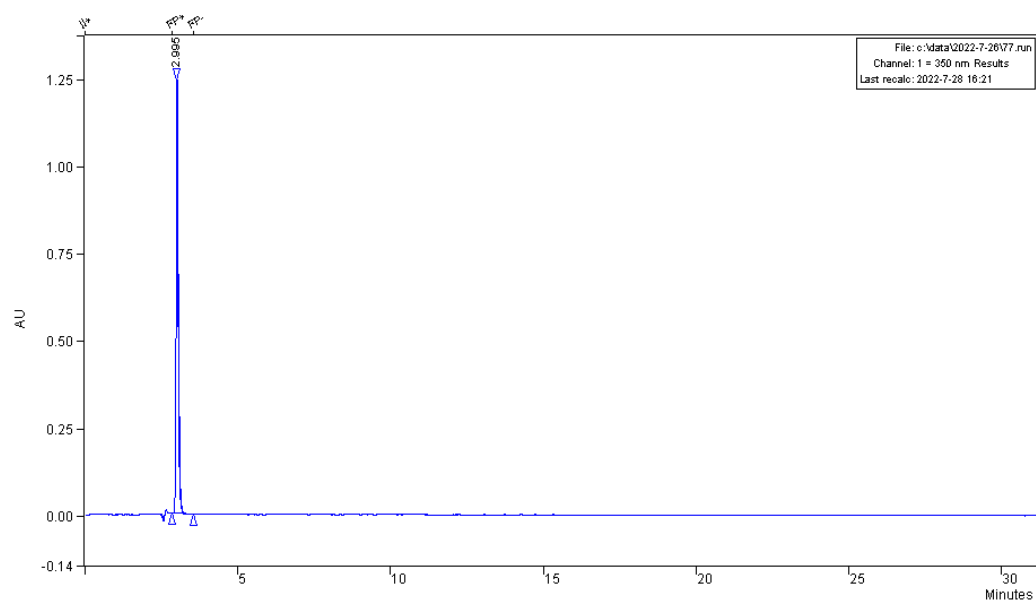


Figure S34. Purity test of compound **C9** by HPLC

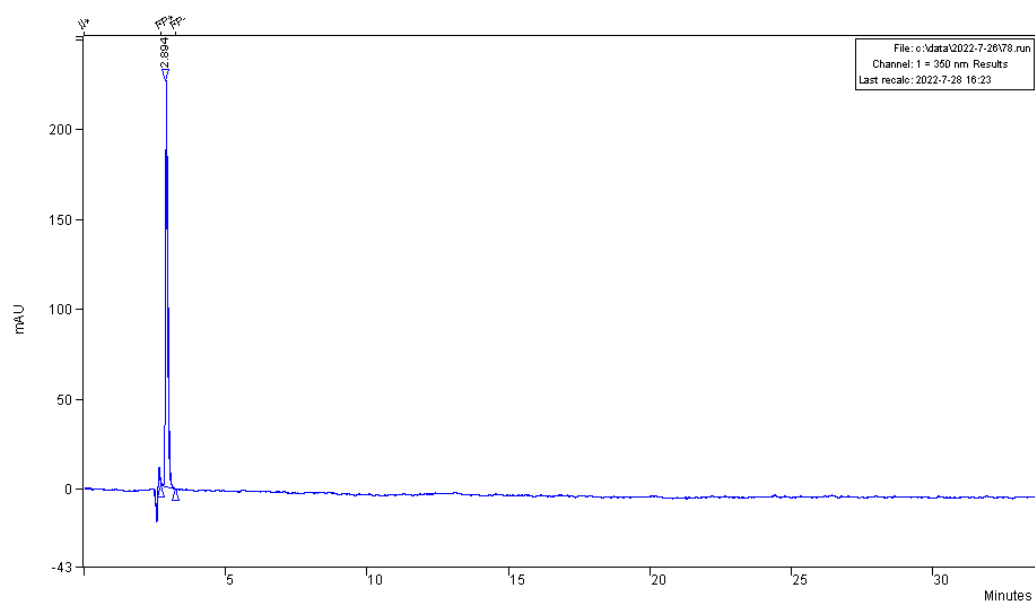


Figure S35. Purity test of compound **C10** by HPLC

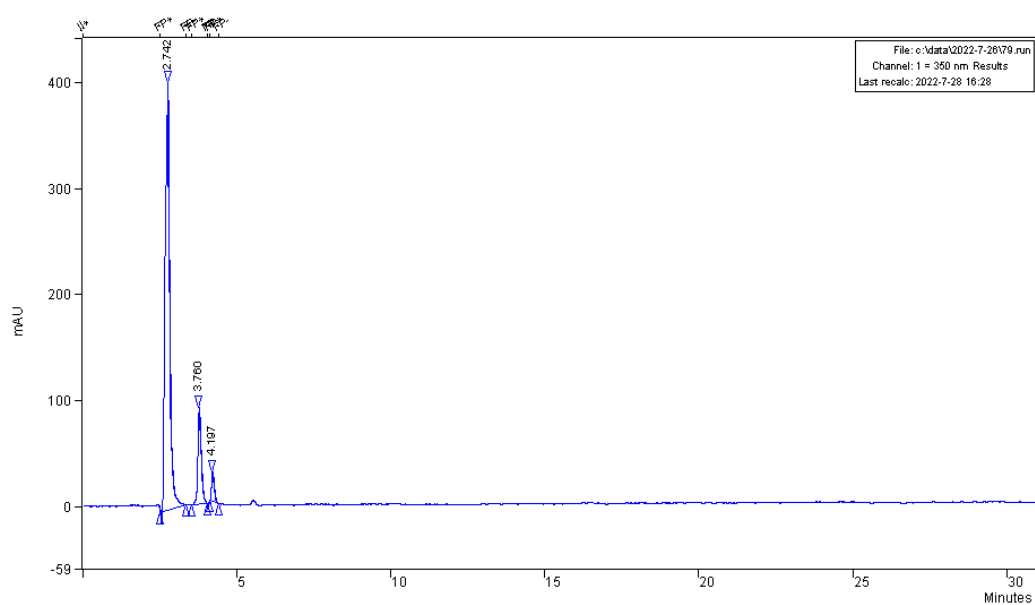


Figure S36. Purity test of compound **D1** by HPLC

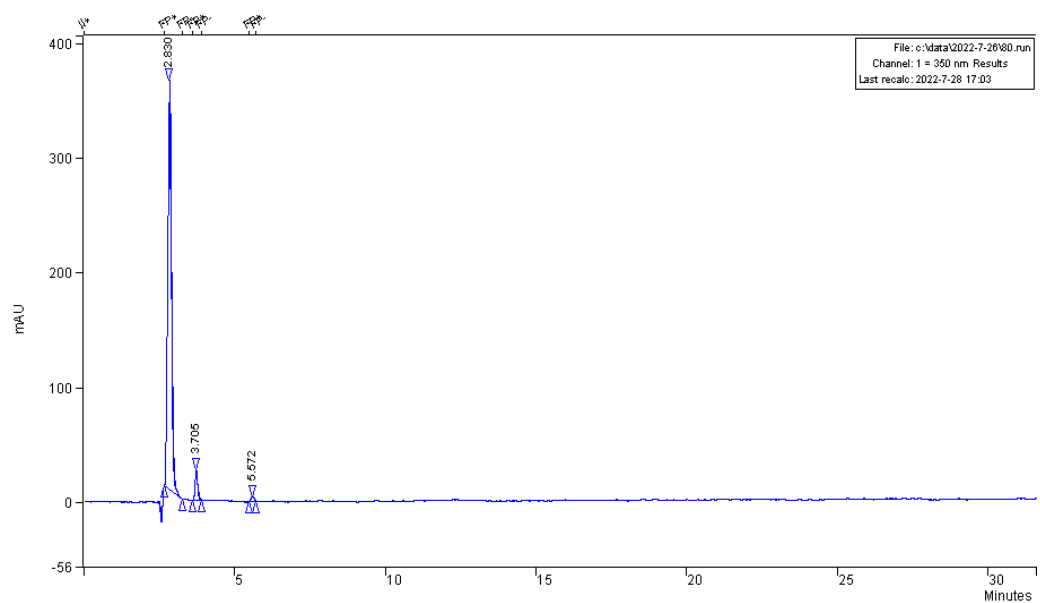


Figure S37. Purity test of compound **D2** by HPLC

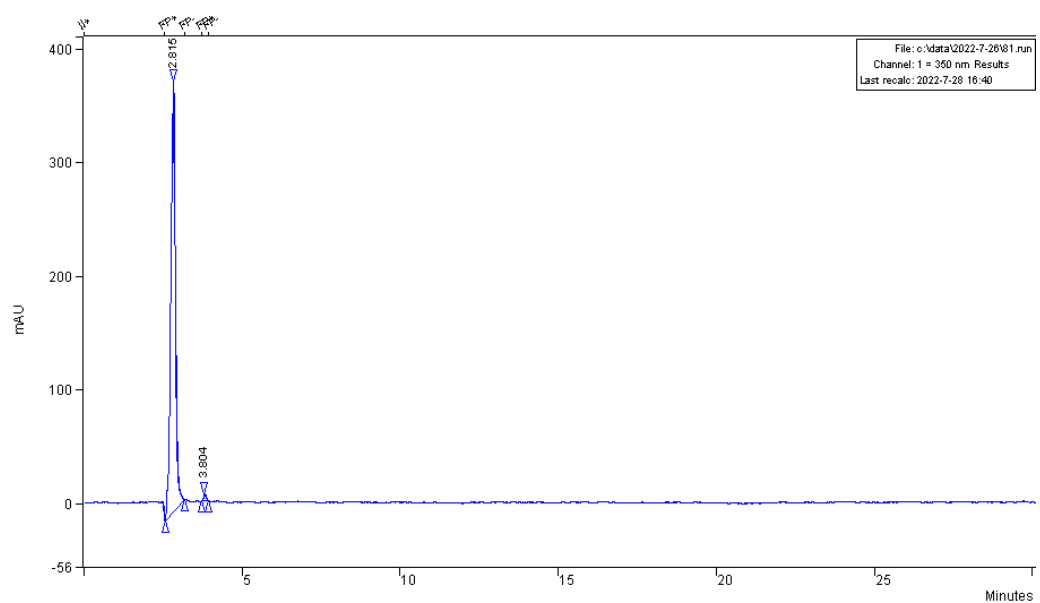


Figure S38. Purity test of compound **D3** by HPLC

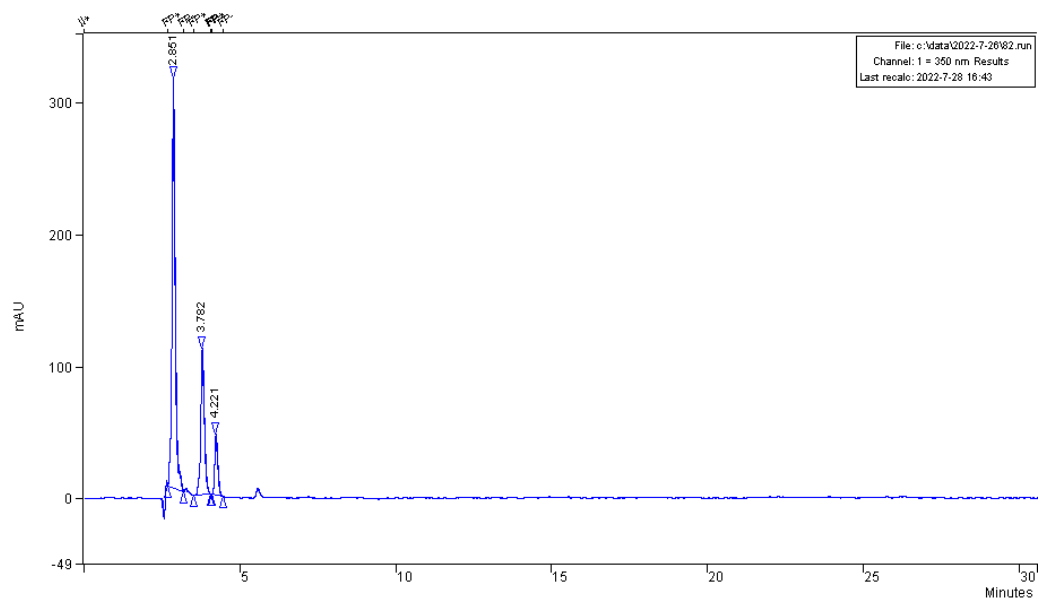


Figure S39. Purity test of compound **D4** by HPLC

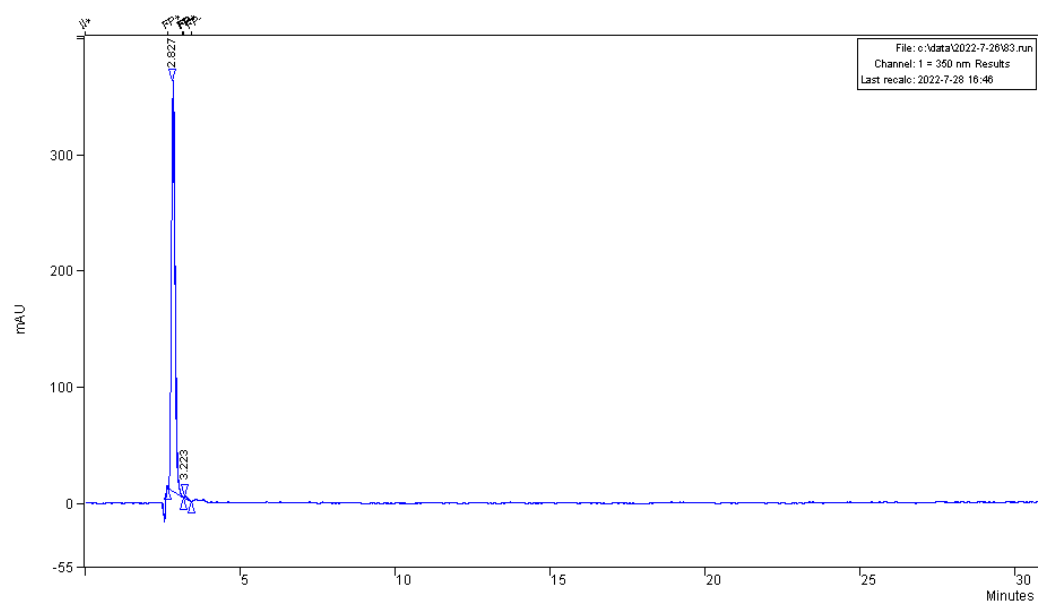


Figure S40. Purity test of compound **D5** by HPLC

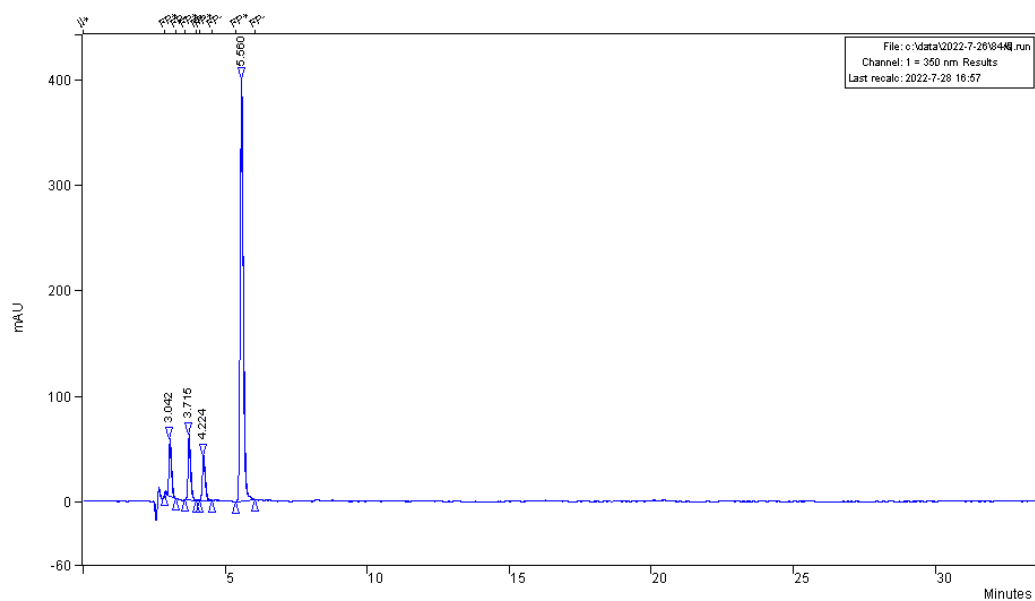


Figure S41. Purity test of compound **D6** by HPLC

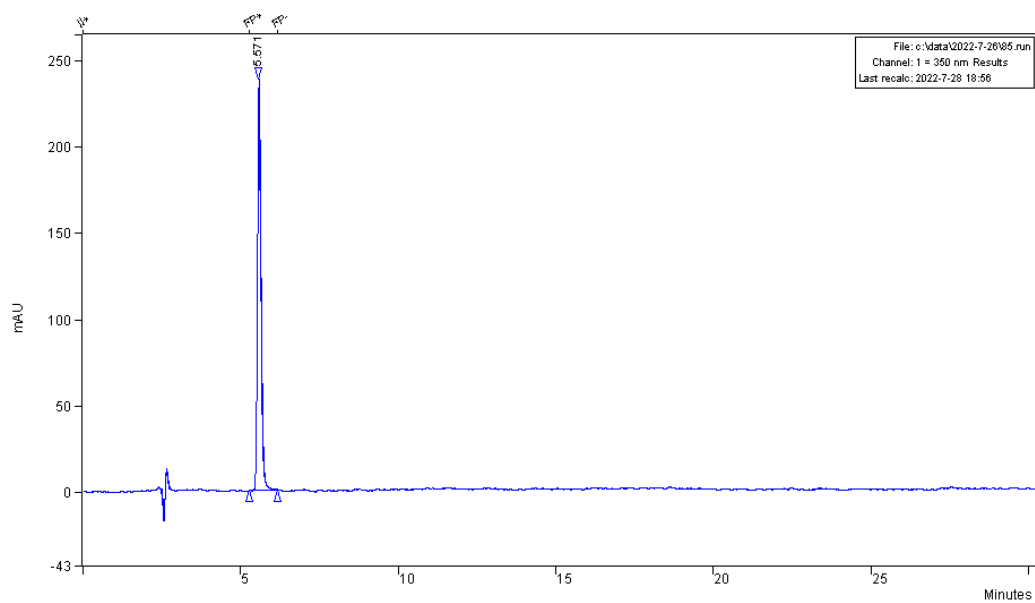


Figure S42. Purity test of compound **E1** by HPLC