Electronic Supplementary Information (ESI)

Synthetic and biochemical studies on the effect of persulfidation on disulfide dimer models of amyloid β42 at position 35 in Alzheimer etiology

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- Figure S1-S3
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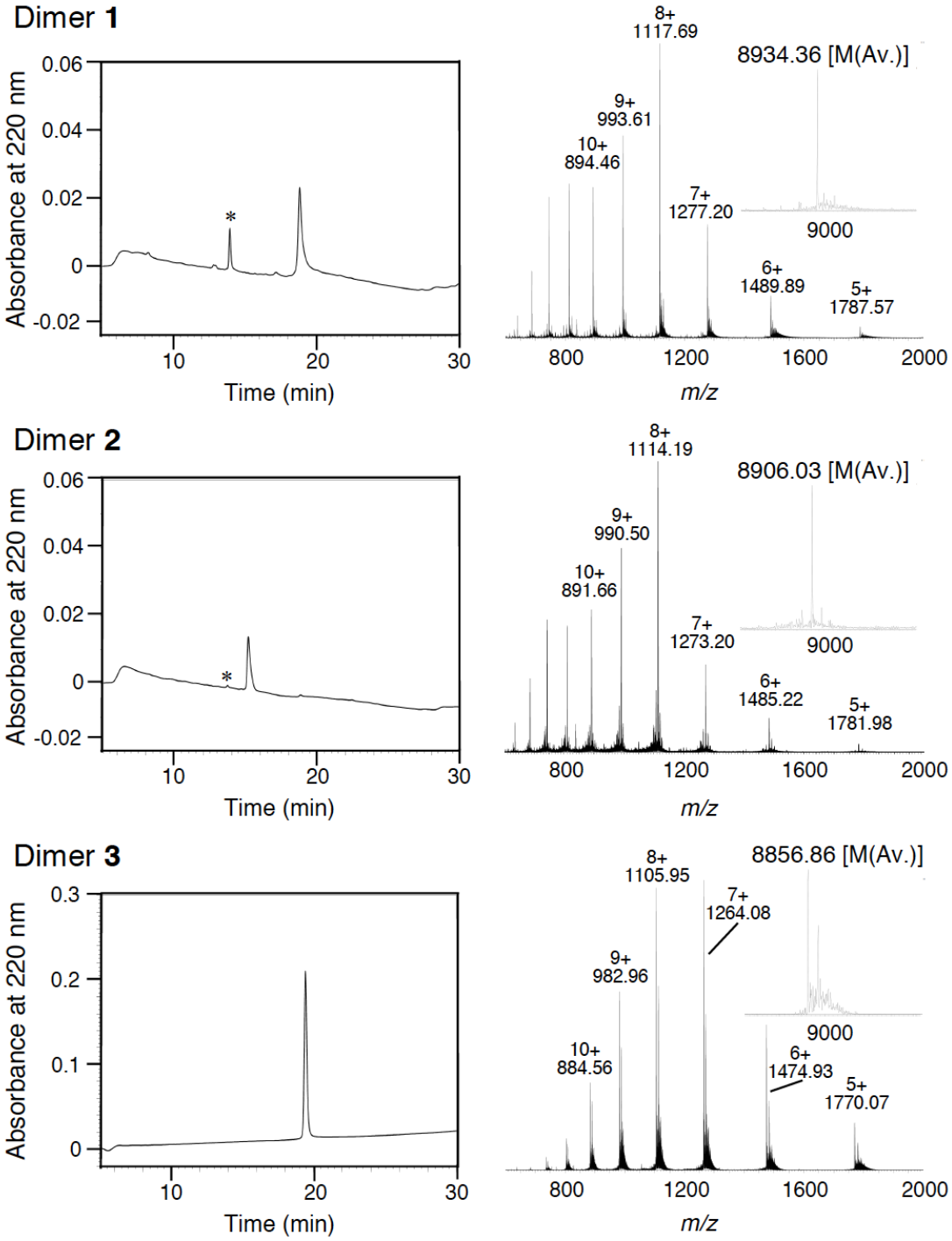

Figure S1 HPLC profiles and ESI-qTOF-MS data of **1**–**3**. HPLC conditions: YMC-Pack ODS–A column (6 mm i.d. x 100 mm), 1 mL/min, UV of 220 nm, 25–60% (**1** and **2**) or 25–50% (**3**) acetonitrile containing 0.1% TFA (30 min linear gradient), 20 µg/20 µL injection (in 0.1% NH_4OH). MS data: (**1**), calculated: 8934.10; observed: 8934.36 [M(ave)]; (**2**), calculated: 8906.14; observed: 8906.03 [M(ave)]; (**3**), calculated: 8856.03; observed: 8856.86 [M(ave)]. Asterisk represents artifact.

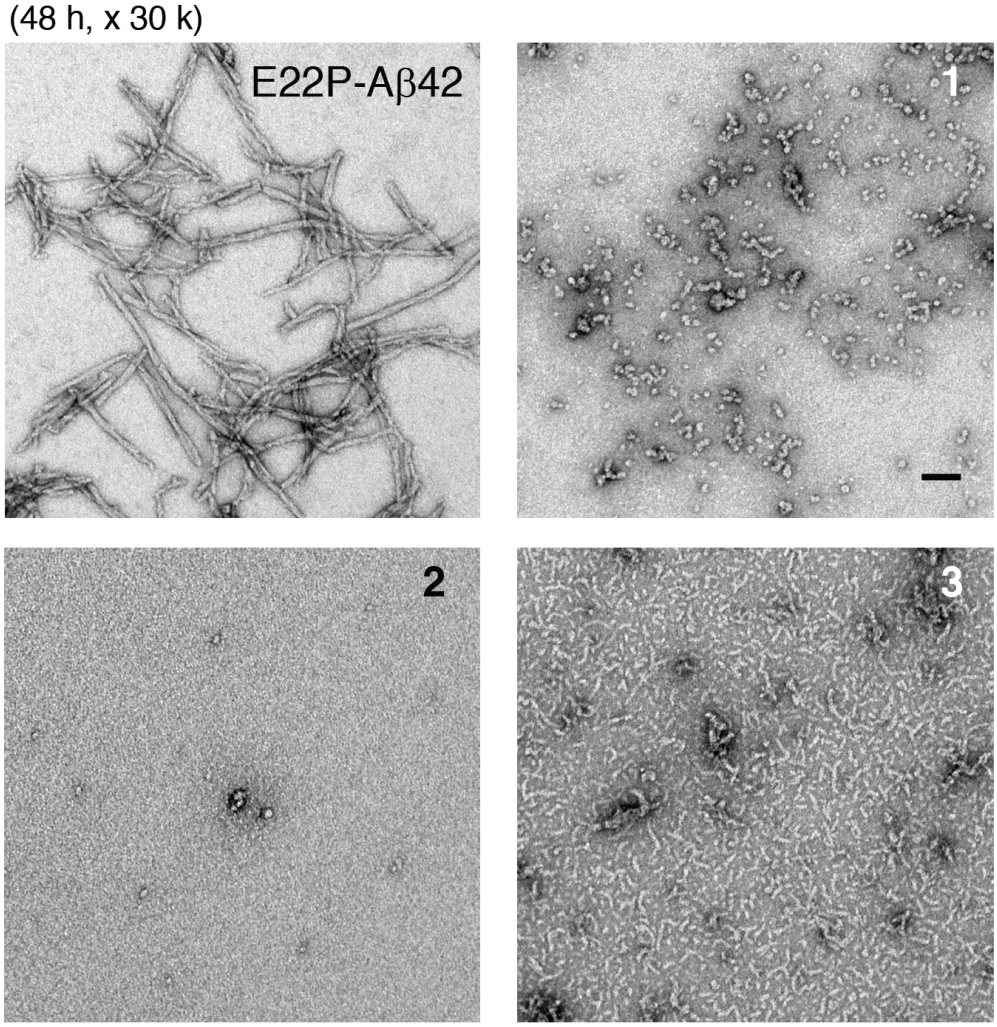

Figure S2 TEM analysis of the aggregates of each Aβ after a 48-h incubation at 37 °C. Scale bar represents 50 nm (magnification: 30 k).

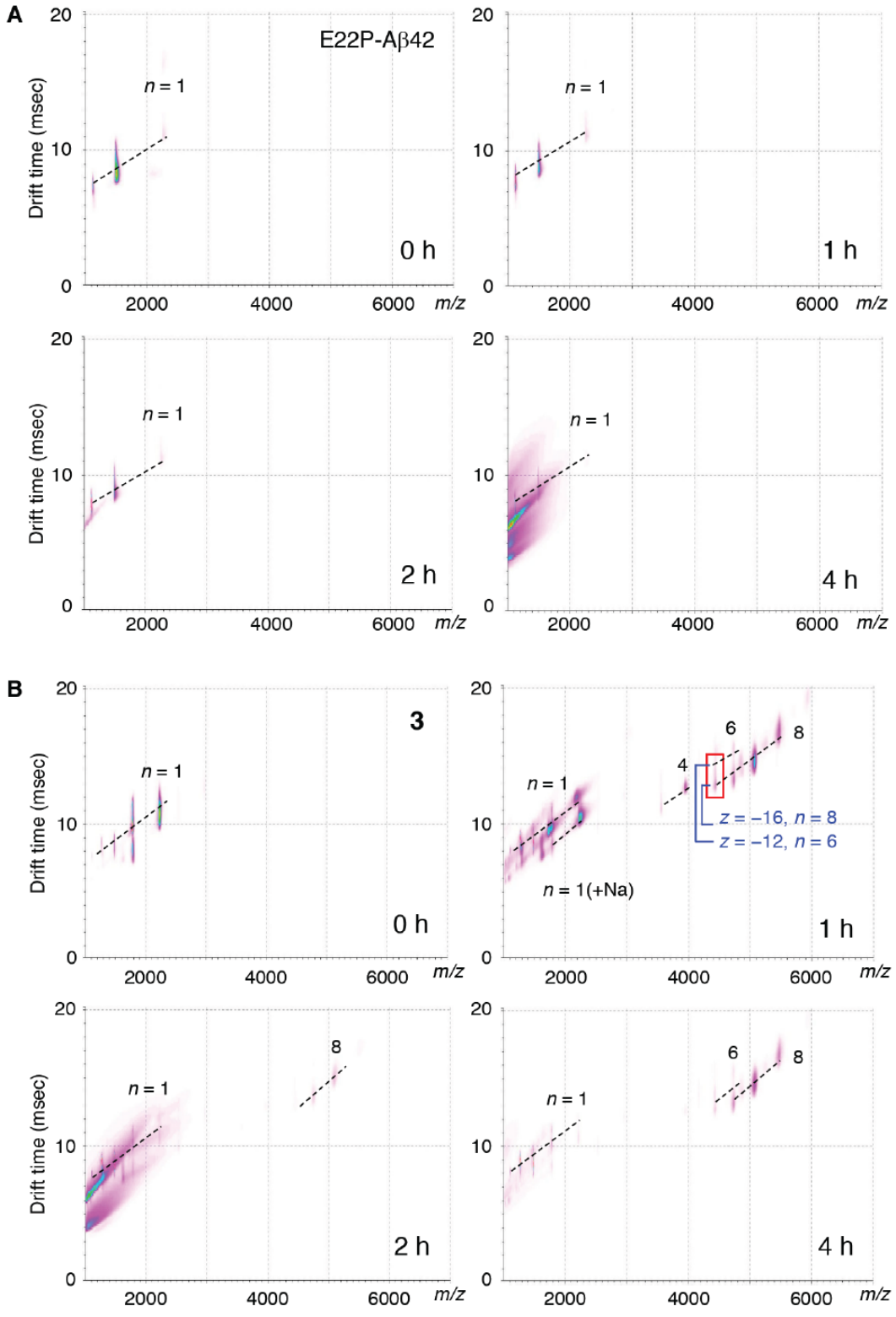

Figure S3 Time-course experiments of IM-MS of E22P-Aβ42 and **3** during 0–4-h incubation in 25 mM ammonium acetate (pH 7.4) at 37 °C. Their spectra during 1-h incubation are also shown in Fig. 3 of the main text. The weak and diffused signals under *m/z* 2000 after a 4-h incubation could be identified from the background signals.

Table S1 The calculated and observed masses of **3** (Figure 3) and E22P-Aβ42 (Figure S2B). The calculated masses matched (*upper table*) and observed masses (*lower table*) are highlighted in yellow.

E22P–M35DAP–Aβ 42 dimer (**3**)

n		1	2	3	4	5	6	7	8	9	10	11
Calculated mass		8856.0	17712.1	26568.1	35424.2	44280.2	53136.2	61992.3	70848.3	79704.4	88560.4	97416.4
z	1	8855.0	17711.1	26567.1	35423.1	44279.2	53135.2	61991.3	70847.3	79703.3	88559.4	97415.4
	2	4427.0	8855.0	13283.1	17711.1	22139.1	26567.1	30995.1	35423.1	39851.2	44279.2	48707.2
	3	2951.0	5903.0	8855.0	11807.0	14759.1	17711.1	20663.1	23615.1	26567.1	29519.1	32471.1
	4	2213.0	4427.0	6641.0	8855.0	11069.0	13283.1	15497.1	17711.1	19925.1	22139.1	24353.1
	5	1770.2	3541.4	5312.6	7083.8	8855.0	10626.2	12397.4	14168.7	15939.9	17711.1	19482.3
	6	1475.0	2951.0	4427.0	5903.0	7379.0	8855.0	10331.0	11807.0	13283.1	14759.1	16235.1
	7	1264.1	2529.3	3794.4	5059.6	6324.7	7589.9	8855.0	10120.2	11385.3	12650.5	13915.6
	8	1106.0	2213.0	3320.0	4427.0	5534.0	6641.0	7748.0	8855.0	9962.0	11069.0	12176.0
	9	983.0	1967.0	2951.0	3935.0	4919.0	5903.0	6887.0	7871.0	8855.0	9839.0	10823.0
	10	884.6	1770.2	2655.8	3541.4	4427.0	5312.6	6198.2	7083.8	7969.4	8855.0	9740.6
	11	804.1	1609.2	2414.3	3219.4	4024.5	4829.6	5634.7	6439.7	7244.8	8049.9	8855.0
	12	737.0	1475.0	2213.0	2951.0	3689.0	4427.0	5165.0	5903.0	6641.0	7379.0	8117.0
	13	680.2	1361.5	2042.7	2723.9	3405.2	4086.4	4767.6	5448.9	6130.1	6811.3	7492.6
	14	631.6	1264.1	1896.7	2529.3	3161.9	3794.4	4427.0	5059.6	5692.2	6324.7	6957.3
	15	589.4	1179.8	1770.2	2360.6	2951.0	3541.4	4131.8	4722.2	5312.6	5903.0	6493.4
	16	552.5	1106.0	1659.5	2213.0	2766.5	3320.0	3873.5	4427.0	4980.5	5534.0	6087.5
	17	519.9	1040.9	1561.8	2082.8	2603.7	3124.7	3645.6	4166.5	4687.5	5208.4	5729.4
	18	491.0	983.0	1475.0	1967.0	2459.0	2951.0	3443.0	3935.0	4427.0	4919.0	5411.0
	19	465.1	931.2	1397.3	1863.4	2329.5	2795.6	3261.7	3727.9	4194.0	4660.1	5126.2
	20	441.8	884.6	1327.4	1770.2	2213.0	2655.8	3098.6	3541.4	3984.2	4427.0	4869.8
	21	420.7	842.4	1264.1	1685.9	2107.6	2529.3	2951.0	3372.7	3794.4	4216.2	4637.9
	22	401.5	804.1	1206.6	1609.2	2011.7	2414.3	2816.8	3219.4	3621.9	4024.5	4427.0
	23	384.0	769.1	1154.1	1539.2	1924.2	2309.3	2694.3	3079.4	3464.4	3849.4	4234.5
	24	368.0	737.0	1106.0	1475.0	1844.0	2213.0	2582.0	2951.0	3320.0	3689.0	4058.0
	25	353.2	707.5	1061.7	1416.0	1770.2	2124.4	2478.7	2832.9	3187.2	3541.4	3895.6
	26	339.6	680.2	1020.8	1361.5	1702.1	2042.7	2383.3	2723.9	3064.5	3405.2	3745.8
	27	327.0	655.0	983.0	1311.0	1639.0	1967.0	2295.0	2623.0	2951.0	3279.0	3607.0
	28	315.3	631.6	947.9	1264.1	1580.4	1896.7	2213.0	2529.3	2845.6	3161.9	3478.2
	29	304.4	609.8	915.1	1220.5	1525.9	1831.3	2136.7	2442.0	2747.4	3052.8	3358.2
	30	294.2	589.4	884.6	1179.8	1475.0	1770.2	2065.4	2360.6	2655.8	2951.0	3246.2

observed	1105.8			3545.8		4432.9		4731.7				
	1264.1			3941.9				5067.4				
	1474.9							5465.0				
	1769.9											
	2212.7											

(continued)

E22P-Aβ42

n		1	2	3	4	5	6	7	8	9	10	11	12
Calculated mass		4482.1	8964.3	13446.4	17928.6	22410.7	26892.8	31375.0	35857.1	40339.3	44821.4	49303.5	53785.7
z	1	4481.1	8963.3	13445.4	17927.6	22409.7	26891.8	31374.0	35856.1	40338.3	44820.4	49302.5	53784.7
	2	2240.1	4481.1	6722.2	8963.3	11204.3	13445.4	15686.5	17927.6	20168.6	22409.7	24650.8	26891.8
	3	1493.0	2987.1	4481.1	5975.2	7469.2	8963.3	10457.3	11951.4	13445.4	14939.5	16433.5	17927.6
	4	1119.5	2240.1	3360.6	4481.1	5601.7	6722.2	7842.7	8963.3	10083.8	11204.3	12324.9	13445.4
	5	895.4	1791.8	2688.3	3584.7	4481.1	5377.6	6274.0	7170.4	8066.8	8963.3	9859.7	10756.1
	6	746.0	1493.0	2240.1	2987.1	3734.1	4481.1	5228.2	5975.2	6722.2	7469.2	8216.2	8963.3
	7	639.3	1279.6	1919.9	2560.2	3200.5	3840.8	4481.1	5121.4	5761.7	6402.1	7042.4	7682.7
	8	559.3	1119.5	1679.8	2240.1	2800.3	3360.6	3920.9	4481.1	5041.4	5601.7	6161.9	6722.2
	9	497.0	995.0	1493.0	1991.1	2489.1	2987.1	3485.1	3983.1	4481.1	4979.1	5477.2	5975.2
	10	447.2	895.4	1343.6	1791.8	2240.1	2688.3	3136.5	3584.7	4032.9	4481.1	4929.3	5377.6
	11	406.5	813.9	1221.4	1628.9	2036.3	2443.8	2851.3	3258.7	3666.2	4073.7	4481.1	4888.6
	12	372.5	746.0	1119.5	1493.0	1866.6	2240.1	2613.6	2987.1	3360.6	3734.1	4107.6	4481.1
	13	343.8	688.6	1033.3	1378.1	1722.9	2067.7	2412.5	2757.2	3102.0	3446.8	3791.6	4136.4
	14	319.1	639.3	959.5	1279.6	1599.8	1919.9	2240.1	2560.2	2880.4	3200.5	3520.7	3840.8
	15	297.8	596.6	895.4	1194.2	1493.0	1791.8	2090.7	2389.5	2688.3	2987.1	3285.9	3584.7
	16	279.1	559.3	839.4	1119.5	1399.7	1679.8	1959.9	2240.1	2520.2	2800.3	3080.5	3360.6
	17	262.6	526.3	790.0	1053.6	1317.3	1580.9	1844.6	2108.2	2371.9	2635.5	2899.2	3162.9
	18	248.0	497.0	746.0	995.0	1244.0	1493.0	1742.0	1991.1	2240.1	2489.1	2738.1	2987.1
	19	234.9	470.8	706.7	942.6	1178.5	1414.4	1650.3	1886.2	2122.1	2358.0	2593.9	2829.8
	20	223.1	447.2	671.3	895.4	1119.5	1343.6	1567.7	1791.8	2016.0	2240.1	2464.2	2688.3
	21	212.4	425.9	639.3	852.7	1066.2	1279.6	1493.0	1706.5	1919.9	2133.3	2346.8	2560.2
	22	202.7	406.5	610.2	813.9	1017.7	1221.4	1425.1	1628.9	1832.6	2036.3	2240.1	2443.8
	23	193.9	388.7	583.6	778.5	973.4	1168.2	1363.1	1558.0	1752.9	1947.7	2142.6	2337.5
	24	185.7	372.5	559.3	746.0	932.8	1119.5	1306.3	1493.0	1679.8	1866.6	2053.3	2240.1
	25	178.3	357.6	536.8	716.1	895.4	1074.7	1254.0	1433.3	1612.6	1791.8	1971.1	2150.4
	26	171.4	343.8	516.2	688.6	860.9	1033.3	1205.7	1378.1	1550.5	1722.9	1895.3	2067.7
	27	165.0	331.0	497.0	663.0	829.0	995.0	1161.0	1327.0	1493.0	1659.0	1825.0	1991.1
	28	159.1	319.1	479.2	639.3	799.4	959.5	1119.5	1279.6	1439.7	1599.8	1759.8	1919.9
	29	153.5	308.1	462.7	617.2	771.8	926.3	1080.9	1235.4	1390.0	1544.6	1699.1	1853.7
	30	148.4	297.8	447.2	596.6	746.0	895.4	1044.8	1194.2	1343.6	1493.0	1642.4	1791.8

observed	2240.1												
	1492.8												
	1191.3												