Supporting information

Materials: Proteasome substrates: Suc-LLVY-AMC, Z-LLE-AMC, Z-VLR-AMC and Ac-ANW-AMC were from Boston Biochem (Cambridge, MA). Human immunoproteasome (isolated from PBMCs) and human constitutive proteasome (isolated from RBCs) were from Boston Biochem Inc. Proteasome-Glo™ Chymotrypsin-Like Cell-Based Assay kit and CellTiter-Glo® Luminescent Cell Viability Assay kits were from Promega (Madison, WI). Human whole blood from 3 TT-responsive donors. Tetanus Toxoid (TT; 0.5mg/ml; LIST Biological Labs 191B). Anti-human CD3 (1.65mg/ml; OKT3; in-house, CR 26Jun2012). Separation Media (SM) is RPMI 1640 (LTI 11875-085) with 2.5mM EDTA (Gibco 15575-038). Lympholyte®-H Lymphocyte Separation Medium (Cedarlane Laboratories CL5020). Complete Media (CM) is RPMI 1640 (LTI 11875-085) with 10% FCS (Gibco 26140), 1% L-glutamine (Gibco 25030-081), 50μg/ml gentamicin (Gibco 15750-060). 96-well round bottom plates (Falcon 3077). Unifilter GF/C plates (Packard 5007185). ^{3}H-thymidine (PerkinElmer Net-027005MC).

IC50 determination

IC_{50} values against β5i and β5c for compounds were carried out in a 96-well format as reported with slight modification.[1] In brief, 1 μL of compound in a 3x series dilution in DMSO at concentration ranging from 100 μM – 0.0017 μM were spotted to the bottom of a black 96-well plate with solid bottom. 100 μL of reaction buffer (20 mM HEPES, 0.5 mM EDTA, pH7.5) containing enzyme (final concentration is 0.2 nM for c-20S, and 0.4 nM for i-20S) and substrate were dispensed into each well, and the plate was then spun at 1000x rpm for 1 minute and followed by shaking on a shaker for 1 minute. Time course of the hydrolysis of each well was followed by recording the fluorescence of product AMC (Ex 360 nm and Em 460 nm) on a SpectraMax M5

plate reader for 1.5 – 2 hours. Initial reaction velocity of each well was fit to a dose-dependent inhibition equation using PRISM to determine the IC50. IC50s were determined only for β5i and β5c. IC50s of compounds < 10 μM were determined three times or more, and IC50s of compounds > 10 μM were determined two times or more. When IC50 is > 100 μM, it is used as 100 μM for the calculation of mean.

Final concentration of activator is 6 nM for PA28α or 0.02% for SDS. Final concentrations of substrates are 15 μM for Ac-WLA-AMC, 12.5 μM for Ac-ANW-AMC, 25 μM for suc-LVY-AMC, 50 μM for Z-VLR-AMC and 50 μM for Z-LLE-AMC. 0.01% BSA was used in the reaction buffer.

Inhibitory activities of β-AA dipeptidomimetics against β1i, β1c, β2i and β2c were tested at 3 concentrations: 100 μM, 33.3 μM and 11.1 μM. All compounds showed < 50% inhibition at 33.3 μM. Hence, the IC50s were presented as > 33.3 μM (Table S1).

Table S1. IC50s of dipeptidomimetics against β1i, β2i, β1c and β2c of human immuno- and constitutive proteasomes

ID	IC50 (μM)			
	β1i Ac-PAL-AMC	β1c Z-LLE-AMC	β2i Z-VLR-AMC	β2c Z-VLR-AMC
P1: β-AA				
PKS2249	> 33.3	> 33.3	> 33.3	> 33.3
PKS2251	> 33.3	> 33.3	> 33.3	> 33.3
PKS2252	> 33.3	> 33.3	> 33.3	> 33.3
PKS2260	> 33.3	> 33.3	> 33.3	> 33.3
PKS2272	> 33.3	> 33.3	> 33.3	> 33.3
PKS2295	> 33.3	> 33.3	> 33.3	> 33.3
PKS3054	> 33.3	> 33.3	> 33.3	> 33.3
P2: β-AA				

PKS2278	> 33.3	> 33.3	> 33.3	> 33.3
PKS2279	> 33.3	> 33.3	> 33.3	> 33.3
P1, P2: β-AAs				
PKS2291	> 33.3	> 33.3	> 33.3	> 33.3
PKS2292	> 33.3	> 33.3	> 33.3	> 33.3

Cytotoxicity of PKS3054

Human peripheral blood mononuclear cells were purified following a reported protocol.[2] PKS3054 and bortezomib (positive control) at designated concentrations in DMSO were spot in wells of a 96-well black plate with clear bottom. 50 µL of plasma were added to each wells, and 50 µL of PBMCs 2 x 10^6 cells / mL in plasma were then added to each well. DMSO was constant at 1% in each well. The cells were incubated at 37°C 5% CO_2 for 5 days. Cell viability was determined with CellTiter-Glo® Luminescent Cell Viability Assay (Promega).

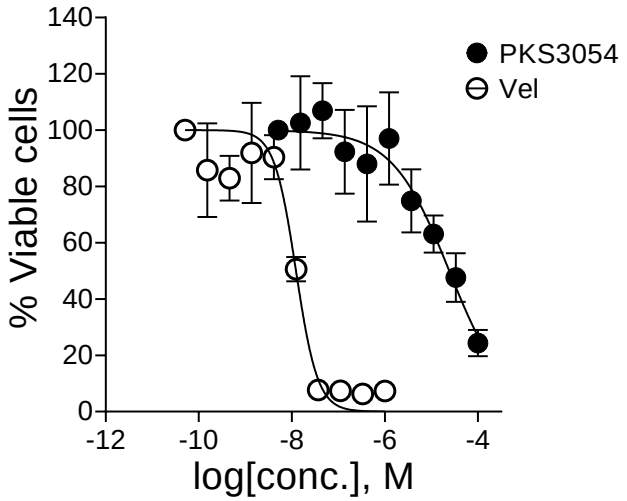


Figure S1. Cytotoxicity of PKS3054 against peripheral blood mononuclear cells. Velcade was used as positive control. Data is a representative of three independent experiments. Cell viability were determined by a CellTiter-Glo® after 5 days.

Human PBMC Proliferation Assay

Informed consents were obtained from blood donors after the nature and possible consequences of the studies were explained.

PBMC Isolation- EDTA-treated blood from donors was separated by Ficoll as follows: The syringes of blood were inverted to mix and divided equally among 50ml tubes (~20ml/tube) containing 20ml SM. 10ml of Ficoll was under laid in each tube. Tubes were spun at 1800 rpm for 20 min (low brake). The interfaces from each two tubes were combined into one 50ml tube, brought up to 45ml with SM and spun at 1700 rpm for 8 min. Supernatant was aspirated; and cells were resuspended in 45ml SM and spun at 1100 rpm (to remove platelets) for 8 min. Cells were then resuspended in CM at 1 x 10^6 cells/mL.

Methods:

PKS3054 was diluted to 10x (3µM final top concentration) 3µl + 7µl DMSO then 6µl + 594µl CM, and then serially diluted 1:3.3333 (135µl + 315µl 1% DMSO/CM). 10µl of each appropriate dilution was added to the appropriate wells (see plate maps). The PBMC cells in CM at 1 x 10^6/mL. 100µl/well (100,000 cells/well) was then added to the appropriate wells of the plates and were incubated for 1hr at 37ºC, 5% CO_2 prior to adding the stimuli: TT was diluted 1:25 to 4x (720µl + 17.3ml 0.1% DMSO/CM = 5µg/ml final), and 50µl/well was then added to the appropriate wells of the plates; or Anti-human CD3 (OKT3) was diluted 1 µg/ml and 50µl/well was then added to the appropriate wells of the plates (0.5 µg/mL final). All wells were brought up to 200µl with 0.1% DMSO/CM. The plates were incubated at 37ºC, 5% CO_2 for 5 days. On the fifth day, 100µl supernatant was removed from each well, and 0.5µCi of ^{3}H-Thymidine in 100µl CM was added to each well of the PBMC assay plates, and incubated for 6 hours. The assay plates were harvested on a Packard Filtermate Harvester according to the manufacturer's instruction. The plates were

dried overnight at room temperature or for 1hr in a 37ºC vacuum oven and then 50µl/well PerkinElmer Microscint-20 scintillant was added. The plates were then counted on a Packard TopCount scintillation counter.

Plate map for assay of Tetanus Toxoid-specific human PBMC Proliferation

33.33333												
11.11111												
3.703704												
1.234568												
0.411523												
0.137174												
0.045725												
0.015242												
0.005081												

Plate map for assay of anti-human CD3 antibody stimulated human PBMC Proliferation

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
A												
B		3000 nM	900 nM	270 nM	81 nM	24 nM	7.29 nM	2.19 nM	0.56 nM	PBMC + xCD3	PBMC only	
C		"	"	"	"	"	"	"	"	"	"	
D		"	"	"	"	"	"	"	"	"	"	
E												
F												
G												
H												

Computational docking study

A homology model of human β5iβ6 dimer was constructed with Modeller,[3] using the crystal structure of mouse i-20S (PDB: 3UNF) as the template. The docking study of compounds PKS2279 and PKS2252 in the binding site of the human β5iβ6 model was carried out with the

core-restrained induce-fit protocol[4] in Schrödinger software (release 2016-1; Schrödinger, LLC: New York, NY), using the OPLS3 force-field.[5] The top ranked poses were further optimized by iterations of manual adjustments using the crystal structure of the yeast 20S with compound 16 as the template [6] and energy minimizations.

Synthesis and characterization

Chemicals and Spectroscopy: Unless otherwise stated, all commercially available materials were purchased from Bachem, Aldrich, P3 BioSystems, or other vendors and were used as received. All non-aqueous reactions were performed under argon in oven-dried glasswares. Routine monitoring of reactions was performed using Waters Acquity Ultra Performance Liquid Chromatography (UPLC). All HPLC purifications were done by Varian PrepStar HPLC system or Waters Autopure (mass directed purification system) using Prep C18 5μm OBD (19 X 150 mm) column. Purity of each final compound was determined on a Waters HPLC equipped with a Waters 2420 ELS (Evaporative Light Scattering) Detector and an XBridge^{TM} C18 5μM 4.6x150 mm column. The purity was calculated by integration of peak area in ELSD spectra and listed in Table S2 (see HPLC). ^{1}H- and ^{13}C- NMR spectra were acquired on a Bruker DRX-500 spectrometer. Chemical shifts δ are expressed in parts per million, with the solvent resonance as an internal standard (chloroform-*d*, ^{1}H: 7.26; ^{13}C: 77.16 ppm; DMSO-*d6*, ^{1}H: 2.50 ppm; ^{13}C: 39.52 ppm). Hexafluorobenzene was used as internal standard for ^{19}F NMR. NMR data are reported as following: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constant, and integration.

General Procedure for HATU Coupling: Carboxylic acid (1.0 eq.), *O*-(7-Azabenzotriazol-1-yl)-*N*,*N*,*N*,*N*'-tetramethyluronium hexafluorophosphate (HATU) (1.2 eq.) and 1-Hydroxy-7-

Azabenzotriazole (HOAt) 0.6M in DMF (1.0 eq.) were dissolved in DMF under argon atmosphere. The solution was cooled to 0 °C and amine was added. After stirring for 5 minutes at 0 °C, Hünig's base (3 - 4 eq.) was added. The reaction mixture was stirred at 0 °C for 1 hr. After completion of reaction (1 h, monitored by LCMS), water (10 mL) was added to quench the reaction and the mixture was further stirred for 30 minutes. Product was isolated either by ethyl acetate extraction or filtering the precipitate.

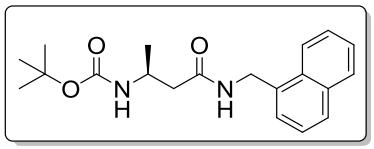
General Procedure for EDC Coupling: Carboxylic acid (1.0 eq.), *N*-(3-Dimethylaminopropyl)-*N′*-ethylcarbodiimide hydrochloride (EDC) (1.2 eq.) and 1-hydroxybenzotriazole (HOBt) (1.3 eq.) were dissolved in DMF under argon atmosphere. The solution was cooled to 0 °C and *t*-butylamine was added. After stirring for 5 minutes at 0 °C, Hünig's base (2 – 3 eq.) was added. The reaction mixture was allowed to warm to room temperature gradually and stirred at room temperature overnight. Product was isolated either by ethyl acetate extraction or filtering the precipitate.

General Procedure for Boc-Deprotection: The substrate was dissolved in dichloromethane and the solution was cooled to 0 °C. Trifluoroacetic acid (20% v/v with respect to dichloromethane) was added to the solution drop wise at 0 °C with constant stirring. The mixture was allowed to warm to room temperature slowly (over a period of 1 hour), and stirred until the completion of reaction (monitored by LCMS). Excess trifluoroacetic acid and dichloromethane were removed under vacuum and crude was dried under vacuum.

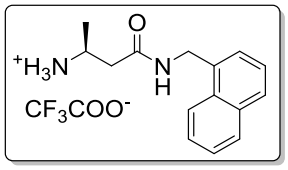
General Procedure for *O*-Debenzylation: The substrate was dissolved in methanol. Palladium on carbon (10%) was added carefully. Residual air from the flask was removed and the mixture was stirred at room temperature for 3 – 4 hours under hydrogen atmosphere using a hydrogen

balloon. After completion of reaction, the mixture was filtered through celite. Filtrate was evaporated and dried under vacuum to give product.

General Procedure for *N*-Sulfonamide Preparation of Amines: The primary amine (generally TFA salt) was dissolved in dichloromethane. The solution was cooled to 0 °C and triethylamine (2.0 – 3.0 eq.) was added. Sulfonyl chloride (1.5 eq.) was added to the solution in one portion and reaction mixture was warmed to room temperature (over 15 minutes). After completion of reaction (2 - 3 h), dichloromethane was evaporated and crude was purified by HPLC to give pure product.

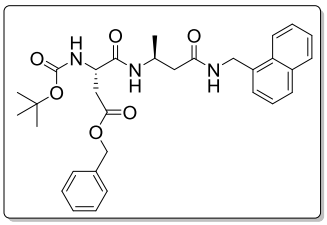


***t*-butyl (*S*)-(4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)carbamate (PKS2261)**: The title compound was synthesized by following the general protocol for HATU mediated coupling of Boc-L-β-homoalanine and 1-naphthylmethylamine on a 1.5 mmol scale. After completion of reaction, water was added to reaction mixture to give white precipitate. Precipitate was filtered, washed with water and dried in air to give product (490 mg, 95%) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.38 (t, J = 5.7 Hz, 1H), 8.06 – 8.04 (m, 1H), 7.95 – 7.93 (m, 1H), 7.86 – 7.84 (m, 1H), 7.56 – 7.52 (m, 2H), 7.48 – 7.42 (m, 2H), 6.72 (d, J = 8.3 Hz, 1H), 4.76 – 4.68 (m, 2H), 3.89 – 3.80 (m, 1H), 2.35 (dd, J = 13.9, 5.7 Hz, 1H), 2.18 (dd, J = 13.9, 8.2 Hz, 1H), 1.37 (s, 9H), 1.01 (d, J = 6.5 Hz, 3H).

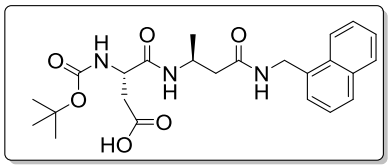


(*S*)-3-amino-*N*-(naphthalen-1-ylmethyl)butanamide 2,2,2-trifluoroacetate (PKS2245): The title compound was prepared by following the general protocol for Boc-deprotection of PKS2261 (480 mg, 1.40 mmol). The crude yellow paste was triturated with diethyl ether and kept standing overnight. The white solid was filtered and dried to give product (480 mg, 96%). ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.69 (t, J = 5.7 Hz, 1H), 8.06 – 8.05 (m, 1H), 7.97 – 7.95 (m, 1H), 7.88 (dd, J = 7.4, 2.0 Hz,

1H), 7.80 (bs, 3H), 7.58 – 7.53 (m, 2H), 7.50 – 7.45 (m, 2H), 4.79 (dd, *J* = 15.0, 5.7 Hz, 1H), 4.73 (dd, *J* = 15.0, 5.5 Hz, 1H), 3.57 – 3.50 (m, 1H), 2.51 – 2.43 (m, 2H), 1.17 (d, *J* = 6.5 Hz, 3H).

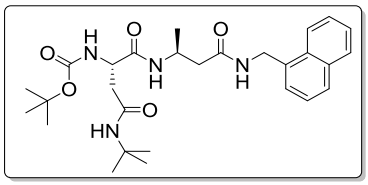


Benzyl (*S*)-3-((*t*-butoxycarbonyl)amino)-4-(((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)amino)-4-oxobutanoate (PKS2265): The title compound was synthesized by following the general protocol for HATU mediated coupling of Boc-Asp(OBn)-OH (142.3 mg, 0.44 mg) and PKS2245 (143 mg, 0.40 mmol). After completion of reaction, water was added to reaction mixture to give white precipitate. Precipitate was filtered, washed with water and dried in air to give product (202 mg, 92%) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.41 (t, *J* = 5.8 Hz, 1H), 8.06 – 8.04 (m, 1H), 7.95 – 7.93 (m, 1H), 7.86 (d, *J* = 8.3 Hz, 1H), 7.84 (d, *J* = 7.7 Hz, 1H), 7.56 – 7.51 (m, 2H), 7.47 – 7.42 (m, 2H), 7.36 – 7.29 (m, 5H), 7.11 (d, *J* = 8.3 Hz, 1H), 5.10 – 5.05 (m, 2H), 4.76 – 4.68 (m, 2H), 4.30 – 4.25 (m, 1H), 4.14 – 4.08 (m, 1H), 2.73 – 2.69 (m, 1H), 2.57 (dd, *J* = 16.1, 8.8 Hz, 1H), 2.34 (dd, *J* = 14.1, 5.6 Hz, 1H), 2.23 (dd, *J* = 14.1, 7.5 Hz, 1H), 1.37 (s, 9H), 1.03 (d, *J* = 6.6 Hz, 3H).

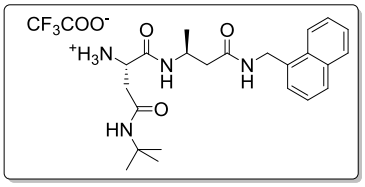


(*S*)-3-((*t*-butoxycarbonyl)amino)-4-(((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)amino)-4-oxobutanoic acid (PKS2267): The title compound was synthesized by following the *O*-debenzylation protocol of PKS2265 (202 mg, 0.37 mmol). Product (168 mg, quant.) was isolated as white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.44 – 8.41 (m, 1H), 8.06 – 8.04 (m, 1H), 7.95 – 7.94 (m, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 8.3 Hz, 1H), 7.57 – 7.52 (m, 2H), 7.48 – 7.43 (m, 2H), 7.02 (d, *J* = 8.2 Hz, 1H), 4.75 (dd, *J* = 15.1, 5.7 Hz, 1H), 4.70 (dd, *J* = 15.1, 5.7 Hz, 1H), 4.21 – 4.16 (m, 1H), 4.13 – 4.08 (m, 1H), 2.58 (dd, *J* = 16.4, 5.1 Hz, 1H), 2.43 (dd, *J*

= 16.4, 8.5 Hz, 1H), 2.35 (dd, *J* = 14.1, 5.4 Hz, 1H), 2.23 (dd, *J* = 14.1, 7.7 Hz, 1H), 1.38 (s, 9H), 1.03 (d, *J* = 6.6 Hz, 3H).

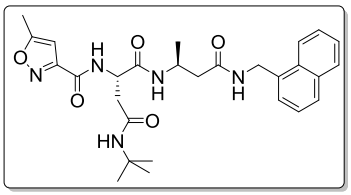


***t*-butyl ((*S*)-4-(*t*-butylamino)-1-(((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)amino)-1,4-dioxobutan-2-yl)carbamate** (PKS2272): The title compound was synthesized following the general protocol of EDC mediated coupling of PKS2267 (168 mg, 0.367 mmol) and *t*-butyl amine (58 μL, 0.551 mmol). A white precipitate appeared which was filtered, washed with water and dried in air to give product (170 mg, 90%) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.43 (t, *J* = 5.6 Hz, 1H), 8.06 – 8.04 (m, 1H), 7.95 – 7.94 (m, 1H), 7.86 – 7.81 (m, 2H), 7.57 – 7.52 (m, 2H), 7.48 – 7.43 (m, 2H), 7.34 (s, 1H), 6.76 (d, *J* = 8.3 Hz, 1H), 4.75 (dd, *J* = 15.1, 5.7 Hz, 1H), 4.70 (dd, *J* = 15.1, 5.5 Hz, 1H), 4.19 – 4.07 (m, 2H), 2.36 – 2.21 (m, 4H), 1.37 (s, 9H), 1.22 (s, 9H), 1.03 (d, *J* = 6.6 Hz, 3H). HRMS calc. for C28H40N4O5Na [M+Na]+: 535.2883. Found: 535.2896.

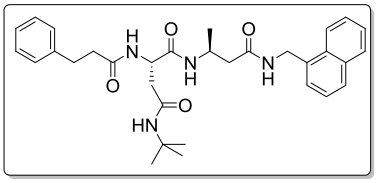


(*S*)-2-amino-*N*^{4}-(*t*-butyl)-*N*^{1}-((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)succinamide 2,2,2-trifluoroacetate (PKS2248): The title compound was prepared by following the general protocol for Boc-Deprotection of PKS2272 (62 mg, 0.12 mmol). The crude was treated with diethyl ether and kept standing 3 hours. The white solid was filtered and dried to give product (60 mg, 95%). ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.47 (t, *J* = 5.6 Hz, 1H), 8.32 (d, *J* = 7.9 Hz, 1H), 8.06 – 8.03 (m, 4H), 7.96 – 7.95 (m, 1H), 7.87 – 7.85 (m, 1H), 7.80 (s, 1H), 7.57 – 7.53 (m, 2H), 7.49 – 7.43 (m, 2H), 4.78 (dd, *J* = 15.1, 5.8 Hz, 1H), 4.69 (dd, *J* = 15.1, 5.4 Hz, 1H),

4.21 – 4.13 (m, 1H), 3.95 (m, 1H), 2.60 (dd, *J* = 16.7, 4.6 Hz, 1H), 2.55 – 2.49 (m, 1H), 2.34 (dd, *J* = 14.1, 5.7 Hz, 1H), 2.26 (dd, *J* = 14.1, 8.0 Hz, 1H), 1.26 (s, 9H), 1.07 (d, *J* = 6.6 Hz, 3H).

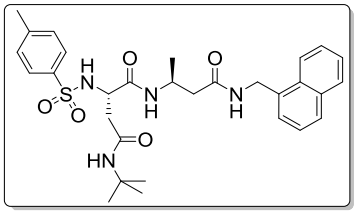


(*S*)-*N*^{4}-(*t*-butyl)-2-(5-methylisoxazole-3-carboxamido)-*N*^{1}-((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)succinamide (PKS2249): The title compound was prepared by following the general protocol for HATU mediated coupling of 5-methylisoxazole-3-carboxylic acid (5.6 mg, 0.044 mmol) and PKS2248 (21.1 mg, 0.04 mmol). After completion of reaction, the mixture was purified by HPLC to give pure product (14.4 mg, 69%) as white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.50 (d, *J* = 8.1 Hz, 1H), 8.41 (t, *J* = 5.7 Hz, 1H), 8.05 – 8.03 (m, 1H), 7.99 (d, *J* = 8.1 Hz, 1H), 7.95 – 7.93 (m, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.57 – 7.51 (m, 2H), 7.48 – 7.42 (m, 3H), 6.53 (s, 1H), 4.74 (dd, *J* = 15.1, 5.7 Hz, 1H), 4.68 (dd, *J* = 15.1, 5.5 Hz, 1H), 4.63 (td, *J* = 8.4, 4.8 Hz, 1H), 4.16 – 4.08 (m, 1H), 2.54 (dd, *J* = 14.3, 8.7 Hz, 1H), 2.45 (s, 3H), 2.41 (dd, *J* = 14.3, 4.8 Hz, 1H), 2.35 (dd, *J* = 14.0, 5.7 Hz, 1H), 2.25 (dd, *J* = 14.0, 7.7 Hz, 1H), 1.18 (s, 9H), 1.04 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (126 MHz, DMSO) δ 171.3, 169.9, 169.2, 168.9, 158.6, 158.2, 134.6, 133.3, 130.9, 128.5, 127.6, 126.2, 125.8, 125.6, 125.4, 123.5, 101.4, 50.5, 50.1, 42.6, 41.6, 40.2, 38.3, 28.4, 20.0, 11.9. HRMS calc. for C28H35N5O5Na [M+Na]+: 544.2536. Found: 544.2537.



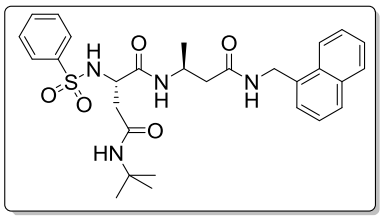
(*S*)-*N*^{4}-(*t*-butyl)-*N*^{1}-((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)-2-(3-phenylpropanamido)succinamide (PKS2251): The title compound was prepared by following the general protocol for HATU mediated coupling of 3-phenylpropanoic acid (5.0 mg, 0.033 mmol) and PKS2248 (15.8 mg, 0.03 mmol). After completion of reaction, the mixture was purified by

HPLC to give pure product (14.3 mg, 88%) as white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.44 (t, *J* = 5.7 Hz, 1H), 8.06 – 8.04 (m, 1H), 7.99 (d, *J* = 8.1 Hz, 1H), 7.95 – 7.93 (m, 1H), 7.86 – 7.83 (m, 2H), 7.57 – 7.53 (m, 2H), 7.49 – 7.43 (m, 2H), 7.33 (s, 1H), 7.26 – 7.23 (m, 2H), 7.20 – 7.14 (m, 3H), 4.75 (dd, *J* = 15.1, 5.7 Hz, 1H), 4.71 (dd, *J* = 15.1, 5.6 Hz, 1H), 4.48 (td, *J* = 8.2, 5.6 Hz, 1H), 4.14 – 4.06 (m, 1H), 2.82 – 2.78 (m, 2H), 2.44 – 2.33 (m, 4H), 2.29 (dd, *J* = 14.6, 8.3 Hz, 1H), 2.23 (dd, *J* = 14.1, 7.8 Hz, 1H), 1.21 (s, 9H), 1.03 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (126 MHz, DMSO) δ 171.1, 170.0, 169.9, 168.7, 141.3, 134.6, 133.3, 130.9, 128.5, 128.3, 128.1, 127.6, 126.2, 125.8, 125.8, 125.6, 125.4, 123.5, 50.1, 50.0, 42.3, 41.5, 40.2, 38.7, 36.9, 31.0, 28.4, 19.9. HRMS calc. for C32H40N4O4Na [M+Na]+: 567.2947. Found: 567.2961.

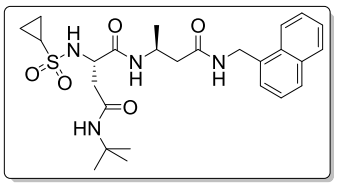


(*S*)-*N*^{4}-(*t*-butyl)-2-((4-methylphenyl)sulfonamido)-*N*^{1}-((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)succinamide (PKS2252): The title compound was prepared by following the general procedure for *N*-sulfonamide formation of PKS2248 (21.1 mg, 0.04 mmol) with tosyl chloride (11.5 mg, 0.06 mmol). The product was isolated as white solid (12.7 mg, 56%) after HPLC purification. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.38 (t, *J* = 5.7 Hz, 1H), 8.05 – 8.03 (m, 1H), 7.95 – 7.93 (m, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.71 (bs, 1H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.56 – 7.52 (m, 2H), 7.48 – 7.41 (m, 2H), 7.32 – 7.29 (m, 3H), 4.73 (dd, *J* = 15.1, 5.7 Hz, 1H), 4.68 (dd, *J* = 15.1, 5.6 Hz, 1H), 4.01 (m, 1H), 3.94 – 3.85 (m, 1H), 2.33 (s, 3H), 2.29 – 2.15 (m, 3H), 2.11 (dd, *J* = 14.1, 8.2 Hz, 1H), 1.18 (s, 9H), 0.83 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (126 MHz, DMSO) δ 169.7, 168.9, 168.0, 142.4, 138.3, 134.6, 133.3, 130.9, 129.2, 128.5, 127.6,

126.6, 126.2, 125.8, 125.6, 125.4, 123.5, 53.6, 50.1, 42.2, 41.5, 40.1, 39.4, 28.4, 20.9, 19.4. HRMS calc. for C30H38N4O5SNa [M+Na]+: 589.2461. Found: 589.2432.

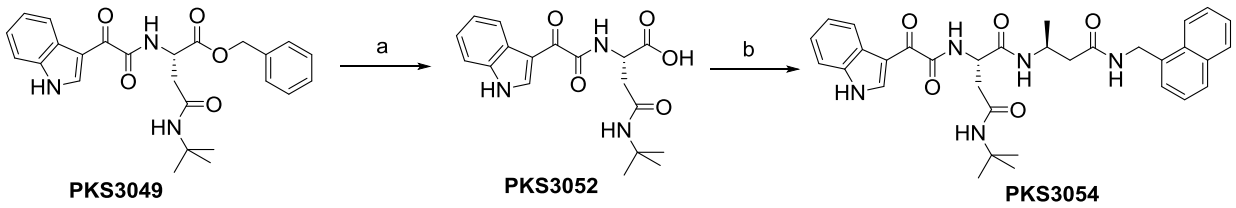


(*S*)-*N*^{4}-(*t*-butyl)-*N*^{1}-((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)-2-(phenylsulfonamido)succinamide (PKS2260): The title compound was prepared by following the general procedure for *N*-sulfonamide formation of PKS2248 (12.1 mg, 0.023 mmol) with phenylsulfonyl chloride (4 μL, 0.028 mmol). The product was isolated as white solid (10.0 mg, 79%) after HPLC purification. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.37 (t, *J* = 5.7 Hz, 1H), 8.04 – 8.02 (m, 1H), 7.95 – 7.93 (m, 1H), 7.85 – 7.81 (m, 3H), 7.77 (d, *J* = 7.6 Hz, 2H), 7.60 – 7.41 (m, 7H), 7.32 (s, 1H), 4.73 (dd, *J* = 15.1, 5.8 Hz, 1H), 4.68 (dd, *J* = 15.1, 5.5 Hz, 1H), 4.07 – 4.03 (m, 1H), 3.92 – 3.86 (m, 1H), 2.28 – 2.17 (m, 3H), 2.12 (dd, *J* = 14.1, 8.3 Hz, 1H), 1.18 (s, 9H), 0.83 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 169.7, 168.8, 168.0, 141.2, 134.6, 133.3, 132.2, 130.9, 128.8, 128.5, 127.6, 126.5, 126.2, 125.8, 125.6, 125.4, 123.5, 53.6, 50.1, 42.2, 41.6, 40.1, 39.7, 28.4, 19.5. HRMS calc. for C29H36N4O5SNa [M+Na]+: 575.2304. Found: 575.2314.

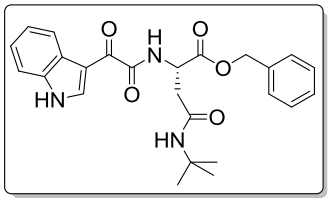


(*S*)-*N*^{4}-(*t*-butyl)-2-(cyclopropanesulfonamido)-*N*^{1}-((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)succinamide (PKS2295): The title compound was prepared by following the general procedure for *N*-sulfonamide formation of PKS2248 (21.1 mg, 0.04 mmol) with cyclopropylsulfonyl chloride (6 μL, 0.06 mmol). The product was isolated as white solid (16.3 mg, 79%) after HPLC purification. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.42 (t, *J* = 5.6 Hz, 1H), 8.06 – 8.04 (m, 1H), 7.97 – 7.94 (m, 2H), 7.85 (d, *J* = 7.9 Hz, 1H), 7.57 – 7.52 (m, 2H), 7.48 – 7.43 (m,

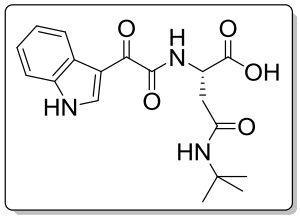
2H), 7.40 (s, 1H), 7.26 (d, *J* = 9.1 Hz, 1H), 4.75 (dd, *J* = 15.1, 5.7 Hz, 1H), 4.70 (dd, *J* = 15.1, 5.5 Hz, 1H), 4.17 – 4.06 (m, 2H), 2.50 – 2.46 (m, 1H), 2.41 – 2.32 (m, 3H), 2.25 (dd, *J* = 14.1, 8.0 Hz, 1H), 1.23 (s, 9H), 1.04 (d, *J* = 6.6 Hz, 3H), 0.90 – 0.82 (m, 4H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 169.9, 169.7, 168.4, 134.6, 133.3, 130.9, 128.5, 127.6, 126.2, 125.8, 125.6, 125.4, 123.5, 53.7, 50.1, 42.4, 41.6, 40.1, 39.8, 30.3, 28.5, 19.8, 5.1, 4.8. HRMS calc. for C28H40N4O5Na [M+Na]+: 535.2896. Found: 535.2883.



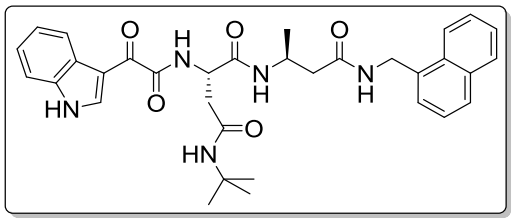
Scheme S1. Synthetic route of PKS3054. Reagents and conditions: a) Pd/C (10%), H_2, methanol; b) **PKS2245**, HATU, HOAt, Hünig's base, DMF



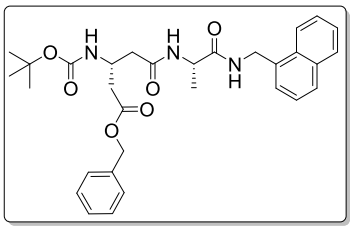
Benzyl N^2-(2-(1H-indol-3-yl)-2-oxoacetyl)-N^4-(*t*-butyl)-*L*-asparaginate (PKS3049): The title compound was synthesized following the general protocol for HATU mediated coupling of 3-indoleglyoxylic acid (189 mg, 1.0 mmol) and H-Asn(*t*-Bu)-OH.TFA salt (432 mg, 1.1 mmol). The compound was isolated by ethyl acetate extraction and purified by column chromatography to give product (270 mg, 60%) as off-white solid. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 10.14 (s, 1H), 9.13 (d, *J* = 3.3 Hz, 1H), 8.42 – 8.34 (m, 2H), 7.47 (dd, *J* = 6.6, 2.3 Hz, 1H), 7.34 – 7.23 (m, 7H), 5.54 (s, 1H), 5.23 (d, *J* = 12.4 Hz, 1H), 5.19 – 5.12 (m, 1H), 5.11 – 5.03 (m, 1H), 2.80 (dd, *J* = 15.2, 5.8 Hz, 1H), 2.74 (dd, *J* = 15.2, 5.3 Hz, 1H), 1.29 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 179.6, 170.8, 168.8, 162.6, 139.3, 136.2, 135.3, 128.7, 128.6, 128.4, 126.9, 124.1, 123.3, 122.4, 113.1, 112.1, 67.7, 52.0, 49.6, 39.2, 28.8.



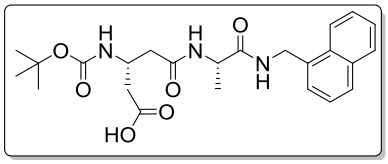
N^2-(2-(1H-indol-3-yl)-2-oxoacetyl)-N^4-(*t*-butyl)-*L*-asparagine (PKS3052): The title compound was synthesized following the general protocol for *O*-debenzylation of PKS3049 (265 mg, 0.59 mmol). Isolated crude was purified by HPLC to give product (112 mg, 53%) as off-white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.81 (s, 1H), 12.27 (d, *J* = 3.3 Hz, 1H), 8.82 – 8.75 (m, 2H), 8.26 – 8.20 (m, 1H), 7.57 (s, 1H), 7.56 – 7.52 (m, 1H), 7.32 – 7.23 (m, 2H), 4.69 – 4.60 (m, 1H), 2.67 (dd, *J* = 15.1, 7.2 Hz, 1H), 2.59 (dd, *J* = 15.1, 5.0 Hz, 1H), 1.22 (s, 9H). ^{13}C NMR (126 MHz, DMSO) δ 181.2, 172.3, 168.8, 162.8, 138.6, 136.2, 126.1, 123.5, 122.7, 121.2, 112.6, 112.1, 50.2, 49.0, 37.2, 28.4.



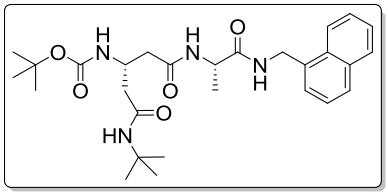
(S)-2-(2-(1H-indol-3-yl)-2-oxoacetamido)-N^4-(*t*-butyl)-N^1-((S)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)succinamide (PKS3054): The title compound was synthesized by following the general protocol for HATU mediated coupling of PKS3052 (7.2 mg, 0.02) and PKS2245 (7.8 mg, 0.022 mmol). The reaction mixture was purified by HPLC to give product (4.0 mg, 34%) as white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.24 (d, *J* = 3.6 Hz, 1H), 8.81 (d, *J* = 3.1 Hz, 1H), 8.70 (d, *J* = 8.4 Hz, 1H), 8.41 (t, *J* = 5.7 Hz, 1H), 8.28 – 8.21 (m, 1H), 8.02 (dd, *J* = 6.3, 3.4 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.93 (dd, *J* = 6.2, 3.4 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.58 – 7.48 (m, 4H), 7.48 – 7.37 (m, 2H), 7.31 – 7.23 (m, 2H), 4.74 (dd, *J* = 15.2, 5.7 Hz, 1H), 4.67 (dd, *J* = 15.2, 5.5 Hz, 1H), 4.62 – 4.54 (m, 1H), 4.20 – 4.09 (m, 1H), 2.59 (dd, *J* = 14.5, 8.4 Hz, 1H), 2.43 (dd, *J* = 14.5, 4.7 Hz, 1H), 2.36 (dd, *J* = 14.0, 5.8 Hz, 1H), 2.26 (dd, *J* = 14.0, 7.7 Hz, 1H), 1.20 (s, 9H), 1.06 (d, *J* = 6.6 Hz, 3H). HRMS calc. for C33H37N5O5Na [M+Na]+: 606.2708. Found: 606.2692.



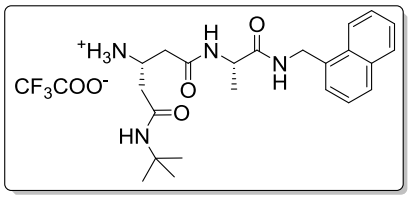
Benzyl (*R*)-3-((*t*-butoxycarbonyl)amino)-5-(((*S*)-1-((naphthalen-1-ylmethyl)amino)-1-oxopropan-2-yl)amino)-5-oxopentanoate (PKS2266): The title compound was synthesized by following the general protocol for HATU mediated coupling of *N*-Boc-L-β-glutamic acid 5-benzyl ester (84 mg, 0.25 mmol) and H-Ala-CH_2-naphth TFA salt (94 mg, 0.275 mmol). After completion of reaction, water was added to reaction mixture to give white precipitate. Precipitate was filtered, washed with water and dried in air to give product (115 mg, 84%) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.40 (t, *J* = 5.6 Hz, 1H), 8.11 (d, *J* = 7.4 Hz, 1H), 8.04 – 8.02 (m, 1H), 7.95 – 7.93 (m, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.56 – 7.51 (m, 2H), 7.47 – 7.41 (m, 2H), 7.37 – 7.30 (m, 5H), 6.82 (d, *J* = 8.3 Hz, 1H), 5.05 (s, 2H), 4.77 – 4.69 (m, 2H), 4.33 – 4.28 (m, 1H), 4.22 – 4.13 (m, 1H), 2.55 (dd, *J* = 15.0, 5.0 Hz, 1H), 2.49 – 2.44 (m, 1H), 2.38 (dd, *J* = 14.6, 6.3 Hz, 1H), 2.32 (dd, *J* = 14.6, 7.5 Hz, 1H), 1.34 (s, 9H), 1.21 (d, *J* = 7.1 Hz, 3H).



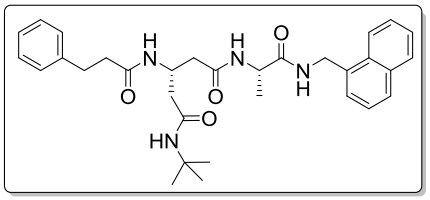
(*R*)-3-((*t*-butoxycarbonyl)amino)-5-(((*S*)-1-((naphthalen-1-ylmethyl)amino)-1-oxopropan-2-yl)amino)-5-oxopentanoic acid (PKS2268): The title compound was synthesized by following the *O*-debenzylation protocol of PKS2266 (110 mg, 0.2 mmol). Product (92 mg, quant.) was isolated as white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.49 (t, *J* = 5.8 Hz, 1H), 8.16 (d, *J* = 7.4 Hz, 1H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.94 (d, *J* = 7.3 Hz, 1H), 7.83 (d, *J* = 7.8 Hz, 1H), 7.56 – 7.51 (m, 2H), 7.48 – 7.42 (m, 2H), 6.74 (d, *J* = 8.2 Hz, 1H), 4.74 – 4.71 (m, 2H), 4.33 – 4.28 (m, 1H), 4.11 – 4.04 (m, 1H), 2.41 – 2.29 (m, 4H), 1.35 (s, 9H), 1.23 (d, *J* = 7.1 Hz, 3H).



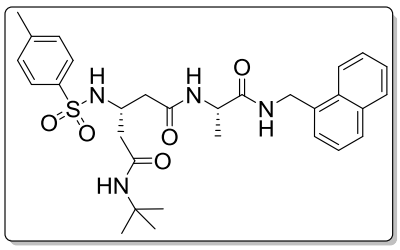
***t*-butyl ((*R*)-1-(*t*-butylamino)-5-(((*S*)-1-((naphthalen-1-ylmethyl)amino)-1-oxopropan-2-yl)amino)-1,5-dioxopentan-3-yl)carbamate** (PKS2271): The title compound was prepared by following the general protocol for EDC mediated coupling of PKS2268 (92 mg, 0.2 mmol) and *t*-butylamine (31.5 μL, 0.3 mmol). After completion of reaction, water was added to reaction mixture to give white precipitate. Precipitate was filtered, washed with water and dried in air to give product (85 mg, 83%) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.44 (t, *J* = 5.9 Hz, 1H), 8.05 – 8.03 (m, 2H), 7.95 – 7.93 (m, 1H), 7.84 (d, *J* = 7.7 Hz, 1H), 7.56 – 7.53 (m, 2H), 7.48 – 7.43 (m, 2H), 7.34 (s, 1H), 6.56 (d, *J* = 8.4 Hz, 1H), 4.78 – 4.69 (m, 2H), 4.34 – 4.28 (m, 1H), 4.10 – 4.00 (m, 1H), 2.36 - 2.12 (m, 4H), 1.35 (s, 9H), 1.23 – 1.22 (m, 12H).



(*R*)-3-amino-*N*^{1}-(*t*-butyl)-*N*^{5}-((*S*)-1-((naphthalen-1-ylmethyl)amino)-1-oxopropan-2-yl)pentanediamide 2,2,2-trifluoroacetate (PKS2273): The title compound was synthesized by following the general protocol for Boc-deprotection of PKS2271 (80 mg, 0.156 mmol). ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.54 (t, *J* = 5.7 Hz, 1H), 8.46 (d, *J* = 7.3 Hz, 1H), 8.05 – 8.03 (m, 1H), 7.96 – 7.94 (m, 1H), 7.89 – 7.82 (m, 5H), 7.56 – 7.54 (m, 2H), 7.49 – 7.43 (m, 2H), 4.78 (dd, *J* = 15.4, 5.9 Hz, 1H), 4.70 (dd, *J* = 15.4, 5.5 Hz, 1H), 4.39 – 4.33 (m, 1H), 3.67 – 3.61 (m, 1H), 2.53 – 2.49 (m, 2H), 2.42 (dd, *J* = 15.9, 5.8 Hz, 1H), 2.36 (dd, *J* = 15.9, 7.2 Hz, 1H), 1.26 - 1.24 (m, 12H).

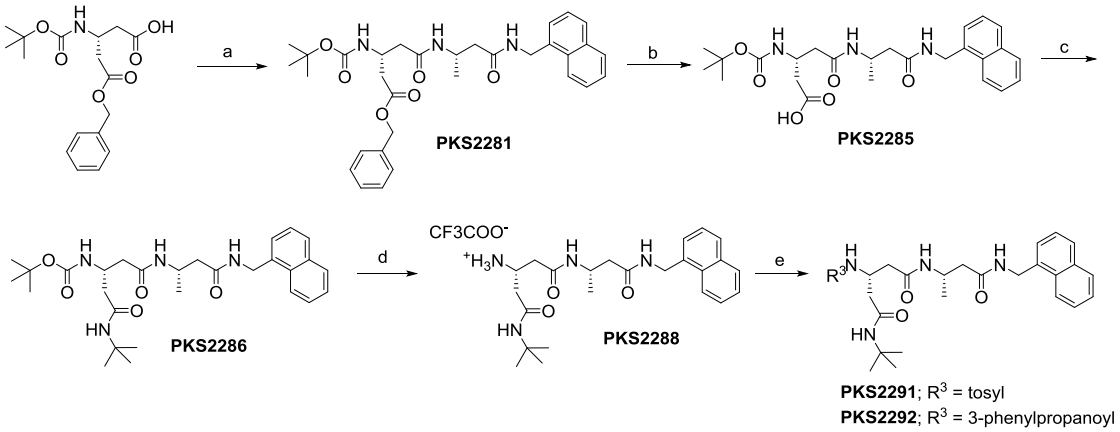


(*R*)-*N*^{1}-(*t*-butyl)-*N*^{5}-((*S*)-1-((naphthalen-1-ylmethyl)amino)-1-oxopropan-2-yl)-3-(3-phenylpropanamido)pentanediamide (PKS2278): The title compound was synthesized by following the general protocol for HATU mediated coupling of 3-phenylproapnoic acid (6.6 mg, 0.044 mmol) and PKS2273 (21.1 mg, 0.04 mmol). After completion of reaction, mixture was purified by HPLC to give pure product (20.7 mg, 95%) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.44 – 8.42 (m, 1H), 8.07 (d, J = 7.3 Hz, 1H), 8.02 – 8.00 (m, 1H), 7.95 – 7.93 (m, 1H), 7.83 (d, J = 7.9 Hz, 1H), 7.68 (d, J = 8.1 Hz, 1H), 7.54 – 7.52 (m, 2H), 7.45 – 7.39 (m, 2H), 7.37 (s, 1H), 7.24 – 7.21 (m, 2H), 7.16 – 7.13 (m, 3H), 4.71 (d, J = 5.7 Hz, 2H), 4.33 – 4.29 (m, 2H), 2.76 – 2.73 (m, 2H), 2.37 – 2.16 (m, 6H), 1.24 – 1.22 (m, 12H). ^{13}C NMR (126 MHz, DMSO) δ 172.4, 170.5, 169.7, 169.4, 141.3, 134.4, 133.2, 130.7, 128.5, 128.2, 128.1, 127.4, 126.1, 125.8, 125.7, 125.4, 124.9, 123.3, 50.0, 48.4, 44.2, 40.7, 40.1, 39.7, 37.2, 31.1, 28.5, 18.2. HRMS calc. for C32H40N4O4Na [M+Na]+: 567.2935. Found: 567.2947.

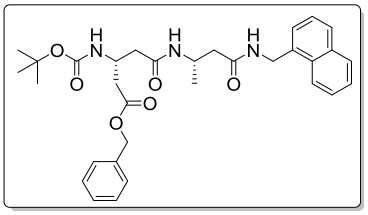


(*R*)-*N*^{1}-(*t*-butyl)-3-(4-methylphenylsulfonamido)-*N*^{5}-((*S*)-1-((naphthalen-1-ylmethyl)amino)-1-oxopropan-2-yl)pentanediamide (PKS2279): The title compound was prepared by following the general procedure for *N*-sulfonamide formation of PKS2273 (21.1 mg, 0.04 mmol) with tosyl chloride (11.4 mg, 0.06 mmol). The product was isolated as white solid (17.8 mg, 78%) after HPLC purification. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.42 (t, J = 5.8 Hz, 1H), 8.08 – 8.03 (m, 2H), 7.95 – 7.94 (m, 1H), 7.84 (d, J = 7.9 Hz, 1H), 7.66 (d, J = 8.4 Hz, 2H), 7.55 – 7.53 (m, 2H), 7.48 – 7.42 (m, 3H), 7.39 (s, 1H), 7.32 (d, J = 8.0 Hz, 2H), 4.78 – 4.70 (m, 2H), 4.28 – 4.23 (m, 1H), 3.81 – 3.74 (m, 1H), 2.35 (s, 3H), 2.29

– 2.20 (m, 2H), 2.13 (d, *J* = 6.6 Hz, 2H), 1.20 – 1.18 (m, 12H). ^{13}C NMR (126 MHz, DMSO) δ 172.2, 169.2, 168.9, 142.4, 138.5, 134.4, 133.2, 130.8, 129.5, 128.5, 127.5, 126.5, 126.1, 125.8, 125.4, 125.1, 123.4, 50.1, 48.5, 48.3, 40.7, 40.1, 40.0, 28.4, 20.9, 18.3. HRMS calc. for C30H38N4O5SNa [M+Na]+: 589.2466. Found: 589.2461.

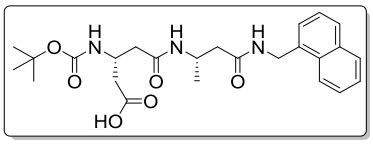


Scheme S2. Synthetic route of P1 and P2 β-aminoacid based peptidomimetics. Reagents and conditions: a) **PKS2245**, HATU, HOAt, Hünig's base, DMF; b) Pd/C (10%), H_2, Methanol; c) t-butyl amine, EDC, HOBt, Hünig base, DMF; d) TFA in DCM (20%); e) R^3COOH, HATU, HOAt, Hünig's base, DMF or R^3Cl, Et_3N, DCM

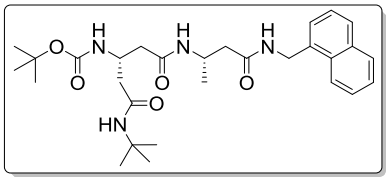


(*R*)-benzyl 3-((*t*-butoxycarbonyl)amino)-5-(((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)amino)-5-oxopentanoate (PKS2281): The title compound was synthesized by following the general protocol for HATU mediated coupling of N-Boc-L-beta-glutamic acid 5-benzyl ester (47 mg, 0.14 mmol) and H-homo-β-Ala-CH_2-naphth TFA salt (50 mg, 0.14 mmol). The reaction mixture was purified by HPLC to give product (73 mg, 93%) as white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.39 (t, *J* = 5.5 Hz, 1H), 8.06 – 8.04 (m, 1H), 7.95 – 7.93 (m, 1H), 7.84 (d, *J* = 7.9 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.56 – 7.51 (m, 2H), 7.48 – 7.42 (m, 2H), 7.37 – 7.30 (m, 5H), 6.79 (d, *J* = 8.5 Hz, 1H), 5.05 (s, 2H), 4.76 – 4.68 (m, 2H), 4.16 – 4.09 (m, 2H), 2.55 –

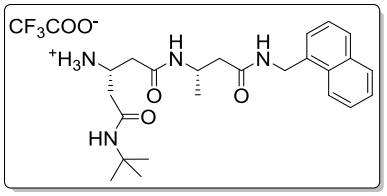
2.43 (m, 2H), 2.36 (dd, *J* = 14.0, 5.7 Hz, 1H), 2.26 – 2.17 (m, 3H), 1.35 (s, 9H), 1.02 (d, *J* = 6.0 Hz, 3H).



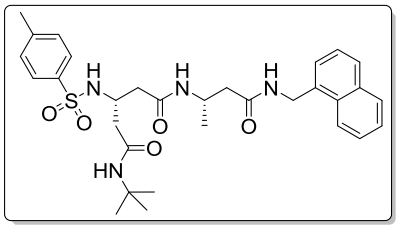
(*R*)-3-((*t*-butoxycarbonyl)amino)-5-(((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)amino)-5-oxopentanoic acid (PKS2285): The title compound was synthesized by following the *O*-debenzylation protocol of PKS2281 (73 mg, 0.13 mmol). Yield 61.0 mg (quant.).^{1}H-NMR (500 MHz, DMSO-d_6) δ 12.12 (s, 1H), 8.39 (t, *J* = 5.6 Hz, 1H), 8.06 – 8.04 (m, 1H), 7.95 – 7.93 (m, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.56 – 7.52 (m, 2H), 7.48 – 7.42 (m, 2H), 6.69 (d, *J* = 8.4 Hz, 1H), 4.77 – 4.68 (m, 2H), 4.15 – 4.01 (m, 2H), 2.38 – 2.34 (m, 3H), 2.26 – 2.16 (m, 3H), 1.36 (s, 9H), 1.02 (d, *J* = 6.6 Hz, 3H).



***t*-butyl ((*R*)-1-(*t*-butylamino)-5-(((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)amino)-1,5-dioxopentan-3-yl)carbamate** (PKS2286): The title compound was prepared by following the general protocol for EDC mediated coupling of PKS2285 (61.0 mg, 0.13 mmol) and *t*-butylamine (20.0 μL, 0.195 mmol). After completion of reaction, mixture was purified by HPLC to give product (13.0 mg, 19%) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.41 (t, *J* = 5.6 Hz, 1H), 8.06 – 8.04 (m, 1H), 7.95 – 7.93 (m, 1H), 7.84 (d, *J* = 7.7 Hz, 1H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.56- 7.51 (m, 2H), 7.48 – 7.43 (m, 2H), 7.31 (s, 1H), 6.50 (d, *J* = 8.7 Hz, 1H), 4.77 – 4.68 (m, 2H), 4.18 – 4.10 (m, 1H), 4.06 – 3.98 (m, 1H), 2.36 (dd, *J* = 13.9, 5.6 Hz, 1H), 2.22 – 2.14 (m, 5H), 1.36 (s, 9H), 1.22 (s, 9H), 1.02 (d, *J* = 6.5 Hz, 3H).

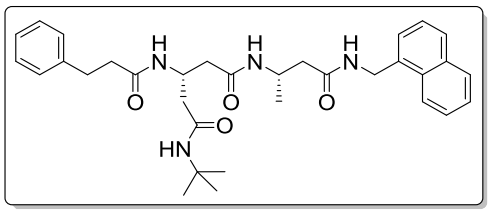


(*R*)-3-amino-*N*^{1}-(*t*-butyl)-*N*^{5}-((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)pentanediamide 2,2,2-trifluoroacetate (PKS2288): The title compound was synthesized by following the general protocol for Boc-deprotection of PKS2286 (13.0 mg, 0.025 mmol). Yield 13.5 mg (quant.). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.65 (bs, 3H), 8.47 (d, *J* = 7.9 Hz, 1H), 7.94 (d, *J* = 8.3 Hz, 1H), 7.86 (d, *J* = 8.1 Hz, 1H), 7.82 – 7.78 (m, 1H), 7.57 – 7.49 (m, 2H), 7.43 – 7.40 (m, 2H), 6.52 (t, *J* = 5.3 Hz, 1H), 5.98 (s, 1H), 4.81 – 4.74 (m, 2H), 4.35 – 4.30 (m, 1H), 3.86 (m, 1H), 2.73 – 2.68 (m, 1H), 2.64 – 2.58 (m, 1H), 2.46 – 2.36 (m, 3H), 2.30 (dd, *J* = 14.2, 8.9 Hz, 1H), 1.32 (s, 9H), 1.18 (d, *J* = 6.6 Hz, 3H).



(*R*)-*N*^{1}-(*t*-butyl)-3-(4-methylphenylsulfonamido)-*N*^{5}-((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)pentanediamide (PKS2291): The title compound was prepared by following the general procedure for N-sulfonamide formation of PKS2288 (6.5 mg, 0.012 mmol) with tosyl chloride (4.6 mg, 0.024 mmol). The product was isolated as white solid (5.2 mg, 74%) after HPLC purification. ^{1}H-NMR (500 MHz, DMSO-d_6) δ 8.40 (t, *J* = 5.6 Hz, 1H), 8.06 – 8.04 (m, 1H), 7.96 – 7.94 (m, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.67 – 7.66 (m, 2H), 7.55 – 7.52 (m, 2H), 7.47- 7.42 (m, 3H), 7.37 – 7.33 (m, 3H), 4.74 (dd, *J* = 15.2, 5.6 Hz, 1H), 4.70 (dd, *J* = 15.2, 5.6 Hz, 1H), 4.11 – 4.05 (m, 1H), 3.80 – 3.73 (m, 1H), 2.34 (s, 3H), 2.31 (dd, *J* = 13.9, 5.5 Hz, 1H), 2.18 – 2.08 (m, 5H), 1.18 (s, 9H), 0.98 (d, *J* = 6.6 Hz, 3H). ^{13}C-NMR (126 MHz, DMSO) δ ^{13}C NMR (126 MHz, DMSO) δ 169.78, 168.9, 168.4, 142.4, 138.6, 134.6, 133.3, 130.9, 129.5, 128.5, 127.6, 126.5,

126.2, 125.8, 125.6, 125.4, 123.5, 50.0, 48.5, 42.2, 41.9, 40.5, 40.1, 40.1, 28.4, 20.9, 20.0. HRMS calc. for C31H40N4O5SNa [M+Na]+: 603.2624. Found: 603.2617.



(*R*)-*N*^{1}-(*t*-butyl)-*N*^{5}-((*S*)-4-((naphthalen-1-ylmethyl)amino)-4-oxobutan-2-yl)-3-(3-phenylpropanamido)pentanediamide (PKS2292): The title compound was synthesized by following the general protocol for HATU mediated coupling of 3-phenylpropanoic acid (2.0 mg, 0.012) and PKS2288 (6.5 mg, 0.012 mmol). The reaction mixture was purified by HPLC to give product (6.0 mg, 90%) as white solid. ^{1}H-NMR (500 MHz, DMSO-d_6) δ 8.40 (t, *J* = 5.6 Hz, 1H), 8.06 – 8.04 (m, 1H), 7.95 – 7.93 (m, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.64 (d, *J* = 8.3 Hz, 1H), 7.56 – 7.51 (m, 2H), 7.48 – 7.42 (m, 2H), 7.33 (s, 1H), 7.26 – 7.23 (m, 2H), 7.18 – 7.14 (m, 3H), 4.76 – 4.68 (m, 2H), 4.31 – 4.24 (m, 1H), 4.19 – 4.10 (m, 1H), 2.78 (t, *J* = 7.9 Hz, 2H), 2.38 – 2.30 (m, 3H), 2.23 – 2.17 (m, 5H), 1.22 (s, 9H), 1.02 (d, *J* = 6.6 Hz, 3H). ^{13}C-NMR (126 MHz, DMSO) δ 170.5, 169.8, 169.4, 168.8, 141.3, 134.6, 133.3, 130.9, 128.5, 128.2, 128.1, 127.6, 126.2, 125.8, 125.8, 125.6, 125.4, 123.5, 49.9, 44.2, 42.2, 42.0, 40.6, 40.1, 40.1, 37.2, 31.2, 28.5, 20.1. HRMS calc. for C33H42N4O4Na [M+Na]+: 581.3112. Found: 581.3104.

Table S2. Purity of compounds determined by integrating peak areas in ELSD spectra.

ID	Purity (%)
PKS2249	97.3
PKS2251	100
PKS2252	95.9
PKS2260	100
PKS2272	100
PKS2295	100
PKS3054	100
PKS2278	100
PKS2279	100
PKS2291	100
PKS2292	97.8

Reference:

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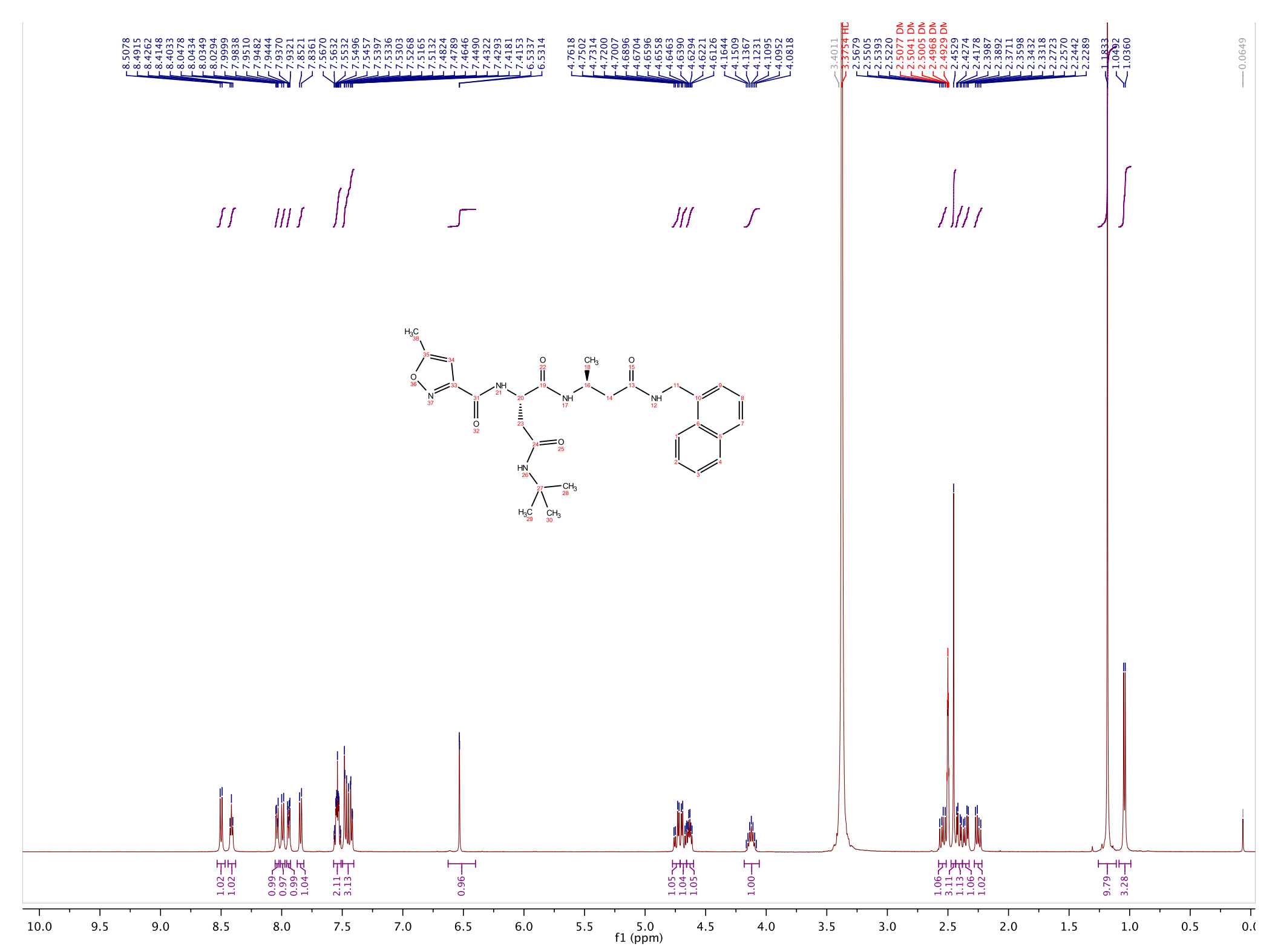
[6] C. Blackburn, K. M. Gigstad, P. Hales, K. Garcia, M. Jones, F. J. Bruzzese, C. Barrett, J. X. Liu, T. A. Soucy, D. S. Sappal, N. Bump, E. J. Olhava, P. Fleming, L. R. Dick, C. Tsu, M. D. Sintchak, J. L. Blank, *Biochem J* **2010**, *430*, 461-476.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1.02
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1.06
1.02
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7.0
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6.0
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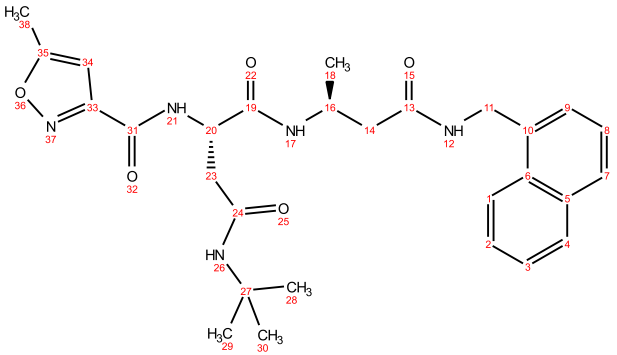
0.5
f1 (ppm)

pks2249.2.fid



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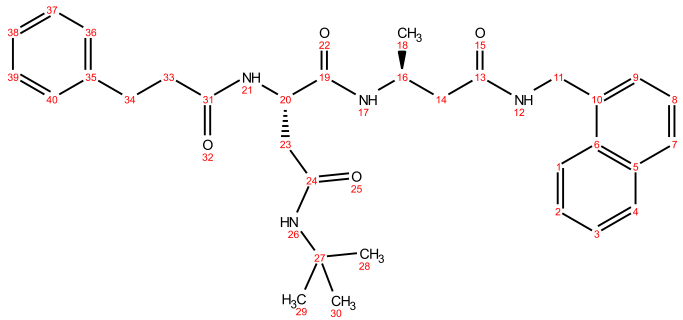
f1 (ppm)

pks2251.1.fid



f1 (ppm)

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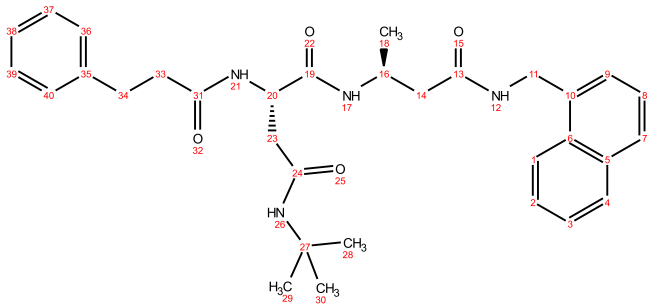

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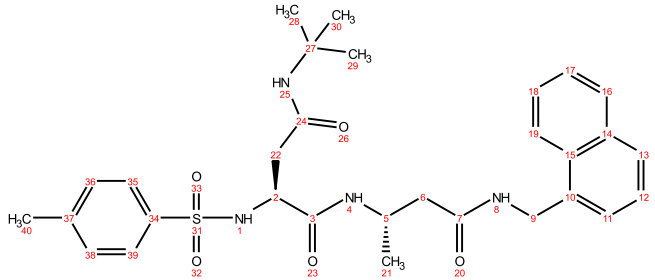

f1 (ppm)

pks2252.2.fid

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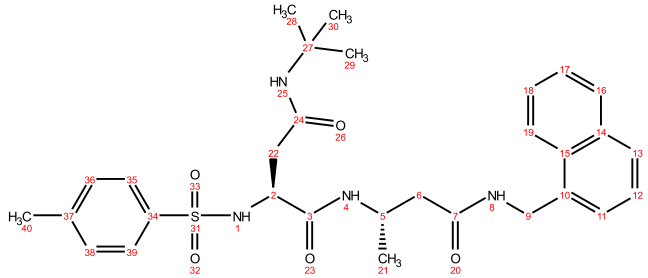

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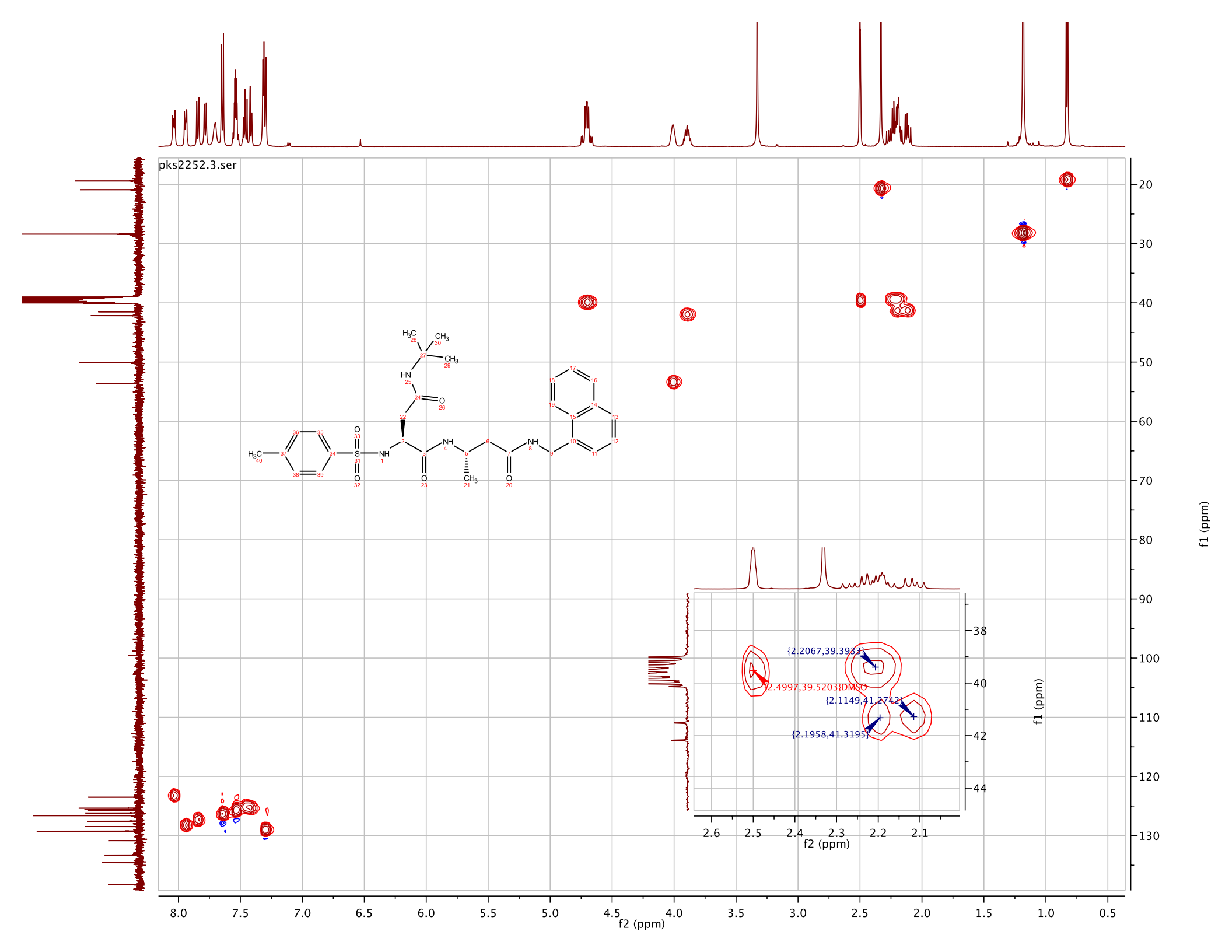
f1 (ppm)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f2 (ppm)
f1 (ppm)

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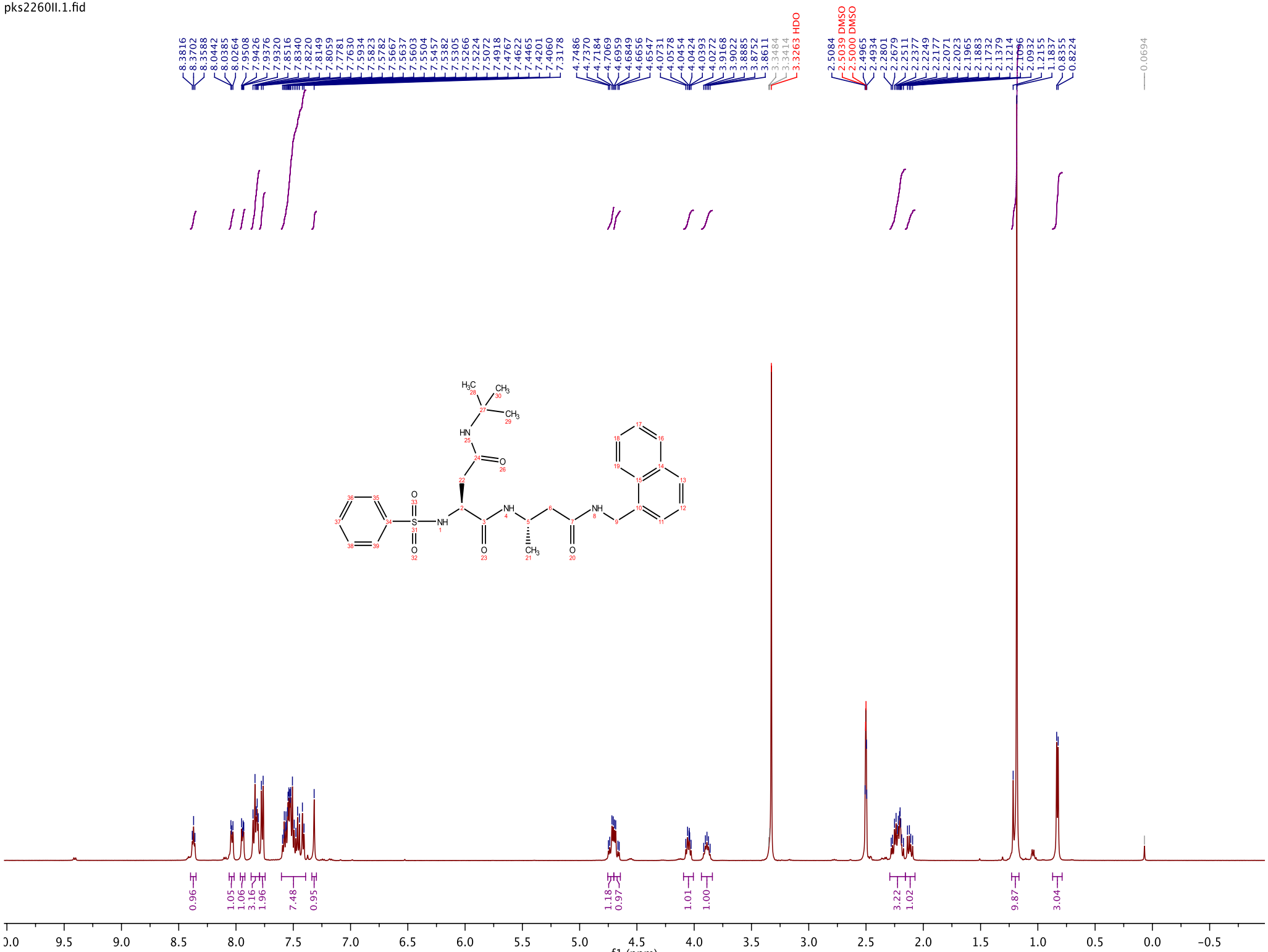

pks2260II.2.fid

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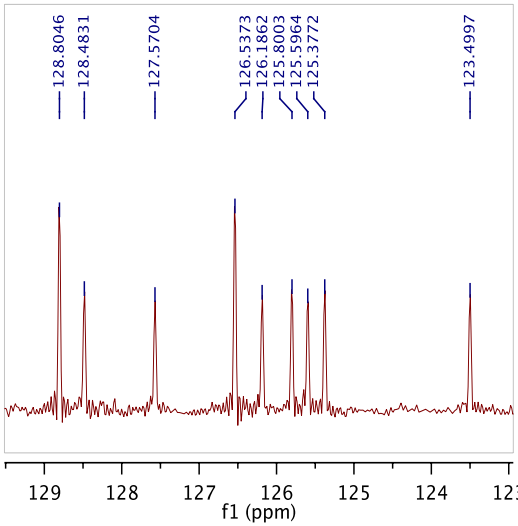

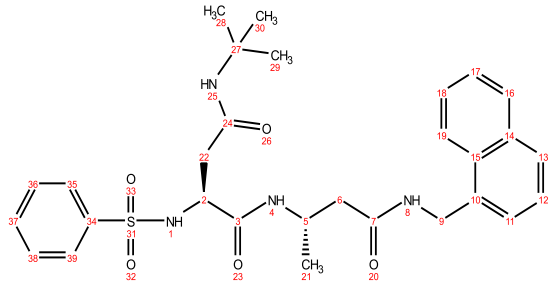

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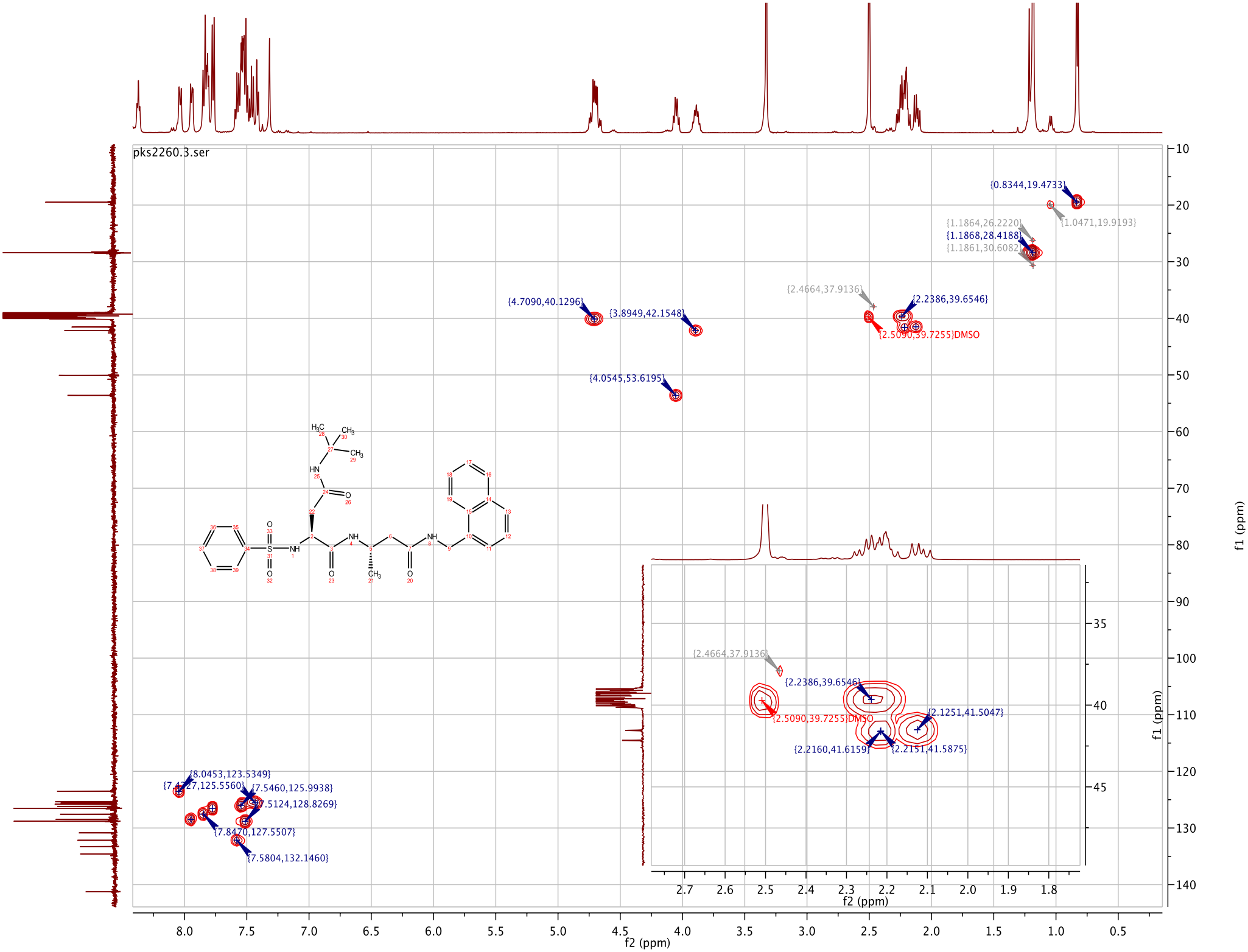
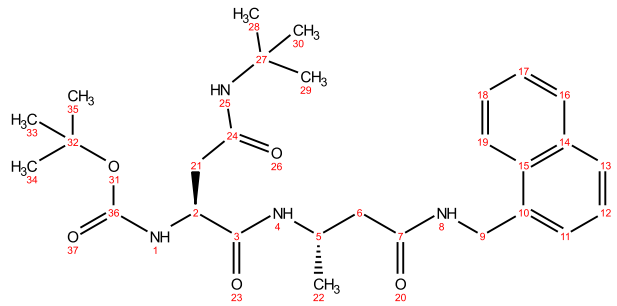
-1
f1 (ppm)

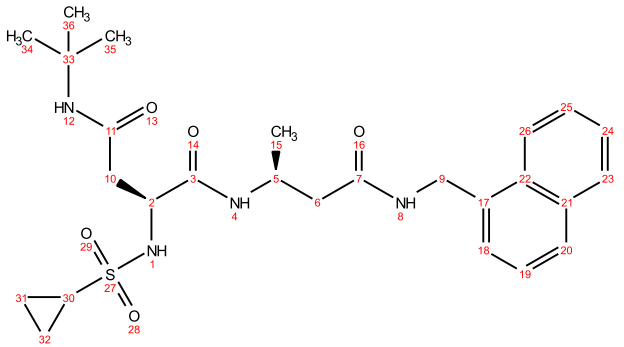

pks2260.3.ser
{0.8344,19.4733}
{1.0471,19.9193}
{1.1864,26.2220}
{1.1868,28.4188}
{1.1861,30.6082}
{2.4664,37.9136}
{2.2386,39.6546}
{2.5090,39.7255}DMSO
{4.7090,40.1296}
{3.8949,42.1548}
{4.0545,53.6195}
{8.0453,123.5349}
{7.4127,125.5560}
{7.5460,125.9938}
{7.5124,128.8269}
{7.8470,127.5507}
{7.5804,132.1460}
{2.4664,37.9136}
{2.2386,39.6546}
{2.5090,39.7255}DMSO
{2.1251,41.5047}
{2.2160,41.6159}
{2.2151,41.5875}
f2 (ppm)
f1 (ppm)

pks2272.2.fid



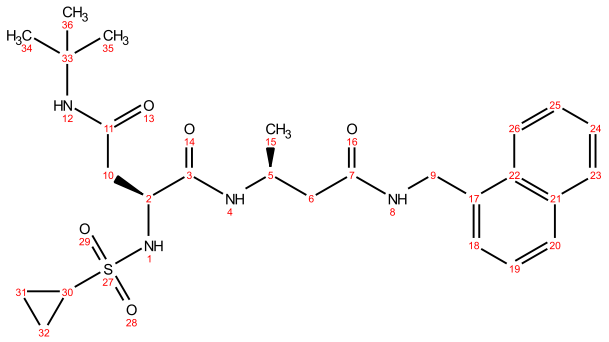
f1 (ppm)

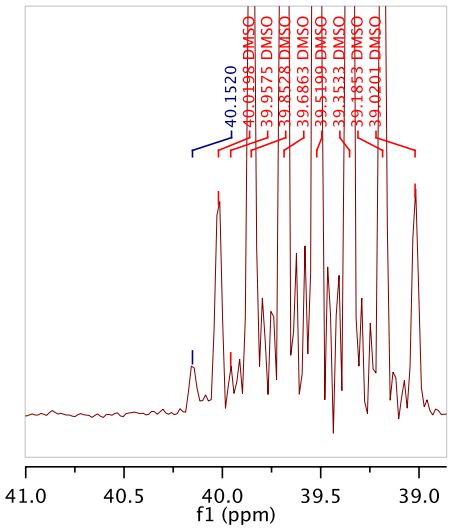
pks2295.1.fid

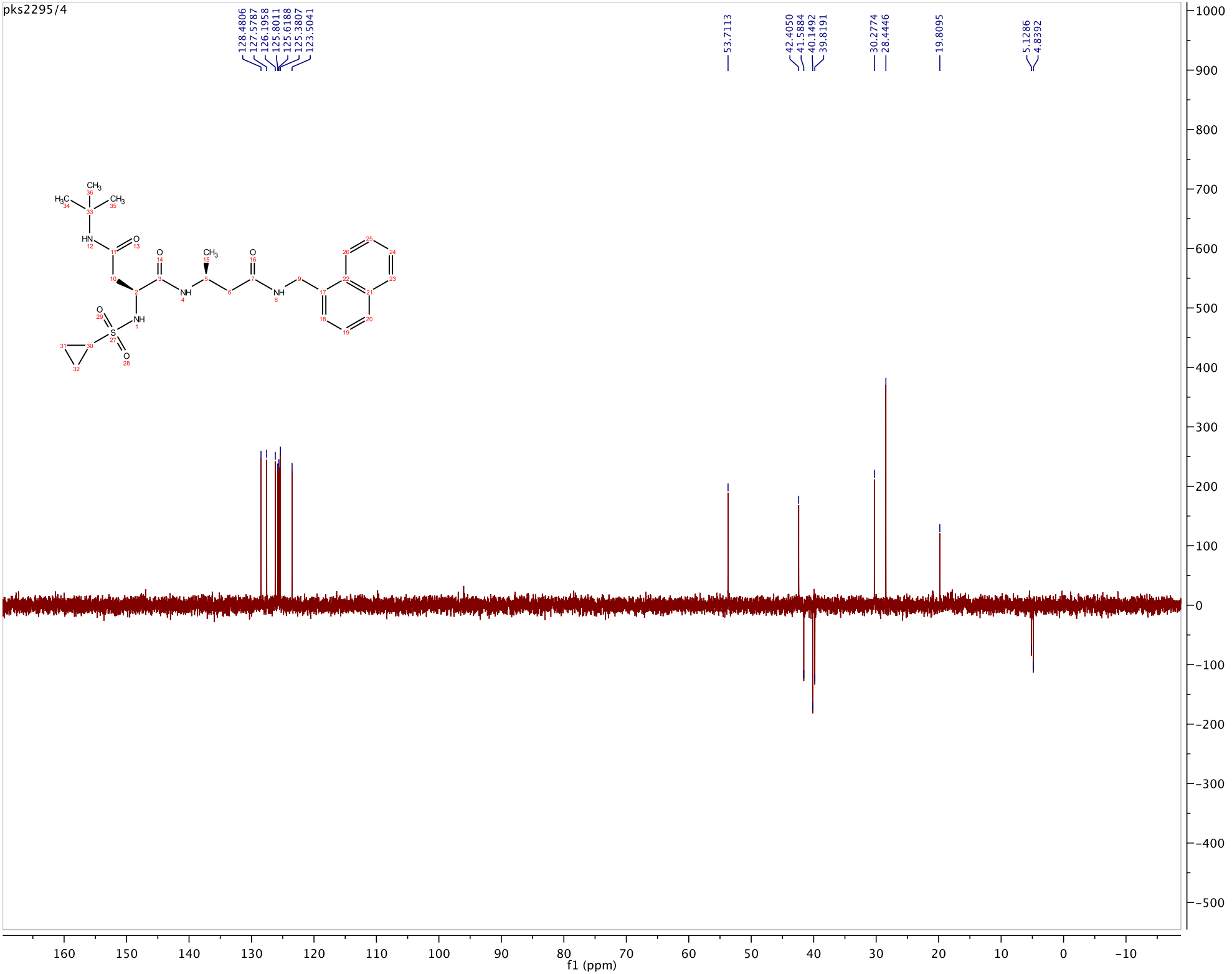


f1 (ppm)

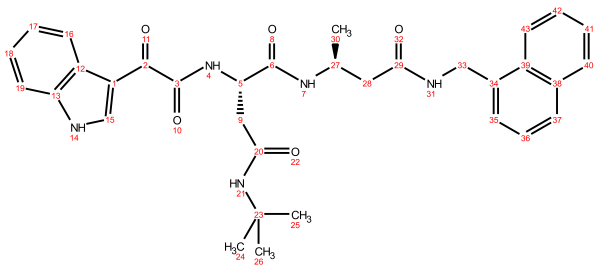
pks2295.2.fid





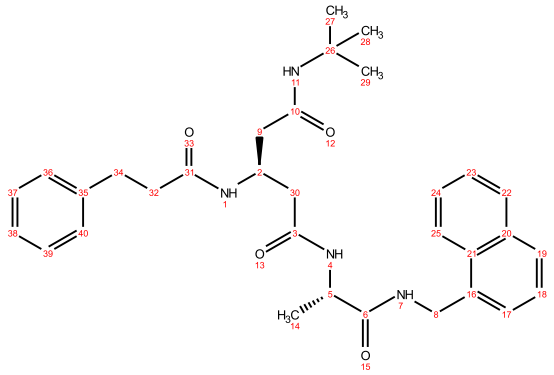

pks2295/4
128.4806
127.5787
126.1958
125.8011
125.6188
125.3807
123.5041
53.7113
42.4050
41.5884
40.1492
39.8191
30.2774
28.4446
19.8095
5.1286
4.8392
f1 (ppm)

pks3054.1.fid



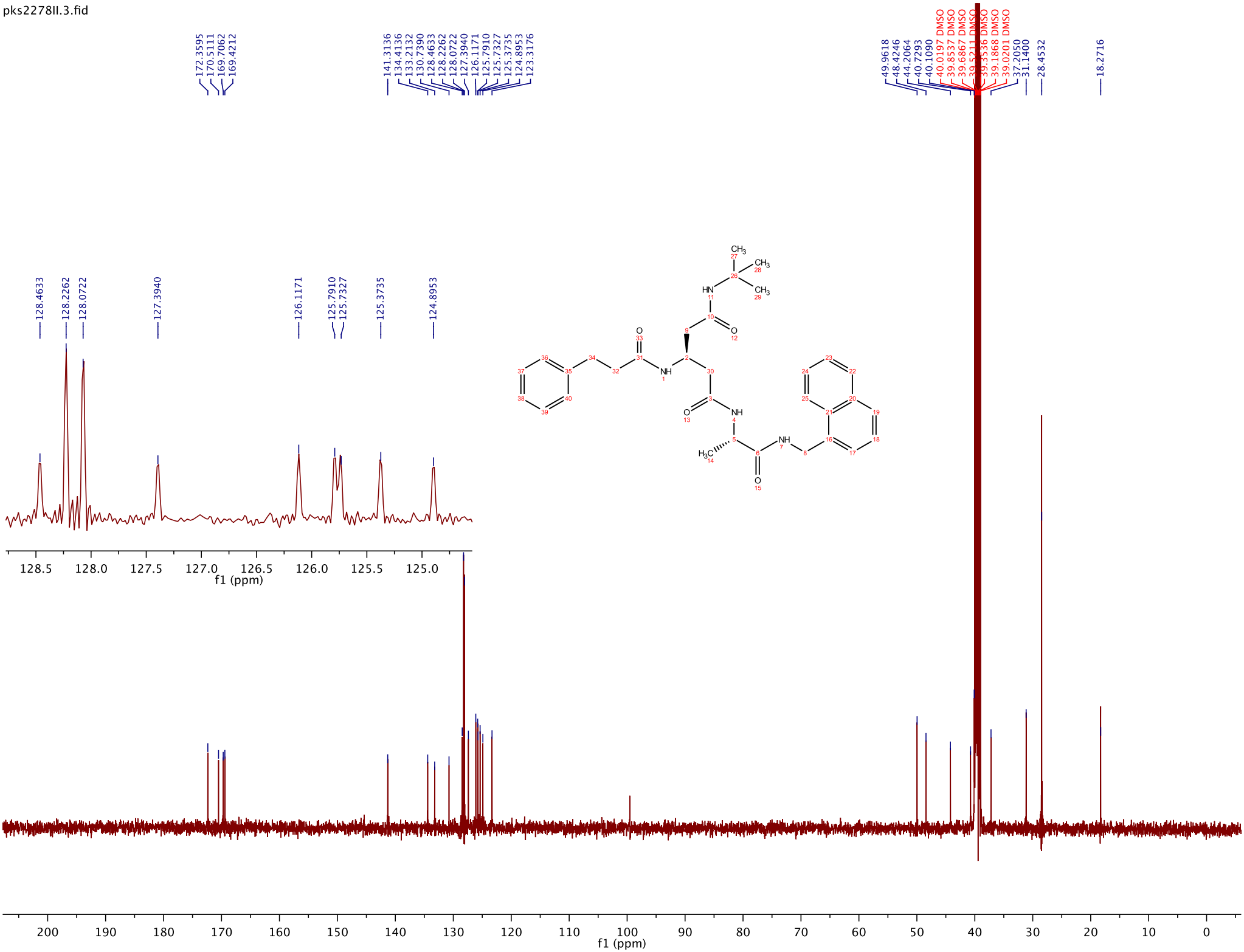
f1 (ppm)

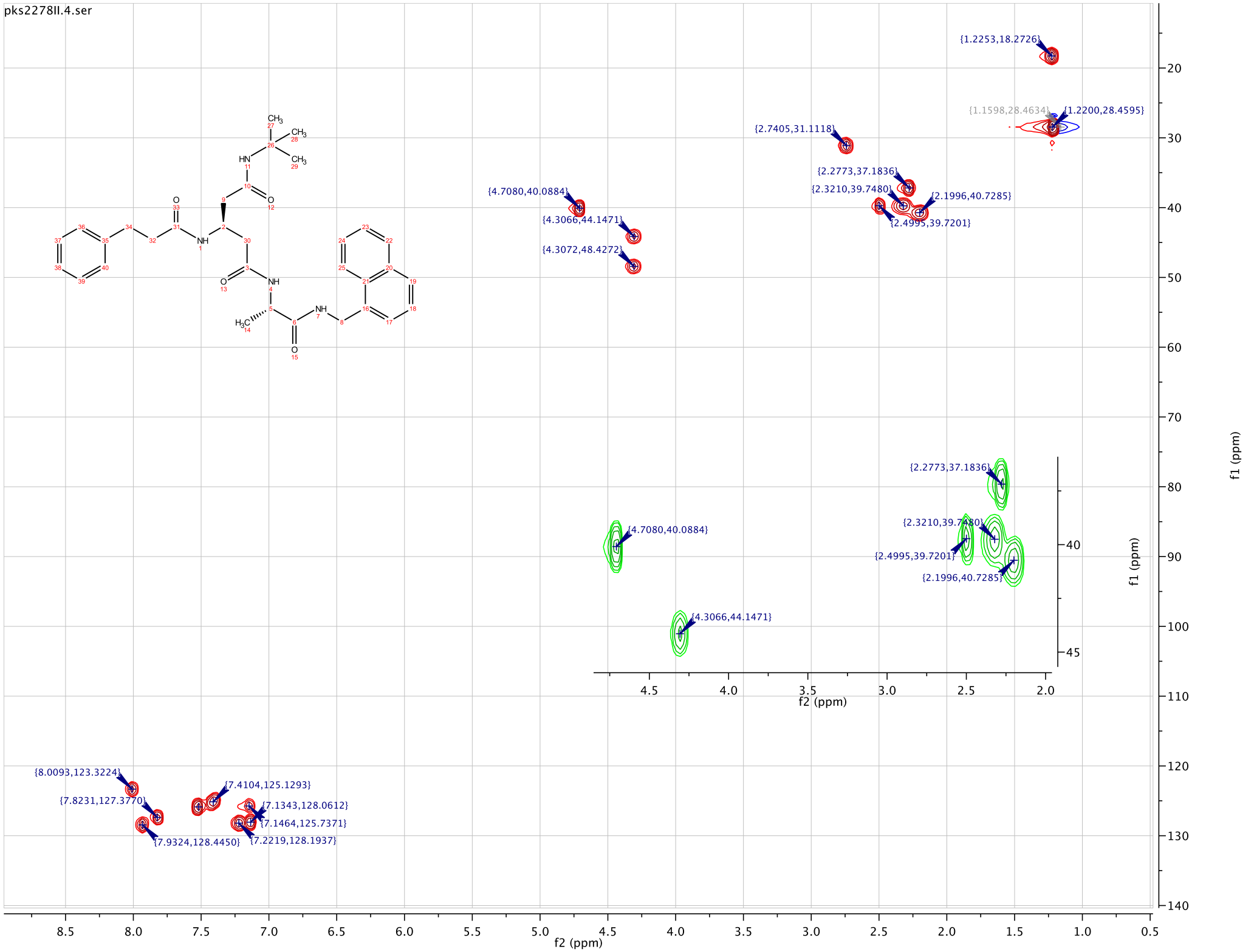
pks2278II.1.fid



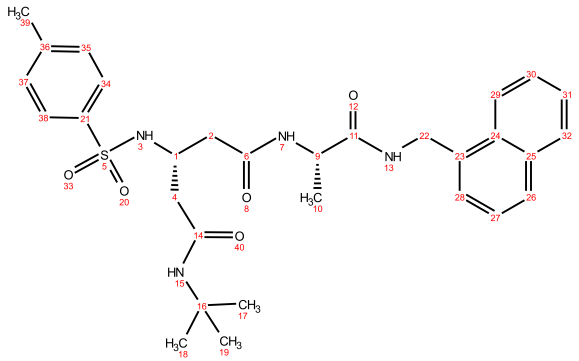
f1 (ppm)

pks2278II.3.fid



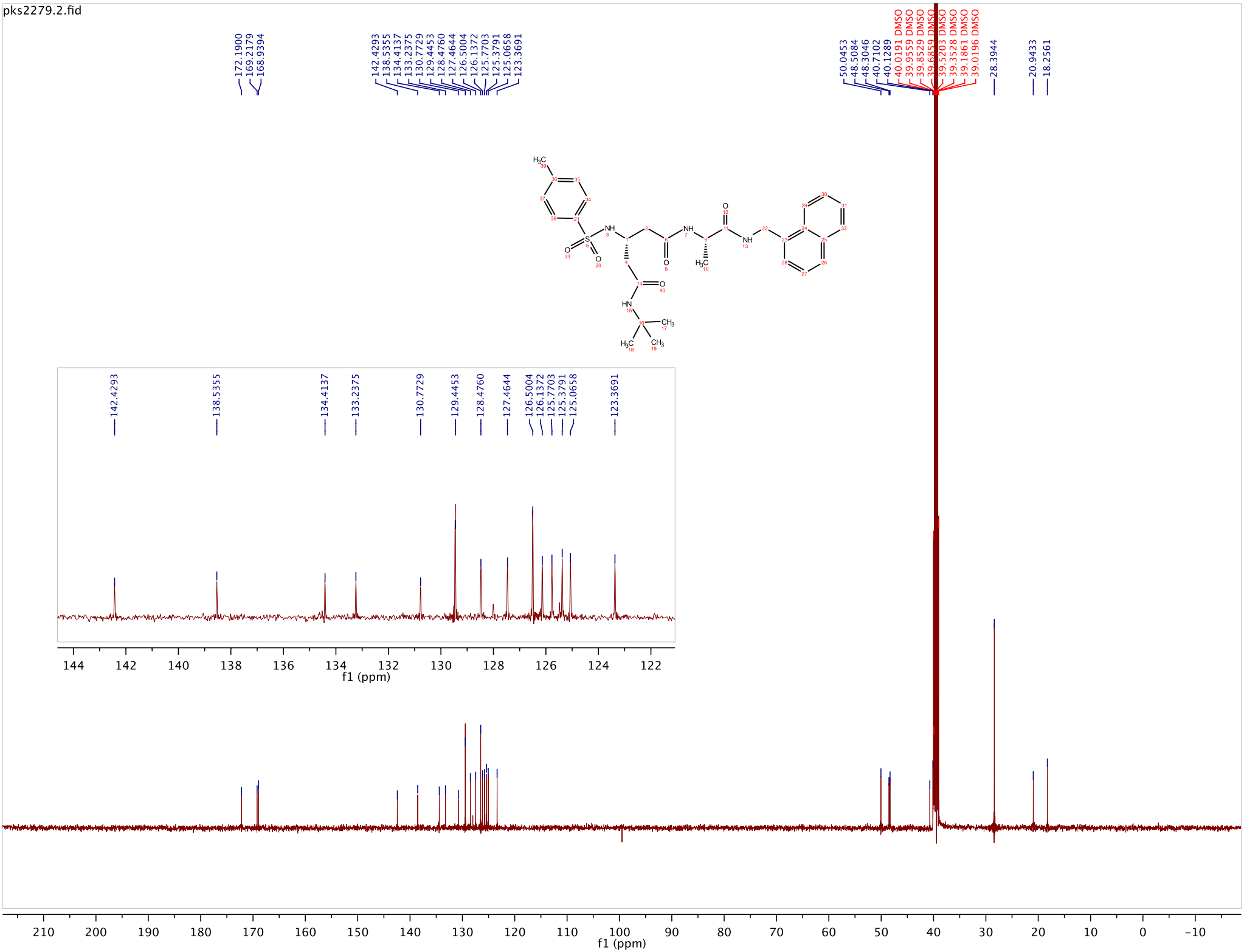

pks2278II.4.ser
{1.2253,18.2726}
{1.1598,28.4634}
{1.2200,28.4595}
{2.7405,31.1118}
{2.2773,37.1836}
{2.3210,39.7480}
{2.1996,40.7285}
{2.4995,39.7201}
{4.7080,40.0884}
{4.3066,44.1471}
{4.3072,48.4272}
{8.0093,123.3224}
{7.8231,127.3770}
{7.9324,128.4450}
{7.4104,125.1293}
{7.1343,128.0612}
{7.1464,125.7371}
{7.2219,128.1937}
f2 (ppm)
f1 (ppm)

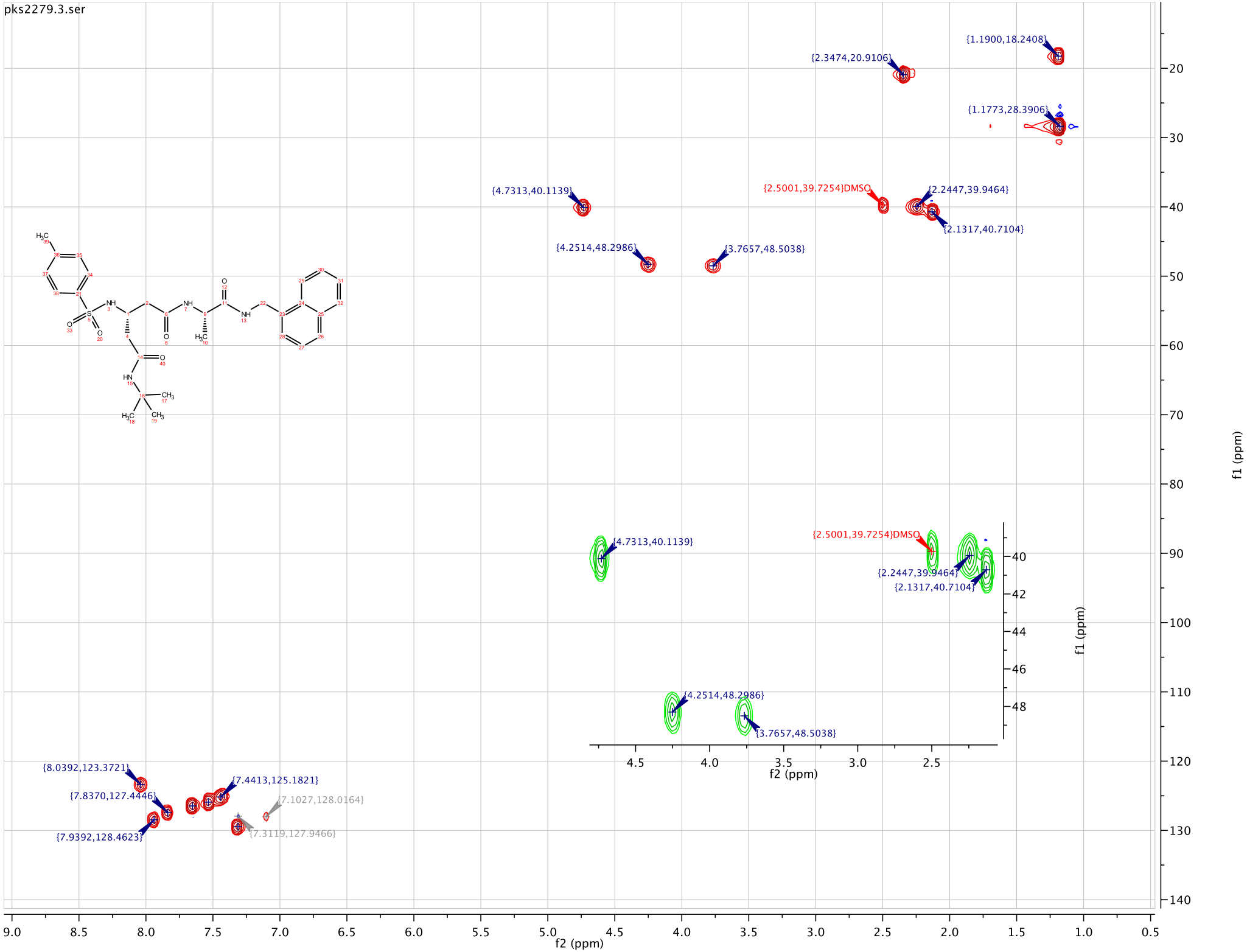
pks2279.1.fid



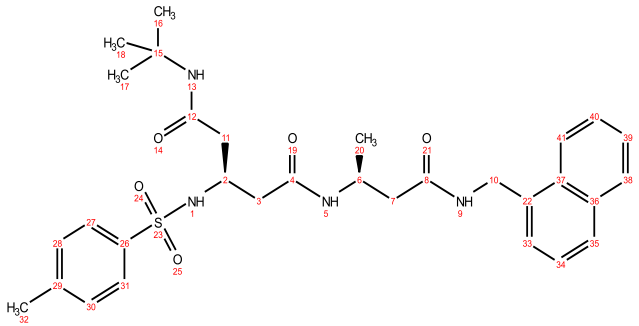
f1 (ppm)

pks2279.2.fid



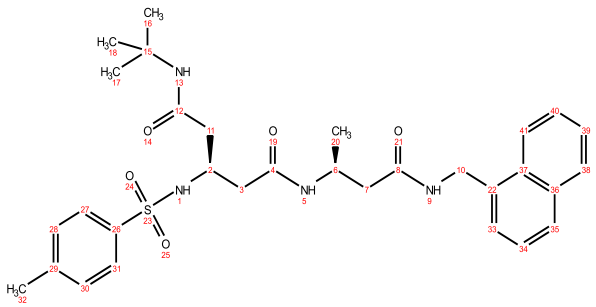

pks2279.3.ser
{1.1900,18.2408}
{2.3474,20.9106}
{1.1773,28.3906}
{4.7313,40.1139}
{2.5001,39.7254}DMSO
{2.2447,39.9464}
{2.1317,40.7104}
{4.2514,48.2986}
{3.7657,48.5038}
{8.0392,123.3721}
{7.4413,125.1821}
{7.8370,127.4446}
{7.1027,128.0164}
{7.9392,128.4623}
{7.3119,127.9466}
f2 (ppm)
f1 (ppm)

pks2291.1.fid



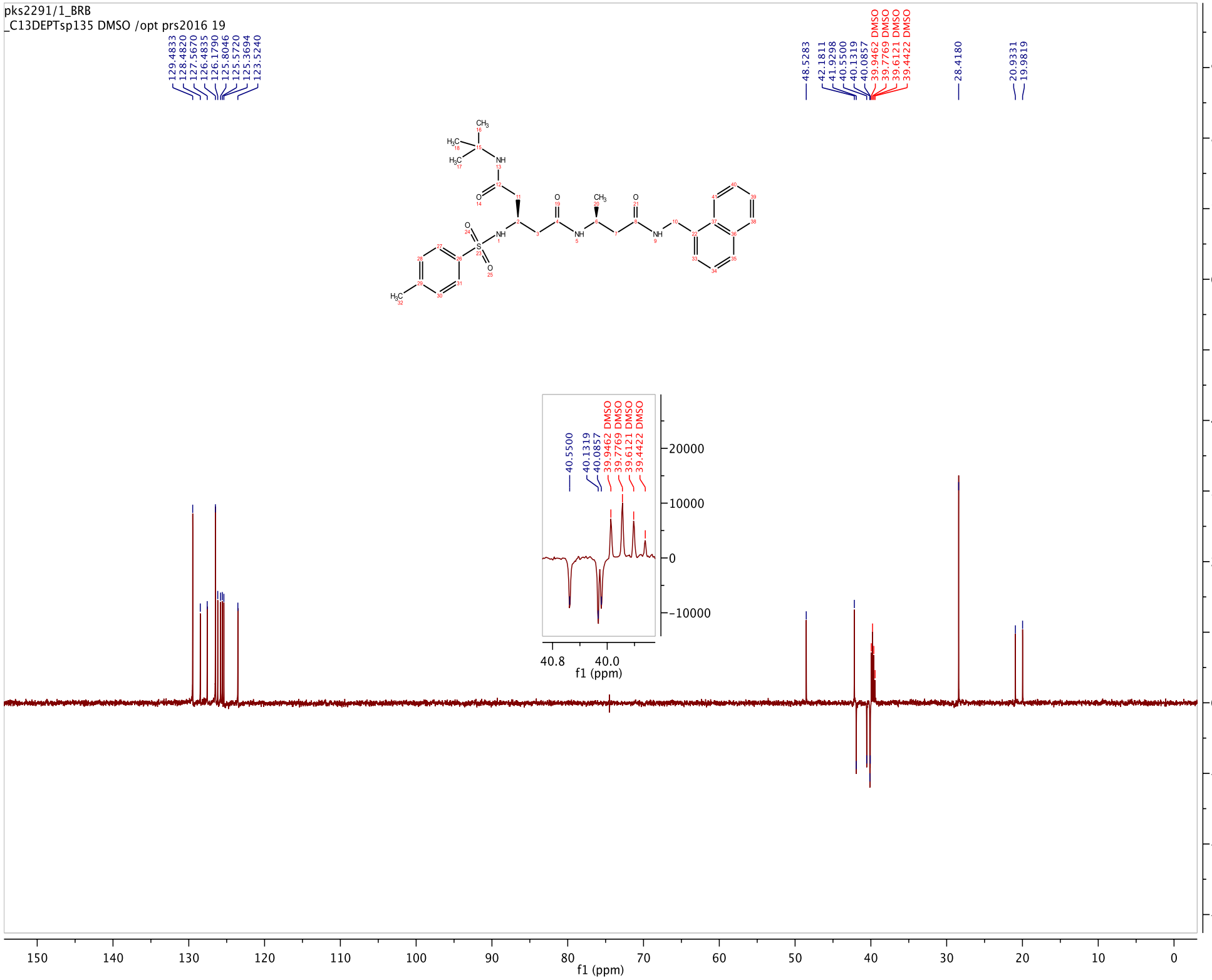
f1 (ppm)

pks2291/2_BRB
C13CPD DMSO /opt prs2016 19

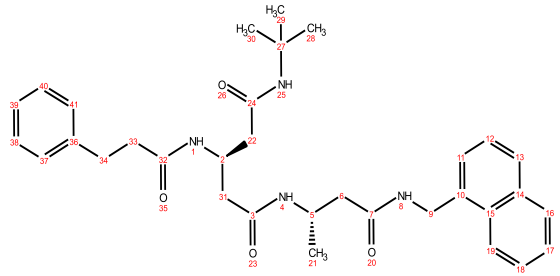


169.7795
168.9418
168.3629
142.4281
138.6550
138.6539
133.2752
130.8618
129.4661
128.4800
127.5575
126.4879
126.1717
125.7954
125.5637
125.3606
123.5162
50.0171
48.5221
42.1875
41.9299
28.4158
20.9328
19.9807

f1 (ppm)

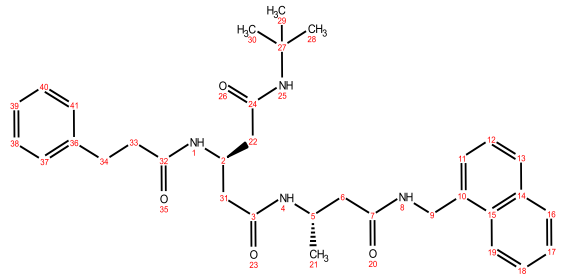

pks2291/1_BRB
_C13DEPTsp135 DMSO /opt prs2016 19
129.4833
128.4820
127.5670
126.4835
126.1790
125.8046
125.5720
125.3694
123.5240
48.5283
42.1811
41.9298
40.5500
40.1319
40.0857
39.9462 DMSO
39.7769 DMSO
39.6121 DMSO
39.4422 DMSO
28.4180
20.9331
19.9819
f1 (ppm)

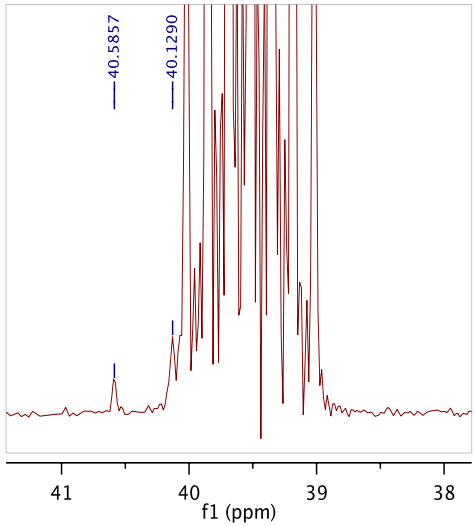
pks2292.1.fid



f1 (ppm)

pks2292.2.fid

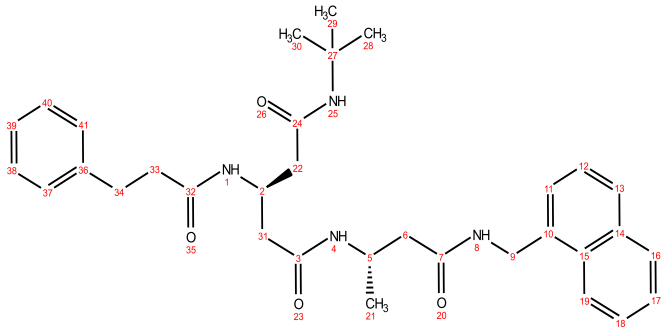


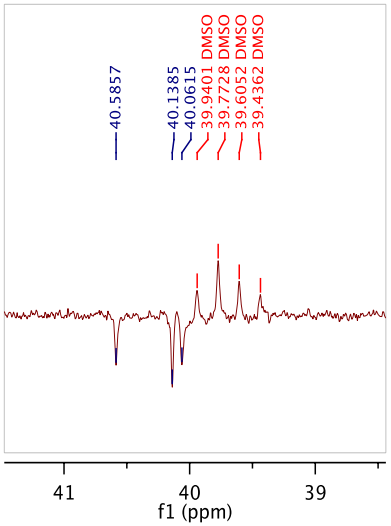


170.4599
169.8357
169.4203
168.7843
141.3108
134.6134
133.2727
130.8692
128.4672
128.2550
128.0889
127.5583
126.1798
125.8024
125.5723
125.3681
123.5114
49.9403
44.2232
42.1647
42.0422
40.5857
40.1290
37.2206
31.1937
28.4750
20.0634

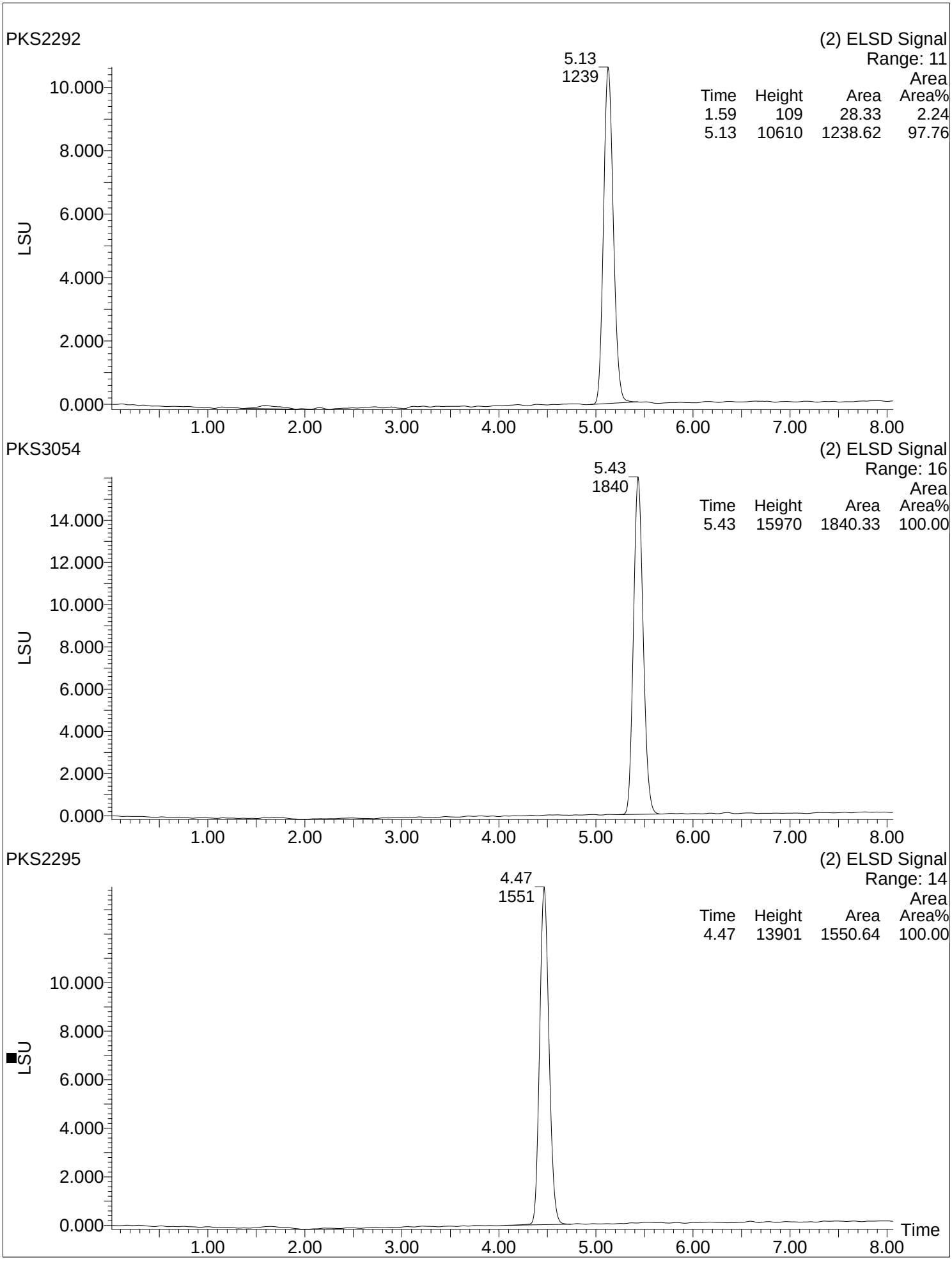
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

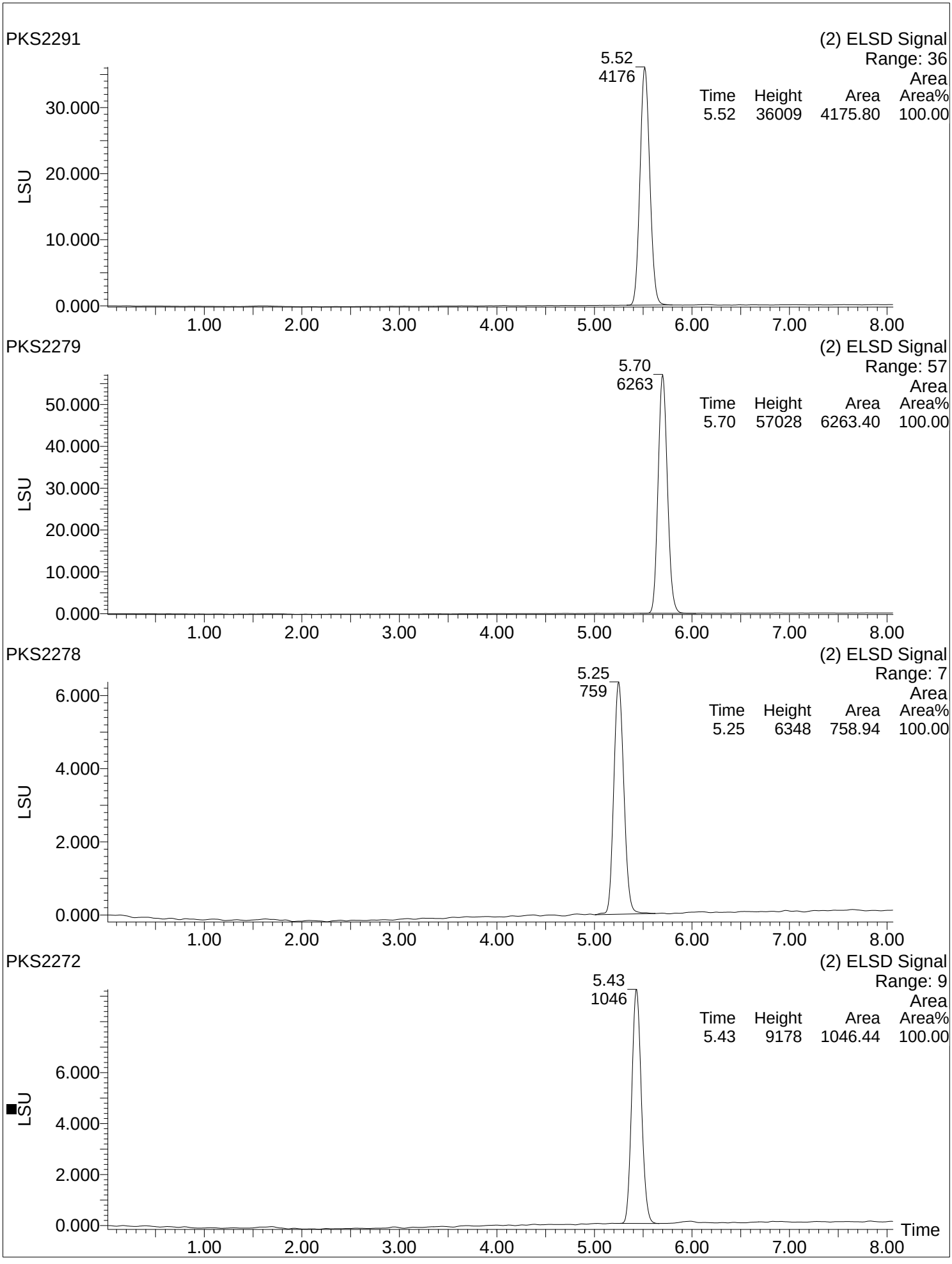
pks2292.3.fid

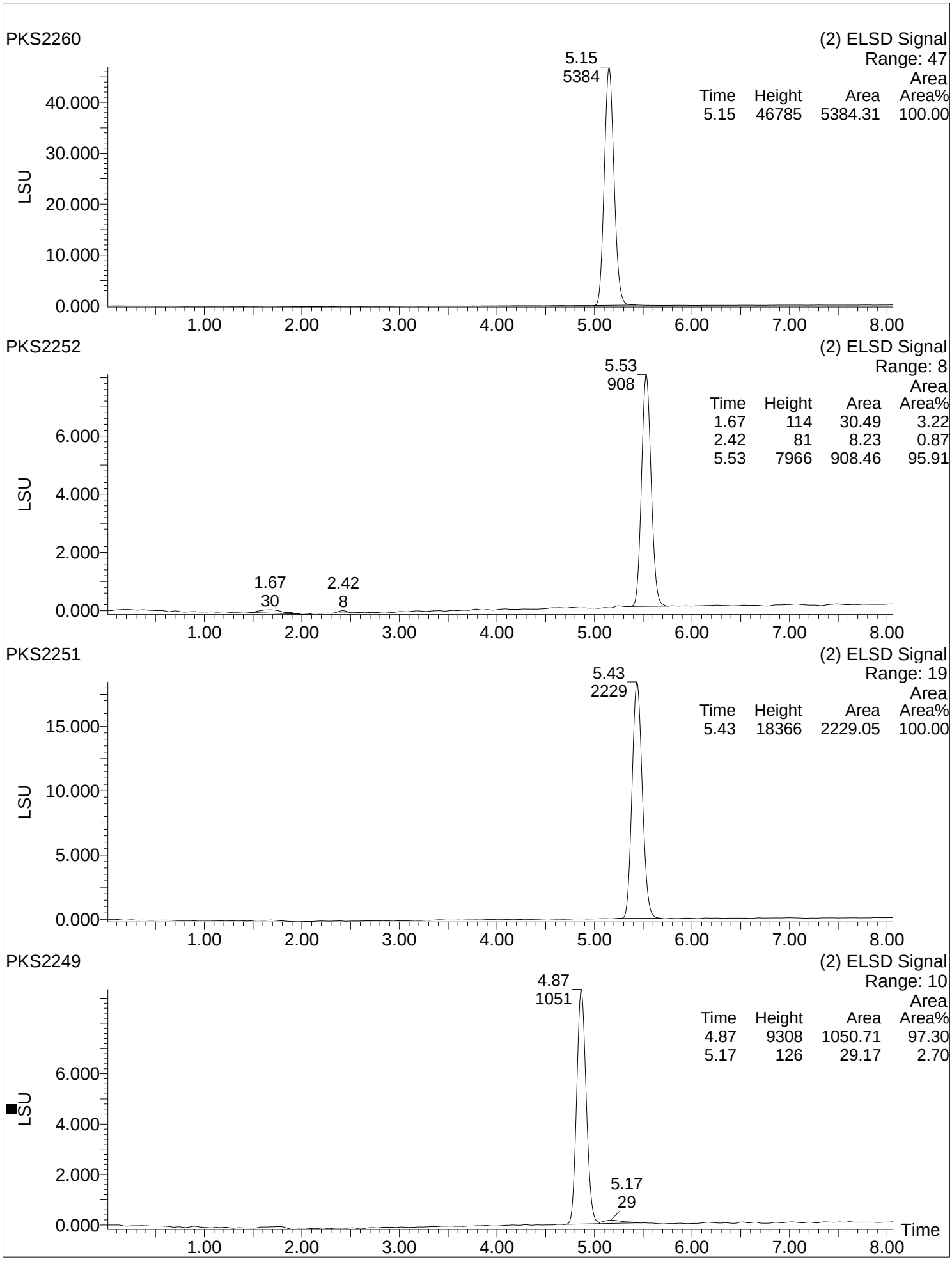


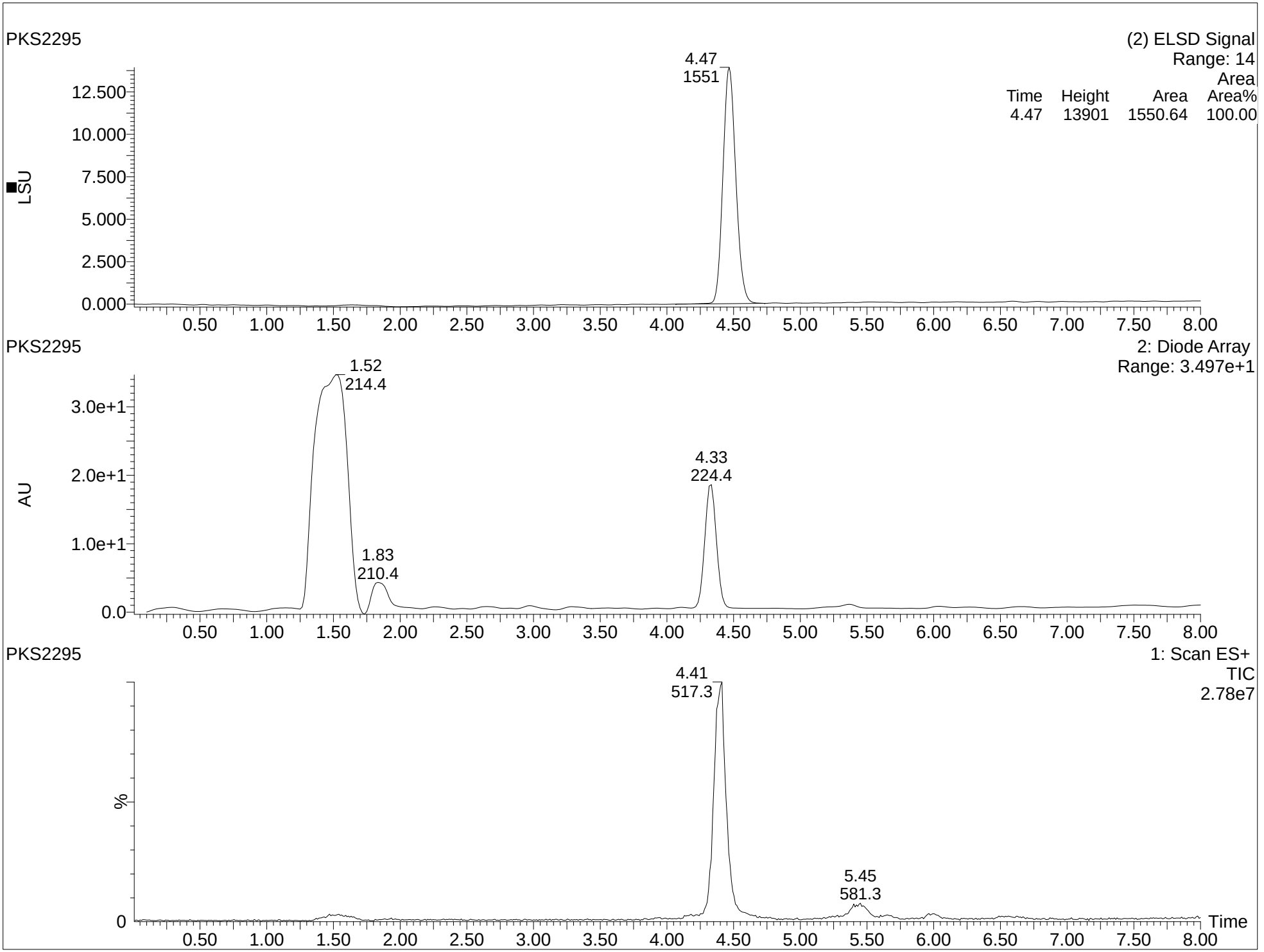


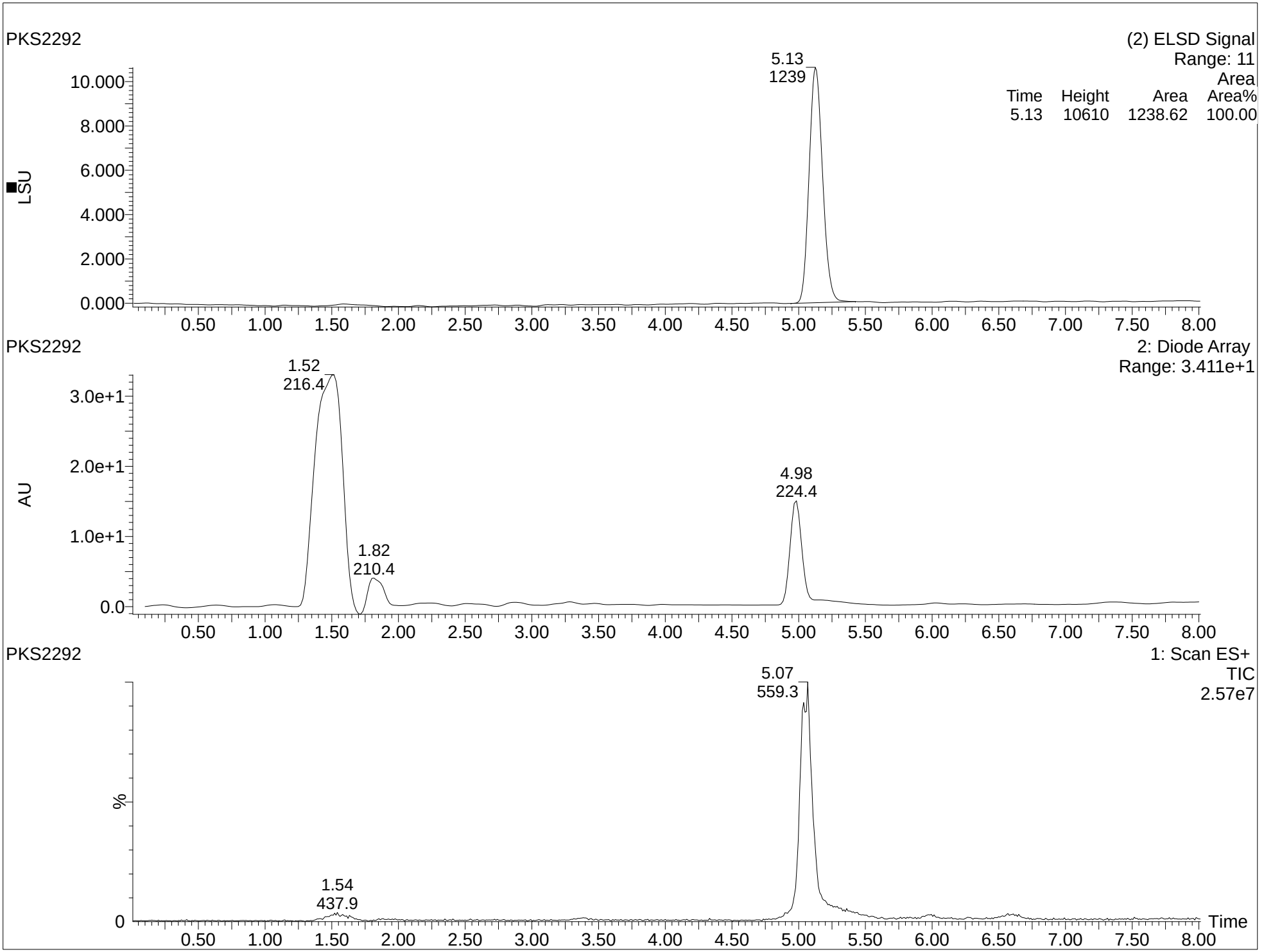
f1 (ppm)

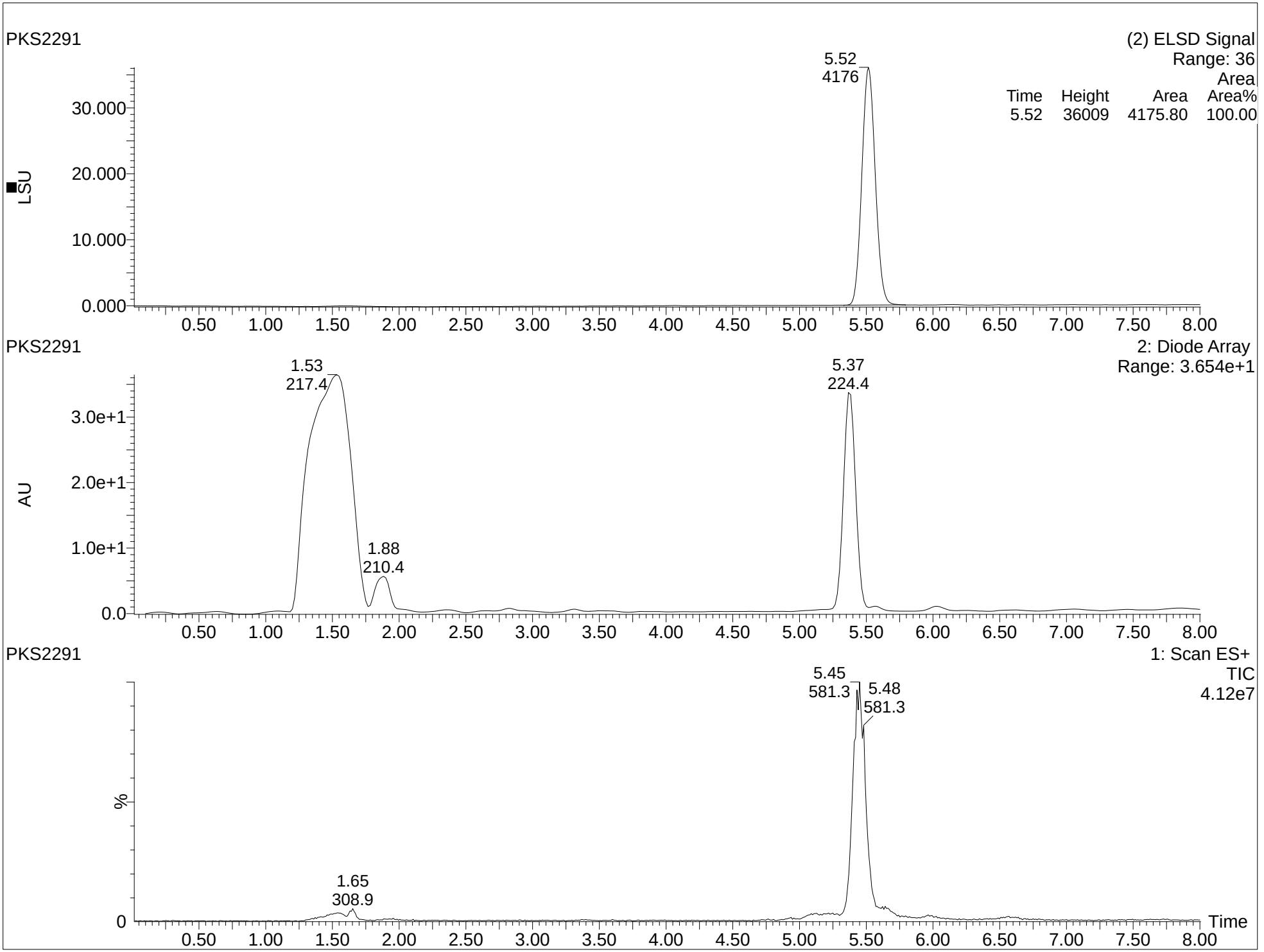

PKS2292
(2) ELSD Signal
Range: 11
Area
5.13
1239
Time Height Area Area%
1.59 109 28.33 2.24
5.13 10610 1238.62 97.76
LSU
10.000
8.000
6.000
4.000
2.000
0.000
1.00 2.00 3.00 4.00 5.00 6.00 7.00 8.00
PKS3054
(2) ELSD Signal
Range: 16
Area
5.43
1840
Time Height Area Area%
5.43 15970 1840.33 100.00
LSU
14.000
12.000
10.000
8.000
6.000
4.000
2.000
0.000
1.00 2.00 3.00 4.00 5.00 6.00 7.00 8.00
PKS2295
(2) ELSD Signal
Range: 14
Area
4.47
1551
Time Height Area Area%
4.47 13901 1550.64 100.00
LSU
10.000
8.000
6.000
4.000
2.000
0.000
Time
1.00 2.00 3.00 4.00 5.00 6.00 7.00 8.00

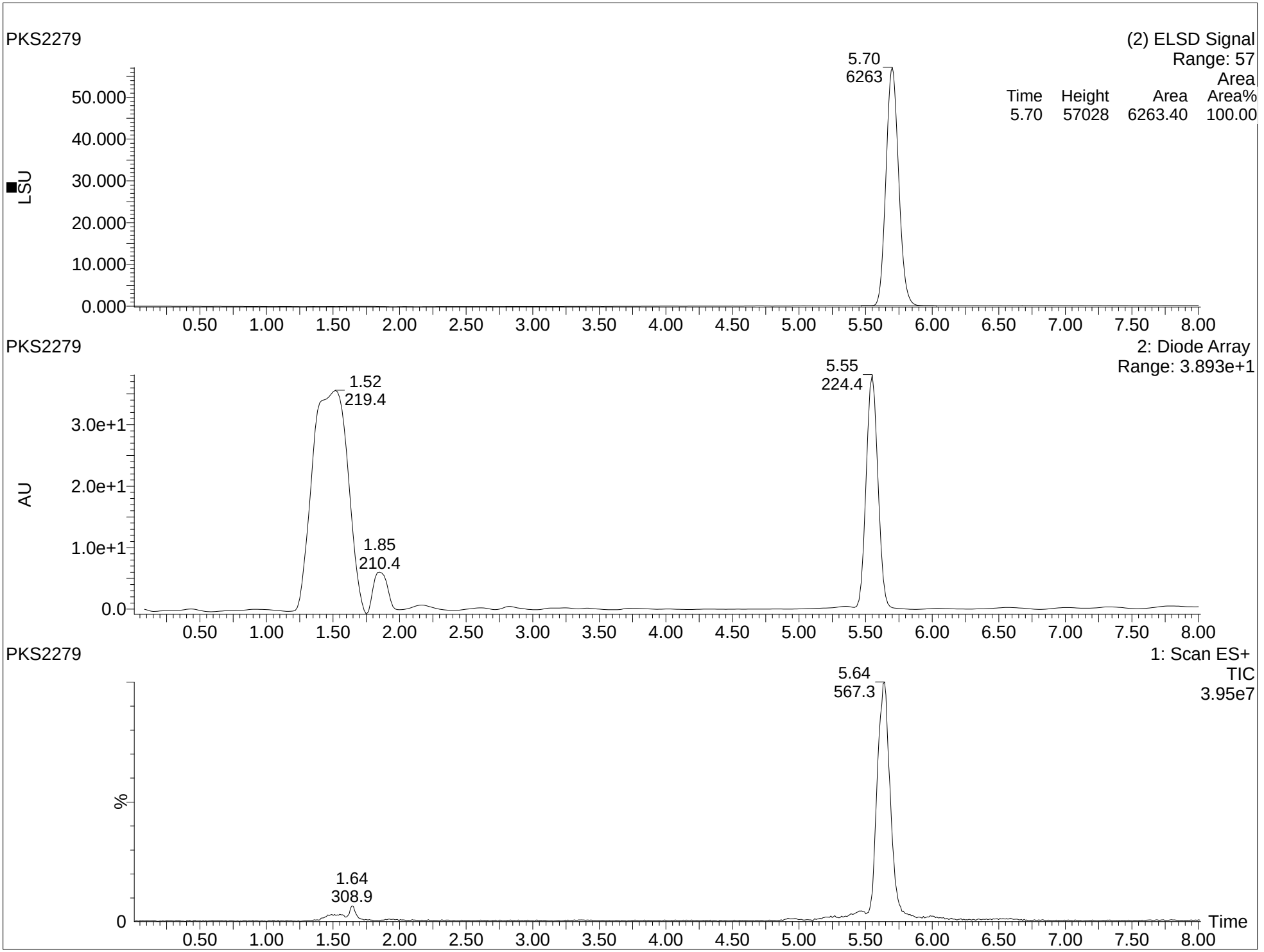

PKS2291
(2) ELSD Signal
Range: 36
Area
5.52
4176
Time Height Area Area%
5.52 36009 4175.80 100.00
LSU
30.000
20.000
10.000
0.000
1.00 2.00 3.00 4.00 5.00 6.00 7.00 8.00
PKS2279
(2) ELSD Signal
Range: 57
Area
5.70
6263
Time Height Area Area%
5.70 57028 6263.40 100.00
LSU
50.000
40.000
30.000
20.000
10.000
0.000
1.00 2.00 3.00 4.00 5.00 6.00 7.00 8.00
PKS2278
(2) ELSD Signal
Range: 7
Area
5.25
759
Time Height Area Area%
5.25 6348 758.94 100.00
LSU
6.000
4.000
2.000
0.000
1.00 2.00 3.00 4.00 5.00 6.00 7.00 8.00
PKS2272
(2) ELSD Signal
Range: 9
Area
5.43
1046
Time Height Area Area%
5.43 9178 1046.44 100.00
LSU
6.000
4.000
2.000
0.000
Time
1.00 2.00 3.00 4.00 5.00 6.00 7.00 8.00

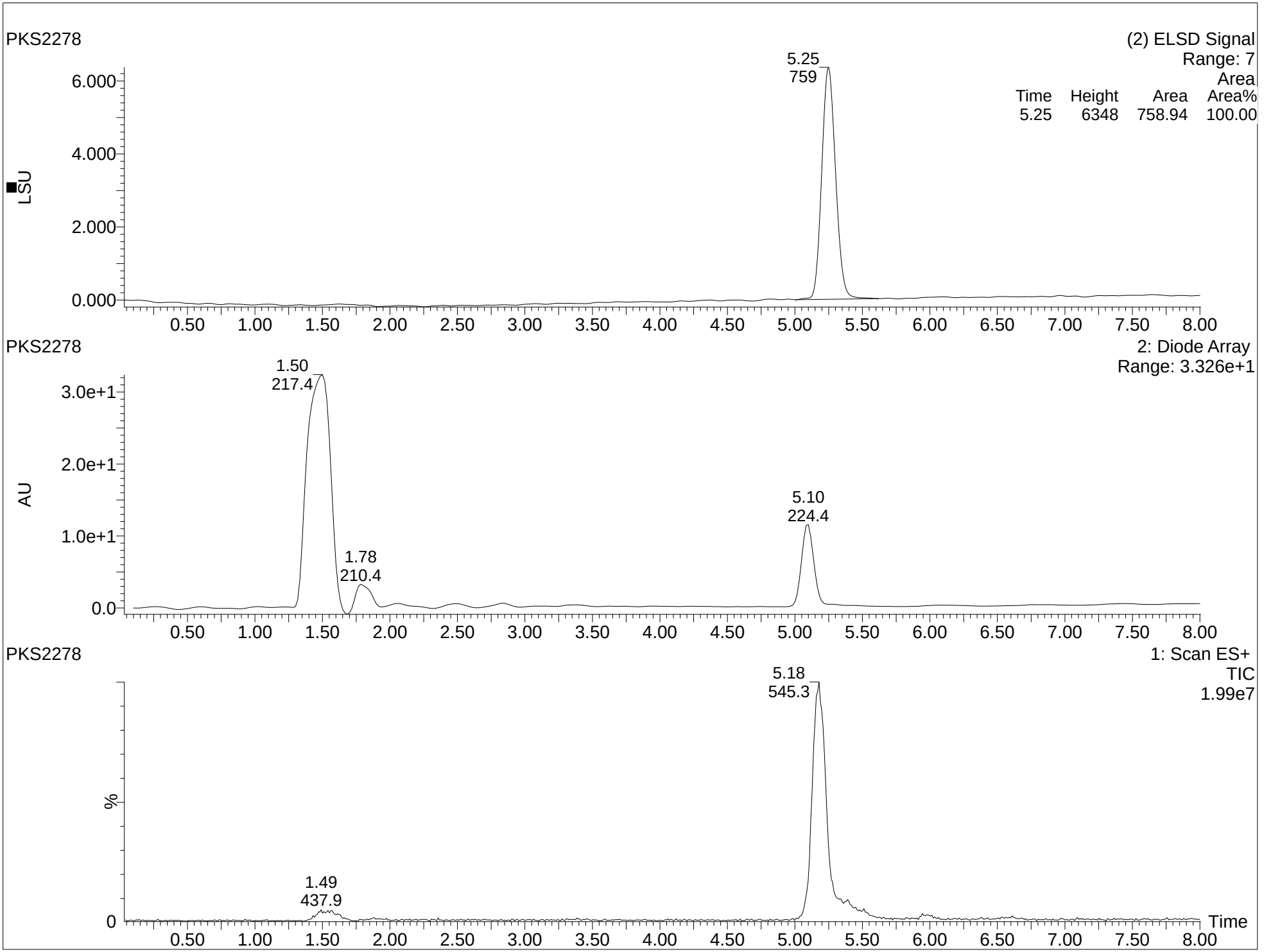

PKS2260
(2) ELSD Signal
Range: 47
Area
5.15
5384
Time Height Area Area%
5.15 46785 5384.31 100.00
LSU
40.000
30.000
20.000
10.000
0.000
1.00 2.00 3.00 4.00 5.00 6.00 7.00 8.00
PKS2252
(2) ELSD Signal
Range: 8
Area
5.53
908
Time Height Area Area%
1.67 114 30.49 3.22
2.42 81 8.23 0.87
5.53 7966 908.46 95.91
LSU
6.000
4.000
2.000
0.000
1.67
30
2.42
8
1.00 2.00 3.00 4.00 5.00 6.00 7.00 8.00
PKS2251
(2) ELSD Signal
Range: 19
Area
5.43
2229
Time Height Area Area%
5.43 18366 2229.05 100.00
LSU
15.000
10.000
5.000
0.000
1.00 2.00 3.00 4.00 5.00 6.00 7.00 8.00
PKS2249
(2) ELSD Signal
Range: 10
Area
4.87
1051
Time Height Area Area%
4.87 9308 1050.71 97.30
5.17 126 29.17 2.70
LSU
6.000
4.000
2.000
0.000
5.17
29
Time
1.00 2.00 3.00 4.00 5.00 6.00 7.00 8.00

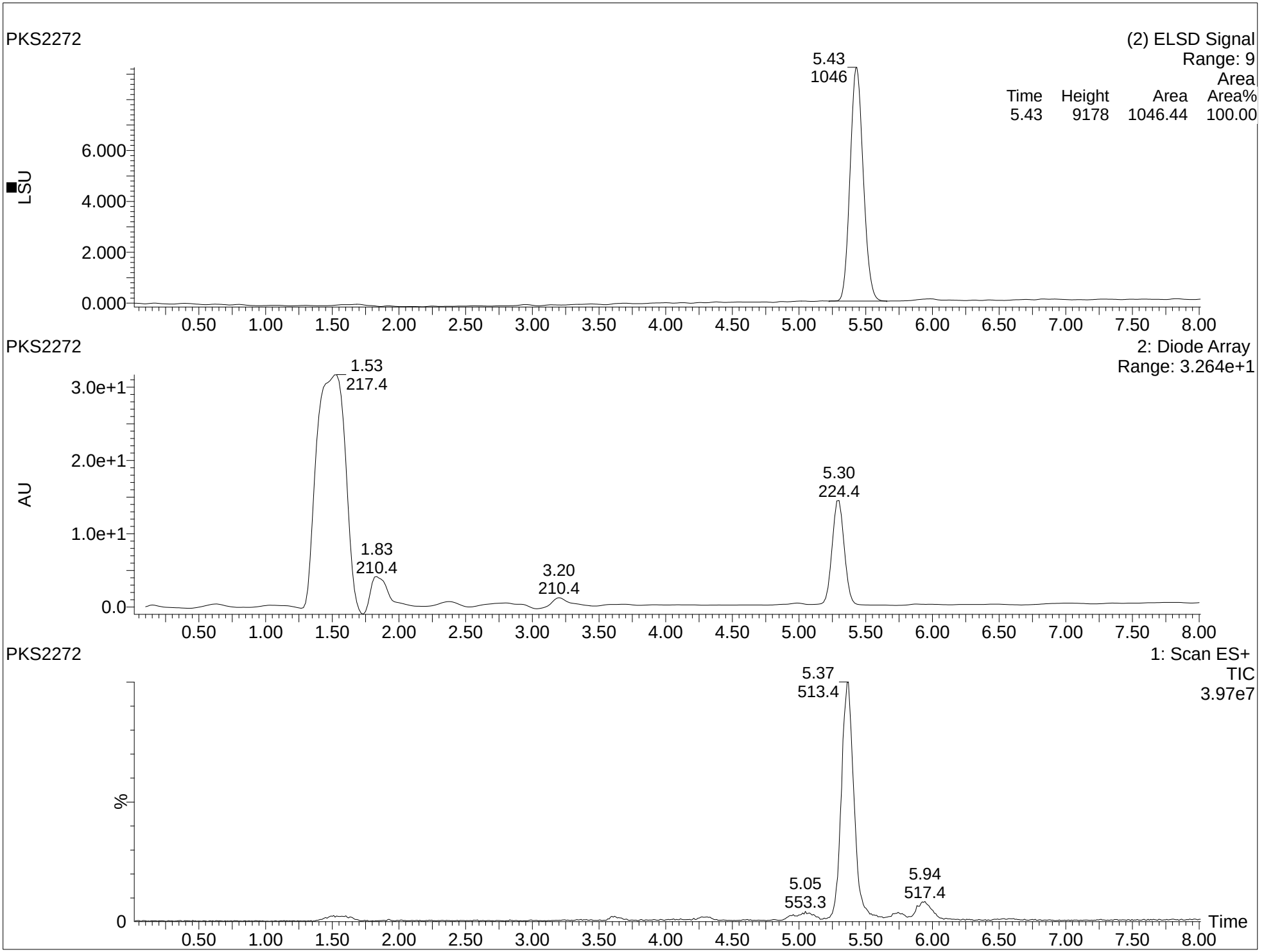

PKS2295
(2) ELSD Signal
Range: 14
Area
Time Height Area Area%
4.47 13901 1550.64 100.00
4.47
1551
LSU
12.500
10.000
7.500
5.000
2.500
0.000
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2295
2: Diode Array
Range: 3.497e+1
1.52
214.4
4.33
224.4
1.83
210.4
AU
3.0e+1
2.0e+1
1.0e+1
0.0
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2295
1: Scan ES+
TIC
2.78e7
4.41
517.3
5.45
581.3
%
0
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00

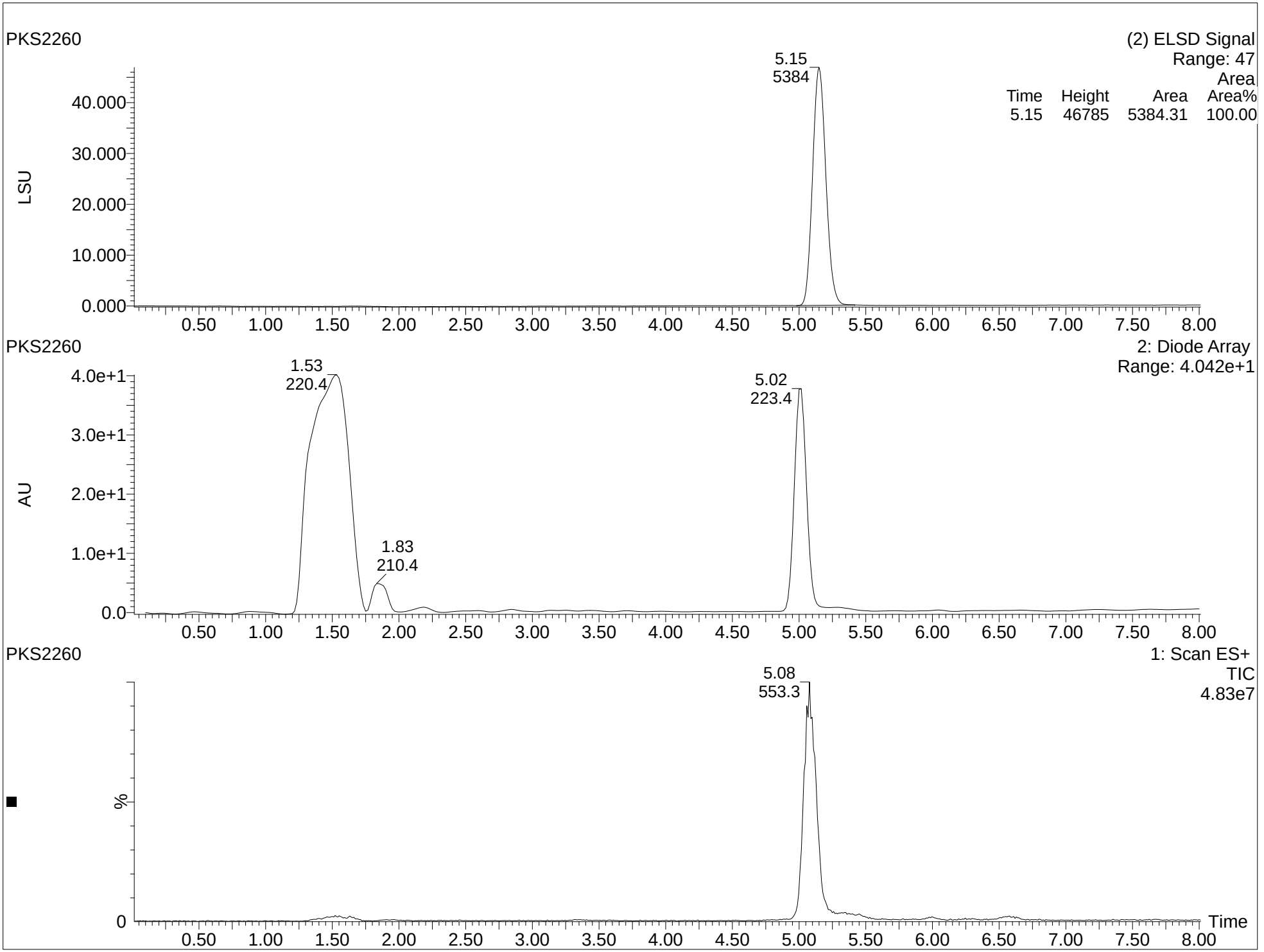

PKS2292
(2) ELSD Signal
Range: 11
Area
Time Height Area Area%
5.13 10610 1238.62 100.00
5.13
1239
LSU
10.000
8.000
6.000
4.000
2.000
0.000
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2292
2: Diode Array
Range: 3.411e+1
1.52
216.4
4.98
224.4
1.82
210.4
AU
3.0e+1
2.0e+1
1.0e+1
0.0
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2292
1: Scan ES+
TIC
2.57e7
5.07
559.3
1.54
437.9
%
0
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00

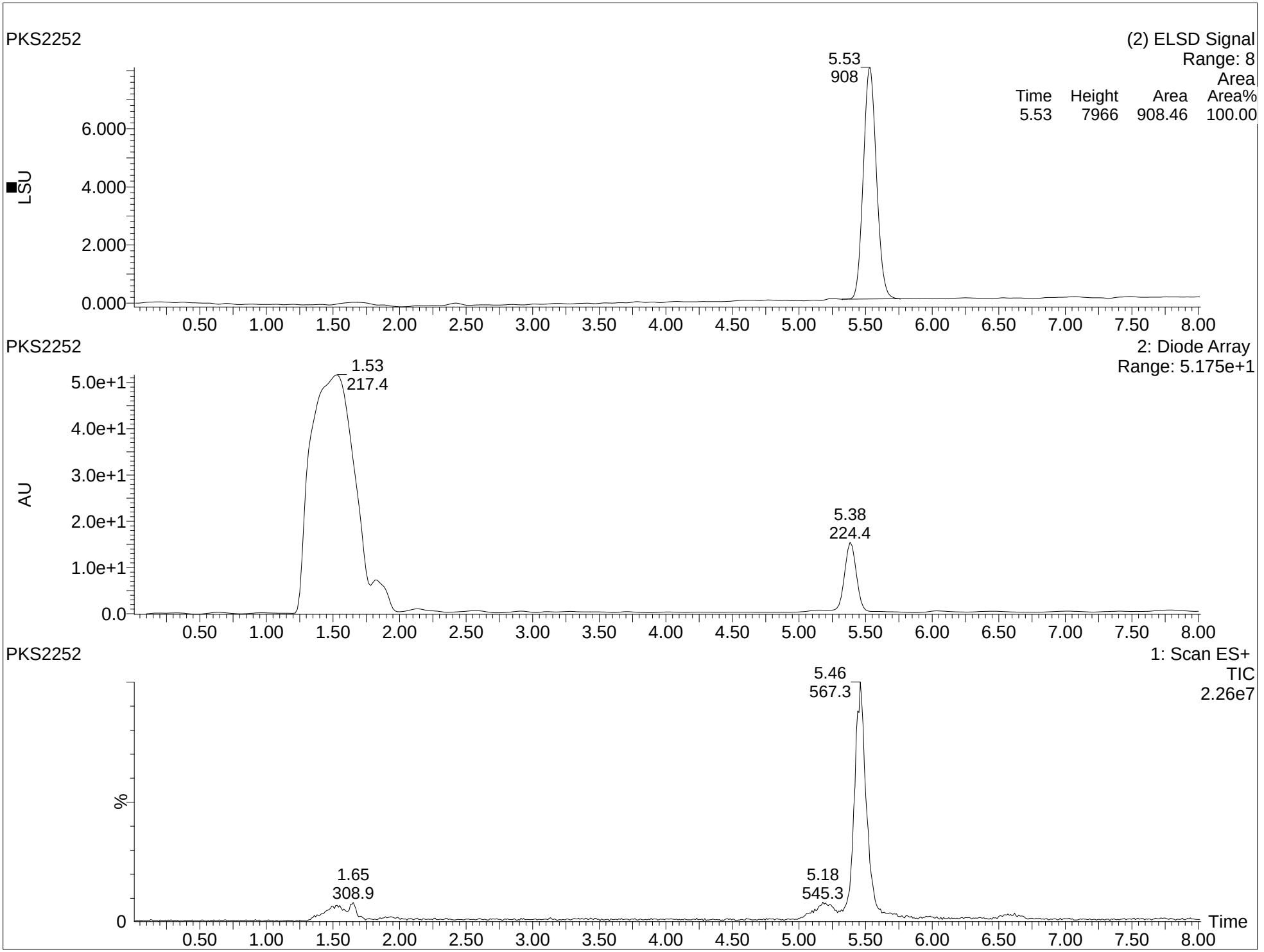

PKS2291
(2) ELSD Signal
Range: 36
Area
Time Height Area Area%
5.52 36009 4175.80 100.00
5.52
4176
LSU
30.000
20.000
10.000
0.000
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2291
2: Diode Array
Range: 3.654e+1
1.53
217.4
5.37
224.4
AU
3.0e+1
2.0e+1
1.0e+1
0.0
1.88
210.4
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2291
1: Scan ES+
TIC
4.12e7
5.45
581.3
5.48
581.3
%
1.65
308.9
0
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00

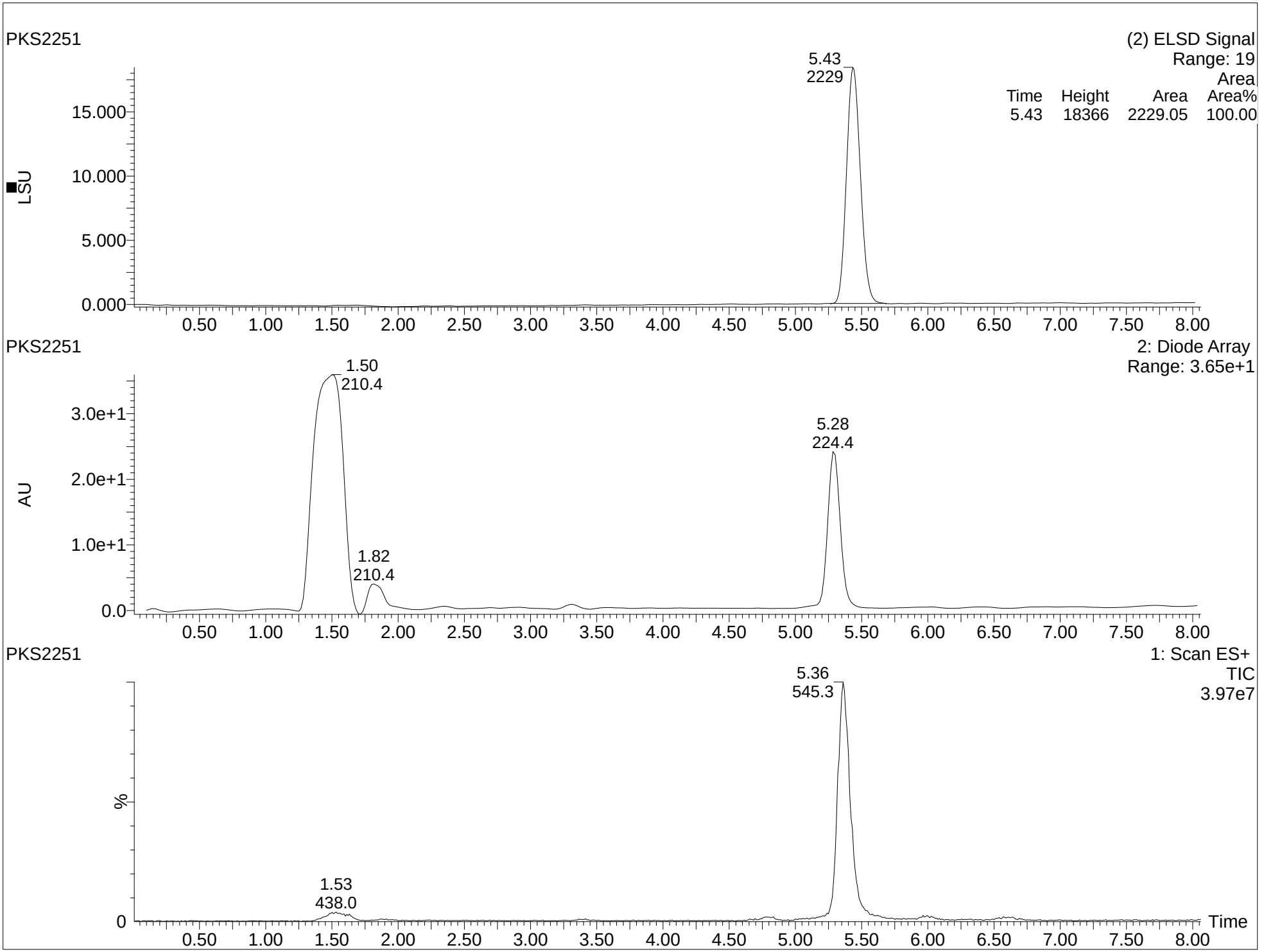

PKS2279
(2) ELSD Signal
Range: 57
Area
Time Height Area Area%
5.70 57028 6263.40 100.00
5.70
6263
LSU
50.000
40.000
30.000
20.000
10.000
0.000
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2279
2: Diode Array
Range: 3.893e+1
1.52
219.4
5.55
224.4
1.85
210.4
AU
3.0e+1
2.0e+1
1.0e+1
0.0
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2279
1: Scan ES+
TIC
3.95e7
5.64
567.3
1.64
308.9
%
0
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00

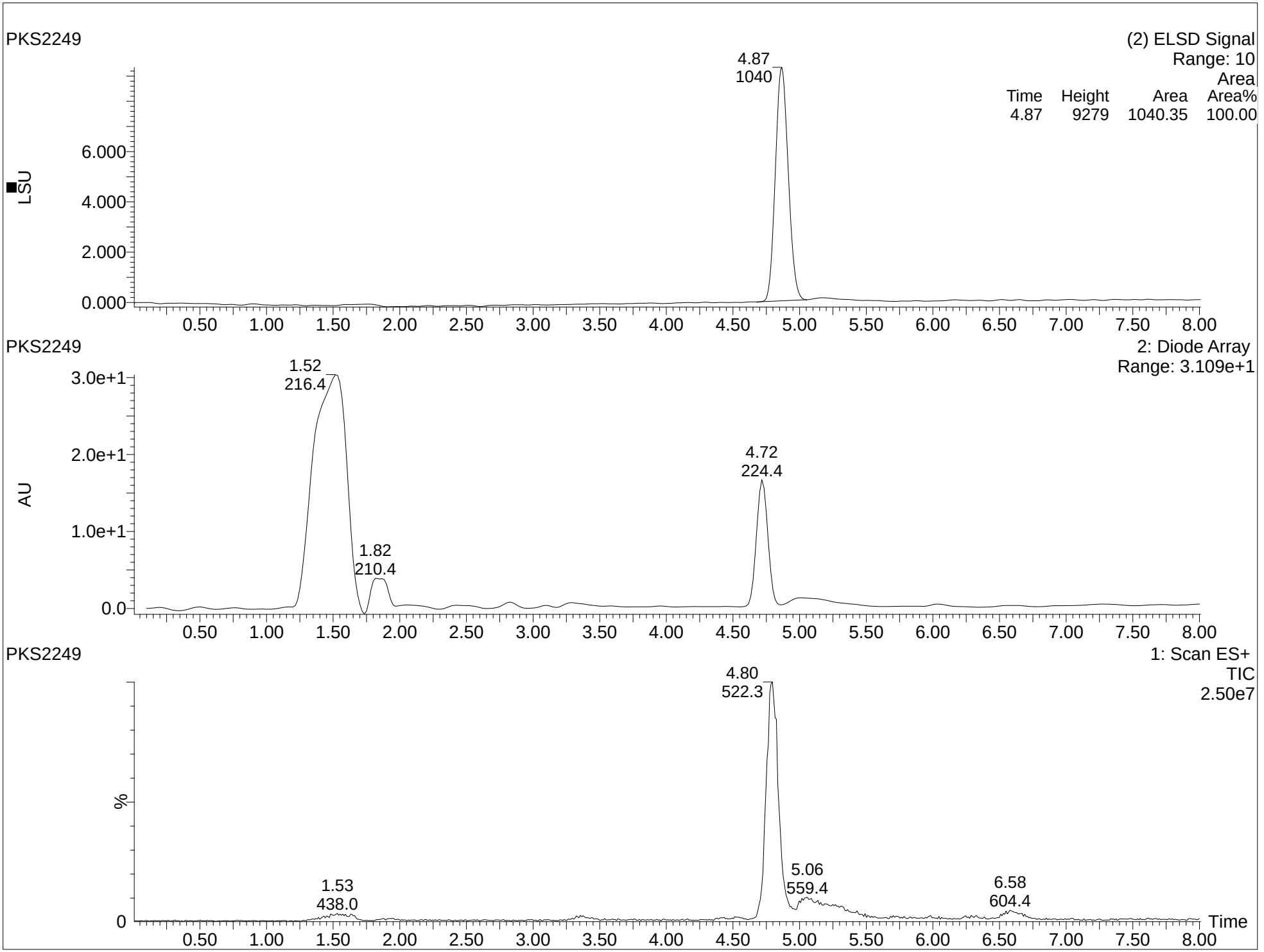

PKS2278
(2) ELSD Signal
Range: 7
Area
Time Height Area Area%
5.25 6348 758.94 100.00
5.25
759
LSU
6.000
4.000
2.000
0.000
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2278
2: Diode Array
Range: 3.326e+1
1.50
217.4
1.78
210.4
5.10
224.4
AU
3.0e+1
2.0e+1
1.0e+1
0.0
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2278
1: Scan ES+
TIC
1.99e7
5.18
545.3
1.49
437.9
%
0
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00

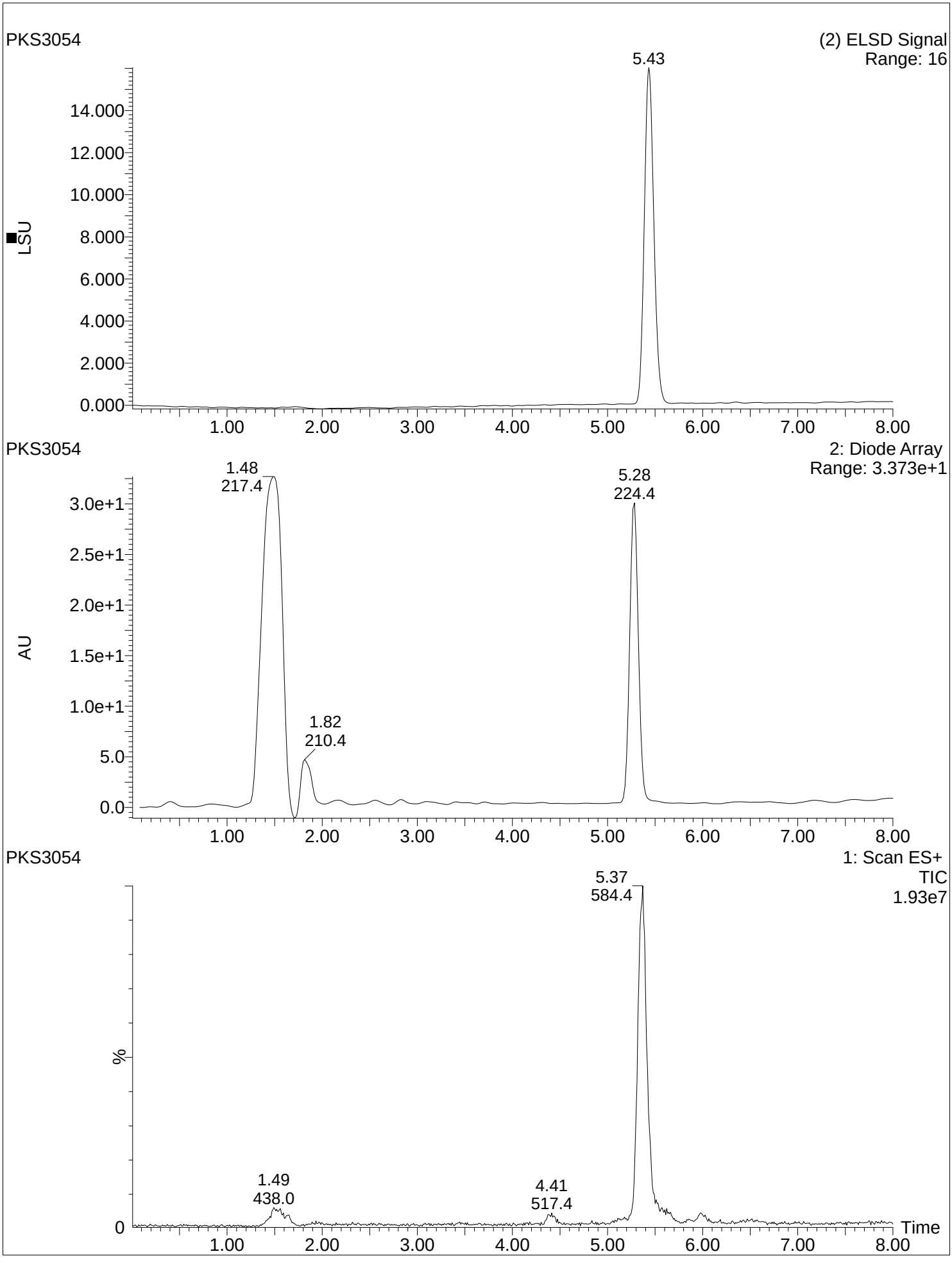

PKS2272
(2) ELSD Signal
Range: 9
Area
Time Height Area Area%
5.43 9178 1046.44 100.00
5.43
1046
LSU
6.000
4.000
2.000
0.000
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2272
2: Diode Array
Range: 3.264e+1
1.53
217.4
AU
3.0e+1
2.0e+1
1.0e+1
0.0
1.83
210.4
3.20
210.4
5.30
224.4
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2272
1: Scan ES+
TIC
3.97e7
5.37
513.4
%
0
5.05
553.3
5.94
517.4
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00


PKS2260
(2) ELSD Signal
Range: 47
Area
Time Height Area Area%
5.15 46785 5384.31 100.00
5.15
5384
LSU
40.000
30.000
20.000
10.000
0.000
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2260
2: Diode Array
Range: 4.042e+1
1.53
220.4
5.02
223.4
1.83
210.4
AU
4.0e+1
3.0e+1
2.0e+1
1.0e+1
0.0
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2260
1: Scan ES+
TIC
4.83e7
5.08
553.3
%
0
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00


PKS2252
(2) ELSD Signal
Range: 8
Area
Time Height Area Area%
5.53 7966 908.46 100.00
5.53
908
LSU
6.000
4.000
2.000
0.000
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2252
2: Diode Array
Range: 5.175e+1
1.53
217.4
5.38
224.4
AU
5.0e+1
4.0e+1
3.0e+1
2.0e+1
1.0e+1
0.0
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2252
1: Scan ES+
TIC
2.26e7
5.46
567.3
1.65
308.9
5.18
545.3
%
0
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00


PKS2251
(2) ELSD Signal
Range: 19
Area
Time Height Area Area%
5.43 18366 2229.05 100.00
5.43
2229
LSU
15.000
10.000
5.000
0.000
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2251
2: Diode Array
Range: 3.65e+1
1.50
210.4
5.28
224.4
1.82
210.4
AU
3.0e+1
2.0e+1
1.0e+1
0.0
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2251
1: Scan ES+
TIC
3.97e7
5.36
545.3
1.53
438.0
%
0
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00


PKS2249
(2) ELSD Signal
Range: 10
Area
Time Height Area Area%
4.87 9279 1040.35 100.00
4.87
1040
LSU
6.000
4.000
2.000
0.000
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2249
2: Diode Array
Range: 3.109e+1
1.52
216.4
4.72
224.4
1.82
210.4
AU
3.0e+1
2.0e+1
1.0e+1
0.0
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00
PKS2249
1: Scan ES+
TIC
2.50e7
4.80
522.3
5.06
559.4
6.58
604.4
1.53
438.0
%
0
Time
0.50 1.00 1.50 2.00 2.50 3.00 3.50 4.00 4.50 5.00 5.50 6.00 6.50 7.00 7.50 8.00


PKS3054
(2) ELSD Signal
Range: 16
5.43
LSU
14.000
12.000
10.000
8.000
6.000
4.000
2.000
0.000
1.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
PKS3054
2: Diode Array
Range: 3.373e+1
1.48
217.4
5.28
224.4
1.82
210.4
AU
3.0e+1
2.5e+1
2.0e+1
1.5e+1
1.0e+1
5.0
0.0
PKS3054
1: Scan ES+
TIC
1.93e7
5.37
584.4
1.49
438.0
4.41
517.4
%
0
Time