

S1: Supporting Information

Small molecule fluorescent ligands for the CXCR4 chemokine receptor

Sebastian Dekkers,¹ Birgit Caspar,^{2,3} Joëlle Goulding,^{2,3} Nicholas D. Kindon¹, Laura E. Kilpatrick,^{1,2} Leigh A Stoddart,^{2,3} Stephen J. Briddon^{2,3} Barrie Kellam,^{1,2} Stephen J. Hill,^{2,3} Michael J. Stocks^{1}*

¹Biodiscovery Institute, School of Pharmacy, University of Nottingham, Nottingham, NG7 2RD, United Kingdom

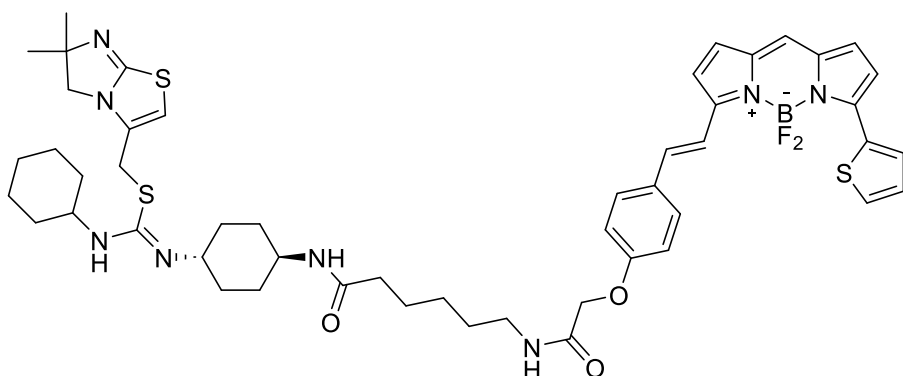
²Centre of Membrane Proteins and Receptors, University of Birmingham and University of Nottingham, The Midlands, NG7 2UH, United Kingdom.

³Division of Physiology, Pharmacology & Neuroscience, Medical School, University of Nottingham, Nottingham, NG7 2UH, UK.

*Corresponding Author: michael.stocks@nottingham.ac.uk

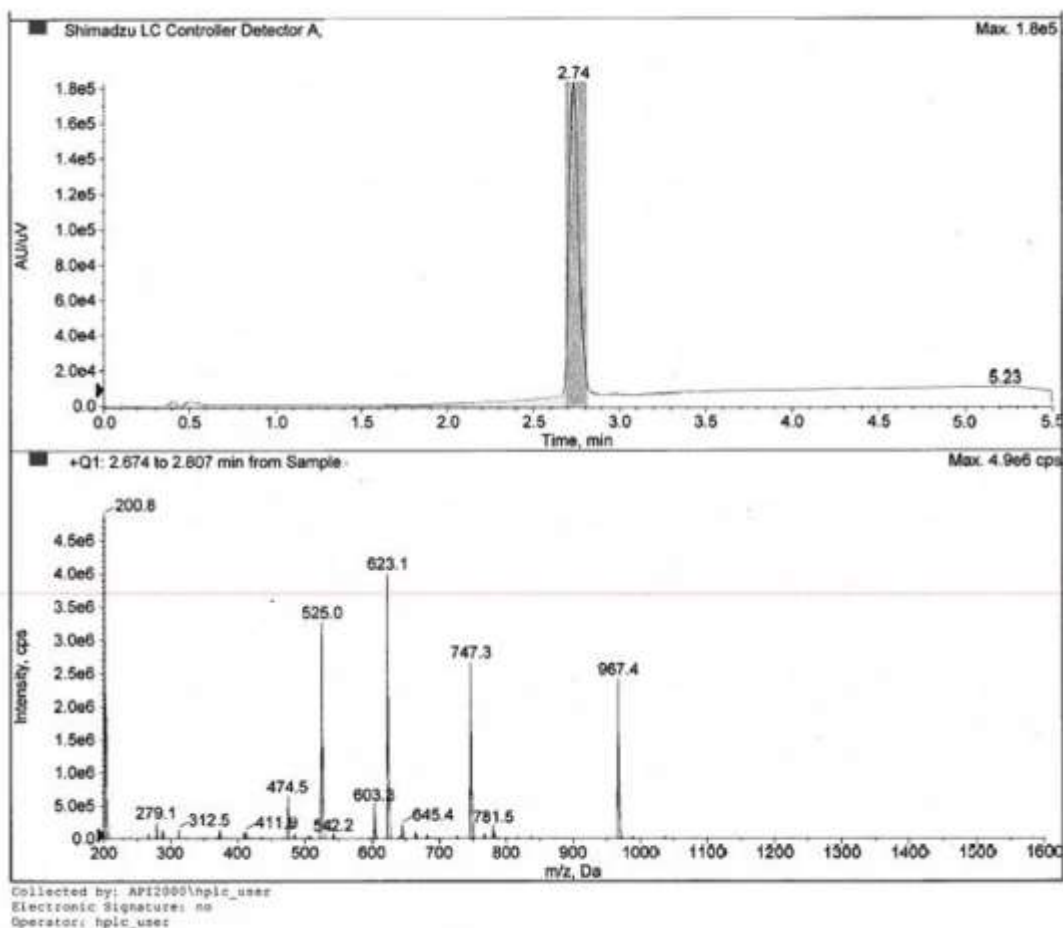
- S2 LCMS purity trace compound **10**
- S3 LCMS purity trace compound **11**
- S4 LCMS purity trace compound **18a**
- S5 LCMS purity trace compound **18b**
- S6 LCMS purity trace compound **24**

LCMS purity trace compound **10**

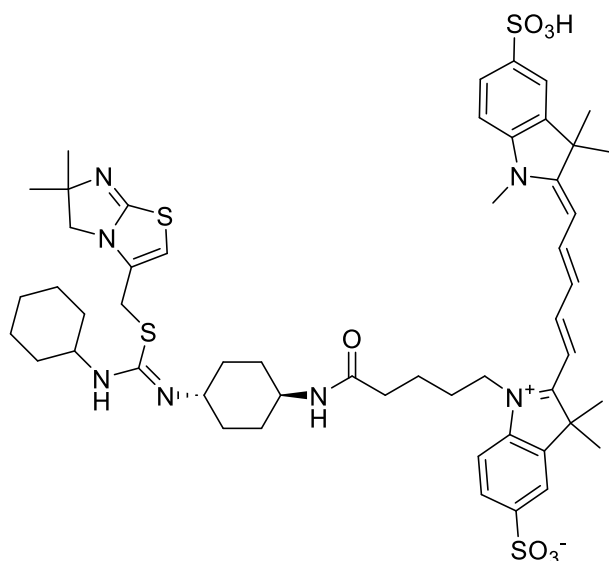


(6,6-Dimethyl-5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl (E)-N-cyclohexyl-N'-((1r,4r)-4-(6-(2-(4-((E)-2-(5,5-difluoro-7-(thiophen-2-yl)-5H-4λ⁴,5λ⁴-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-3-yl)vinyl)phenoxy)acetamido)hexanamido)cyclohexyl)carbamimidothioate

C₅₀H₆₂BF₂N₈O₃S₃: [M+H]⁺ found: 967.4

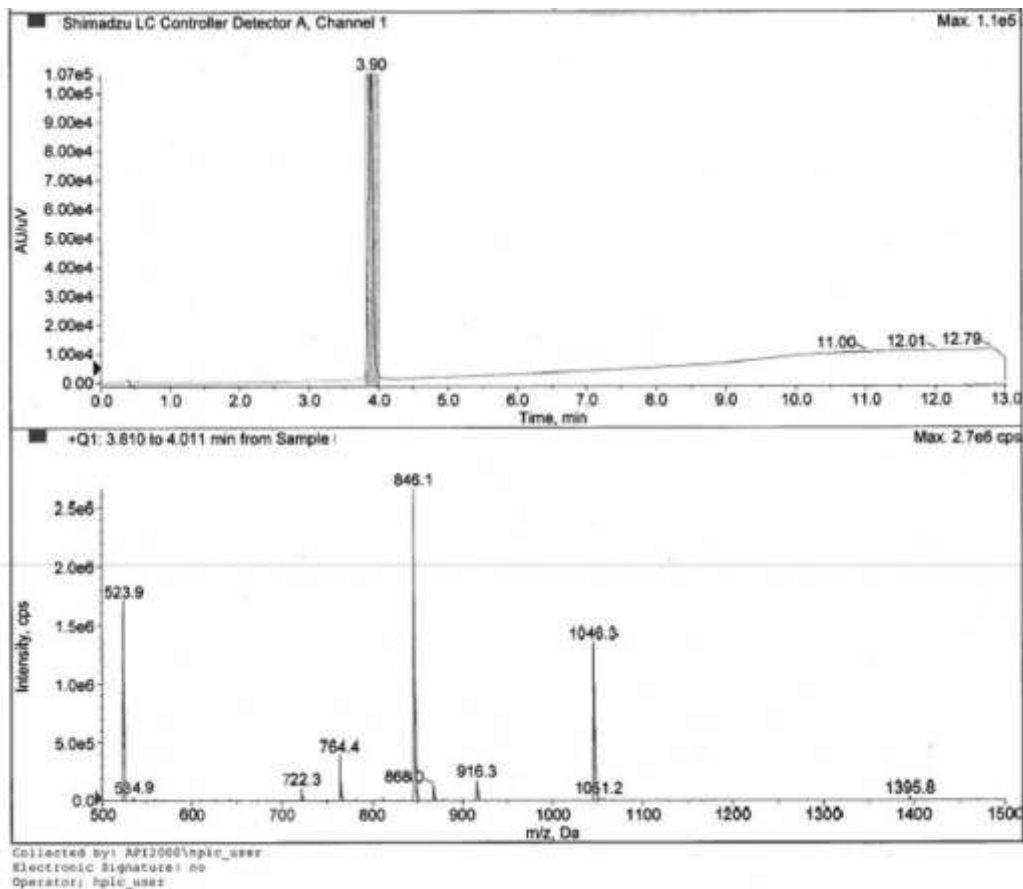


LCMS purity trace compound **11**

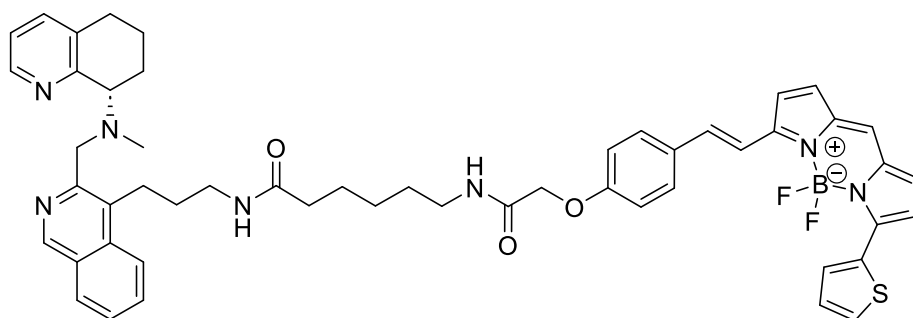


1-(6-(((1r,4r)-4-(((Z)-(cyclohexylamino)(((6,6-dimethyl-5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl)thio)methylene)amino)cyclohexyl)amino)-6-oxohexyl)-3,3-dimethyl-2-((1E,3E)-5-((Z)-1,3,3-trimethyl-5-sulfoindolin-2-ylidene)penta-1,3-dien-1-yl)-3H-indol-1-ium-5-sulfonate

$C_{53}H_{72}N_7O_7S_4$: $[M+H]^+$ found: 1046.4

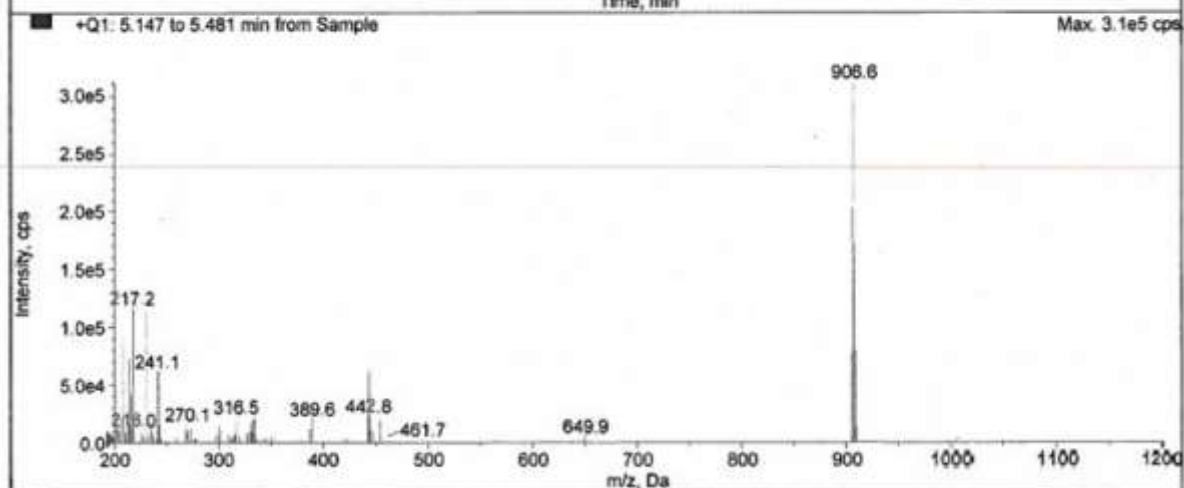
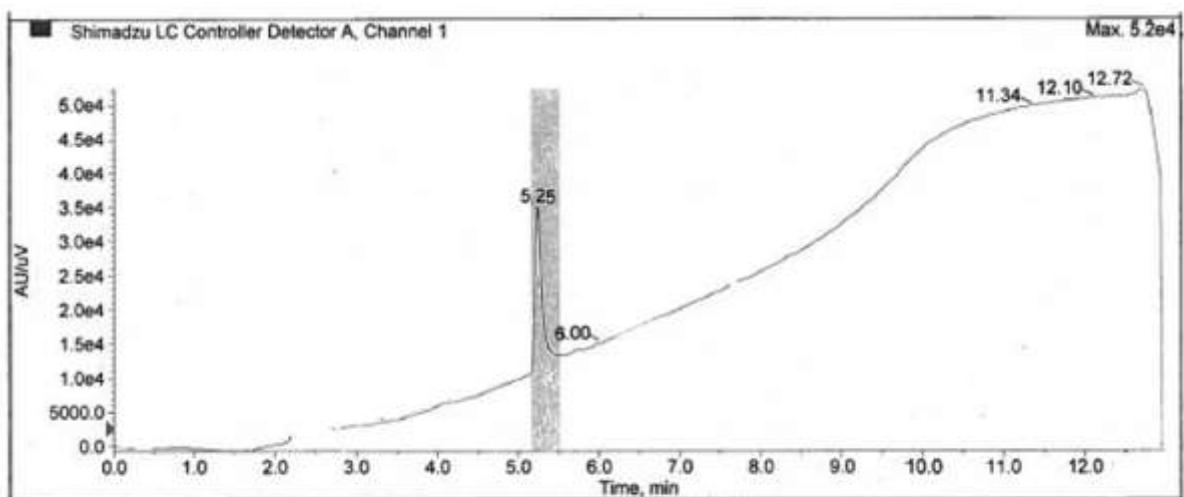


LCMS purity trace compound **18a**



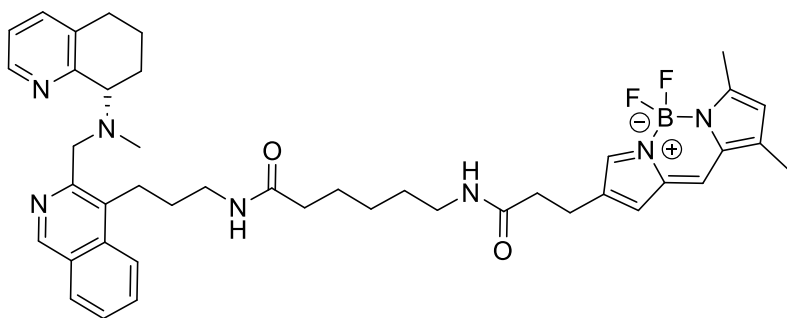
(S,E)-6-(2-(4-(2-(5,5-Difluoro-7-(thiophen-2-yl)-5H-4 λ^4 ,5 λ^4 -dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-3-yl)vinyl)phenoxy)acetamido)-N-(3-(3-(methyl(5,6,7,8-tetrahydroquinolin-8-yl)amino)methyl)isoquinolin-4-yl)propyl)hexanamide

C₅₂H₅₅BF₂N₇O₃S [M+H]⁺: found: 906.6



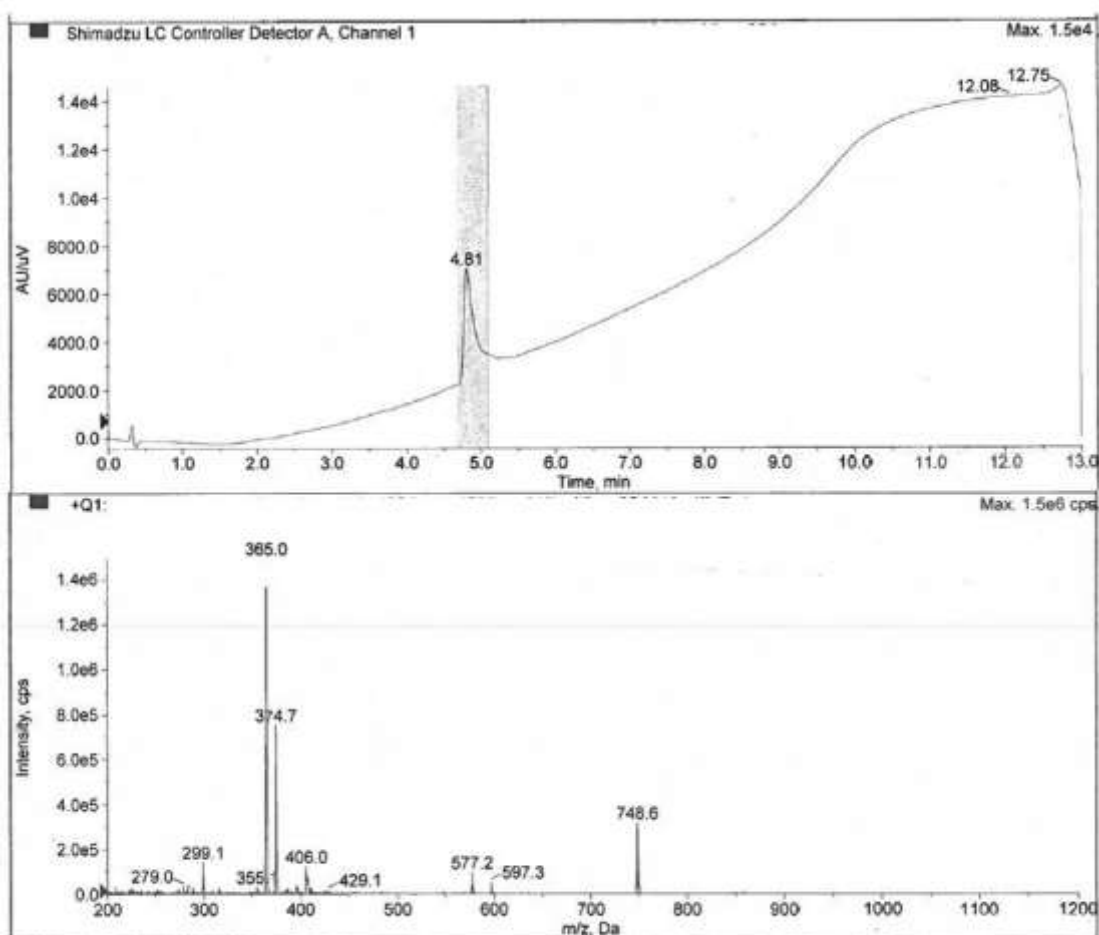
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LCMS purity trace compound **18b**



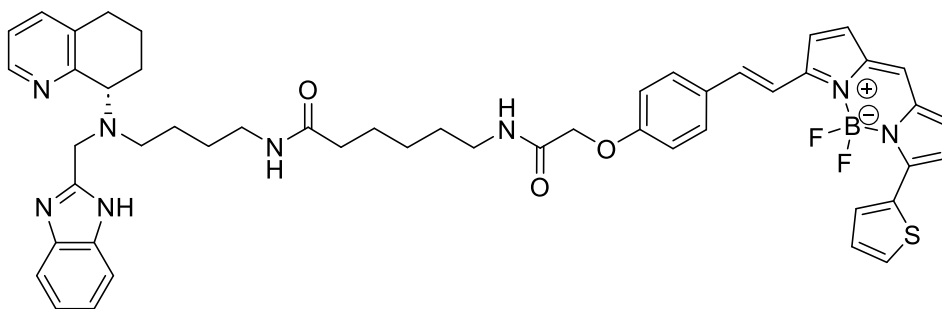
(S)-6-(3-(5,5-Difluoro-7,9-dimethyl-5H-4λ⁴,5λ⁴-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-2-yl)propanamido)-N-(3-(3-((methyl(5,6,7,8-tetrahydroquinolin-8-yl)amino)methyl)isoquinolin-4-yl)propyl)hexanamide

C₄₃H₅₃BF₂N₇O₂ [M+H]⁺: found: 748.6



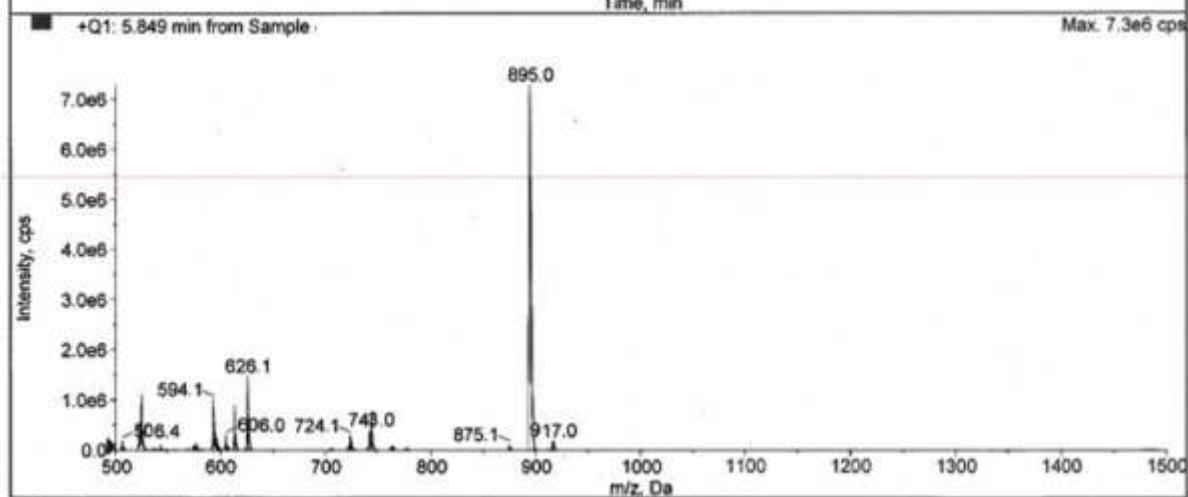
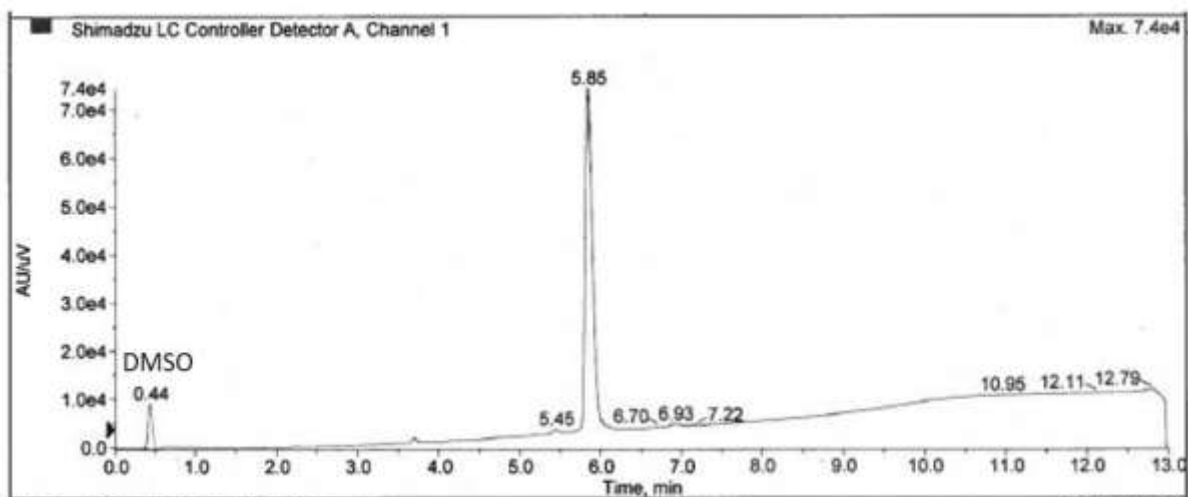
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LCMS purity trace compound **24**



(S,E)-N-(4-(((1H-Benzo[d]imidazol-2-yl)methyl)(5,6,7,8-tetrahydroquinolin-8-yl)amino)butyl)-6-(2-(4-(2-(5,5-difluoro-7-(thiophen-2-yl)-5H-4λ4,5λ4-dipyrrolo [1,2-c:2',1'-f][1,3,2]diazaborinin-3-yl)vinyl)phenoxy)acetamido)hexanamide

$C_{50}H_{53}BF_2N_8O_3S$ $[M+H]^+$: found: 895.5



Collected by: API2000\hplc_user
Electronic Signature: no
Operator: hplc_user