

Supplementary Materials:

Mechanistic Insights into Binding of Ligands with Thiazolidinedione warhead to human histone deacetylase 4

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Tab. S1: SMILES Strings and IC₅₀-values of all tested TZD ligands.

Ligand Name	IC ₅₀ / μ M	Smiles Code
8b	0,33	<chem>O=C(COc1cc2ccc(/C=C(/C(N3)=O)\SC3=O)cc2cc1)N(C(C1)c(cccc2)c2Cl)N=C1c1ccccc1</chem>
8i	0,34	<chem>O=C(COc1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)N(C(C1)c2cccs2)N=C1c1ccccc1</chem>
16b	0,42	<chem>O=C(COc1cc2ccc(/C=C(/C(N3)=O)\SC3=O)cc2cc1)N(C(C1)c(cccc2)c2Cl)N=C1c(cc1)ccc1F</chem>
16g	0,46	<chem>Cc1ccc(C(C2)N(C(COc3ccc(cc(/C=C(/C(N4)=O)\SC4=O)cc4)c4c3)=O)N=C2c(cc2)ccc2F)cc1</chem>
7l	0,54	<chem>Cc(cc(cc1)Br)c1NC(COc1cc2ccc(/C=C(/C(N3)=O)\SC3=O)cc2cc1)=O</chem>
4j	0,67	<chem>O=C(COc1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cc2)cc(Cl)c2Cl)N=C1c1ccccc1</chem>
24g	0,71	<chem>Cc1ccc(C(C2)N(C(COc3ccc(cc(/C=C(/C(N4)=O)\SC4=O)cc4)c4c3)=O)N=C2c(ccc(F)c2)c2F)cc1</chem>
24e	0,73	<chem>O=C(COc1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)N(C(C1)c(cc2)ccc2F)N=C1c(ccc(F)c1)c1F</chem>
8g	0,76	<chem>Cc1ccc(C(C2)N(C(COc3ccc(cc(/C=C(/C(N4)=O)\SC4=O)cc4)c4c3)=O)N=C2c2ccccc2)cc1</chem>
8a	0,77	<chem>O=C(COc1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)N(C(C1)c2ccccc2)N=C1c1ccccc1</chem>
7s	0,78	<chem>O=C(COc1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)Nc1ncccc1F</chem>
4d	0,79	<chem>O=C(COc1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c2ccc(C(F)(F)F)cc2)N=C1c1ccccc1</chem>
12j	0,83	<chem>O=C(COc1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cc2)cc(Cl)c2Cl)N=C1c(cc1)ccc1F</chem>
5w	0,90	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)Nc1nc(cccc2)c2s1</chem>

20e	1,0	<chem>O=C(COC1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cc2)ccc2F)N=C1c(ccc(F)c1)c1F</chem>
8e	1,1	<chem>O=C(COC1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)N(C(C1)c(cc2)ccc2F)N=C1c1ccccc1</chem>
16a	1,1	<chem>O=C(COC1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)N(C(C1)c2ccccc2)N=C1c(cc1)ccc1F</chem>
8c	1,2	<chem>O=C(COC1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)N(C(C1)c2ccco2)N=C1c1ccccc1</chem>
7x	1,2	<chem>Cc1cccc2c1nc(NC(COC1cc3ccc(/C=C(/C(N4)=O)\SC4=O)cc3cc1)=O)s2</chem>
16e	1,3	<chem>O=C(COC1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)N(C(C1)c(cc2)ccc2F)N=C1c(cc1)ccc1F</chem>
7i	1,3	<chem>O=C(COC1cc2ccc(/C=C(/C(N3)=O)\SC3=O)cc2cc1)Nc(c(F)cc(F)c1)c1Br</chem>
4k	1,4	<chem>O=C(COC1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cc2)ccc2Br)N=C1c1ccccc1</chem>
16c	1,4	<chem>O=C(COC1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)N(C(C1)c2ccco2)N=C1c(cc1)ccc1F</chem>
22g	1,5	<chem>Cc1ccc(C(C2)N(C(COc3ccc(/C=C(/C(N4)=O)\SC4=O)cc3)=O)N=C2c(ccc(F)c2)c2F)cc1</chem>
12d	1,5	<chem>O=C(COC1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c2ccc(C(F)(F)F)cc2)N=C1c(cc1)ccc1F</chem>
12a	1,6	<chem>O=C(COC1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c2ccccc2)N=C1c(cc1)ccc1F</chem>
7w	1,6	<chem>O=C(COC1cc2ccc(/C=C(/C(N3)=O)\SC3=O)cc2cc1)Nc1nc(cccc2)c2s1</chem>
12f	1,6	<chem>O=C(COC1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(ccc(F)c2)c2F)N=C1c(cc1)ccc1F</chem>
4g	1,8	<chem>Cc1ccc(C(C2)N(C(COc3ccc(/C=C(/C(N4)=O)\SC4=O)cc3)=O)N=C2c2ccccc2)cc1</chem>
12g	1,8	<chem>Cc1ccc(C(C2)N(C(COc3ccc(/C=C(/C(N4)=O)\SC4=O)cc3)=O)N=C2c(cc2)ccc2F)cc1</chem>
7q	1,8	<chem>[O-][N+](c(cc1)ccc1NC(COC1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)=O)=O</chem>
4b	1,9	<chem>O=C(COC1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cccc2)c2Cl)N=C1c1ccccc1</chem>
22d	1,9	<chem>O=C(COC1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c2ccc(C(F)(F)F)cc2)N=C1c(ccc(F)c1)c1F</chem>
5z	2,1	<chem>[O-][N+](c(cc1)cc2c1nc(NC(COc1ncc(/C=C(/C(N3)=O)\SC3=O)cc1)=O)s2)=O</chem>
14d	2,2	<chem>O=C(COC1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c2ccc(C(F)(F)F)cc2)N=C1c(cc1)ccc1F</chem>
7g	2,2	<chem>COc1cccc(NC(COc2ccc(cc(/C=C(/C(N3)=O)\SC3=O)cc3)c3c2)=O)c1</chem>
12e	2,3	<chem>O=C(COC1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cc2)ccc2F)N=C1c(cc1)ccc1F</chem>
14b	2,3	<chem>O=C(COC1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cccc2)c2Cl)N=C1c(cc1)ccc1F</chem>
4f	2,5	<chem>O=C(COC1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(ccc(F)c2)c2F)N=C1c1ccccc1</chem>
7u	2,9	<chem>Cc(ccc(NC(COC1cc2ccc(/C=C(/C(N3)=O)\SC3=O)cc2cc1)=O)c1)c1Cl</chem>
4e	2,9	<chem>O=C(COC1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cc2)ccc2F)N=C1c1ccccc1</chem>
7o	2,9	<chem>O=C(COC1cc2ccc(/C=C(/C(N3)=O)\SC3=O)cc2cc1)Nc(cc1)ccc1Br</chem>
7n	3,1	<chem>Cc1cccnc1NC(COC1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)=O</chem>
22f	3,4	<chem>O=C(COC1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(ccc(F)c2)c2F)N=C1c(ccc(F)c1)c1F</chem>

5y	3,4	<chem>CCOc(cc1)cc2c1nc(NC(COc1ncc(/C=C(/C(N3)=O)\SC3=O)cc1)=O)s2</chem>
7p	3,5	<chem>O=C(COc1cc2ccc(/C=C(/C(N3)=O)\SC3=O)cc2cc1)Nc1cc(C(F)(F)F)cc(Cl)c1</chem>
7b	3,6	<chem>O=C(COc1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)Nc(cc1)ccc1F</chem>
7y	3,6	<chem>CCOc(cc1)cc2c1nc(NC(COc1cc3ccc(/C=C(/C(N4)=O)\SC4=O)cc3cc1)=O)s2</chem>
14e	3,8	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cc2)ccc2F)N=C1c(cc1)ccc1F</chem>
7a	3,9	<chem>O=C(COc1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)Nc1ccccc1</chem>
7j	4,0	<chem>O=C(COc1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)Nc(cccc1)c1Oc1ccccc1</chem>
6e	4,2	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cc2)ccc2F)N=C1c1ccccc1</chem>
5x	4,3	<chem>Cc1ccc2c1nc(NC(COc1ncc(/C=C(/C(N3)=O)\SC3=O)cc1)=O)s2</chem>
6h	4,3	<chem>[O-][N+](c1cccc(C(C2)N(C(COc3ncc(/C=C(/C(N4)=O)\SC4=O)cc3)=O)N=C2c2ccccc2)c1)=O</chem>
7t	4,4	<chem>Cc1cc(NC(COc2ccc(cc(/C=C(/C(N3)=O)\SC3=O)cc3)c3c2)=O)no1</chem>
7c	4,5	<chem>Cc(cc1)ccc1NC(COc1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)=O</chem>
7r	4,6	<chem>O=C(COc1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)Nc(ccc(S)c1)c1F</chem>
14c	4,7	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c2ccco2)N=C1c(cc1)ccc1F</chem>
7e	4,8	<chem>O=C(COc1ccc(cc(/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)Nc1cc(C(F)(F)F)ccc1</chem>
5o	5,0	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)Nc(cc1)ccc1Br</chem>
7v	5,2	<chem>O=C(COc1cc2ccc(/C=C(/C(N3)=O)\SC3=O)cc2cc1)Nc(cc1)cc(Br)c1Br</chem>
22e	5,2	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cc2)ccc2F)N=C1c(ccc(F)c1)c1F</chem>
6d	5,3	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c2ccc(C(F)(F)F)cc2)N=C1c1ccccc1</chem>
22b	5,6	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cccc2)c2Cl)N=C1c(ccc(F)c1)c1F</chem>
6a	5,7	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c2ccccc2)N=C1c1ccccc1</chem>
5h	5,7	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)Nc(cc1)cc(Cl)c1Cl</chem>
14f	5,8	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(ccc(F)c2)c2F)N=C1c(cc1)ccc1F</chem>
6i	5,9	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c2cccs2)N=C1c1ccccc1</chem>
7h	6,2	<chem>O=C(COc1cc2ccc(/C=C(/C(N3)=O)\SC3=O)cc2cc1)Nc(cc1)cc(Cl)c1Cl</chem>
6b	6,3	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cccc2)c2Cl)N=C1c1ccccc1</chem>
5v	7,0	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)Nc(cc1)cc(Br)c1Br</chem>
12c	7,0	<chem>O=C(COc1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c2ccco2)N=C1c(cc1)ccc1F</chem>
12b	8,0	<chem>O=C(COc1ccc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c(cccc2)c2Cl)N=C1c(cc1)ccc1F</chem>
22c	8,1	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)N(C(C1)c2ccco2)N=C1c(ccc(F)c1)c1F</chem>
5u	8,4	<chem>Cc1cc(Cl)cc(NC(COc2ncc(/C=C(/C(N3)=O)\SC3=O)cc2)=O)c1</chem>

7k	8,4	<chem>O=C(COc1ccc(cc/C=C/C(N2)=O)/SC2=O)cc2)c2c1)Nc(ccc(F)c1)c1F</chem>
6f	8,9	<chem>O=C(COc1ncc(/C=C/C(N2)=O)\SC2=O)cc1)N(C(C1)c(ccc(F)c2)c2F)N=C1c1cccc1</chem>
7f	9,4	<chem>O=C(COc1cc2ccc(/C=C/C(N3)=O)\SC3=O)cc2cc1)Nc1cccc(Cl)c1</chem>
5f	11	<chem>O=C(COc1ncc(/C=C/C(N2)=O)\SC2=O)cc1)Nc1cccc(Cl)c1</chem>
4a	12	<chem>O=C(COc1ccc(/C=C/C(N2)=O)\SC2=O)cc1)N(C(C1)c2cccc2)N=C1c1cccc1</chem>
5c	12	<chem>Cc(cc1)ccc1NC(COc1ncc(/C=C/C(N2)=O)\SC2=O)cc1)=O</chem>
5e	13	<chem>O=C(COc1ncc(/C=C/C(N2)=O)\SC2=O)cc1)Nc1cc(C(F)(F)F)ccc1</chem>
3k	15	<chem>[O-][N+](c(cc1)ccc1NC(COc1c(/C=C/C(N2)=O)\SC2=O)c2cccc2cc1)=O)=O</chem>
20c	15	<chem>O=C(COc1ccc(/C=C/C(N2)=O)\SC2=O)cc1)N(C(C1)c2ccco2)N=C1c(ccc(F)c1)c1F</chem>
5r	15	<chem>O=C(COc1ncc(/C=C/C(N2)=O)\SC2=O)cc1)Nc(ccc(Br)c1)c1F</chem>
5k	19	<chem>O=C(COc1ncc(/C=C/C(N2)=O)\SC2=O)cc1)Nc(ccc(F)c1)c1F</chem>
5s	19	<chem>O=C(COc1ncc(/C=C/C(N2)=O)\SC2=O)cc1)Nc1ncccc1F</chem>
7m	20	<chem>O=C(COc1ccc(cc/C=C/C(N2)=O)\SC2=O)cc2)c2c1)Nc1ncccc1</chem>
14a	21	<chem>O=C(COc1ncc(/C=C/C(N2)=O)\SC2=O)cc1)N(C(C1)c2cccc2)N=C1c(cc1)ccc1F</chem>
5n	21	<chem>Cc1cccnc1NC(COc1ncc(/C=C/C(N2)=O)\SC2=O)cc1)=O</chem>
5m	22	<chem>O=C(COc1ncc(/C=C/C(N2)=O)\SC2=O)cc1)Nc1ncccc1</chem>
5d	25	<chem>COc(cc1)ccc1NC(COc1ncc(/C=C/C(N2)=O)\SC2=O)cc1)=O</chem>
5p	34	<chem>O=C(COc1ncc(/C=C/C(N2)=O)\SC2=O)cc1)Nc(c(C(F)(F)F)ccc1)c1Cl</chem>
GB24	35	<chem>Cc(c(C)c1)cc2c1sc(NC(CN(C(/C(/S1)=C/c(cc3)ccc3Cl)=O)C1=O)=O)n2</chem>
P10	43	<chem>CC(N(C)N(C1=O)c2cccc2)=C1NC(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)=O</chem>
3a	> 50	<chem>O=C(COc1c(/C=C/C(N2)=O)\SC2=O)c2cccc2cc1)Nc1cccc1</chem>
3b	> 50	<chem>O=C(COc1c(/C=C/C(N2)=O)\SC2=O)c2cccc2cc1)Nc(cc1)ccc1F</chem>
3c	> 50	<chem>Cc(cc1)ccc1NC(COc1c(/C=C/C(N2)=O)\SC2=O)c2cccc2cc1)=O</chem>
3d	> 50	<chem>COc(cc1)ccc1NC(COc1c(/C=C/C(N2)=O)\SC2=O)c2cccc2cc1)=O</chem>
3e	> 50	<chem>O=C(COc1c(/C=C/C(N2)=O)\SC2=O)c2cccc2cc1)Nc(cc1)cc(Cl)c1Cl</chem>
3f	> 50	<chem>O=C(COc1c(/C=C/C(N2)=O)\SC2=O)c2cccc2cc1)Nc(c(F)cc(F)c1)c1Br</chem>
3g	> 50	<chem>O=C(COc1c(/C=C/C(N2)=O)\SC2=O)c2cccc2cc1)Nc(ccc(F)c1)c1F</chem>
3h	> 50	<chem>Cc(cc(cc1)Br)c1NC(COc1c(/C=C/C(N2)=O)\SC2=O)c2cccc2cc1)=O</chem>
3i	> 50	<chem>O=C(COc1c(/C=C/C(N2)=O)\SC2=O)c2cccc2cc1)Nc(cc1)ccc1Br</chem>
3j	> 50	<chem>O=C(COc1c(/C=C/C(N2)=O)\SC2=O)c2cccc2cc1)Nc1cc(C(F)(F)F)ccc1</chem>
5a	> 50	<chem>O=C(COc1ncc(/C=C/C(N2)=O)\SC2=O)cc1)Nc1cccc1</chem>

5b	> 50	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)Nc(cc1)ccc1F</chem>
5g	> 50	<chem>COc1cccc(NC(COc2ncc(/C=C(/C(N3)=O)\SC3=O)cc2)=O)c1</chem>
5i	> 50	<chem>O=C(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)Nc(c(F)cc(F)c1)c1Br</chem>
5j	> 50	<chem>Cc1ncc(NC(COc2ncc(/C=C(/C(N3)=O)\SC3=O)cc2)=O)s1</chem>
5l	> 50	<chem>Cc(cc(cc1)Br)c1NC(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)=O</chem>
5q	> 50	<chem>[O-][N+](c(cc1)ccc1NC(COc1ncc(/C=C(/C(N2)=O)\SC2=O)cc1)=O)=O</chem>
5t	> 50	<chem>Cc1cc(NC(COc2ncc(/C=C(/C(N3)=O)\SC3=O)cc2)=O)no1</chem>
7d	> 50	<chem>COc(cc1)ccc1NC(COc1ccc(cc1/C=C(/C(N2)=O)\SC2=O)cc2)c2c1)=O</chem>
F1	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc1cccc1</chem>
F10	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc(cc(C(F)(F)F)cc1)c1Cl</chem>
F11	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc(ccc(Br)c1)c1F</chem>
F12	> 50	<chem>COc(cc1)ccc1NC(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)=O</chem>
F13	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc(cc1)ccc1F</chem>
F14	> 50	<chem>[O-][N+](c(cc1)ccc1NC(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)=O)=O</chem>
F15	> 50	<chem>Cc1cc(NC(CN(C(/C(/S2)=C/c3ccco3)=O)C2=O)=O)no1</chem>
F16	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc1nccs1</chem>
F17	> 50	<chem>Cc(ccc(NC(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)=O)c1)c1Cl</chem>
F18	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc1nc(cccc2)c2s1</chem>
F19	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc(cc1)cc(Cl)c1Cl</chem>
F2	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc(cccc1)c1F</chem>
F21	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc(cc1)ccc1Br</chem>
F22	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc1ncccc1</chem>
F23	> 50	<chem>Cc(cc1)ccc1NC(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)=O</chem>
F24	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc(cc1)cc(Br)c1Br</chem>
F25	> 50	<chem>Cc1csc(NC(CN(C(/C(/S2)=C/c3ccco3)=O)C2=O)=O)n1</chem>
F3	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc1cc(F)ccc1</chem>
F4	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc(c(F)cc(Br)c1)c1F</chem>
F5	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc(ccc(F)c1)c1F</chem>
F6	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc1cc(C(F)(F)F)ccc1</chem>
F7	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc(cc1)c(C(F)(F)F)cc1Cl</chem>
F8	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ccco2)=O)C1=O)Nc(cc1)c(C(F)(F)F)cc1Cl</chem>

F9	> 50	<chem>O=C(CN(C/C(/S1)=C/c2ccco2)=O)C1=O)Nc(cc1)ccc1Oc1ccccc1</chem>
G1	> 50	<chem>O=C(CN(C/C(/S1)=C/c(cc2)ccc2Br)=O)C1=O)Nc(cc1)c(C(F)(F)F)cc1Cl</chem>
G10	> 50	<chem>O=C(CN(C/C(/S1)=C/c(cc2)ccc2F)=O)C1=O)Nc(ccc(F)c1)c1F</chem>
G11	> 50	<chem>Cc1ccc/C=C/C(N2CC(Nc(cc3)c(C(F)(F)F)cc3Cl)=O)=O)\SC2=O)cc1</chem>
G12	> 50	<chem>Cc1ccc/C=C/C(N2CC(Nc(ccc(F)c3)c3F)=O)=O)\SC2=O)cc1</chem>
G13	> 50	<chem>O=C(CN(C/C(/S1)=C/c2ccccc2)=O)C1=O)Nc(cc1)c(C(F)(F)F)cc1Cl</chem>
G14	> 50	<chem>O=C(CN(C/C(/S1)=C/c2ccccc2)=O)C1=O)Nc(ccc(F)c1)c1F</chem>
G15	> 50	<chem>O=C(CN(C/C(/S1)=C/c(ccc(F)c2)c2F)=O)C1=O)Nc1cc(C(F)(F)F)ccc1</chem>
G16	> 50	<chem>O=C(CN(C/C(/S1)=C/c(cc2)ccc2F)=O)C1=O)Nc1cc(C(F)(F)F)ccc1</chem>
G2	> 50	<chem>O=C(CN(C/C(/S1)=C/c(cc2)ccc2Br)=O)C1=O)Nc(ccc(F)c1)c1F</chem>
G3	> 50	<chem>Cc1c(C)cc/C=C/C(N2CC(Nc(cc3)c(C(F)(F)F)cc3Cl)=O)=O)\SC2=O)cc1</chem>
G4	> 50	<chem>Cc1c(C)cc/C=C/C(N2CC(Nc(ccc(F)c3)c3F)=O)=O)\SC2=O)cc1</chem>
G5	> 50	<chem>O=C(CN(C/C(/S1)=C/c(cc2)ccc2Cl)=O)C1=O)Nc(cc1)c(C(F)(F)F)cc1Cl</chem>
G6	> 50	<chem>O=C(CN(C/C(/S1)=C/c(cc2)ccc2Cl)=O)C1=O)Nc(ccc(F)c1)c1F</chem>
G7	> 50	<chem>O=C(CN(C/C(/S1)=C/c(ccc(F)c2)c2F)=O)C1=O)Nc(cc1)c(C(F)(F)F)cc1Cl</chem>
G8	> 50	<chem>O=C(CN(C/C(/S1)=C/c(ccc(F)c2)c2F)=O)C1=O)Nc(ccc(F)c1)c1F</chem>
G9	> 50	<chem>O=C(CN(C/C(/S1)=C/c(cc2)ccc2F)=O)C1=O)Nc(cc1)c(C(F)(F)F)cc1Cl</chem>
GB01	> 50	<chem>O=C(CN(C/C(/S1)=C/c2ccccc2)=O)C1=O)Nc(sc1ccc2)nc1c2Cl</chem>
GB02	> 50	<chem>Cc1ccc/C=C/C(N2CC(Nc(sc3ccc4)nc3c4Cl)=O)=O)\SC2=O)cc1</chem>
GB03	> 50	<chem>O=C(CN(C/C(/S1)=C/c(cc2)ccc2Cl)=O)C1=O)Nc(sc1ccc2)nc1c2Cl</chem>
GB04	> 50	<chem>O=C(CN(C/C(/S1)=C/c(cc2)ccc2Br)=O)C1=O)Nc1nc(c(Cl)ccc2)c2s1</chem>
GB05	> 50	<chem>O=C(CN(C/C(/S1)=C/c(ccc(F)c2)c2F)=O)C1=O)Nc(sc1ccc2)nc1c2Cl</chem>
GB06	> 50	<chem>Cc1c(C)cc/C=C/C(N2CC(Nc(sc3ccc4)nc3c4Cl)=O)=O)\SC2=O)cc1</chem>
GB07	> 50	<chem>O=C(CN(C/C(/S1)=C/c(cc2)ccc2Br)=O)C1=O)Nc1nc(c(F)cc(F)c2)c2s1</chem>
GB08	> 50	<chem>COc1cccc2c1nc(NC(CN(C/C(/S1)=C/c3ccccc3)=O)C1=O)=O)s2</chem>
GB09	> 50	<chem>Cc1cccc2c1nc(NC(CN(C/C(/S1)=C/c3ccccc3)=O)C1=O)=O)s2</chem>
GB10	> 50	<chem>Cc1cccc2c1nc(NC(CN(C/C(/S1)=C/c(cc3)ccc3F)=O)C1=O)=O)s2</chem>
GB11	> 50	<chem>O=C(CN(C/C(/S1)=C/c(cc2)ccc2Cl)=O)C1=O)Nc1nc(c(F)cc(F)c2)c2s1</chem>
GB12	> 50	<chem>O=C(CN(C/C(/S1)=C/c2ccccc2)=O)C1=O)Nc1nc(c(F)cc(F)c2)c2s1</chem>
GB13	> 50	<chem>Cc(cc1)cc2c1nc(NC(CN(C/C(/S1)=C/c(ccc(F)c3)c3F)=O)C1=O)=O)s2</chem>
GB14	> 50	<chem>Cc1ccc/C=C/C(N2CC(Nc3nc(ccc(C)c4)c4s3)=O)=O)\SC2=O)cc1</chem>

GB15	> 50	<chem>Cc(cc1)cc2c1nc(NC(CN(C(C/S1)=C/c3cc(C)c(C)cc3)=O)C1=O)=O)s2</chem>
GB16	> 50	<chem>Cc(cc1)cc2c1nc(NC(CN(C(C/S1)=C/c(cc3)ccc3Cl)=O)C1=O)=O)s2</chem>
GB17	> 50	<chem>CCOc(cc1)cc2c1nc(NC(CN(C(C/S1)=C/c(cc3)ccc3Cl)=O)C1=O)=O)s2</chem>
GB18	> 50	<chem>O=C(CN(C(C/S1)=C/c(cc2)ccc2F)=O)C1=O)Nc1nc(c(F)cc(F)c2)c2s1</chem>
GB19	> 50	<chem>Cc1ccc/C=C/C(N2CC(Nc3nc(c(F)cc(F)c4)c4s3)=O)=O)\SC2=O)cc1</chem>
GB20	> 50	<chem>Cc1c(C)cc/C=C/C(N2CC(Nc3nc(c(F)cc(F)c4)c4s3)=O)=O)\SC2=O)cc1</chem>
GB21	> 50	<chem>Cc1ccc/C=C/C(N2CC(Nc3nc(cc(C)c(C)c4)c4s3)=O)=O)\SC2=O)cc1</chem>
GB23	> 50	<chem>Cc(c(C)c1)cc2c1sc(NC(CN(C(C/S1)=C/c(cc3)ccc3Br)=O)C1=O)=O)n2</chem>
GB25	> 50	<chem>Cc(c(C)c1)cc2c1sc(NC(CN(C(C/S1)=C/c(cc3)ccc3F)=O)C1=O)=O)n2</chem>
GB26	> 50	<chem>Cc1c(C)cc/C=C/C(N2CC(Nc3nc(cc(C)c(C)c4)c4s3)=O)=O)\SC2=O)cc1</chem>
GB27	> 50	<chem>Cc1ccc/C=C/C(N2CC(Nc3nc(c(OC)ccc4)c4s3)=O)=O)\SC2=O)cc1</chem>
GB28	> 50	<chem>Cc1cccc2c1nc(NC(CN(C(C/S1)=C/c3cccc3)=O)C1=O)=O)s2</chem>
GB29	> 50	<chem>O=C(CN(C(C/S1)=C/c(ccc(F)c2)c2F)=O)C1=O)Nc1nc(c(F)cc(F)c2)c2s1</chem>
GB30	> 50	<chem>O=C(CN(C(C/S1)=C/c2cccc2)=O)C1=O)Nc1nc(c(F)ccc2)c2s1</chem>
GB31	> 50	<chem>Cc(cc1)cc2c1nc(NC(CN(C(C/S1)=C/c(cc3)ccc3Br)=O)C1=O)=O)s2</chem>
GB32	> 50	<chem>Cc1ccc/C=C/C(N2CC(Nc3nc(ccc(F)c4)c4s3)=O)=O)\SC2=O)cc1</chem>
GB33	> 50	<chem>O=C(CN(C(C/S1)=C/c(cc2)ccc2Cl)=O)C1=O)Nc1nc(ccc(F)c2)c2s1</chem>
GB34	> 50	<chem>O=C(CN(C(C/S1)=C/c(cc2)ccc2F)=O)C1=O)Nc1nc(ccc(F)c2)c2s1</chem>
GB35	> 50	<chem>COc1cccc2c1nc(NC(CN(C(C/S1)=C/c(cc3)ccc3F)=O)C1=O)=O)s2</chem>
GB36	> 50	<chem>CCOc(cc1)cc2c1nc(NC(CN(C(C/S1)=C/c3cccc3)=O)C1=O)=O)s2</chem>
P1	> 50	<chem>O=C(CN(C(C/S1)=C/c2ncccc2)=O)C1=O)Nc1cccc1</chem>
P11	> 50	<chem>O=C(CN(C(C/S1)=C/c2ncccc2)=O)C1=O)Nc(cc1)ccc1F</chem>
P12	> 50	<chem>Cc(cc1)ccc1NC(CN(C(C/S1)=C/c2ncccc2)=O)C1=O)=O</chem>
P13	> 50	<chem>O=C(CN(C(C/S1)=C/c2ncccc2)=O)C1=O)Nc(cccc1)c1Oc1cccc1</chem>
P14	> 50	<chem>COc(cc1)ccc1NC(CN(C(C/S1)=C/c2ncccc2)=O)C1=O)=O</chem>
P15	> 50	<chem>O=C(CN(C(C/S1)=C/c2ncccc2)=O)C1=O)Nc(c(F)cc(Br)c1)c1F</chem>
P16	> 50	<chem>[O-][N+](c(cc1)ccc1NC(CN(C(C/S1)=C/c2ncccc2)=O)C1=O)=O)=O</chem>
P17	> 50	<chem>Cc(ccc(NC(CN(C(C/S1)=C/c2ncccc2)=O)C1=O)=O)c1)c1Cl</chem>
P18	> 50	<chem>Cc1conc1NC(CN(C(C/S1)=C/c2ncccc2)=O)C1=O)=O</chem>
P19	> 50	<chem>O=C(CN(C(C/S1)=C/c2ncccc2)=O)C1=O)Nc1nc(cccc2)c2s1</chem>
P2	> 50	<chem>O=C(CN(C(C/S1)=C/c2ncccc2)=O)C1=O)Nc(cccc1)c1F</chem>

P20	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc1nccs1</chem>
P21	> 50	<chem>Cc1cnc(NC(CN(C(/C(/S2)=C/c3ncccc3)=O)C2=O)=O)s1</chem>
P22	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc(cc1)ccc1Br</chem>
P23	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc1ncccc1</chem>
P24	> 50	<chem>COc1cccc(NC(CN(C(/C(/S2)=C/c3ncccc3)=O)C2=O)=O)c1</chem>
P25	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc(cc1)cc(Br)c1Br</chem>
P3	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc1cc(F)ccc1</chem>
P4	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc(ccc(Br)c1)c1F</chem>
P5	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc(ccc(F)c1)c1F</chem>
P6	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc1cc(C(F)(F)F)ccc1</chem>
P7	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc(cc1)c(C(F)(F)F)cc1Cl</chem>
P8	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc(cc1)cc(Cl)c1Cl</chem>
P9	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc(cc(C(F)(F)F)cc1)c1Cl</chem>
PB01	> 50	<chem>[O-][N+](c(cc1)cc2c1nc(NC(CN(C(/C(/S1)=C/c3ncccc3)=O)C1=O)=O)s2)=O</chem>
PB02	> 50	<chem>Cc1cccc2c1nc(NC(CN(C(/C(/S1)=C/c3ncccc3)=O)C1=O)=O)s2</chem>
PB05	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc1nc(cc(c(F)c2)F)c2s1</chem>
PB07	> 50	<chem>COc1cccc2c1nc(NC(CN(C(/C(/S1)=C/c3ncccc3)=O)C1=O)=O)s2</chem>
PB08	> 50	<chem>CCOc(cc1)cc2c1nc(NC(CN(C(/C(/S1)=C/c3ncccc3)=O)C1=O)=O)s2</chem>
PB09	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc1nc(ccc(F)c2)c2s1</chem>
F20	> 50	<chem>CC(N(C)N(C1=O)c2cccc2)=C1NC(CN(C(/C(/S1)=C/c2cccc2)=O)C1=O)=O</chem>
GB22	> 50	<chem>Cc(c(C)c1)cc2c1sc(NC(CN(C(/C(/S1)=C/c3cccc3)=O)C1=O)=O)n2</chem>
PB03	> 50	<chem>Cc(cc1)cc2c1nc(NC(CN(C(/C(/S1)=C/c3ncccc3)=O)C1=O)=O)s2</chem>
PB04	> 50	<chem>O=C(CN(C(/C(/S1)=C/c2ncccc2)=O)C1=O)Nc(sc1ccc2)nc1c2Cl</chem>
PB06	> 50	<chem>Cc(c(C)c1)cc2c1sc(NC(CN(C(/C(/S1)=C/c3ncccc3)=O)C1=O)=O)n2</chem>
SAHA	40	<chem>ONC(CCCCCC(Nc1cccc1)=O)=O</chem>

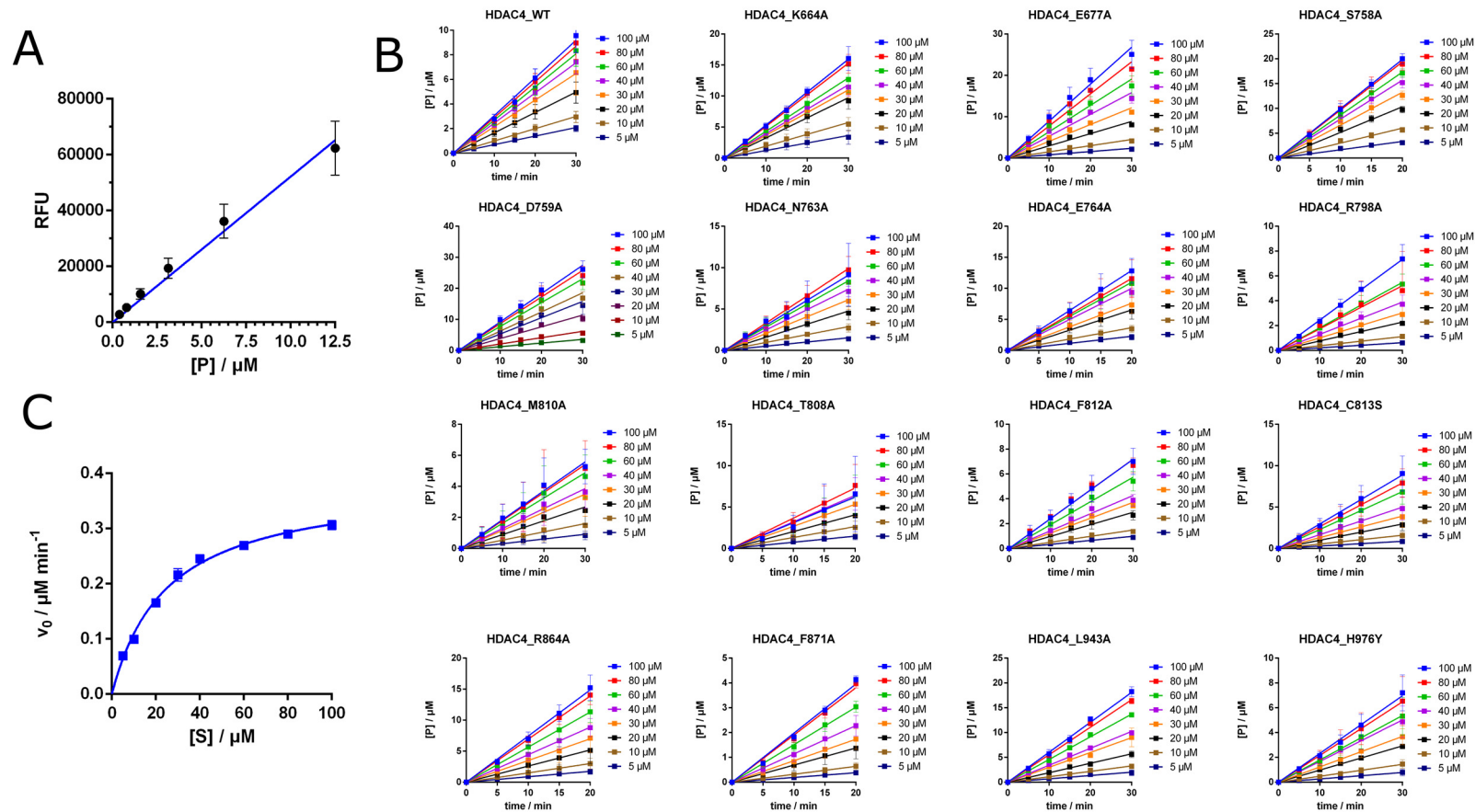


Fig. S2: Determination of Michaelis-Menten Parameters. (A) Calibration curve for the artificial substrate Boc-Lys{TFA}-AMC. A serial dilution of 7-Amino-4-methycoumarin was prepared and the slope of linear regression was calculated in RFU/ μM . (B) Time progress curves for the HDAC4 wildtype and mutant variants with varying substrate concentrations. Y-axis was converted from RFU to product concentration using the slope of calibration from experiment A. Afterwards, the slope was calculated in $\mu\text{M}/\text{min}$ which is the initial velocity of substrate conversion v_0 . (C) Finally v_0 was plotted against substrate concentration for each HDAC4 variant. K_m was calculated using a Michaelis-Menten fit in GraphPad Prism.

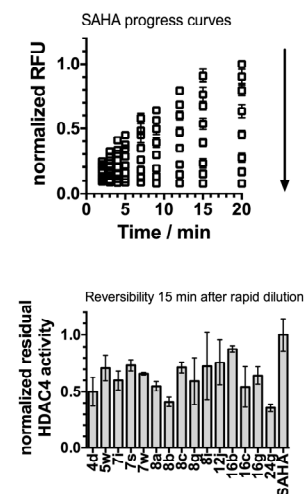
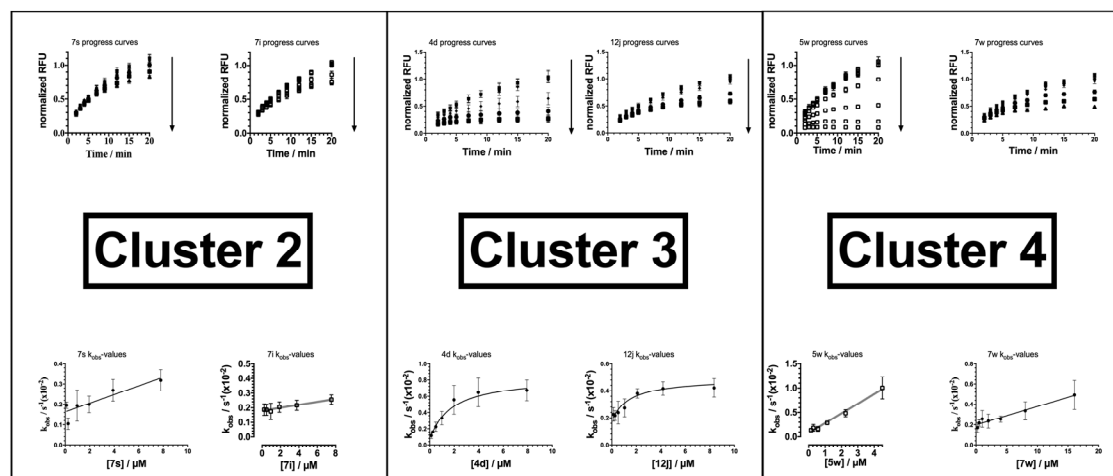
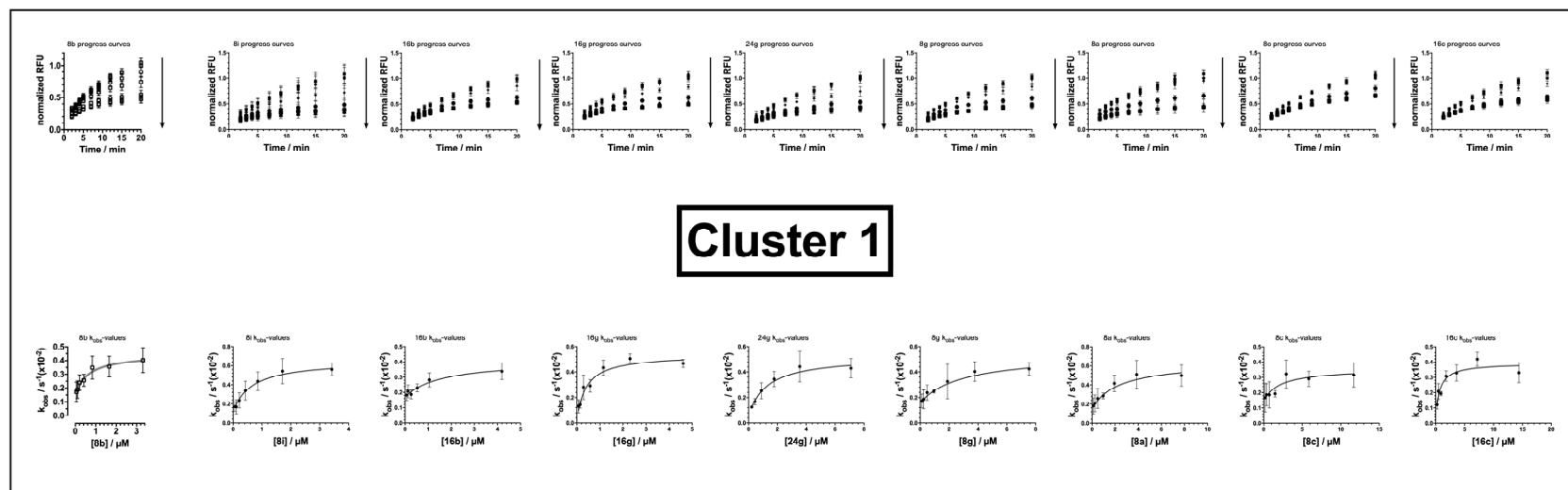


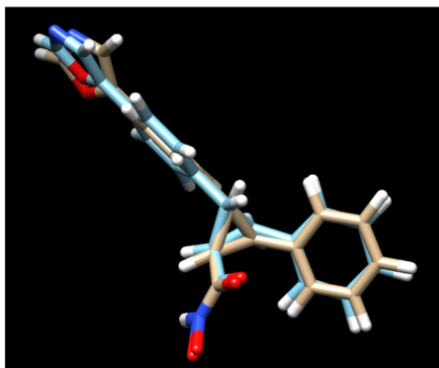
Fig. S3: Kinetic data plots of TZD ligands. Compound identifiers are displayed in the respective figures. Arrows indicate increasing TZD ligand concentration. Shown data represent means and standard deviations, N=3. Zoomable, high resolution picture (1200 dpi).

Tab. S4: IC₅₀-values in μ M for indicated TZD ligands towards cdHDAC4_{wt} and corresponding mutants .

TZD ligand	WT	S758A	F871A	T808A	R864A	D759A	M810A	F812A	C813S	L943A	H976Y	K664A	E764A	N763A	R798A	E677A
12d	1,25	8,63	5,86	6,66	17,84	2,40	5,07	31,22	3,23	>50	1,64	3,30	>50	0,91	7,40	1,05
12e	1,13	35,01	38,64	29,43	12,38	5,81	6,28	>50	3,97	>50	4,79	12,41	>50	1,26	8,10	1,35
12j	1,42	28,85	14,61	16,76	8,01	4,84	15,99	28,85	8,83	44,92	6,21	2,91	>50	4,83	4,04	4,19
14d	1,66	20,54	26,93	34,53	11,16	10,17	7,58	49,09	3,69	>50	9,44	5,96	>50	1,87	1,95	0,85
16a	1,06	32,44	9,98	10,63	10,33	2,33	8,67	>50	25,31	>50	15,35	17,31	>50	2,84	14,31	2,01
16b	0,47	14,50	5,48	5,31	21,63	1,24	28,24	>50	4,01	28,74	29,17	2,39	>50	5,65	5,33	0,84
16c	1,66	26,25	7,61	10,42	11,61	3,14	7,78	>50	3,95	>50	26,42	6,53	>50	1,70	2,47	0,88
16e	0,78	16,16	6,19	7,59	29,73	4,27	20,11	>50	25,43	>50	7,46	27,85	>50	20,02	29,69	>50
16g	2,04	11,91	6,34	7,70	11,09	2,09	9,29	>50	4,61	>50	15,10	2,96	>50	1,41	2,91	2,24
20e	1,23	43,60	11,10	10,97	32,78	3,33	5,95	46,73	3,94	>50	3,47	4,19	>50	0,77	1,73	2,42
24e	0,69	41,36	3,85	13,85	20,07	2,38	7,45	>50	4,11	>50	28,45	7,15	>50	2,12	5,85	0,58
24g	1,18	6,19	4,04	4,30	9,82	1,61	8,47	>50	3,87	>50	6,49	3,27	>50	2,62	3,84	1,43
4d	0,49	5,02	2,43	4,44	8,61	1,75	4,23	43,61	6,95	>50	4,03	3,99	>50	0,68	2,26	0,76
4j	0,41	10,48	9,12	14,32	6,12	2,08	13,27	28,15	14,11	>50	2,79	5,50	>50	4,39	4,15	4,27
4k	1,17	23,60	9,29	4,20	4,15	2,26	8,81	48,59	3,97	>50	4,12	3,67	>50	0,72	4,14	0,41
5w	0,78	3,04	8,66	2,02	7,36	1,93	4,43	25,47	4,04	>50	3,60	4,92	33,24	1,81	7,20	11,00
7b	0,73	21,37	>50	28,98	29,25	6,73	13,77	34,75	26,32	>50	8,53	8,56	>50	5,31	7,38	>50
7i	1,04	31,05	4,90	38,94	28,93	1,99	19,85	>50	23,95	>50	26,72	37,15	>50	6,10	2,77	4,55
7l	0,47	16,16	2,55	11,70	28,93	2,17	20,07	>50	23,07	>50	26,72	6,89	>50	3,54	2,77	3,26
7n	0,45	26,53	10,53	29,76	29,31	1,61	4,95	>50	9,24	>50	25,27	7,42	>50	4,67	2,40	4,29
7s	1,41	20,26	34,79	18,55	16,47	6,42	9,25	>50	26,44	>50	27,38	8,49	49,16	12,83	6,29	>50
7w	0,47	22,36	13,69	34,02	6,41	0,63	21,39	>50	>50	>50	0,44	4,68	>50	2,99	3,58	8,00
8a	0,90	>50	32,23	30,02	39,30	6,00	26,58	>50	25,33	>50	15,61	32,61	>50	9,80	21,24	>50
8b	0,44	3,21	3,55	1,93	5,16	1,09	4,27	25,85	2,50	>50	9,00	2,51	33,51	1,74	3,91	2,96
8c	0,51	>50	5,40	33,57	11,29	4,22	9,22	>50	4,03	37,56	26,77	6,36	>50	1,41	1,46	2,89
8e	0,54	11,03	1,99	4,21	29,49	1,50	7,39	>50	6,55	>50	11,52	5,72	>50	1,26	7,55	1,17
8g	0,22	13,07	4,99	11,89	11,60	1,97	6,37	>50	4,69	>50	2,84	5,03	>50	1,18	5,23	2,11
8i	0,17	3,15	3,50	2,90	6,93	0,91	2,88	40,56	25,73	>50	1,93	2,34	>50	1,03	1,04	11,81

DOCKING

A)



B)

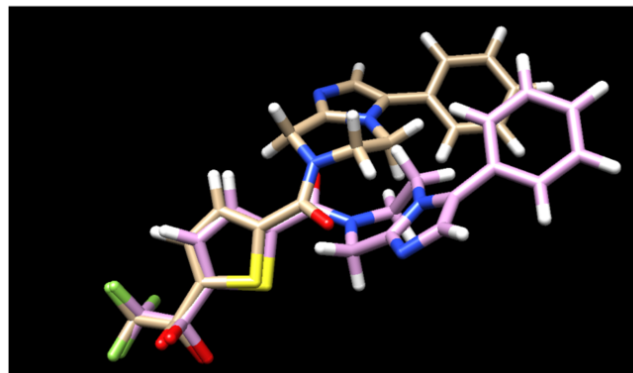


Fig. S5: Overlay of crystallized and redocked ligands in complex with A) HDAC4_c (PDB-ID: 4CBY) and B) HDAC4_o (PDB-ID: 2VQJ).

Overlay: closed (4CBY) and open (2VQJ) HDAC4 - intact structures:

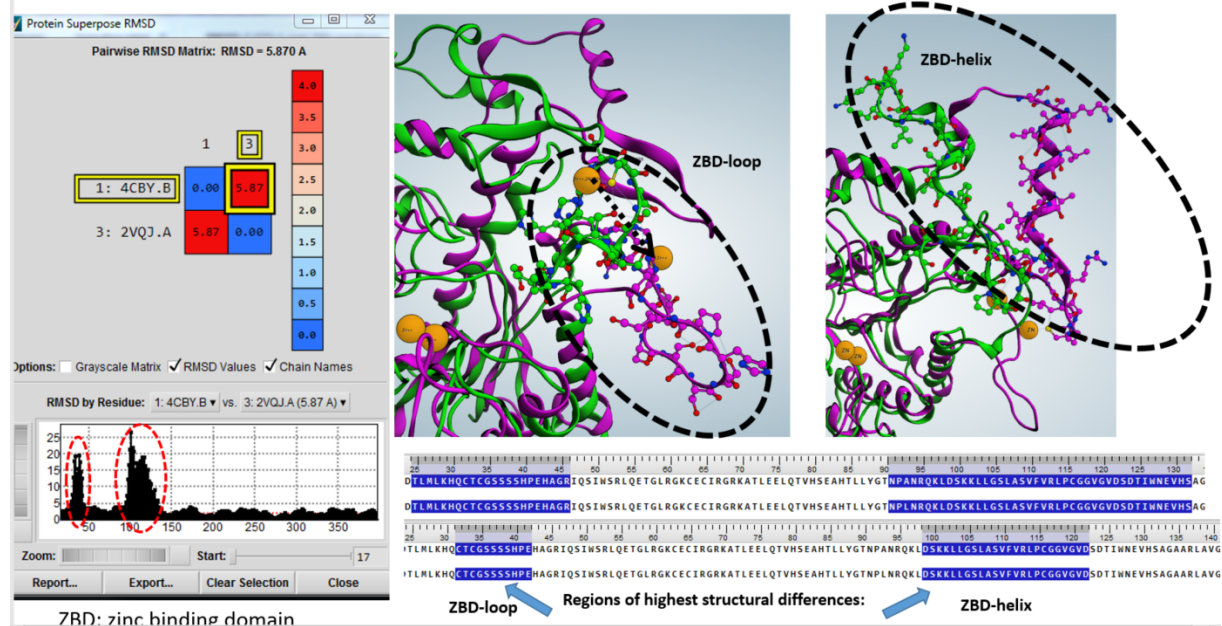


Fig. S6: Regions of largest structural shifts for the transition from *closed* to *open* conformation of HDAC4.

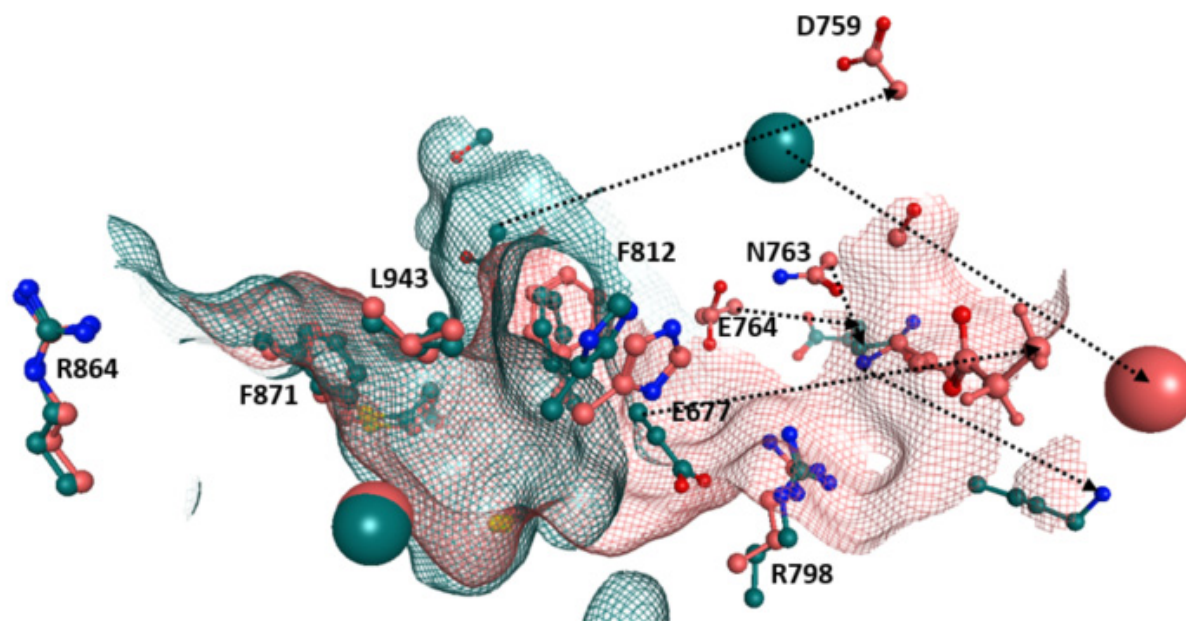


Fig. S7: Overlay of HDAC4c (4CBY, dark cyan) and HDAC4o (2VQJ, dark pink) showing the amino acids that are mutated in this study. Larger shifts upon the transition from open to closed conformation are indicated by dotted black arrows. The bigger beads represent the catalytic and structural zinc ions.

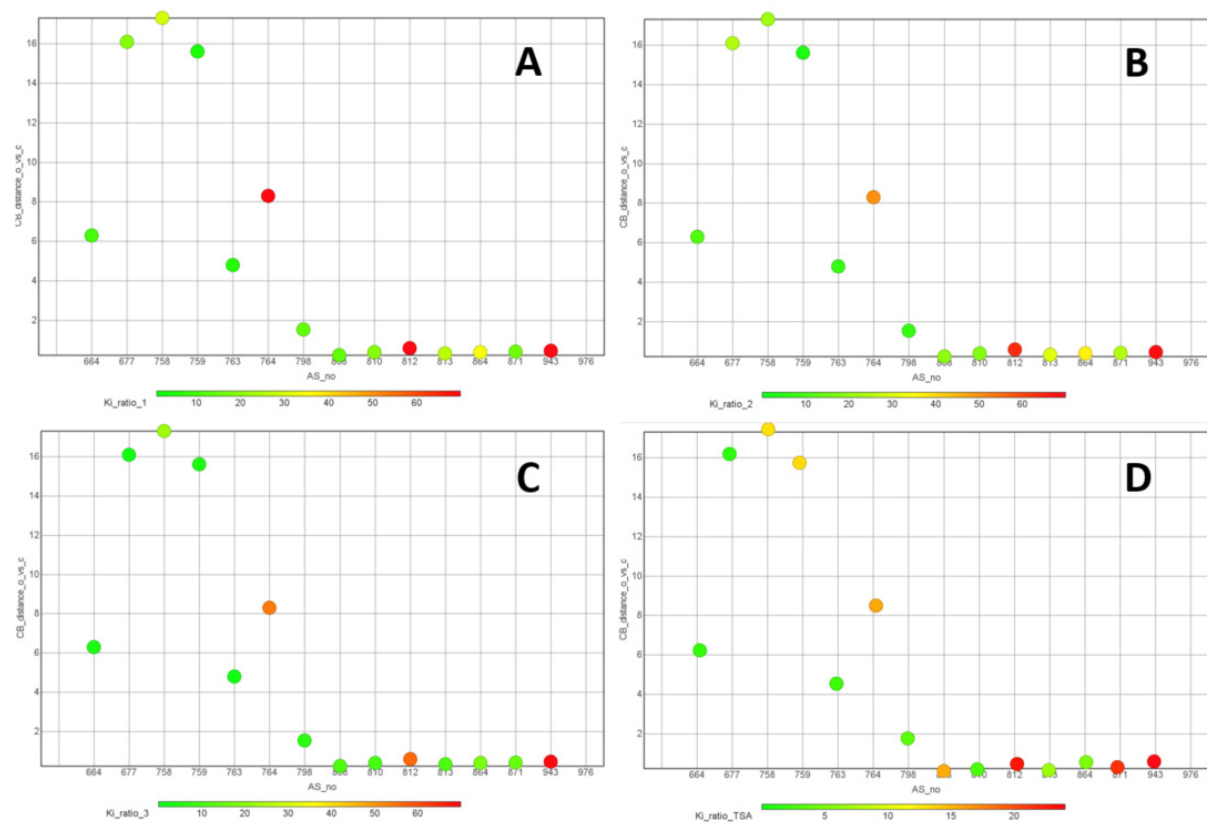


Fig. S8: The distance between C β -atoms is plotted versus the number of the mutated amino acids. Coloring is according to the Ki-ratio for docking poses in A) cluster 1, B) cluster 2, C) cluster 3 and D) TSA.

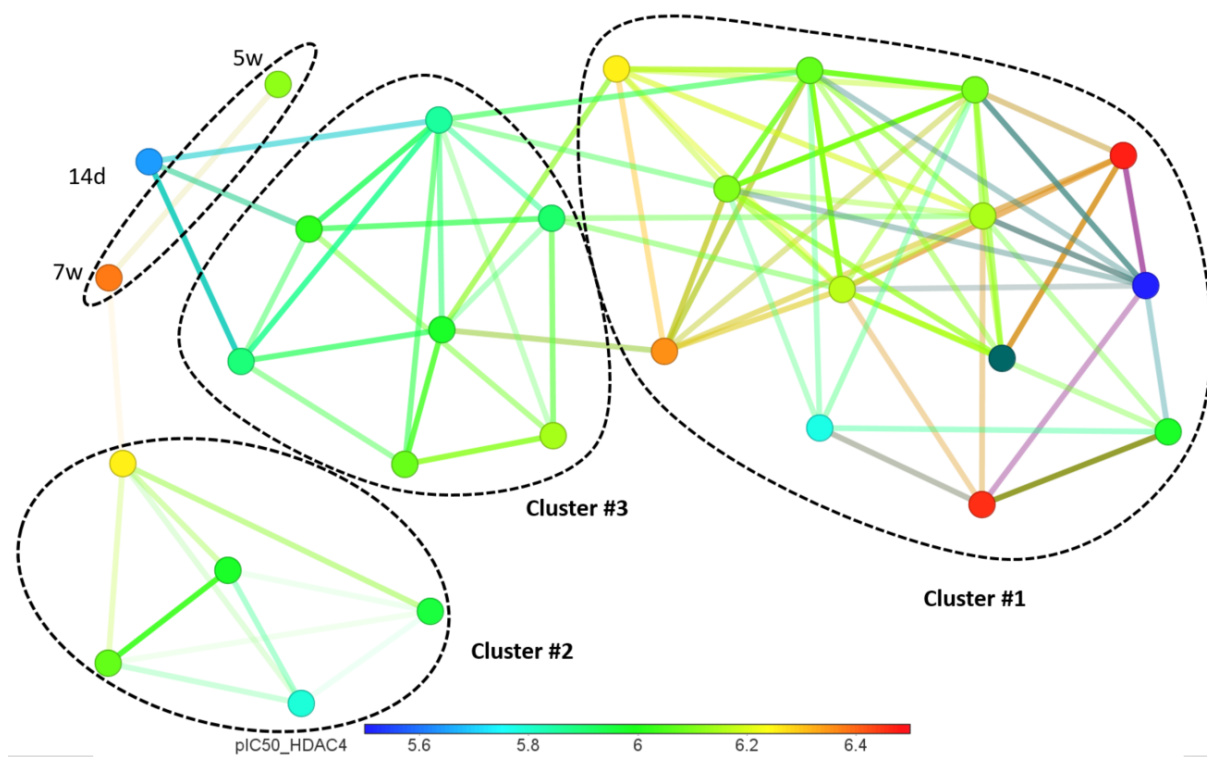


Fig. S9: Cluster analysis of most active TZA analogs. Each dot represents one compound. The dots are colored according to experimental pIC_{50} against $cdHDAC4_{wt}$. Structurally nearest neighbours are connected by lines.

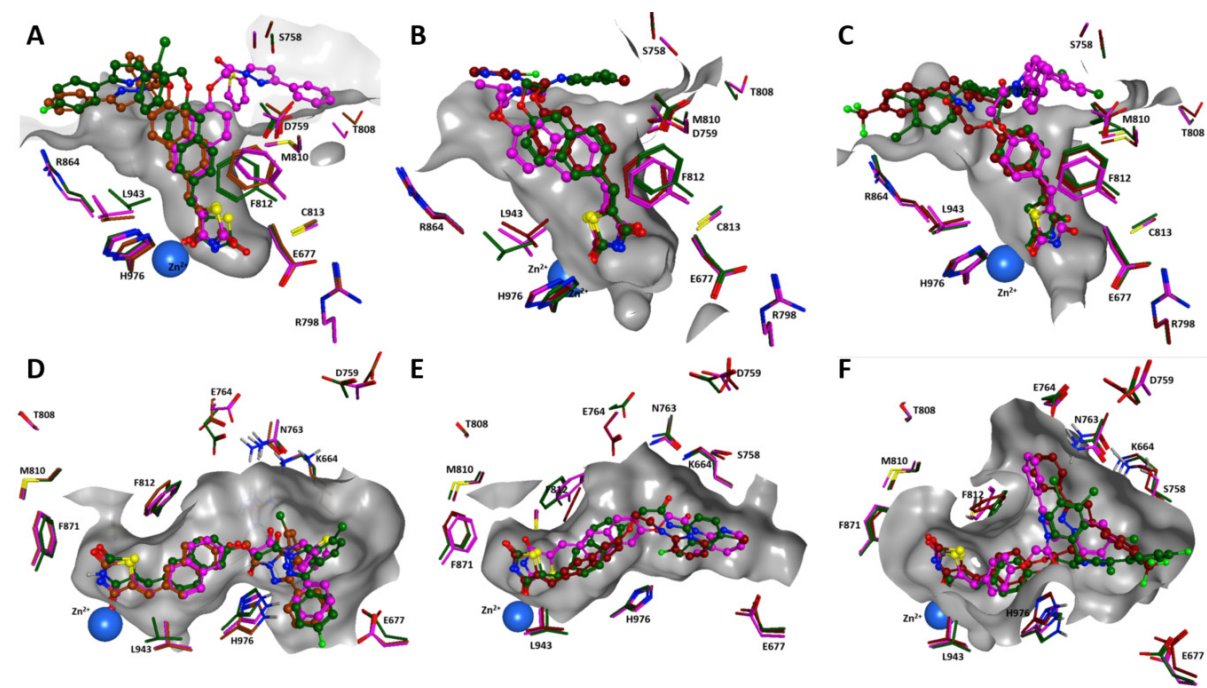


Fig. S10: Overlap of docking poses of TZD analogs to A)-C) HDAC4_c (PDB-ID: 4CBY) and D)-F) HDAC4_o (PDB-ID: 2VQJ). Docking poses of cluster 1 containing (S)-16b [green], (S)-8i [magenta] and (S)-8b [brown] are shown in A and D, cluster 2 containing 7l [green], 7n [magenta] and 7s [brown] in B and E, and cluster 3 containing (R)-12j [green], (R)-4d [brown] and (R)-4j [magenta] are shown in C and F. The catalytic zinc ion at the bottom of the binding pocket is colored blue and the surface of the pocket light gray.

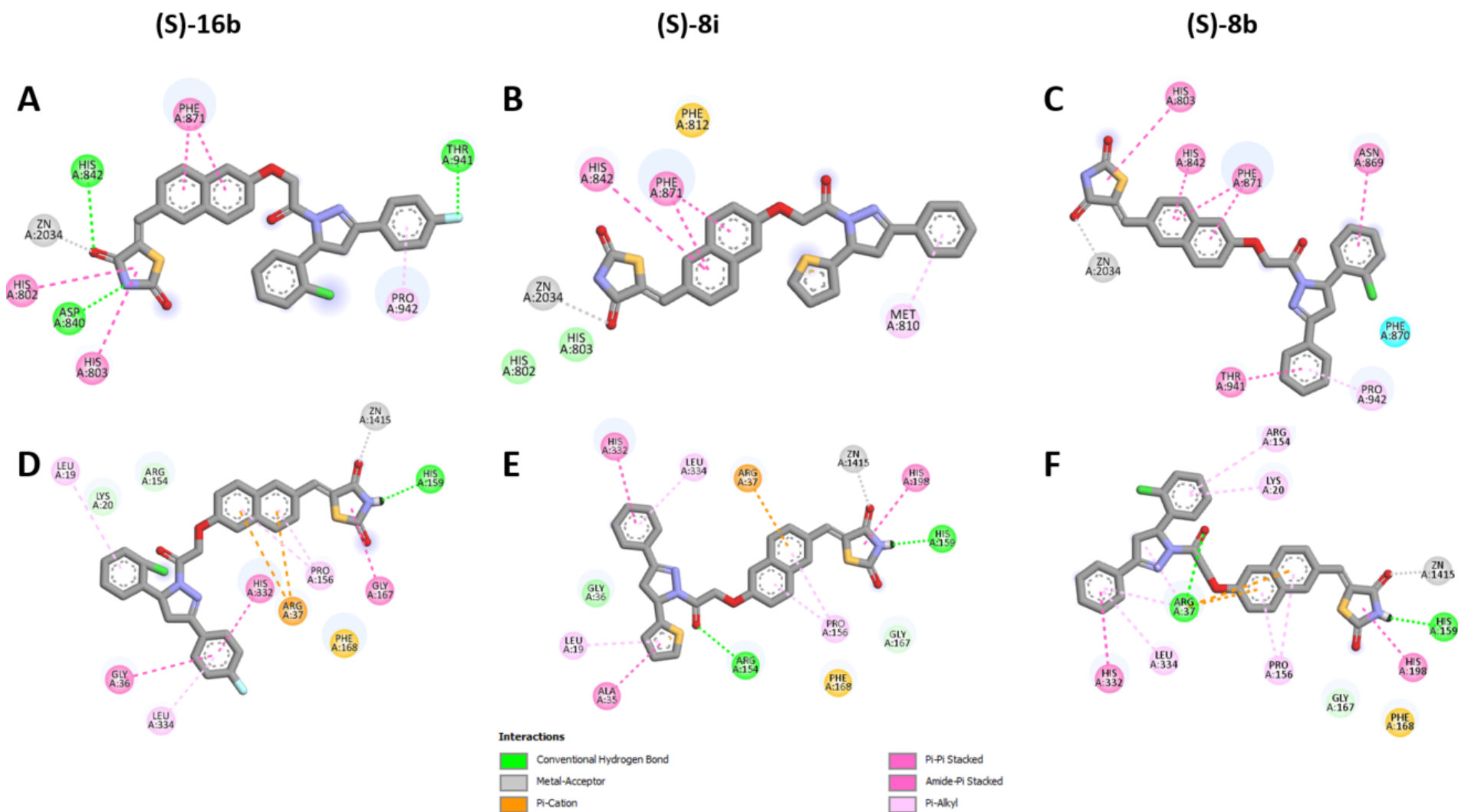


Fig. S11: 2D ligand interactions of (S)-16b, (S)-8i and (S)-8b in the binding pocket of A)-C) HDAC4_c (PDB-ID: 4CBY) and D)-F) HDAC4_o (PDB-ID: 2VQJ).

Tab. S11: Open reading frame of cdHDAC4_{wt} in pET14b for recombinant protein expression.

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START

His₆-SUMO

cHDAC4_{wt}

Strep(II)-tag

STOP

Tab. S12: Mutant to cdHDAC4_{wt} (WT) IC50 ratios. Mutant HDAC4 variants were generated using splicing by overlap extension PCR (SOE-PCR) with the following primers and cloned into a pET14b vector (Novagen, EMD Millipore) consists of a n-terminal His6-SUMO-tag and c-terminal Strep(II)-tag with NdeI and BamHI restriction enzymes.

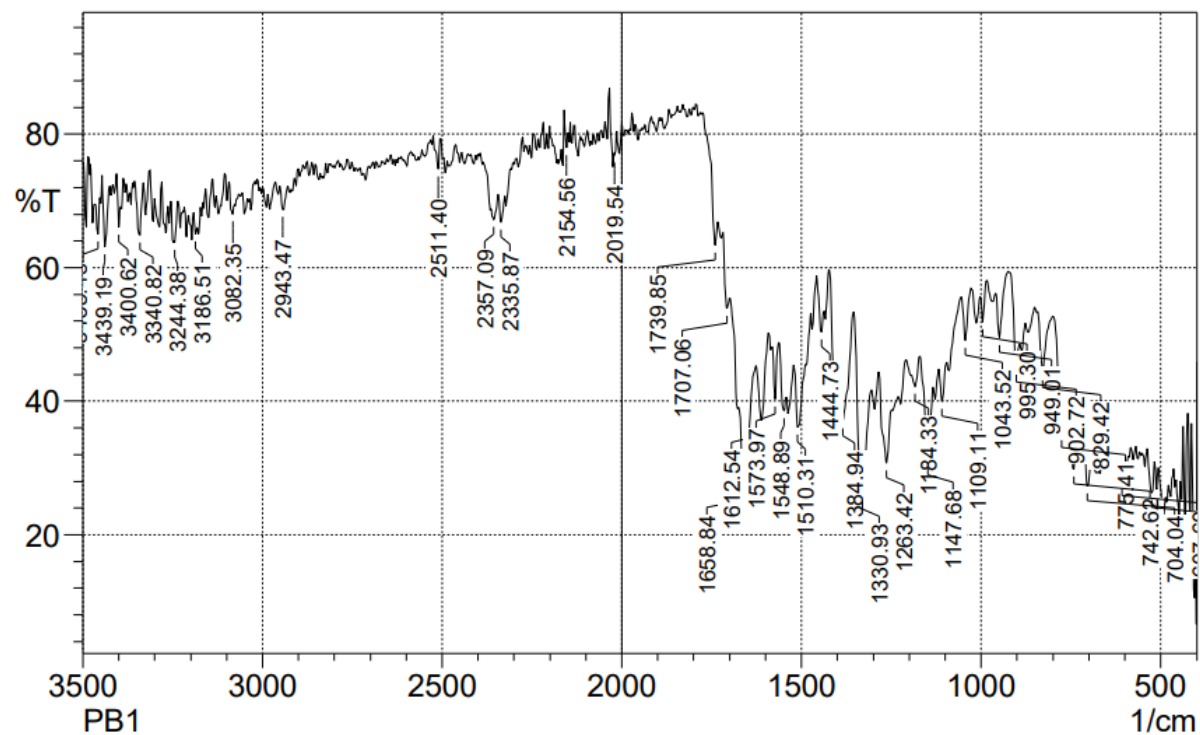
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K664A_rev	GGTGCATTGGTGAGCCAGCATCAGCGT
E677A_for	TCCTCACATCCGGCTCATGCAGGCCGC
E677A_rev	GCGGCCTGCATGAGCCGGATGTGAGGA
S758A_for	GTTGGTGTCTGATGCTGACACCATCTGG
S758A_rev	CCAGATGGTGTCTCAGCATCGACACCAAC
D759A_for	GGTGTCTGATTCTGCTACCATCTGGAAC
D759A_rev	GTTCCAGATGGTAGCAGAATCGACACC
N763A_for	GACACCATCTGGGCTGAAGTGCACAGT
N763A_rev	ACTGTGCACTTCAGCCCAGATGGTGTC
E764A_for	ACCATCTGGAACGCTGTGCACAGTGCA
E764A_rev	TGCACTGTGCACAGCGTTCCAGATGGT
R798A_for	TTCGCAGTCGTGGCTCCGCCGGGTCAT
R798A_rev	ATGACCCGGCGGAGCCACGACTGCGAA
T808A_for	GCAGAAGAATCGGCTCCGATGGGTTTT
T808A_rev	AAAACCCATCGGAGCCGATTCTTCTGC
M810A_for	GAATCGACGCCGGCTGGTTTTTGCTAT
M810A_rev	ATAGCAAAAACCAGCCGGCGTCGATTC
F812A_for	ACGCCGATGGGTGCTTGCTATTTCAAT
F812A_rev	ATTGAAATAGCAAGCACCCATCGGCGT
C813S_for	ACGCCGATGGGTTTTTCTTATTTCAATAGCGTG
C813S_rev	CACGCTATTGAAATAAGAAAAACCCATCGGCGT
R864A_for	ATGTCTCTGCATGCTTACGATGACGGC
R864A_rev	GCCGTCATCGTAAGCATGCAGAGACAT
F871A_for	GACGGCAACTTTGCTCCGGGCAGTGGT

F871A_rev	ACCACTGCCCCGGAGCAAAGTTGCCGTC
L943A_for	CATCCGACCCCGGCTGGCGGTTATAAC
L943A_rev	GTTATAACCGCCAGCCGGGGTCGGATG
H976Y_for	GCTCTGGAAGGCGGTTATGATCTGACCGCTATC
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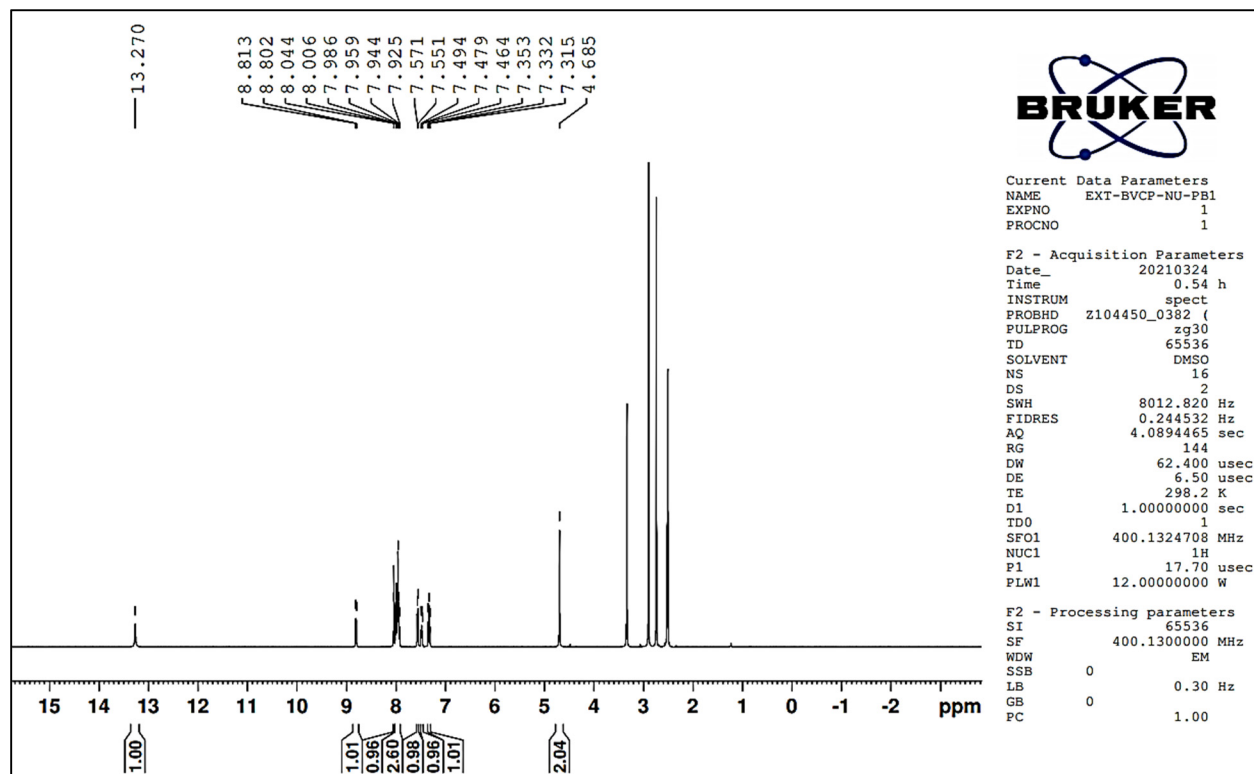
Structural characterization

2-(2,4-dioxo-5-(pyridin-2-ylmethylene)thiazolidin-3-yl)-N-(6-nitrobenzo[d]thiazol-2-yl)acetamide (PB1)

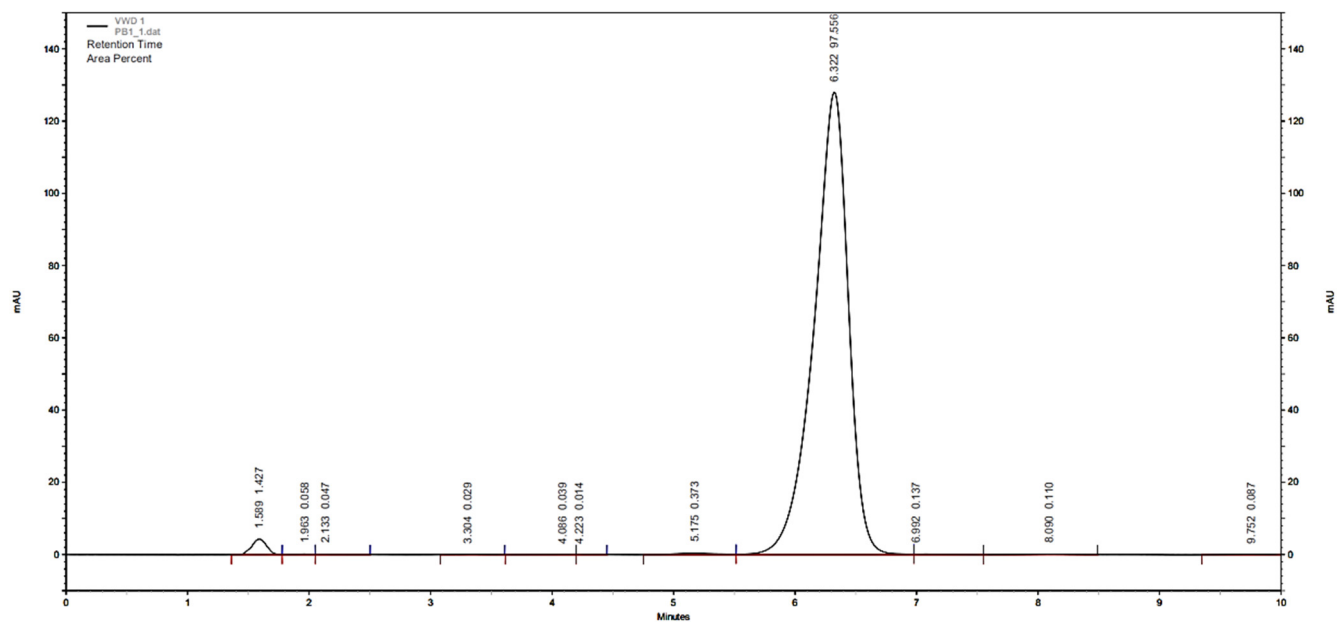
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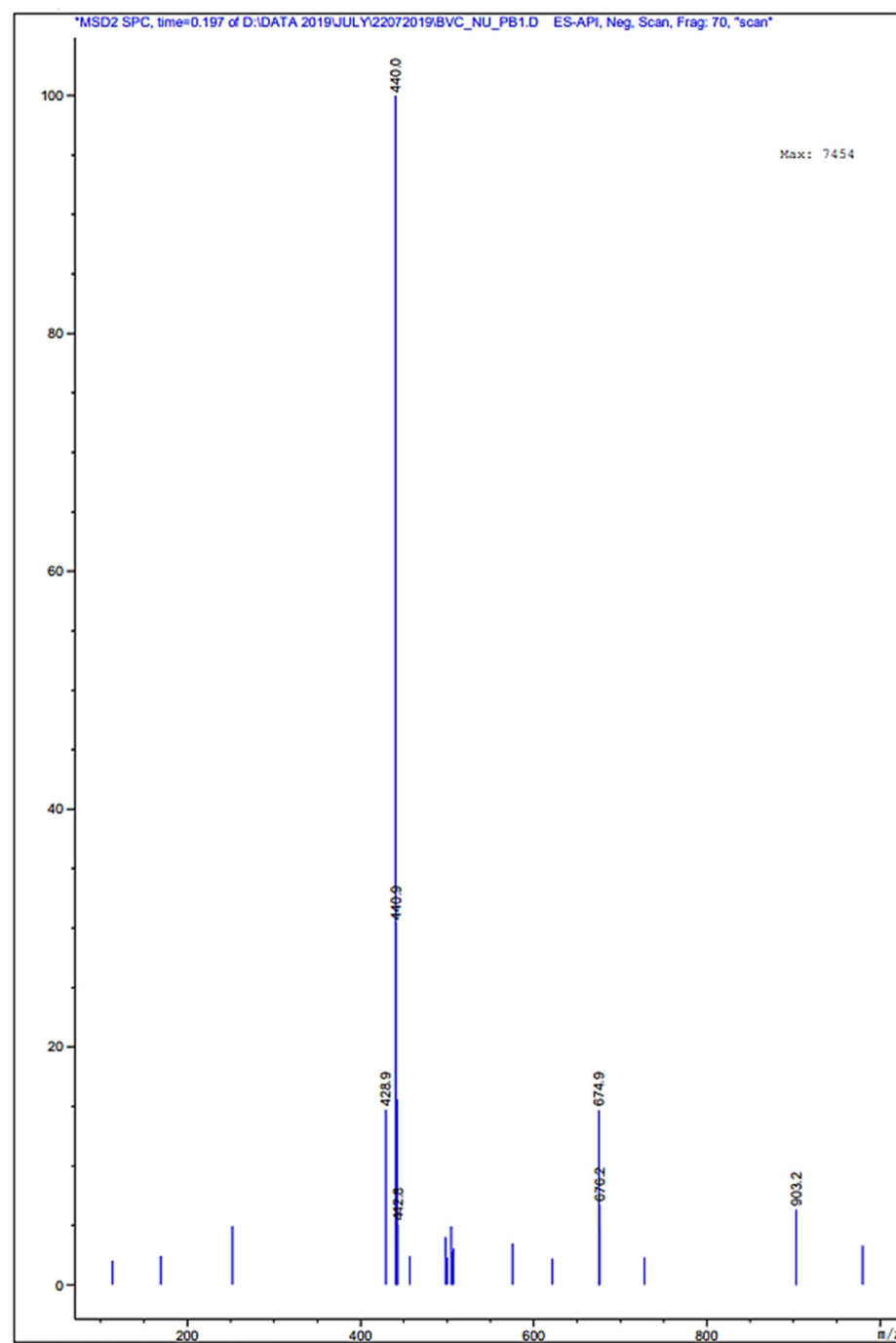
2. ¹H-NMR



3. 13C-NMR

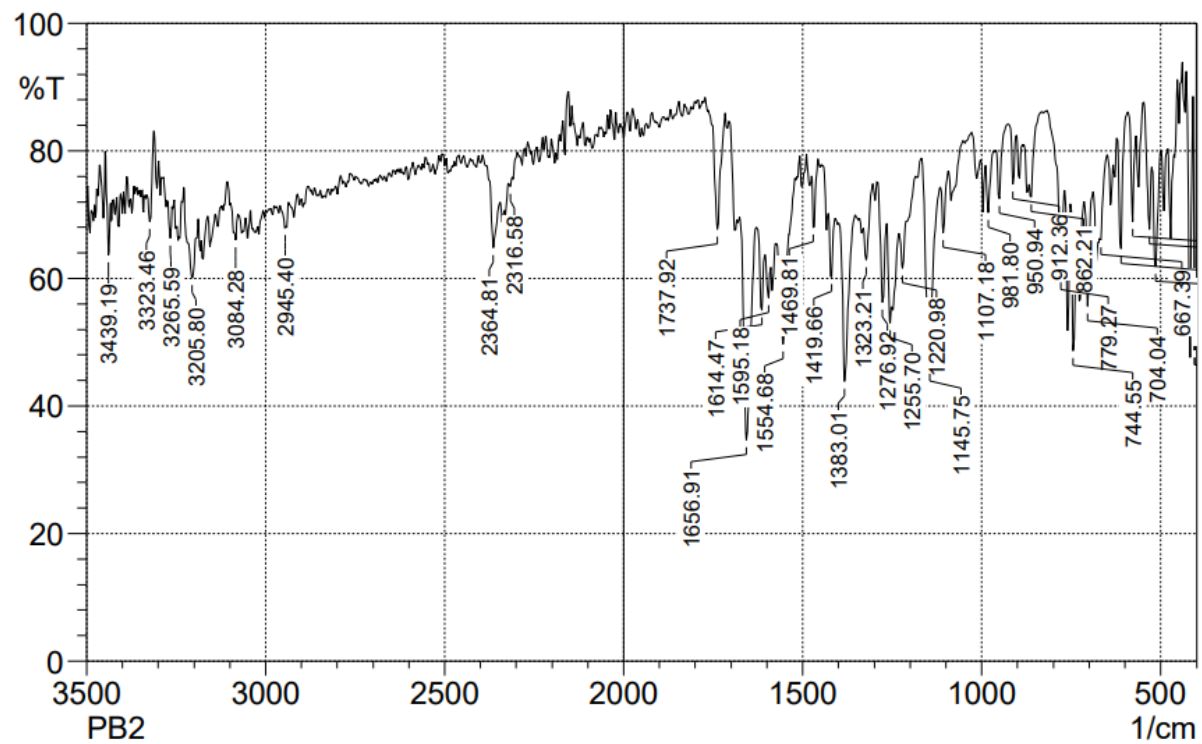


5. Mass

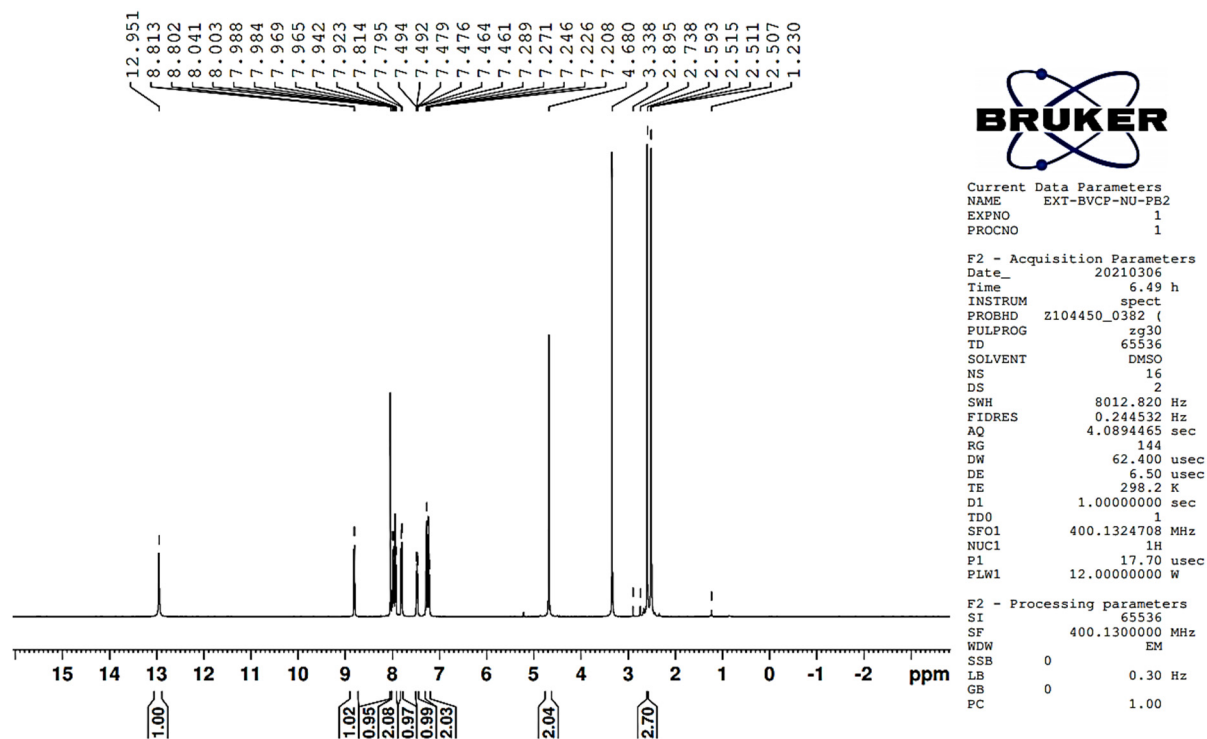


2-(2,4-dioxo-5-(pyridin-2-ylmethylene)thiazolidin-3-yl)-N-(4-methylbenzo[d]thiazol-2-yl)acetamide (PB2)

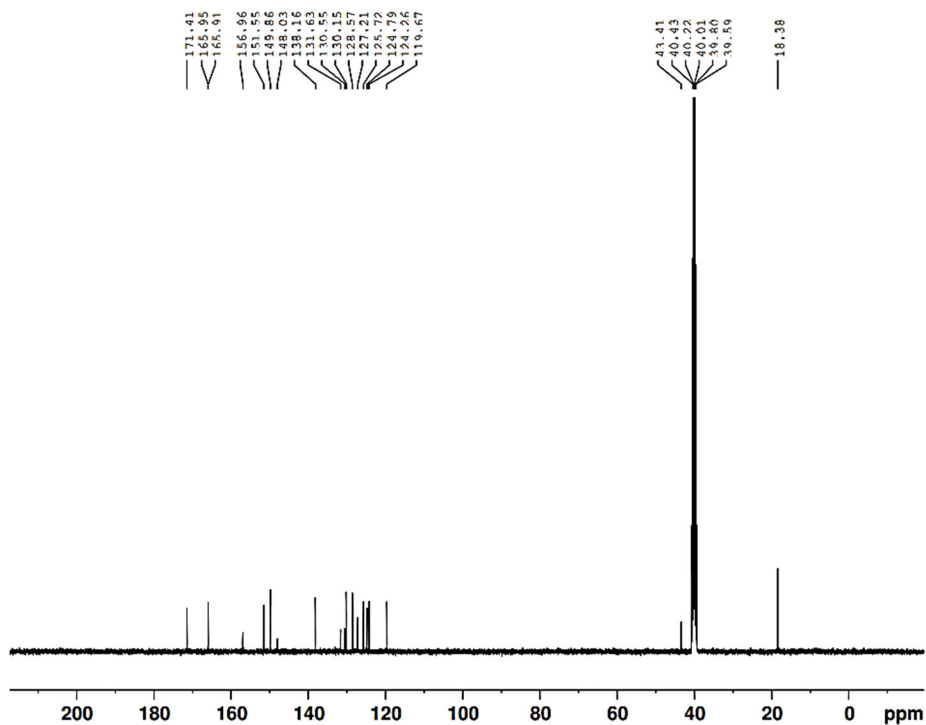
1. FTIR



2. $^1\text{H-NMR}$



3. 13C-NMR

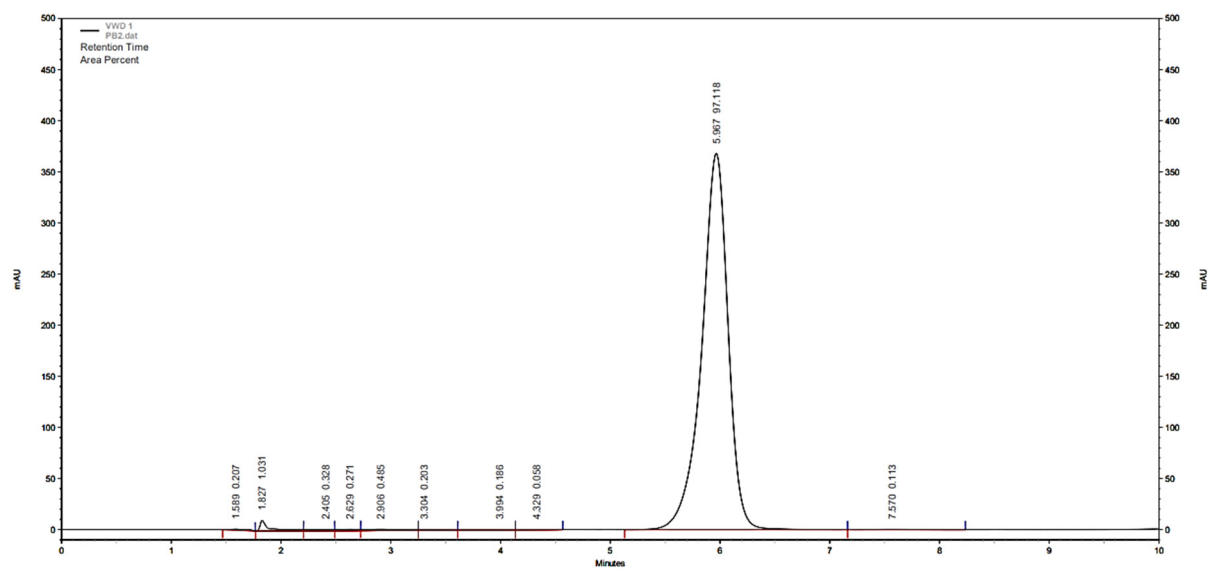


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PROCNO 1

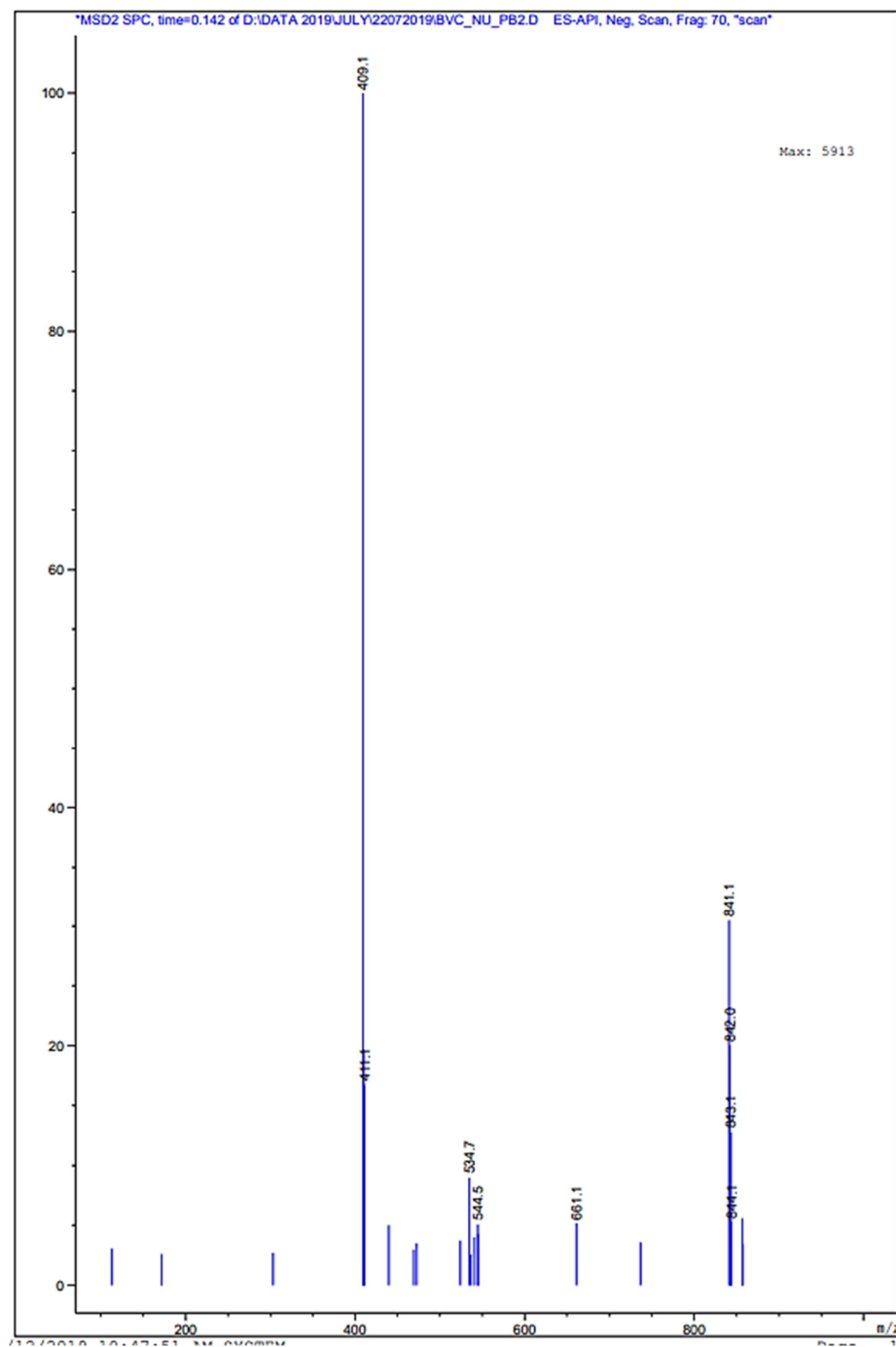
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SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 11.00 usec
PLW1 58.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
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PLW2 12.00000000 W
PLW12 0.46413001 W
PLW13 0.23345999 W

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4. HPLC

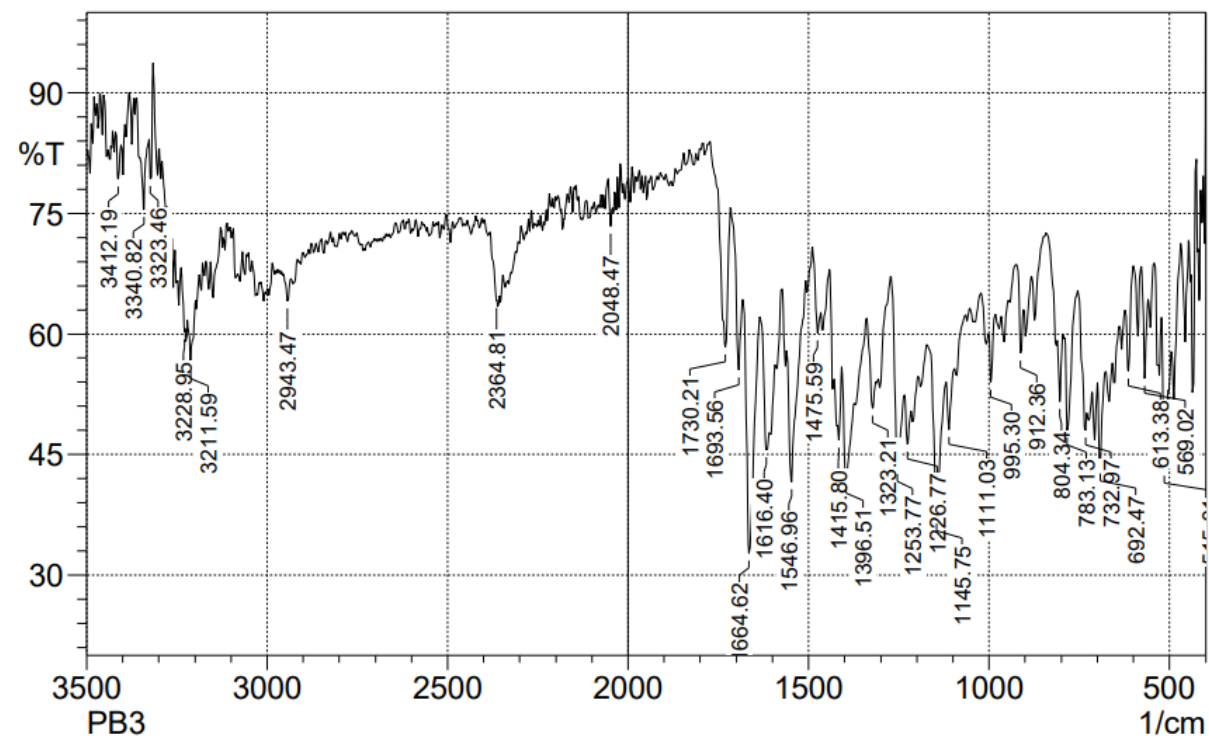


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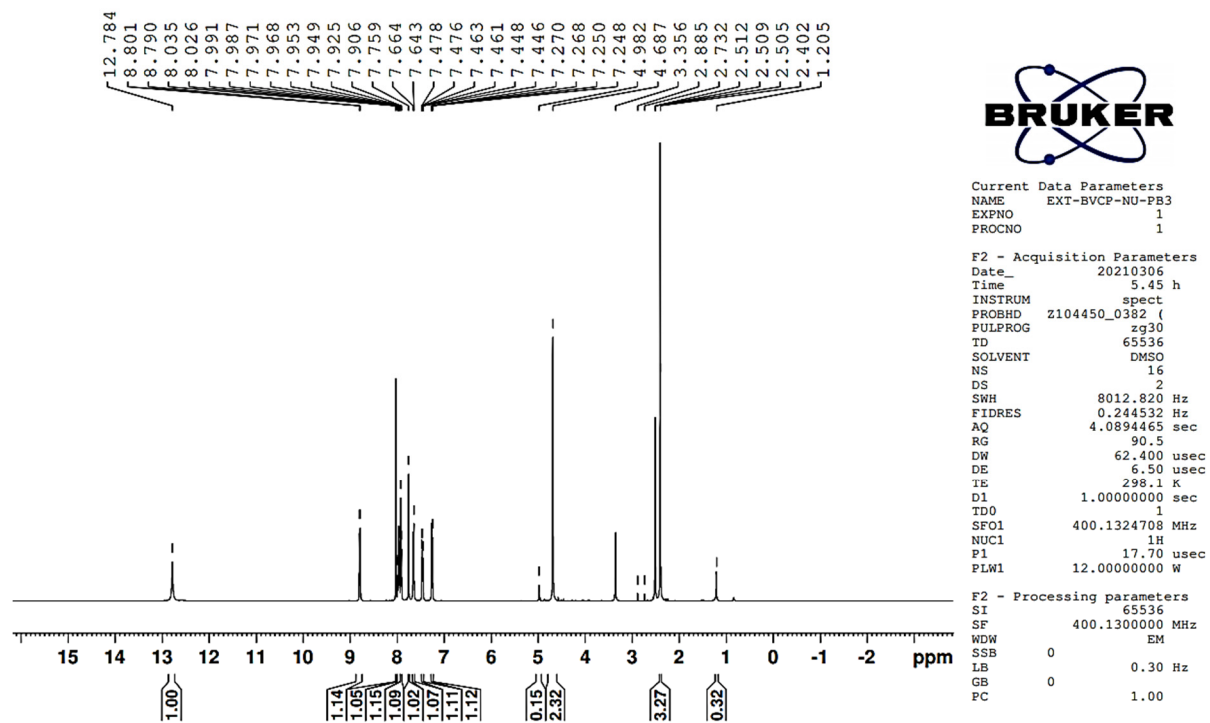


2-(2,4-dioxo-5-(pyridin-2-ylmethylene)thiazolidin-3-yl)-N-(6-methylbenzo[d]thiazol-2-yl)acetamide (PB3)

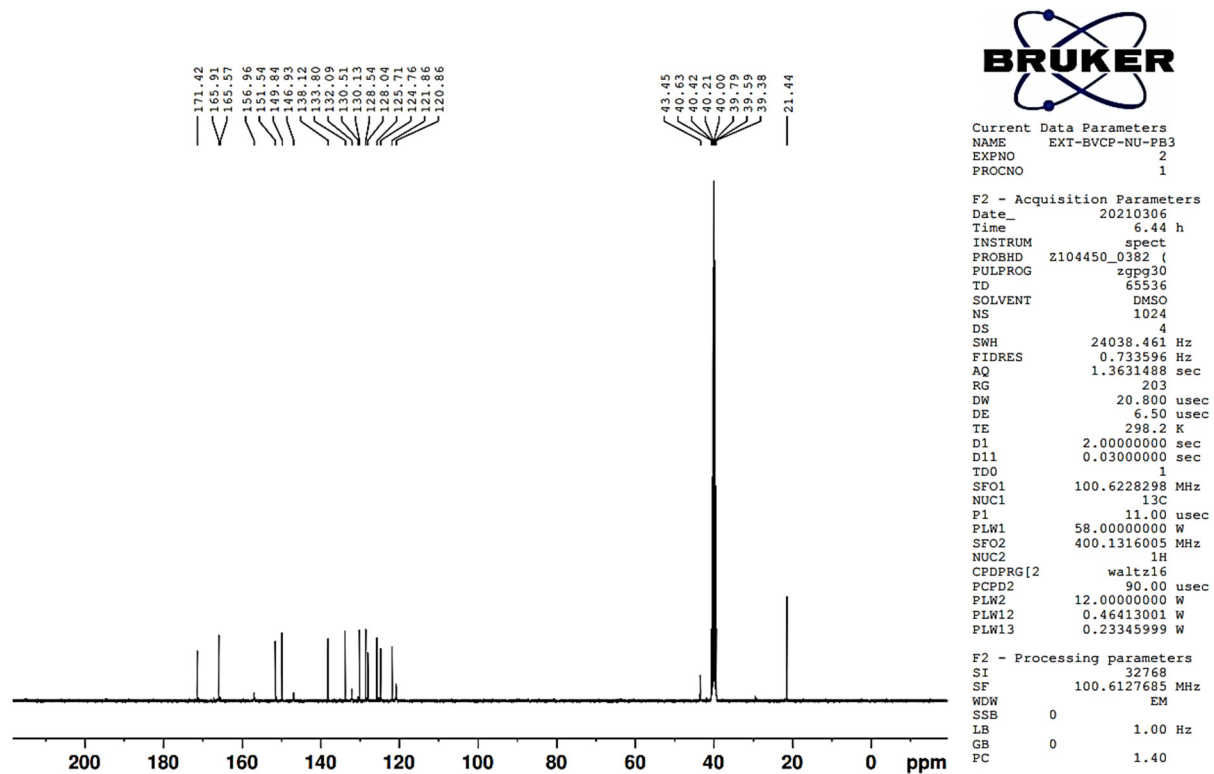
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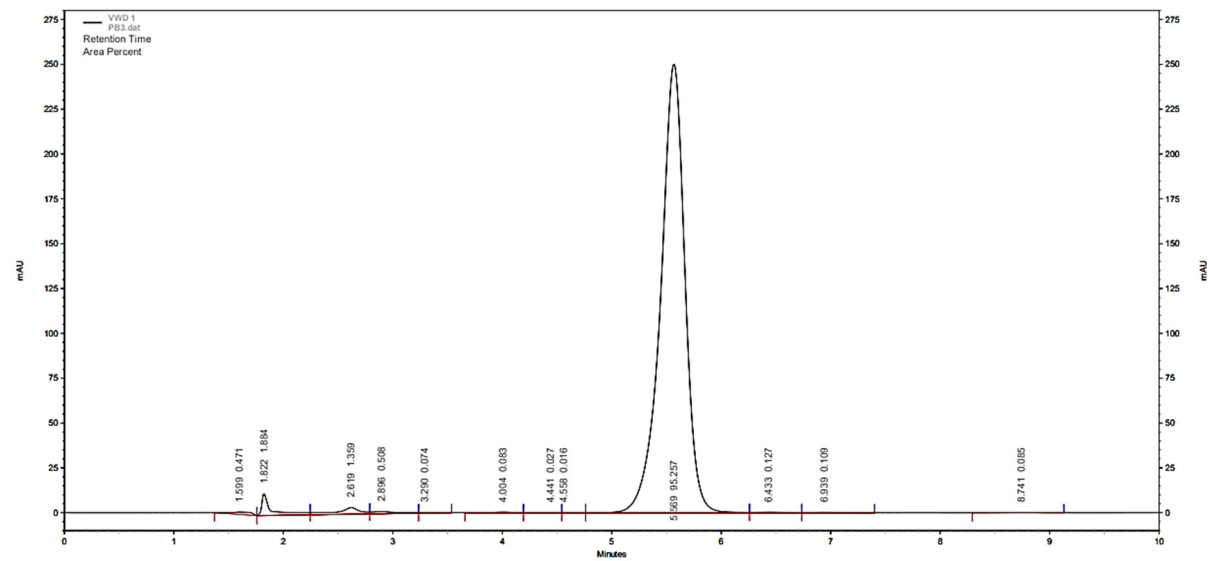
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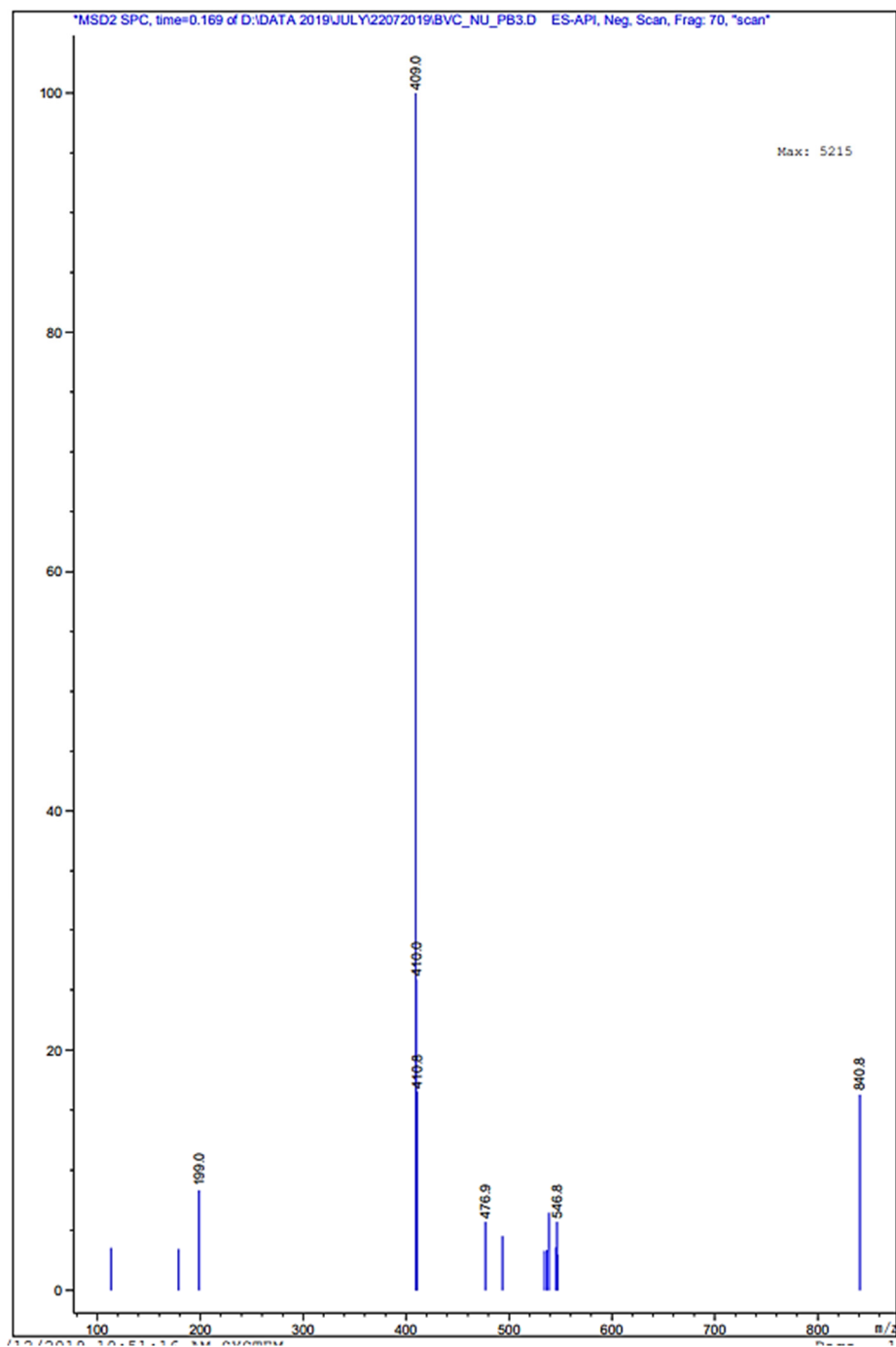
3. 13C-NMR



4. HPLC

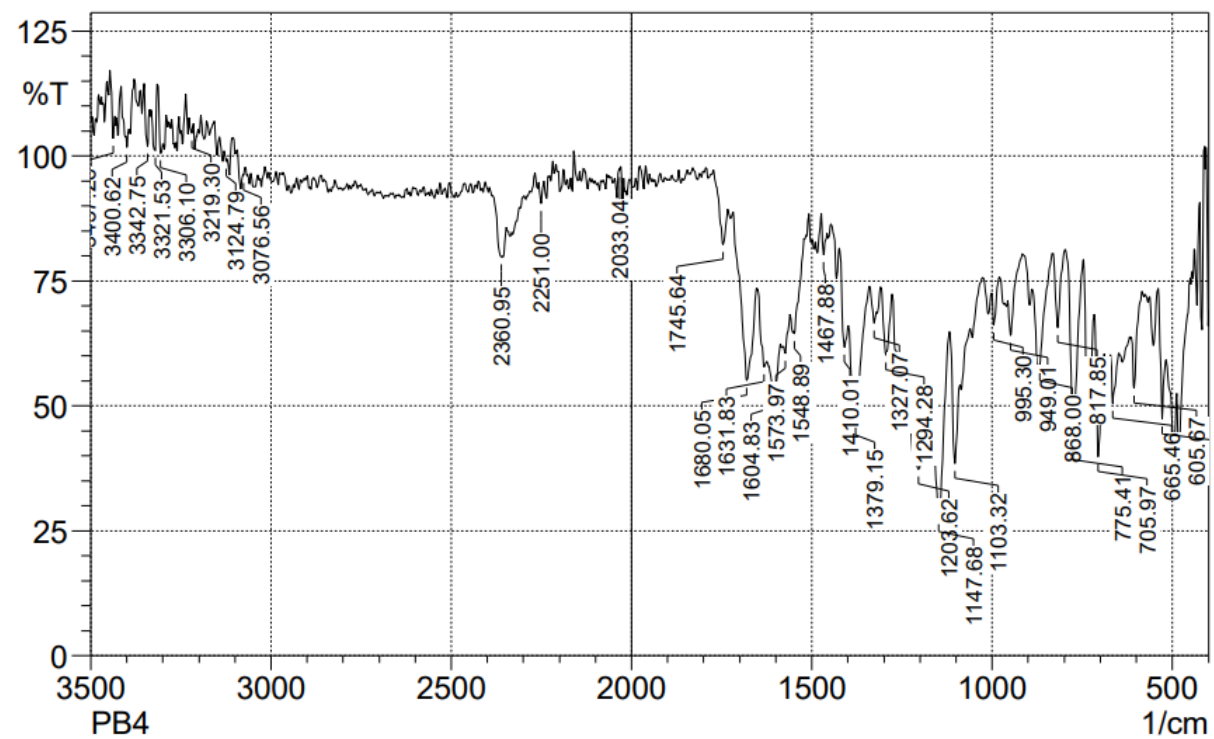


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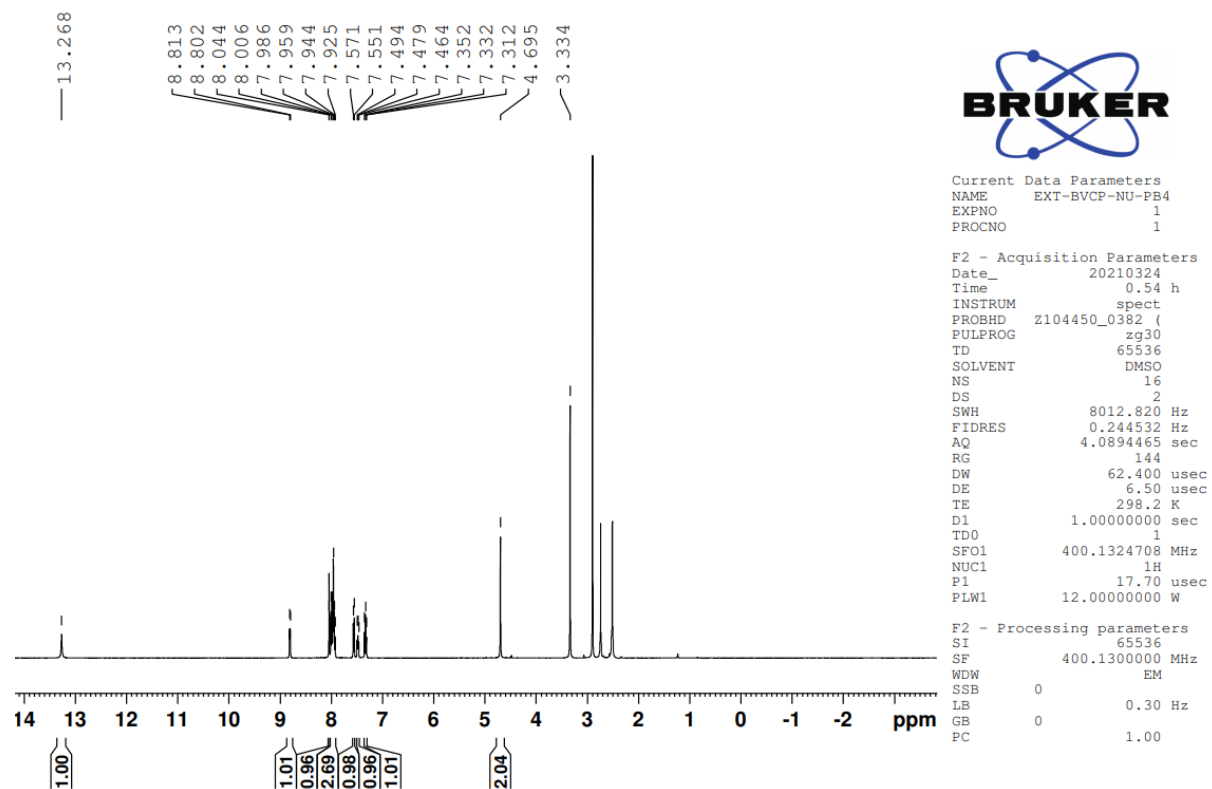


N-(4-chlorobenzo[d]thiazol-2-yl)-2-(2,4-dioxo-5-(pyridin-2-ylmethylene)thiazolidin-3-yl)acetamide (PB4)

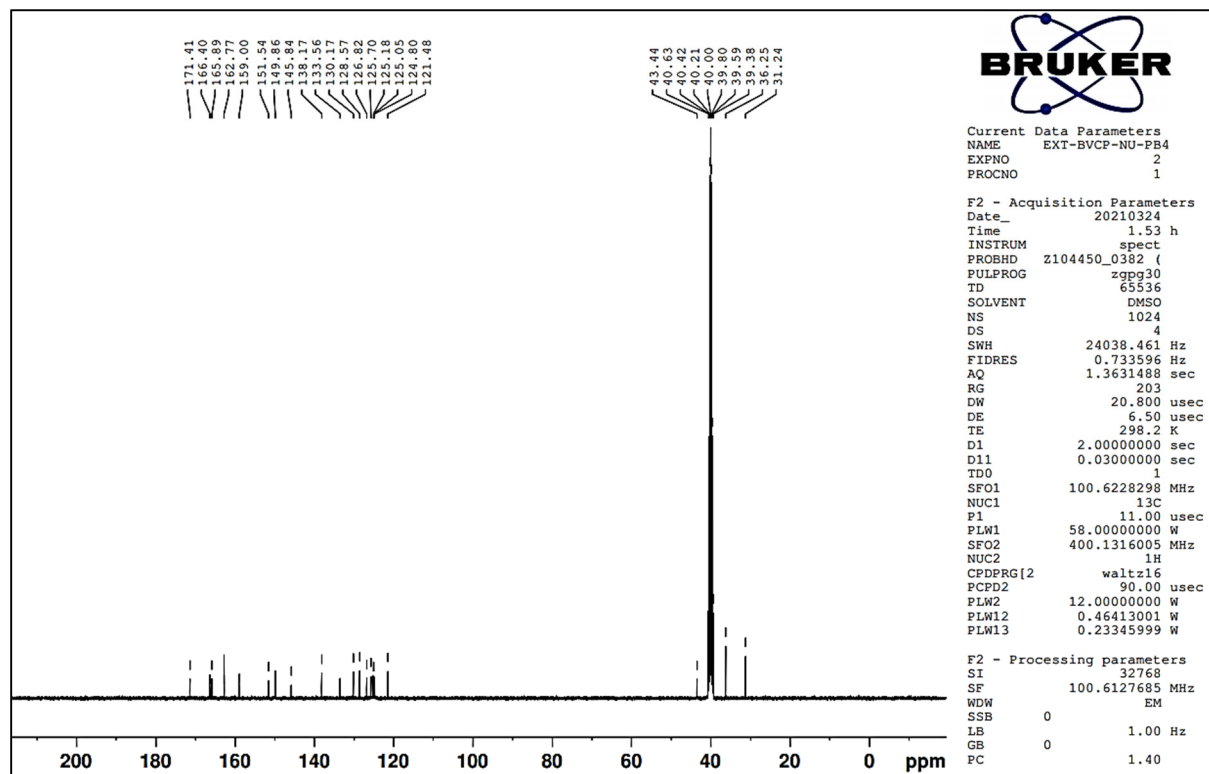
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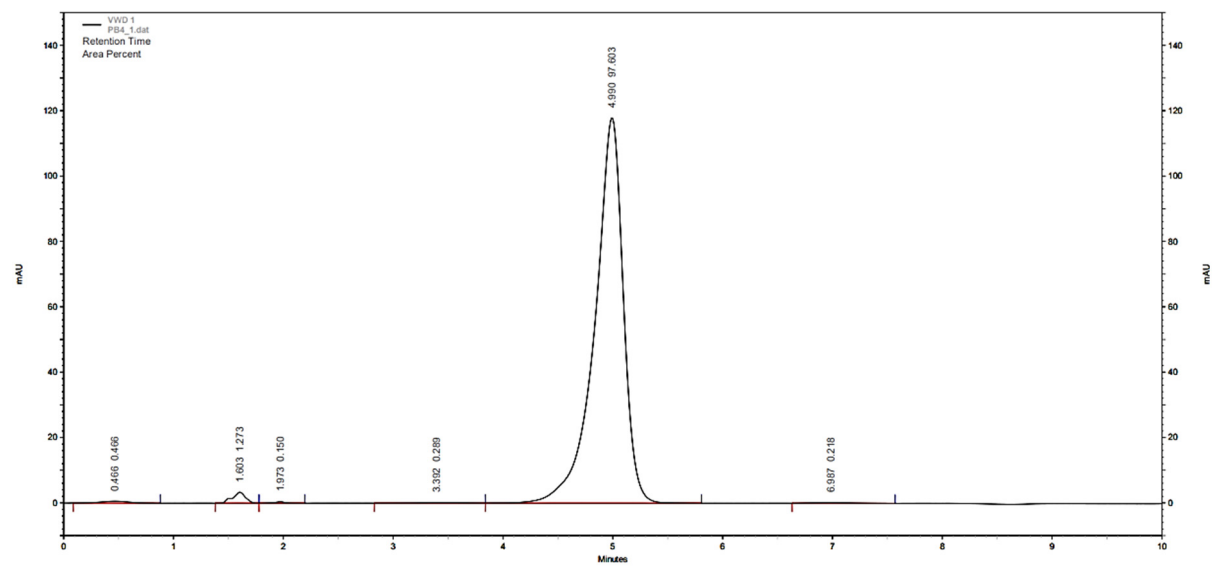
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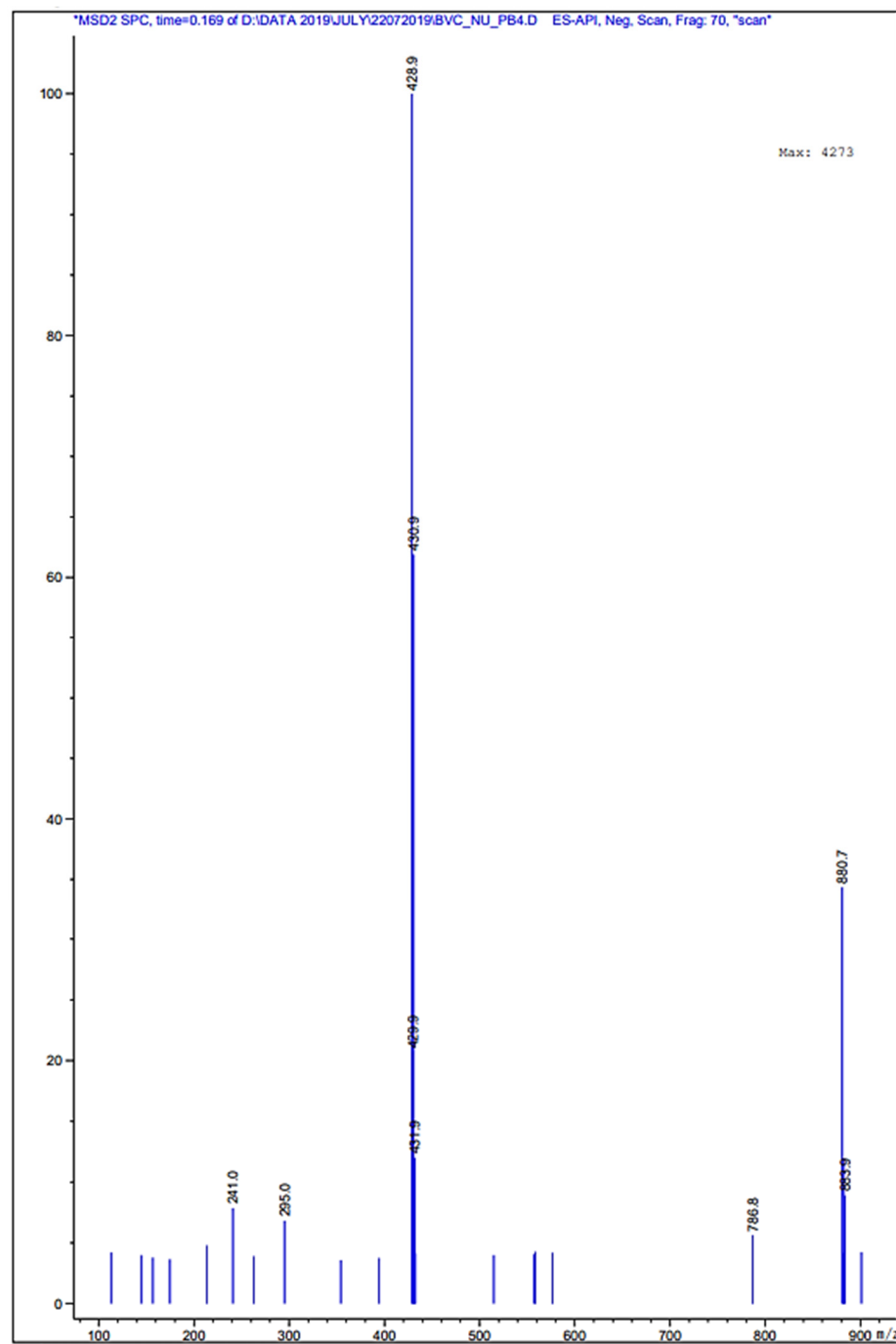
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4. HPLC

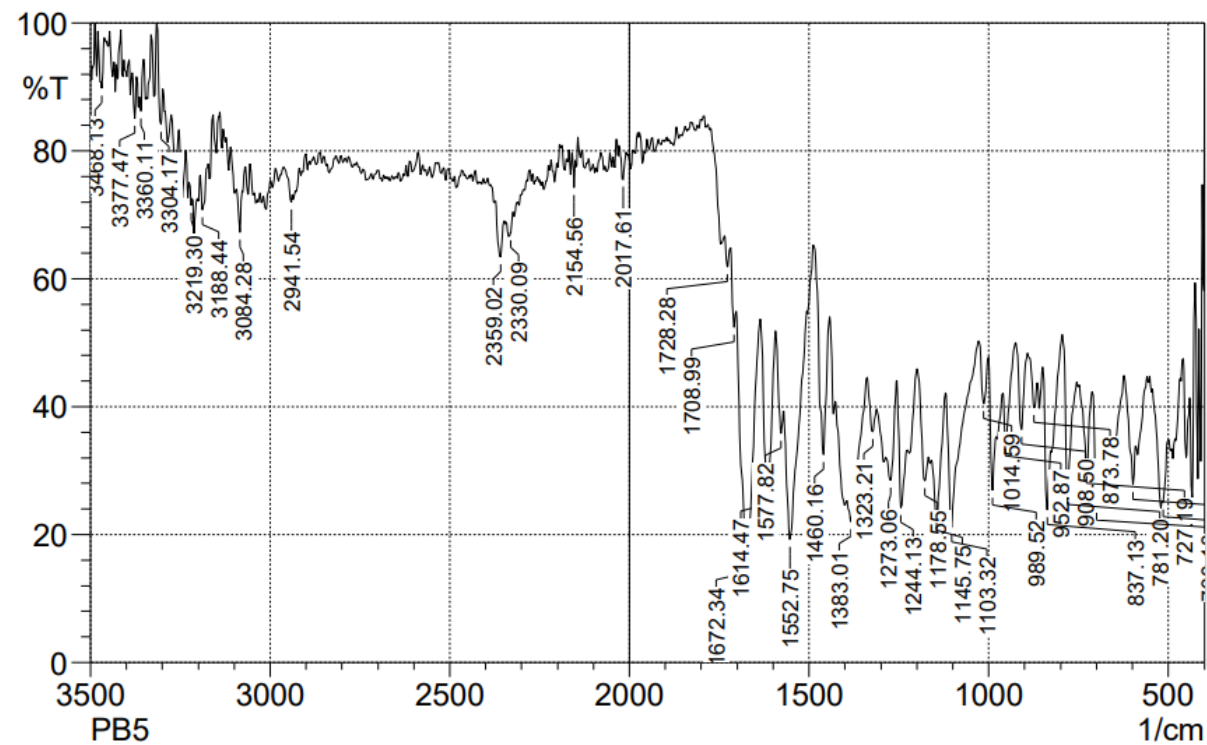


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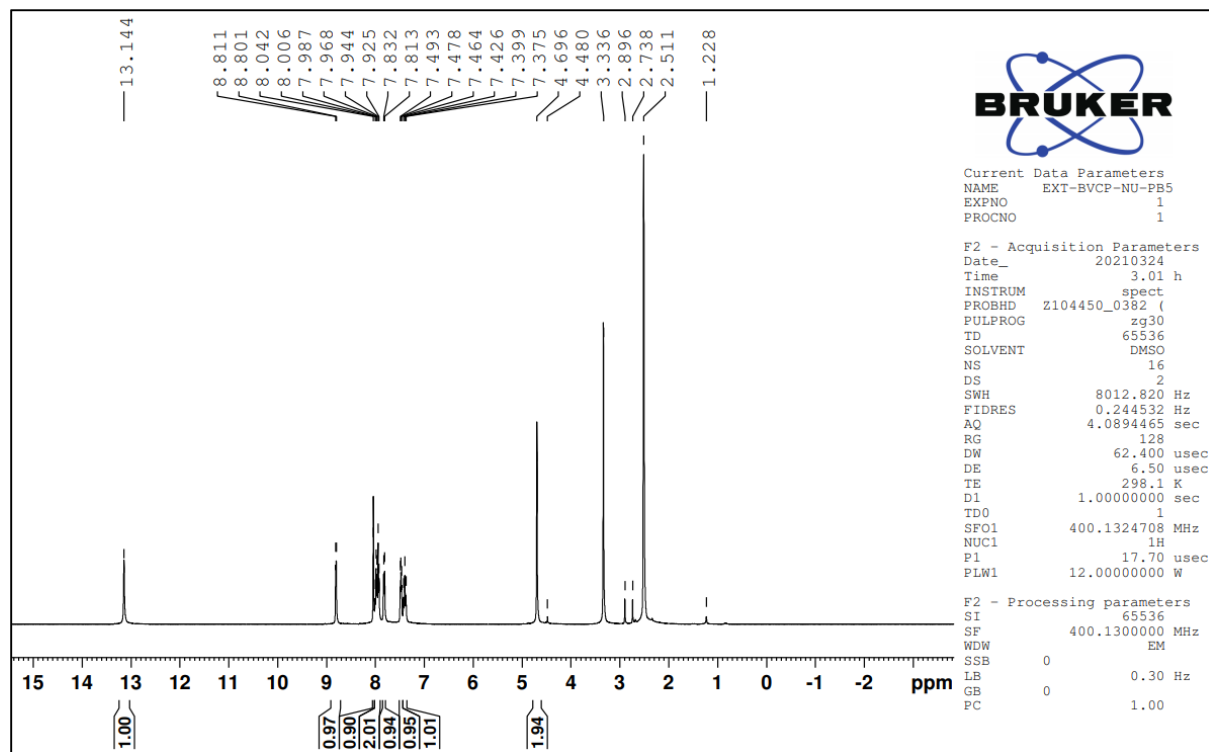


N-(4,6-difluorobenzo[d]thiazol-2-yl)-2-(2,4-dioxo-5-(pyridin-2-ylmethylene)thiazolidin-3-yl)acetamide (PB5)

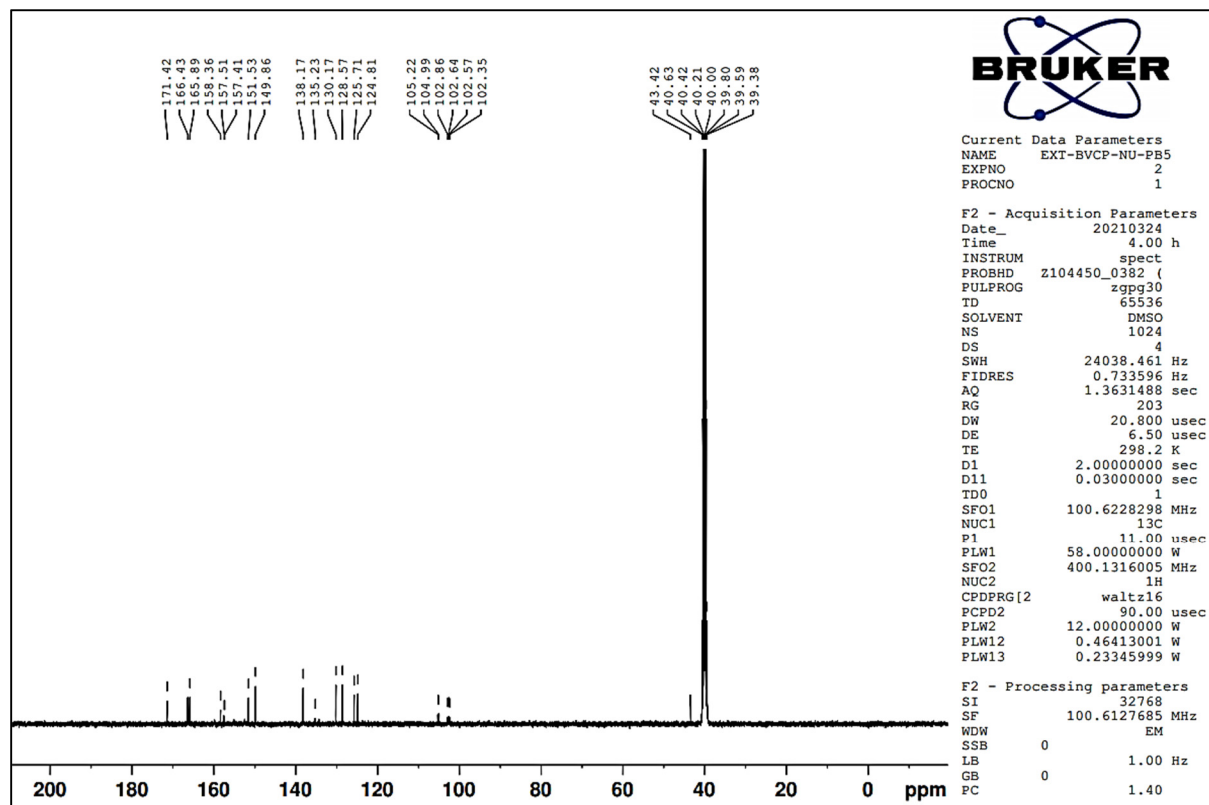
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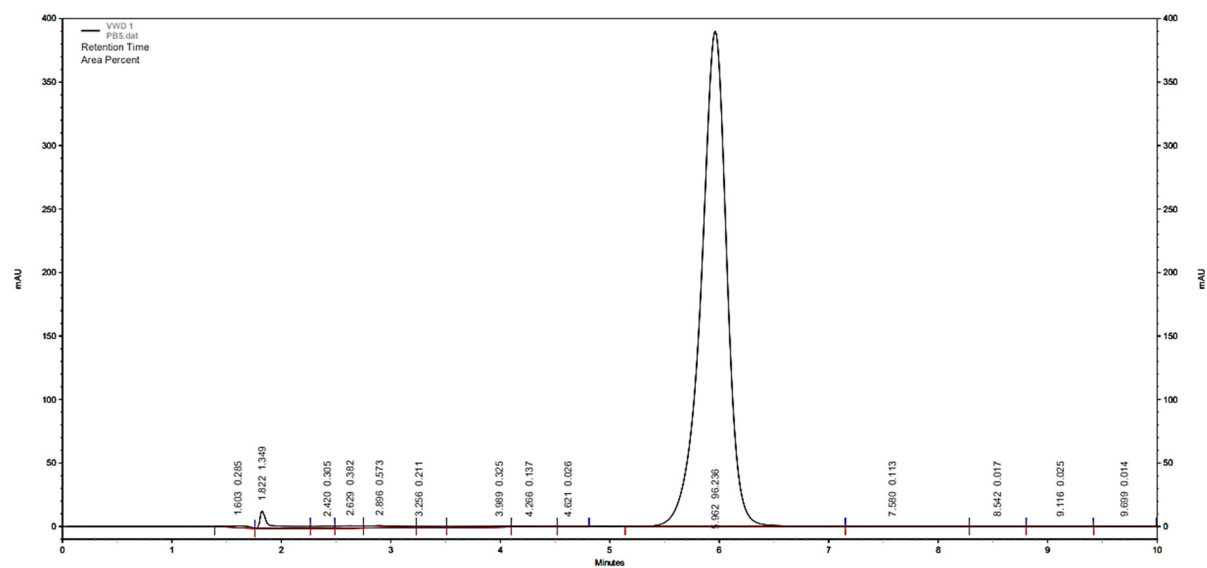
2. $^1\text{H-NMR}$



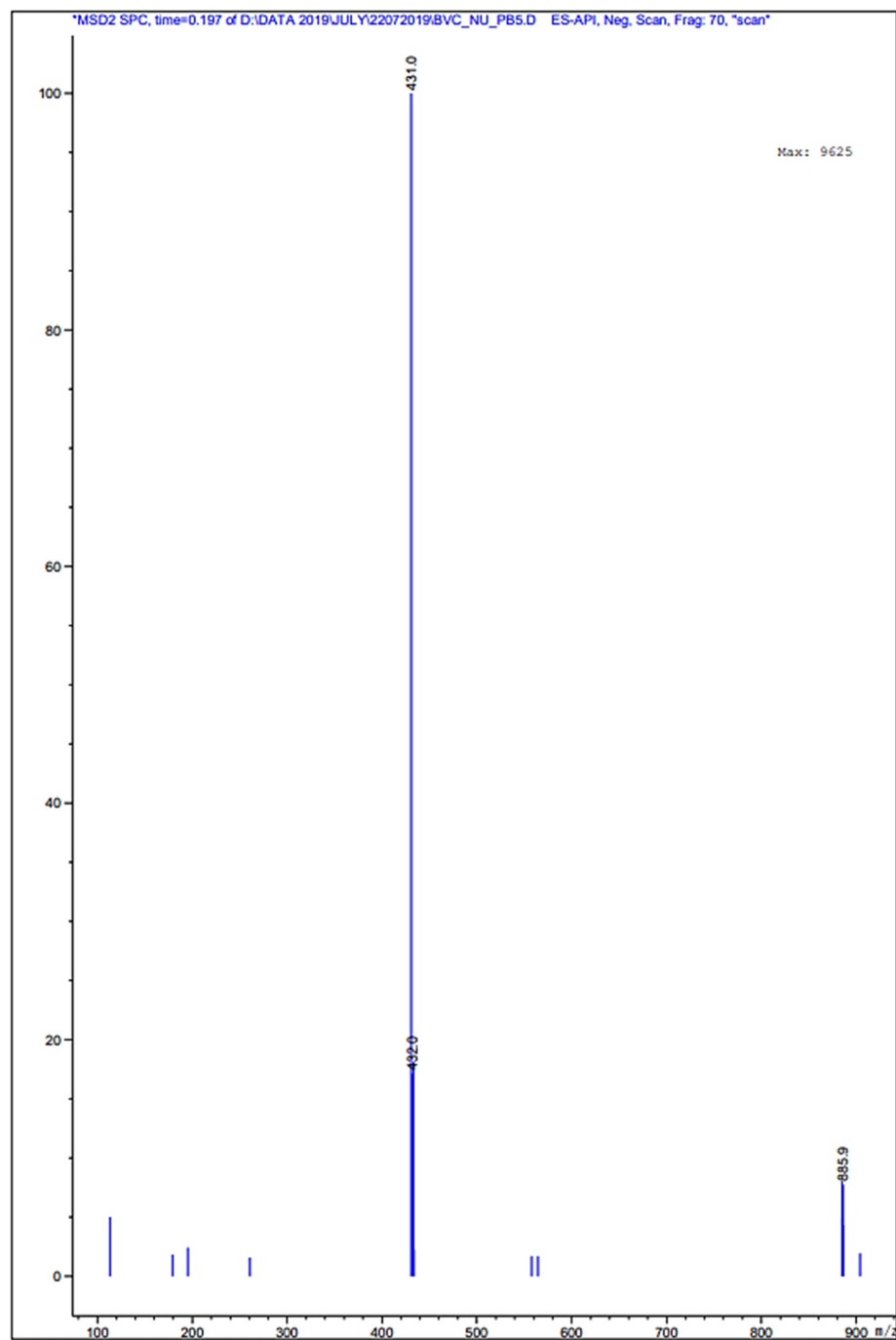
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4. HPLC

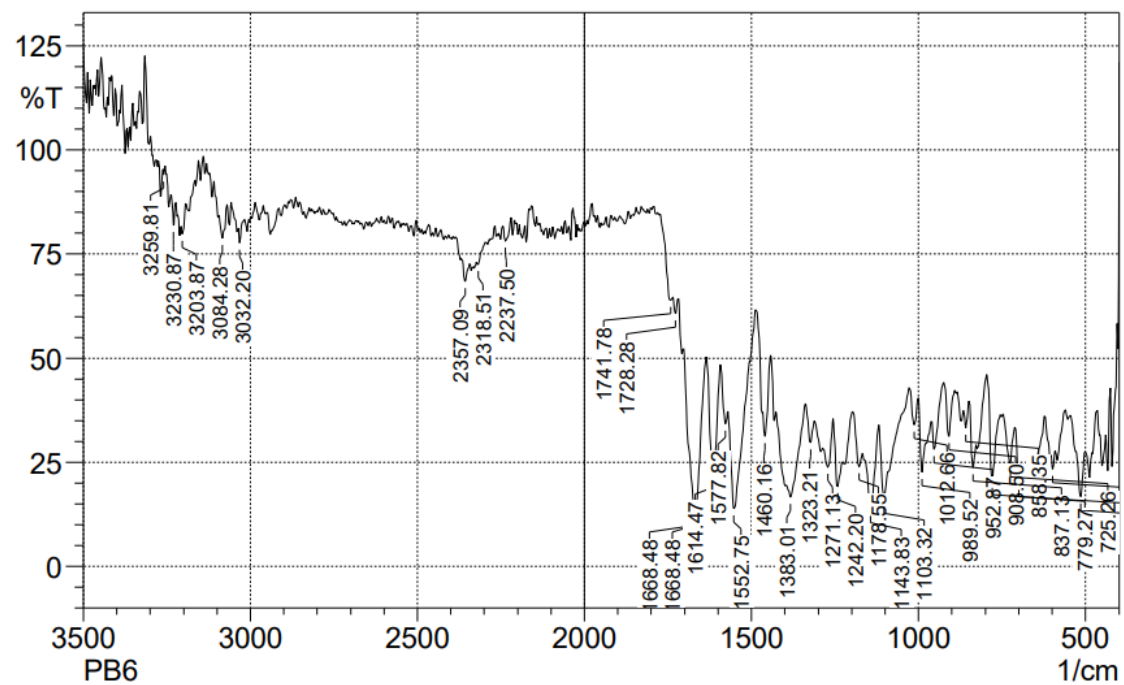


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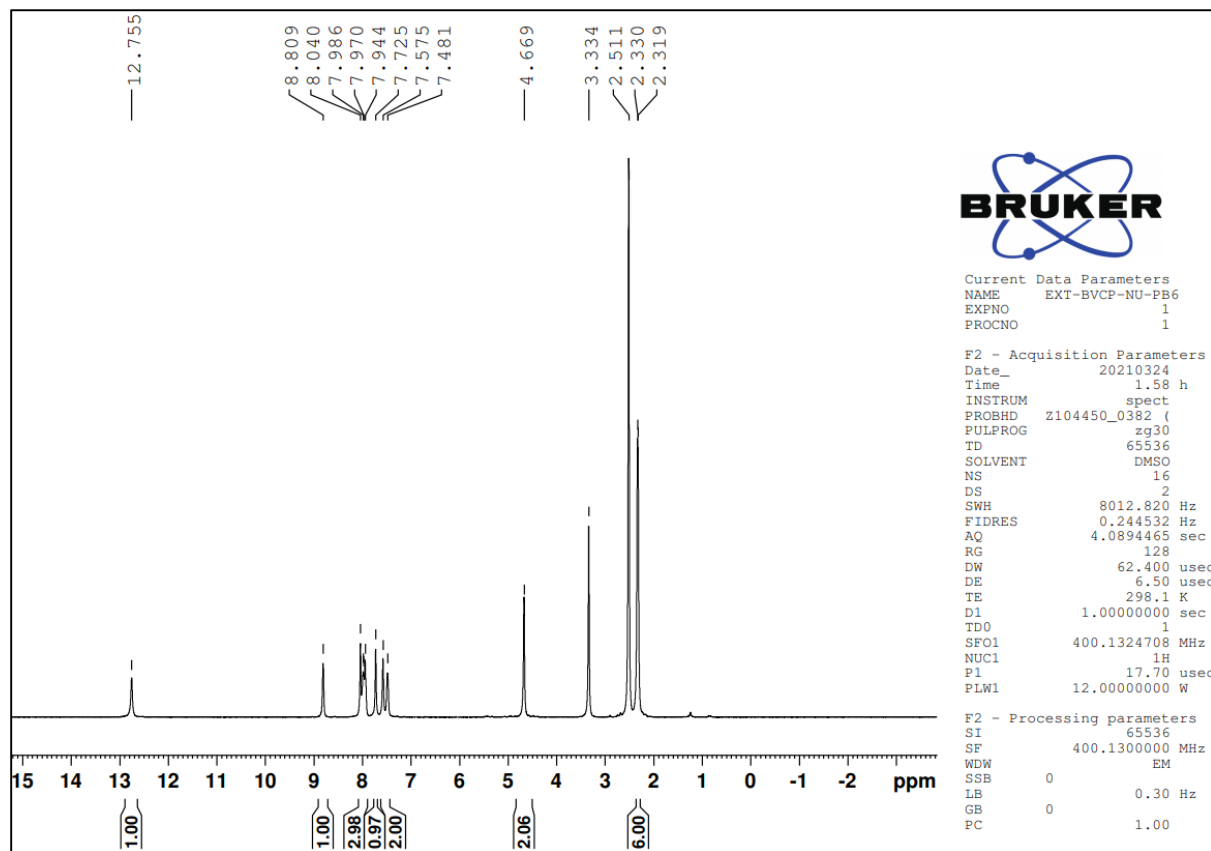


N-(5,6-dimethylbenzo[d]thiazol-2-yl)-2-(2,4-dioxo-5-(pyridin-2-ylmethylene)thiazolidin-3-yl)acetamide (PB6)

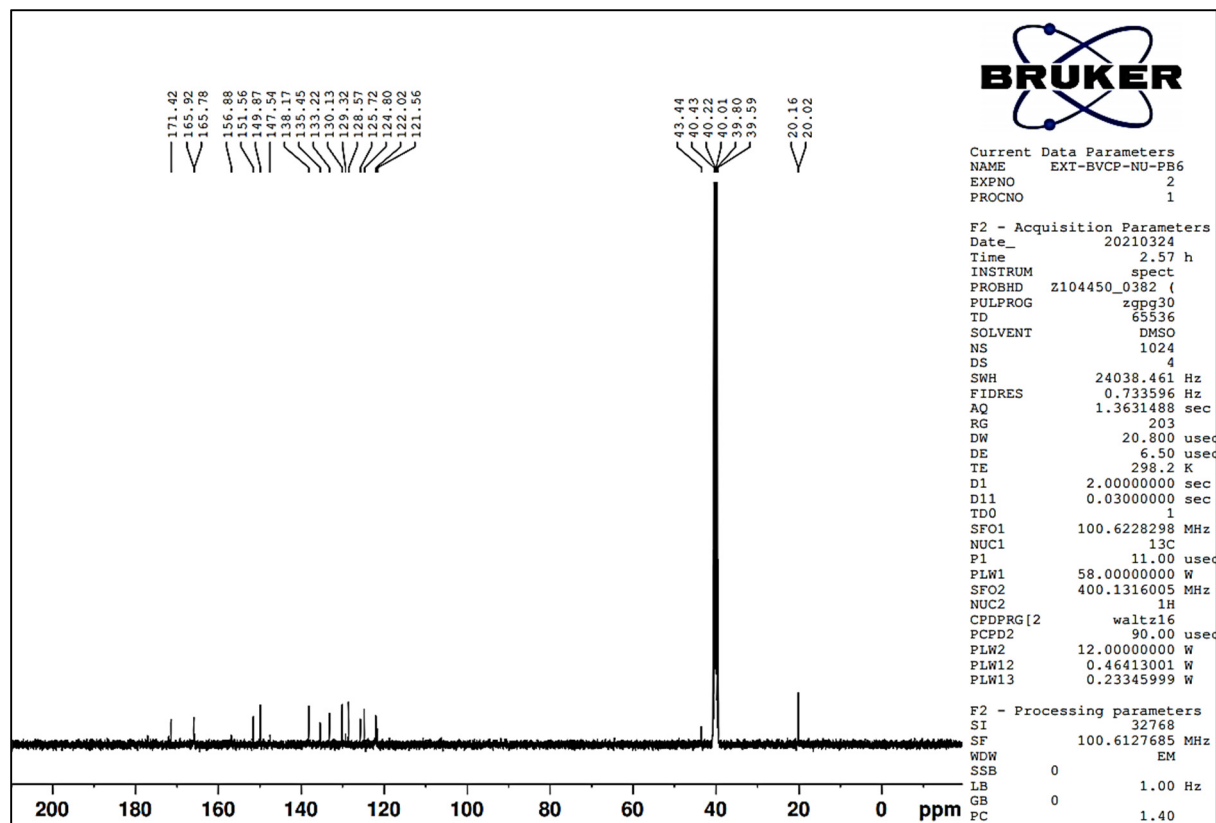
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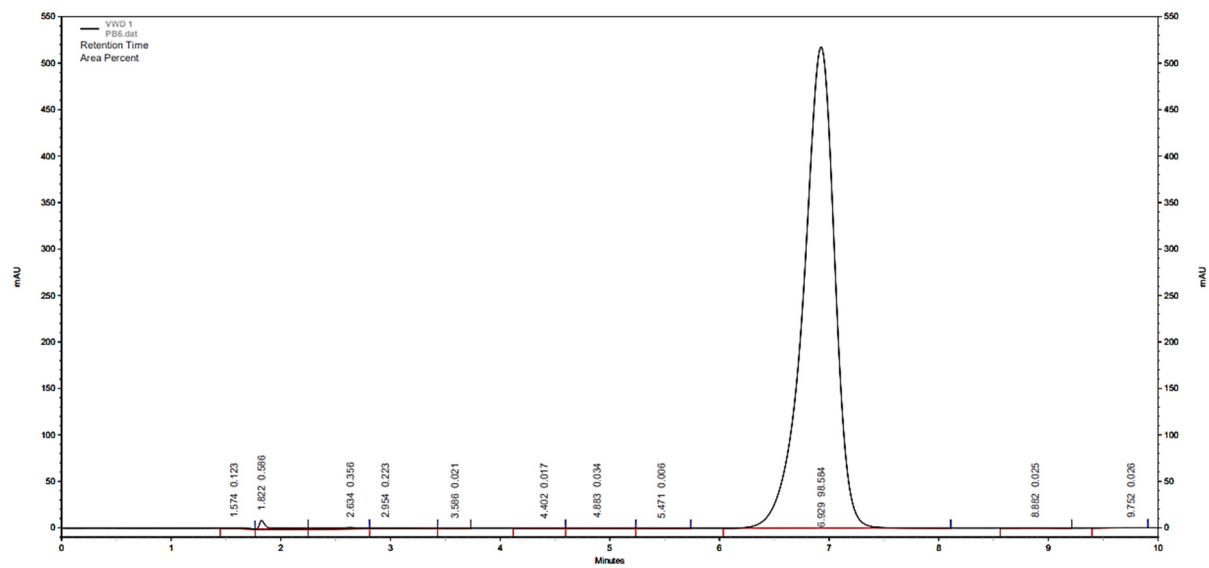
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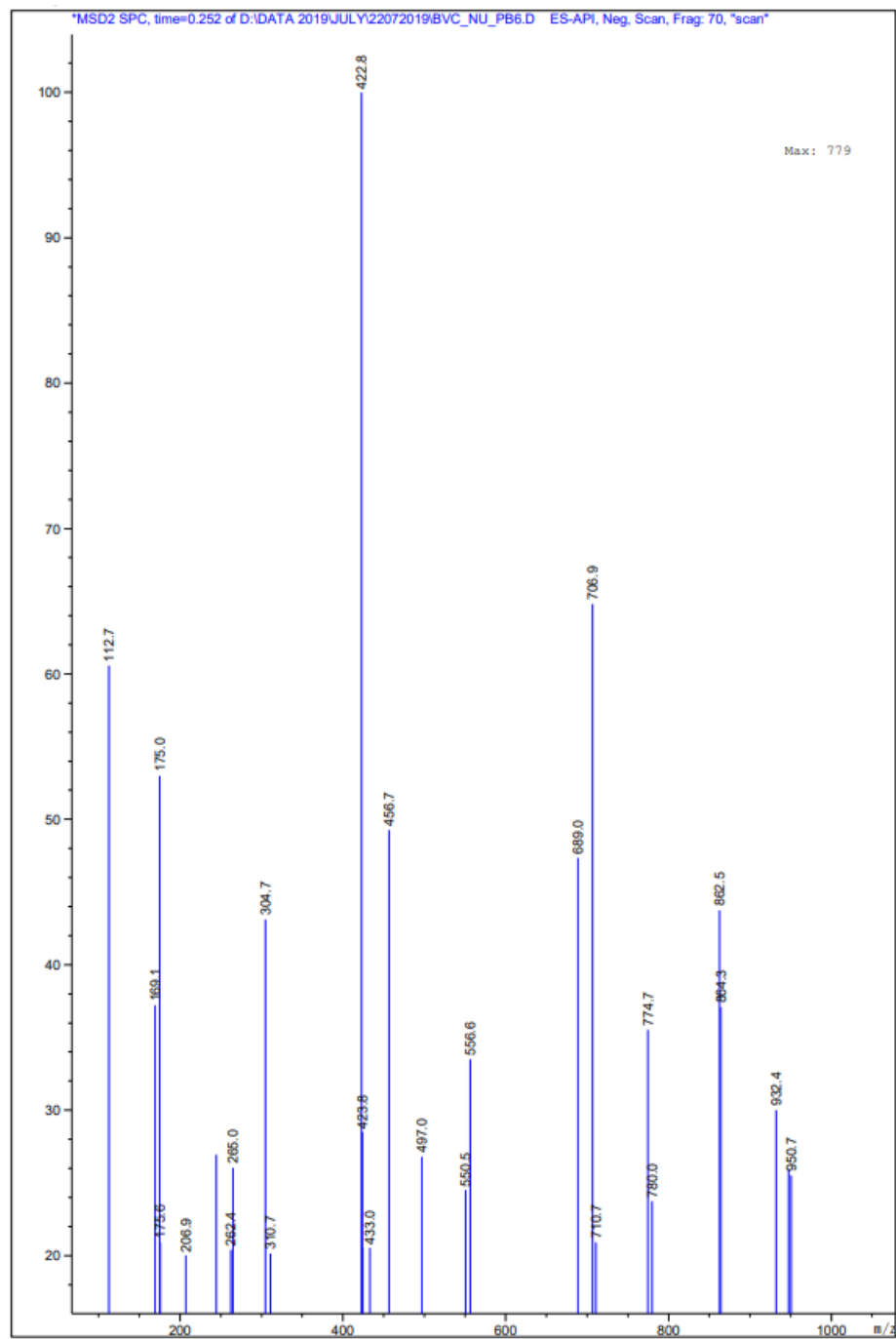
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4. HPLC

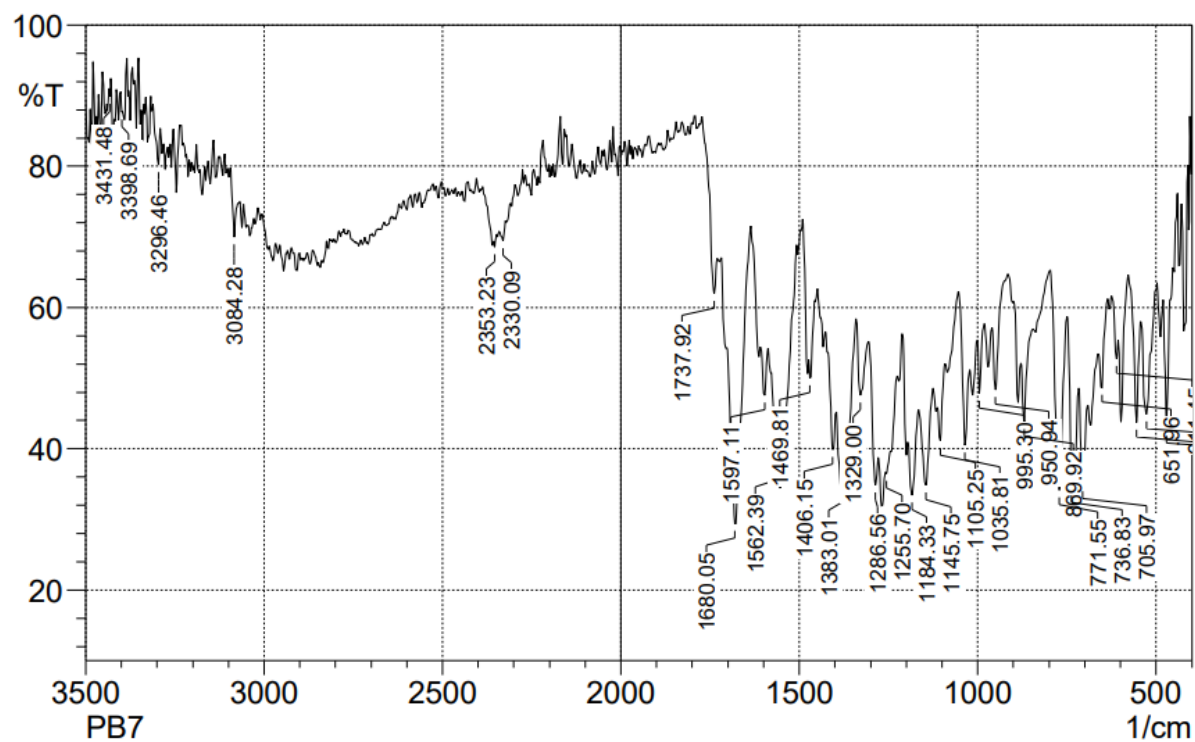


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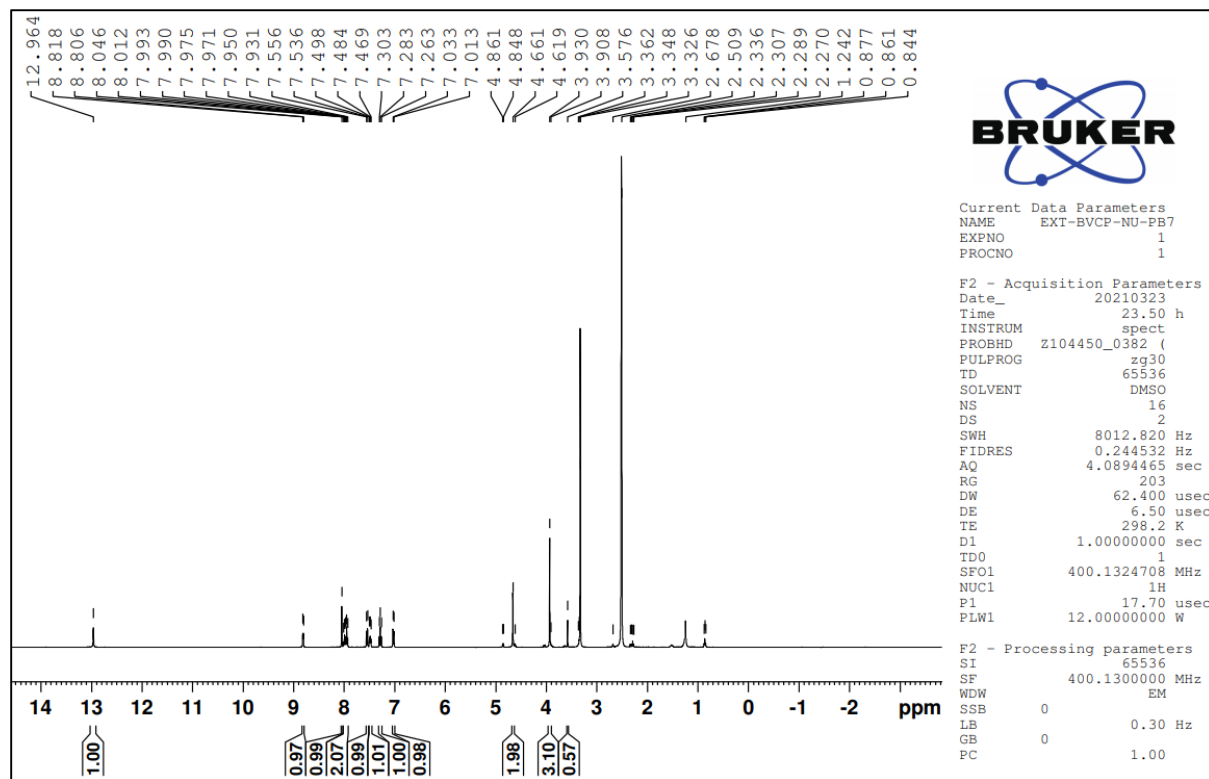


2-(2,4-dioxo-5-(pyridin-2-ylmethylene)thiazolidin-3-yl)-N-(4-methoxybenzo[d]thiazol-2-yl)acetamide (PB7)

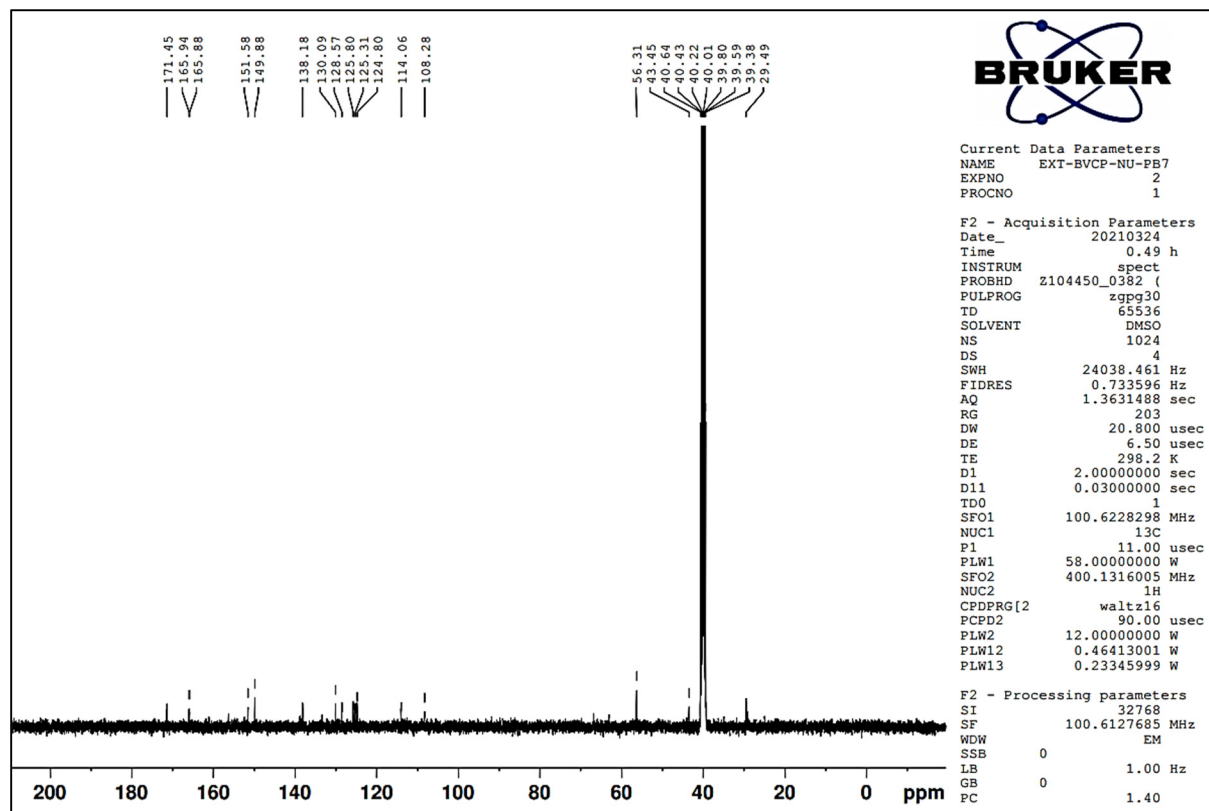
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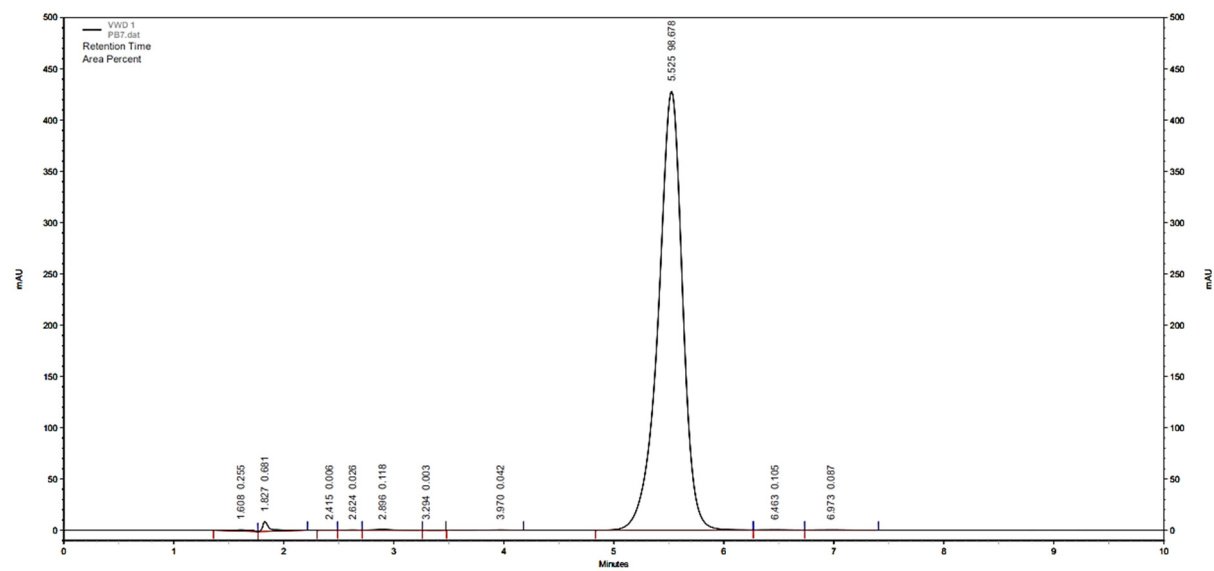
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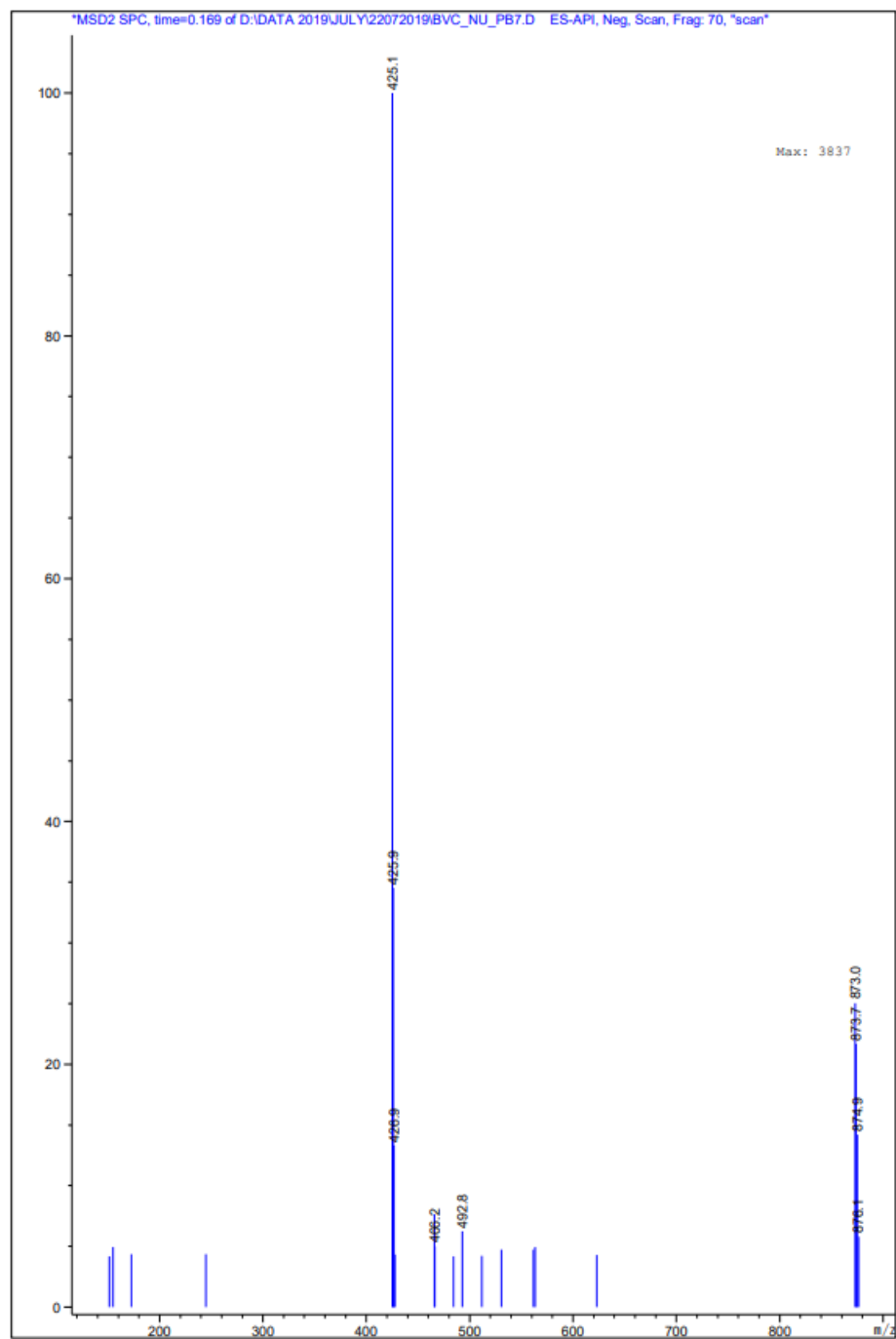
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4. HPLC

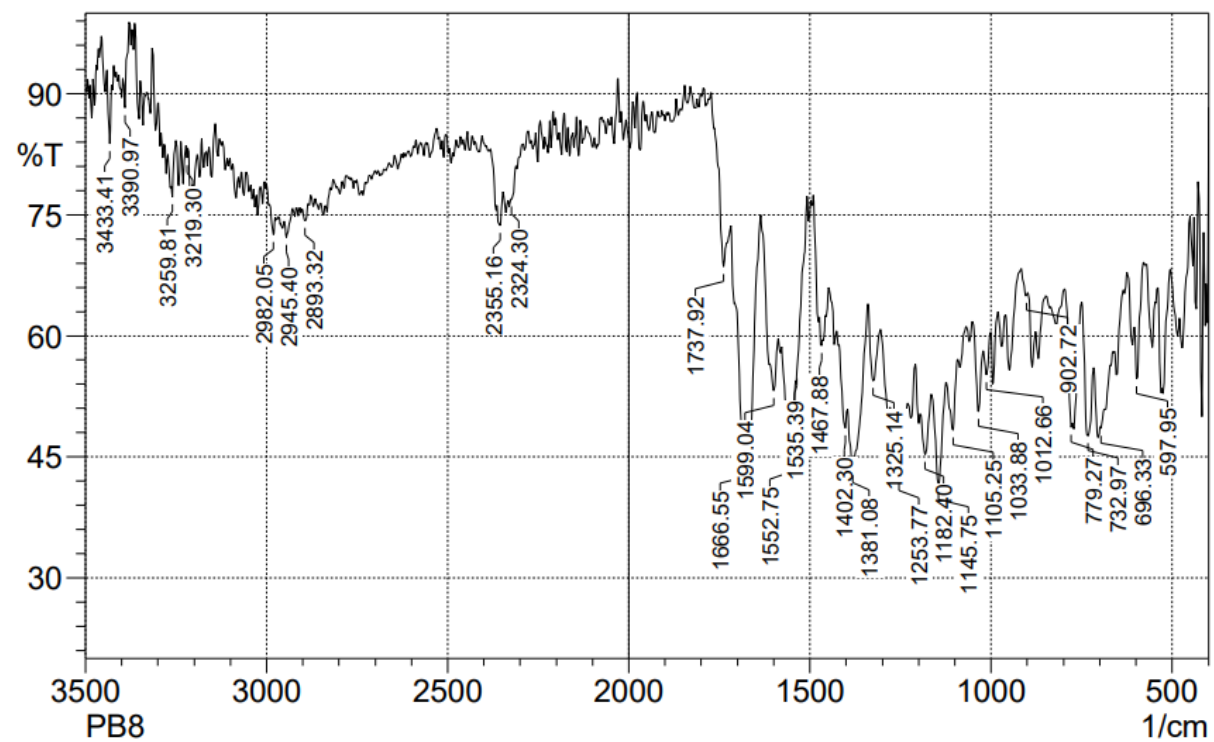


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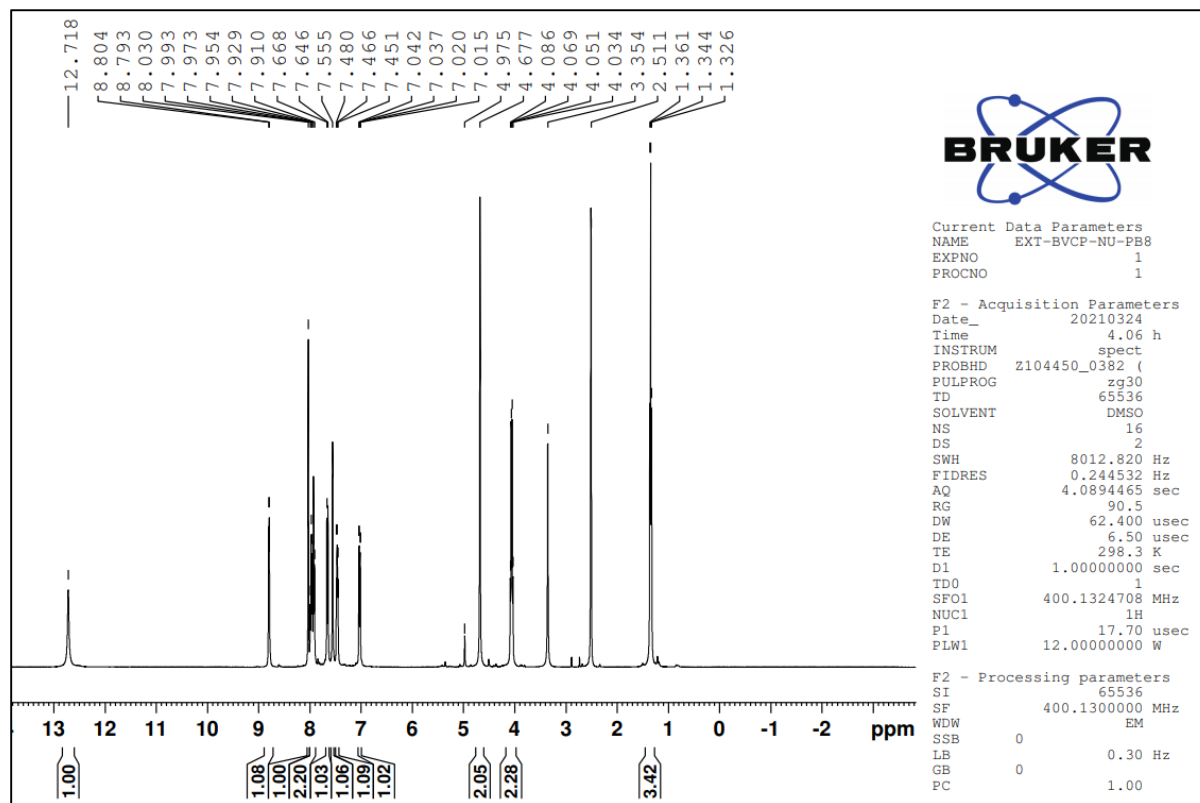


2-(2,4-dioxo-5-(pyridin-2-ylmethylene)thiazolidin-3-yl)-N-(6-ethoxybenzo[d]thiazol-2-yl)acetamide (PB8)

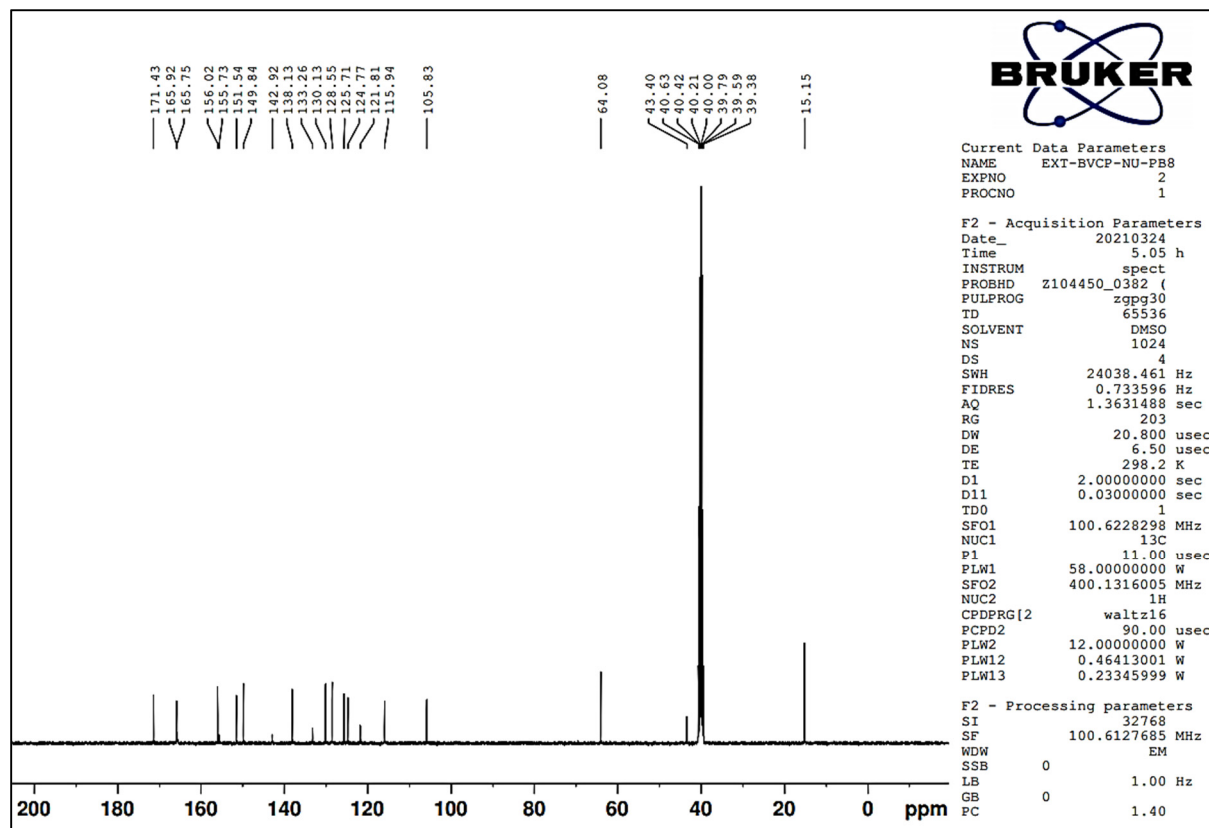
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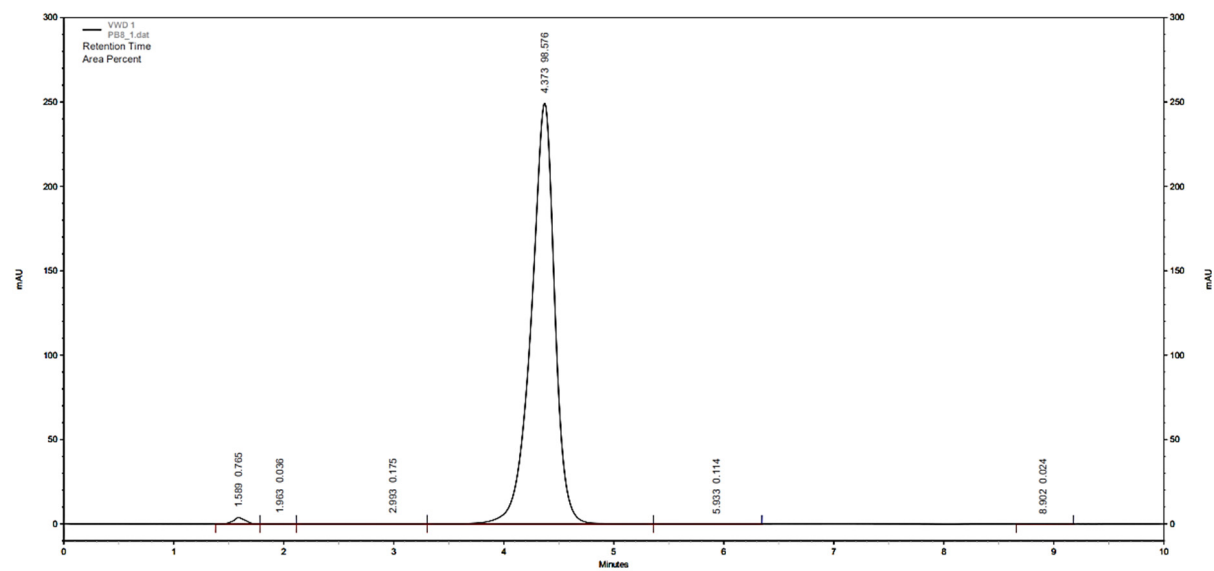
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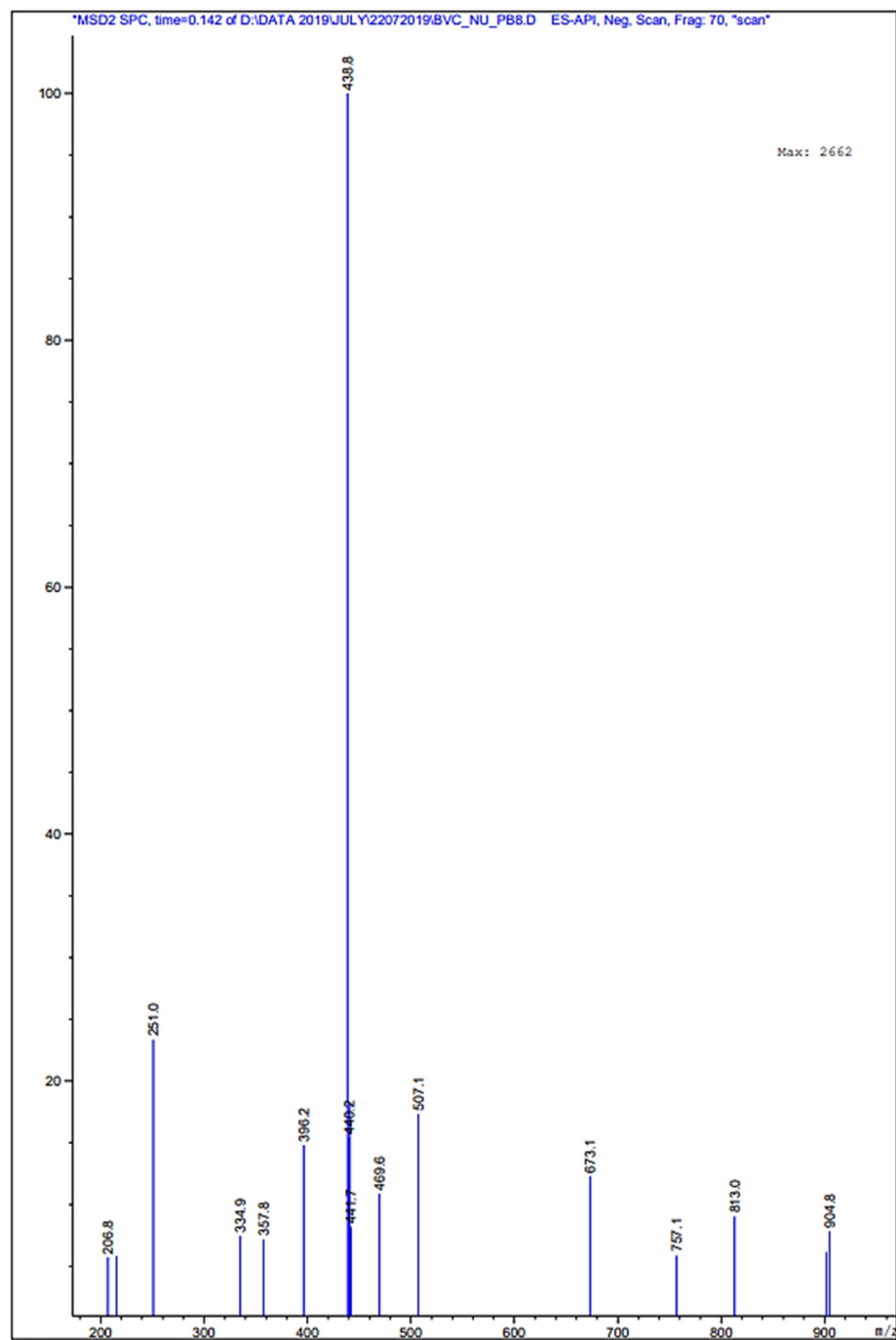
3. 13C-NMR



4. HPLC

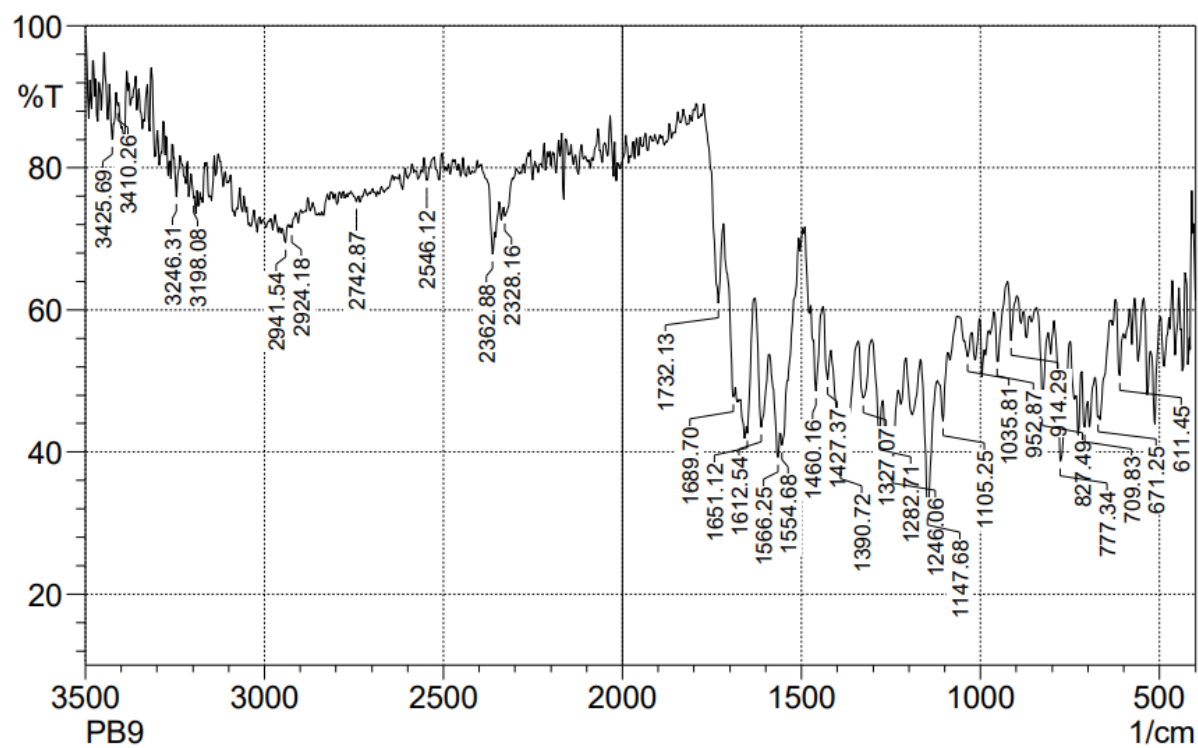


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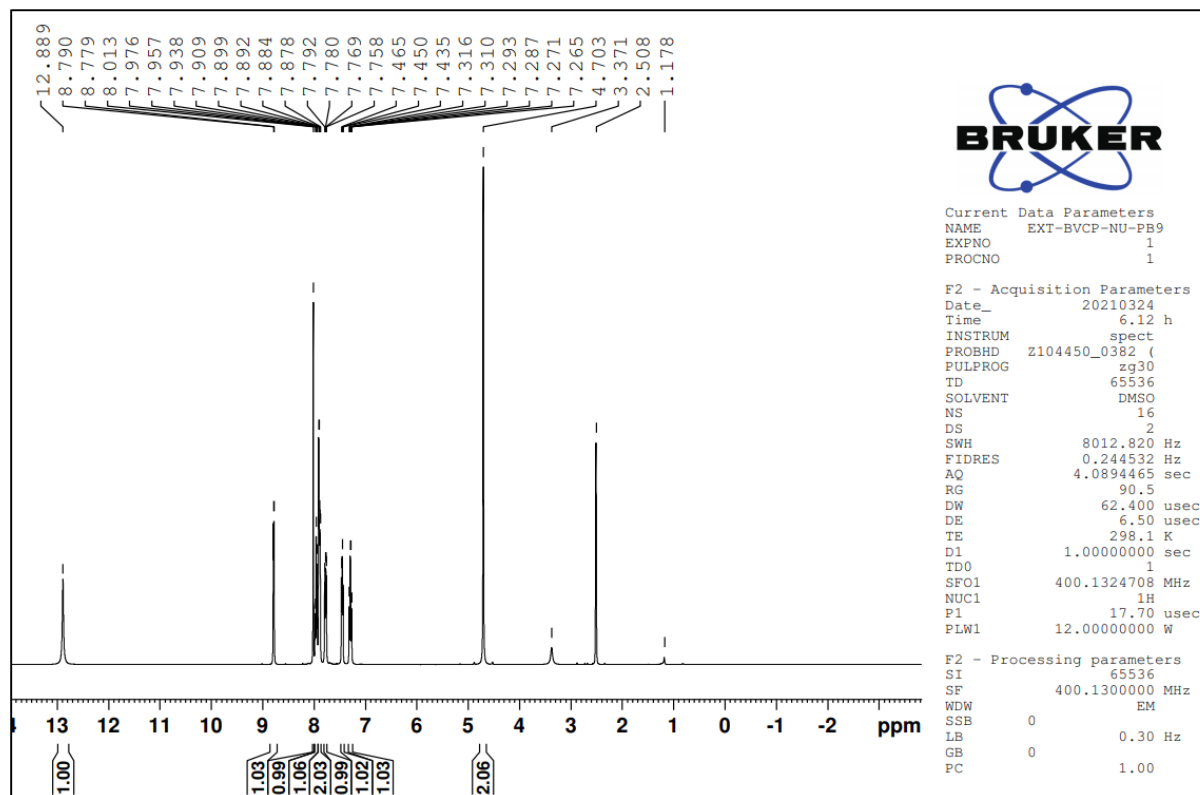


2-(2,4-dioxo-5-(pyridin-2-ylmethylene)thiazolidin-3-yl)-N-(6-fluorobenzo[d]thiazol-2-yl)acetamide (PB9)

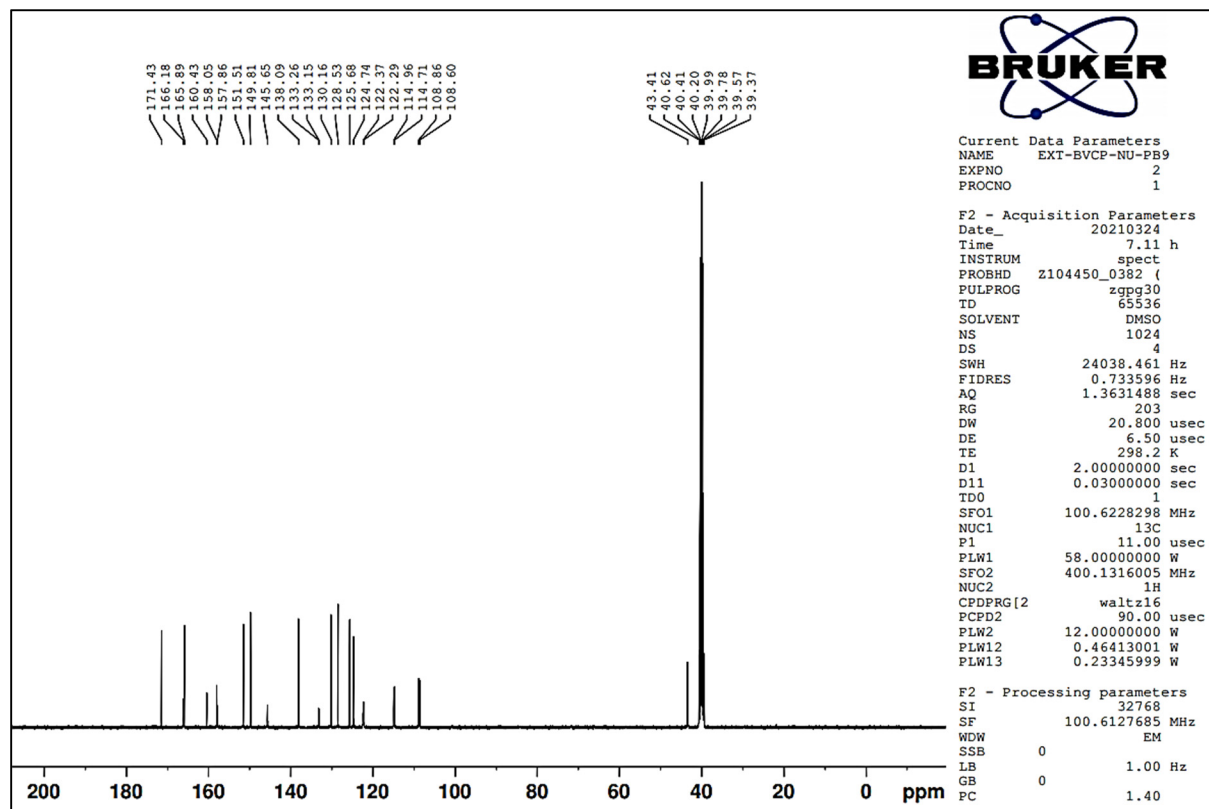
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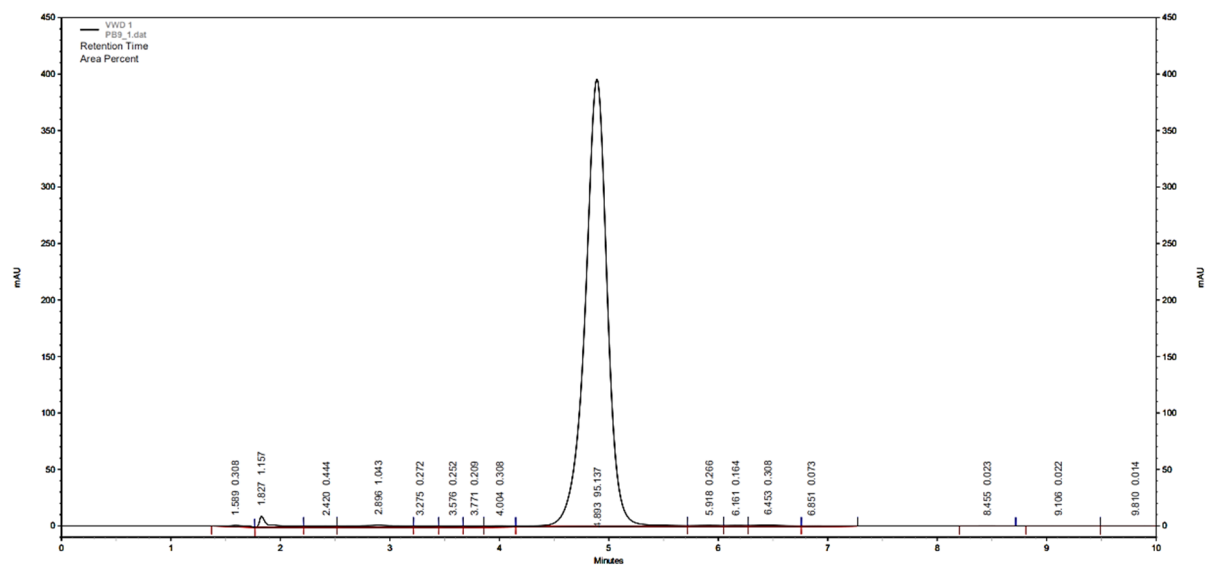
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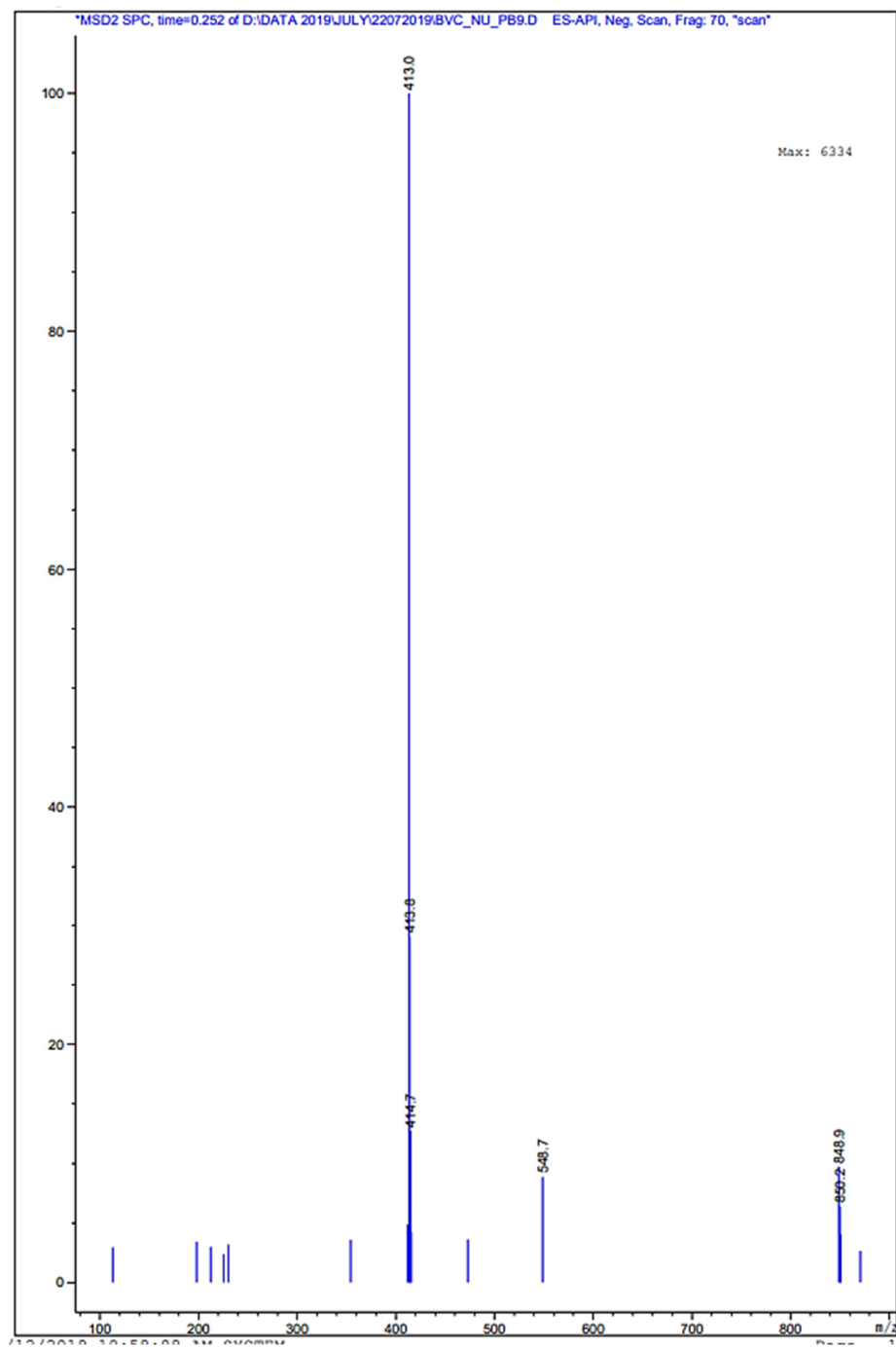
3. 13C-NMR



4. HPLC

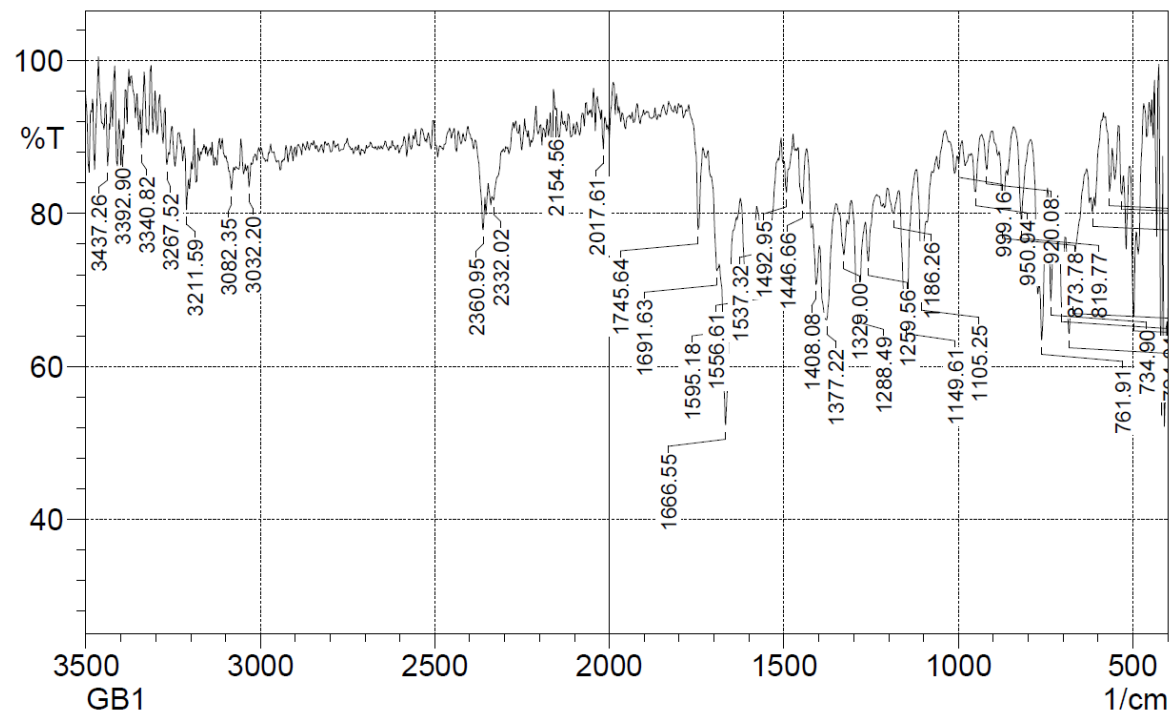


5. Mass



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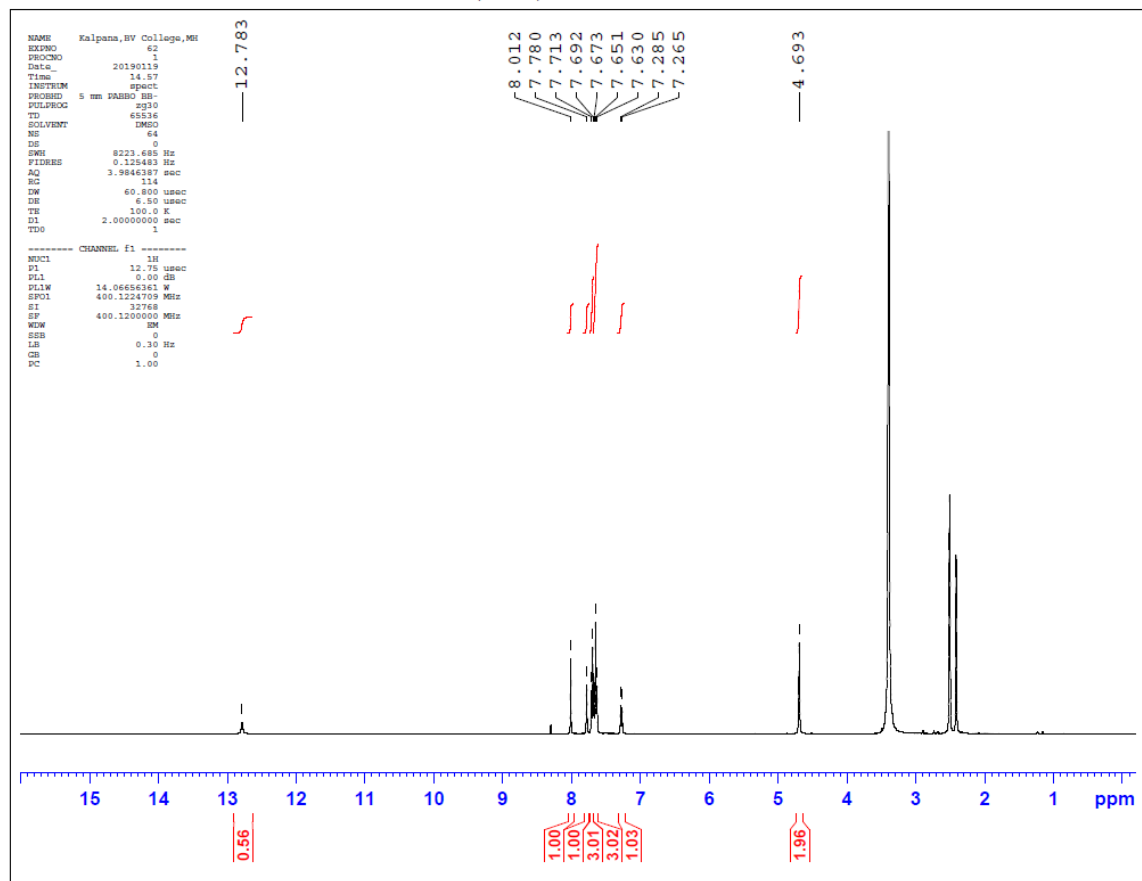
1. FTIR



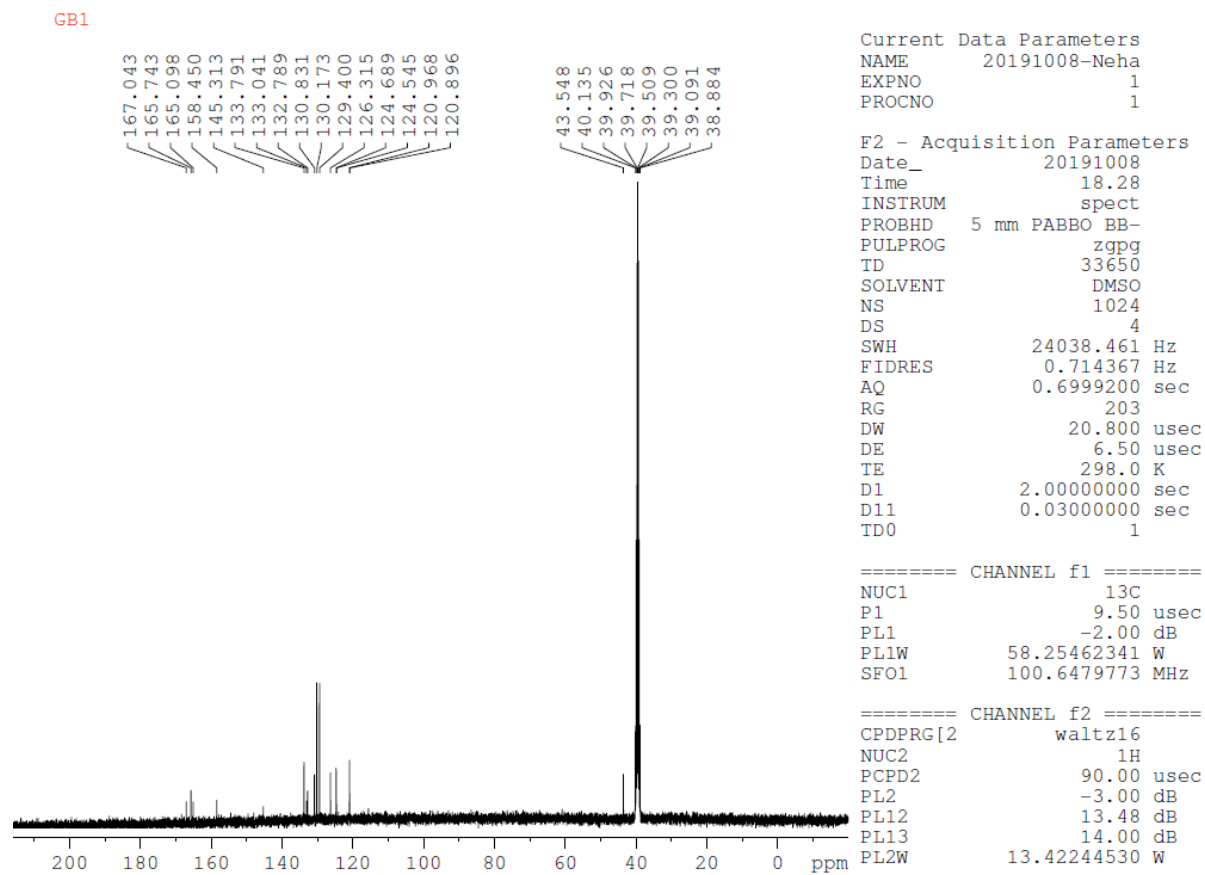
2. $^1\text{H-NMR}$

SAIFNM190114A-45(GS-1)

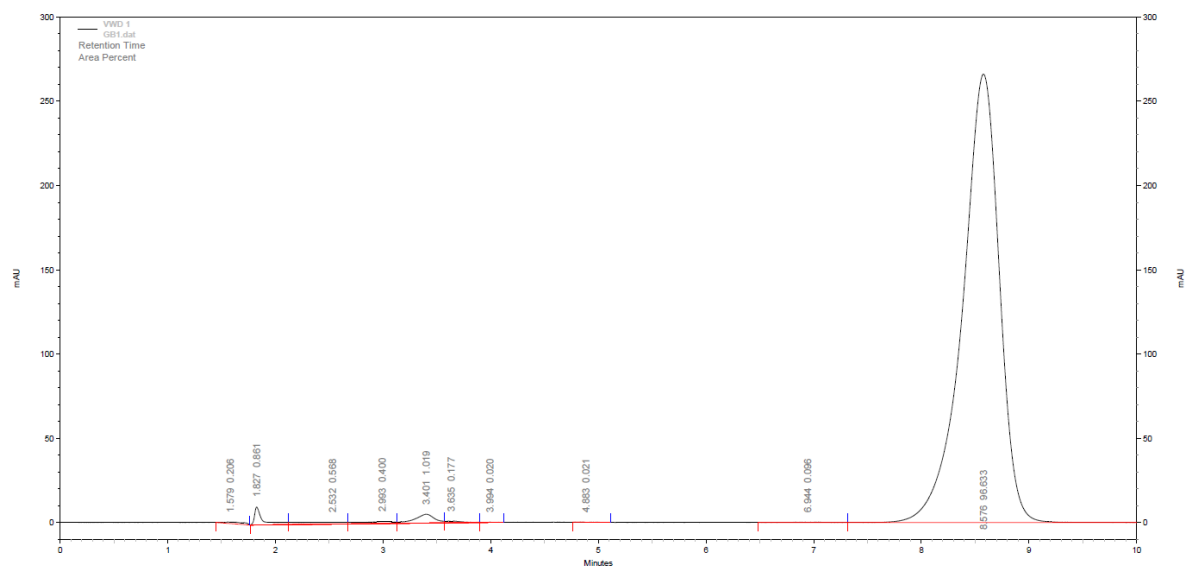
SAIF Cochin



3. 13C-NMR

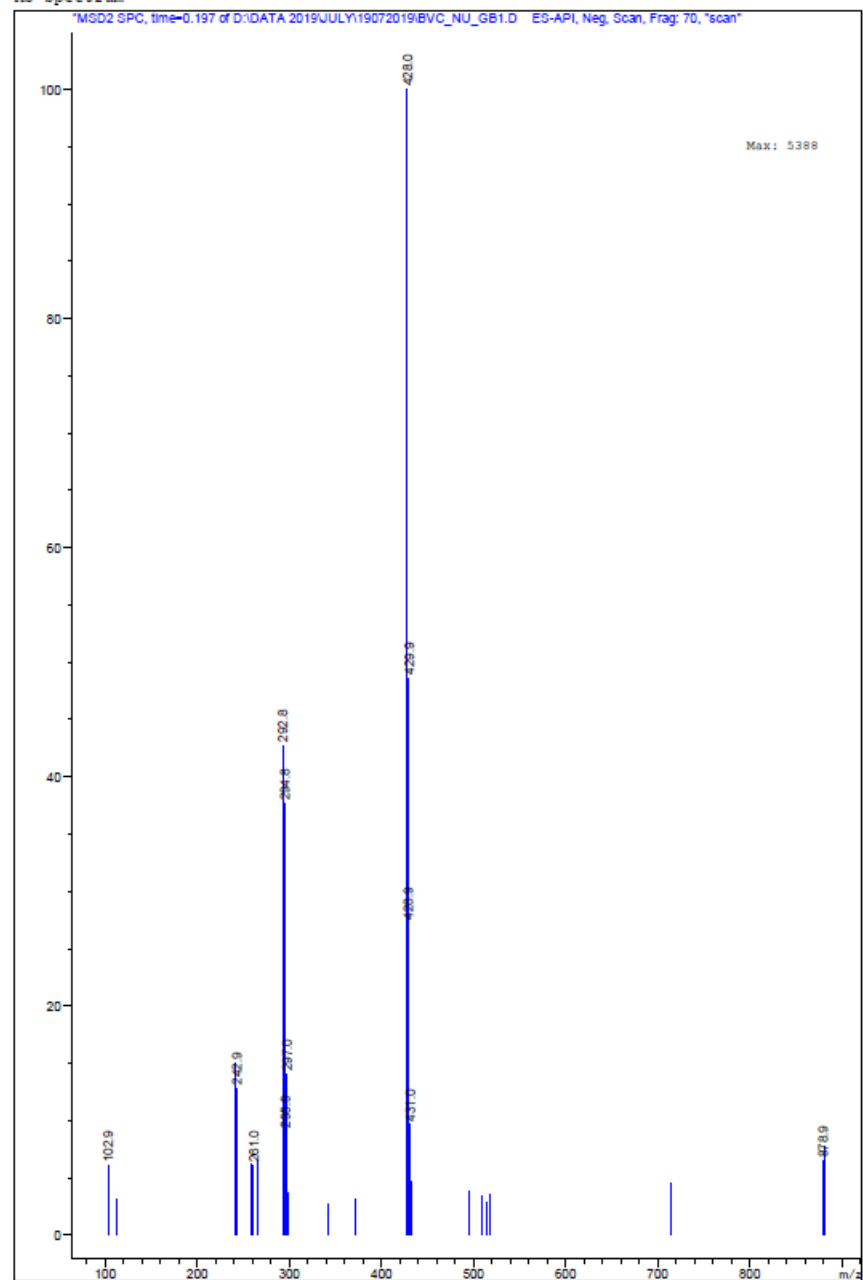


4. HPLC



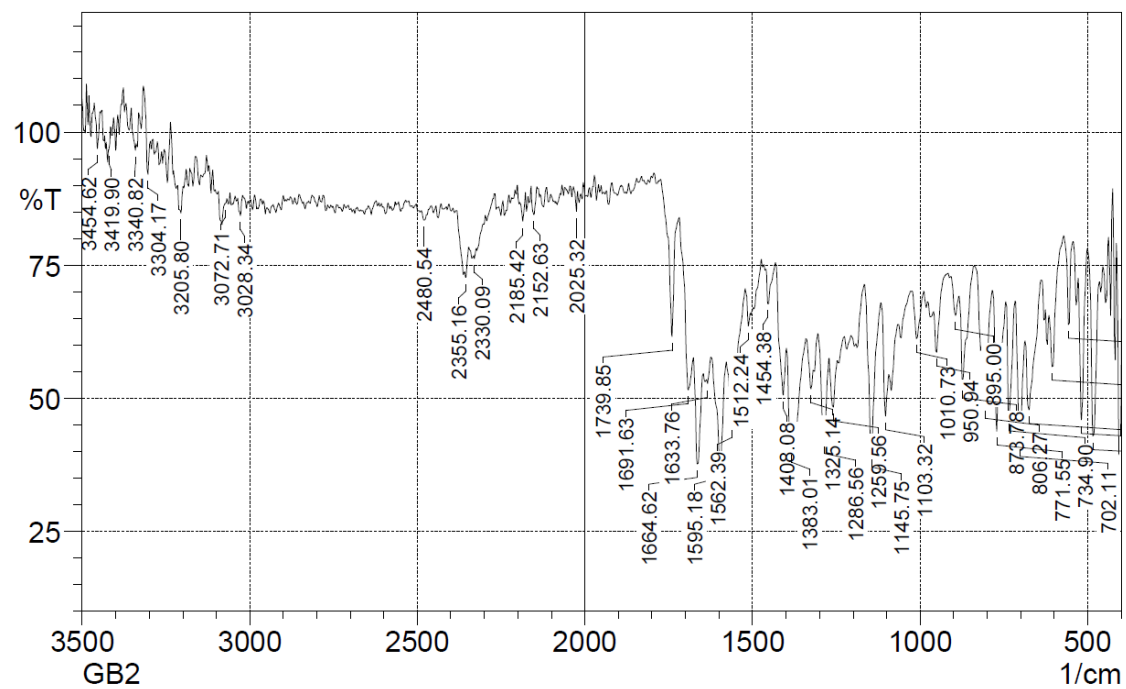
5. Mass

MS Spectrum



N-(4-chlorobenzo[d]thiazol-2-yl)-2-(5-(4-methylbenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB2)

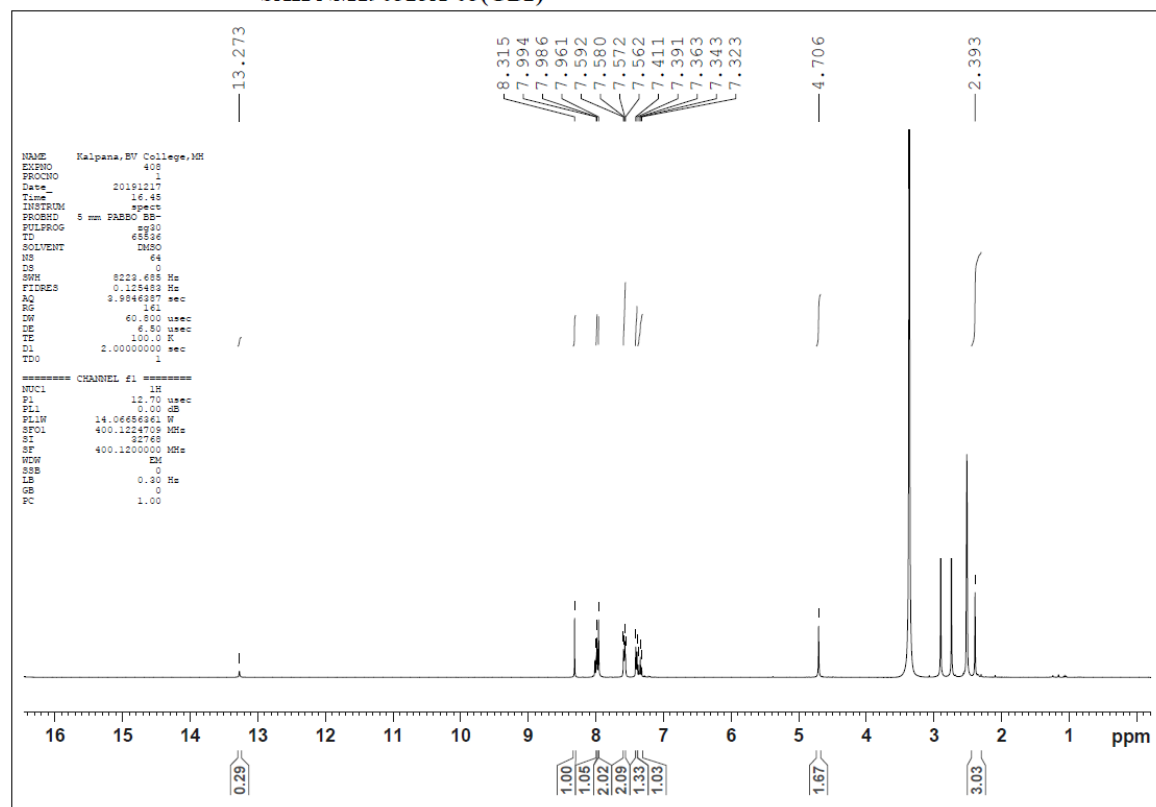
1. FTIR



2. ¹H-NMR

SAIFNM190323A-05(GB2)

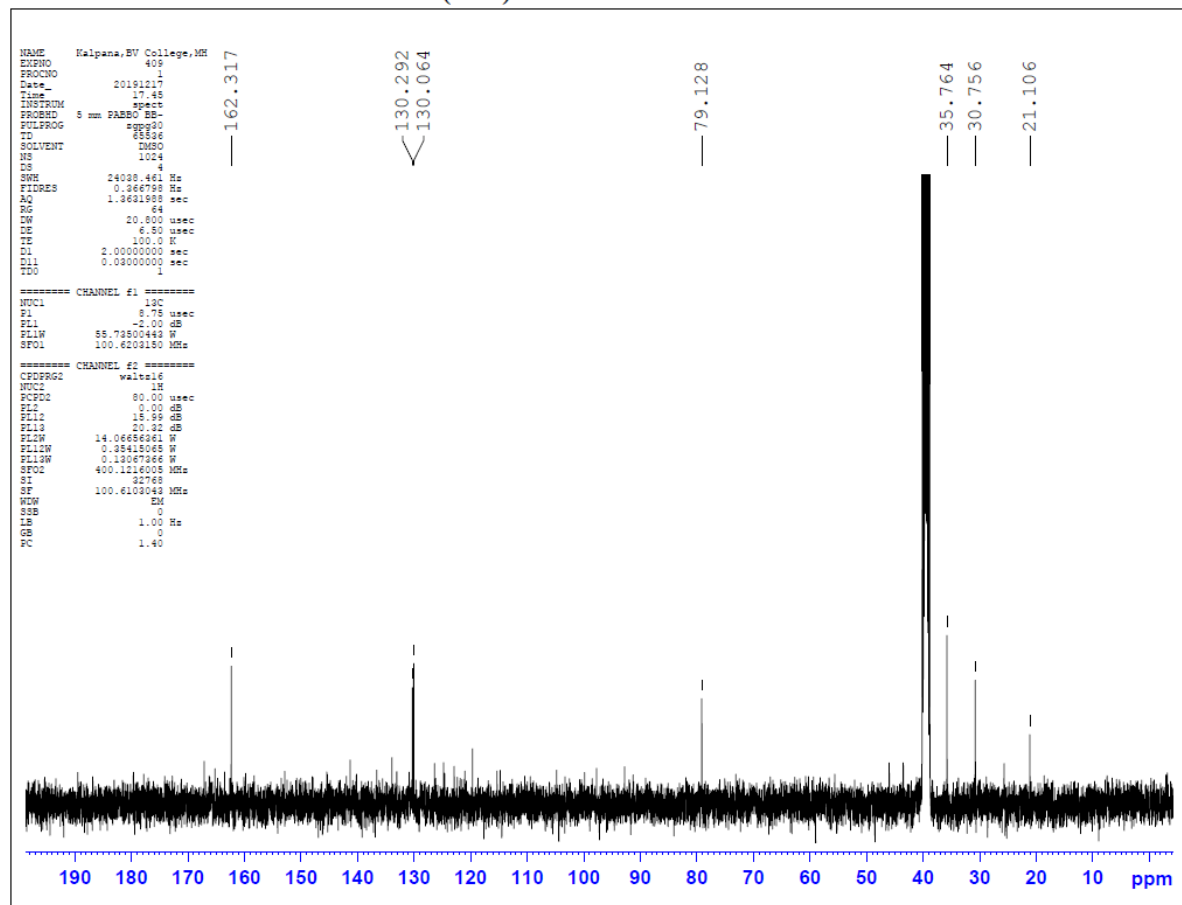
SAIF Cochin



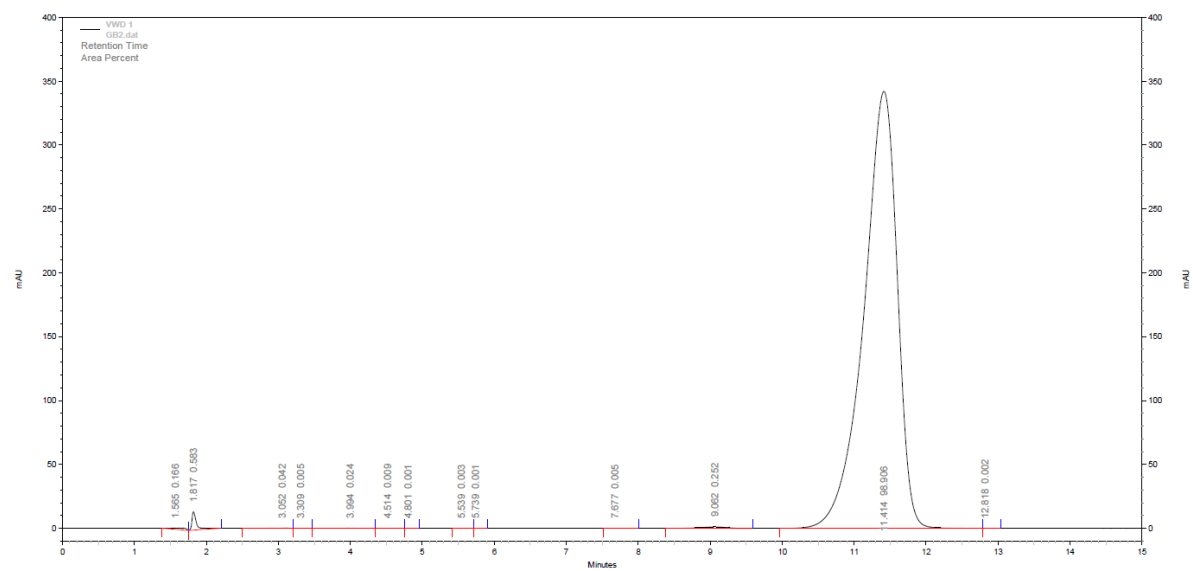
3. 13C-NMR

SAIFNM190323A-06(GB2)

SAIF Cochin

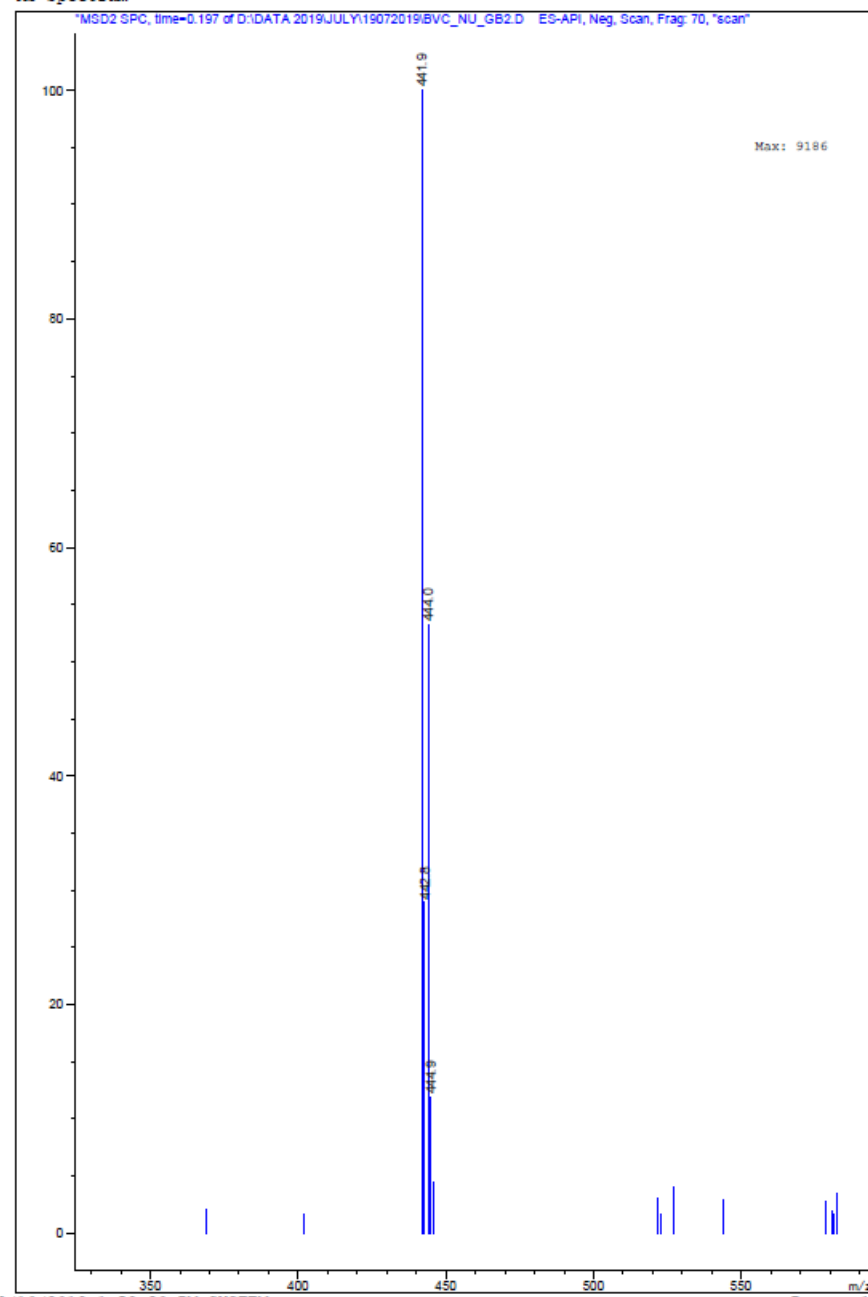


4. HPLC



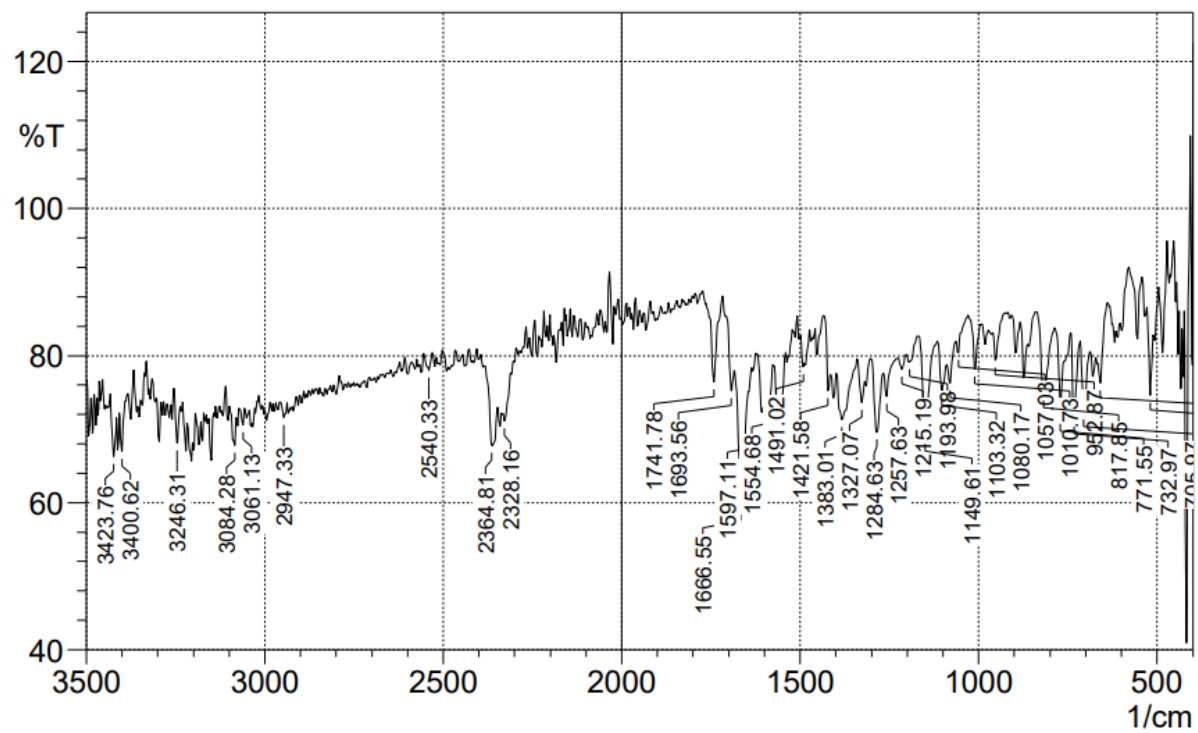
5. Mass

MS Spectrum

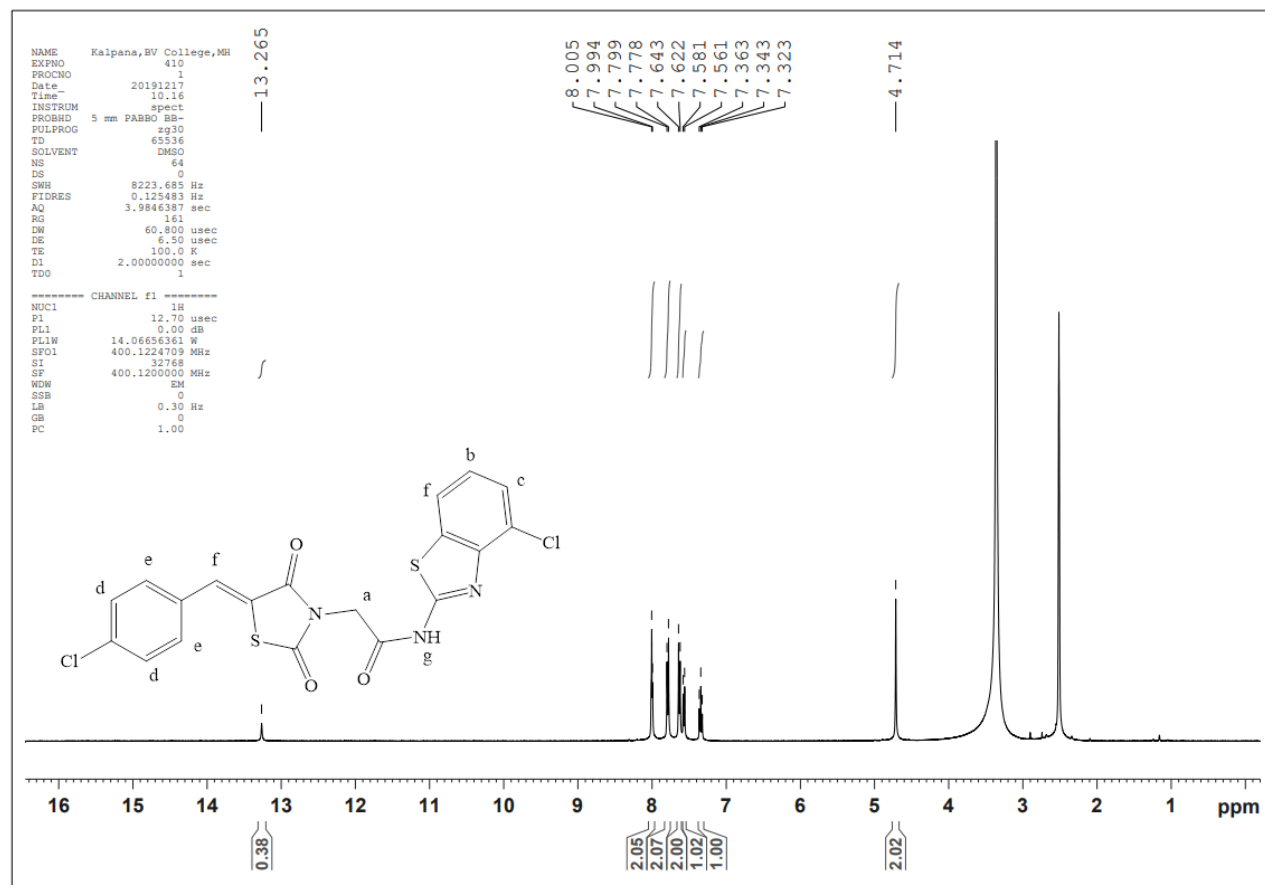


N-(4-chlorobenzo[d]thiazol-2-yl)-2-(5-(4-chlorobenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB3)

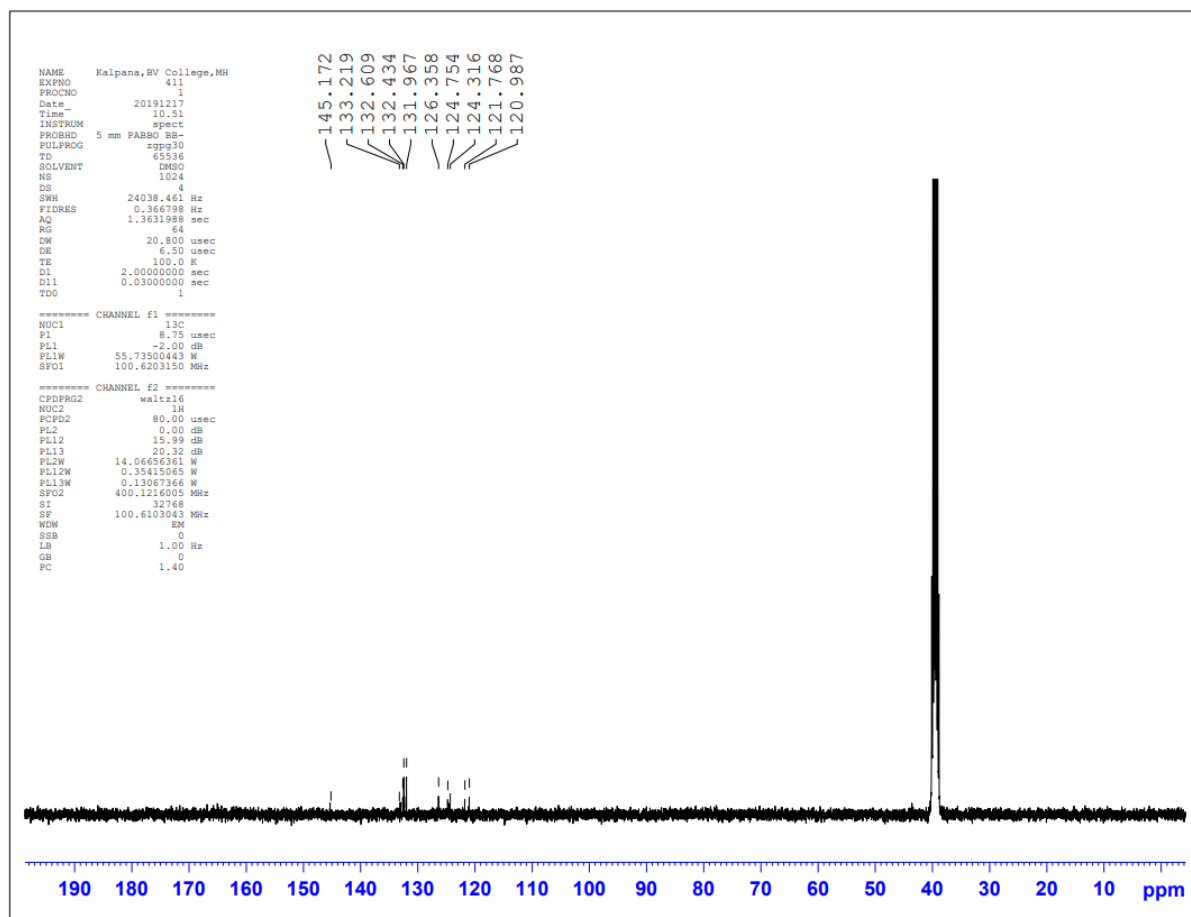
1. FTIR -



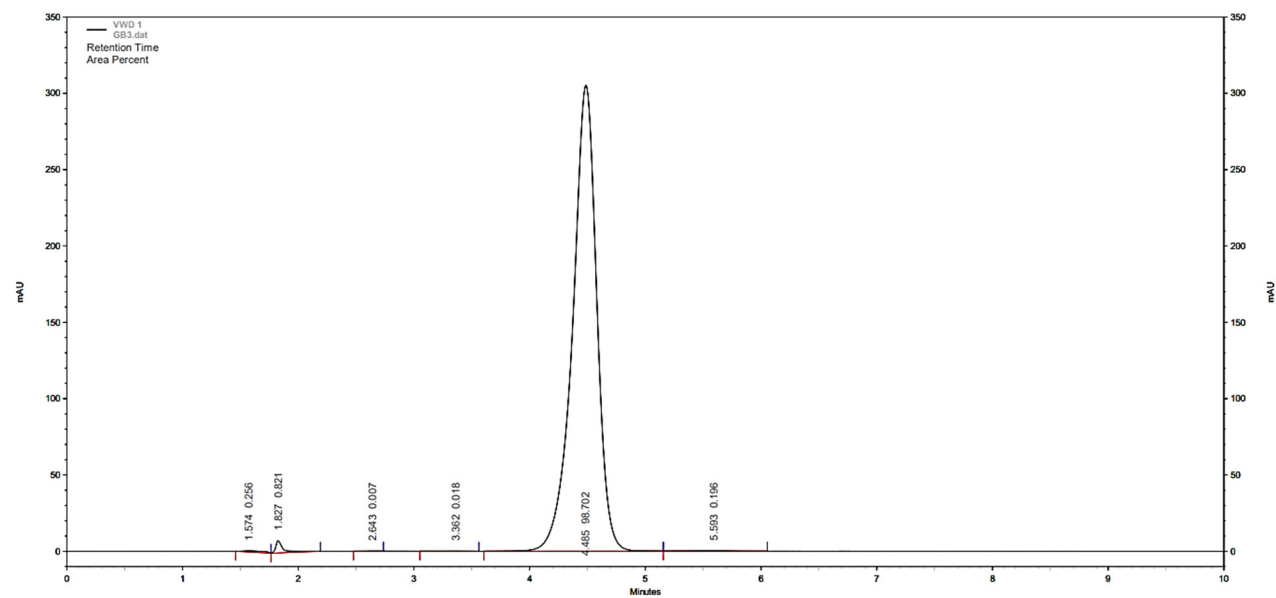
2. ¹H-NMR



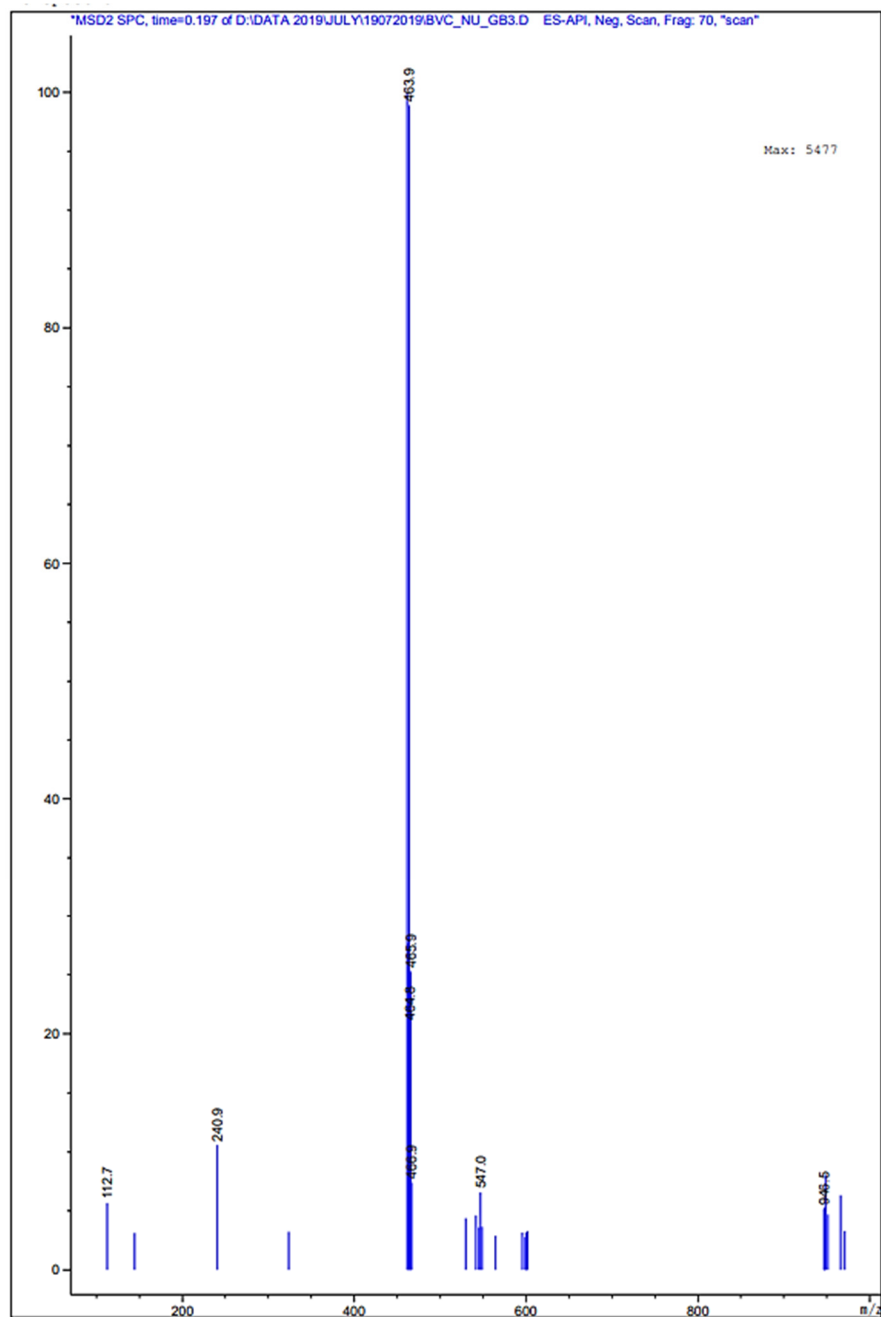
3. ¹³C-NMR



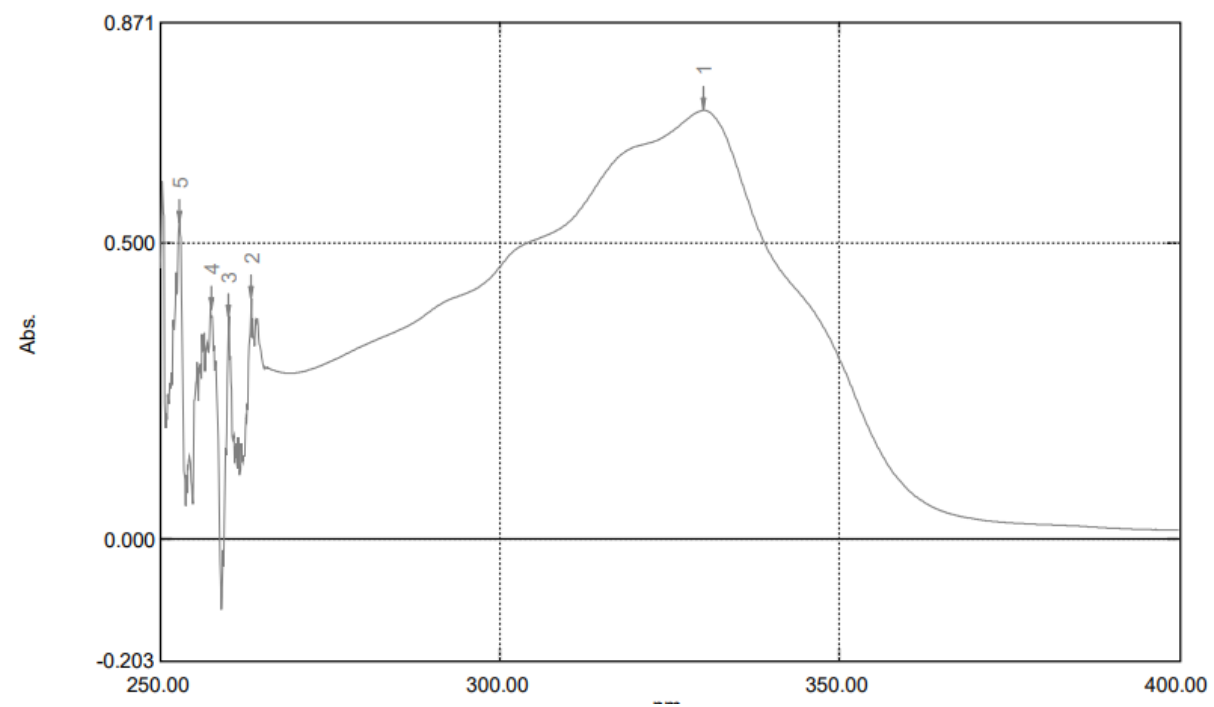
4. HPLC Analysis



5. Mass Spectrometry

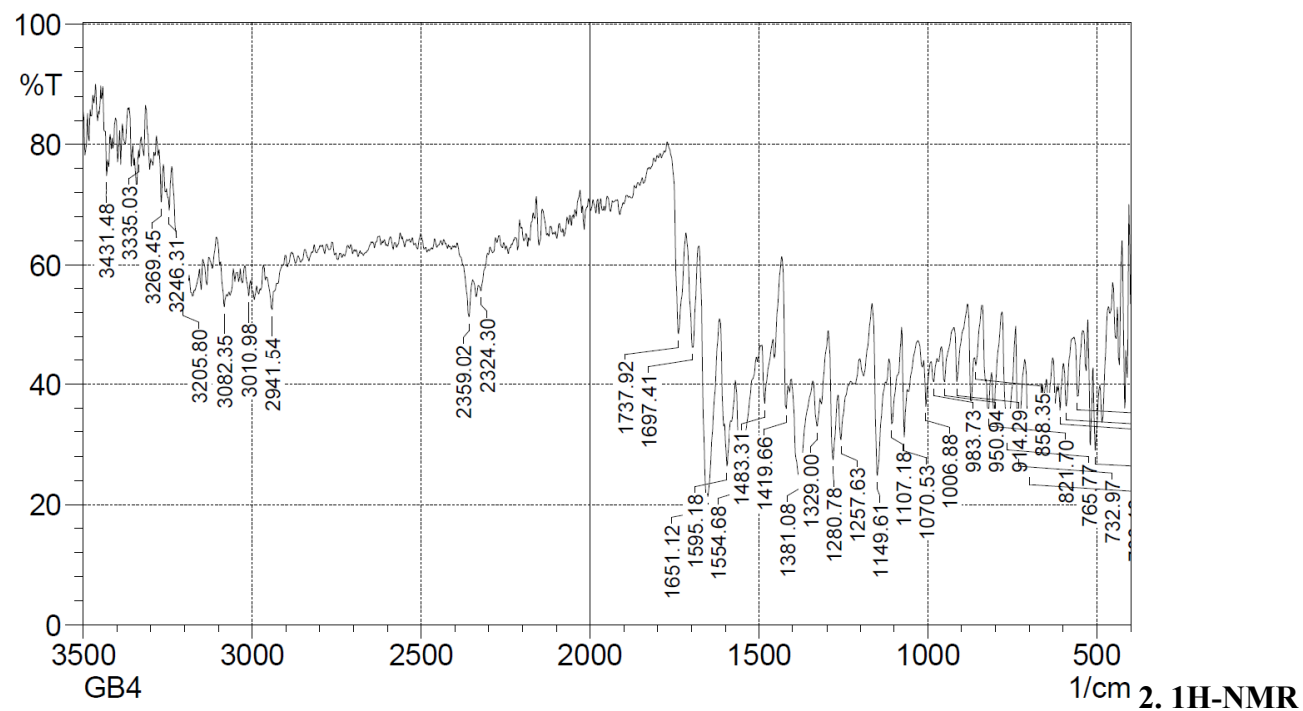


6. UV



2-(5-(4-bromobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-(4-chlorobenzo[d]thiazol-2-yl)acetamide (GB4)

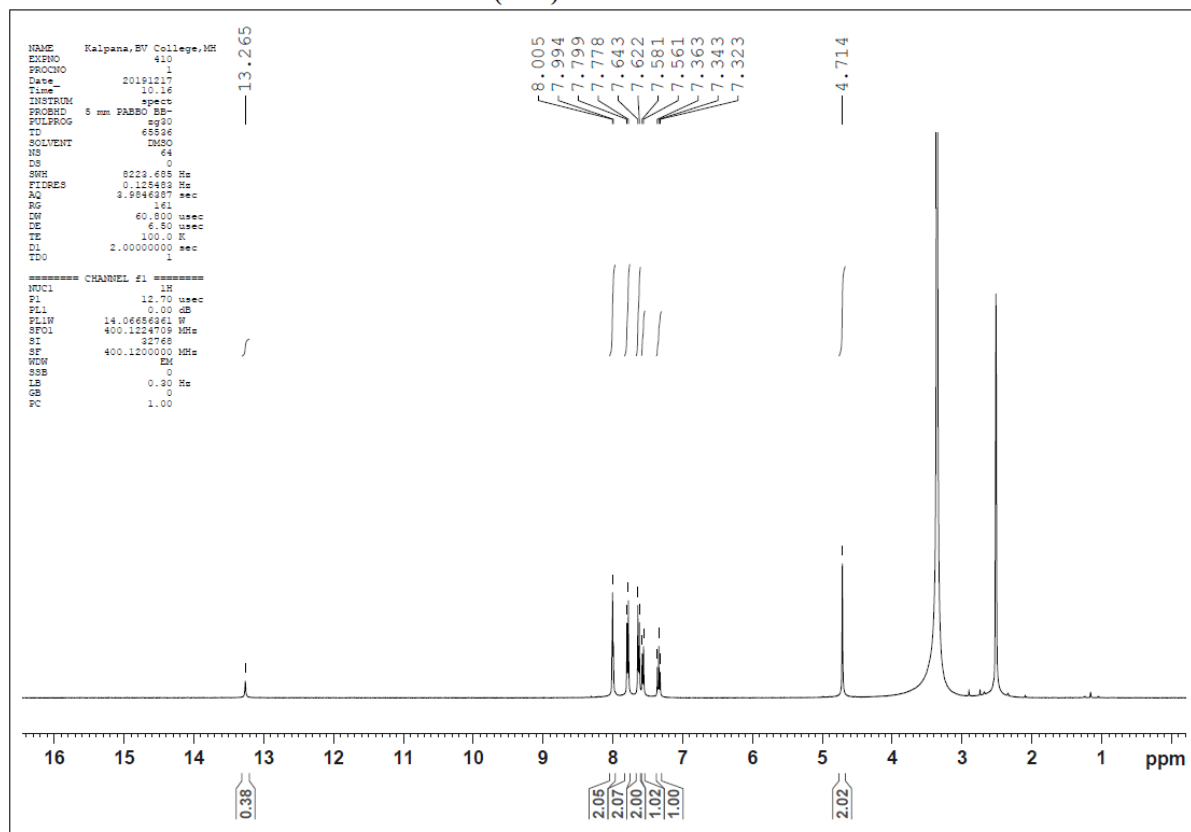
1. FTIR



2. ¹H-NMR

SAIFNM190323A-07(GB4)

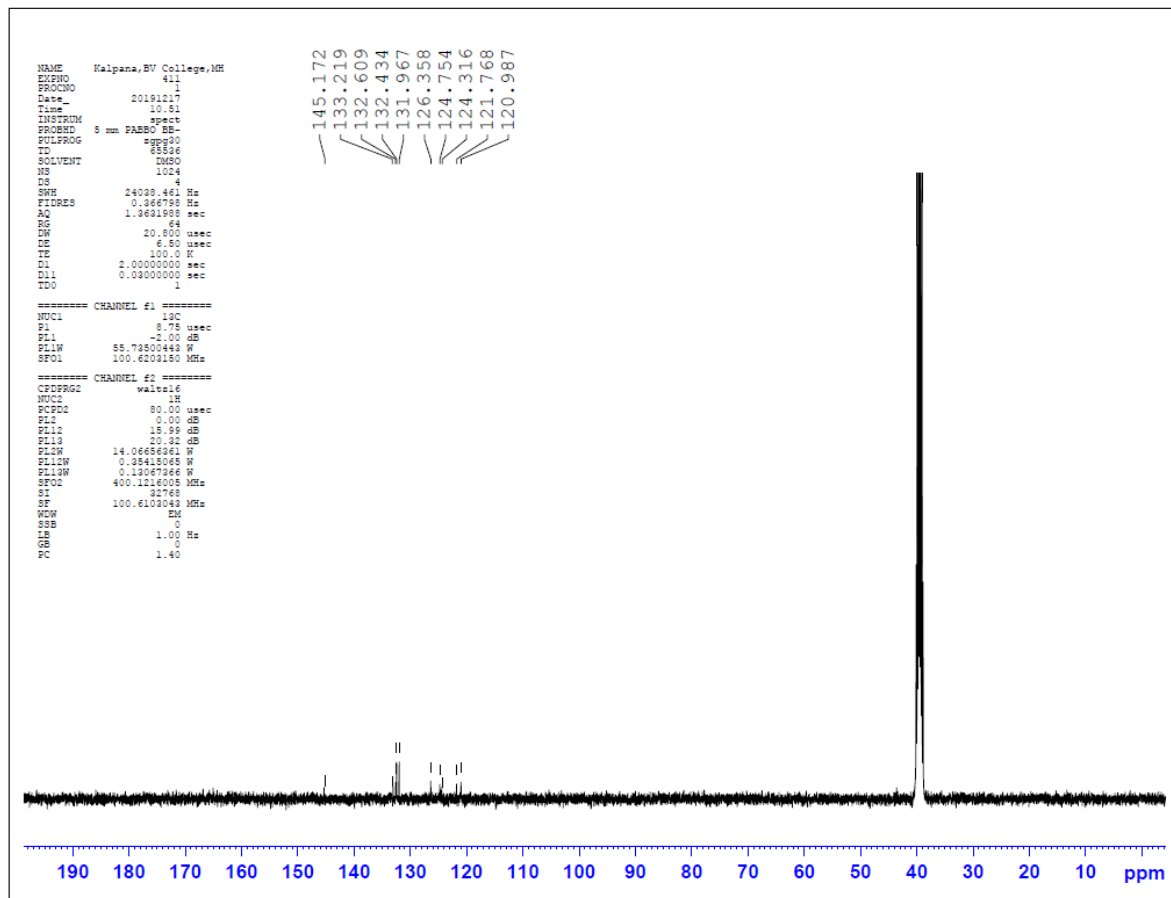
SAIF Cochin



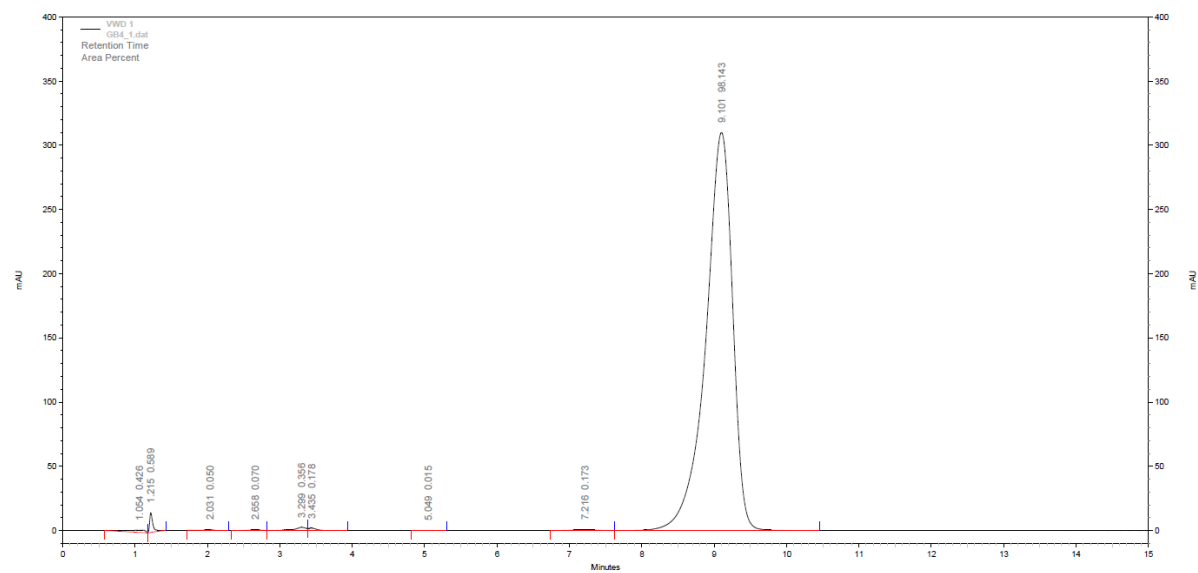
3. 13C-NMR

SAIFNM190323A-08(GB4)

SAIF Cochin

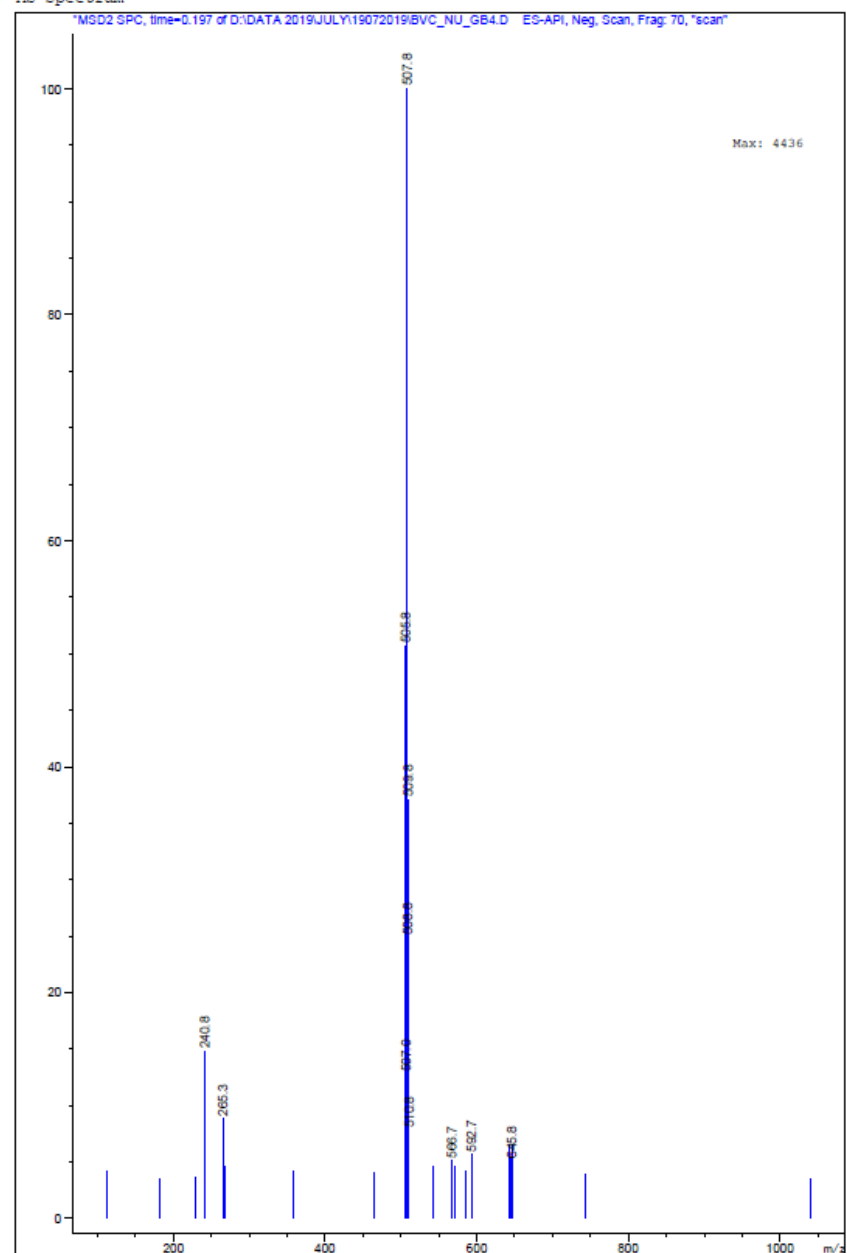


5. HPLC



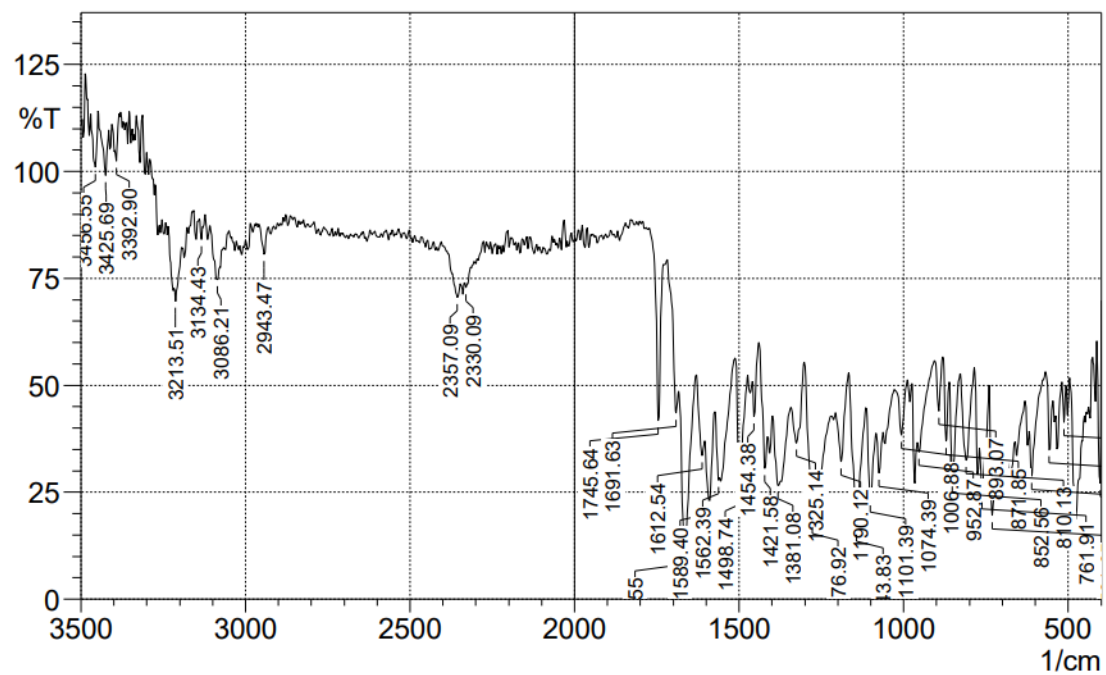
5. Mass

MS Spectrum

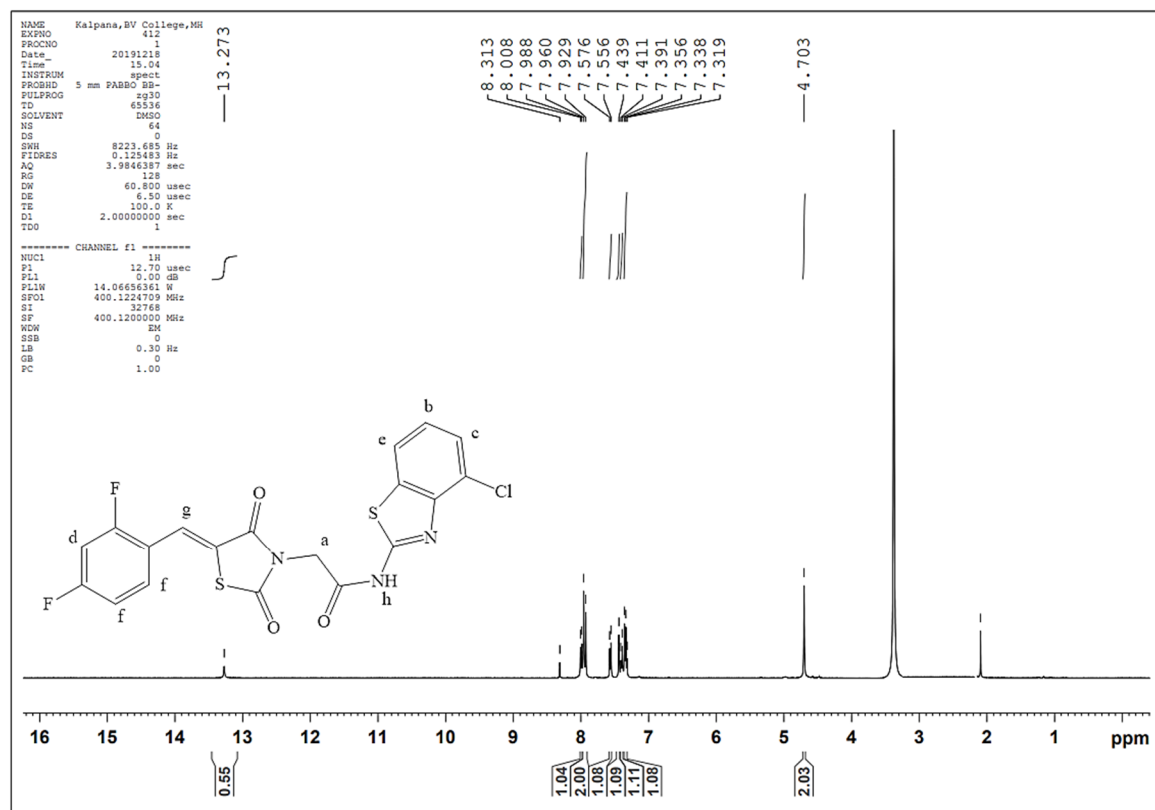


N-(4-chlorobenzo[d]thiazol-2-yl)-2-(5-(2,4-difluorobenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB5)

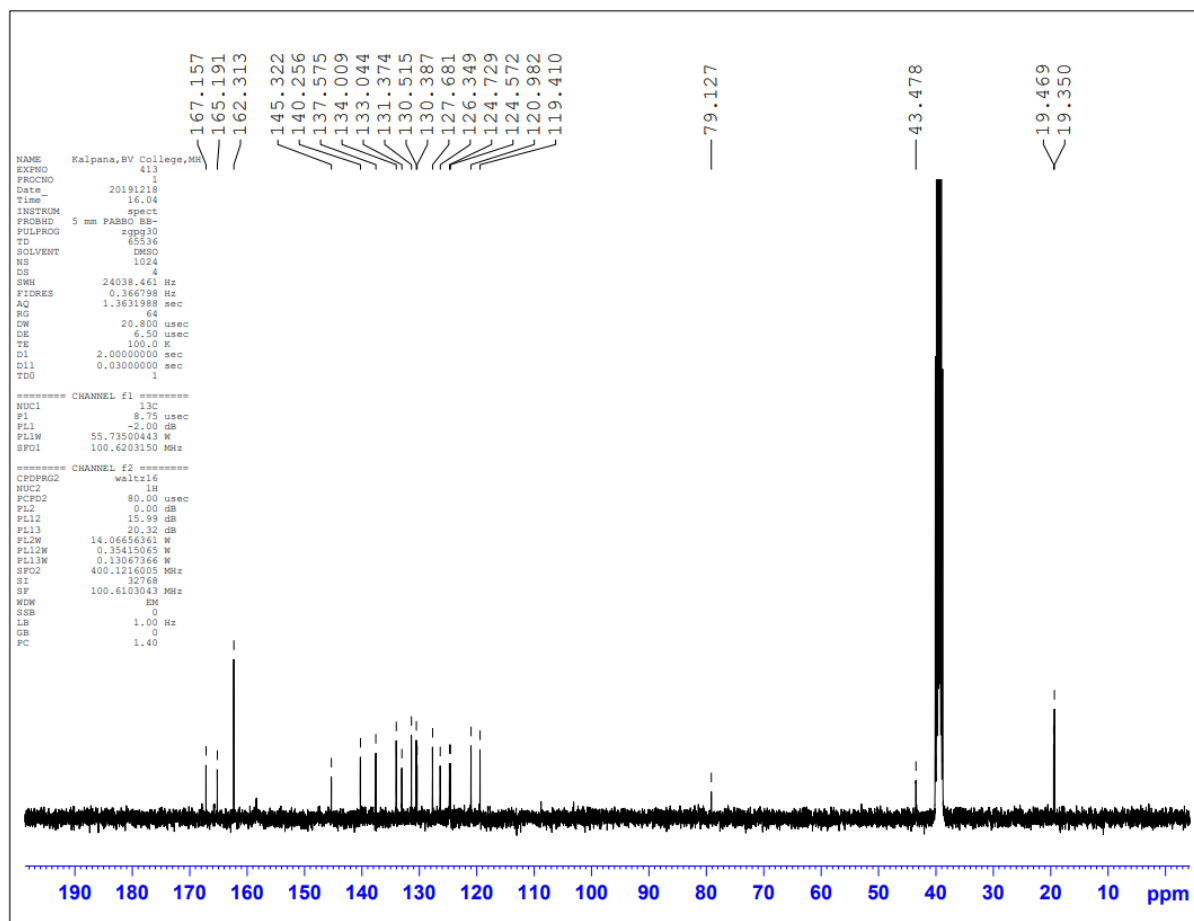
1. FTIR -



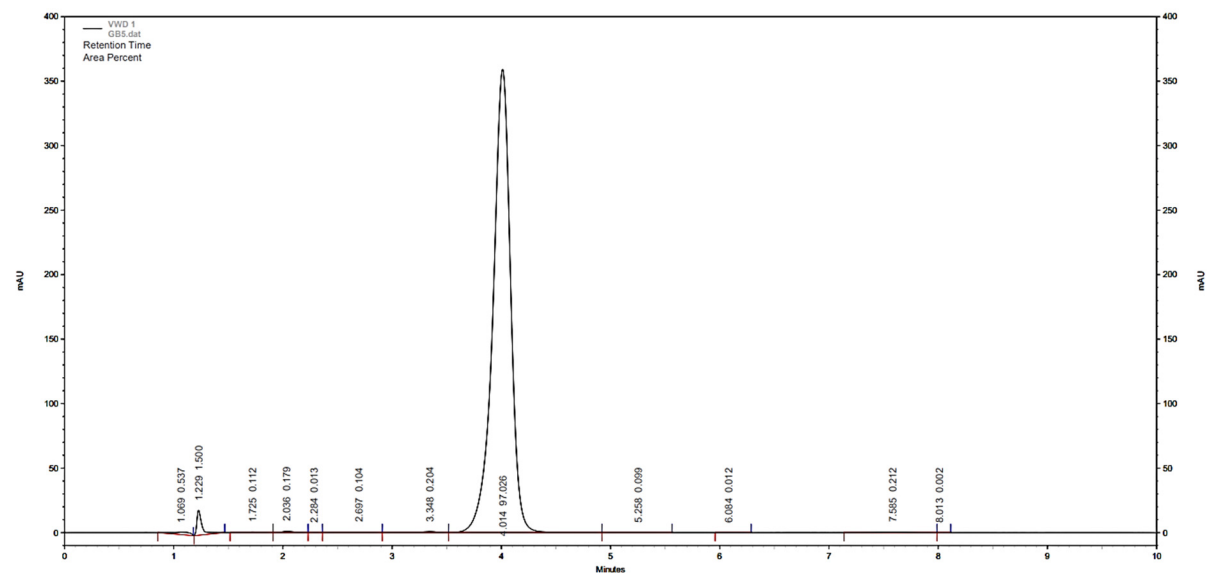
2. ¹H-NMR



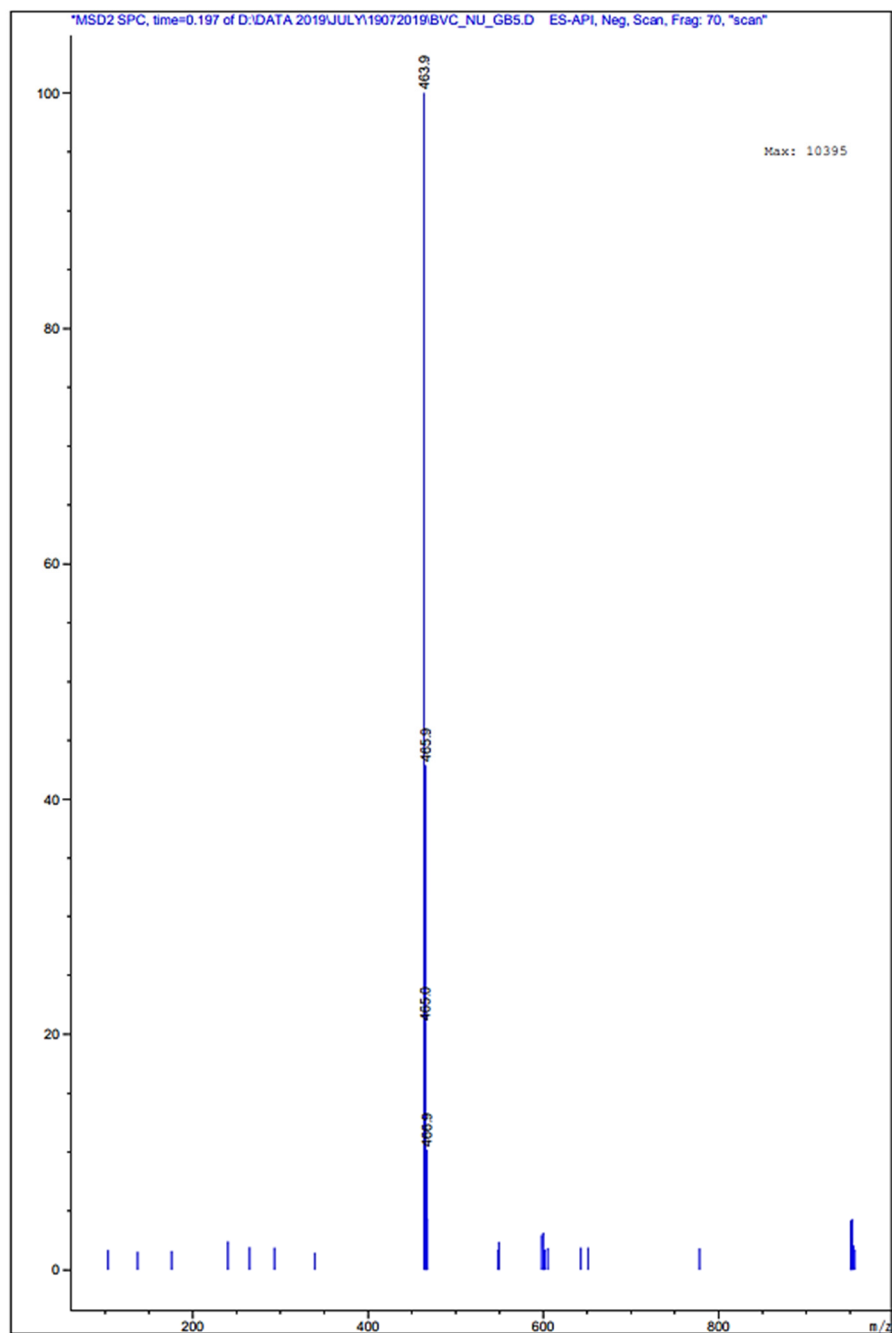
3. ¹³C-NMR



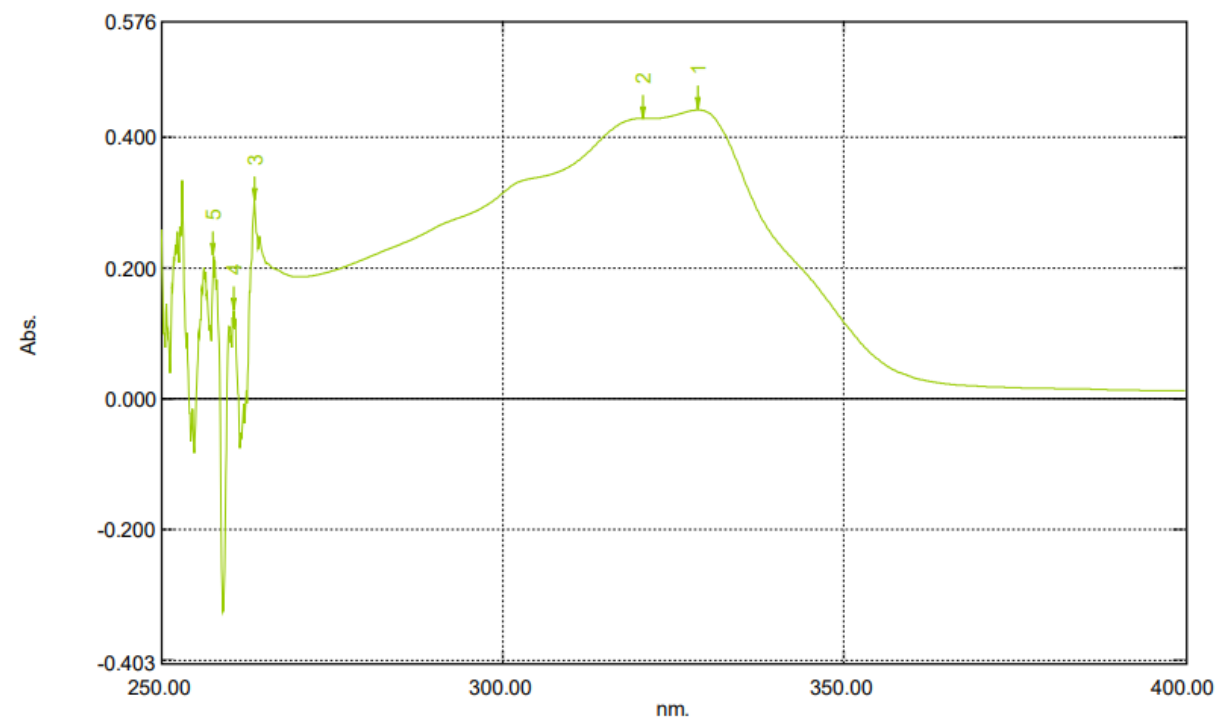
4. HPLC



5. Mass Spectrometry

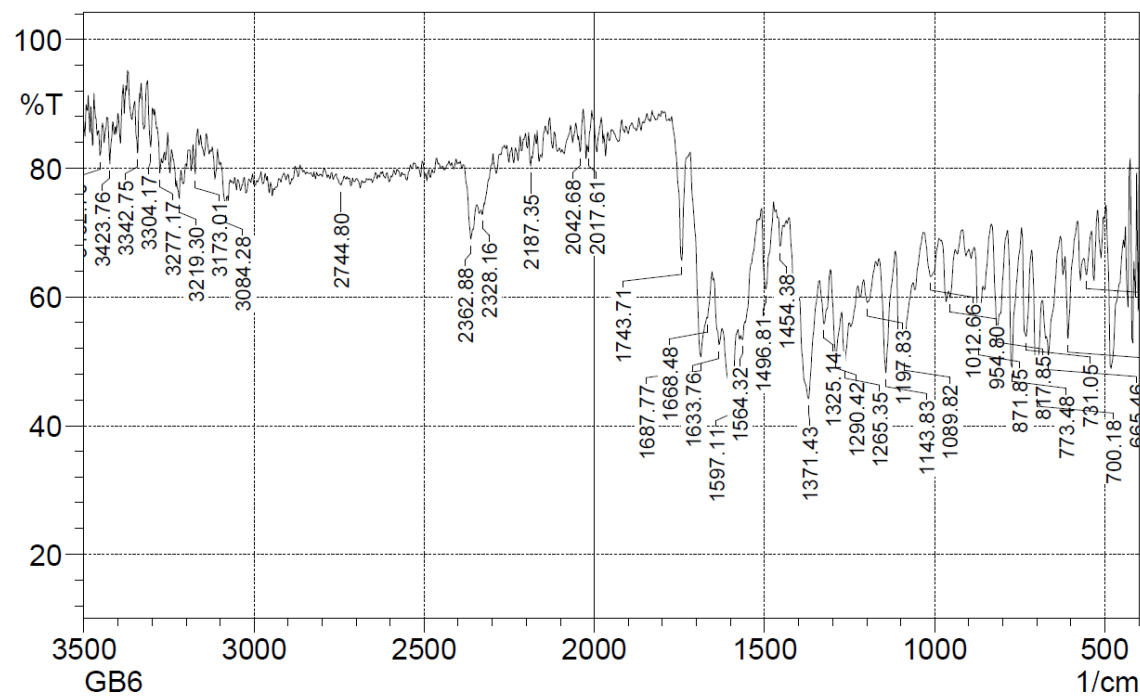


6. UV



N-(4-chlorobenzo[d]thiazol-2-yl)-2-(5-(3,4-dimethylbenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB6)

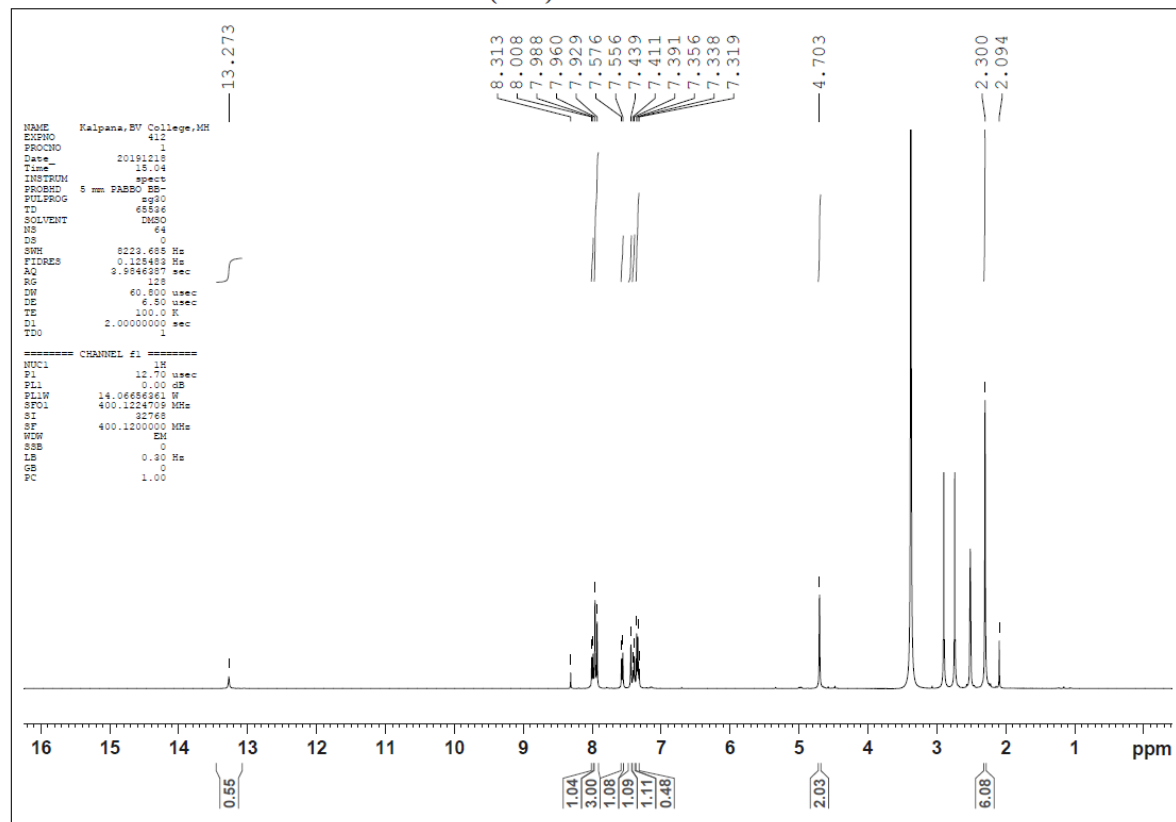
1. FTIR



2. 1H-NMR

SAIFNM190323A-09(GB6)

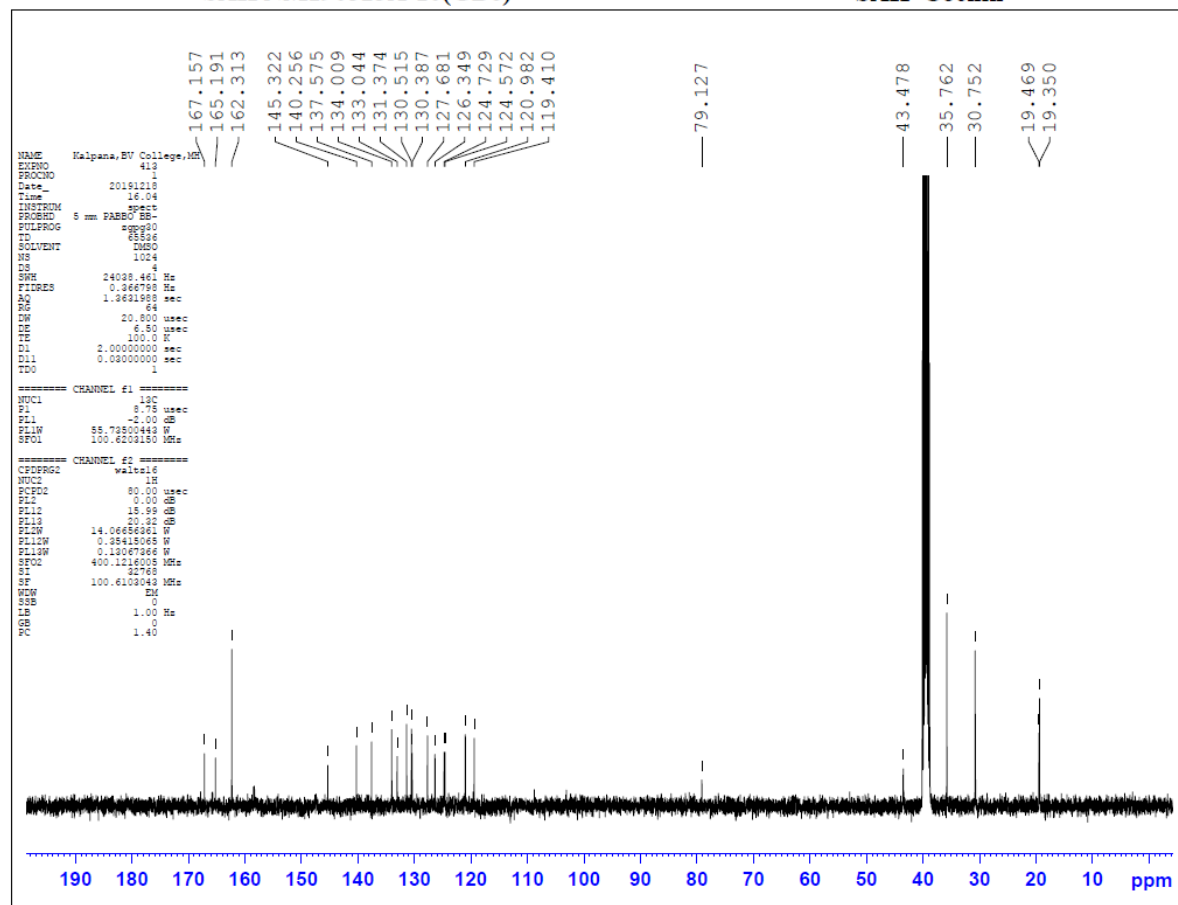
SAIF Cochin



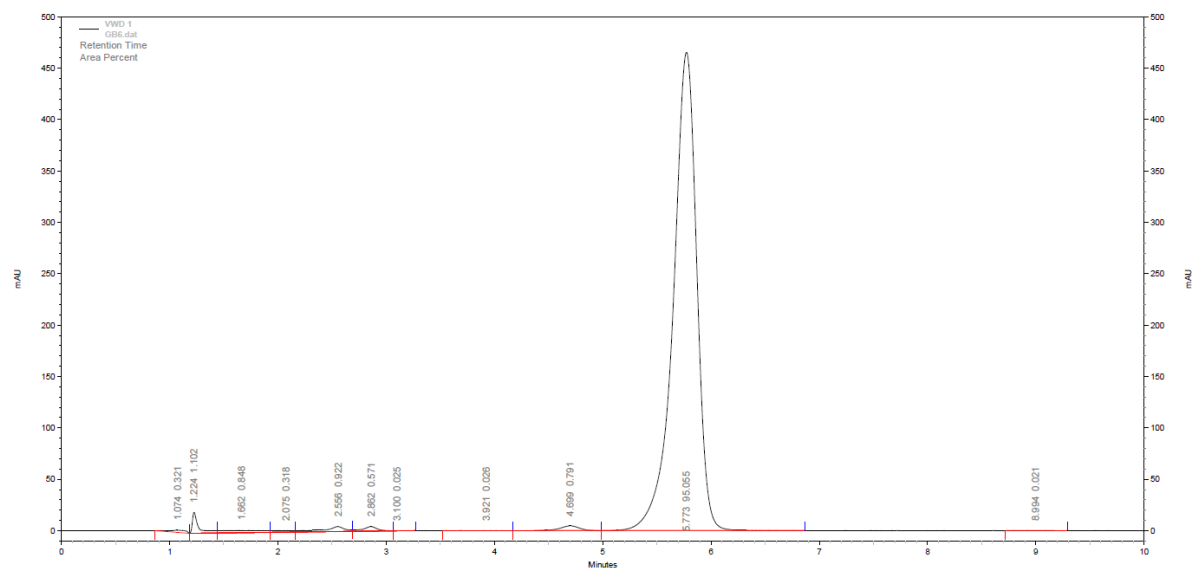
3. 13C-NMR

SAIFNM190323A-10(GB6)

SAIF Cochlin

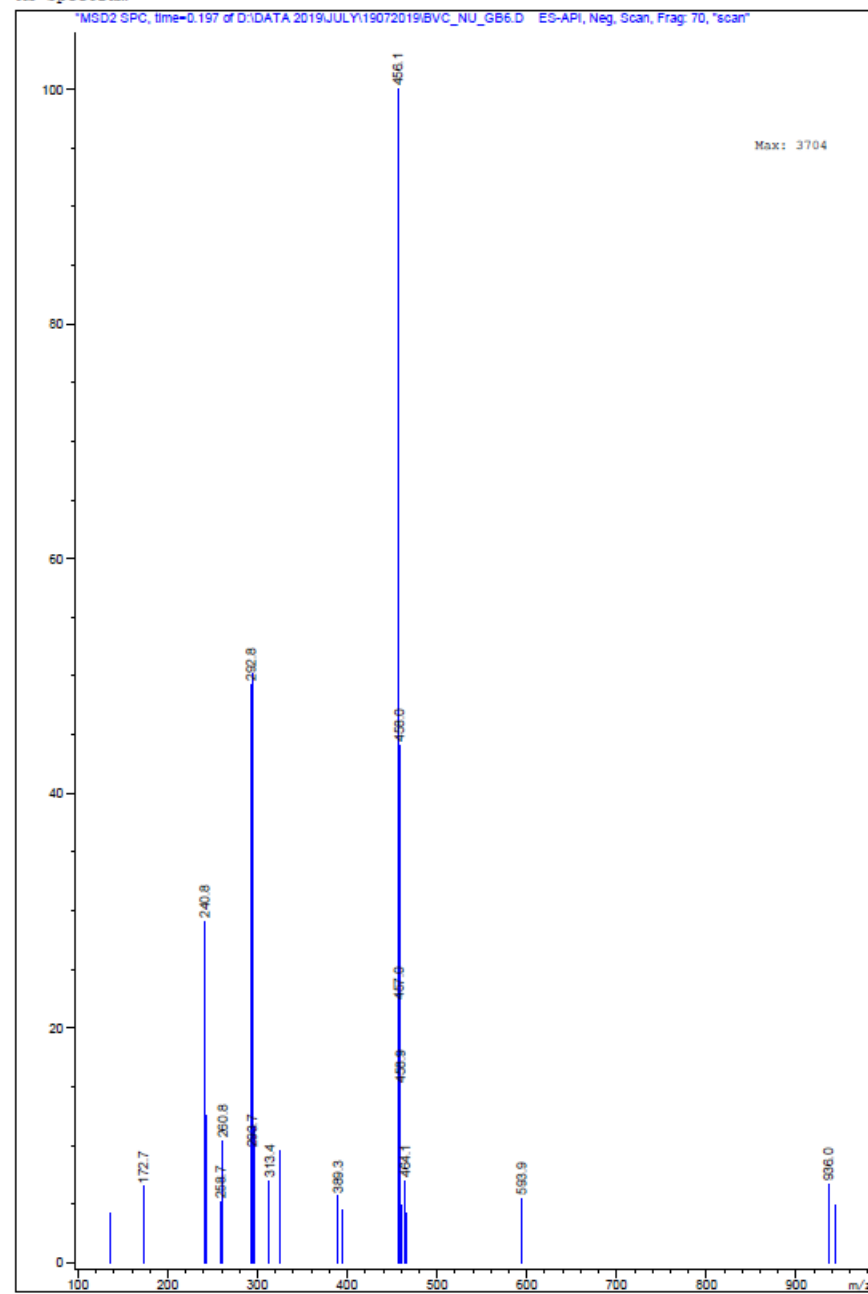


4. HPLC



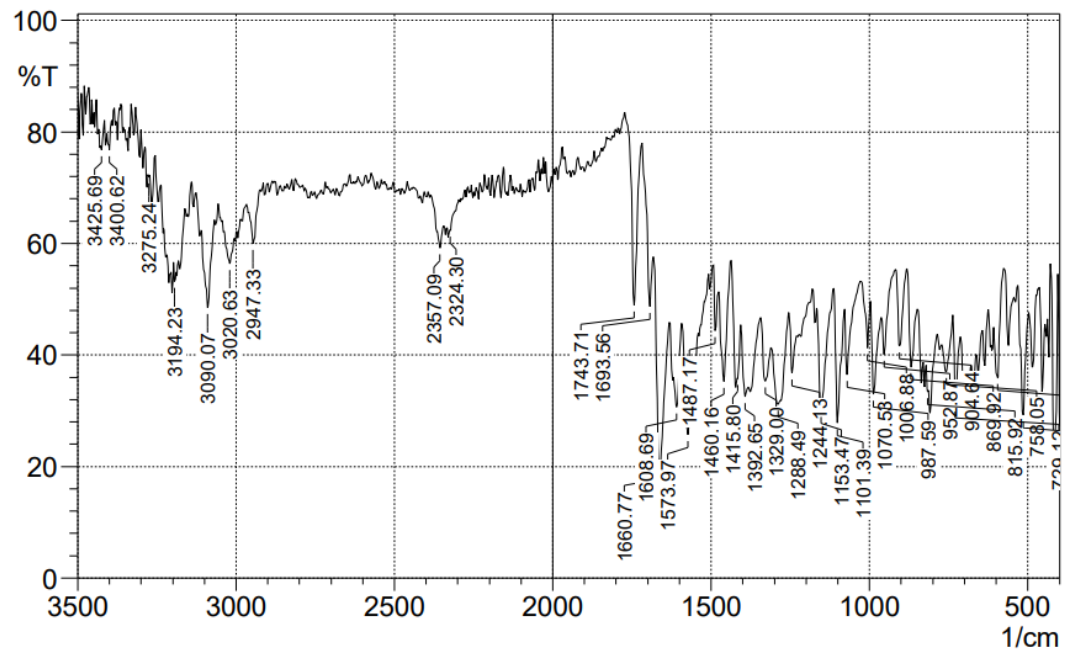
5. Mass

MS Spectrum

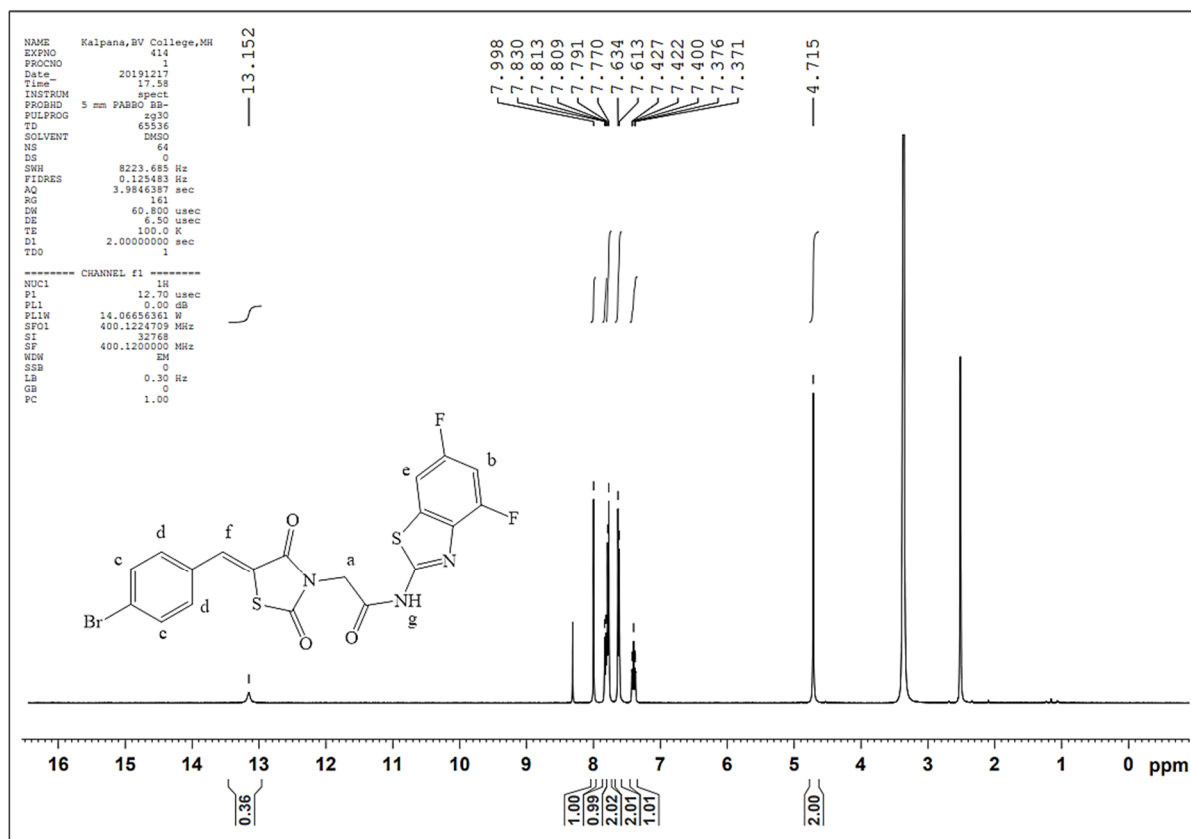


2-(5-(4-bromobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-(4,6-difluorobenzo[d]thiazol-2-yl)acetamide (GB7)

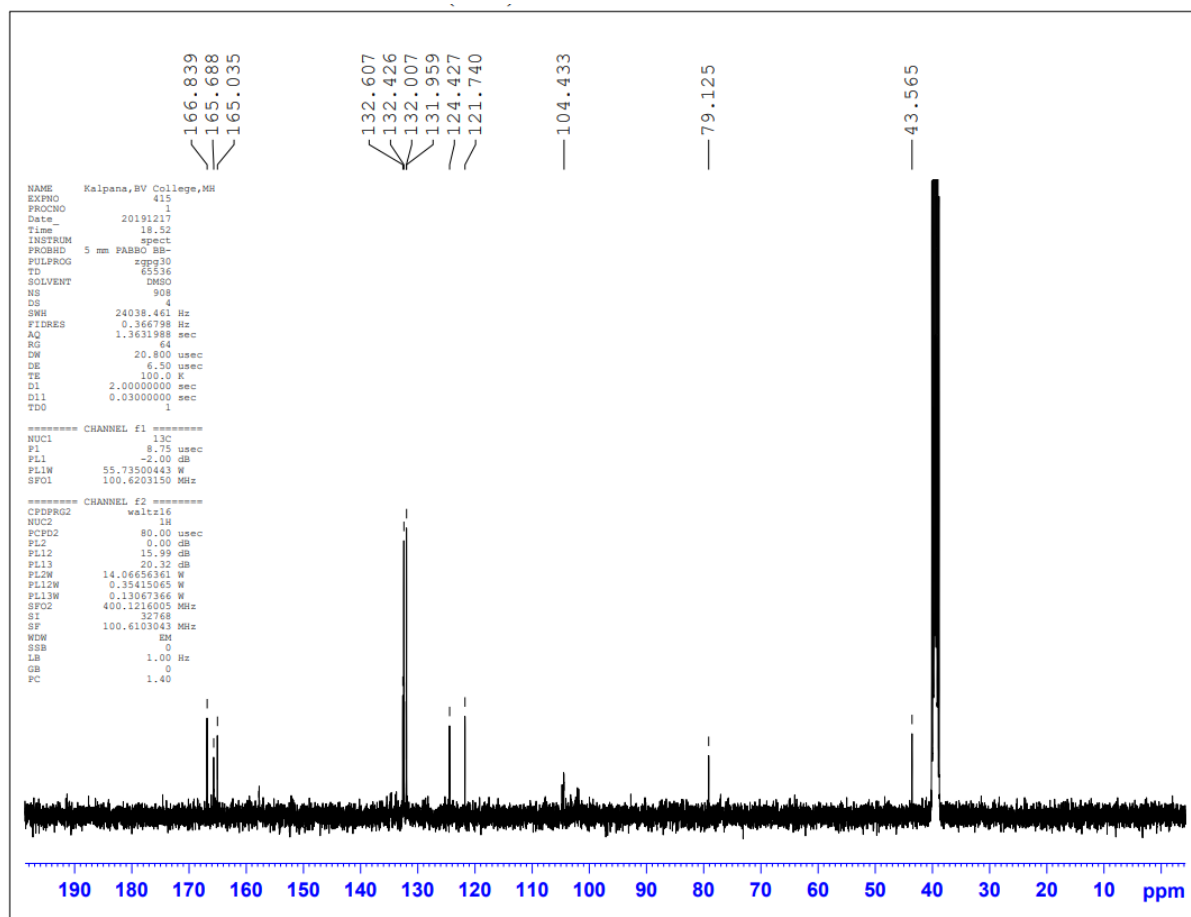
1. FTIR –



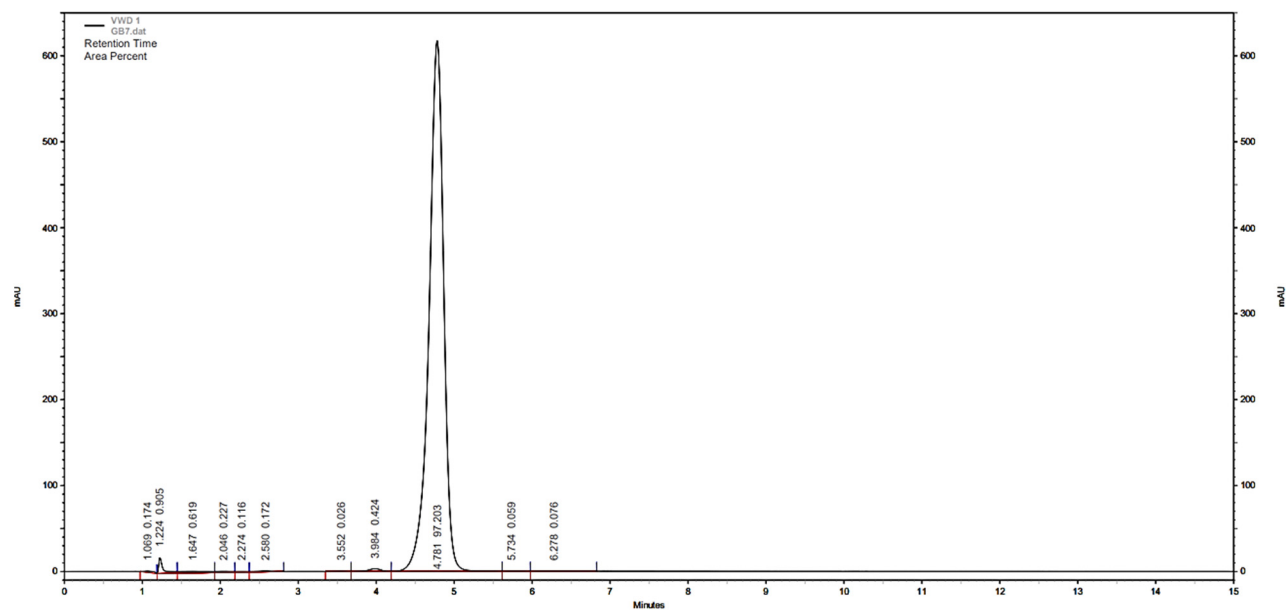
2. ¹H-NMR



3. ¹³C-NMR

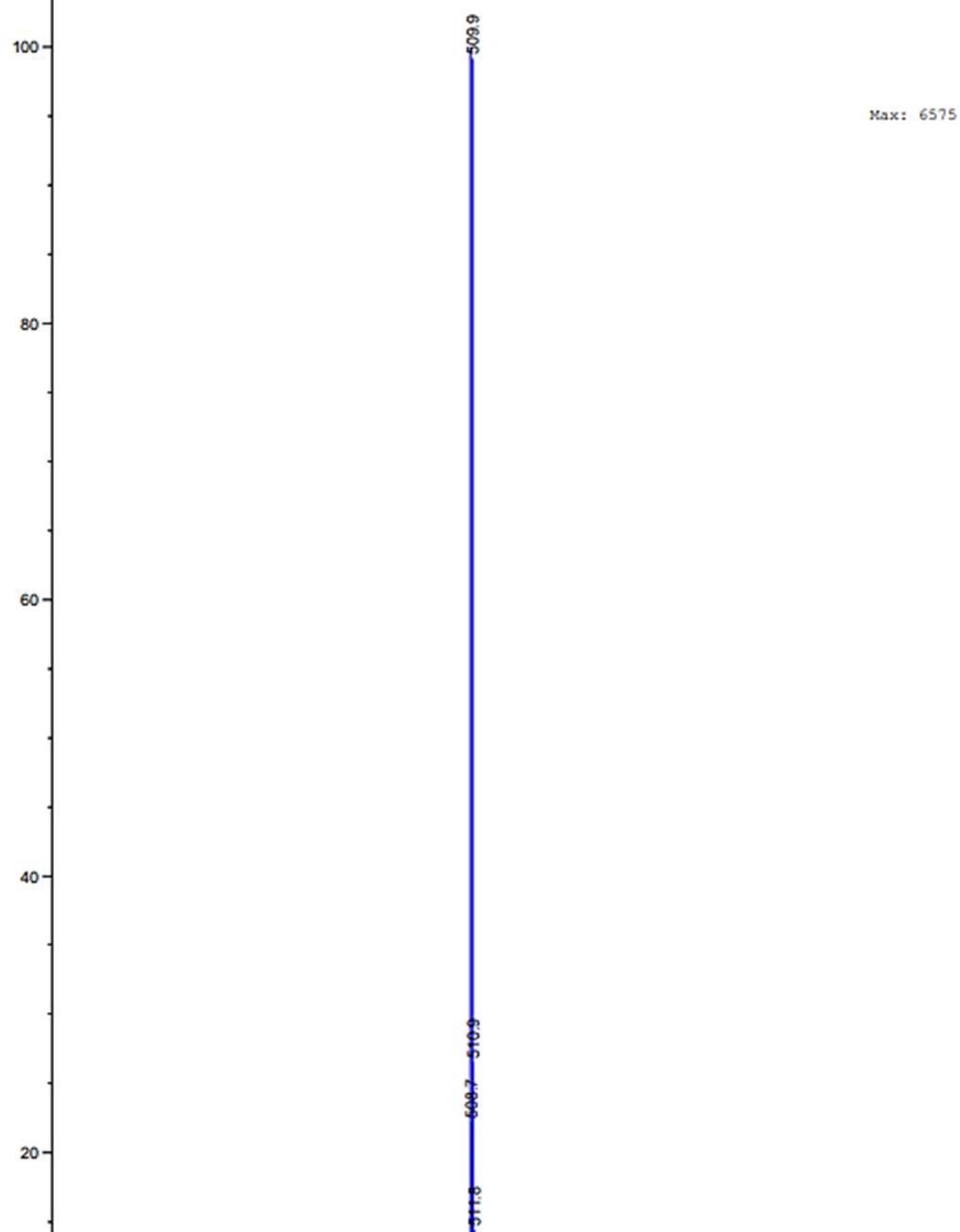


4. HPLC Analysis

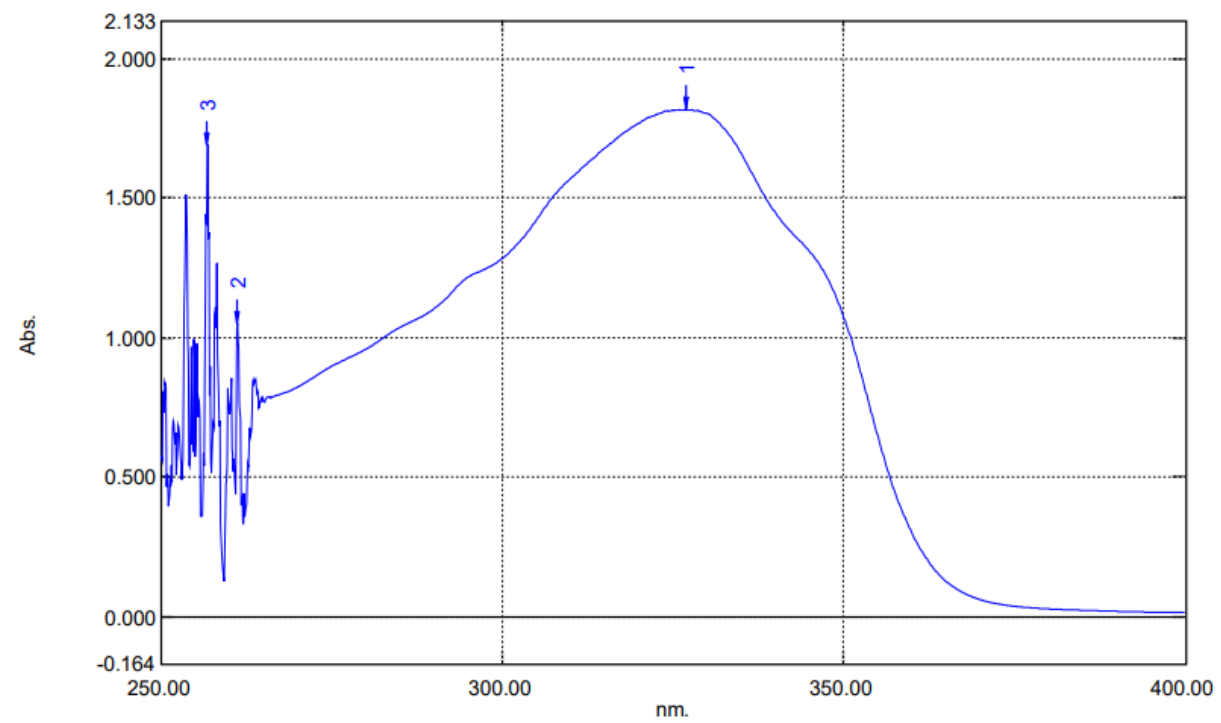


5. Mass Spectrometry

*MSD2 SPC, time=0.169 of D:\DATA 2019\JULY\19072019\BVC_NU_GB7.D ES-API, Neg, Scan, Frag: 70, "scan"

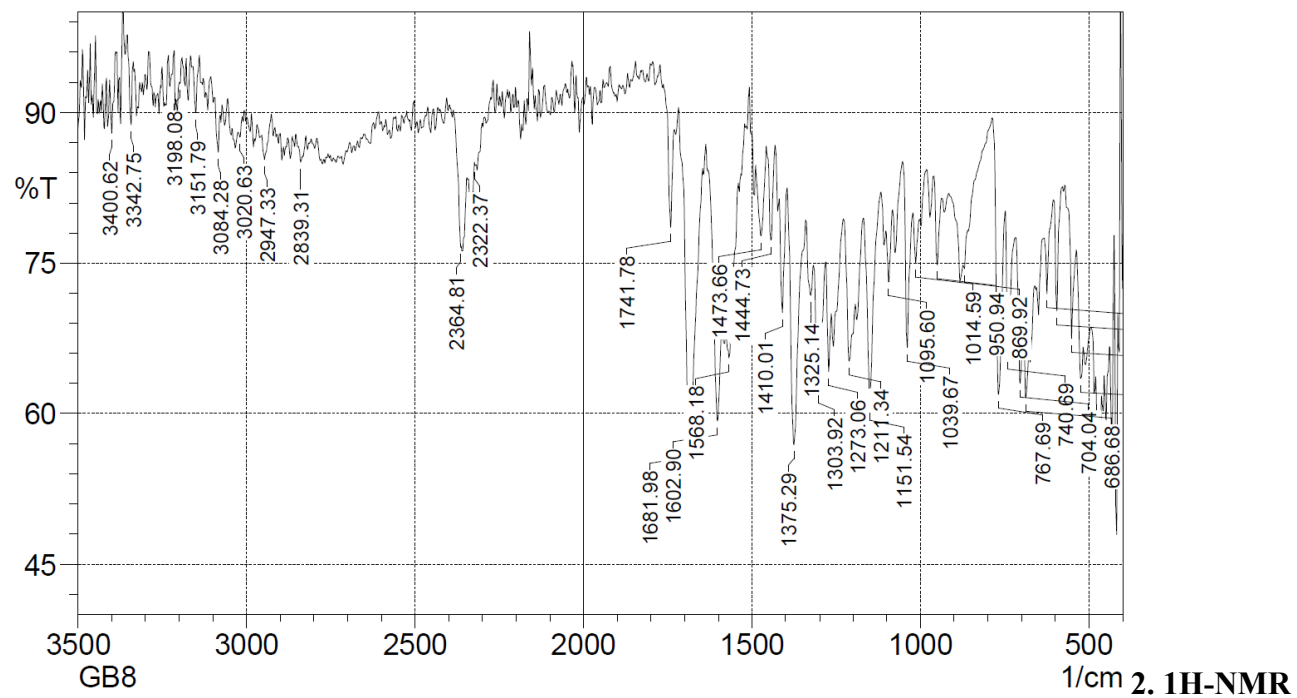


6. UV



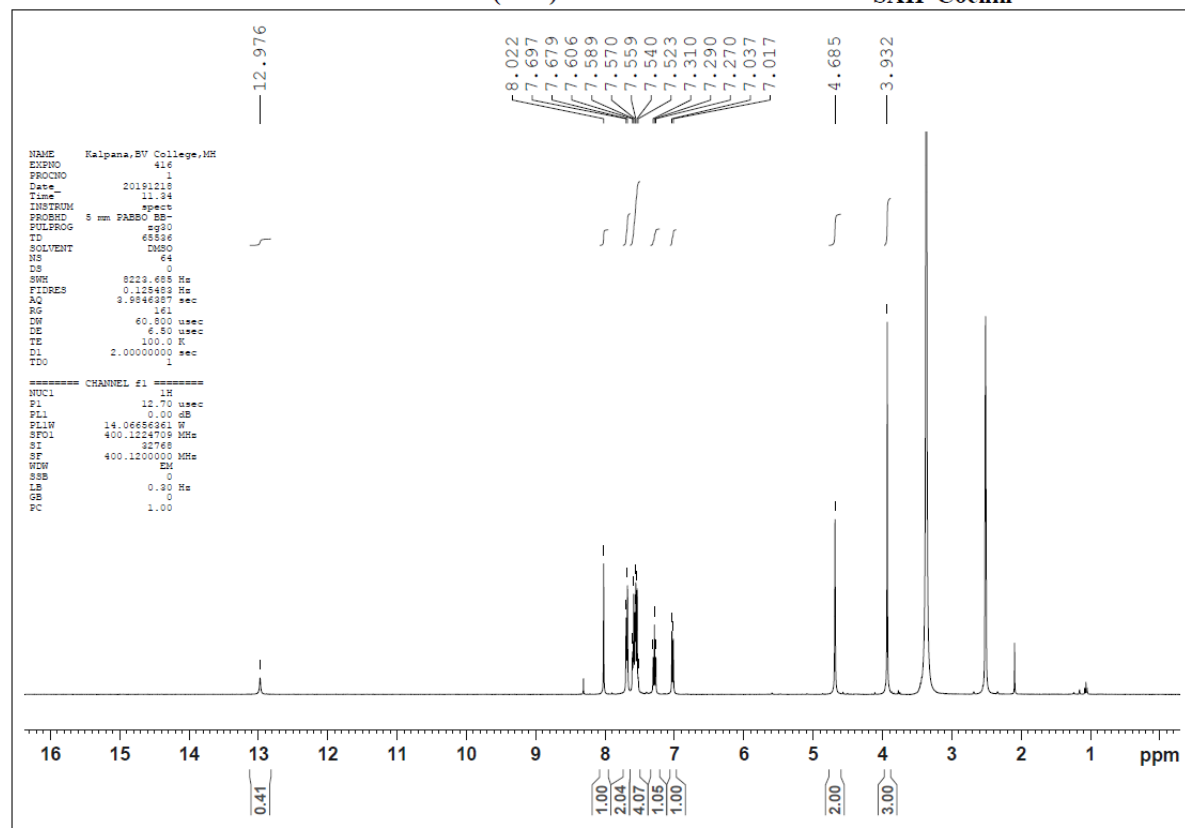
2-(5-benzylidene-2,4-dioxothiazolidin-3-yl)-N-(4-methoxybenzo[d]thiazol-2-yl)acetamide (GB8)

1. FTIR



SAIFNM190323A-13(GB8)

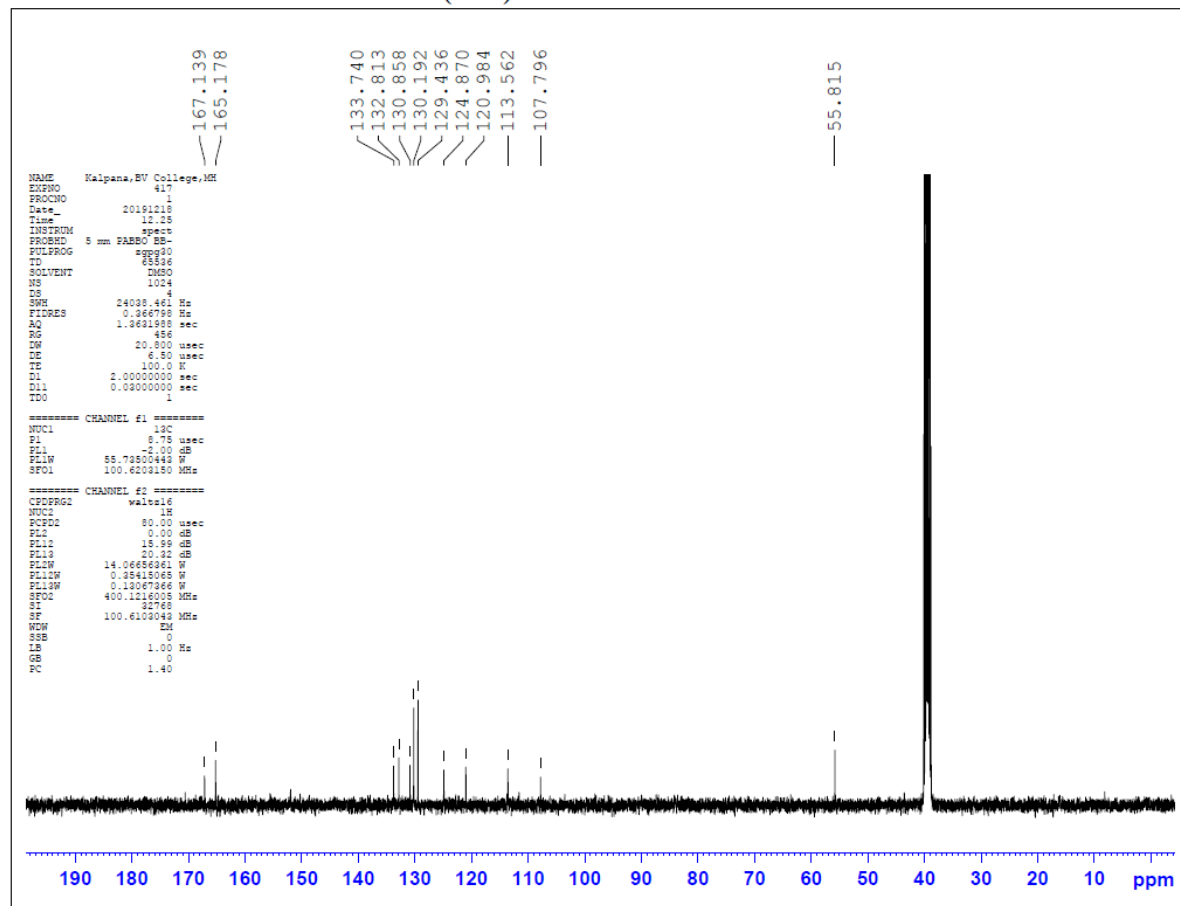
SAIF Cochin



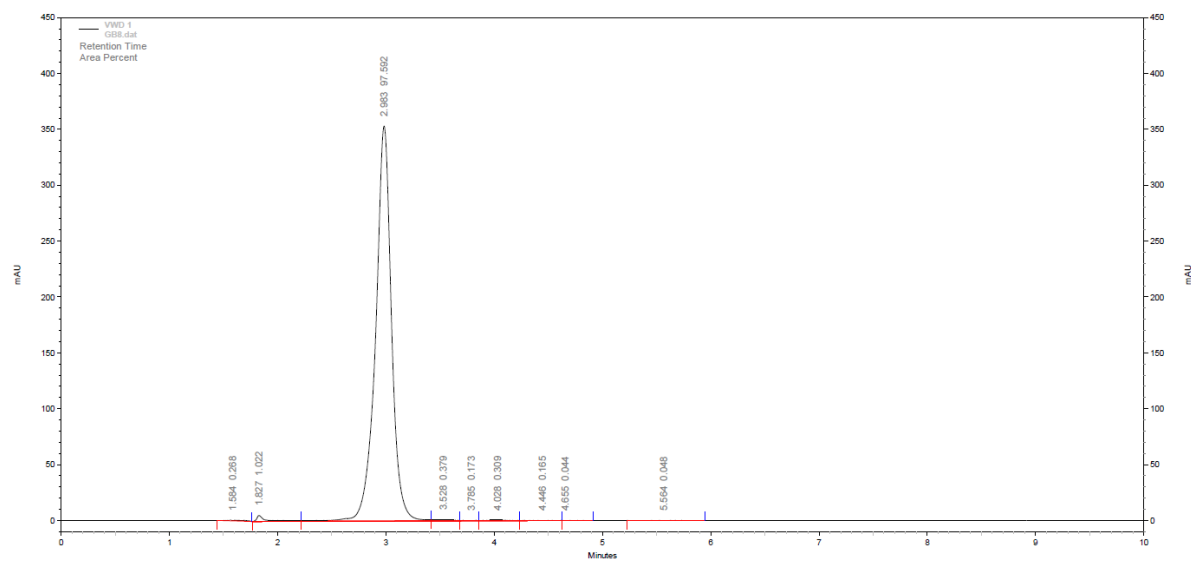
3. 13C-NMR

SAIFNM190323A-14(GB8)

SAIF Cochin

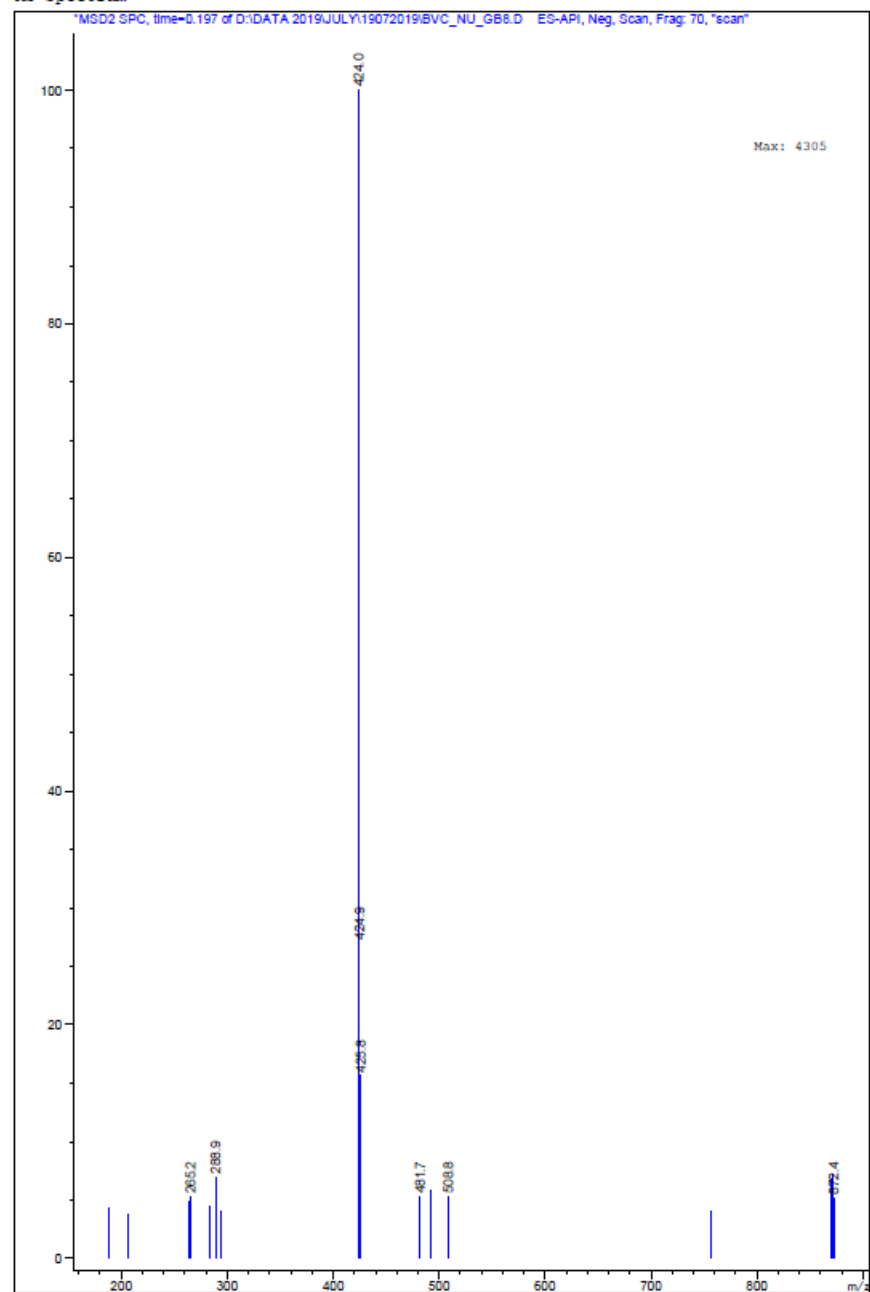


4. HPLC



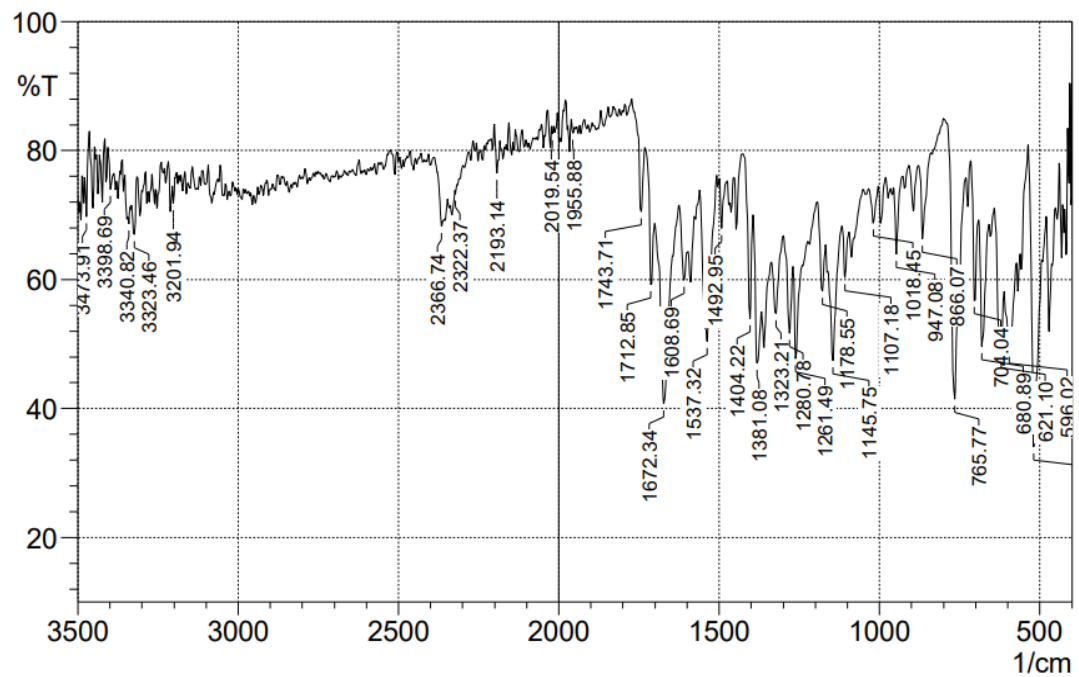
4. Mass

MS Spectrum

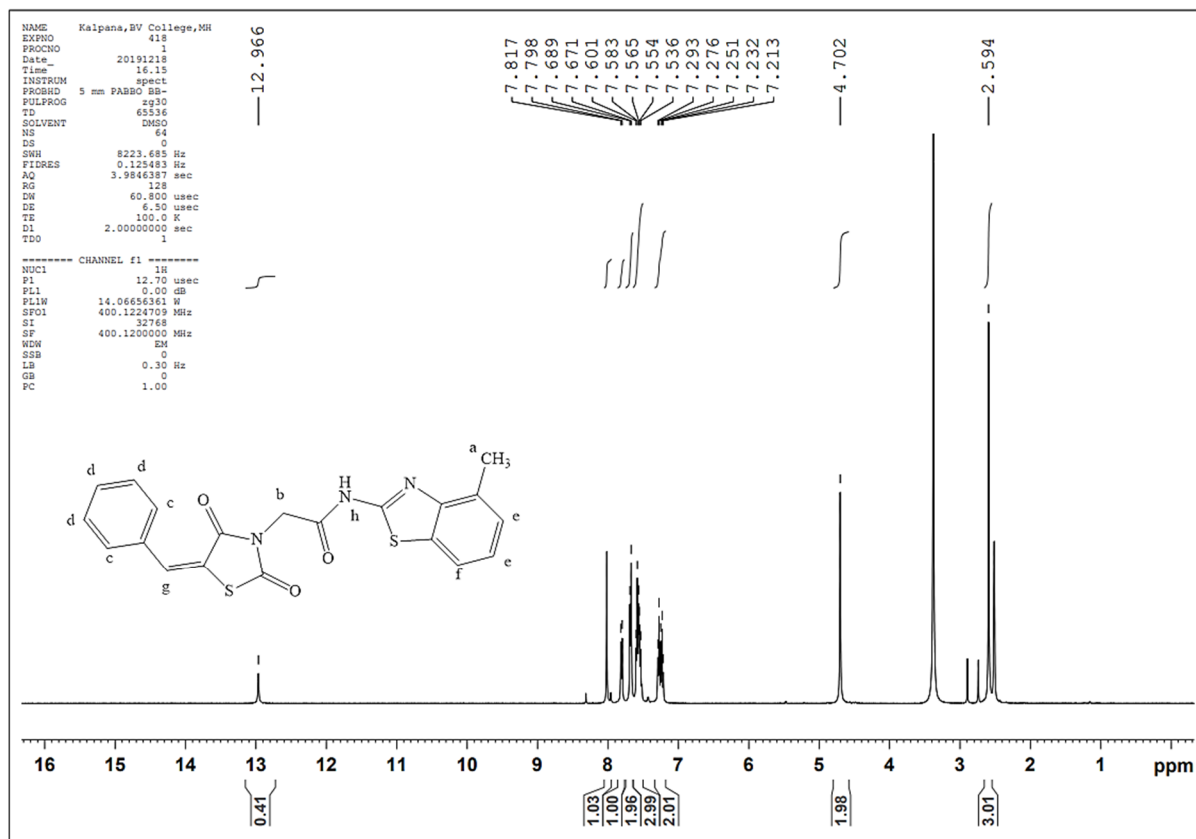


2-(5-benzylidene-2,4-dioxothiazolidin-3-yl)-N-(4-methylbenzo[d]thiazol-2-yl)acetamide (GB9)

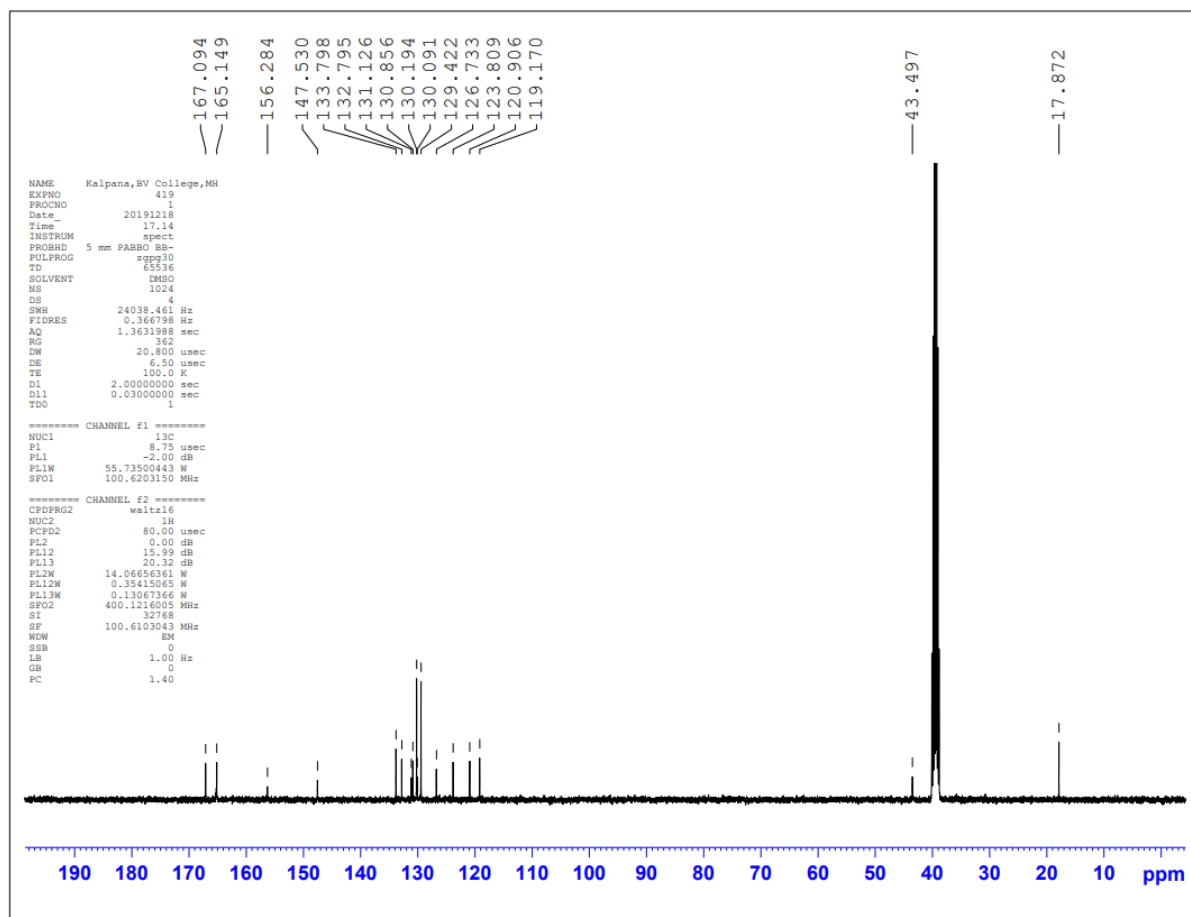
1. FTIR –



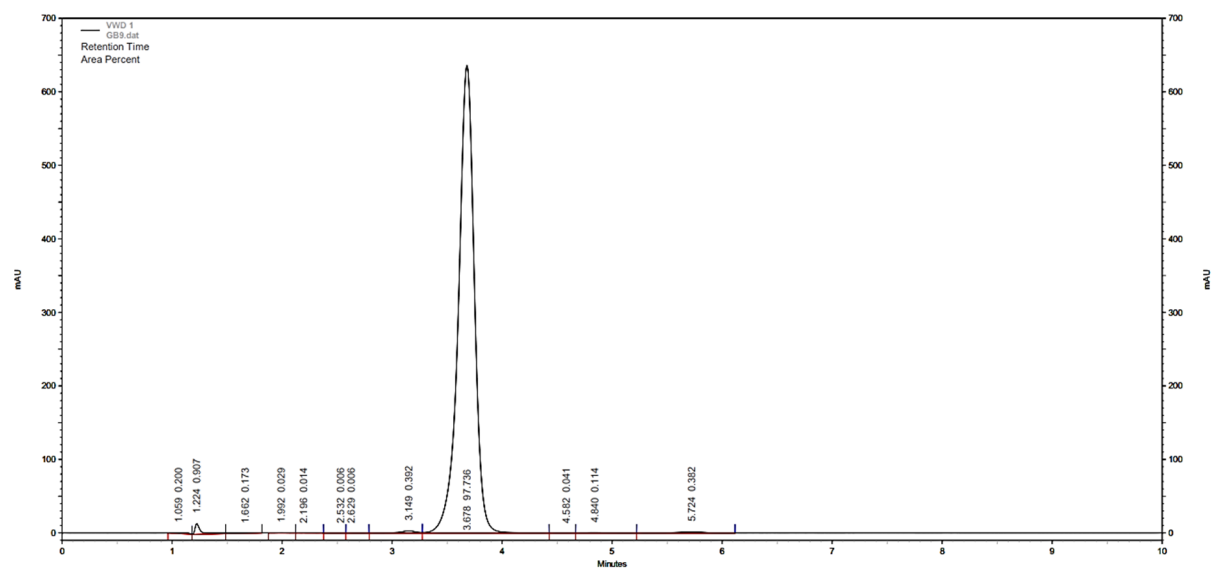
2. ¹H-NMR



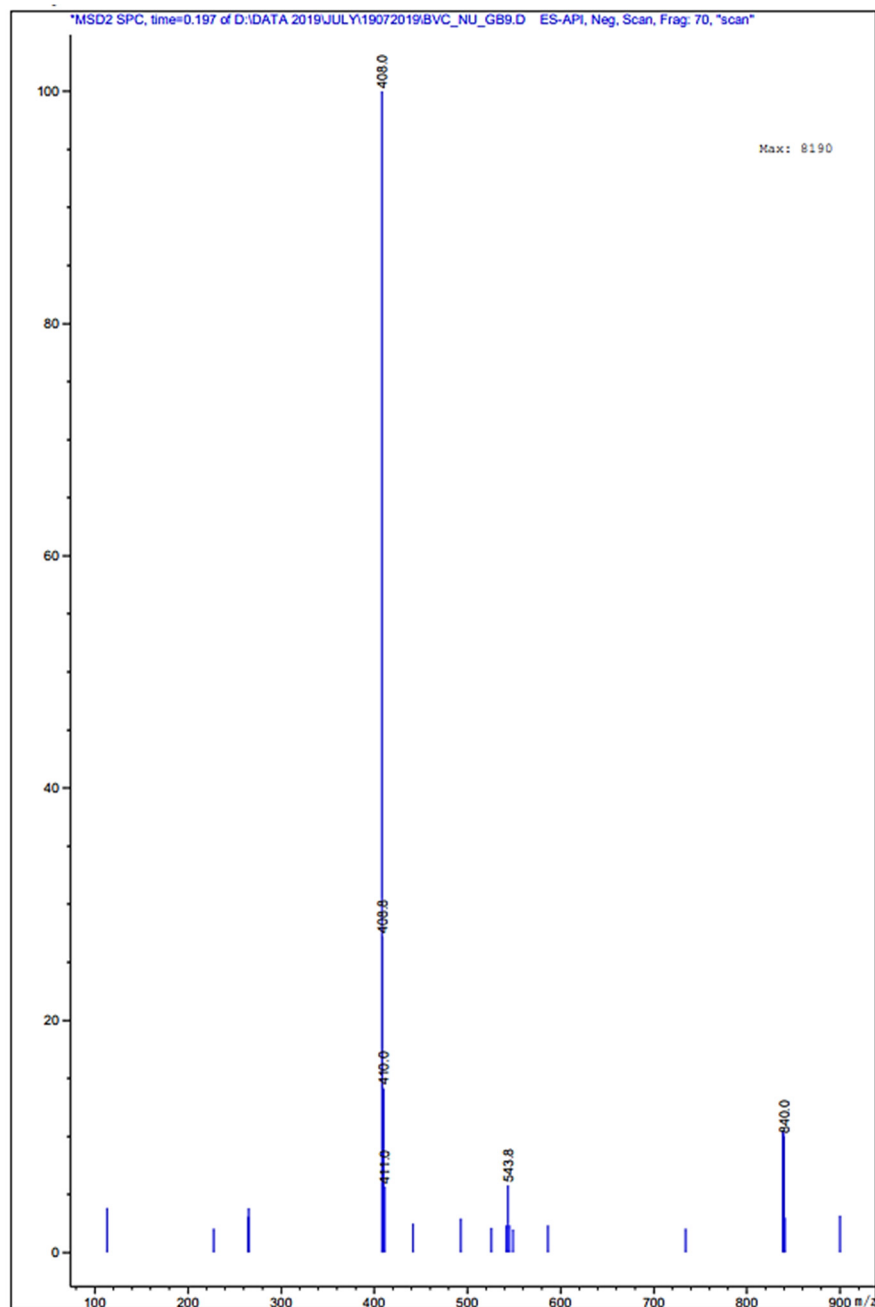
3. ¹³C-NMR



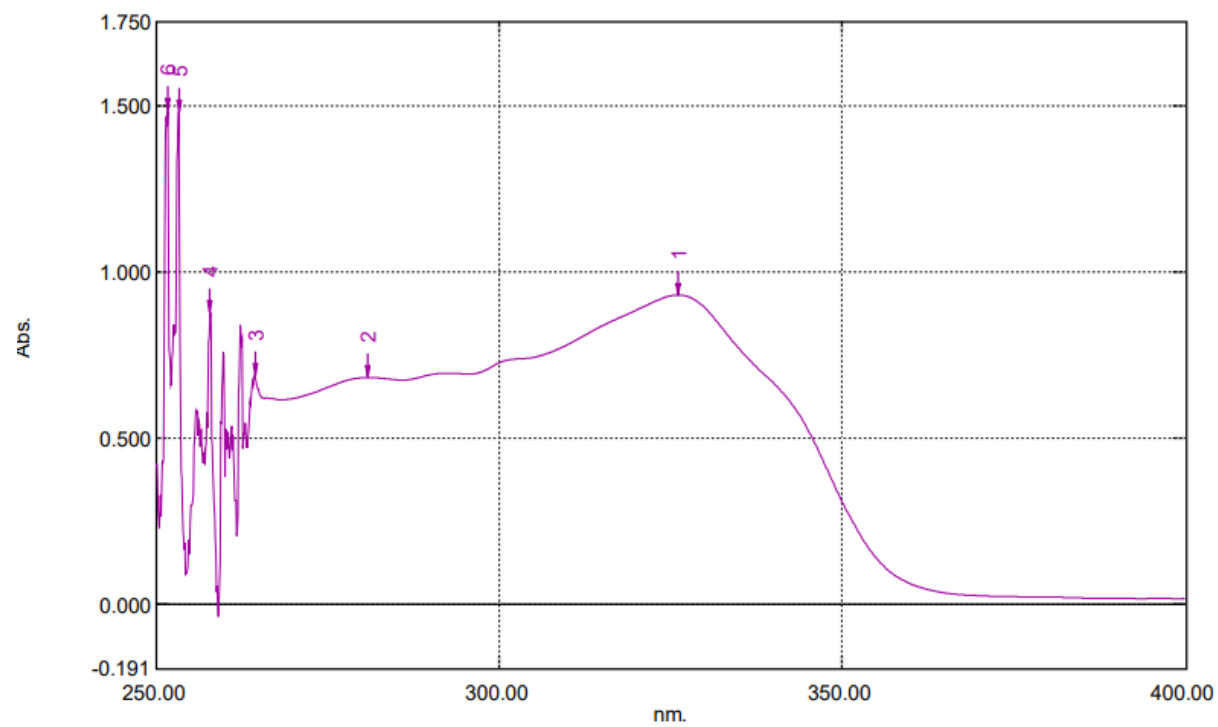
4. HPLC Analysis



5. Mass Spectrometry

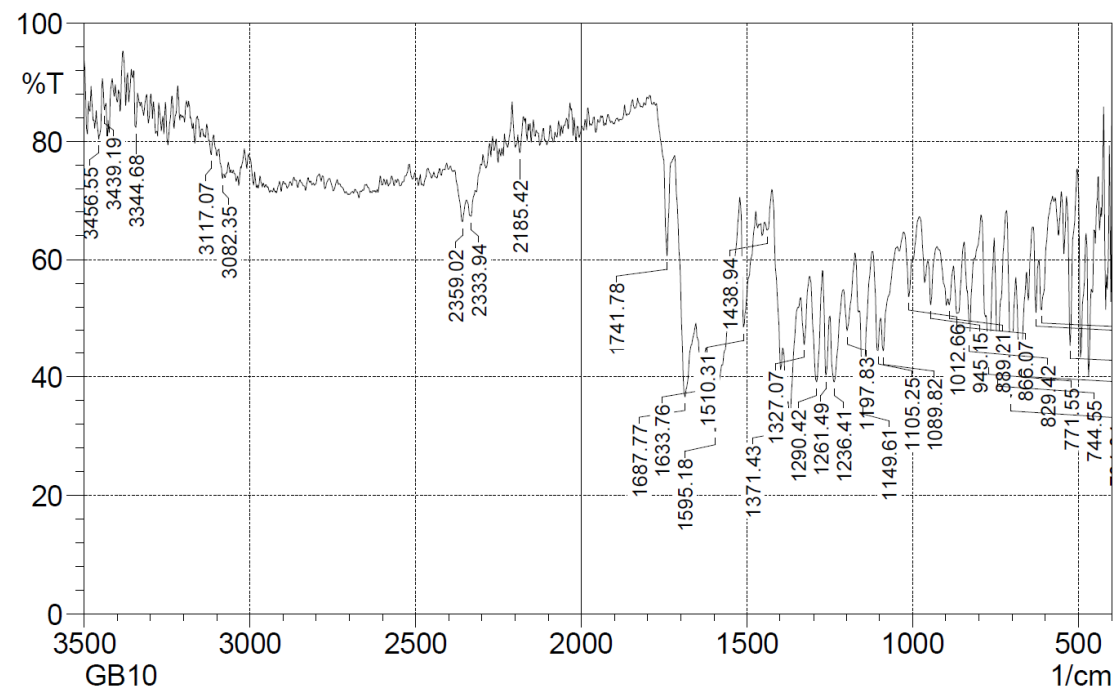


6. UV



2-(5-(4-fluorobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-(4-methylbenzo[d]thiazol-2-yl)acetamide (GB10)

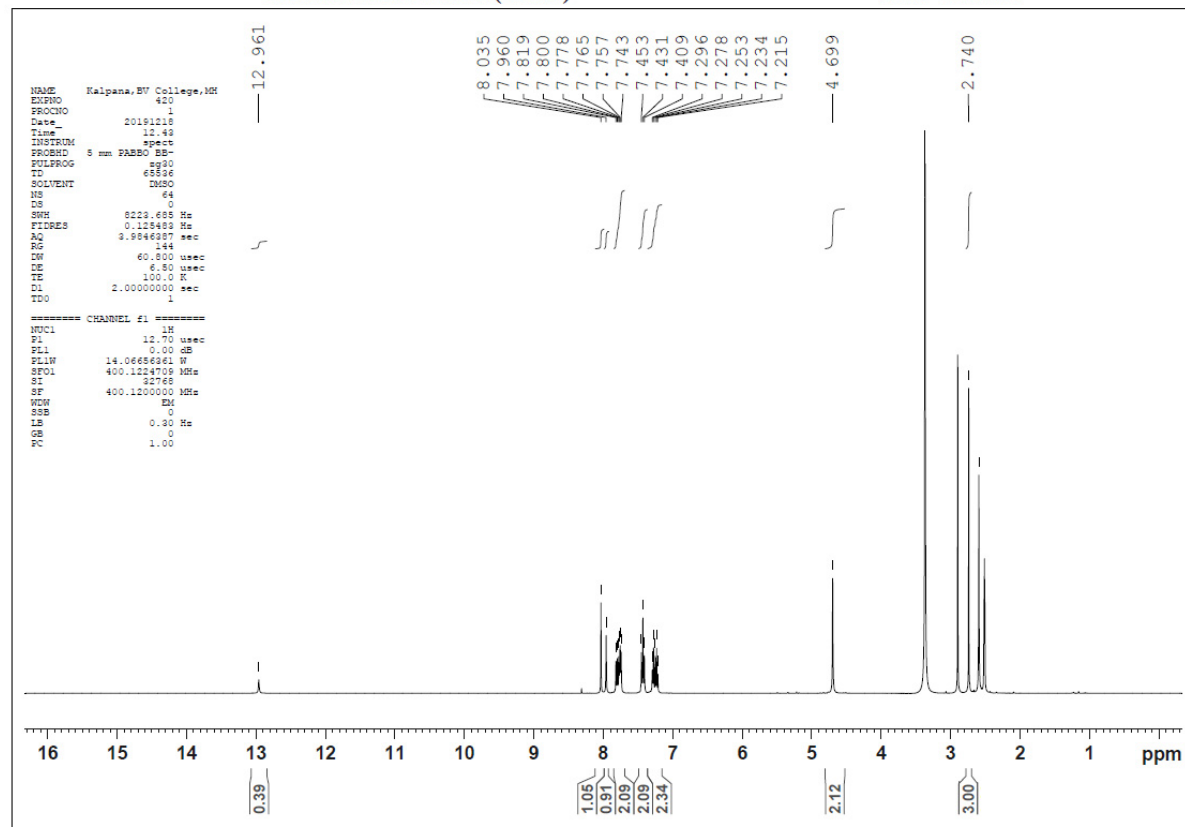
1. FTIR



2. ¹H-NMR

SAIFNM190323A-17(GB10)

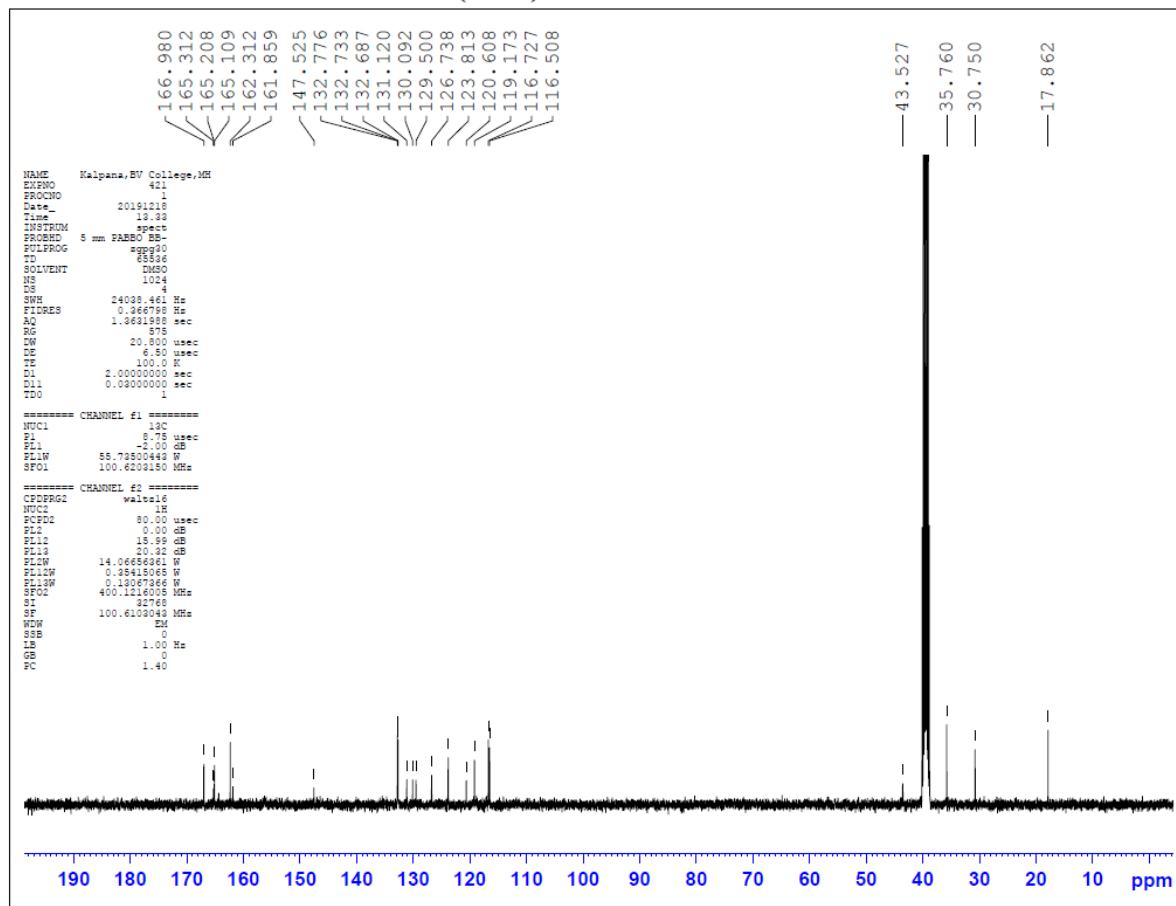
SAIF Cochin



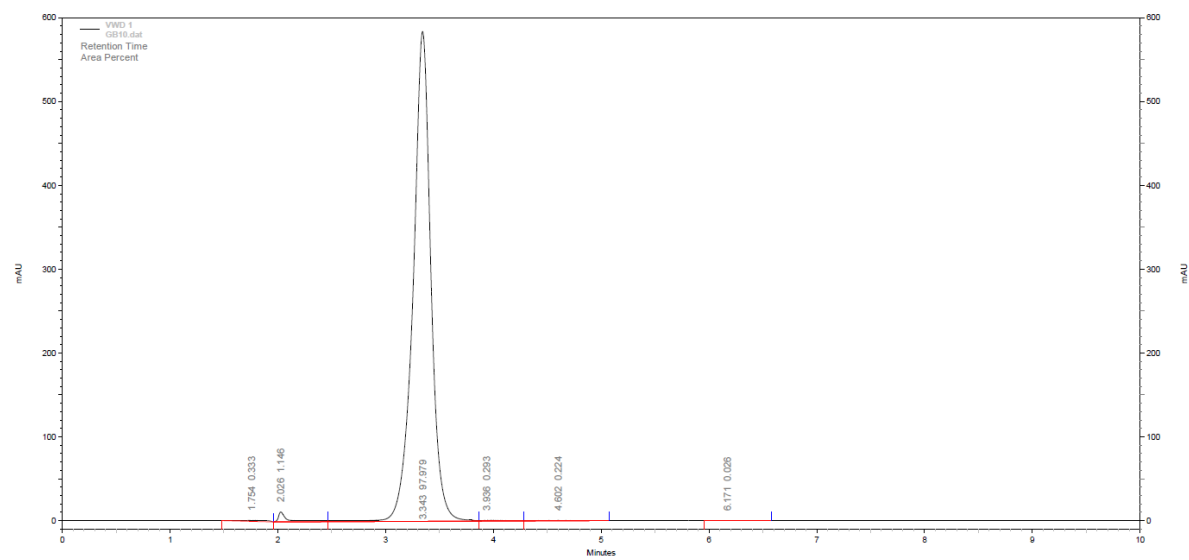
3. 13C-NMR

SAIFNM190323A-18(GB10)

SAIF Cochin

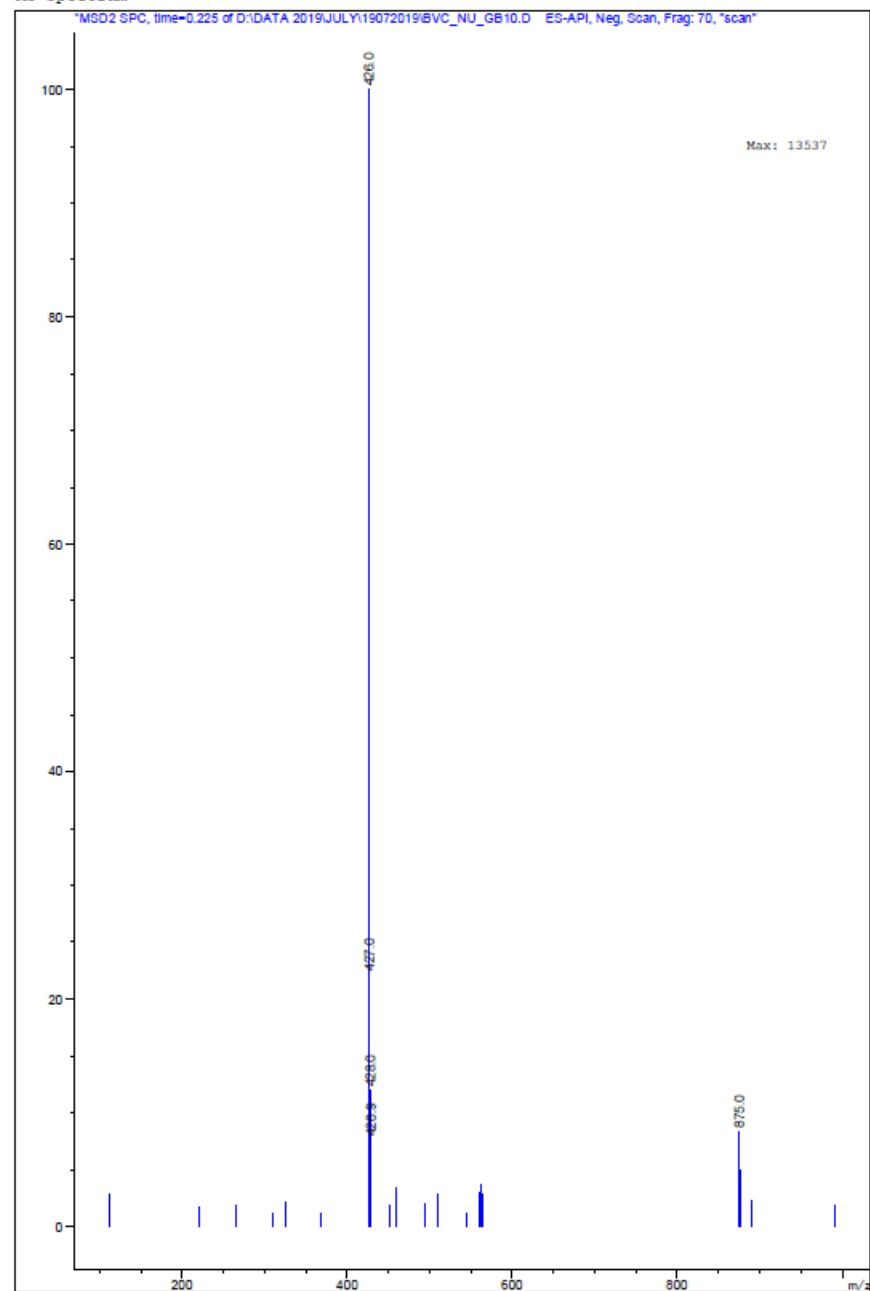


4. HPLC



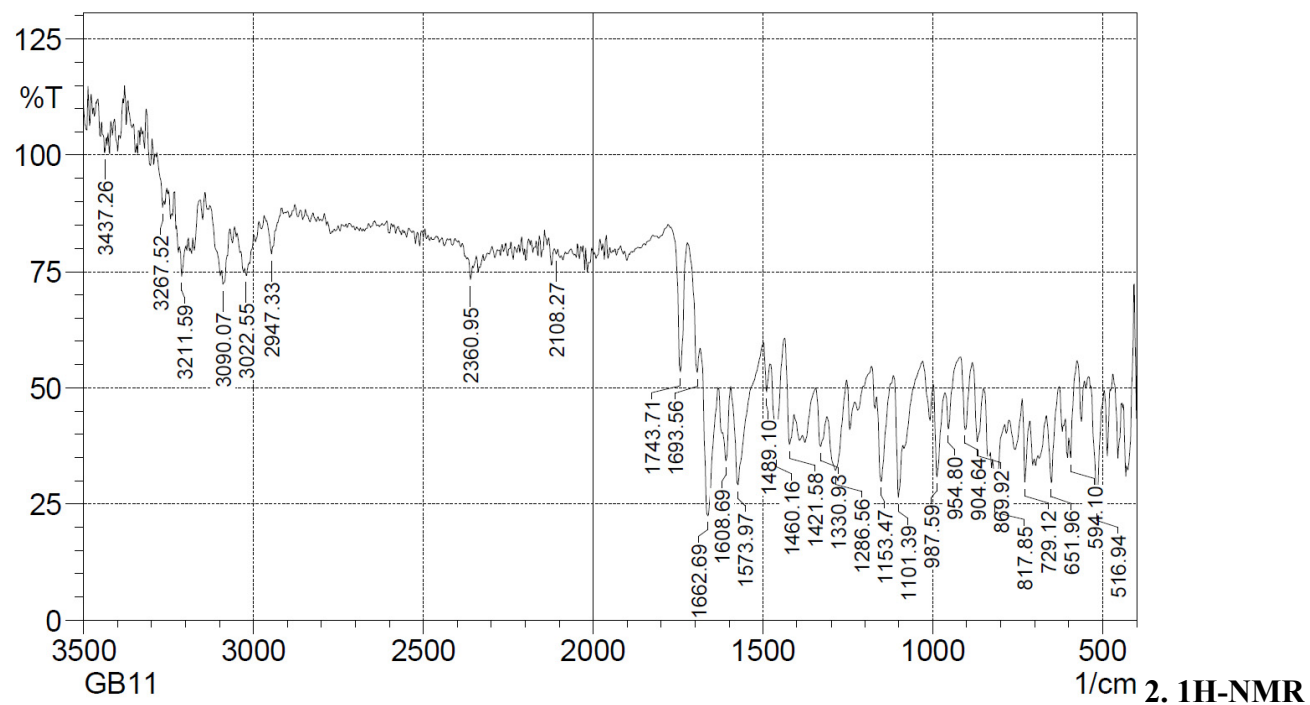
4. Mass

MS Spectrum



2-(5-(4-chlorobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-(4,6-difluorobenzo[d]thiazol-2-yl)acetamide (GB11)

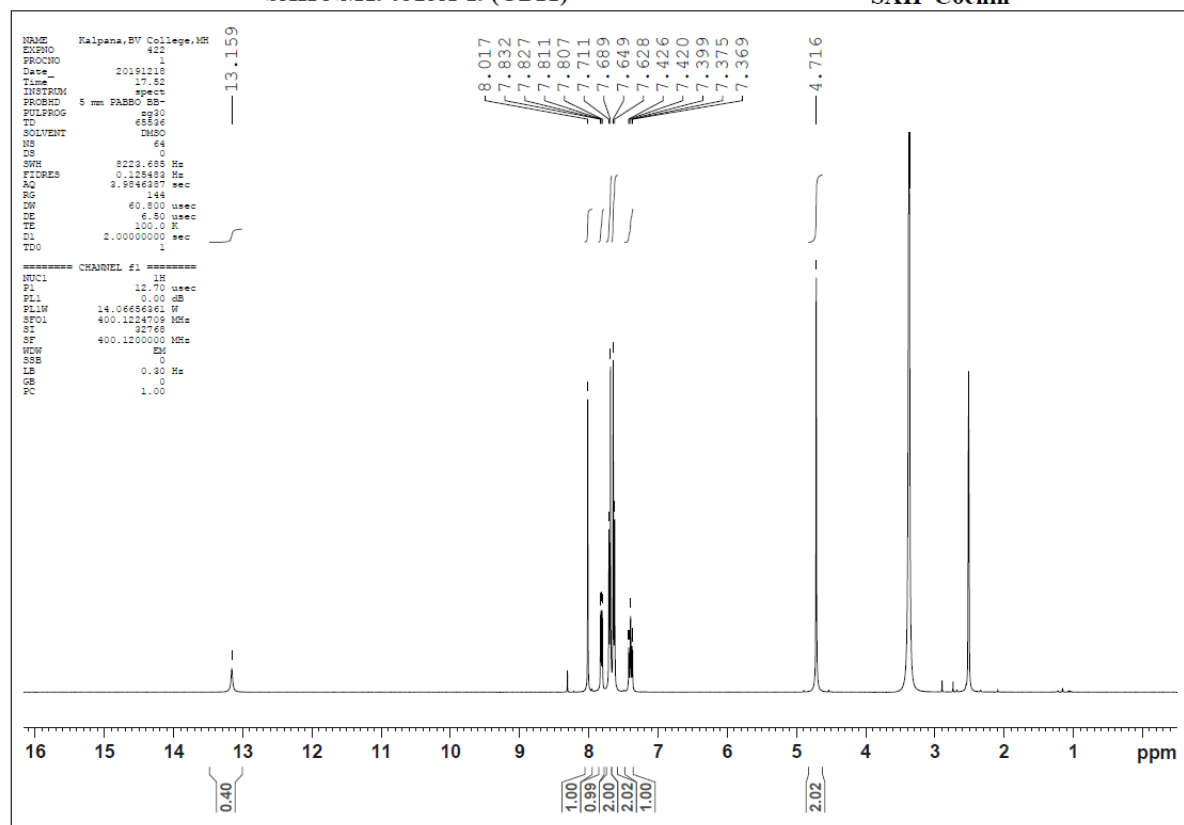
1. FTIR



2. $^1\text{H-NMR}$

SAIFNM190323A-19(GB11)

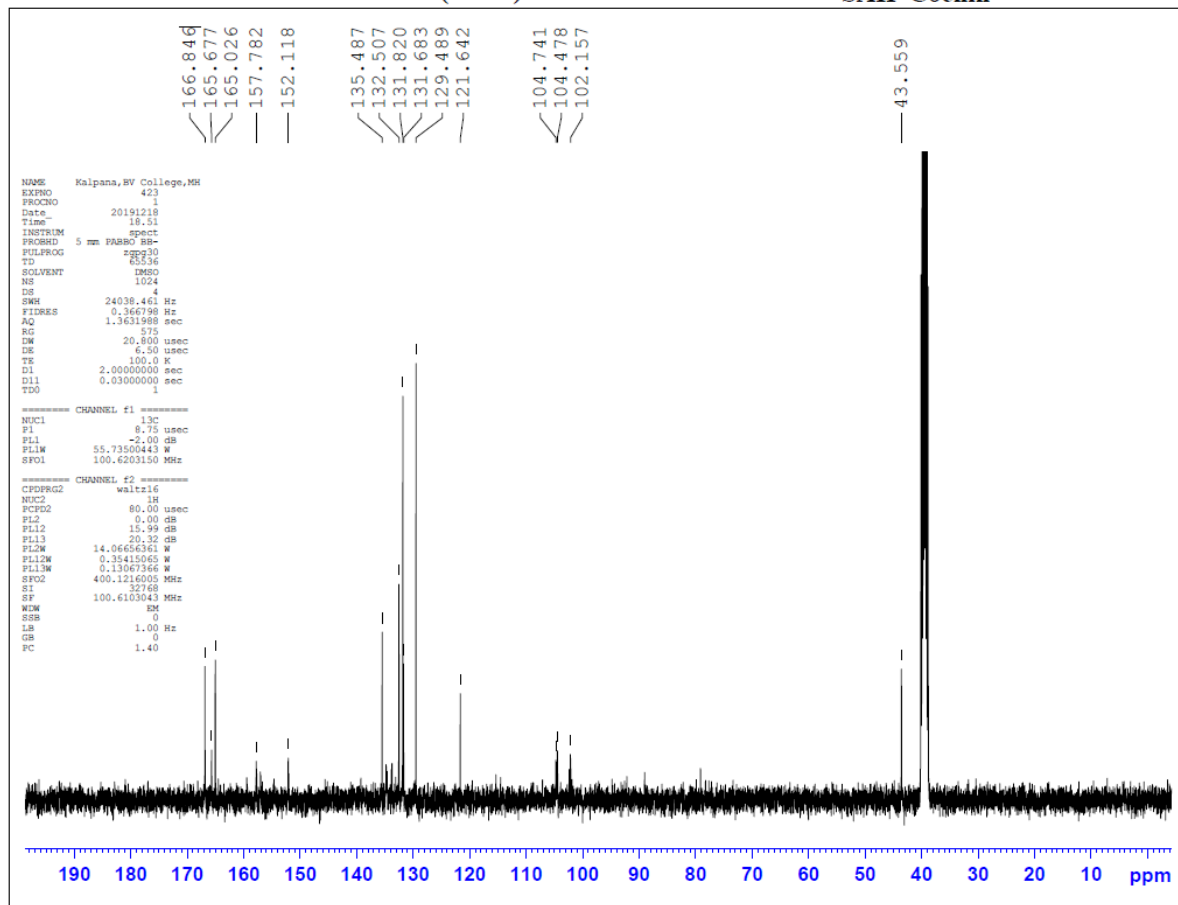
SAIF Cochin



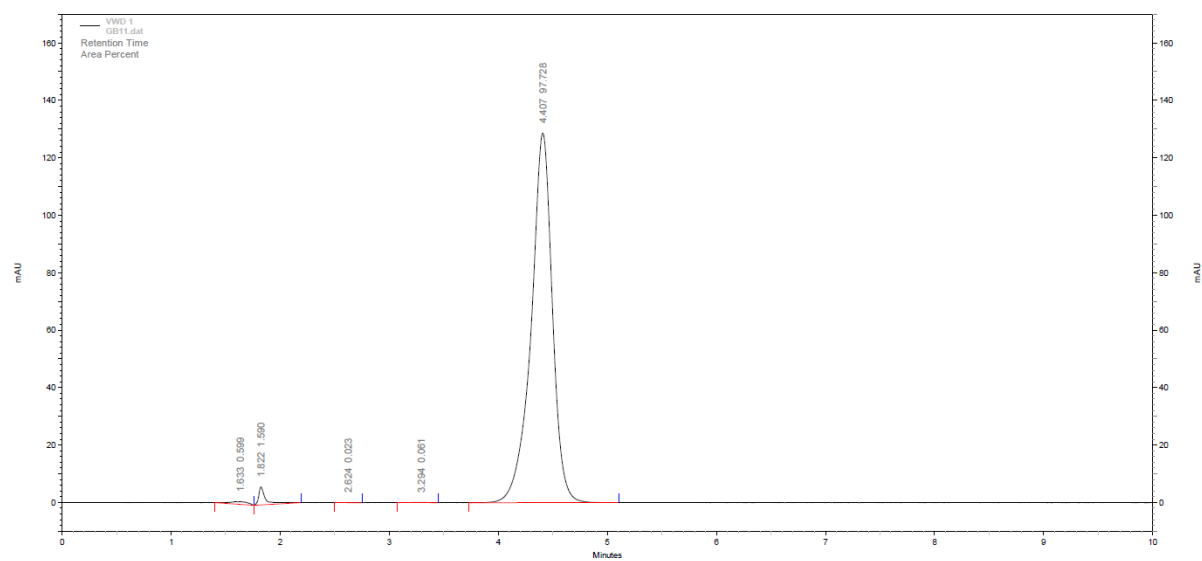
3. 13C-NMR

SAIFNM190323A-20(GB11)

SAIF Cochin

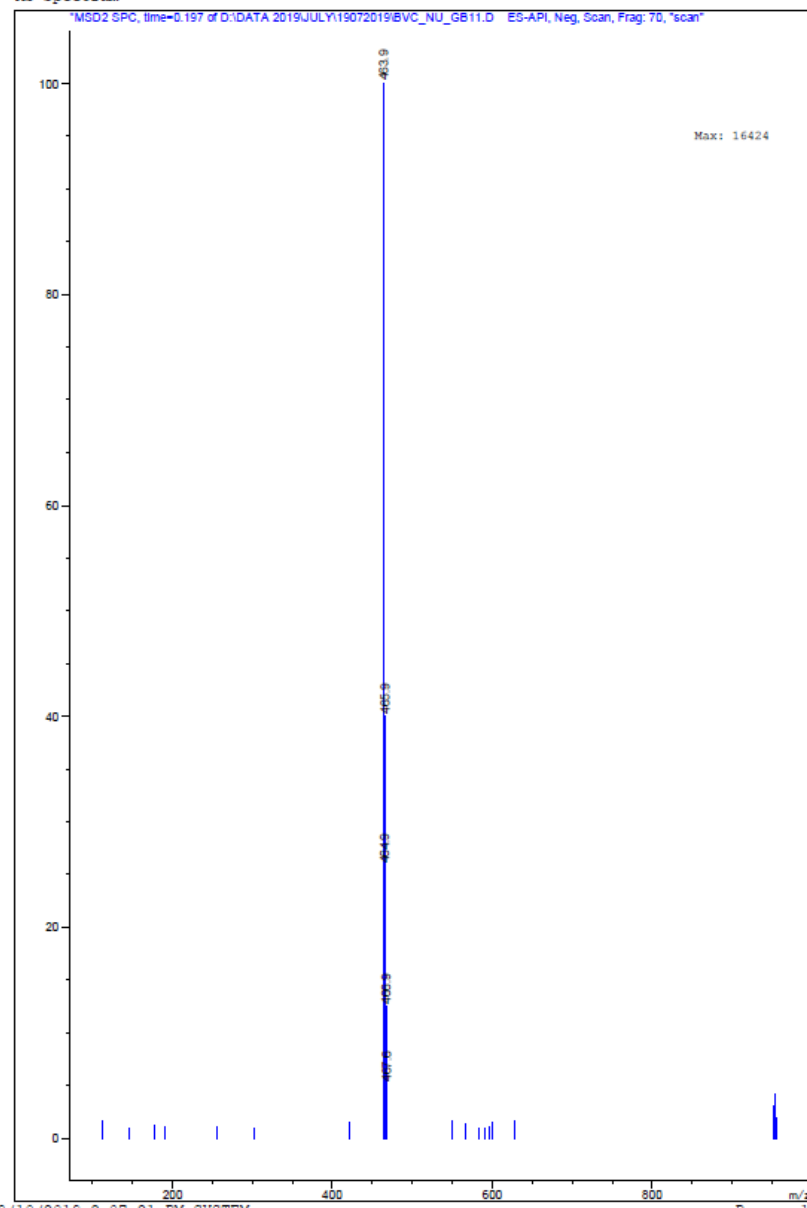


4. HPLC



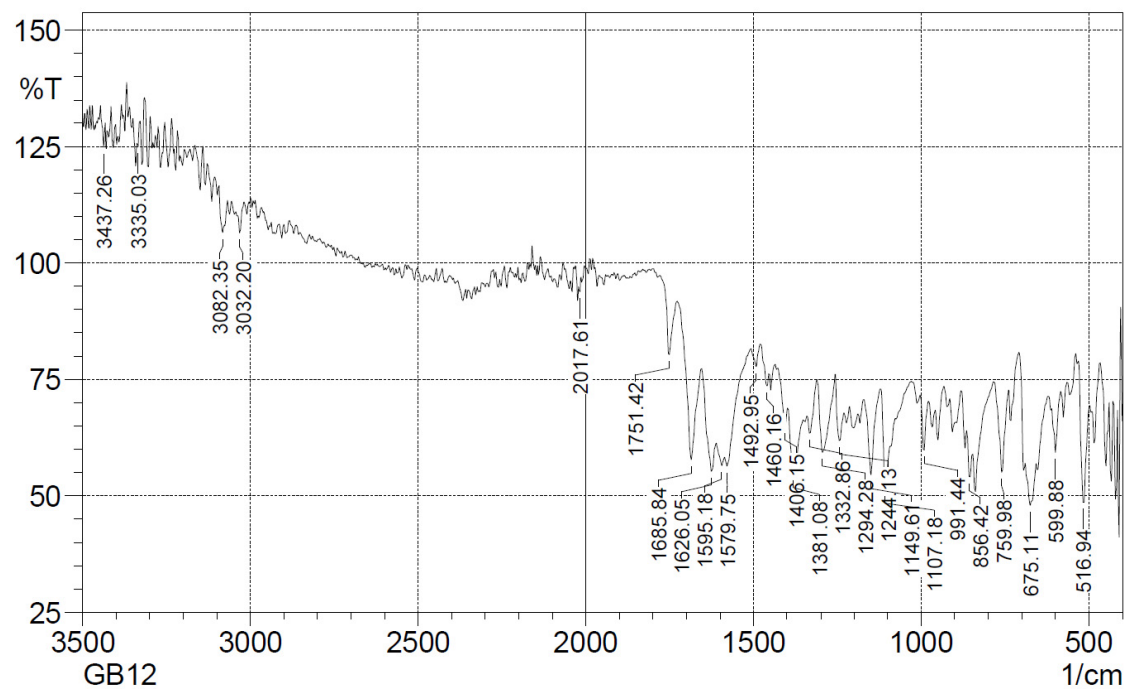
5. Mass

MS Spectrum



2-(5-benzylidene-2,4-dioxothiazolidin-3-yl)-N-(4,6-difluorobenzo[d]thiazol-2-yl)acetamide (GB12)

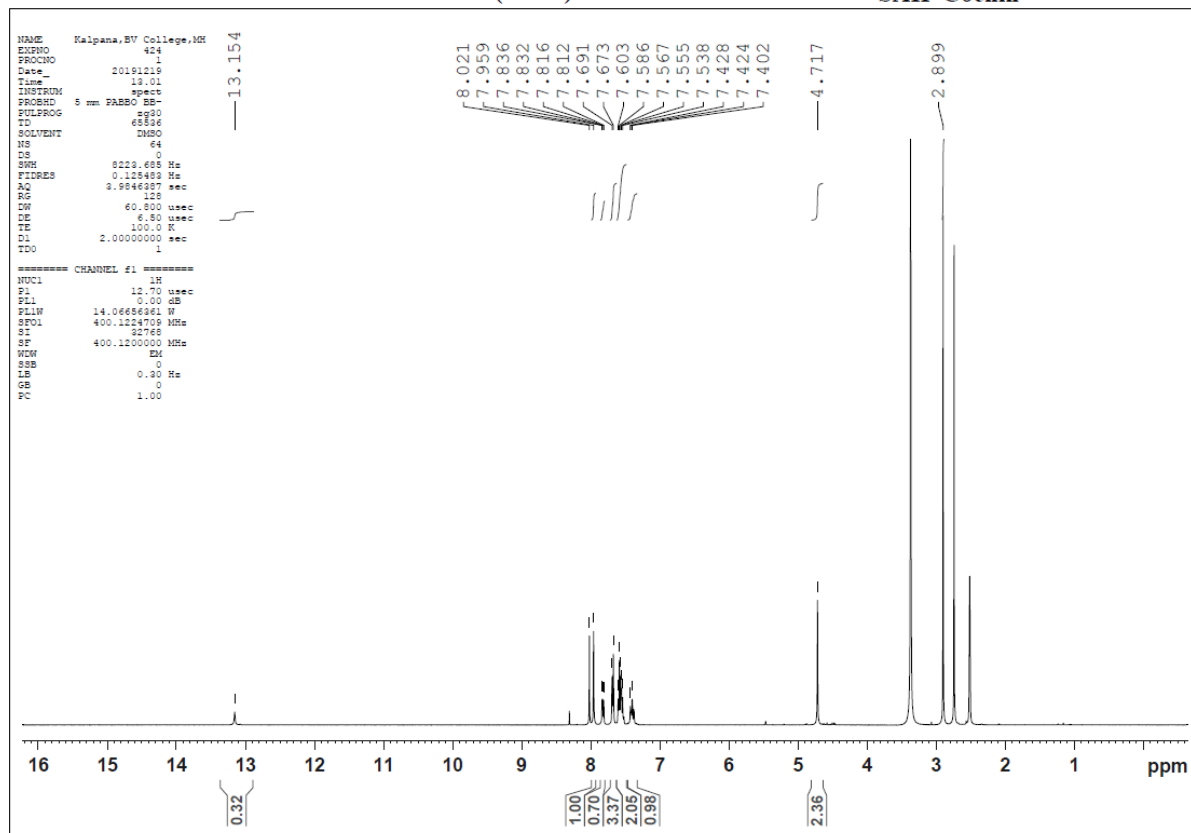
1. FTIR



2. $^1\text{H-NMR}$

SAIFNM190323A-21(GB12)

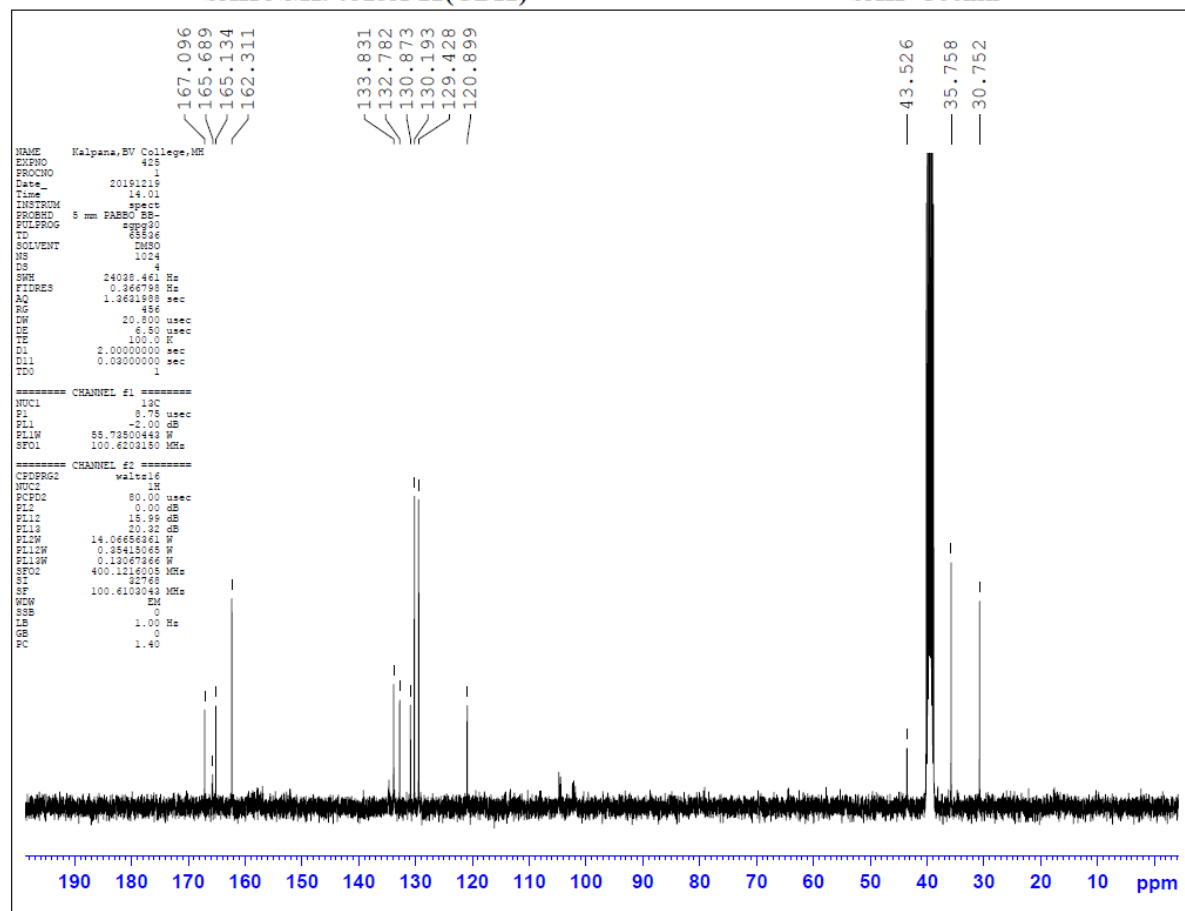
SAIF Cochin



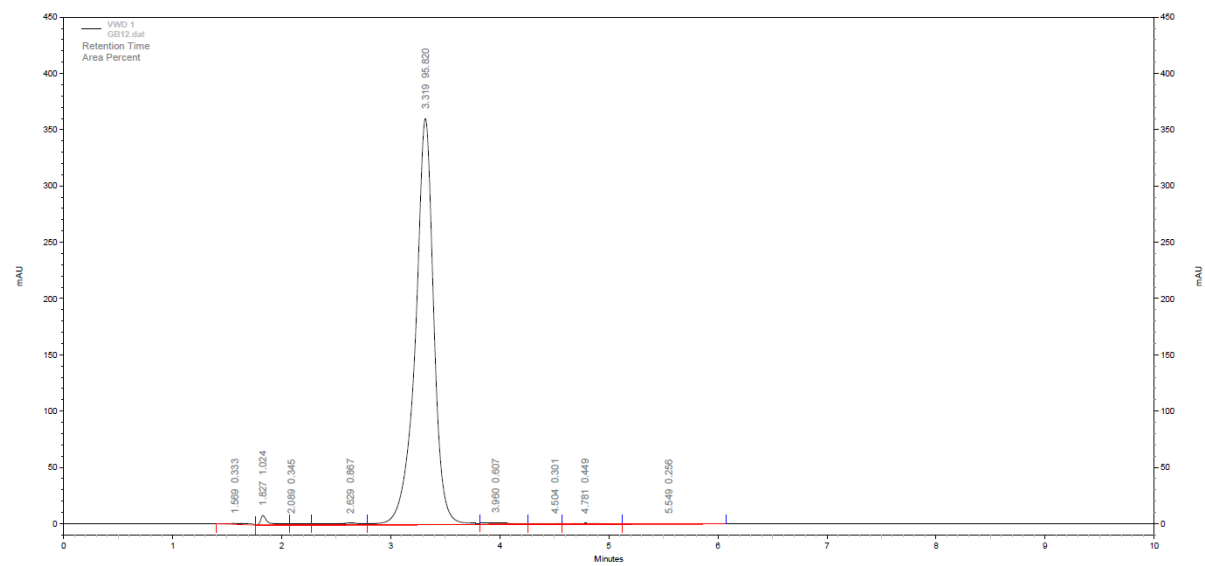
3. ¹³C-NMR

SAIFNM190323A-22(GB12)

SAIF Cochin

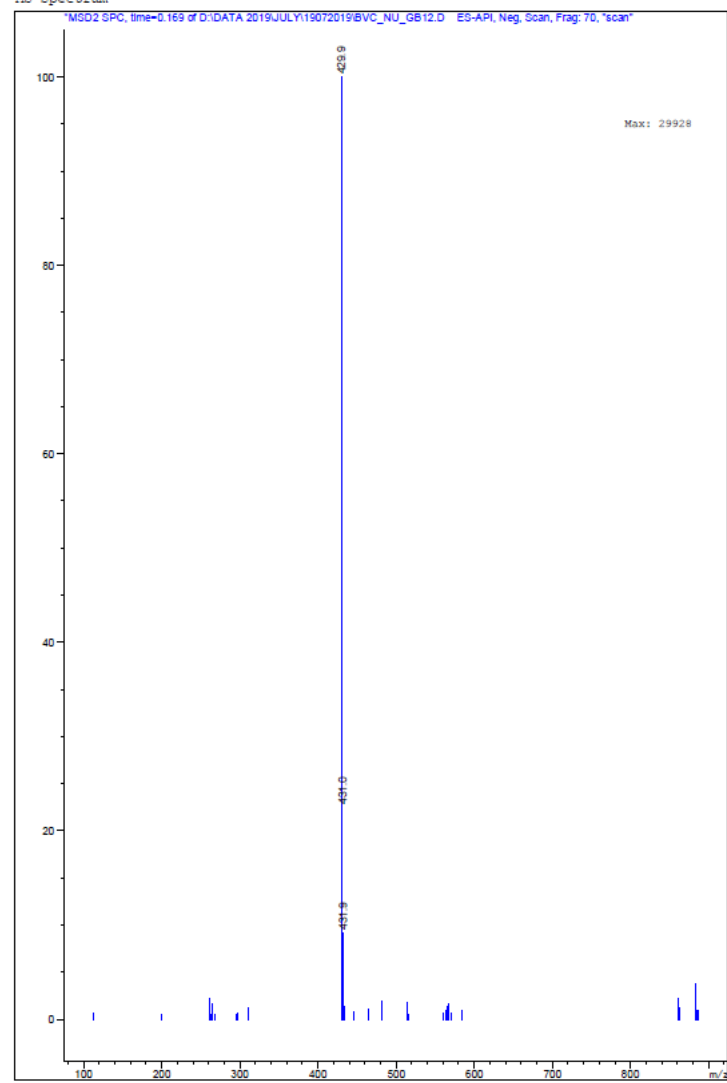


4. HPLC



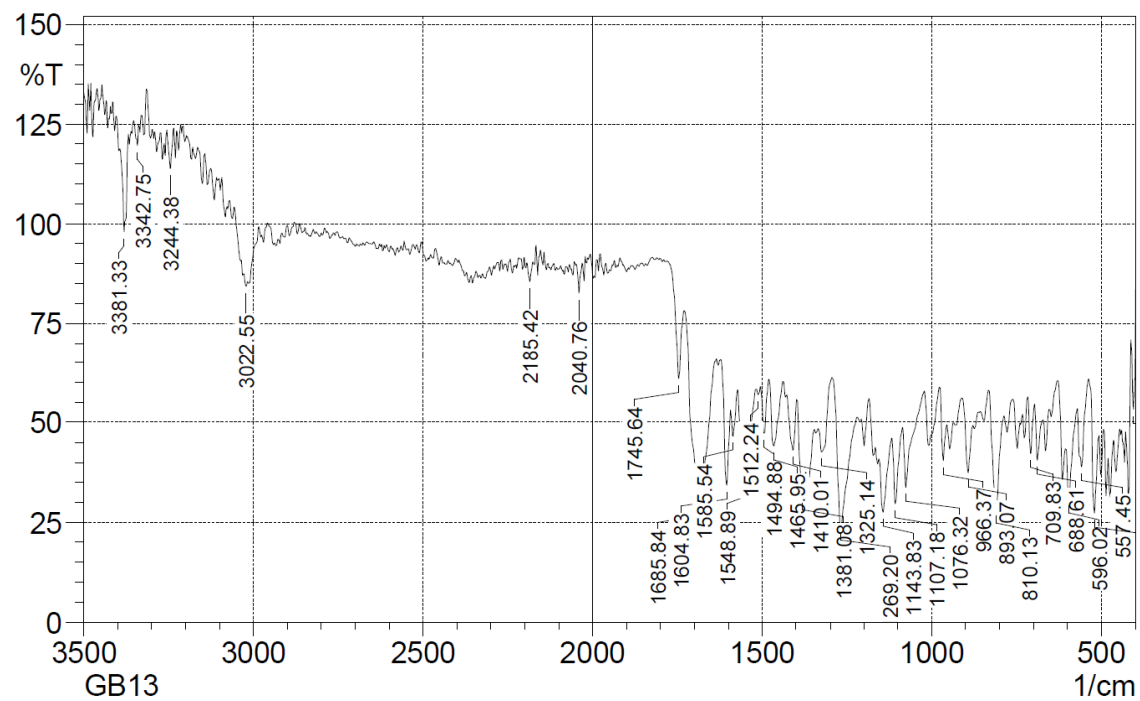
5. Mass

MS Spectrum



2-(5-(2,4-difluorobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-(6-methylbenzo[d]thiazol-2-yl)acetamide (GB13)

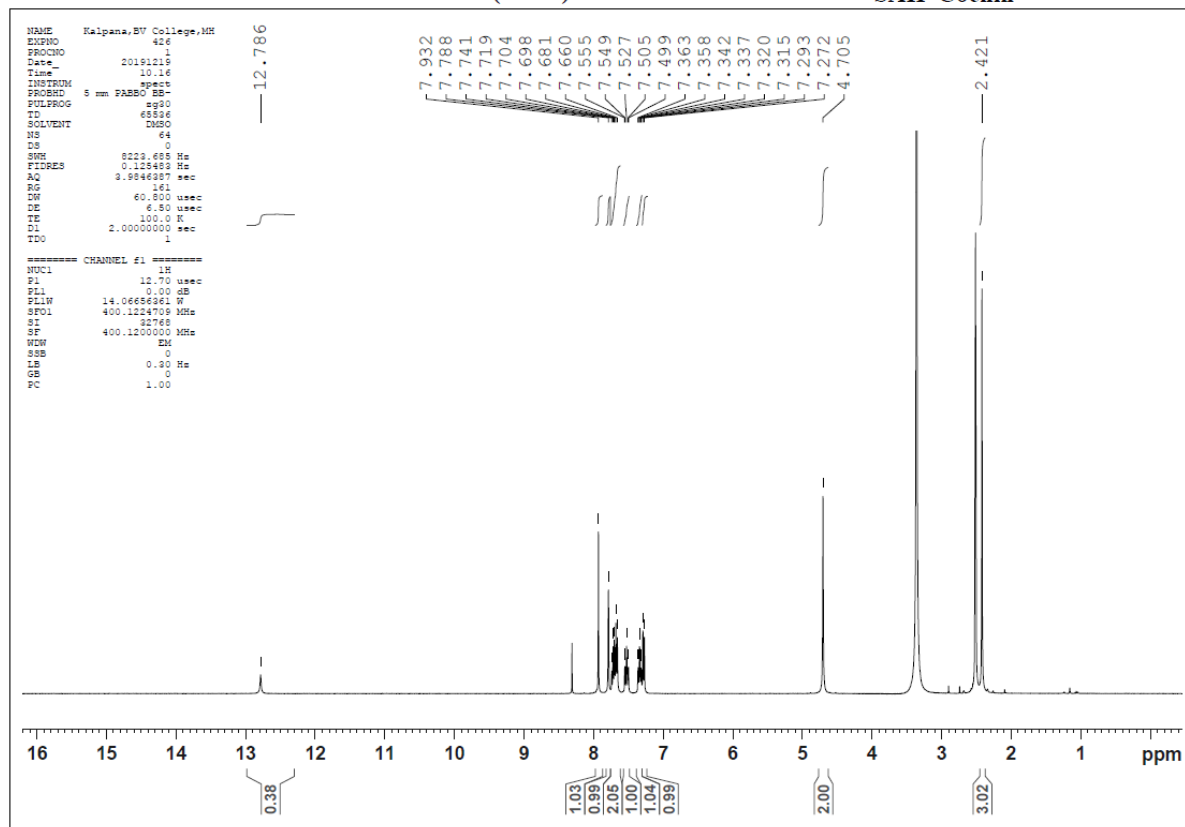
1. FTIR



2. ^1H -NMR

SAIFNM190323A-23(GB13)

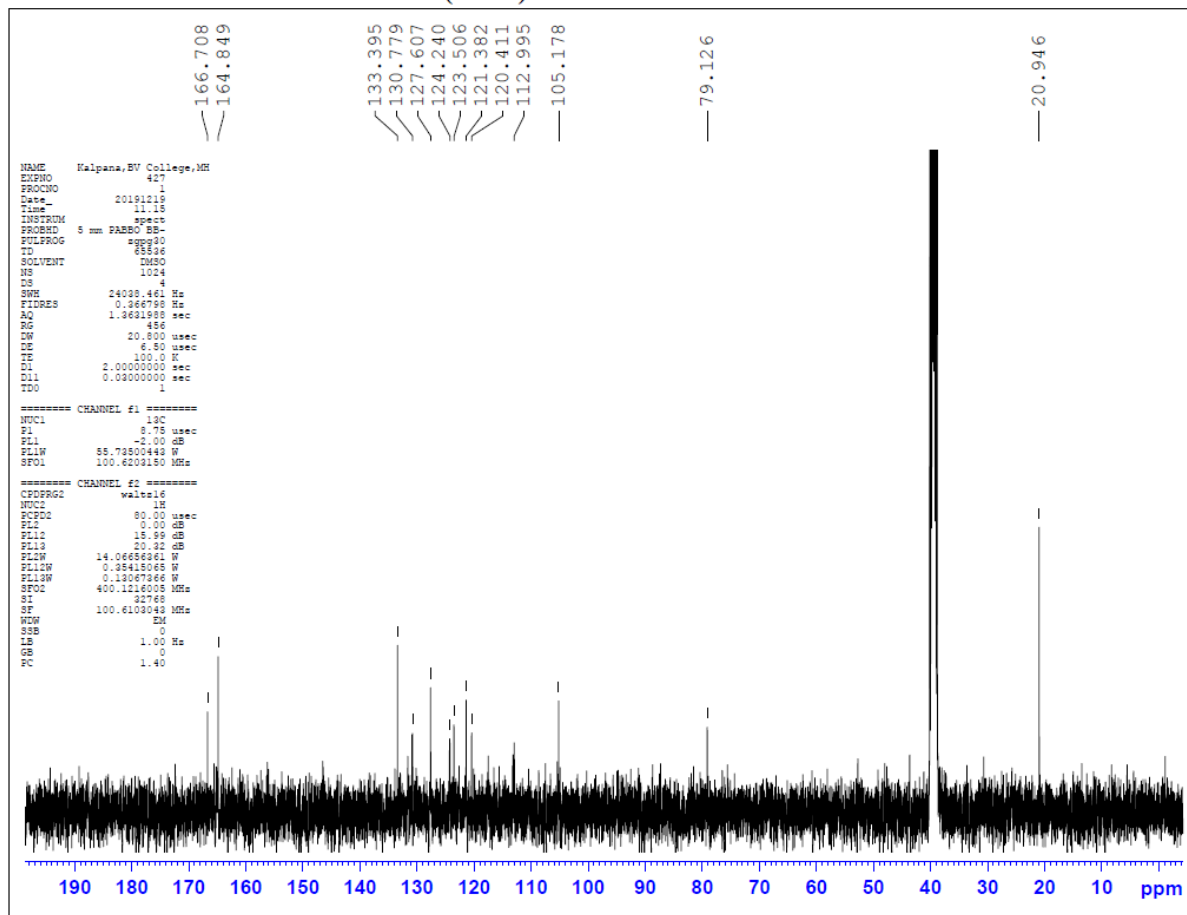
SAIF Cochin



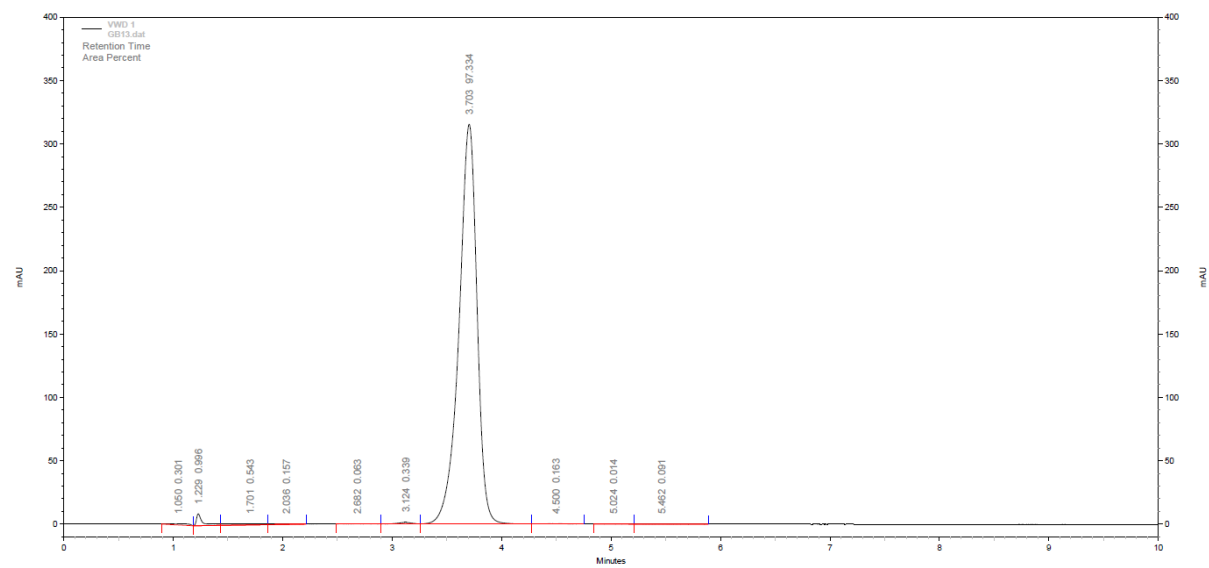
3. 13C-NMR

SAIFNM190323A-24(GB13)

SAIF Cochin



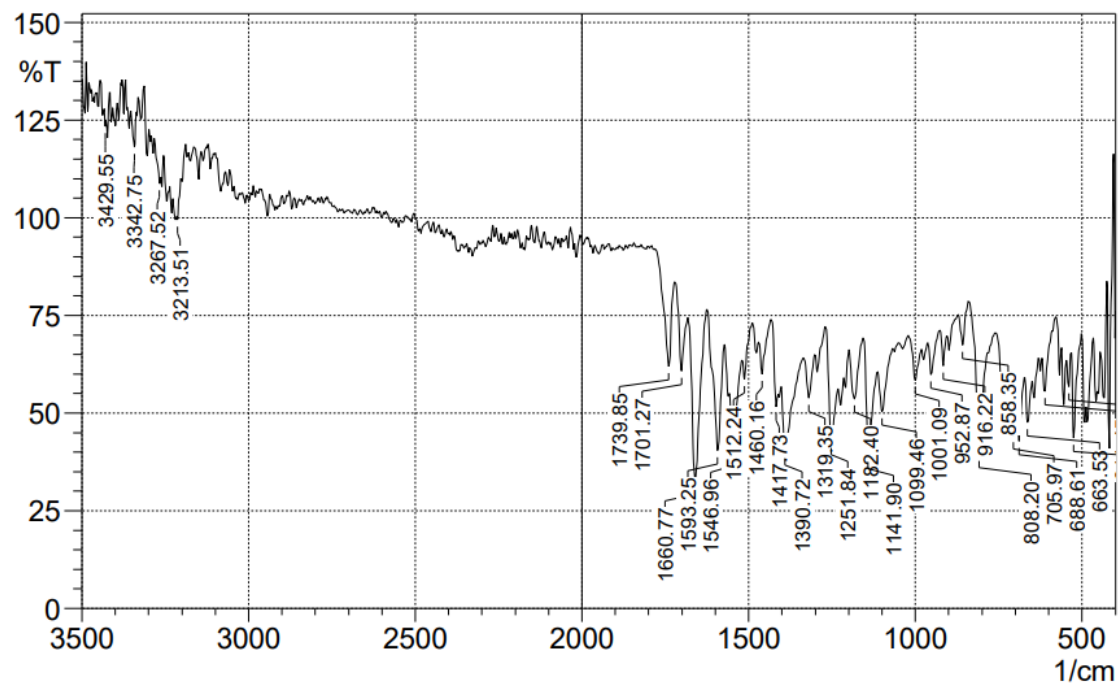
4. HPLC



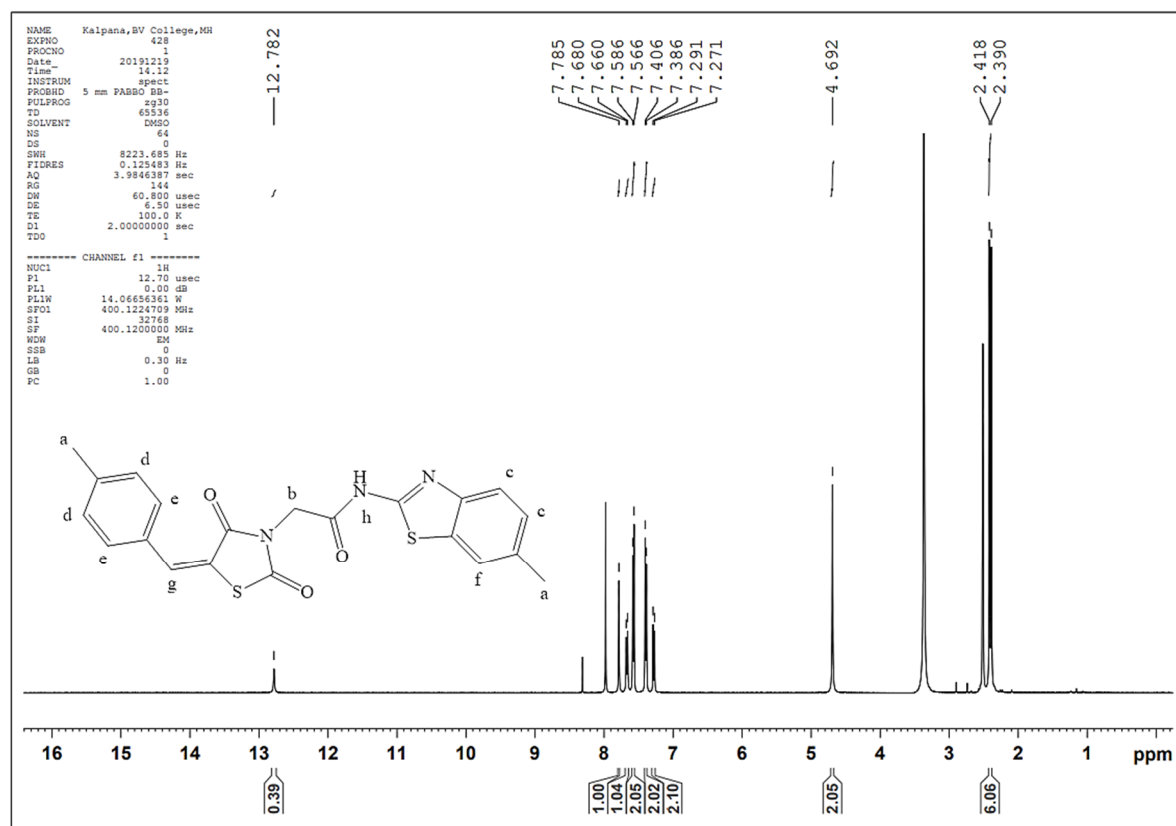
5. Mass

N-(6-methylbenzo[d]thiazol-2-yl)-2-(5-(4-methylbenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB14)

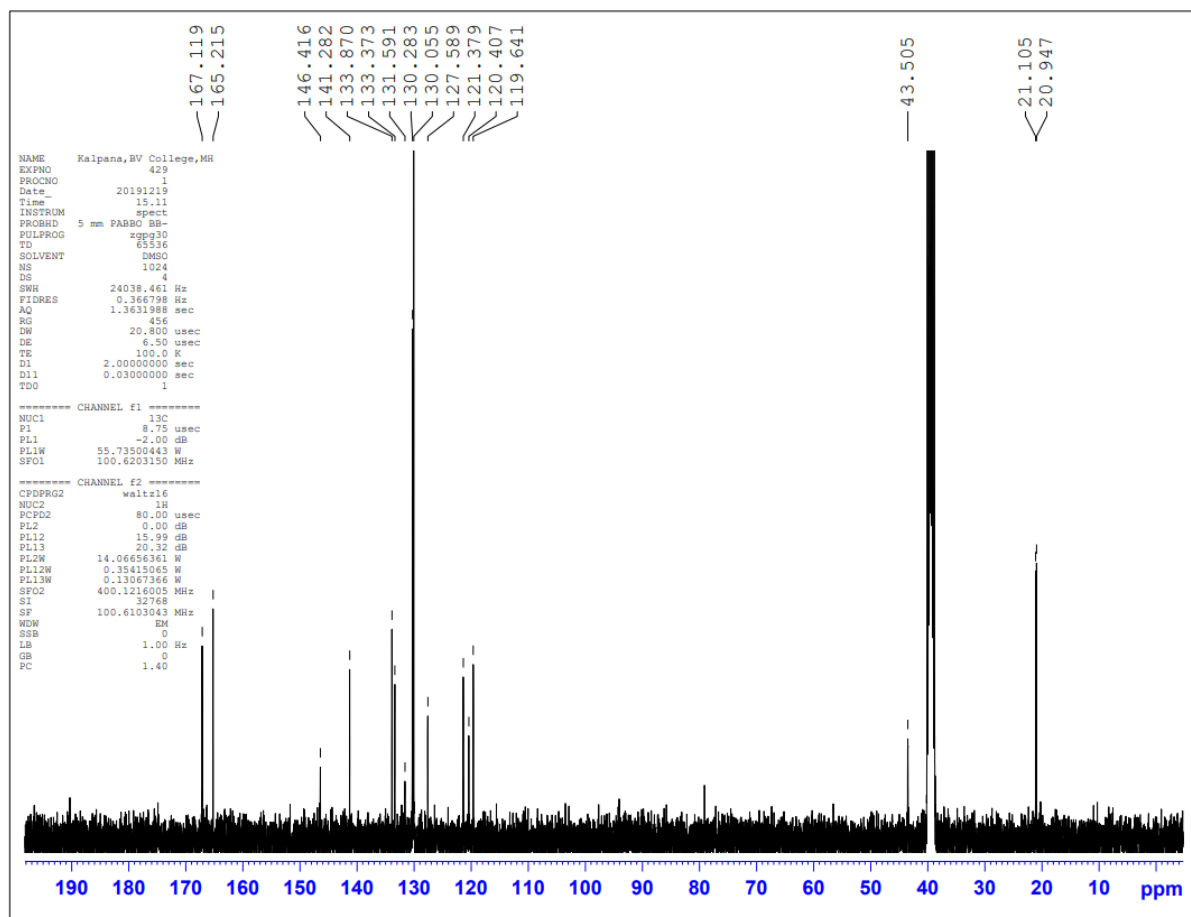
1. FTIR



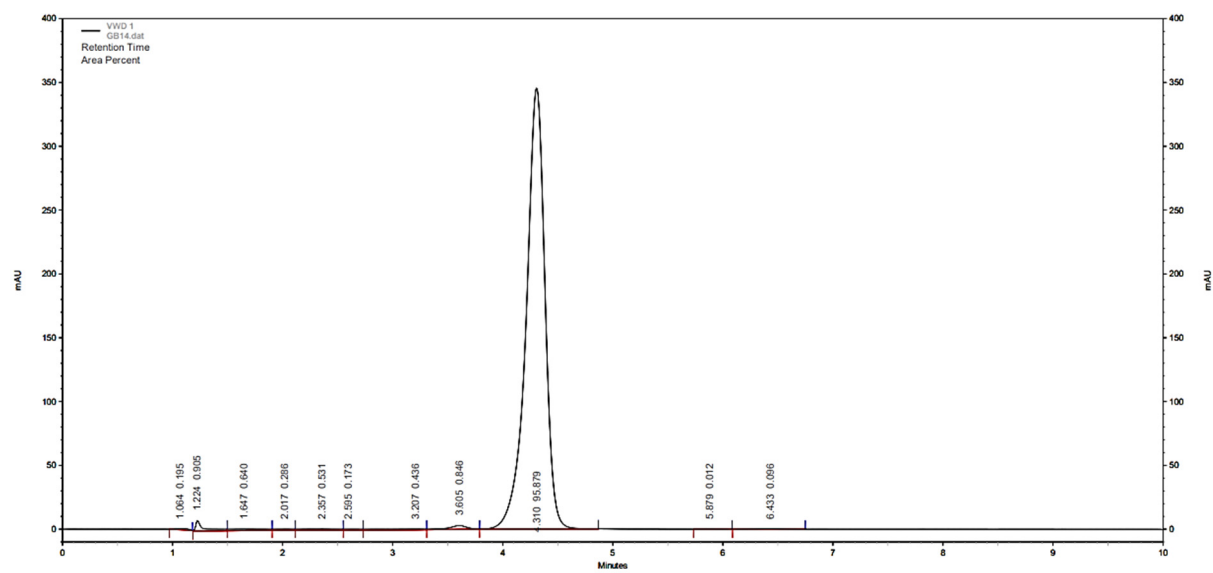
2. ¹H-NMR



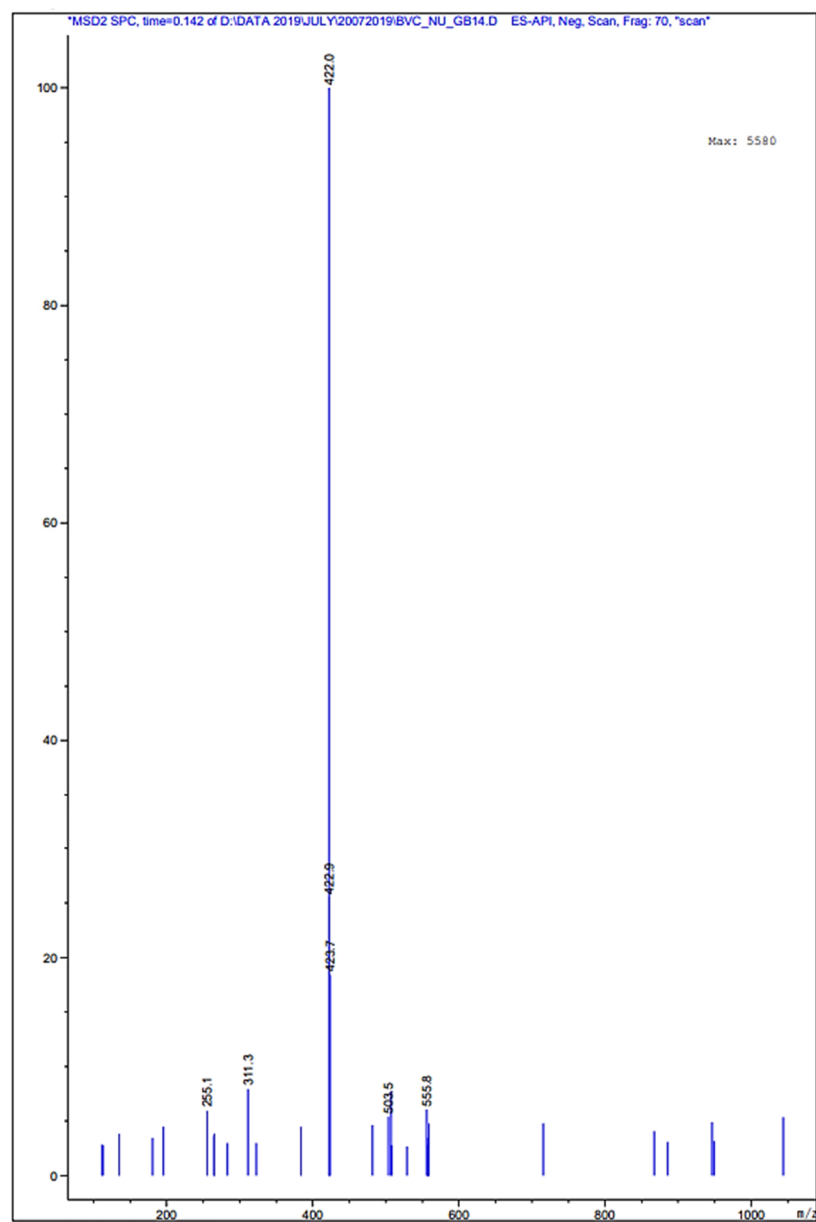
3. ^{13}C -NMR



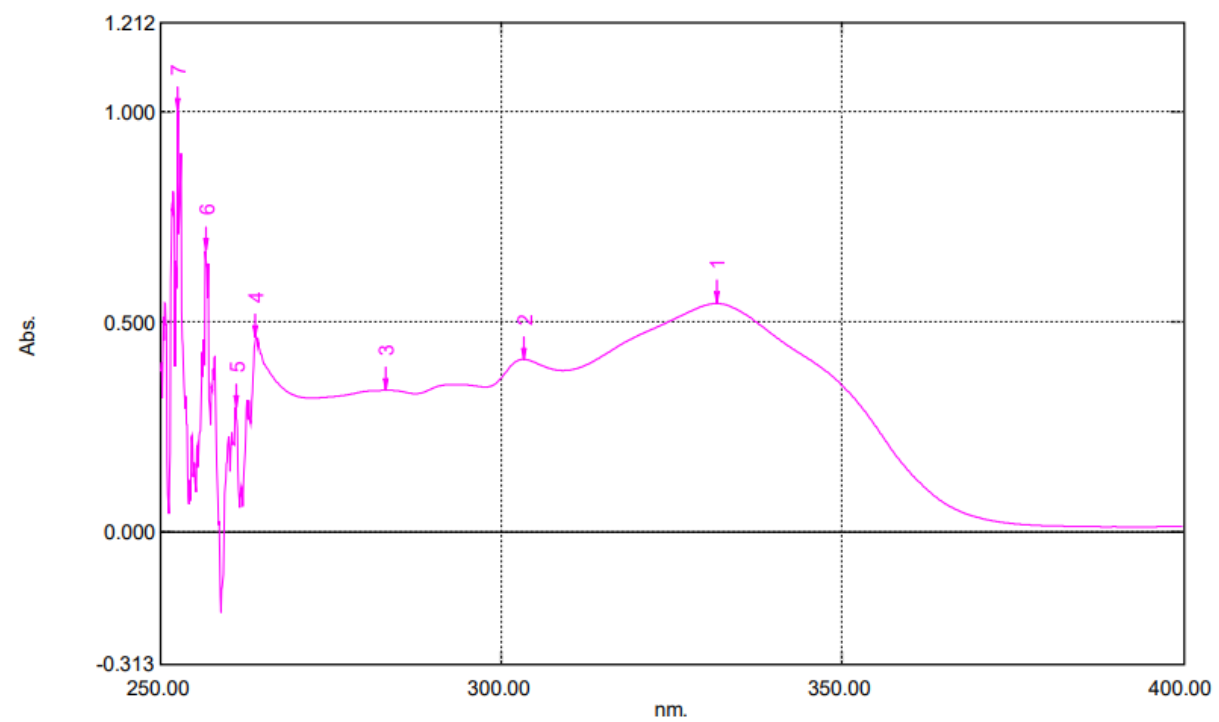
4. HPLC Analysis



5. Mass Spectrometry

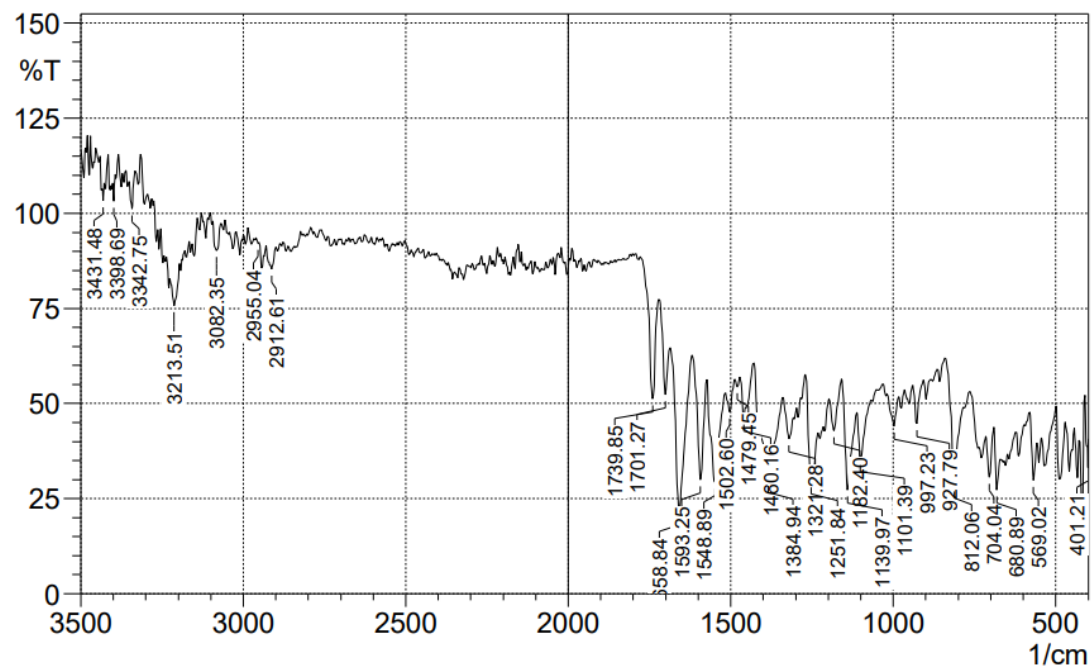


6. UV

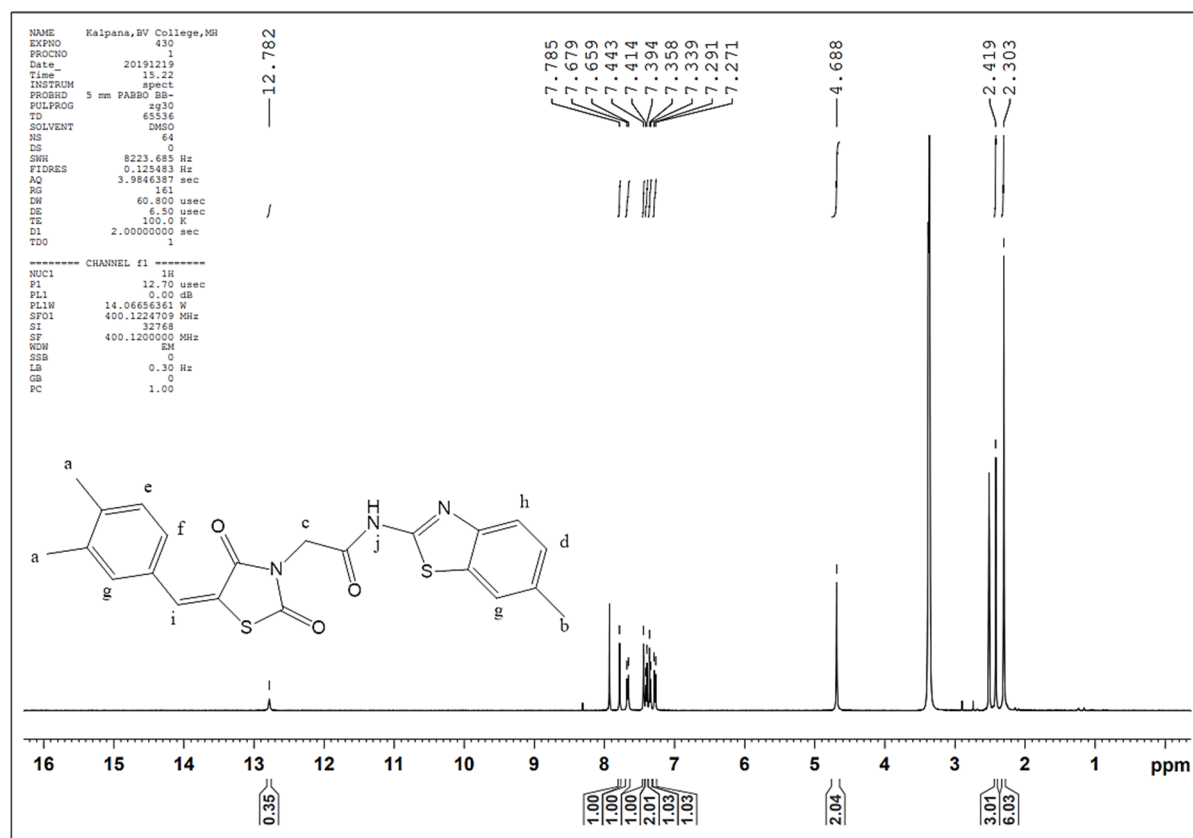


2-(5-(3,4-dimethylbenzylidene)-2,4-dioxothiazolidin-3-yl)-N-(6-methylbenzo[d]thiazol-2-yl)acetamide (GB15)

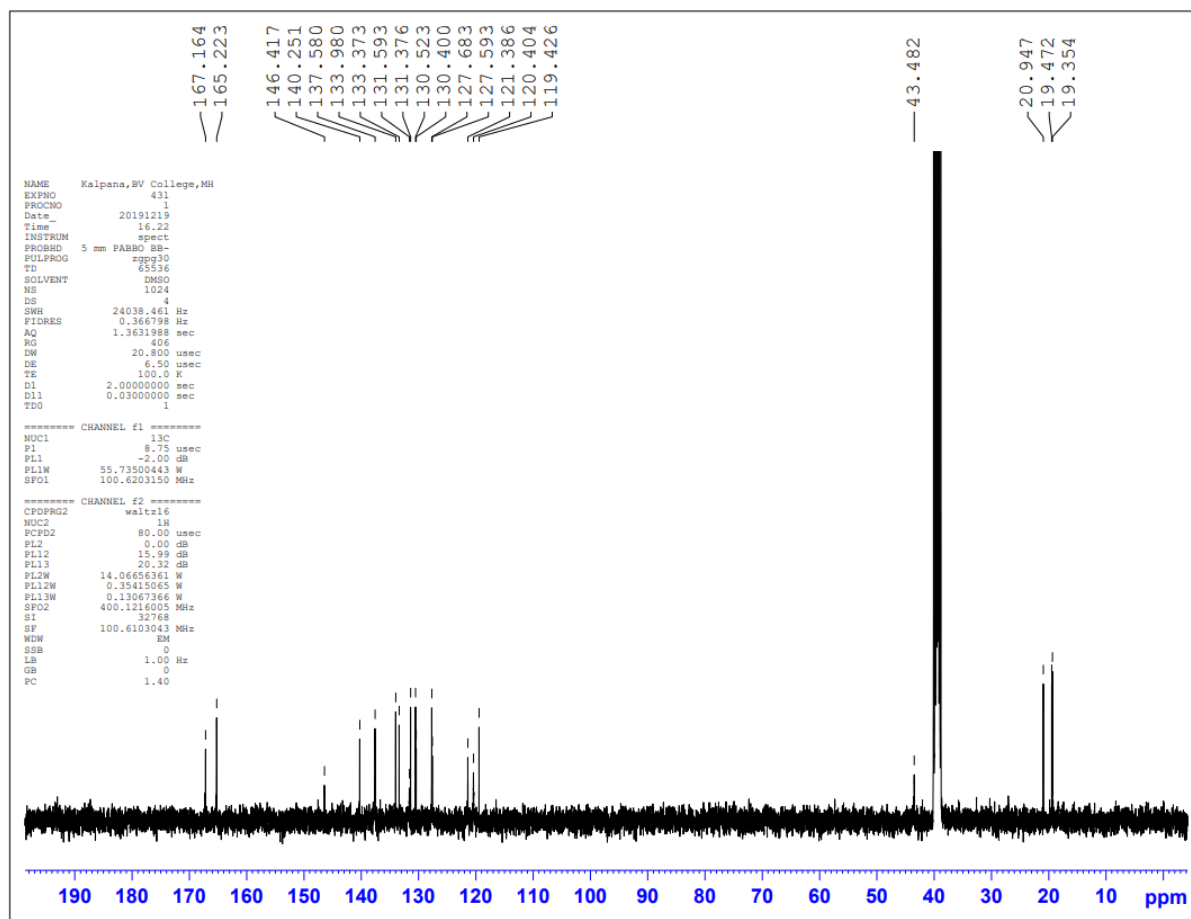
1. FTIR –



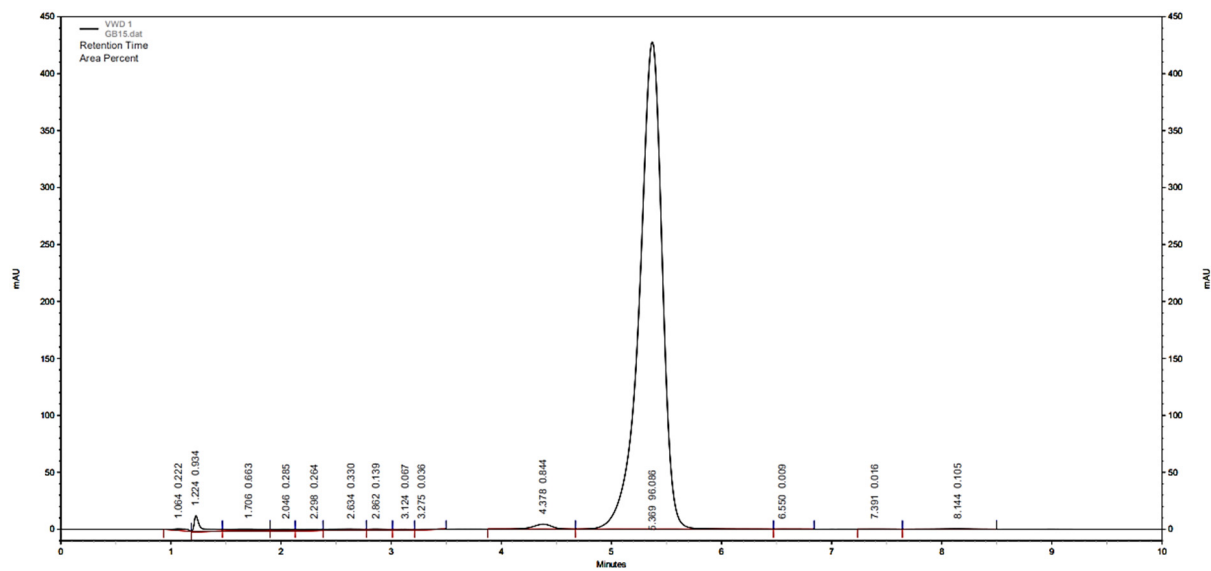
2. ¹H-NMR



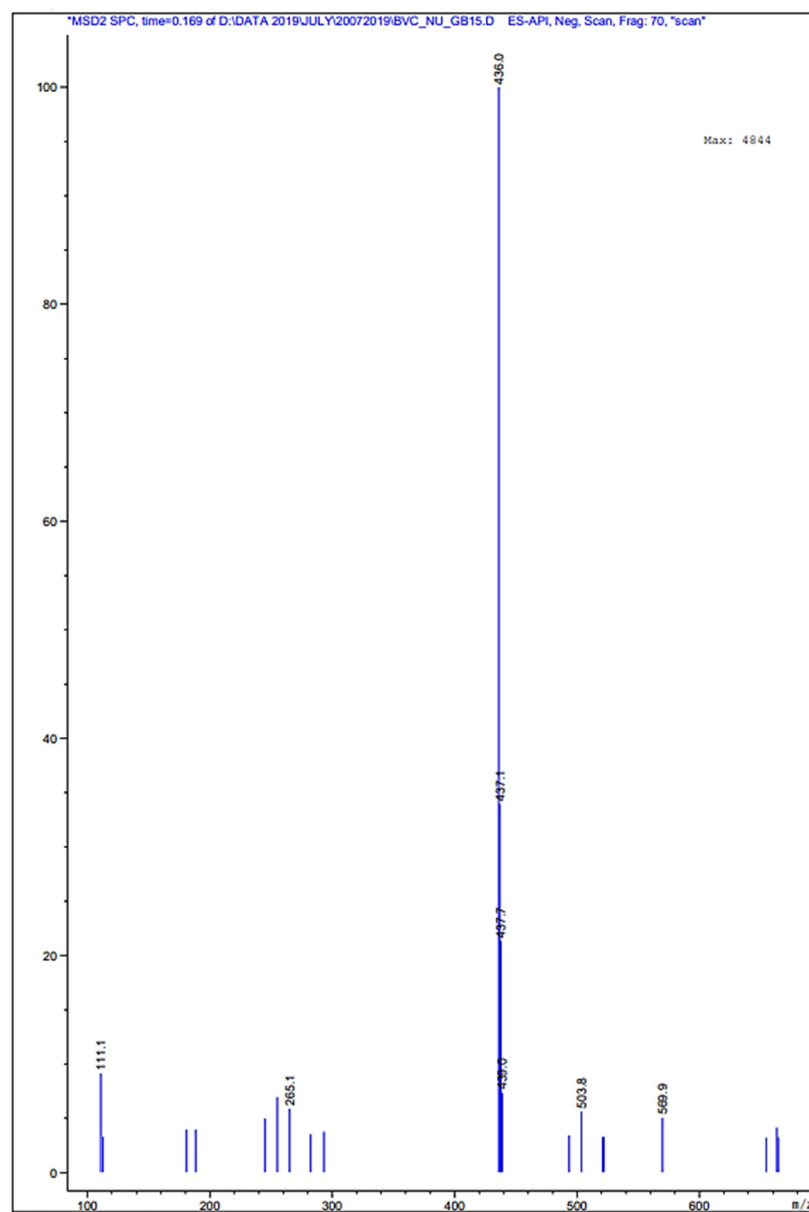
3. ¹³C-NMR



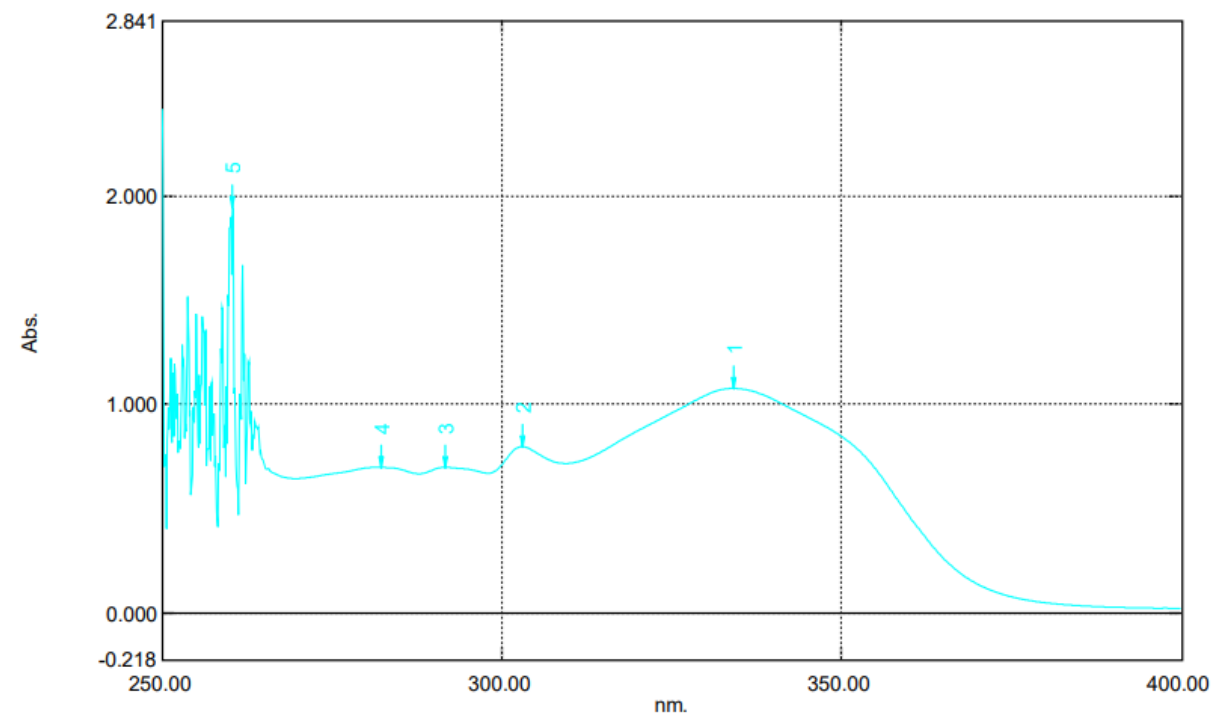
4. HPLC Analysis



5. Mass Spectrometry

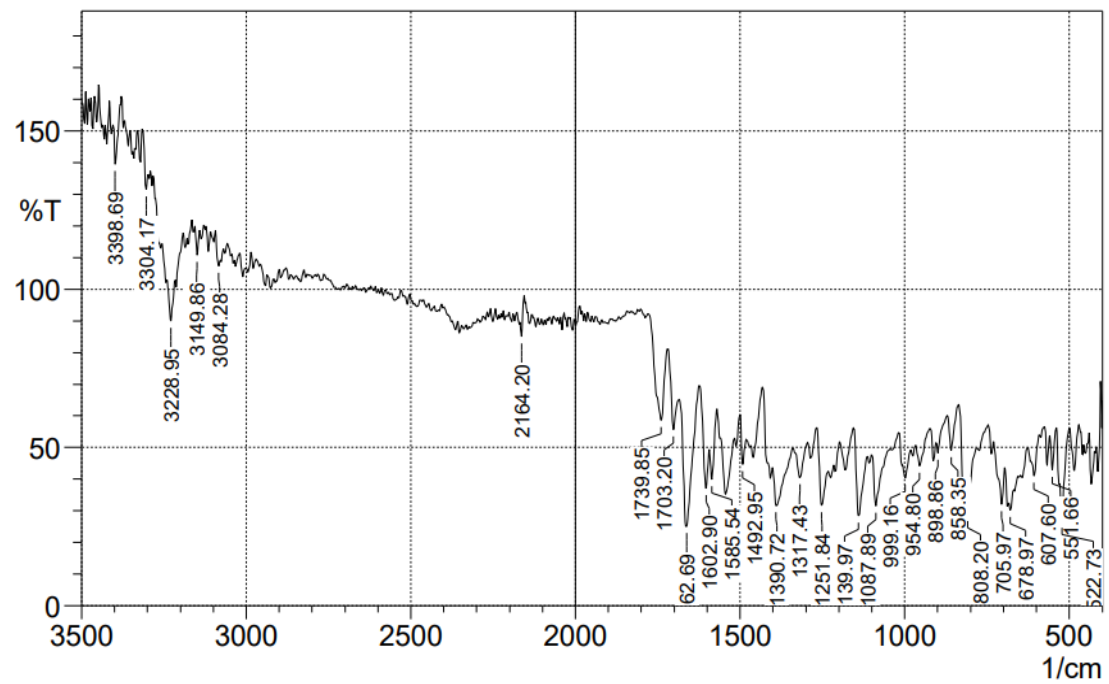


6. UV

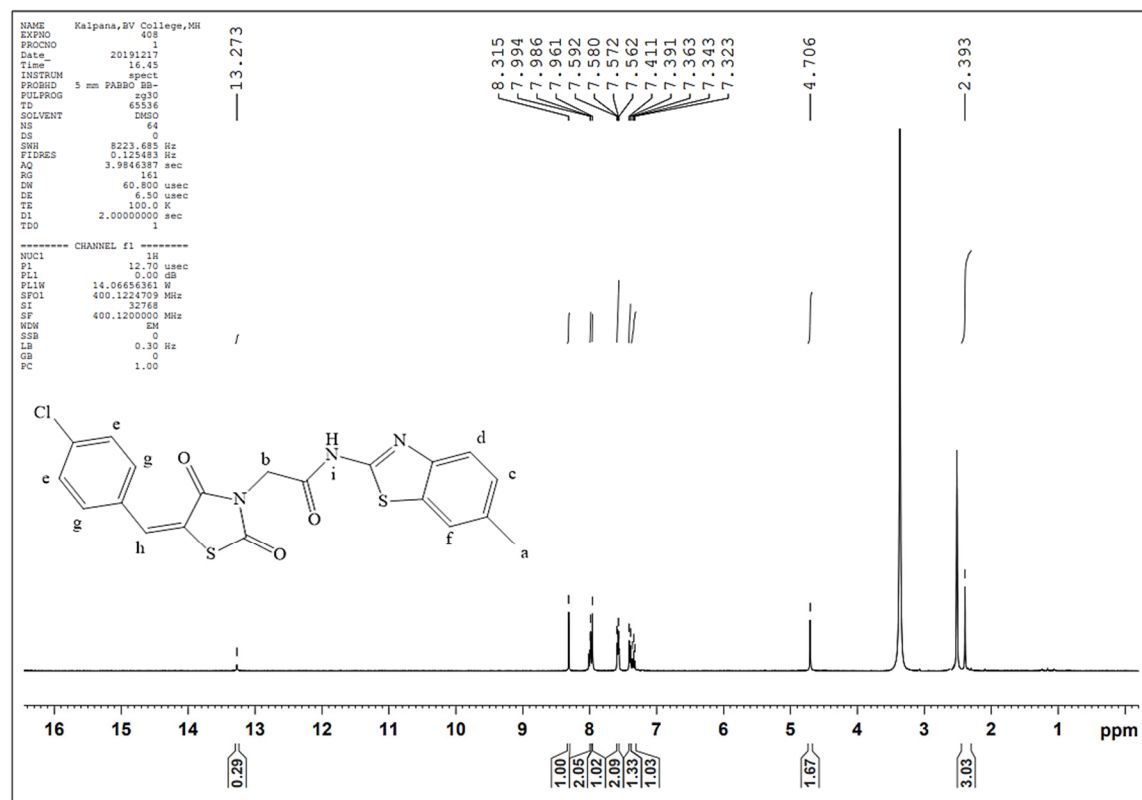


2-(5-(4-chlorobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-(6-methylbenzo[d]thiazol-2-yl)acetamide (GB16)

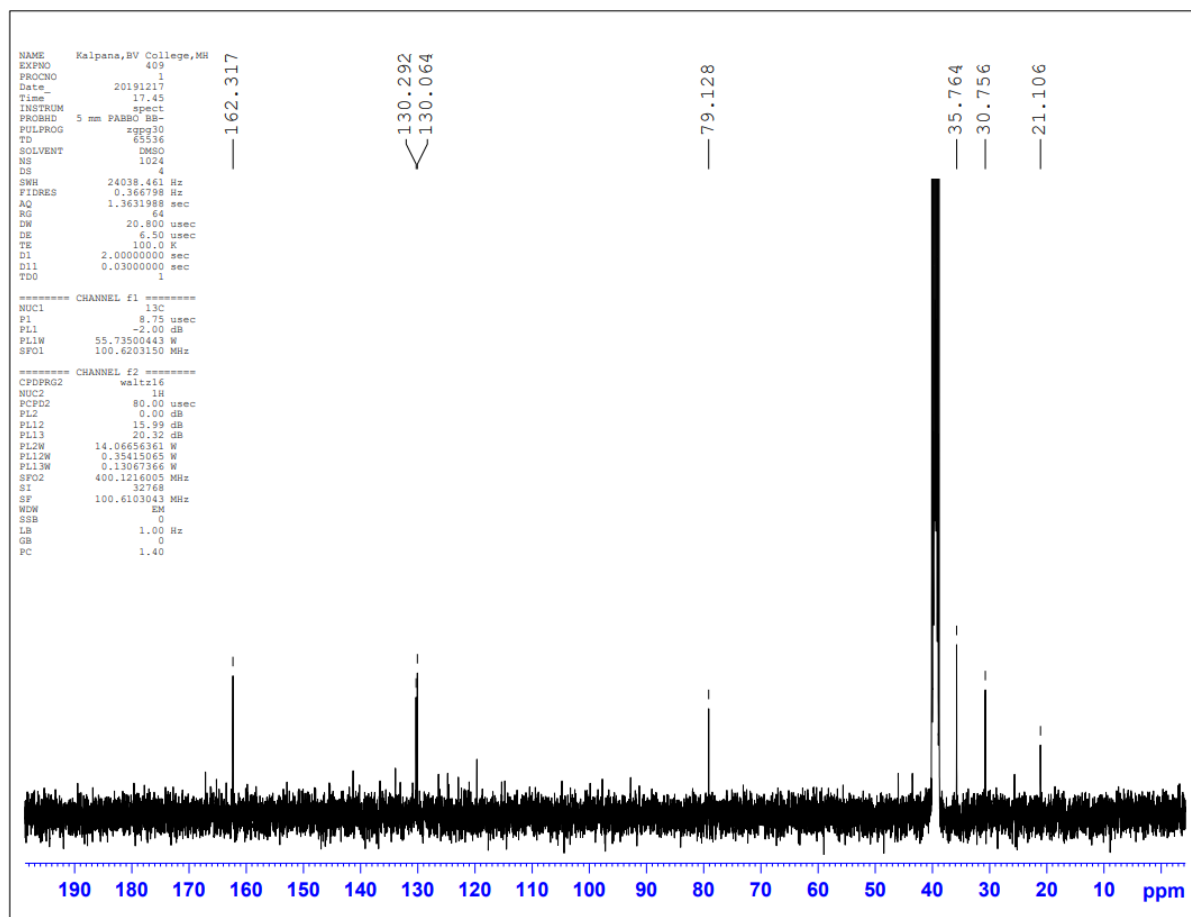
1. FTIR –



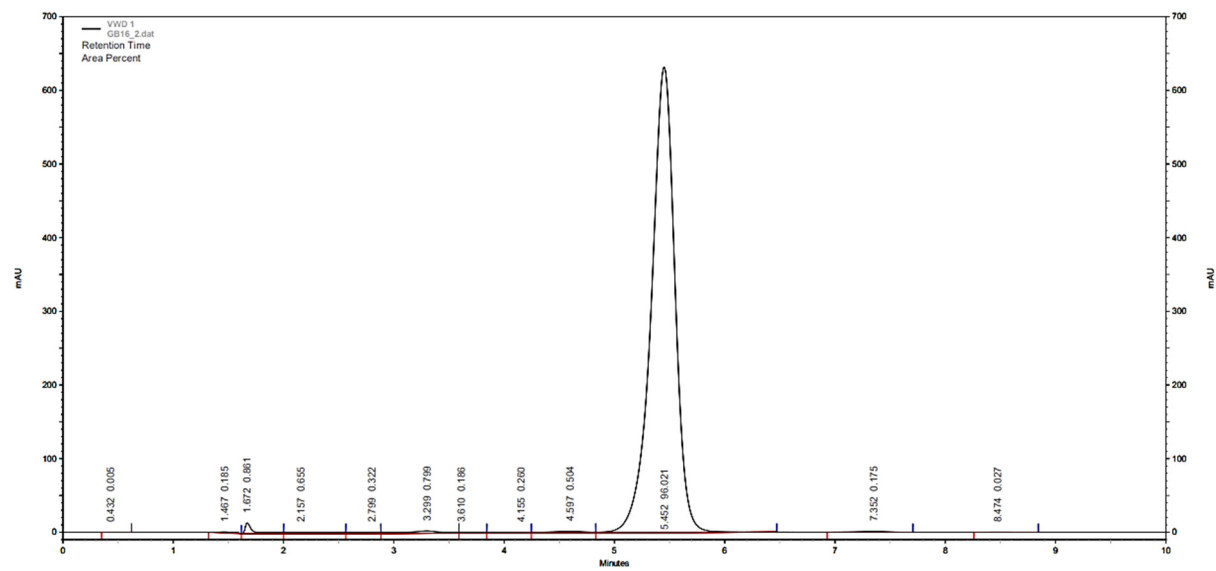
2. ¹H-NMR



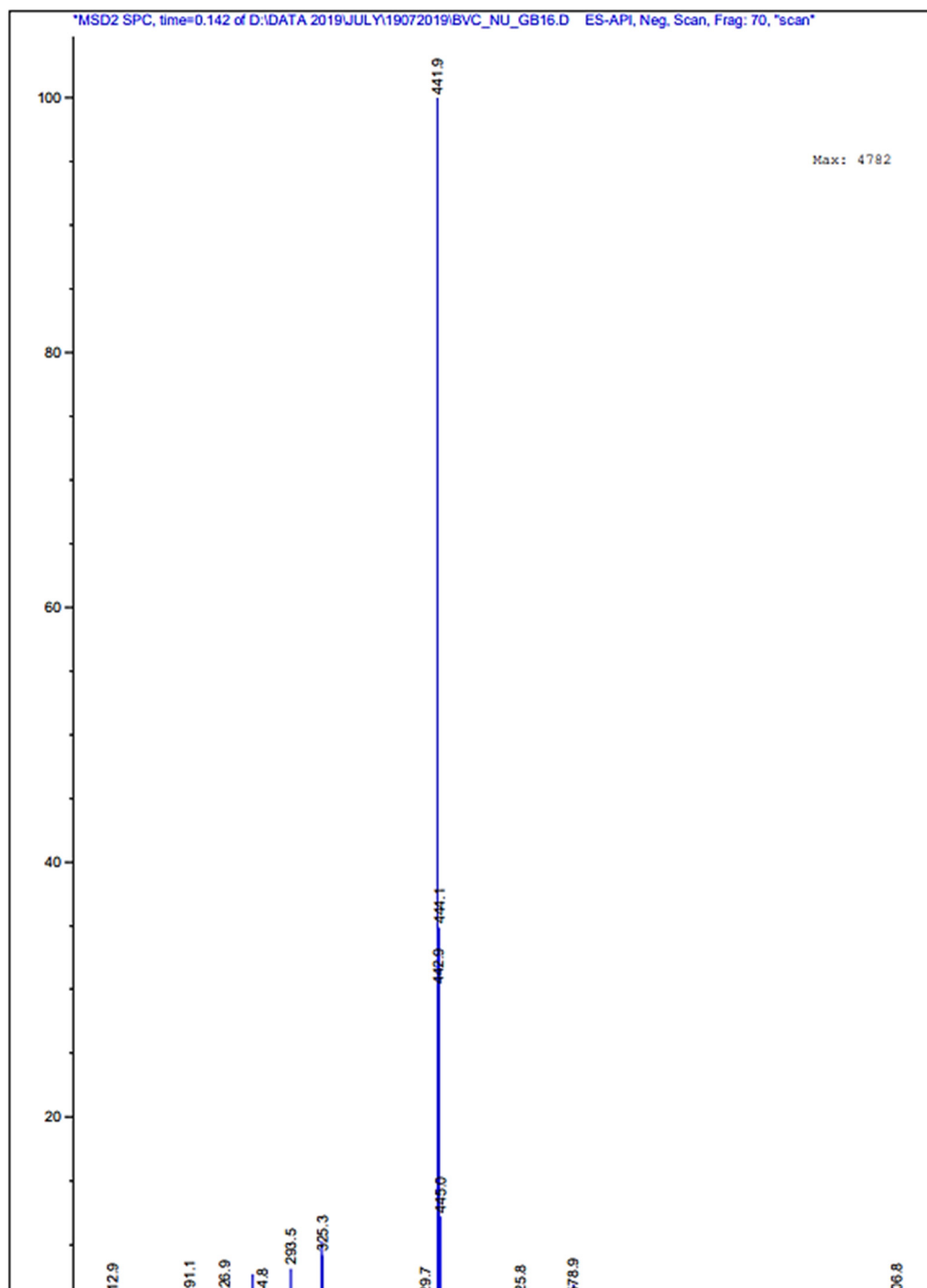
3. ¹³C-NMR



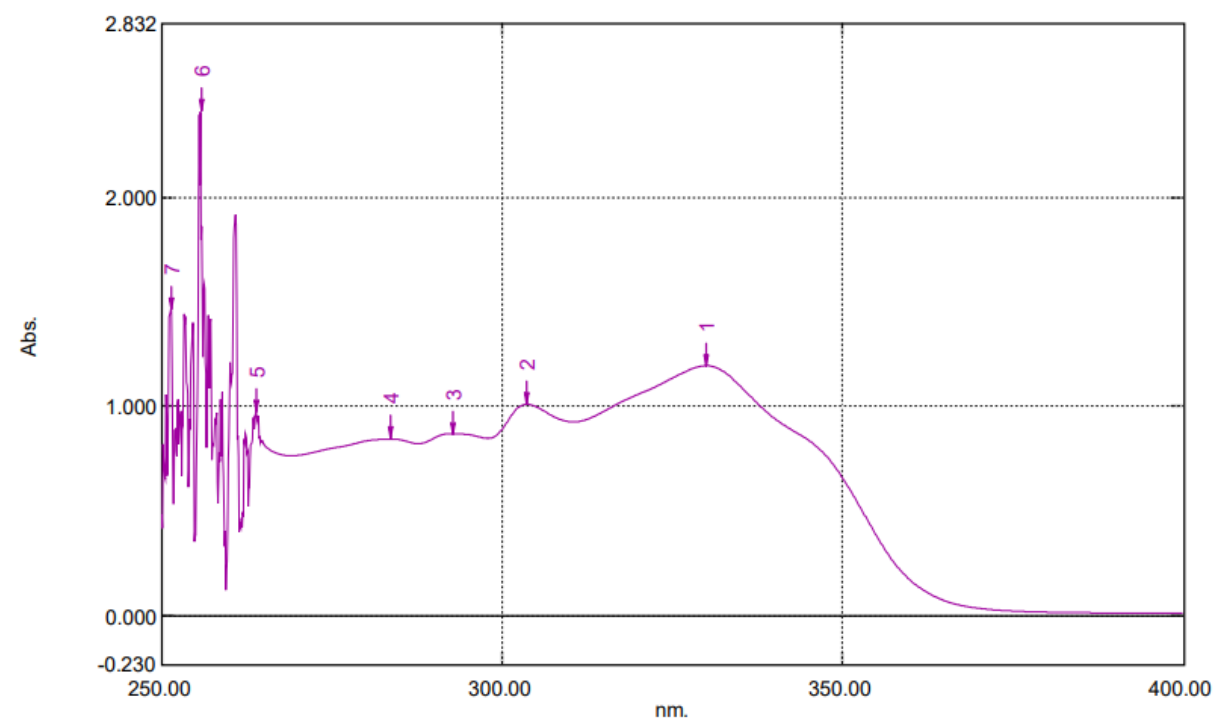
4. HPLC Analysis



5. Mass Spectrometry

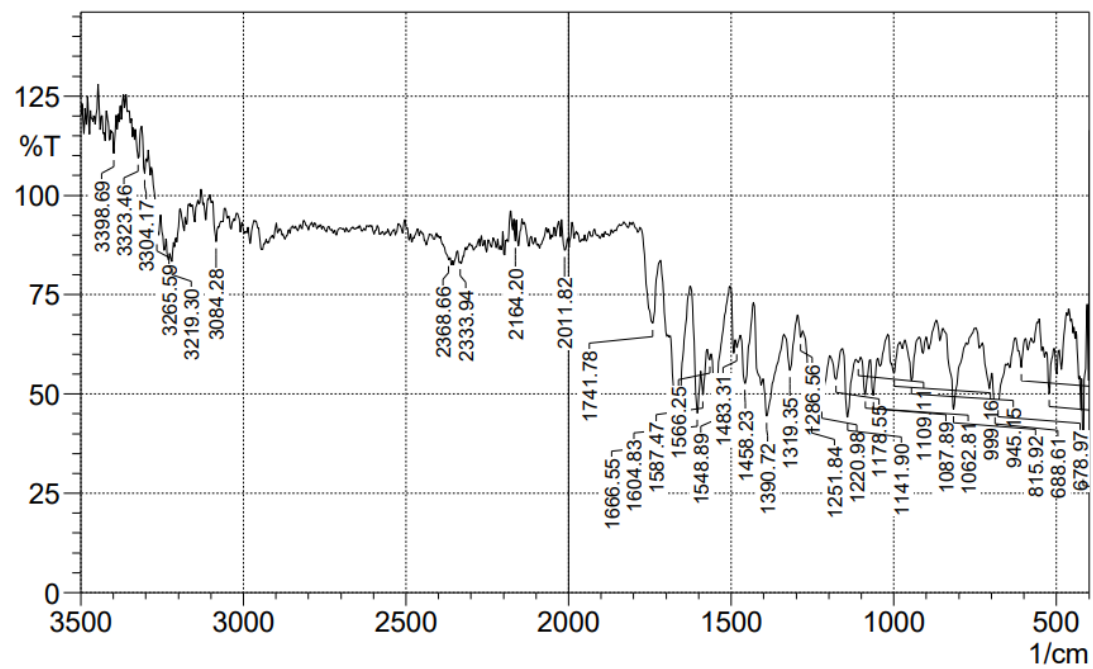


6. UV

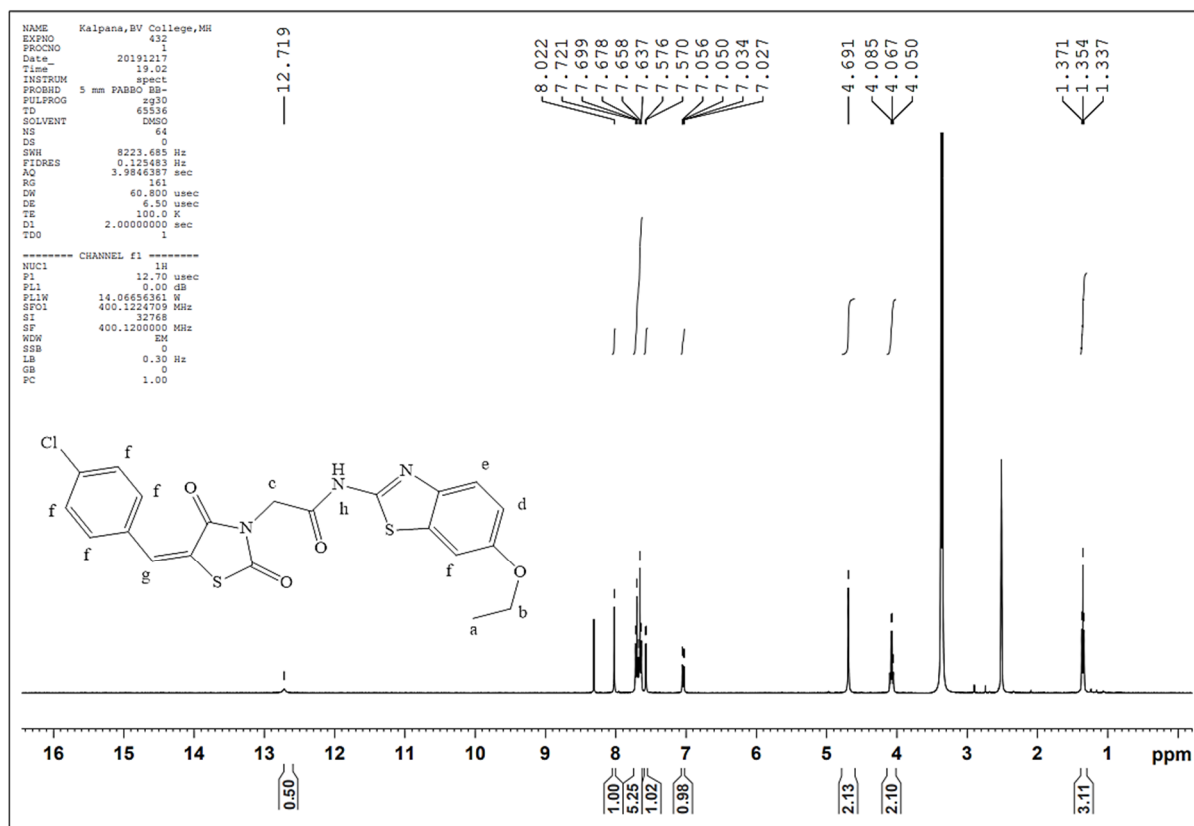


2-(5-(4-chlorobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-(6-ethoxybenzo[d]thiazol-2-yl)acetamide (GB17)

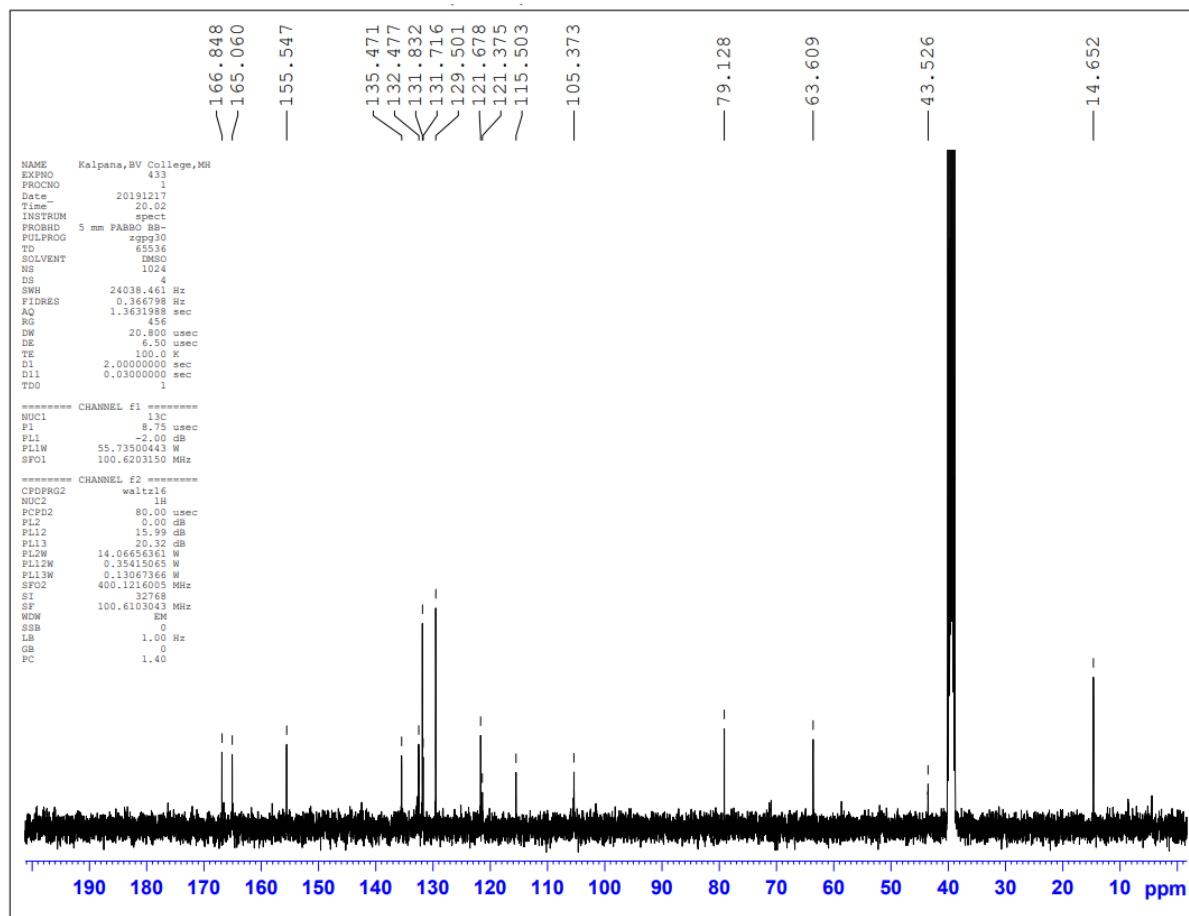
1. FTIR –



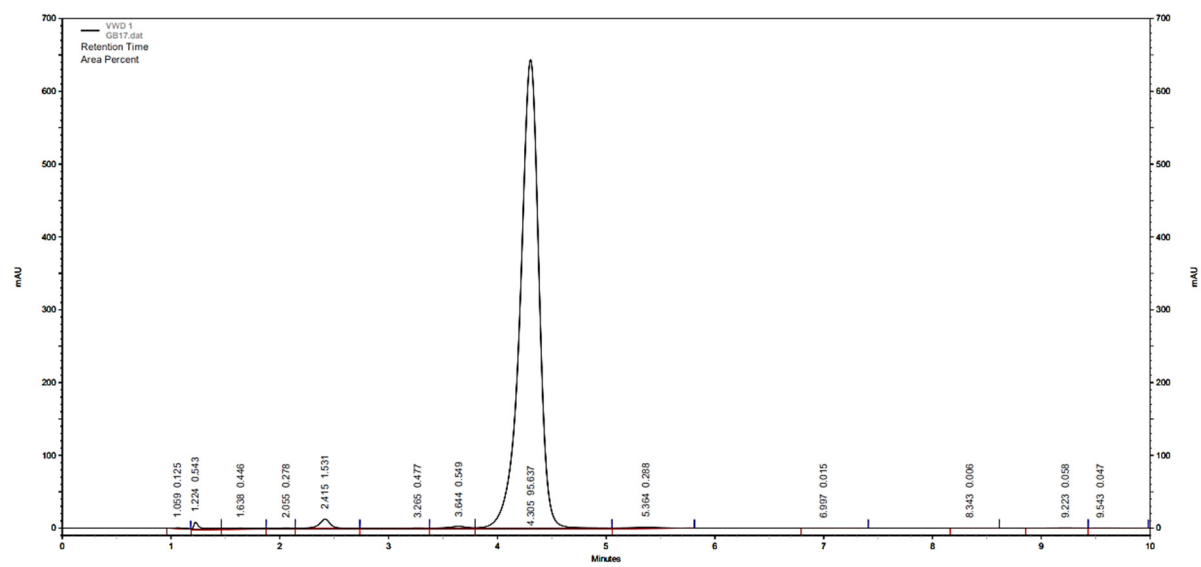
2. ¹H-NMR



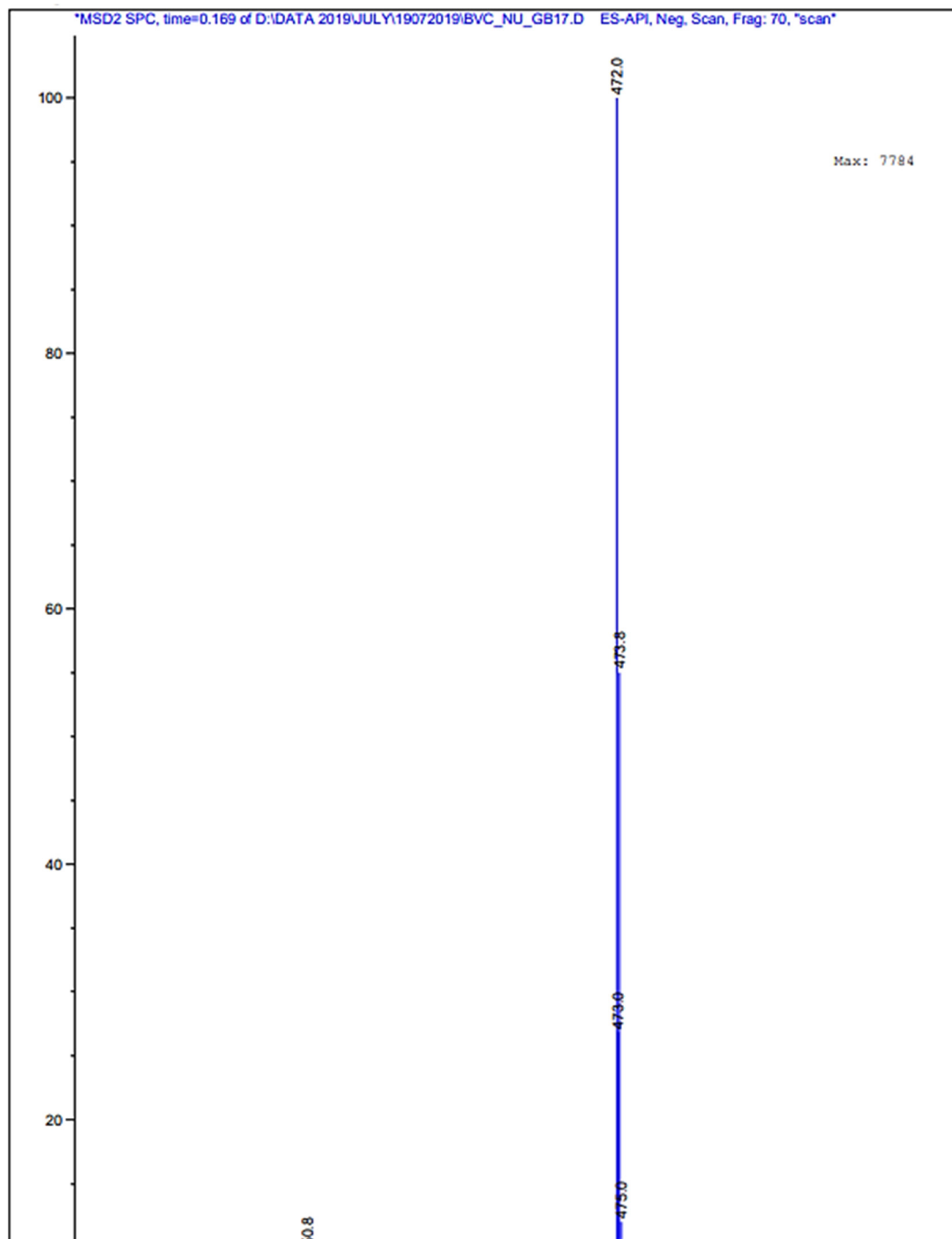
3. ¹³C-NMR



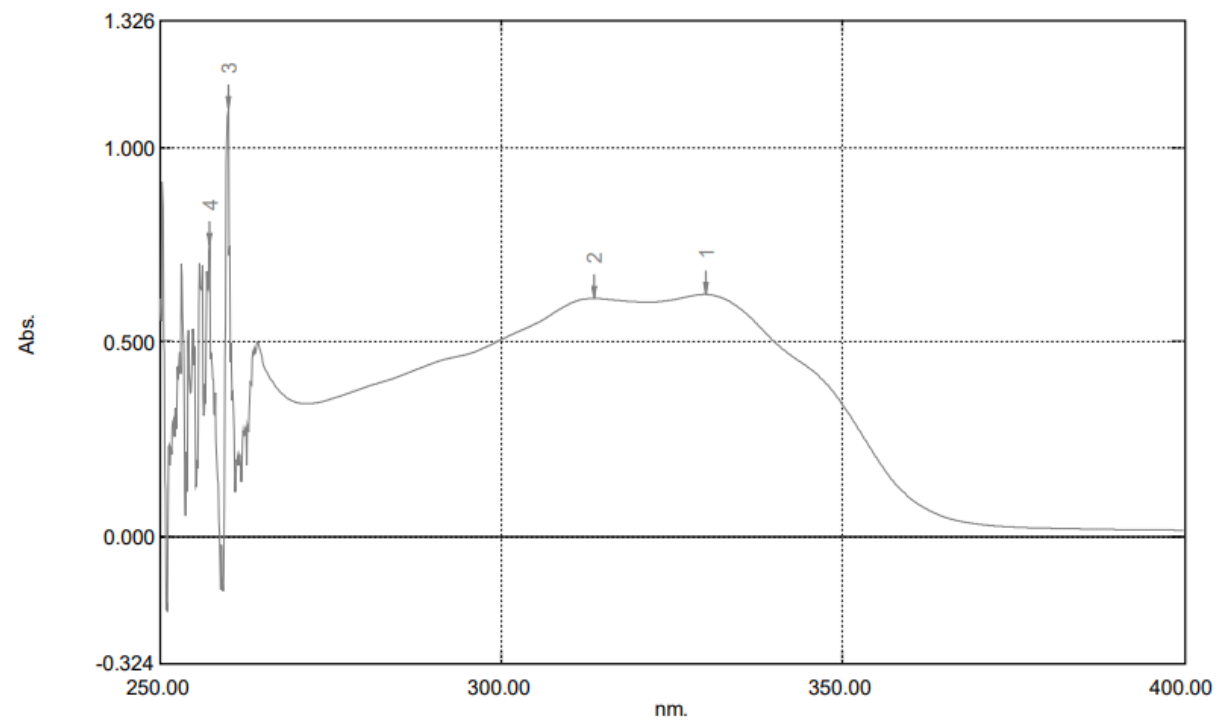
4. HPLC Analysis



5. Mass Spectrometry

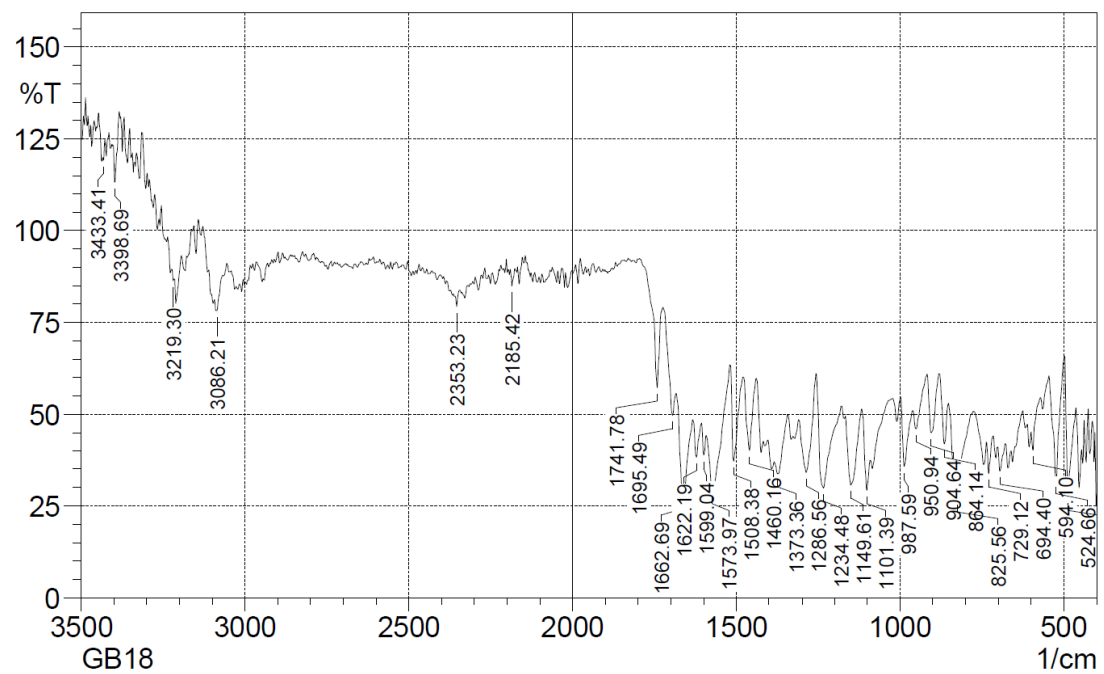


6. UV



N-(4,6-difluorobenzo[d]thiazol-2-yl)-2-(5-(4-fluorobenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB18)

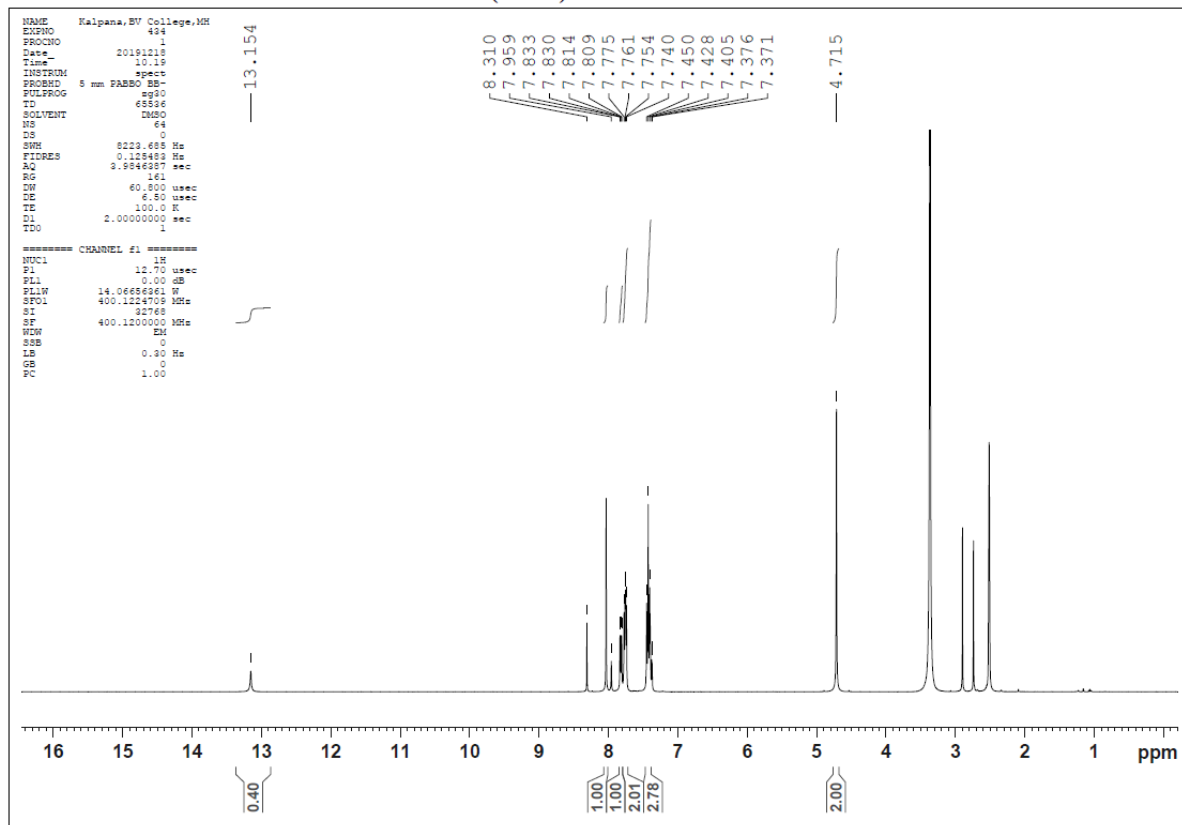
1. FTIR



2. 1H-NMR

SAIFNM190323A-31(GB18)

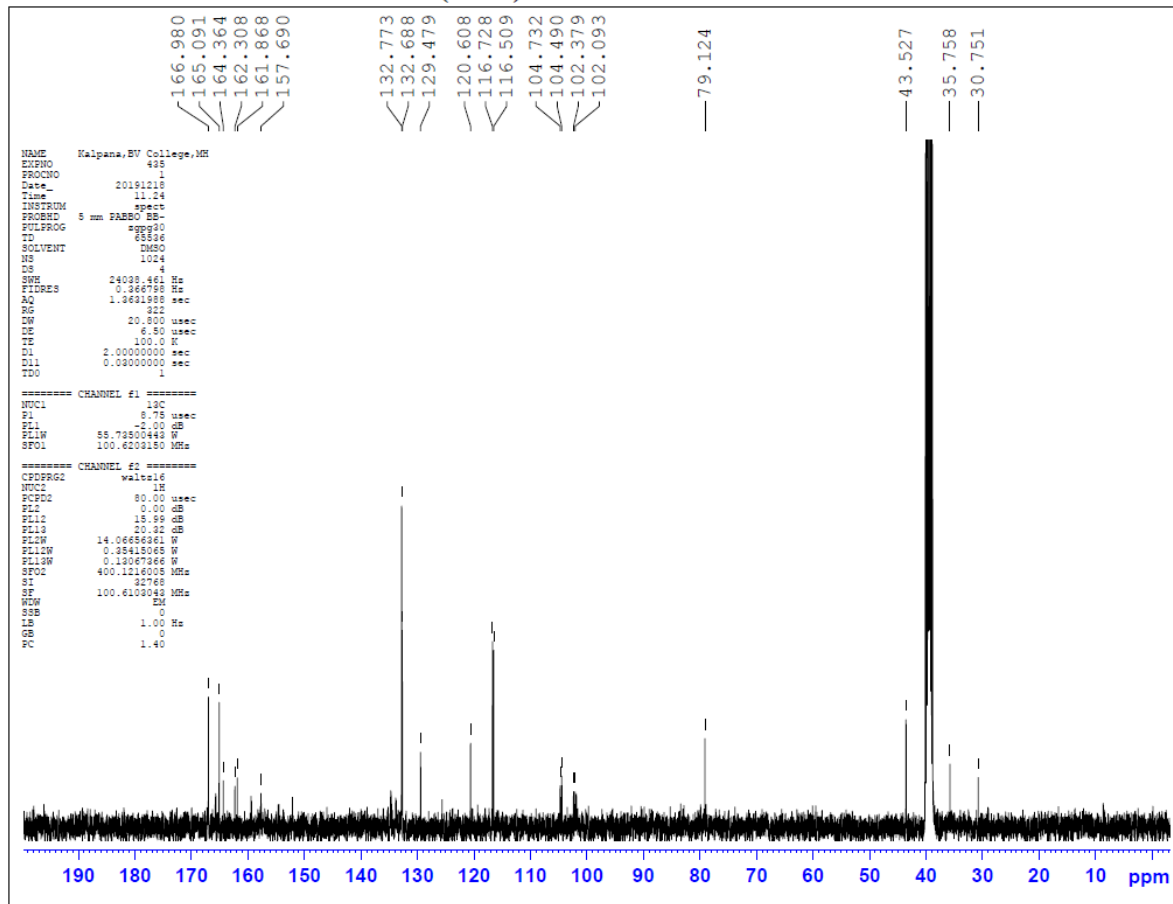
SAIF Cochin



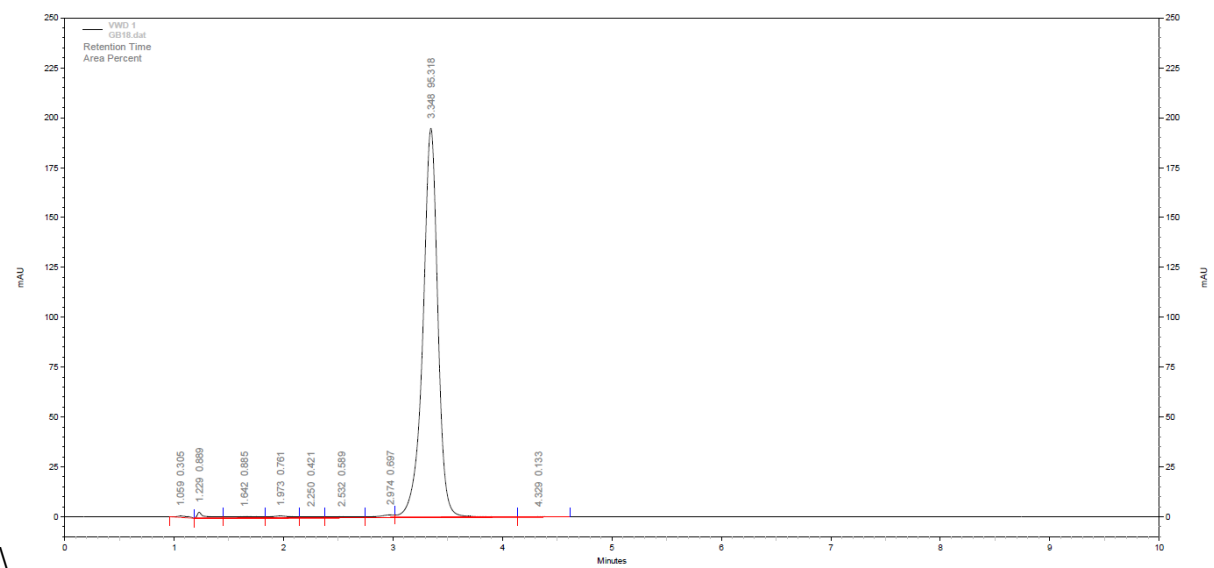
3. 13C-NMR

SAIFNM190323A-32(GB18)

SAIF Cochin

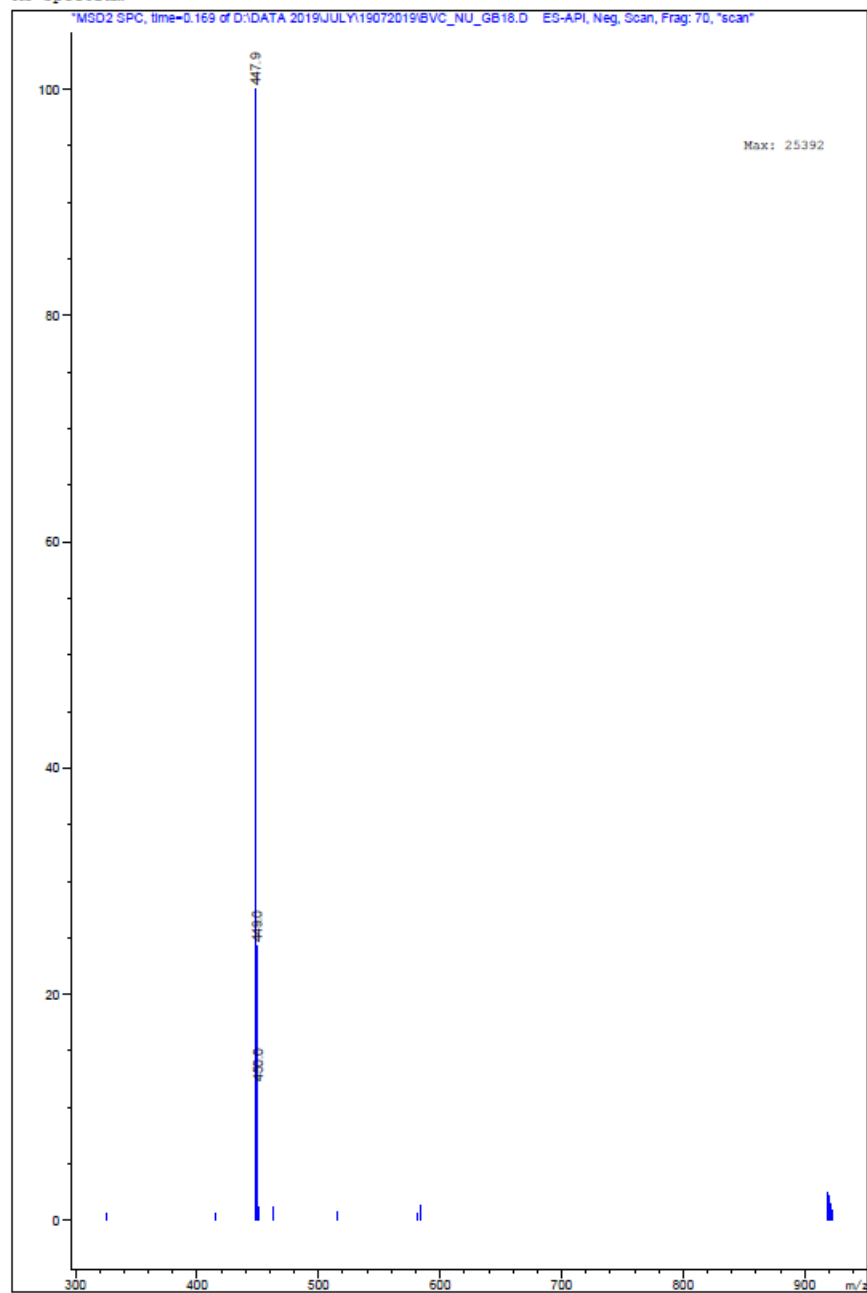


4. HPLC



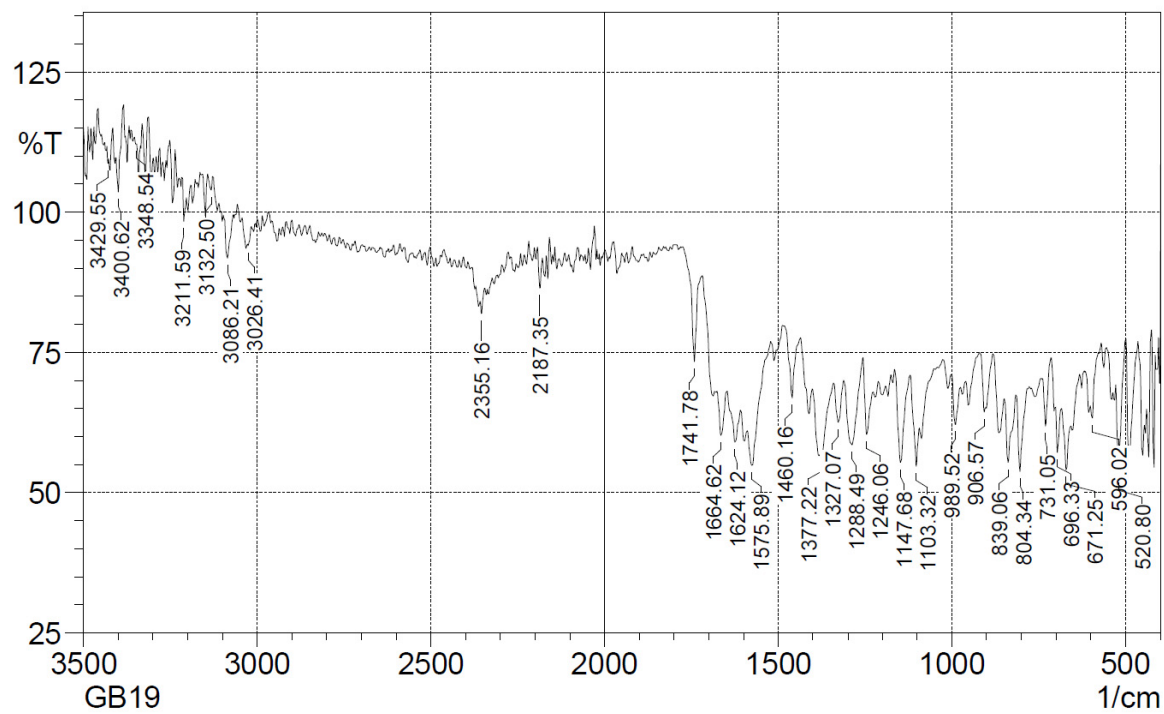
5. Mass

MS Spectrum



N-(4,6-difluorobenzo[d]thiazol-2-yl)-2-(5-(4-methylbenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB19)

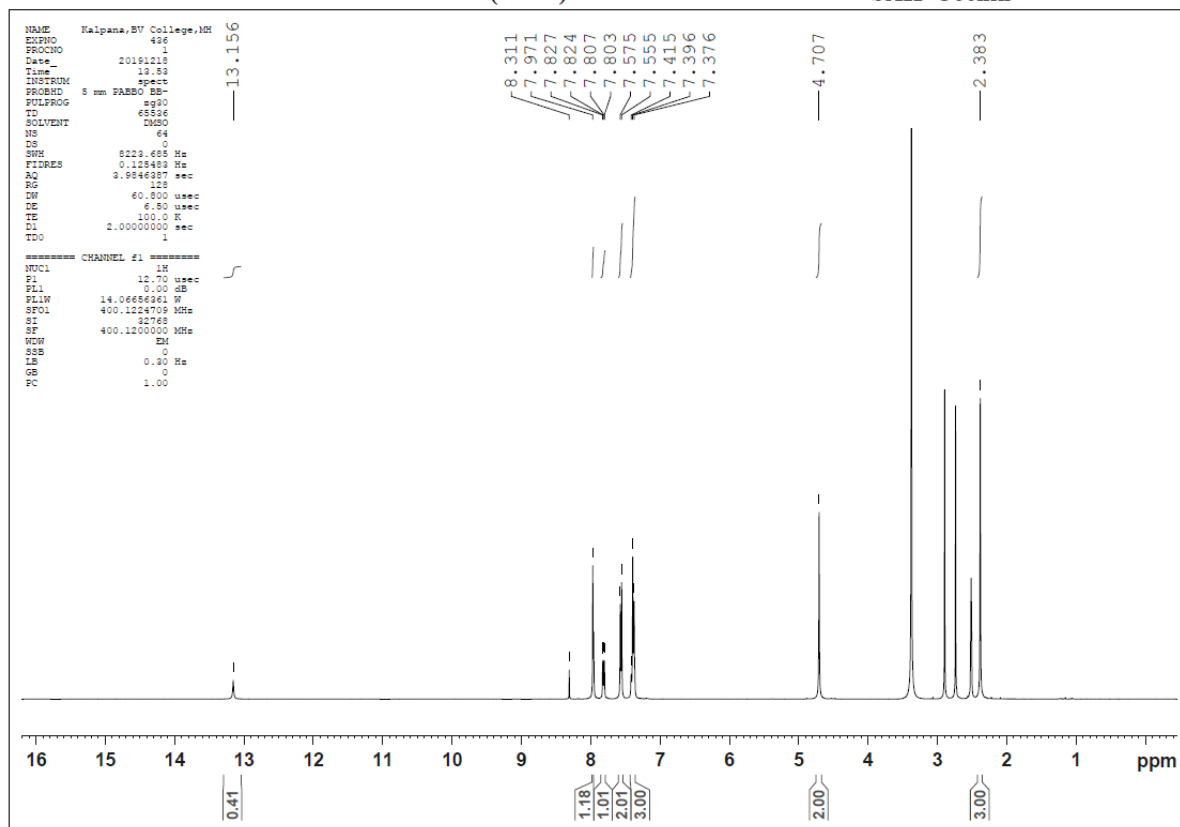
1. FTIR



2. 1H-NMR

SAIFNM190323A-33(GB19)

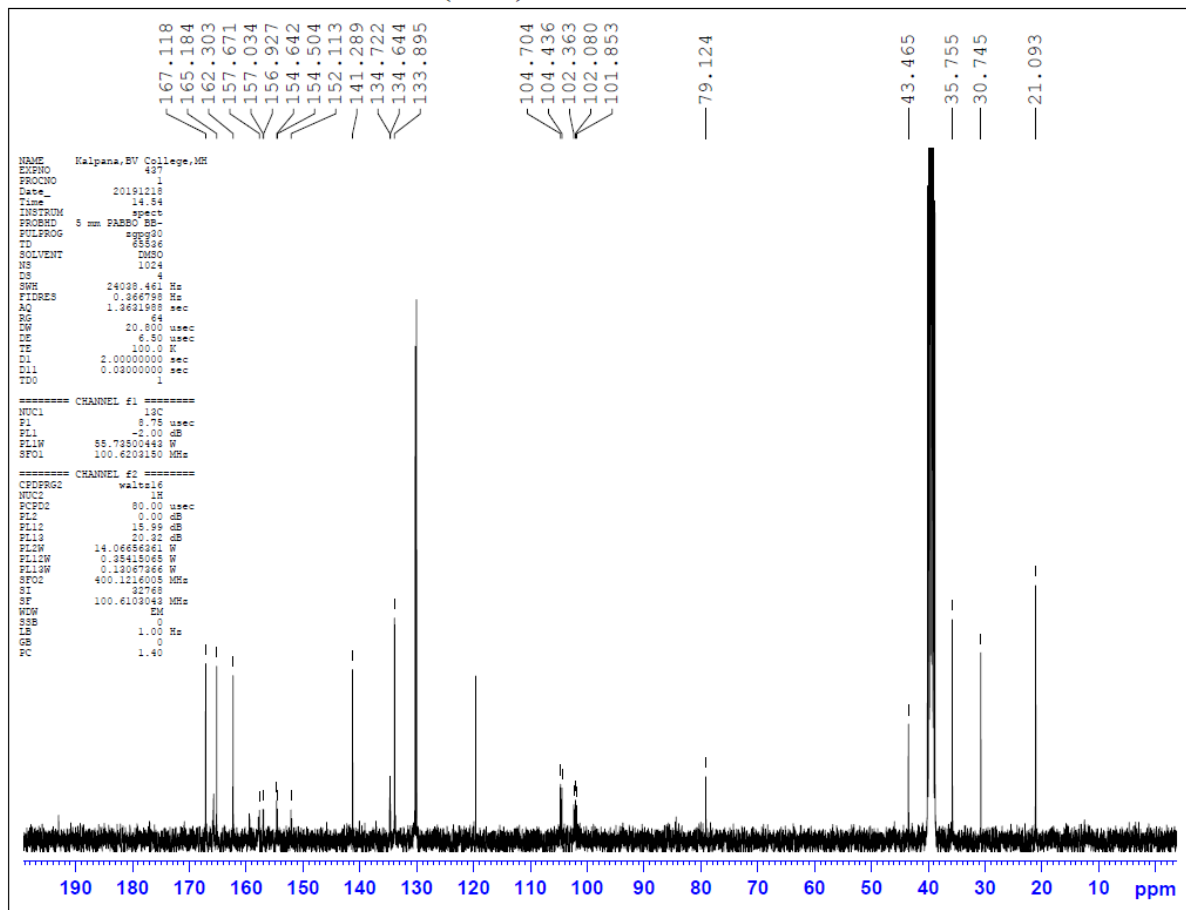
SAIF Cochin



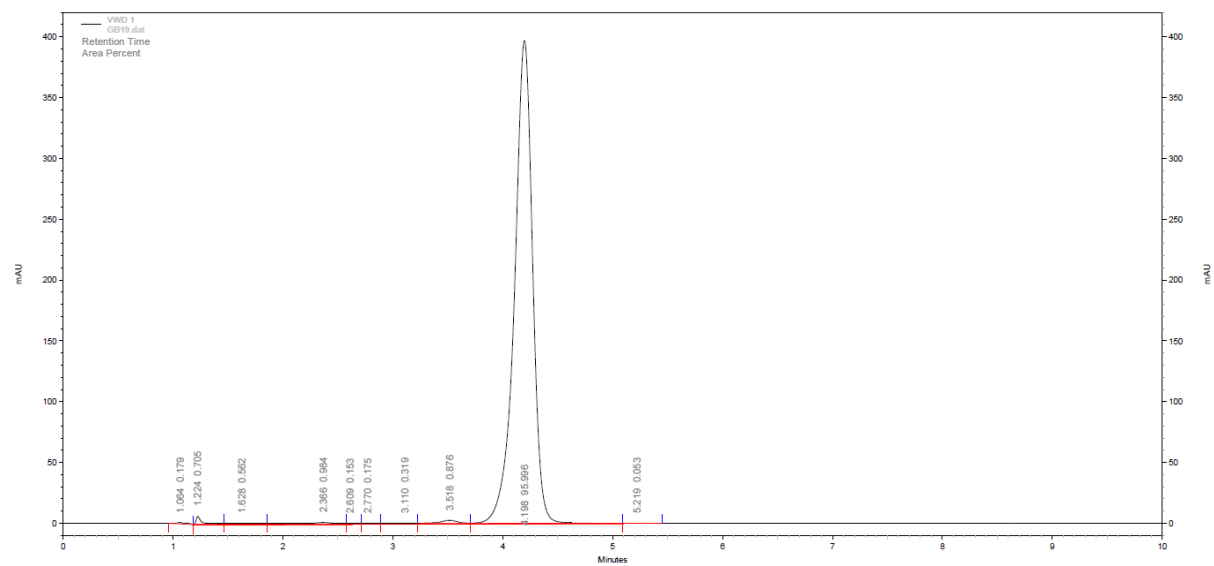
3. 13C-NMR

SAIFNM190323A-34(GB19)

SAIF Cochin

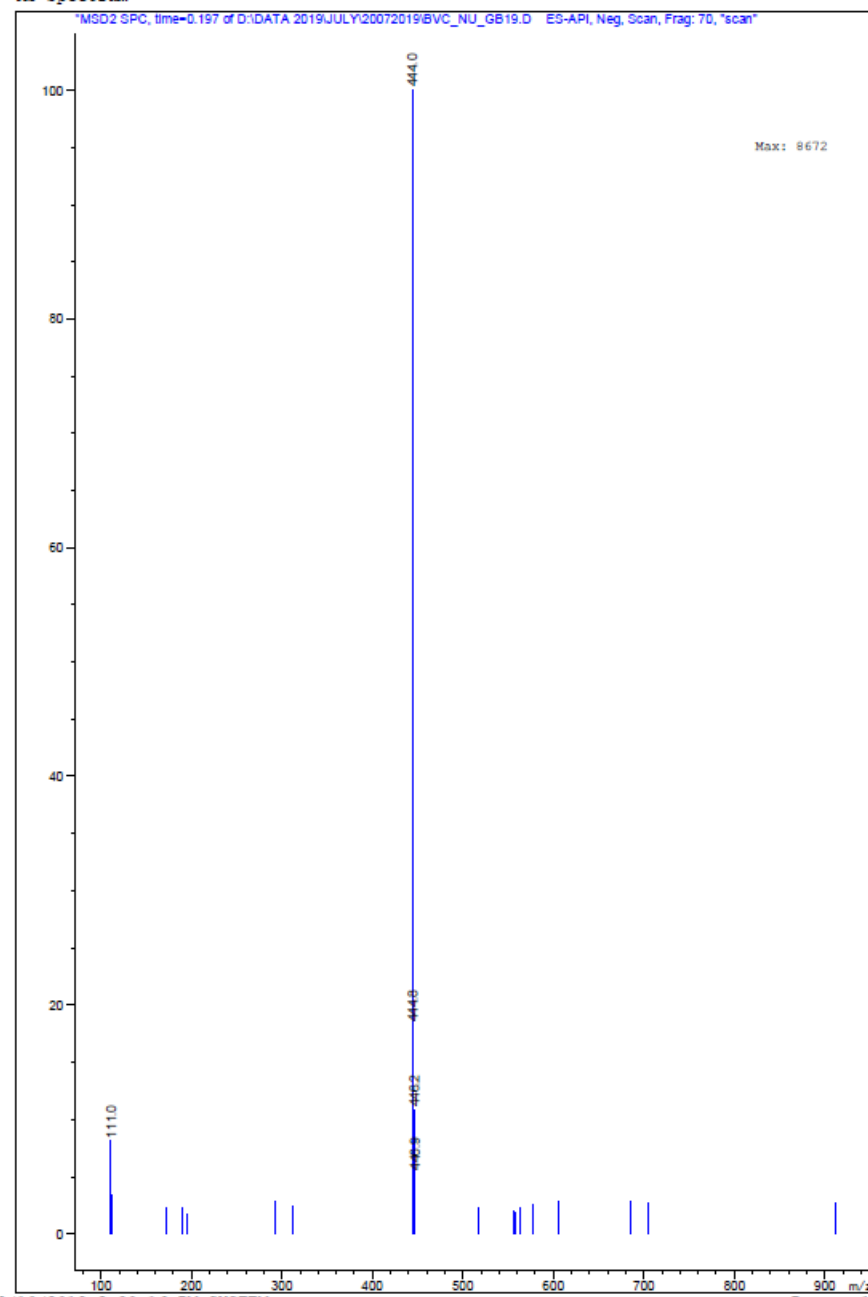


4. HPLC



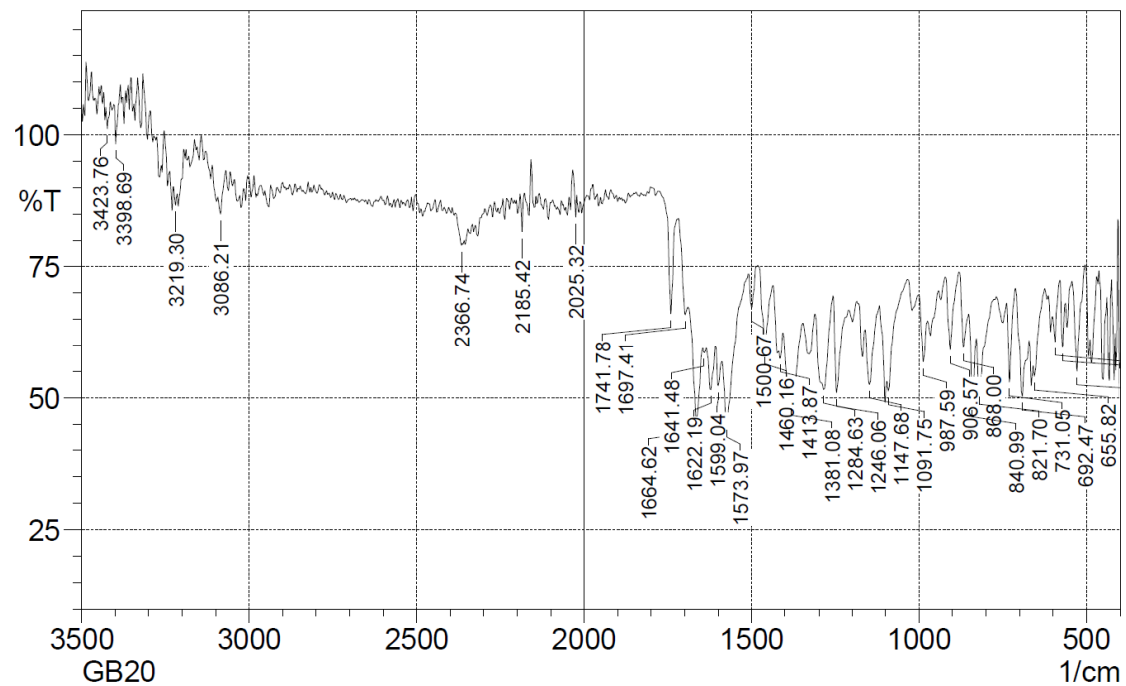
5. Mass

MS Spectrum



N-(4,6-difluorobenzo[d]thiazol-2-yl)-2-(5-(3,4-dimethylbenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB20)

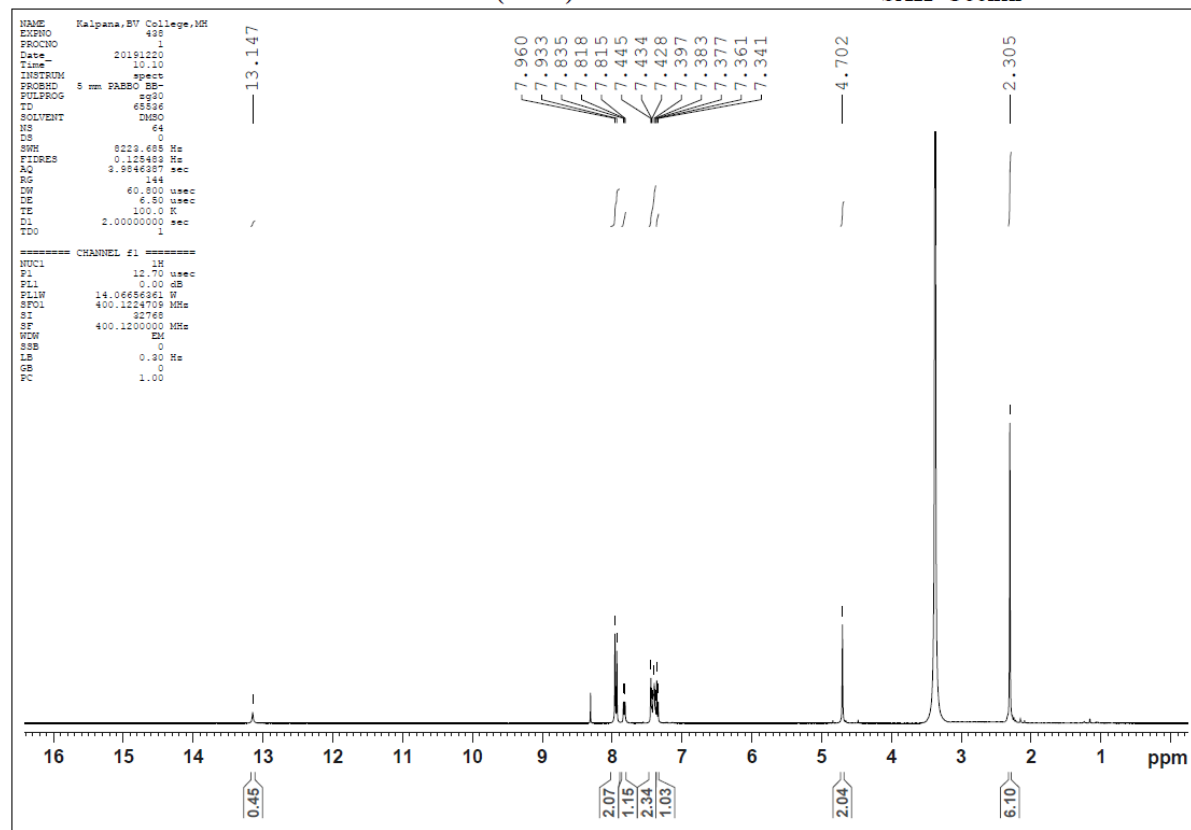
1. FTIR



2. 1H-NMR

SAIFNM190323A-35(GB20)

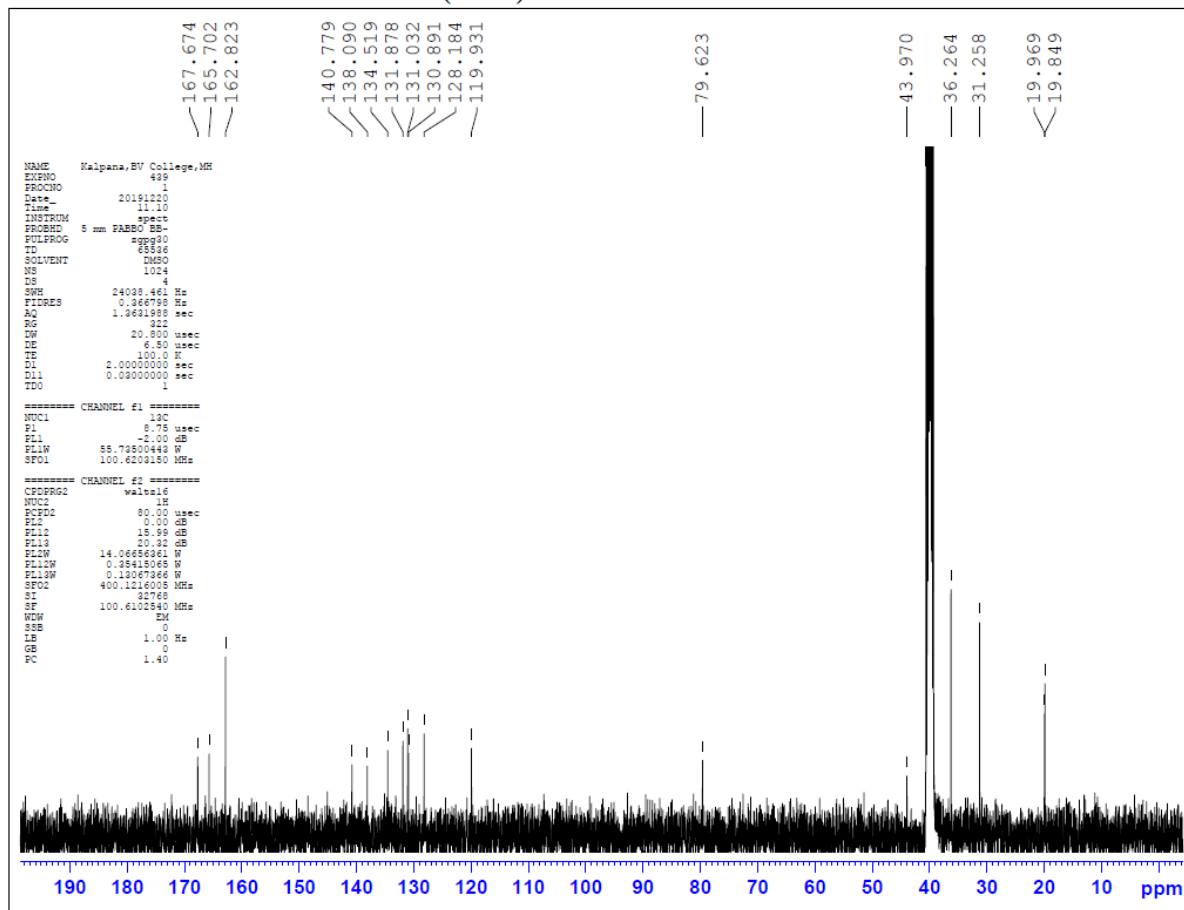
SAIF Cochin



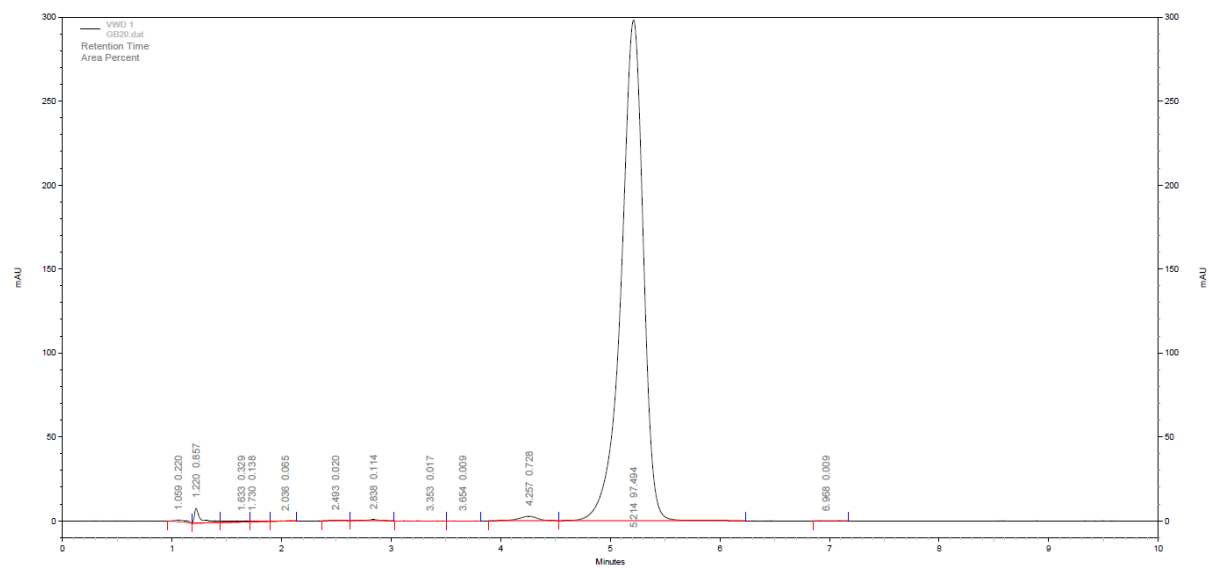
3. 13C-NMR

SAIFNM190323A-36(GB20)

SAIF Cochin

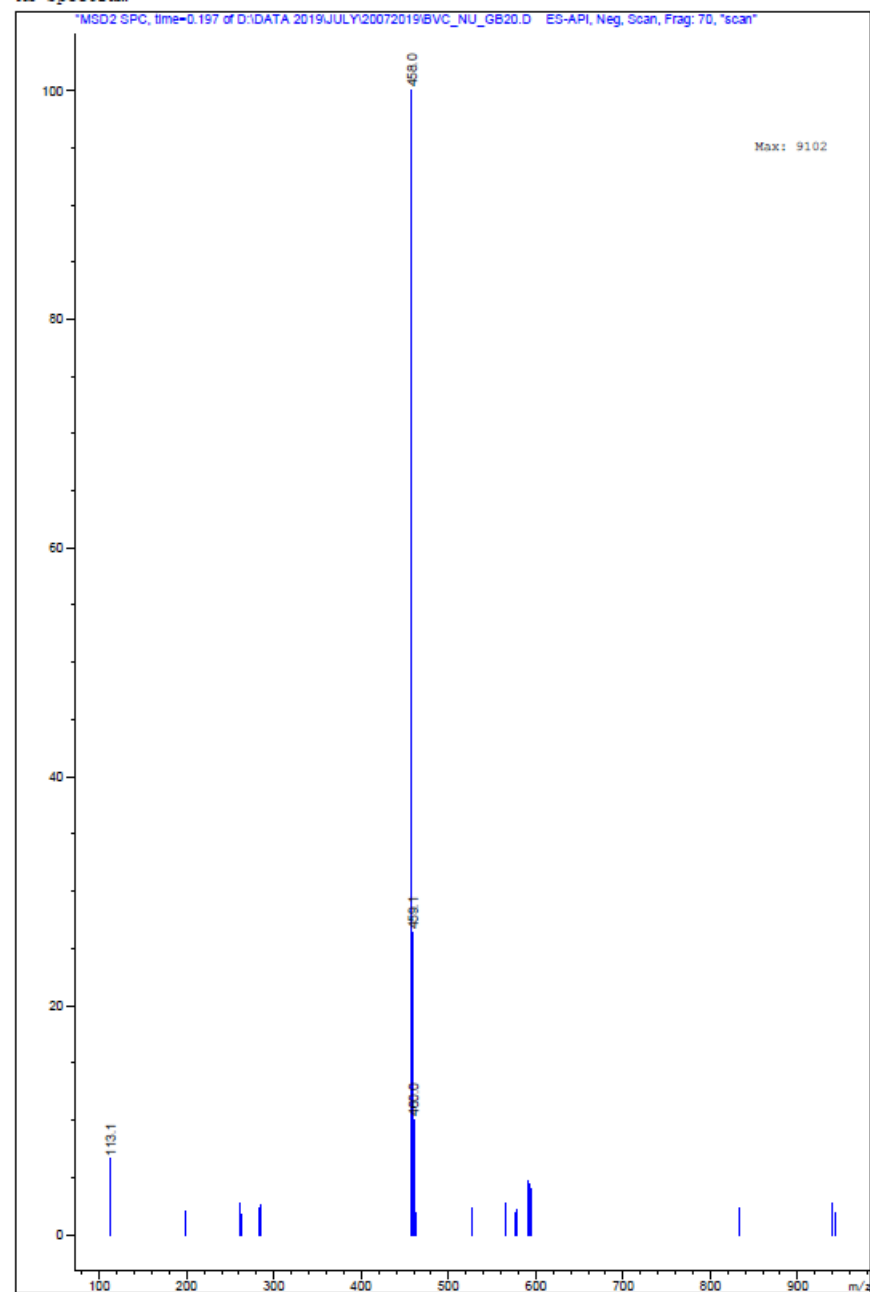


4. HPLC



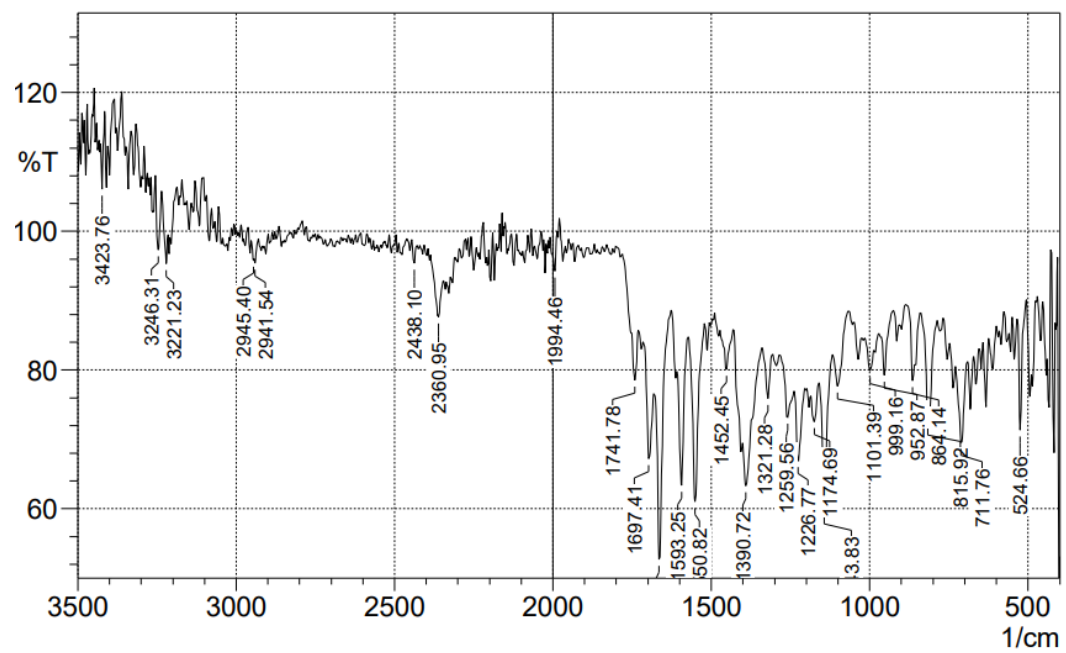
5. Mass

MS Spectrum

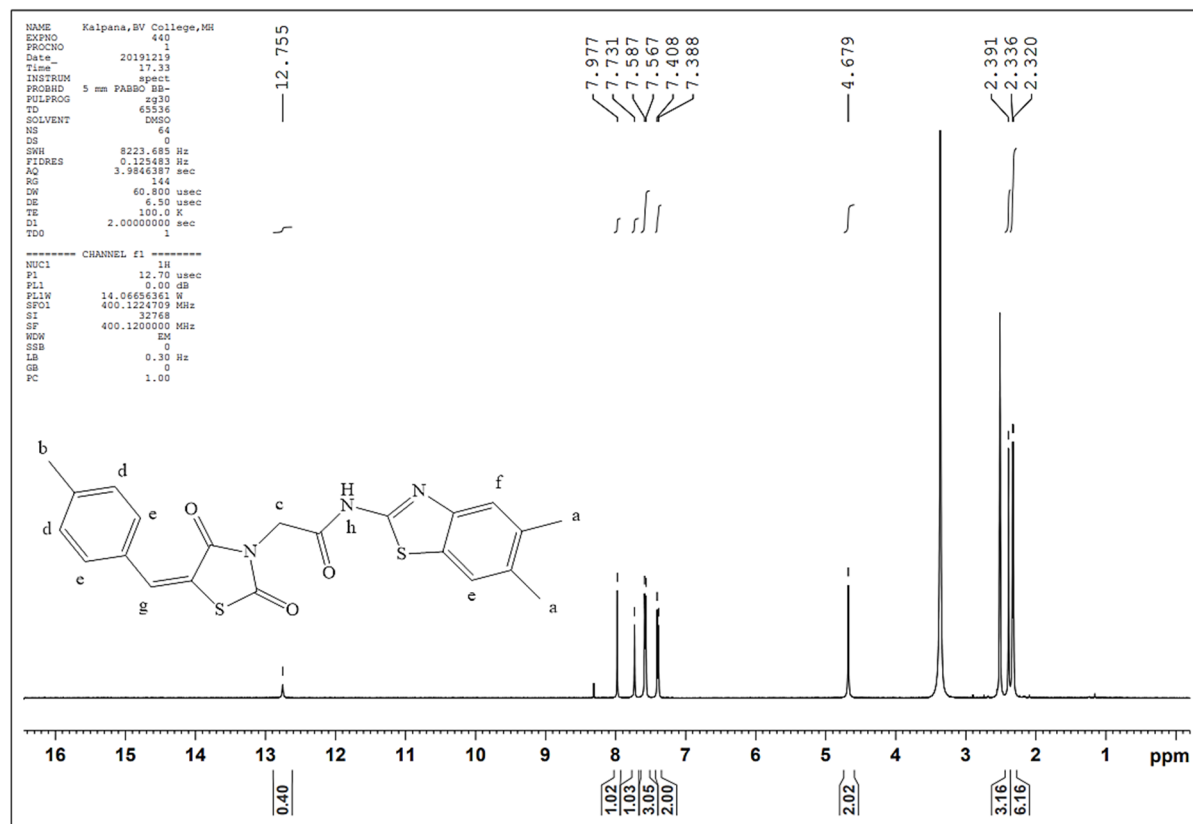


N-(5,6-dimethylbenzo[d]thiazol-2-yl)-2-(5-(4-methylbenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB21)

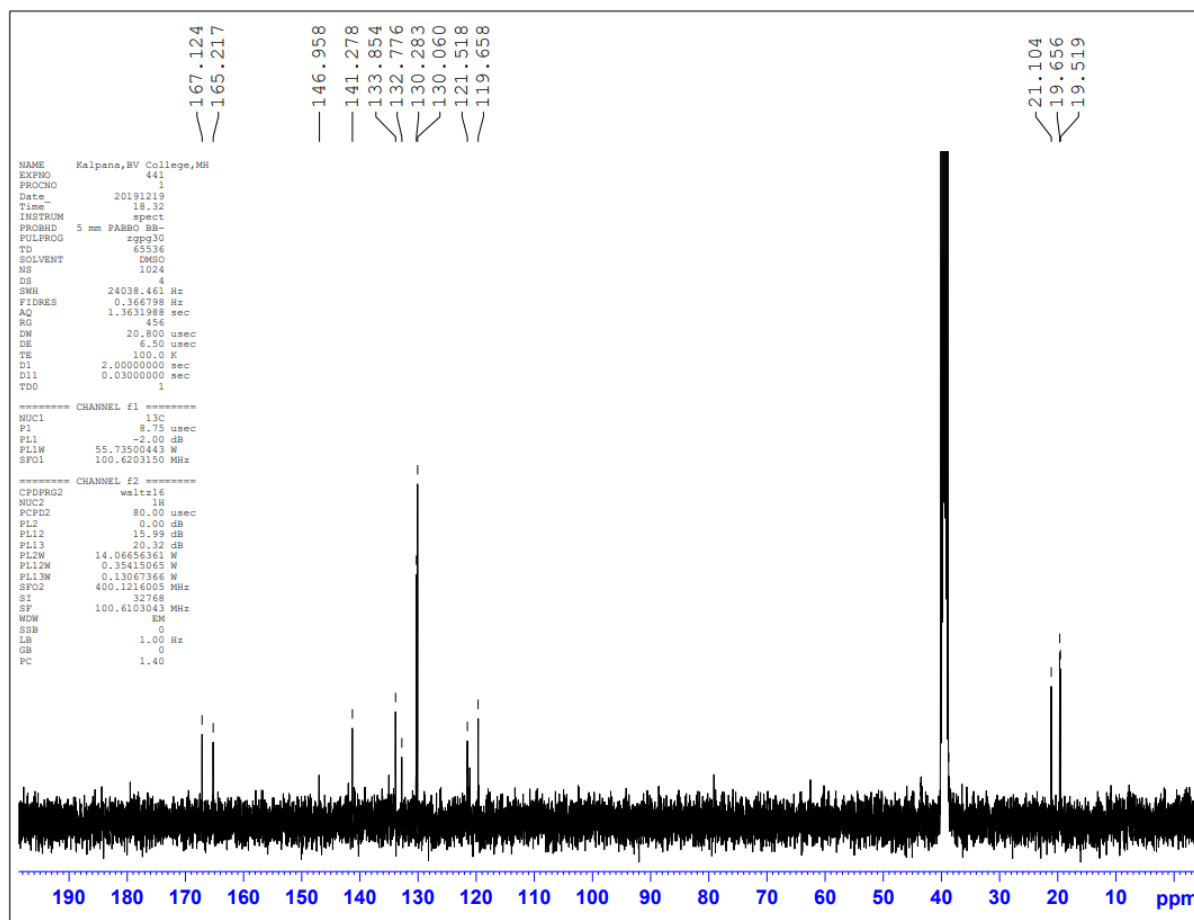
1. FTIR



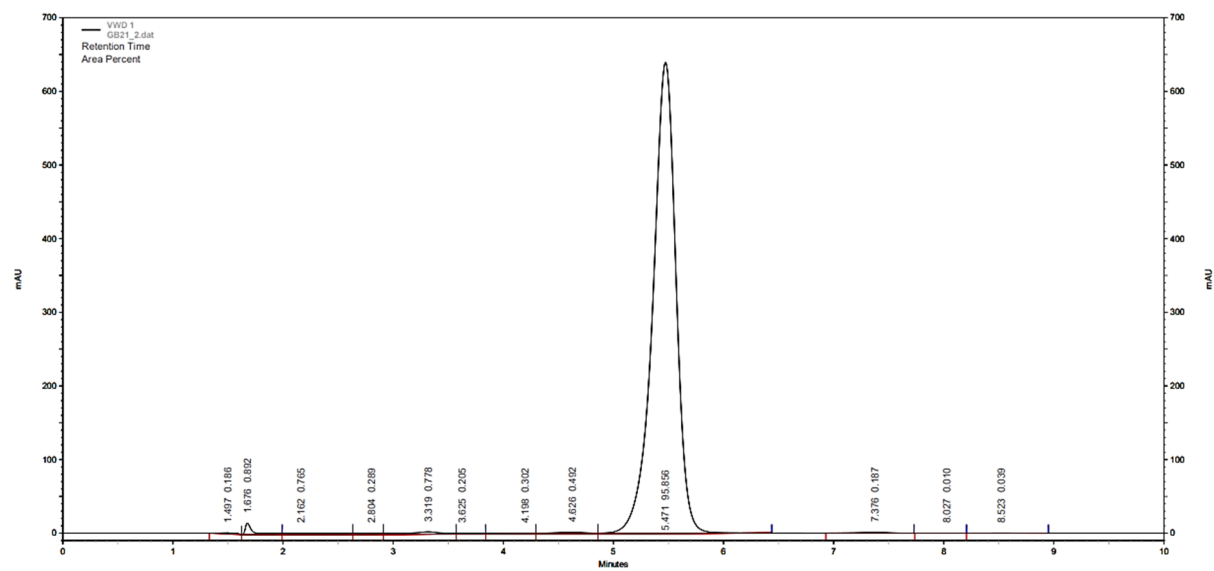
2. ¹H-NMR



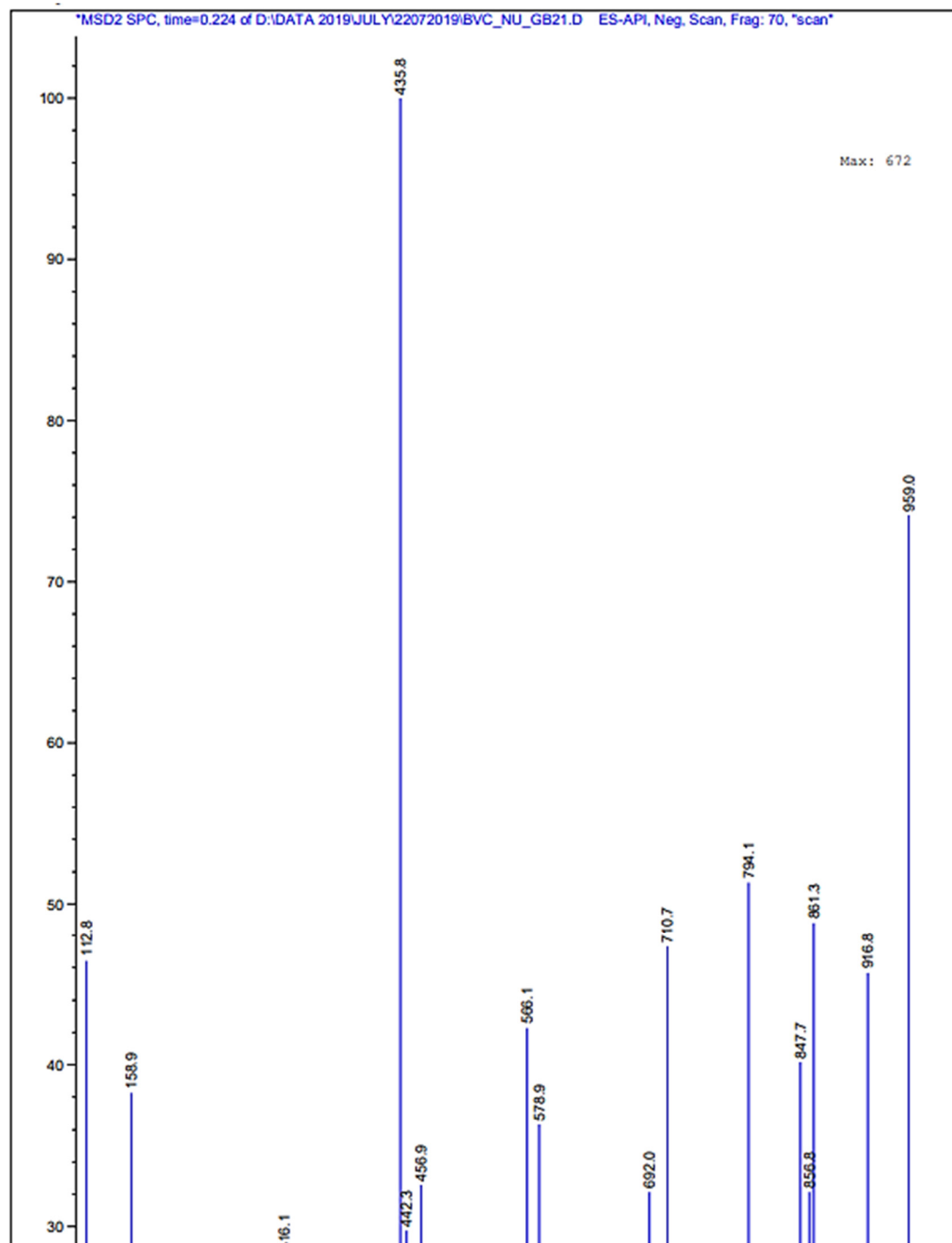
3. ¹³C-NMR



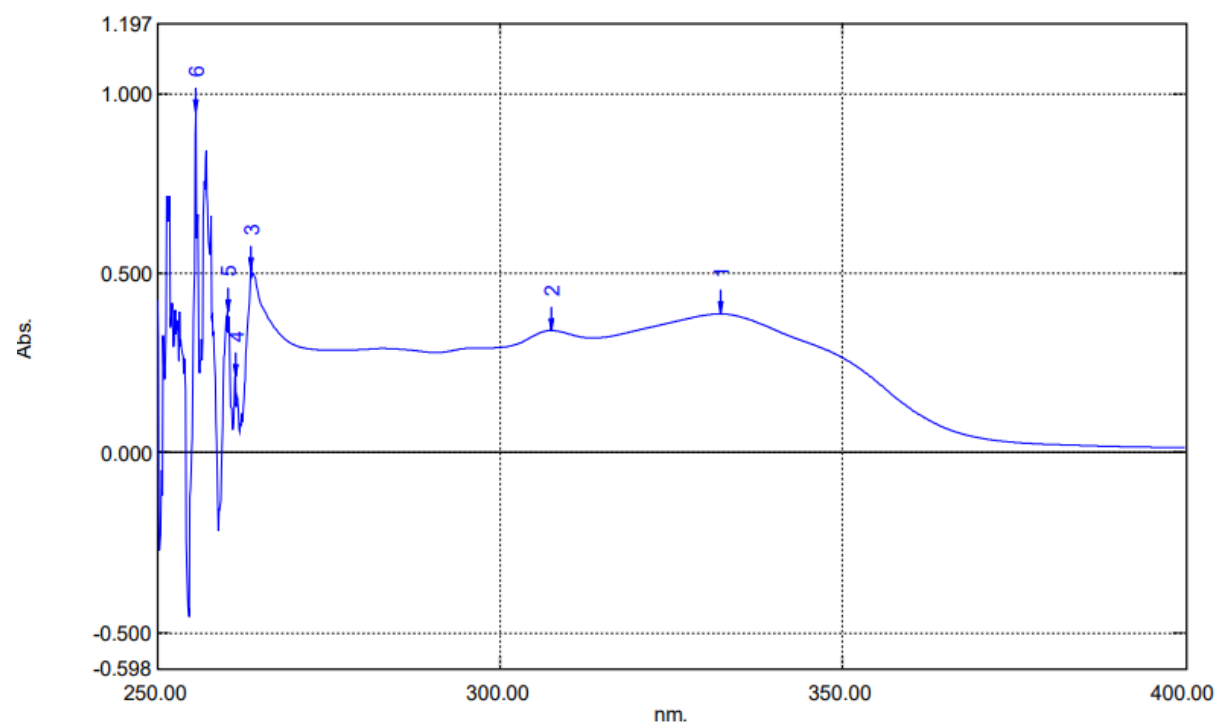
4. HPLC Analysis



5. Mass Spectrometry

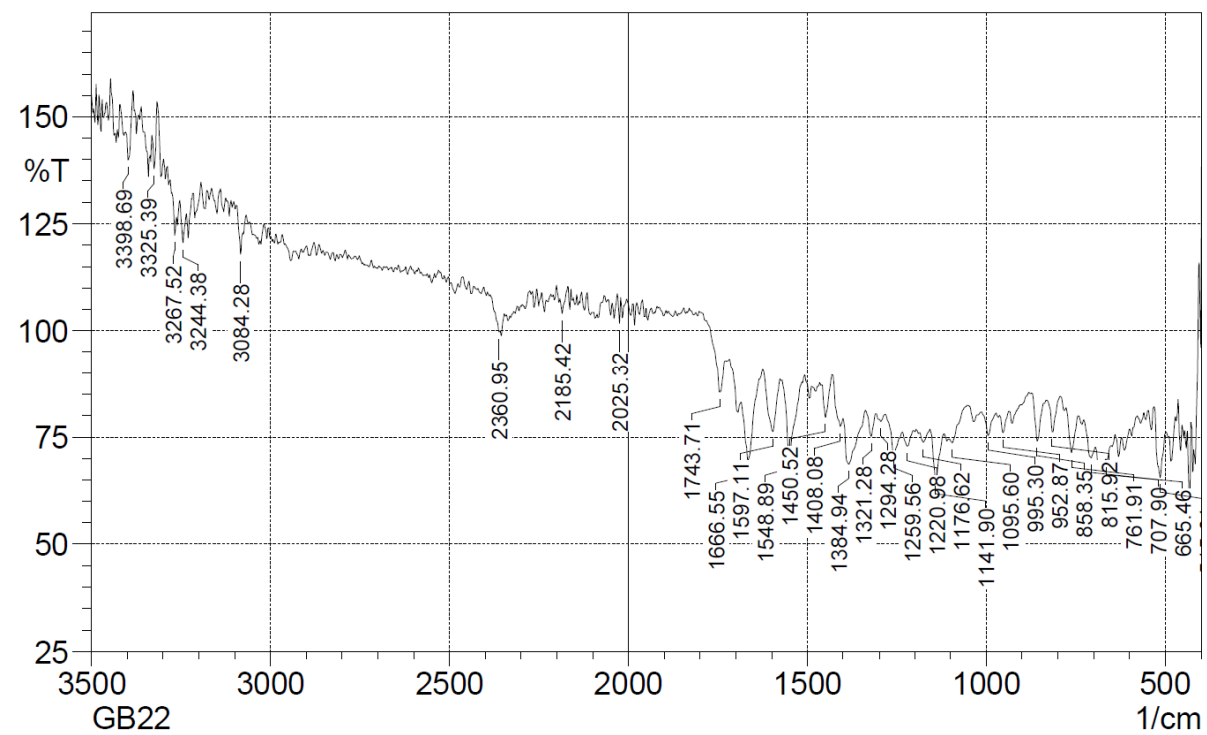


6. UV

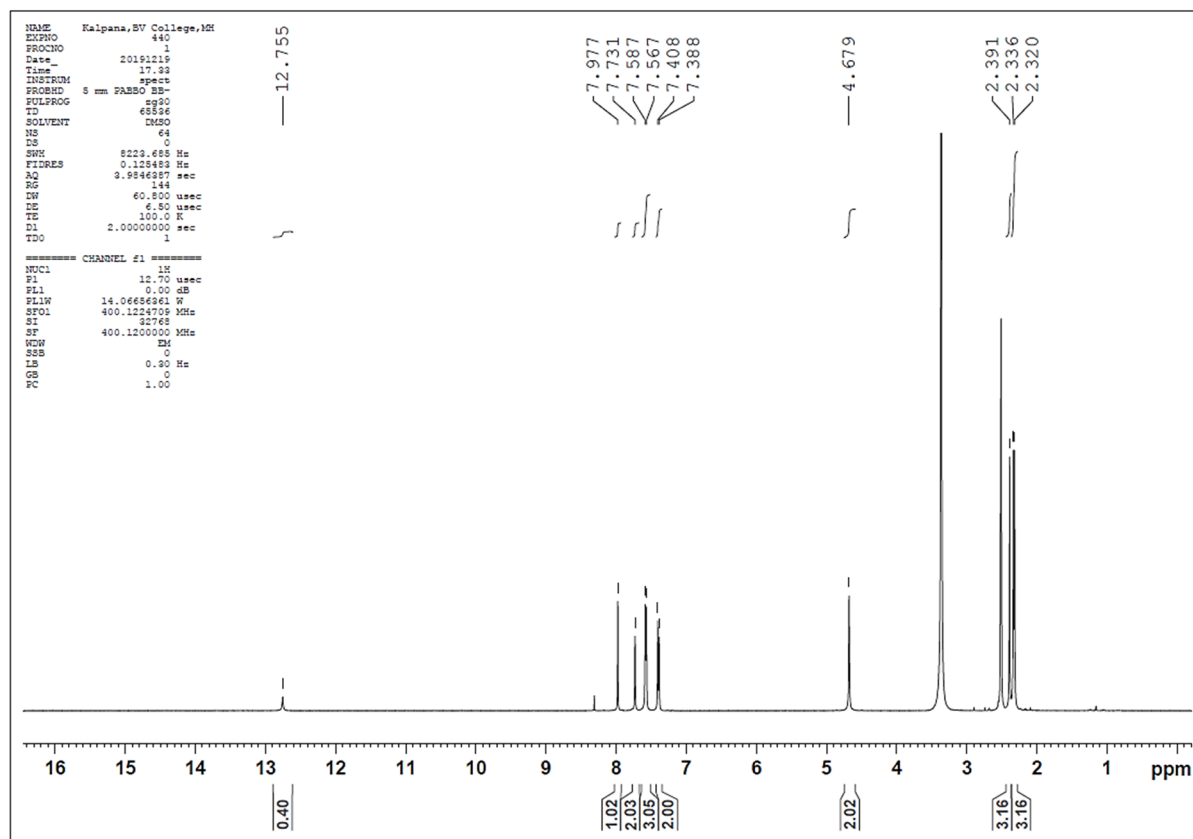


2-(5-benzylidene-2,4-dioxothiazolidin-3-yl)-N-(5,6-dimethylbenzo[d]thiazol-2-yl)acetamide (GB22)

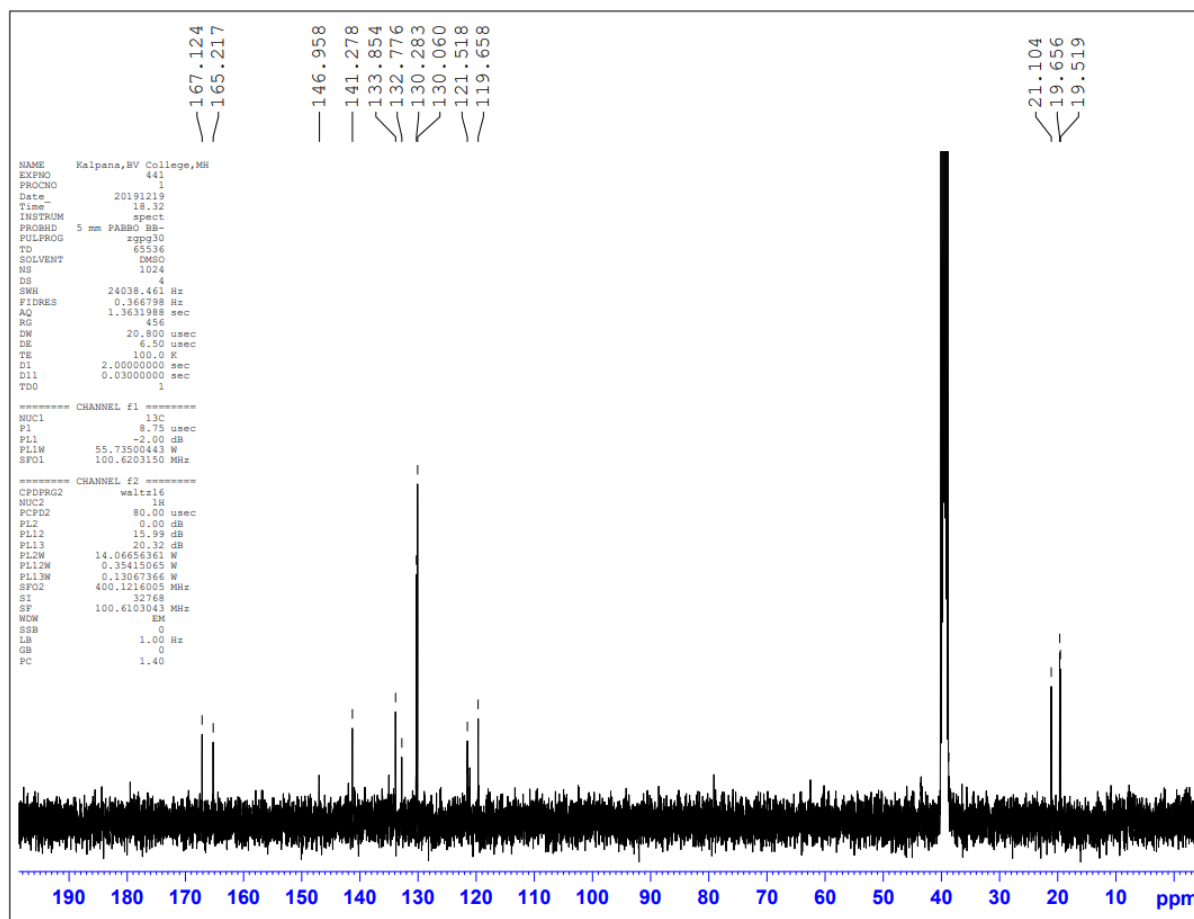
1. FTIR



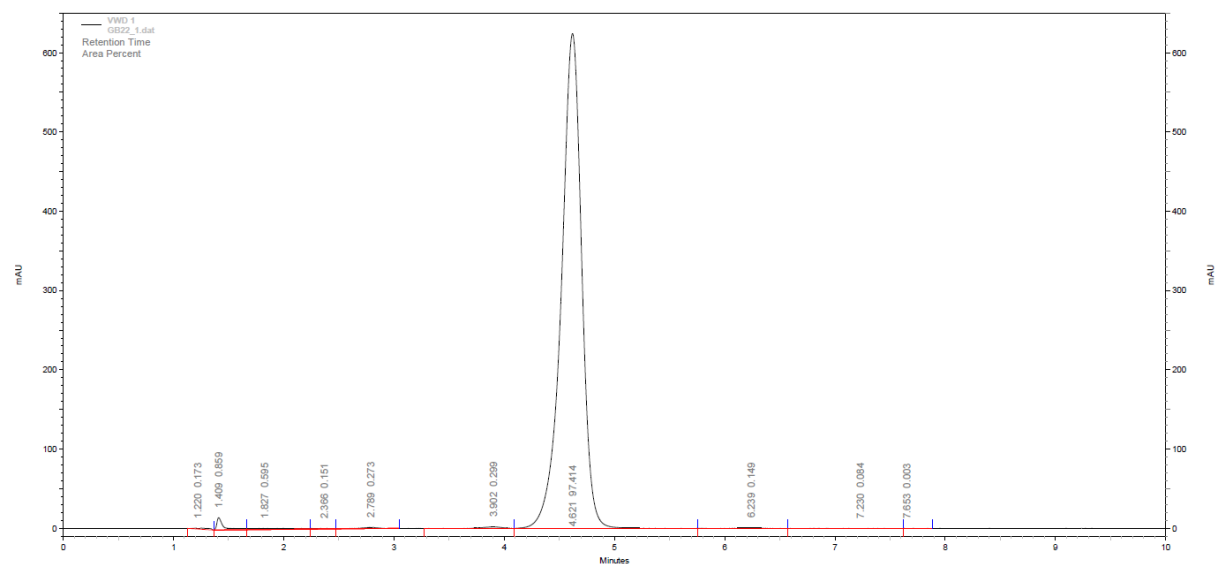
2. ^1H -NMR



3. ¹³C-NMR

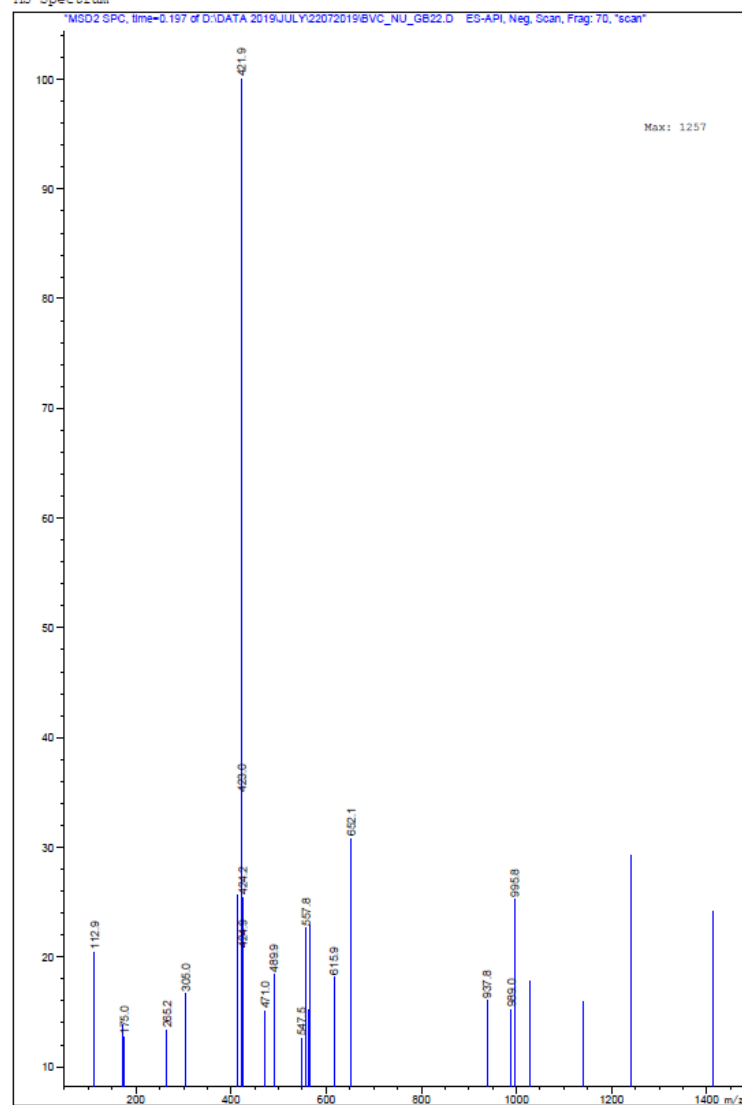


4. HPLC



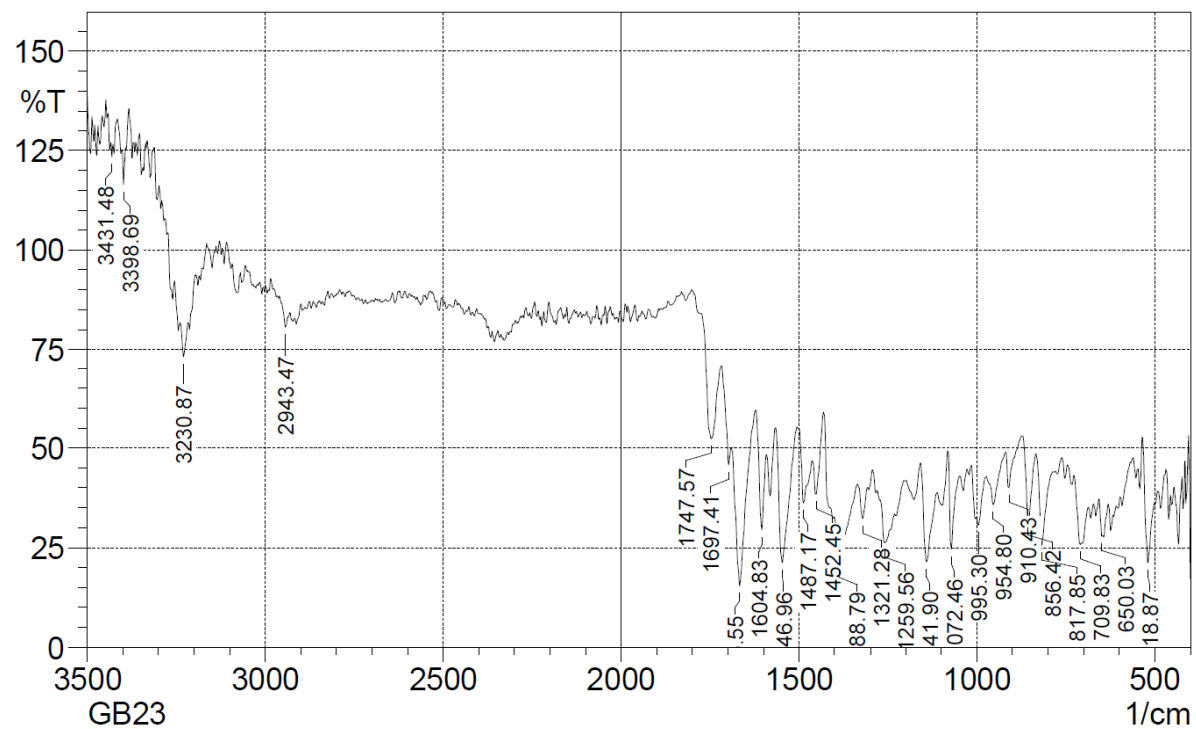
5. Mass

MS Spectrum

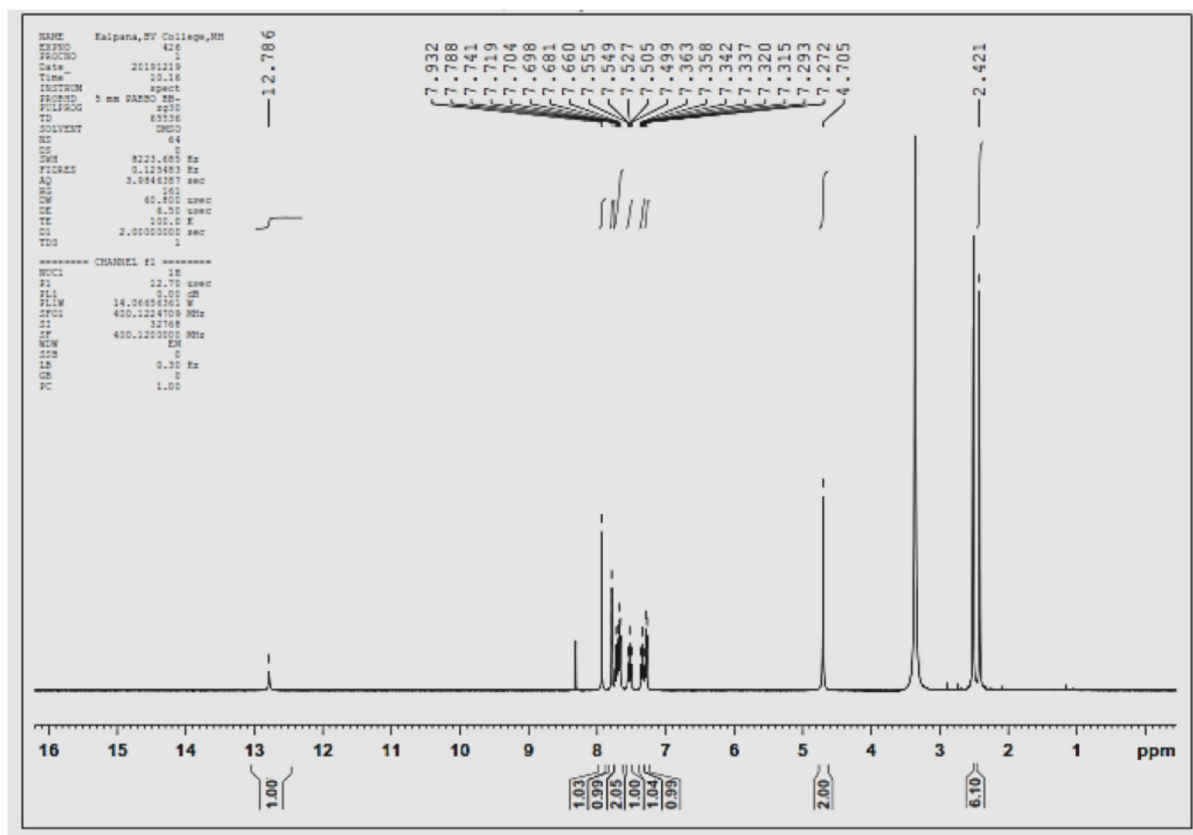


2-(5-(4-bromobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-(5,6-dimethylbenzo[d]thiazol-2-yl)acetamide (GB23)

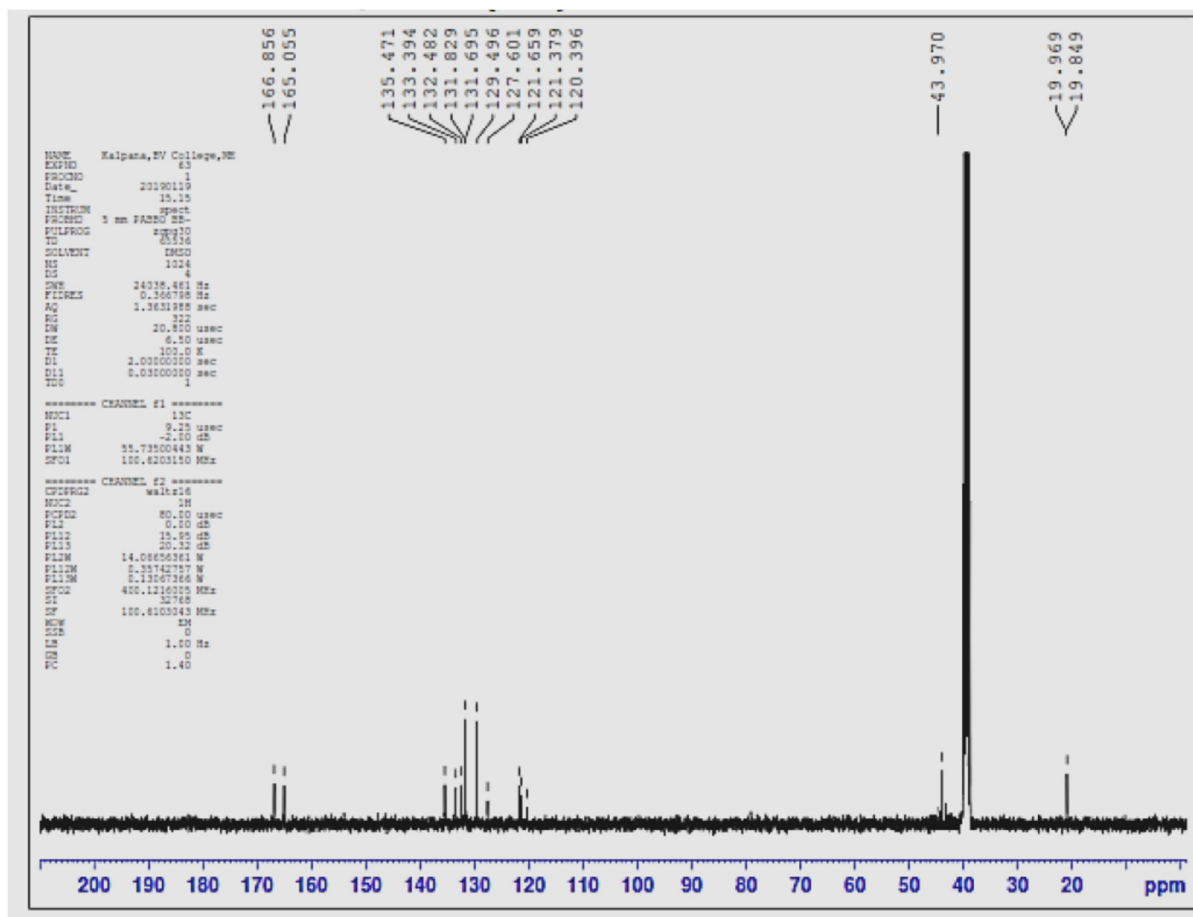
1. FTIR



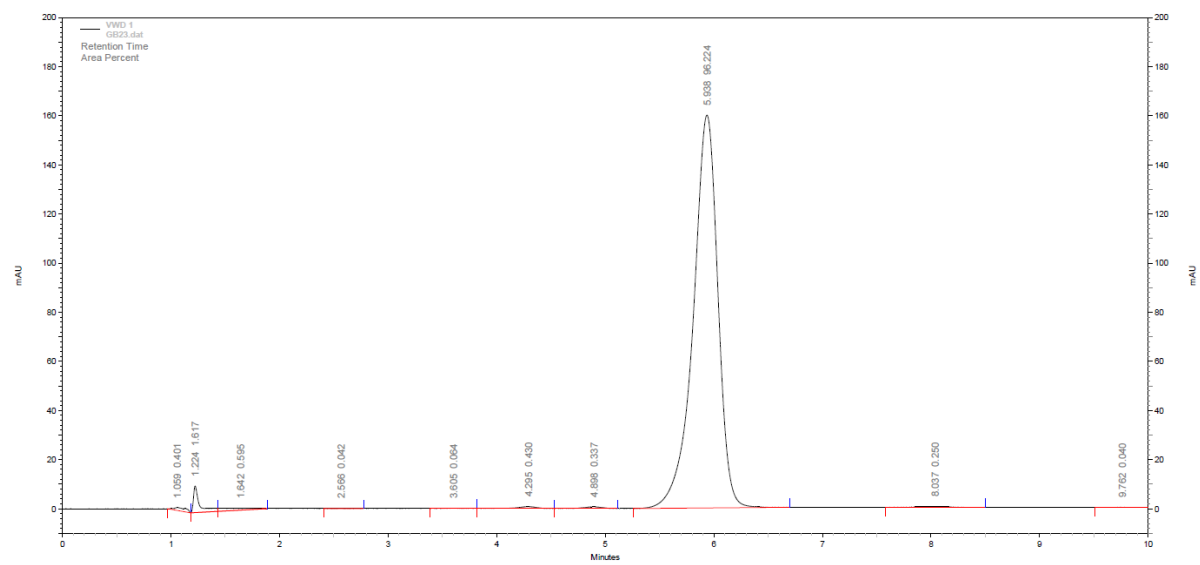
2. ¹HNMR



3. ^{13}C NMR

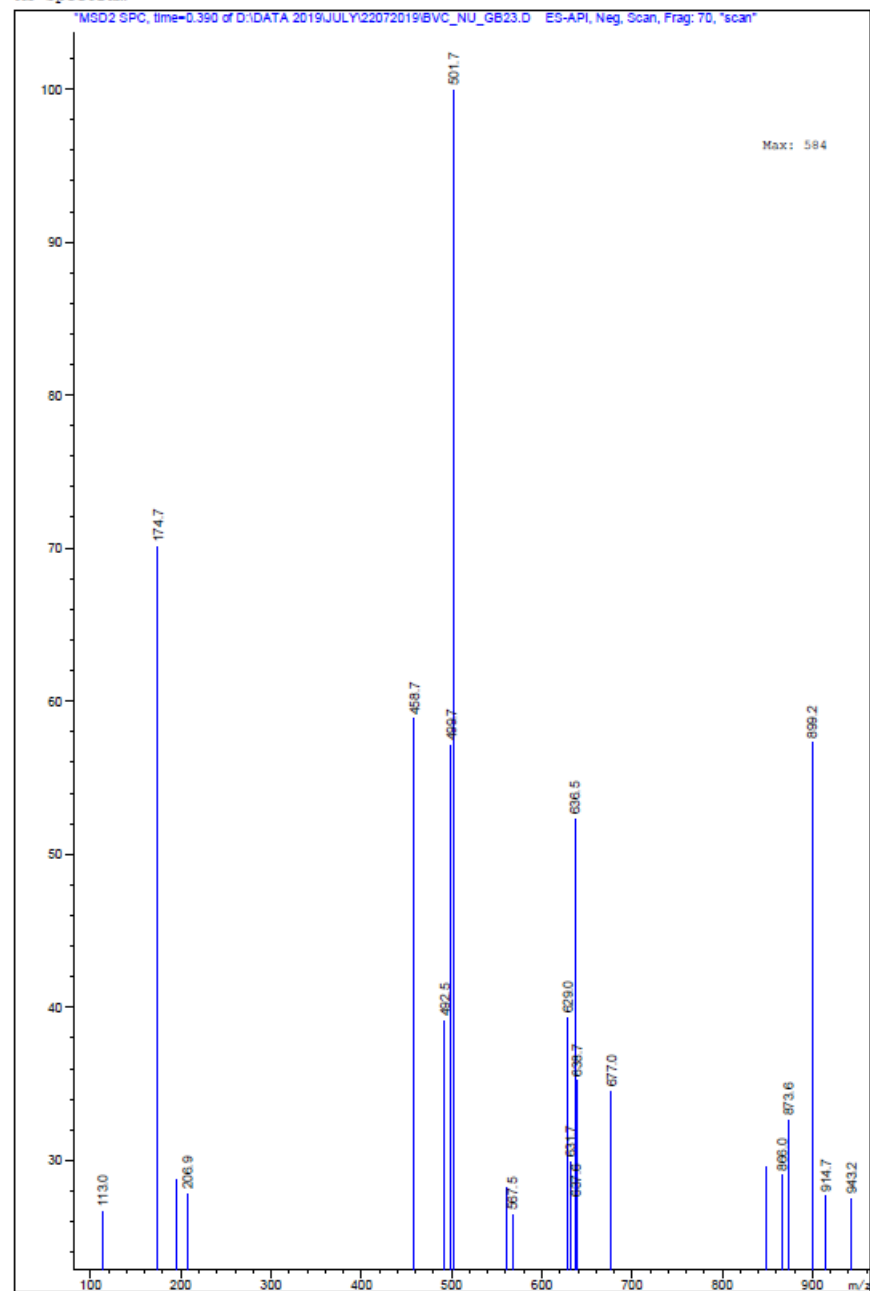


4. HPLC



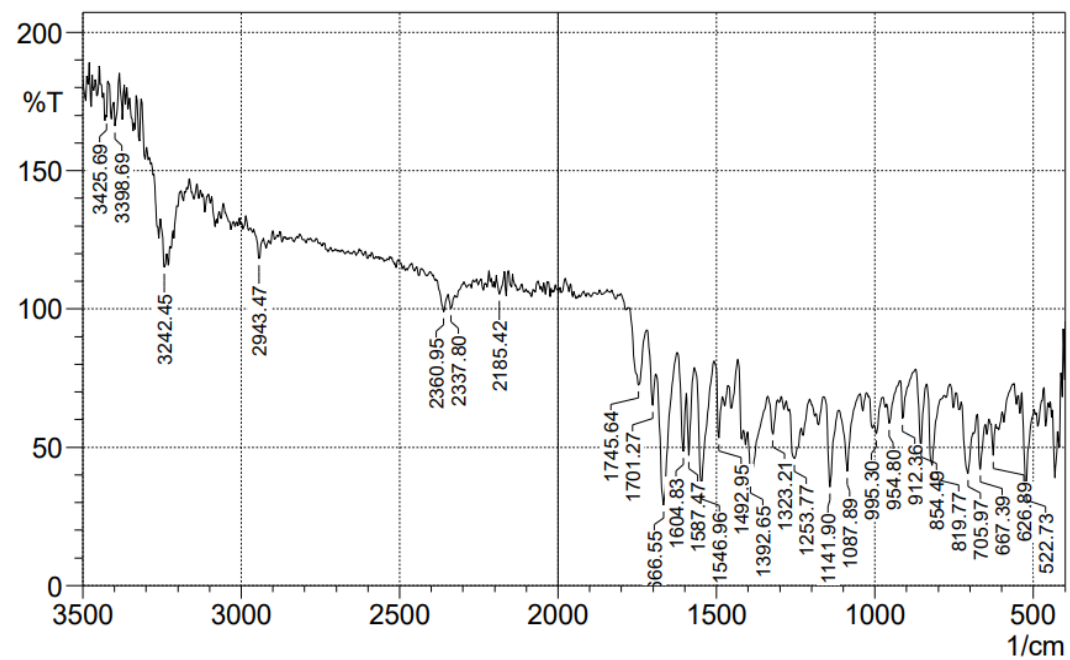
5. Mass

MS Spectrum

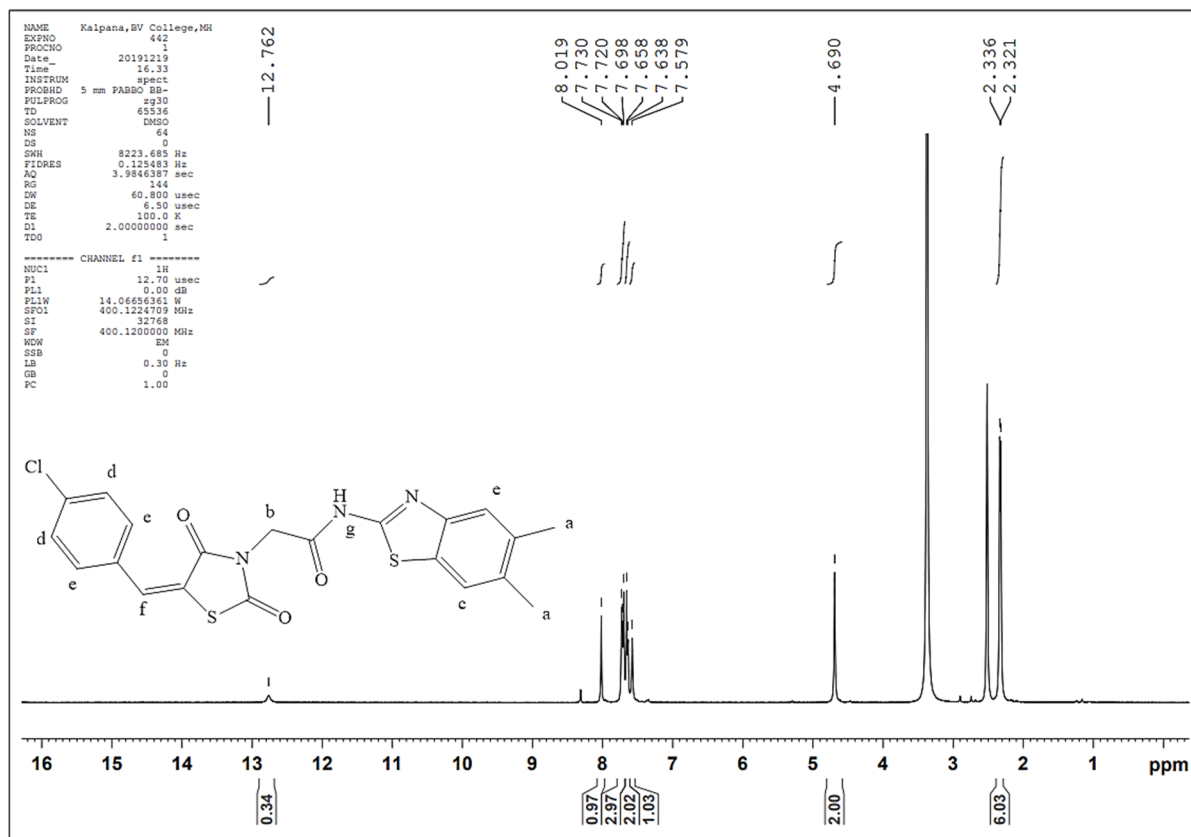


2-(5-(4-chlorobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-(5,6-dimethylbenzo[d]thiazol-2-yl)acetamide (GB24)

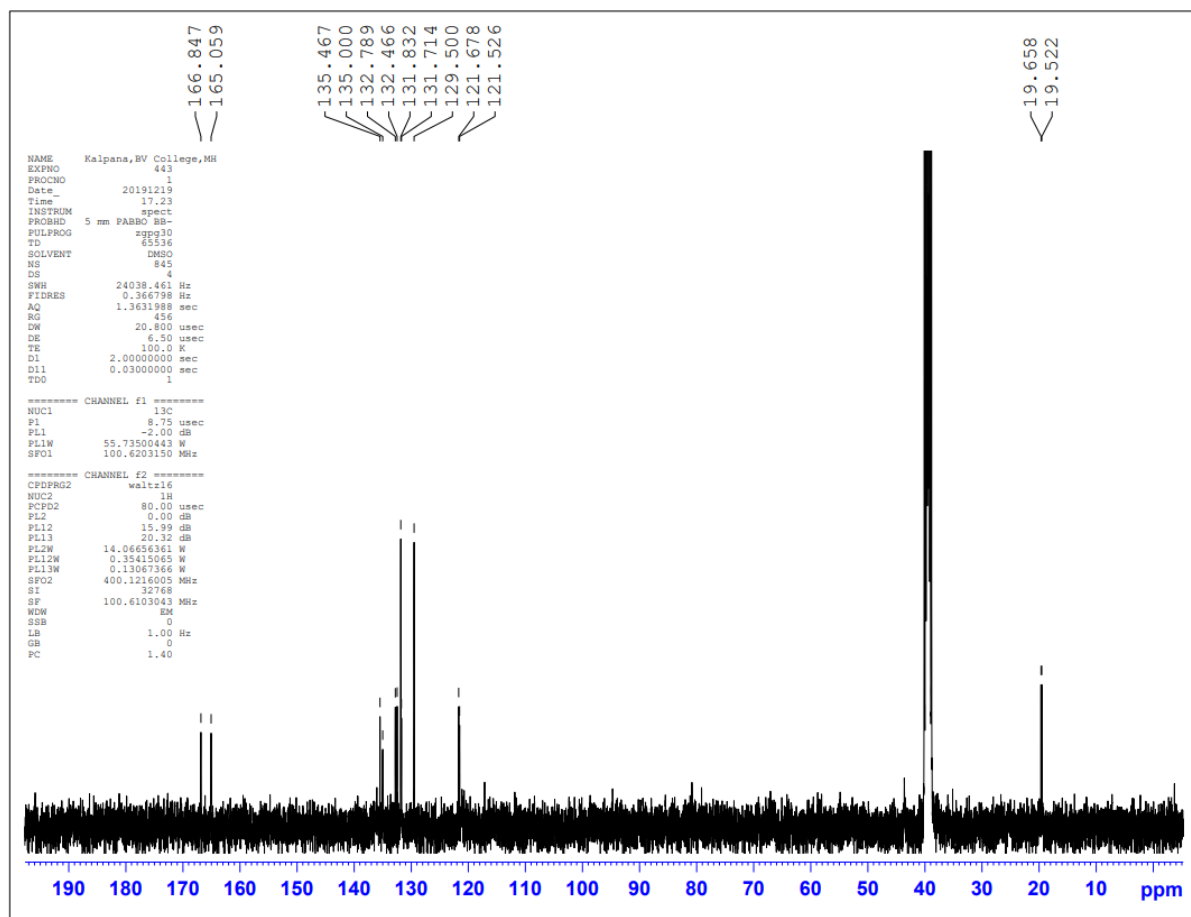
1. FTIR –



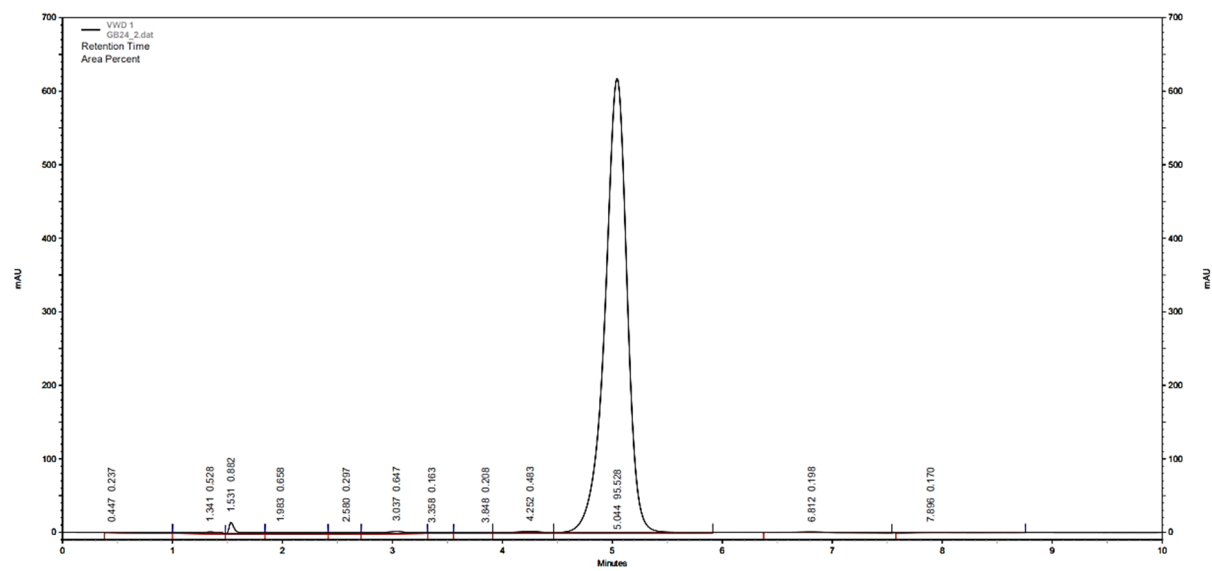
2. ¹H-NMR



3. ¹³C-NMR

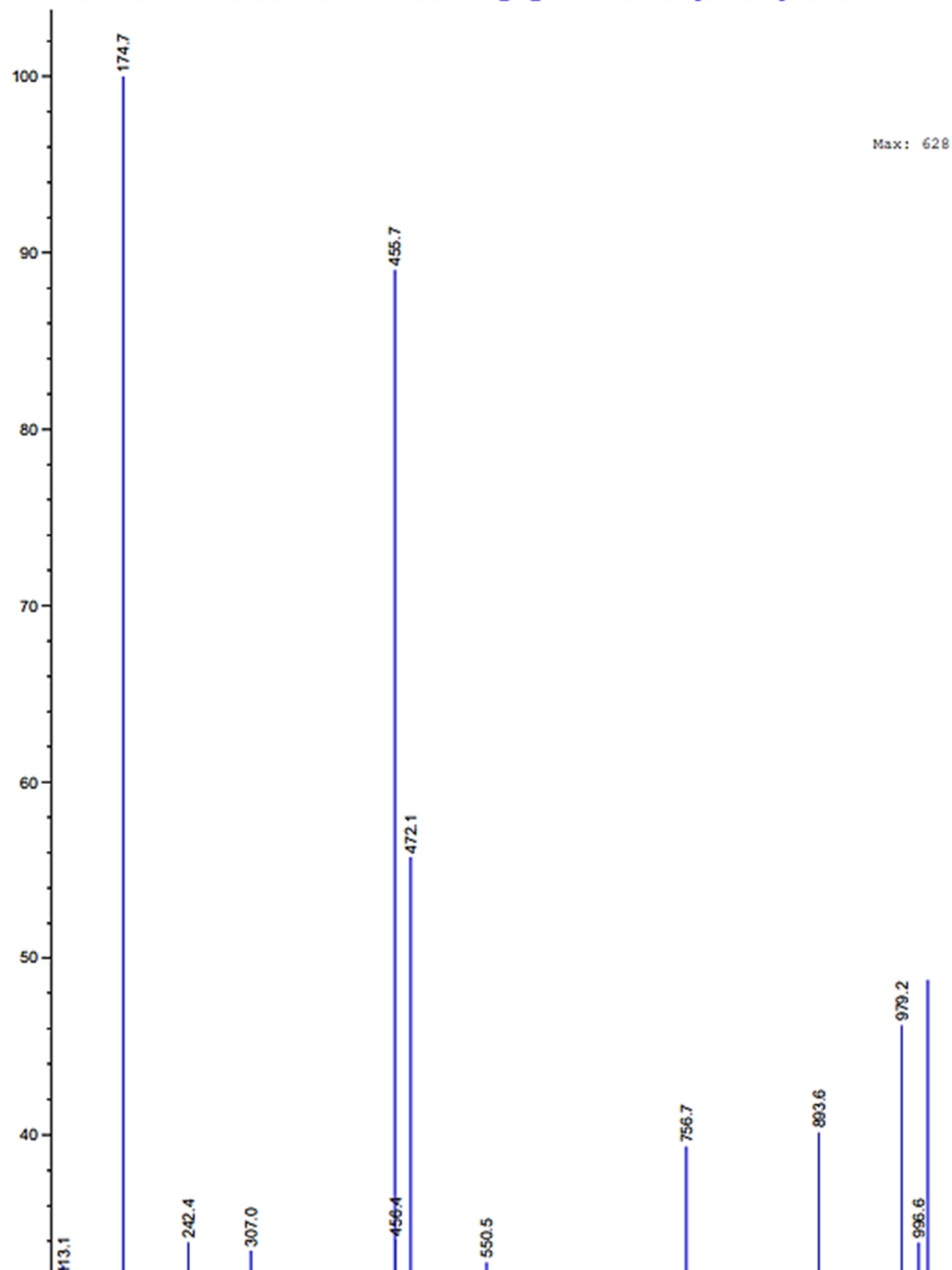


4. HPLC Analysis

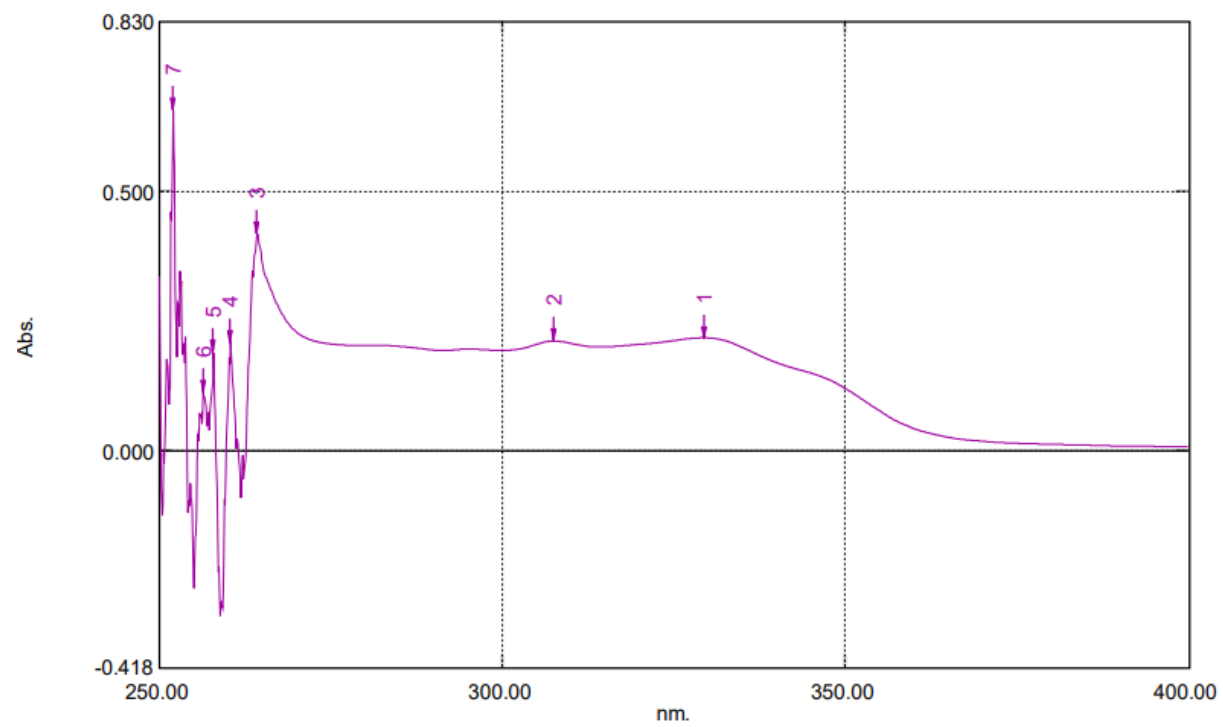


5. Mass Spectrometry

*MSD2 SPC, time=0.252 of D:\DATA 2019\JULY\22072019\BVC_NU_GB24.D ES-API, Neg. Scan, Frag: 70, "scan"

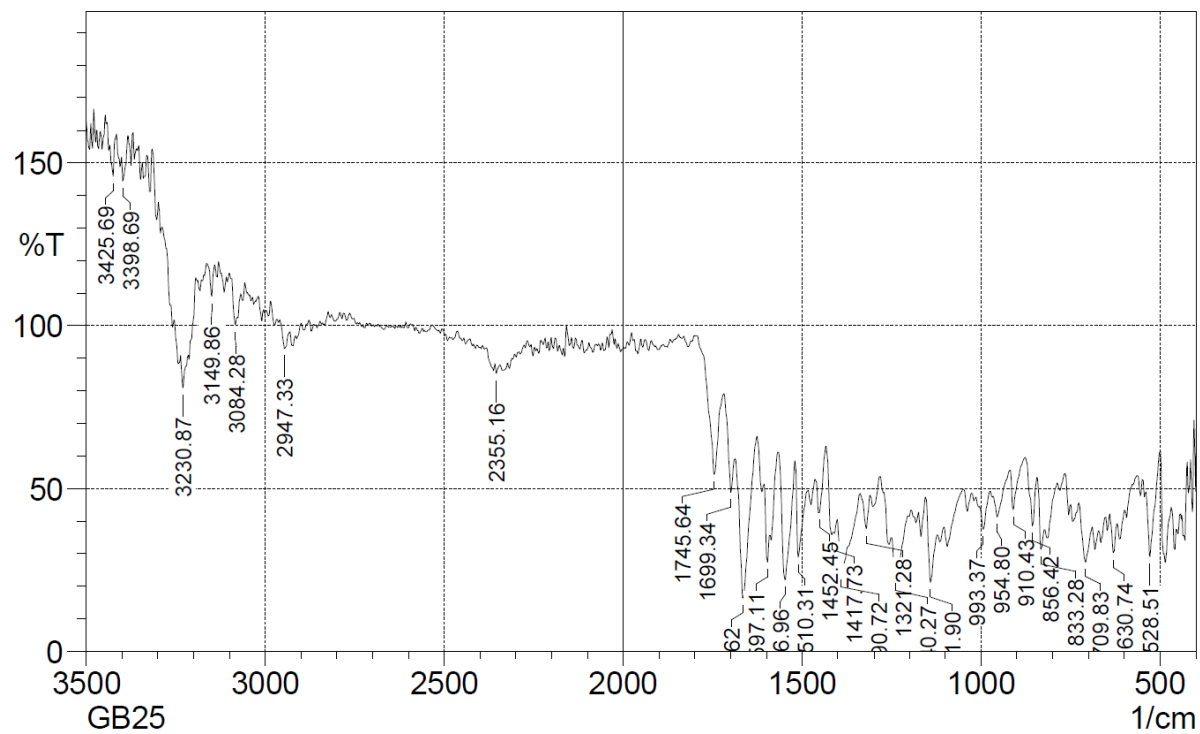


6. UV

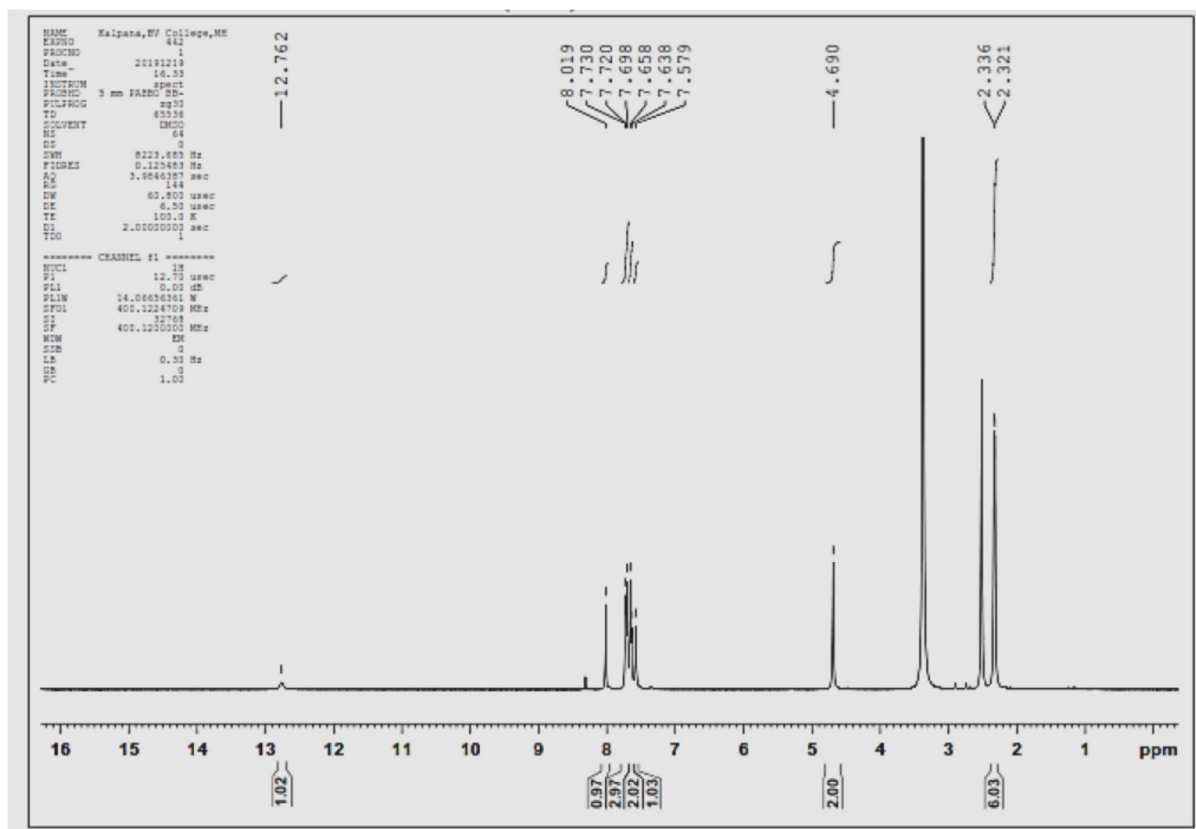


N-(5,6-dimethylbenzo[d]thiazol-2-yl)-2-(5-(4-fluorobenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB25)

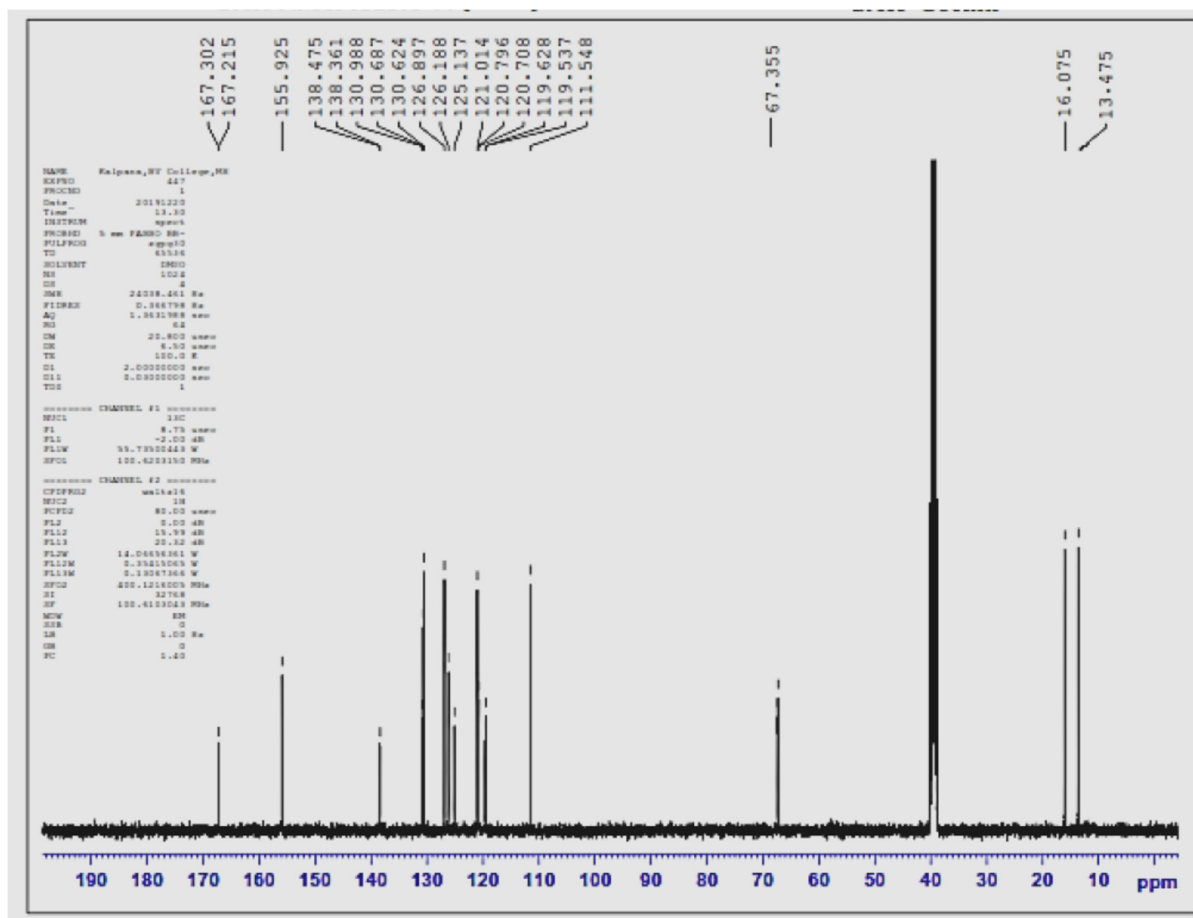
1. FTIR



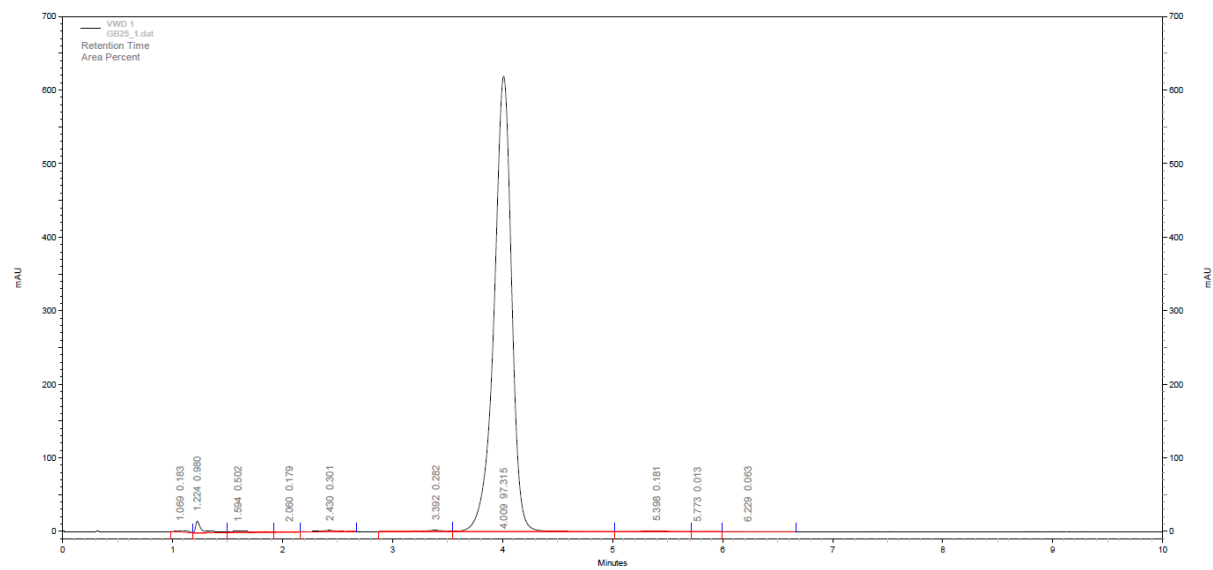
2. ¹H NMR



3. ^{13}C NMR

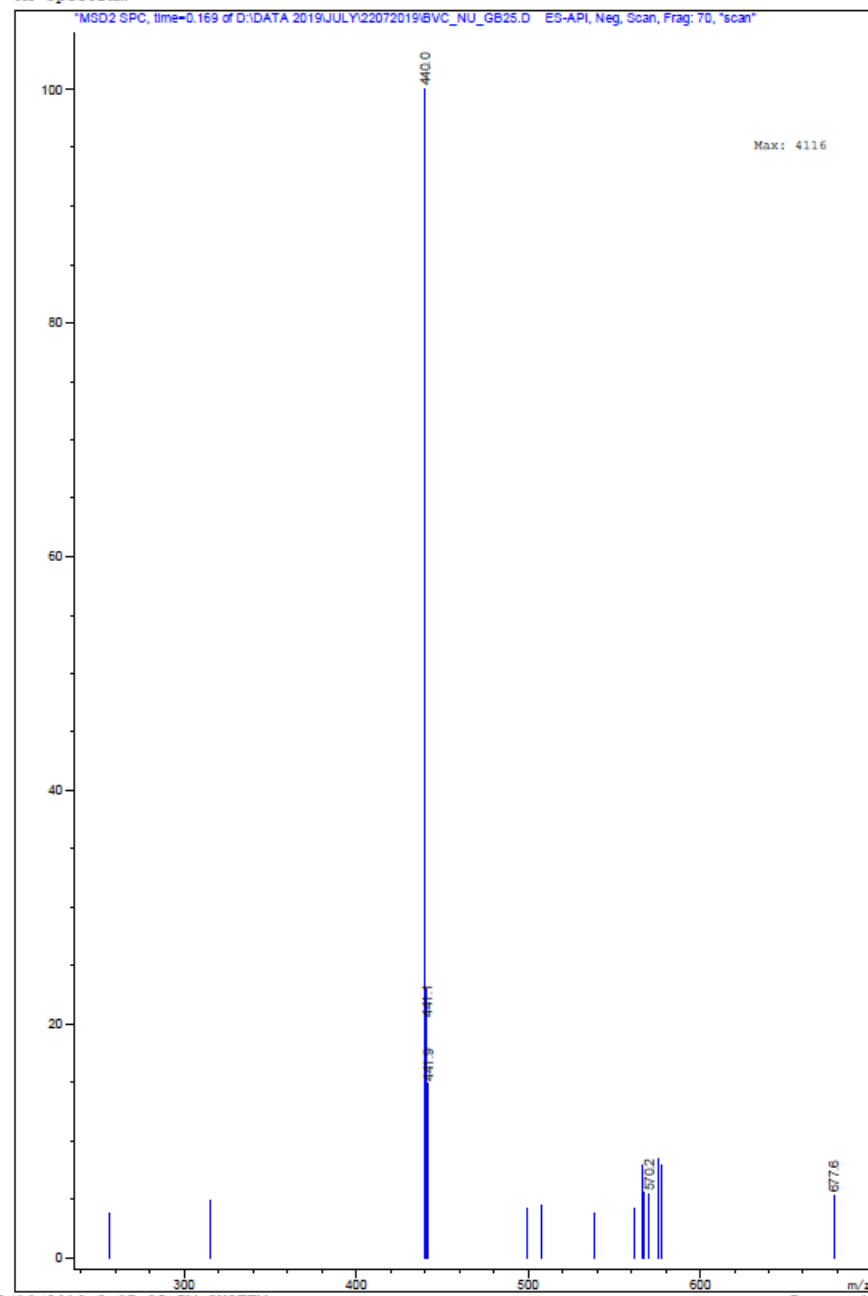


4. HPLC



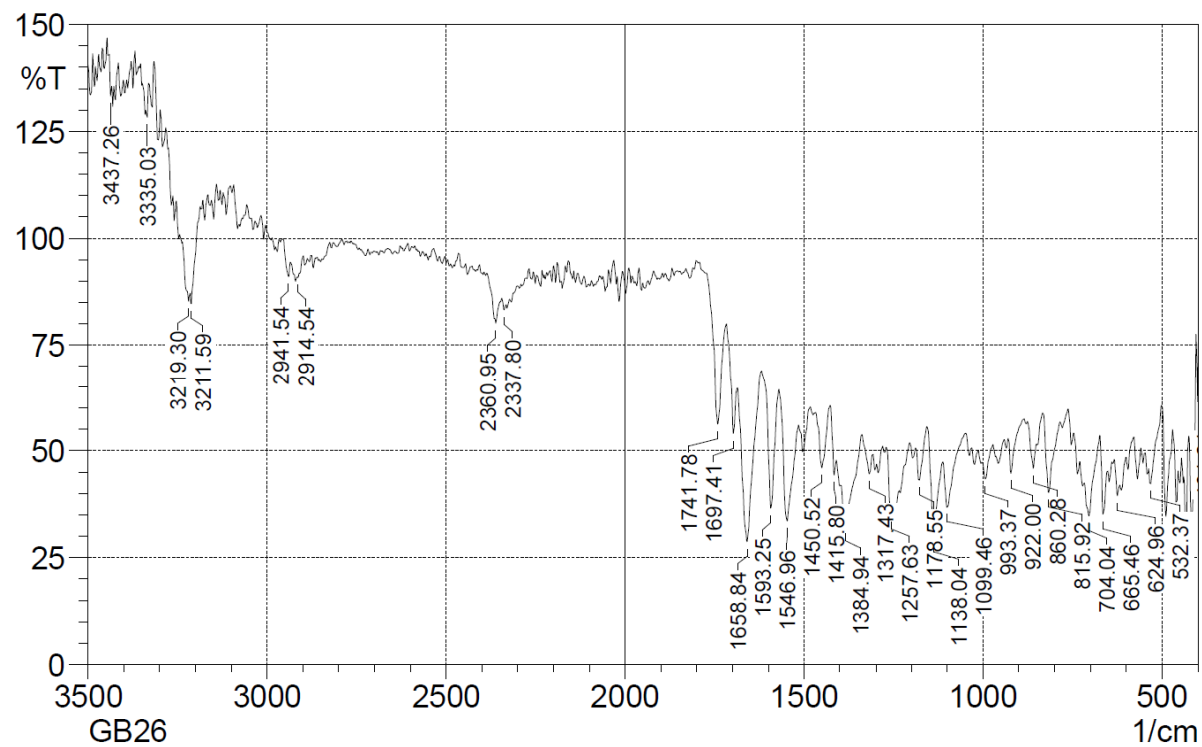
5. Mass

MS Spectrum

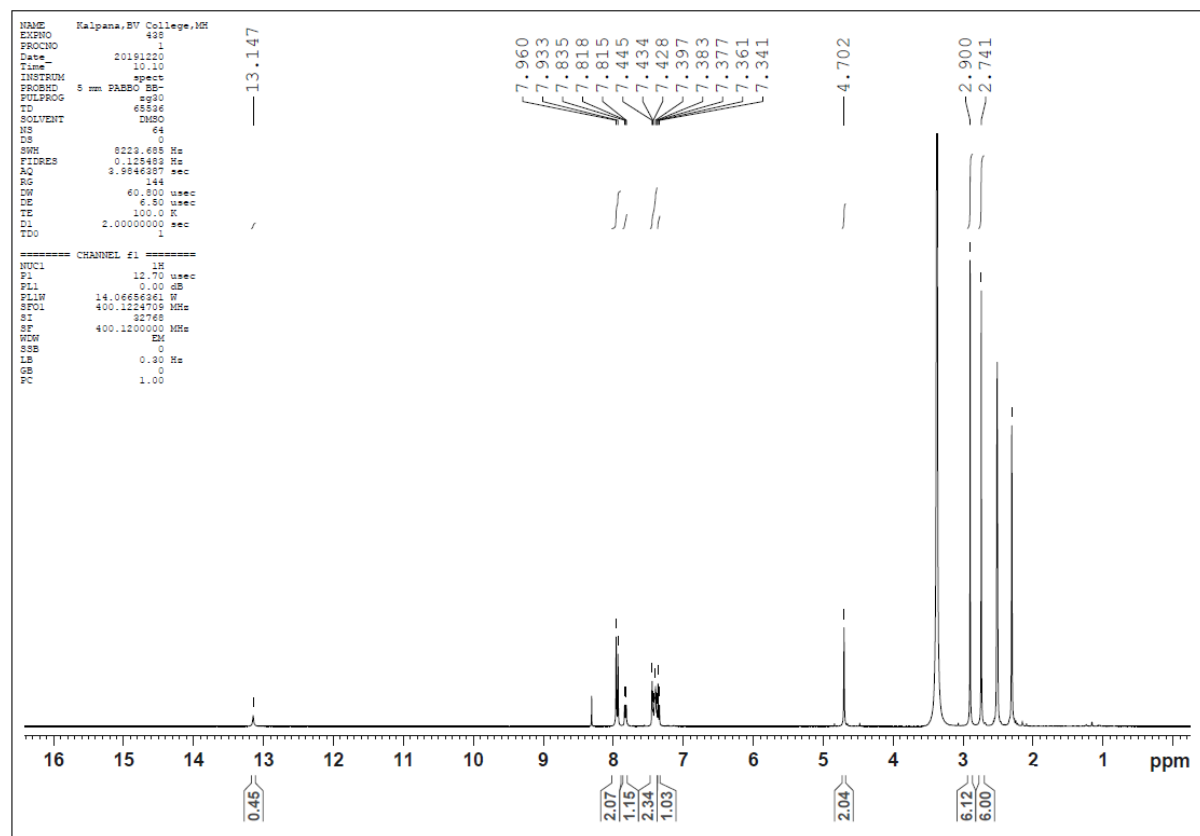


N-(5,6-dimethylbenzo[d]thiazol-2-yl)-2-(5-(3,4-dimethylbenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB26)

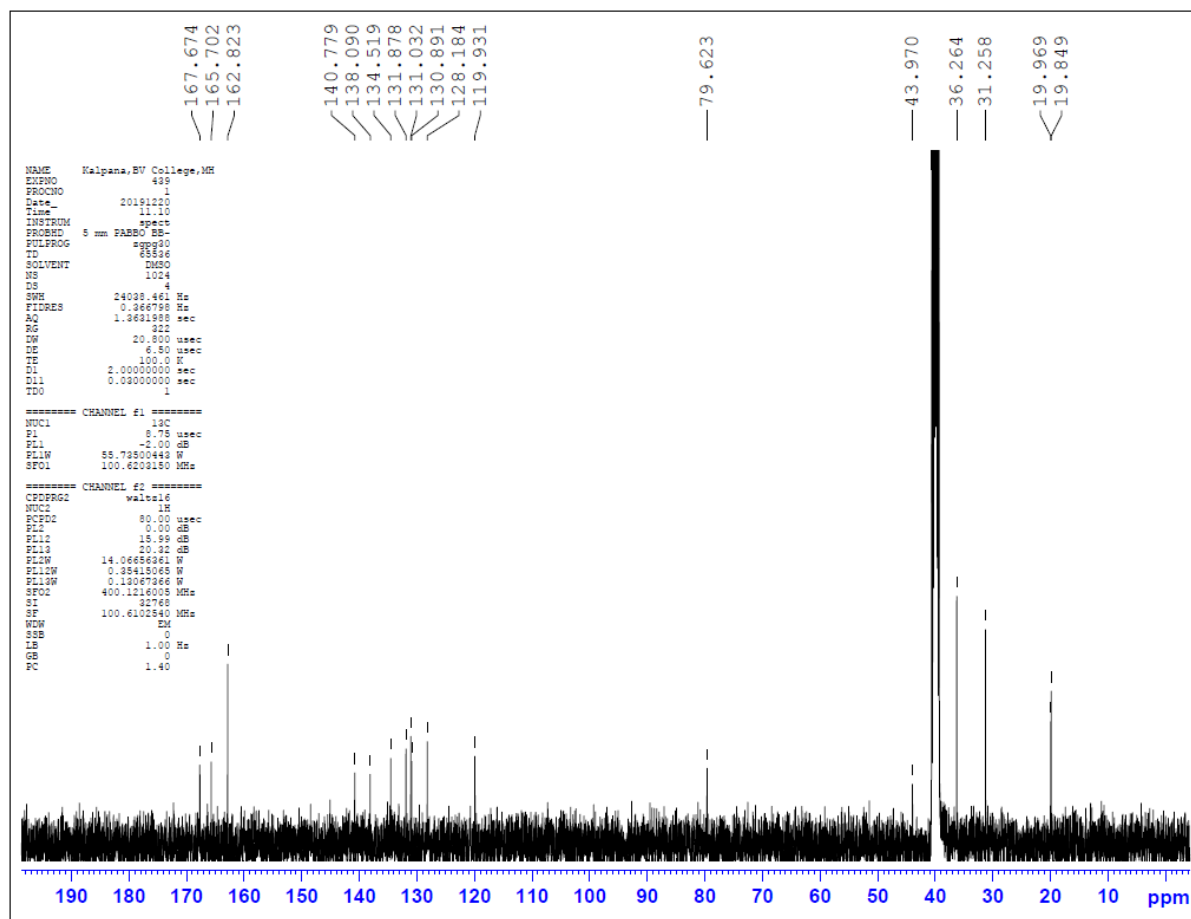
1. FTIR



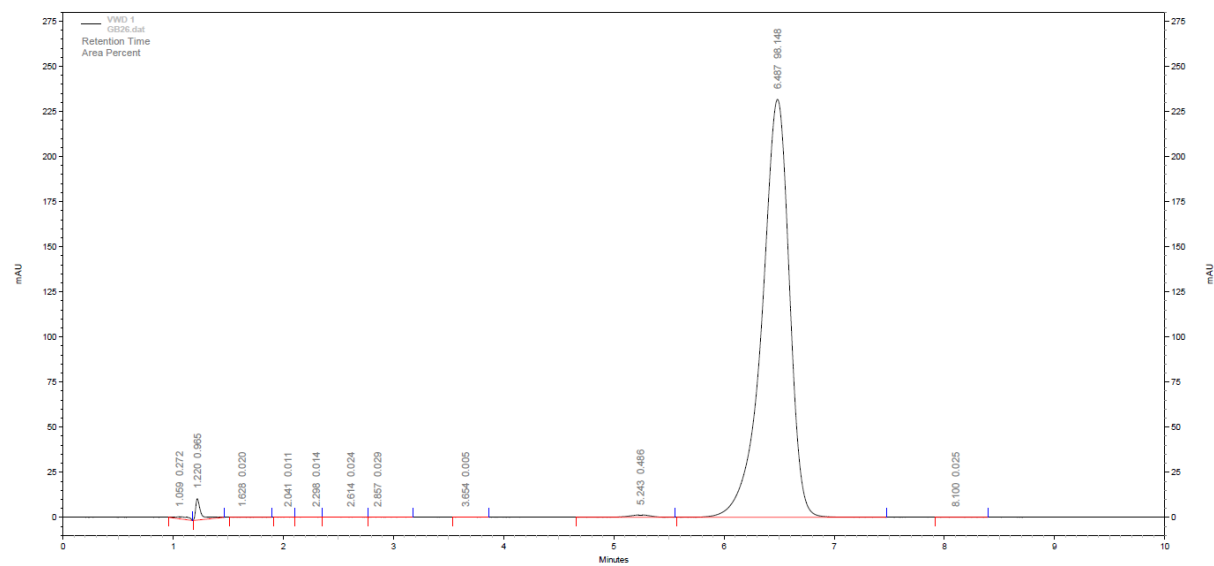
2. ¹H-NMR



3. 13C-NMR

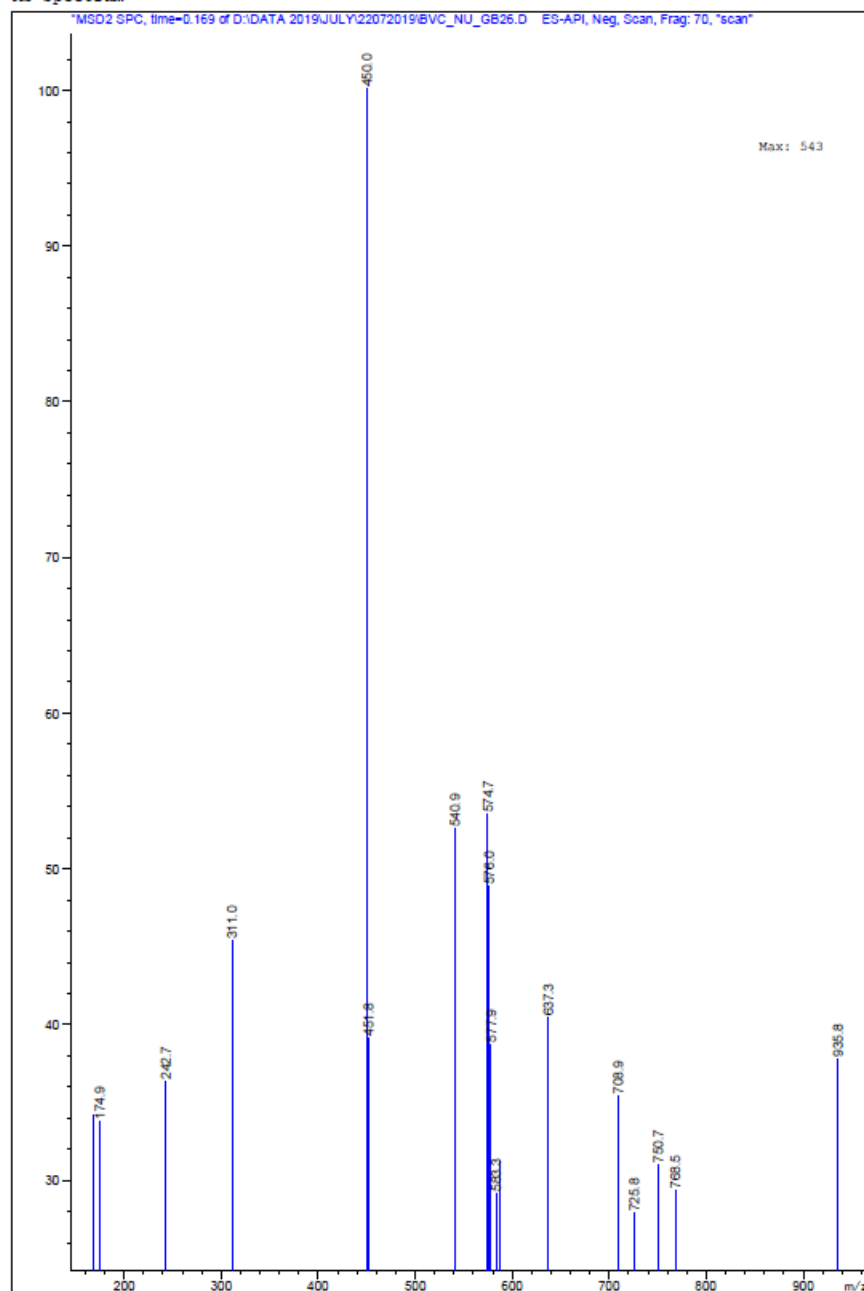


4. HPLC



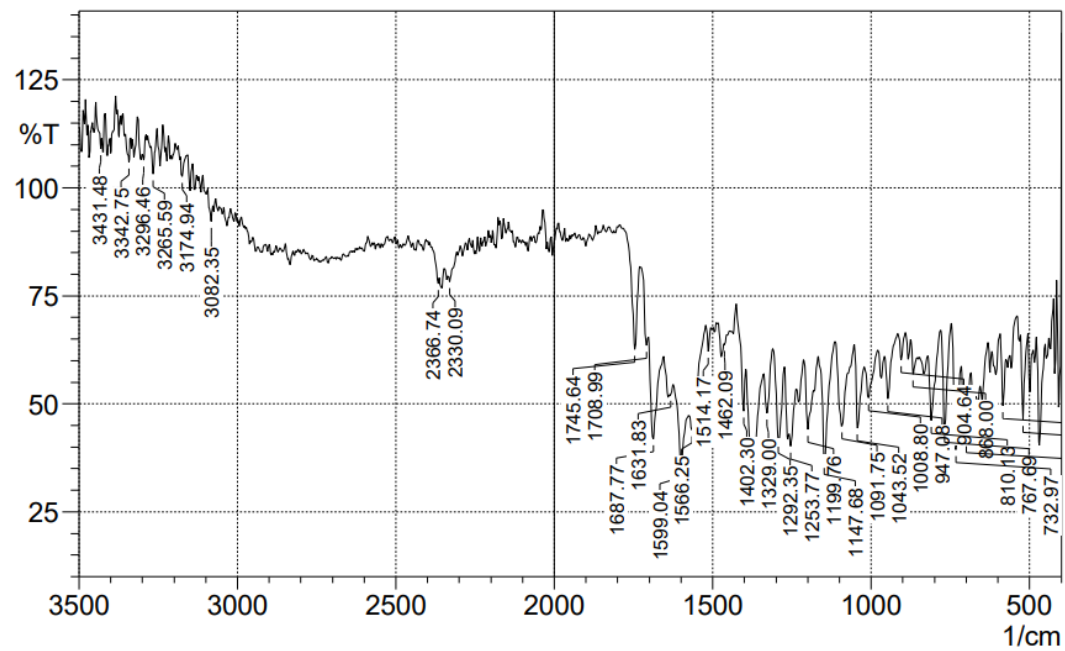
5. Mass

MS Spectrum

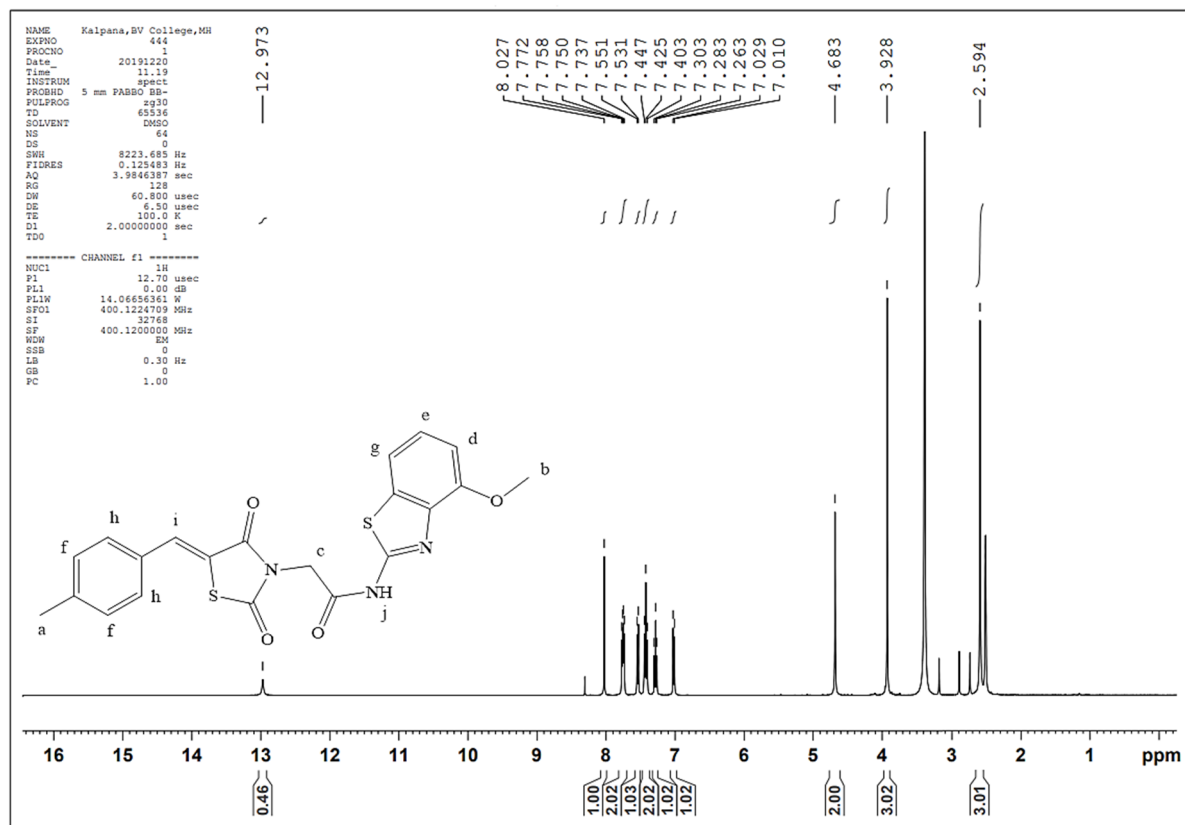


N-(4-methoxybenzo[d]thiazol-2-yl)-2-(5-(4-methylbenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB27)

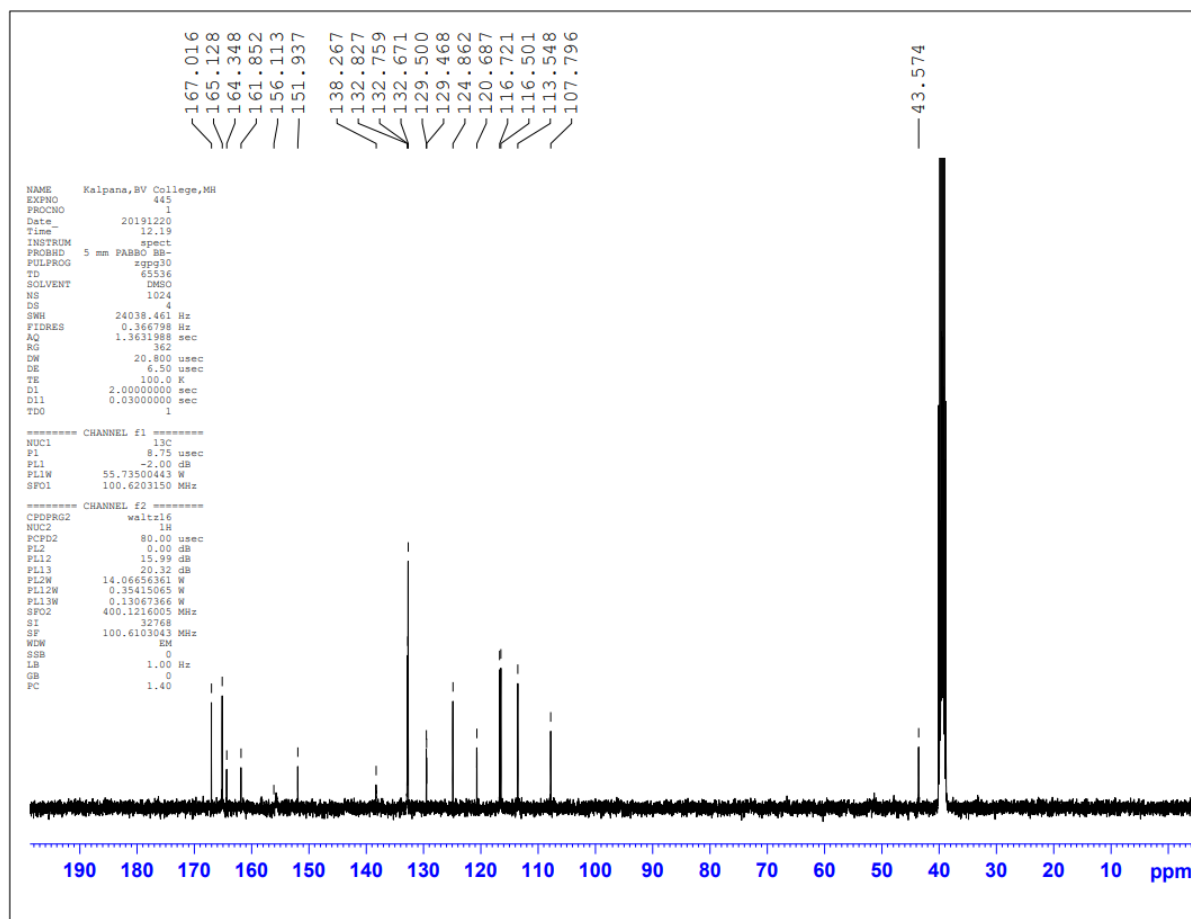
1. FTIR



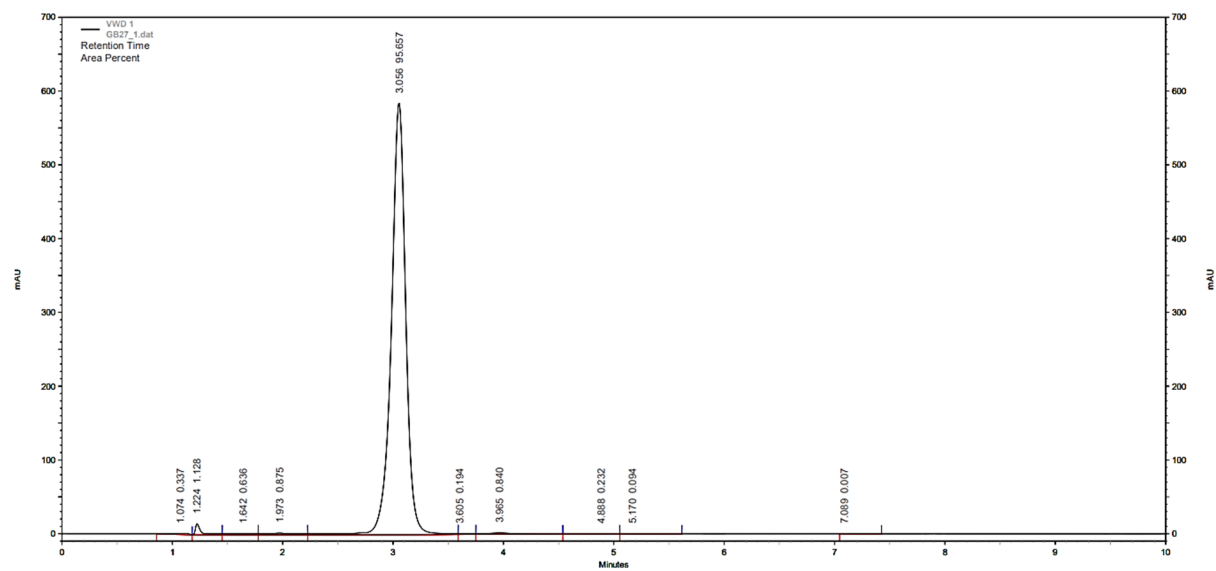
2. ¹H-NMR



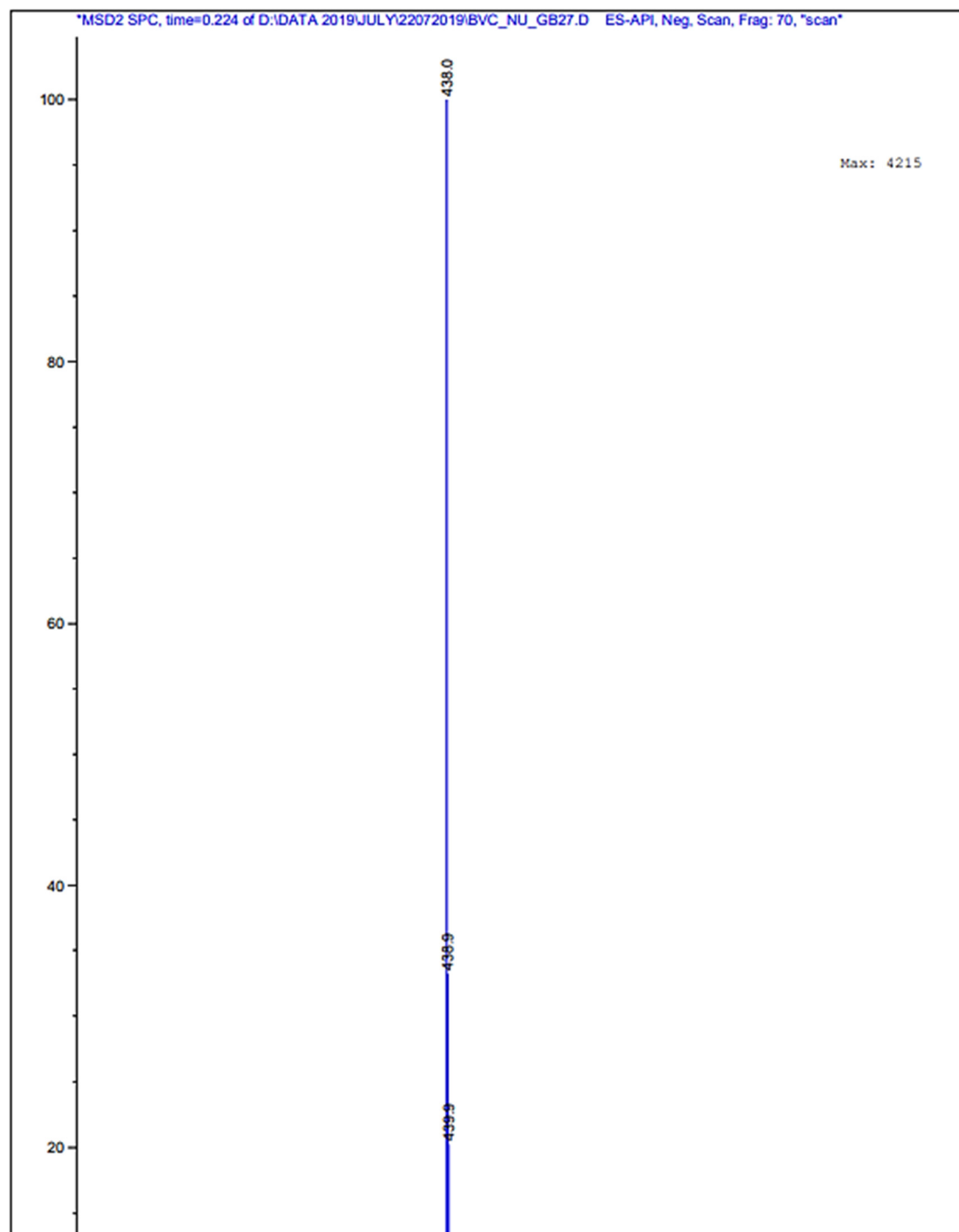
3. ¹³C-NMR



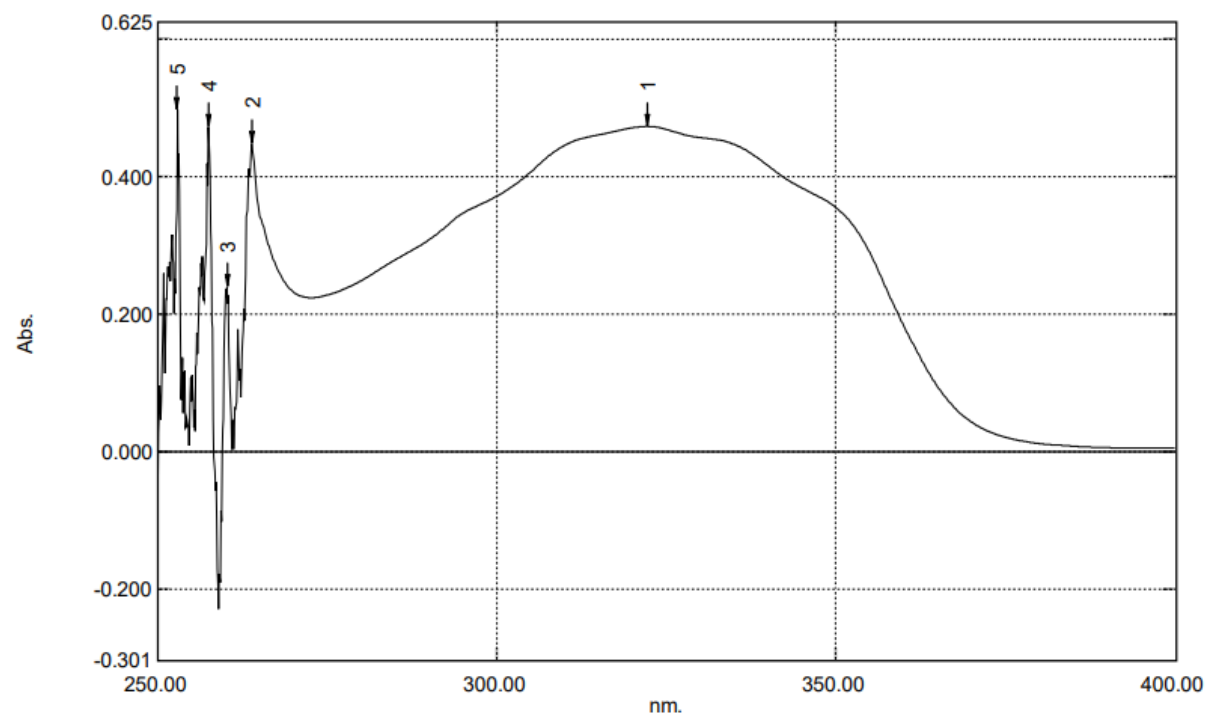
4. HPLC Analysis



5. Mass Spectrometry

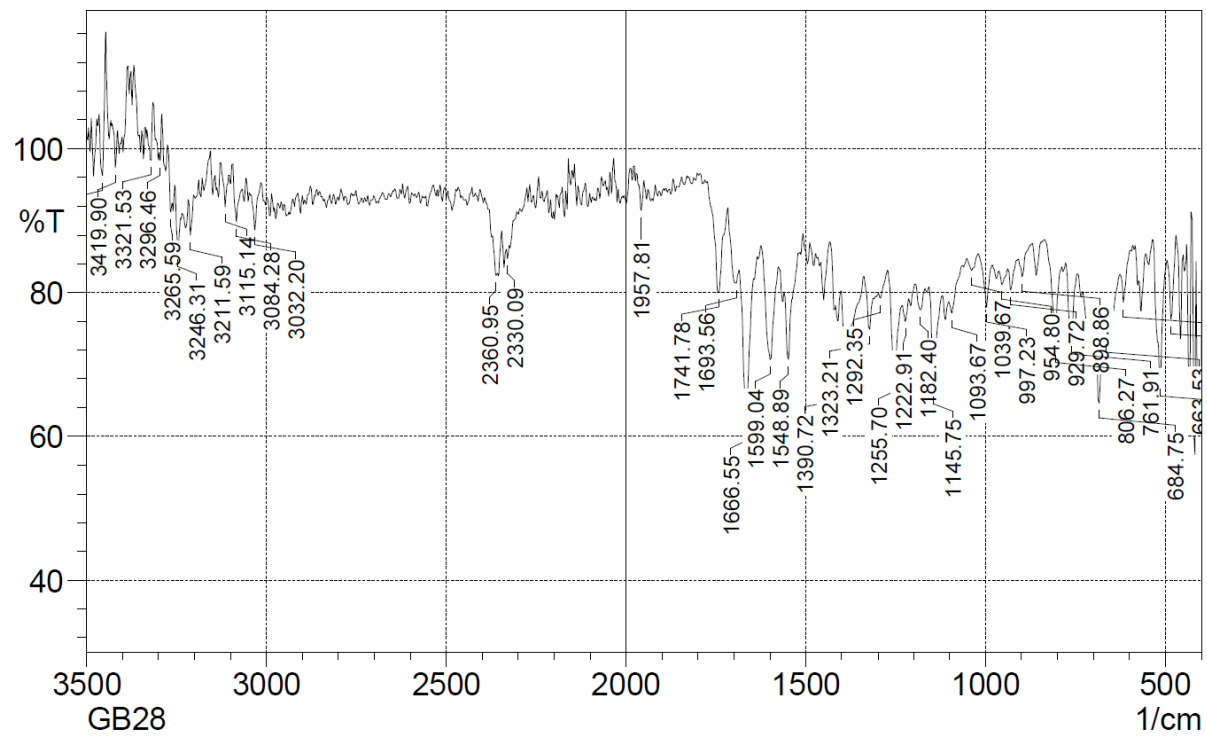


6. UV

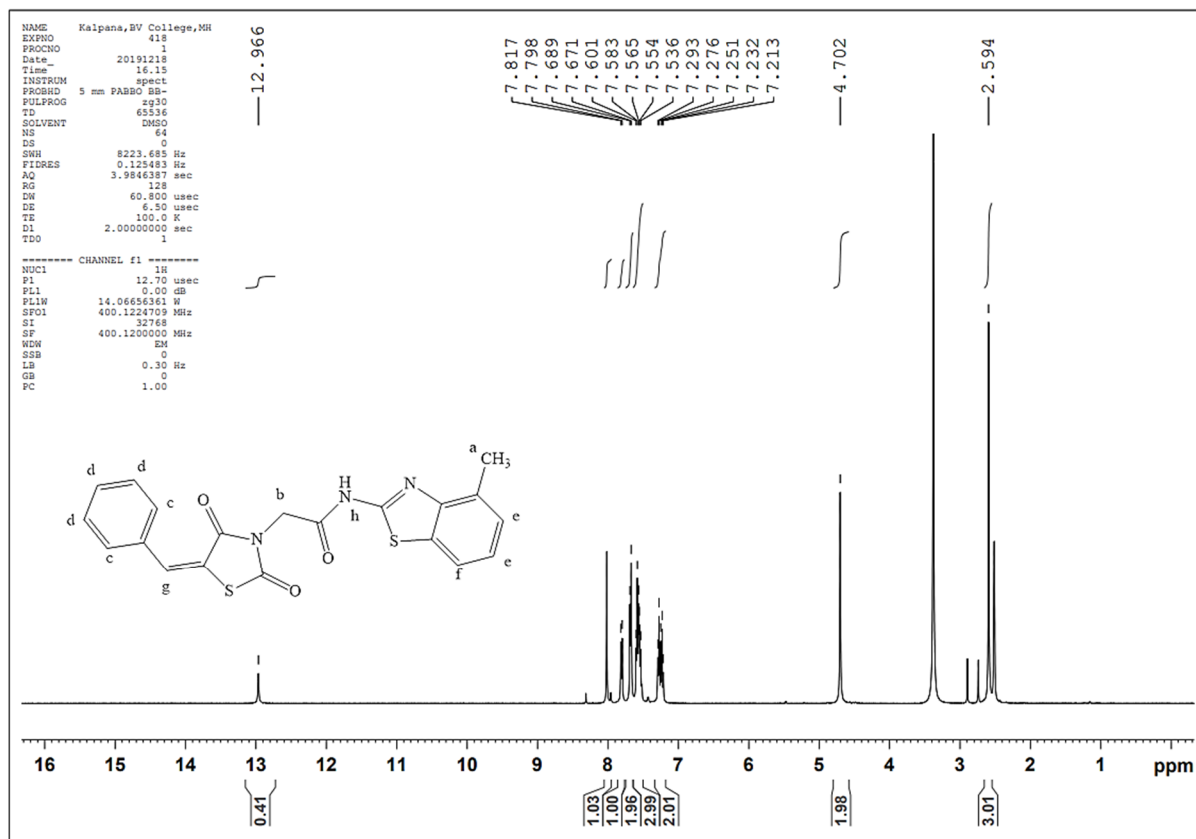


2-(5-benzylidene-2,4-dioxothiazolidin-3-yl)-N-(4-methylbenzo[d]thiazol-2-yl)acetamide (GB28)

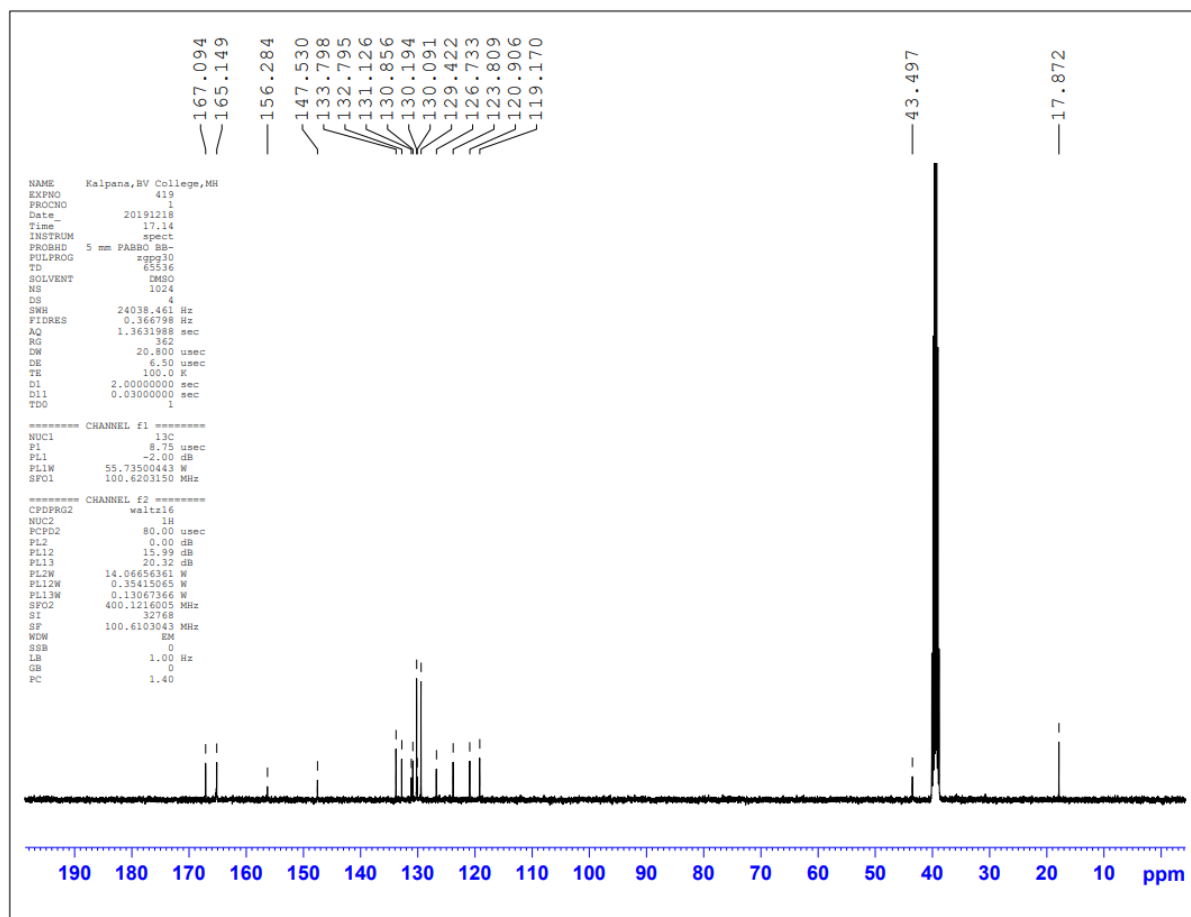
1. FTIR



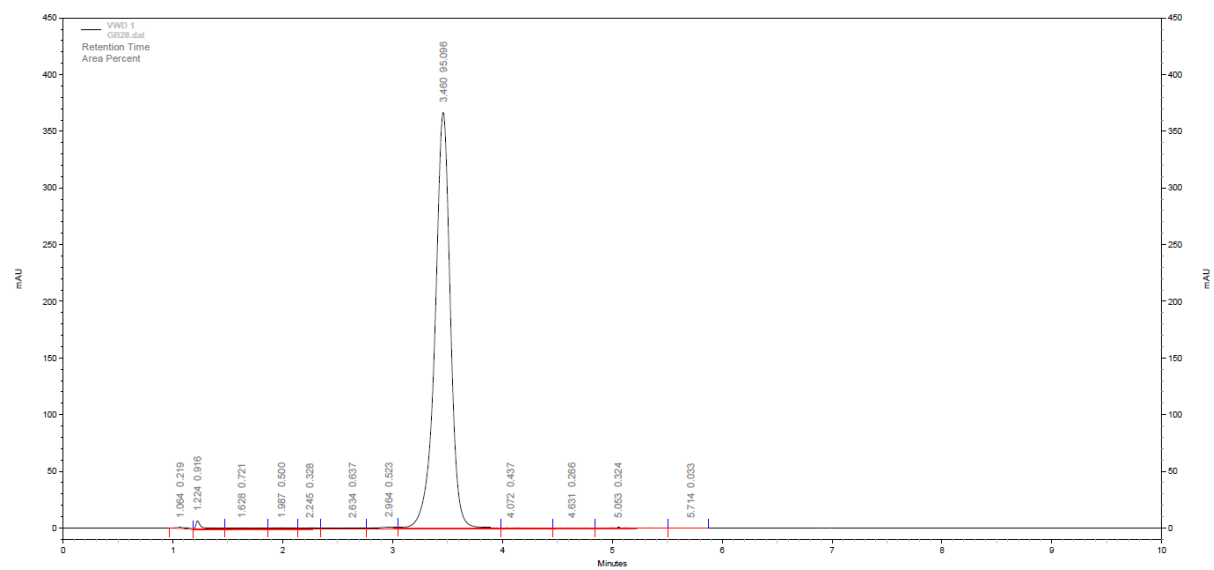
2. ^1H -NMR



3. ¹³C-NMR

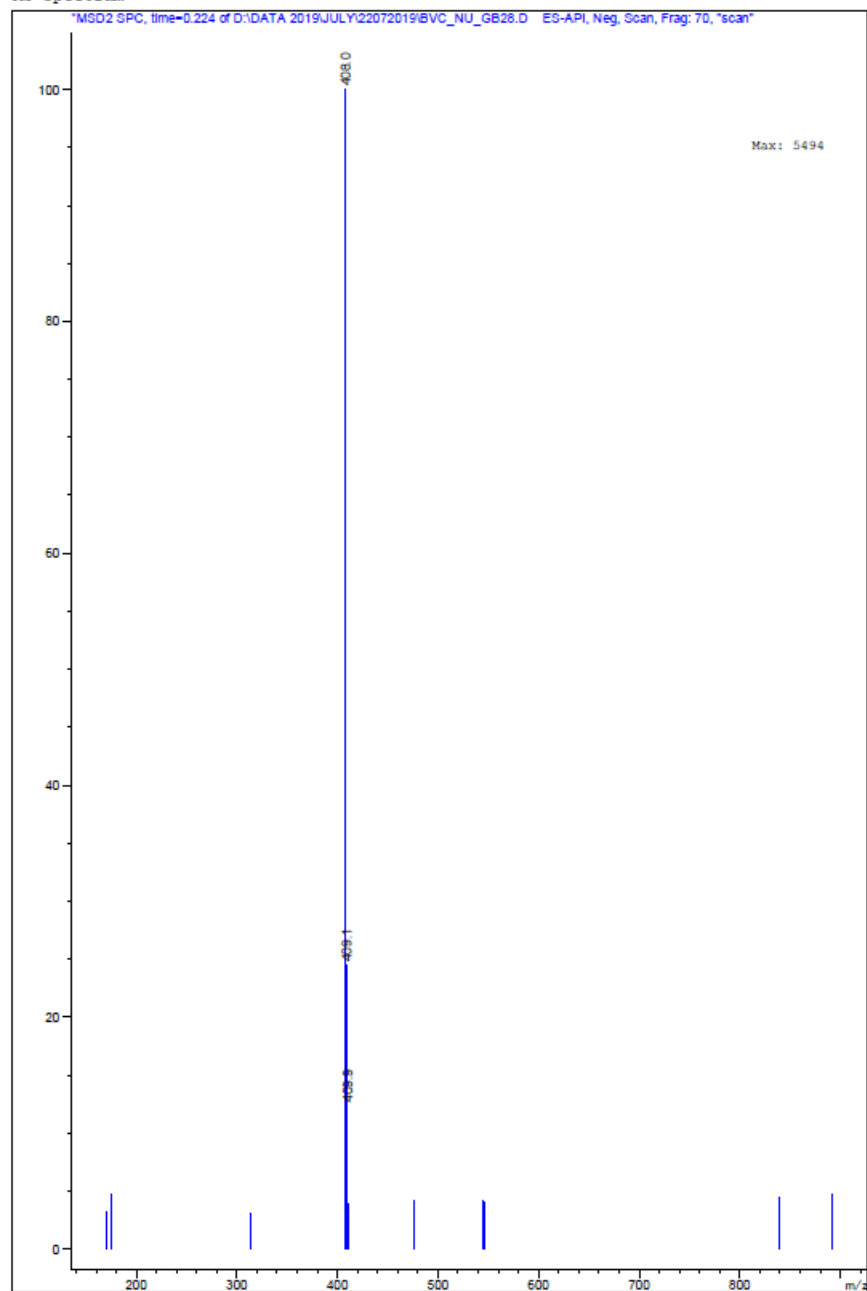


4. HPLC



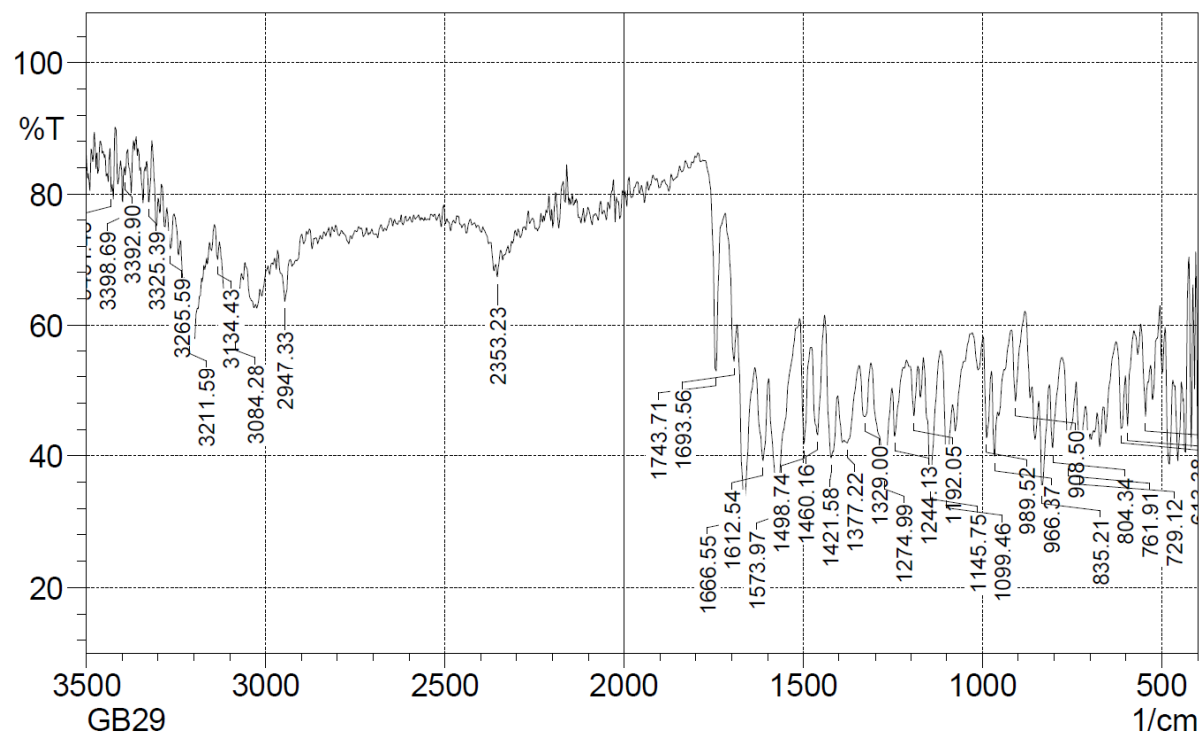
5. Mass

MS Spectrum

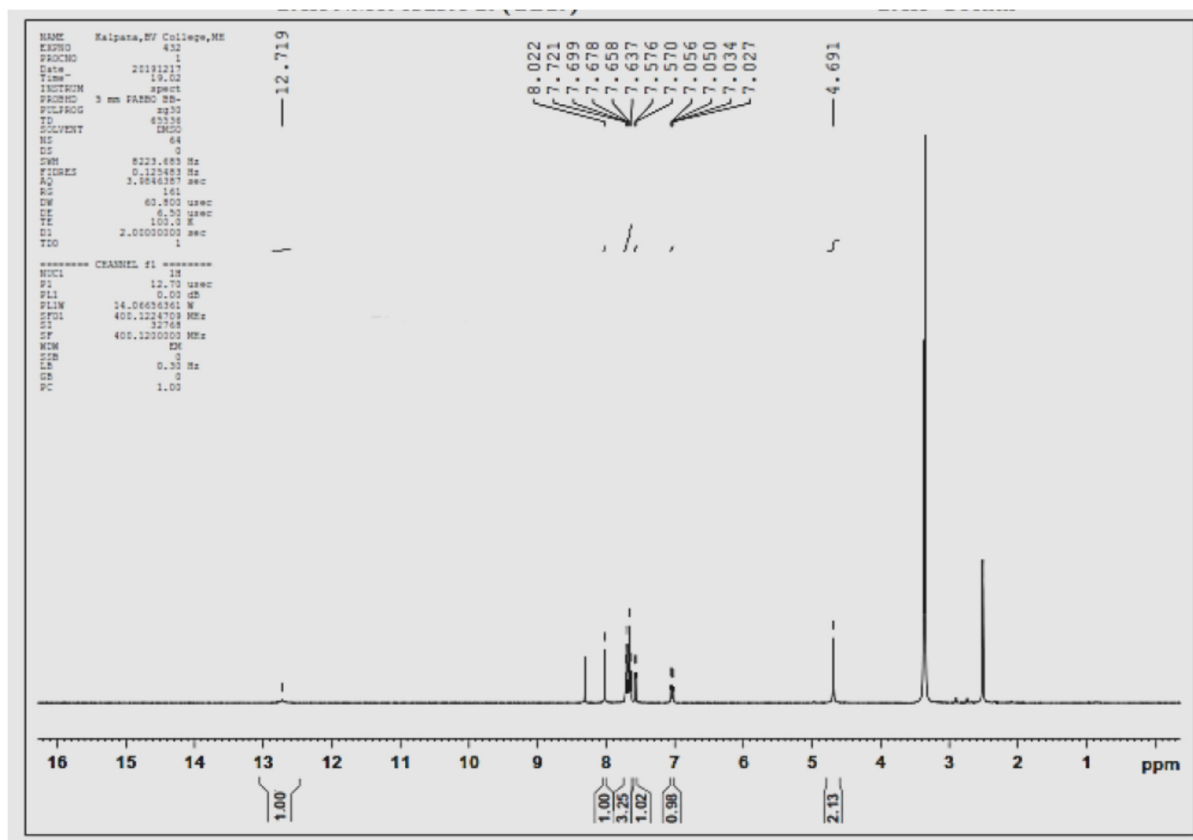


N-(4,6-difluorobenzo[d]thiazol-2-yl)-2-(5-(2,4-difluorobenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB29)

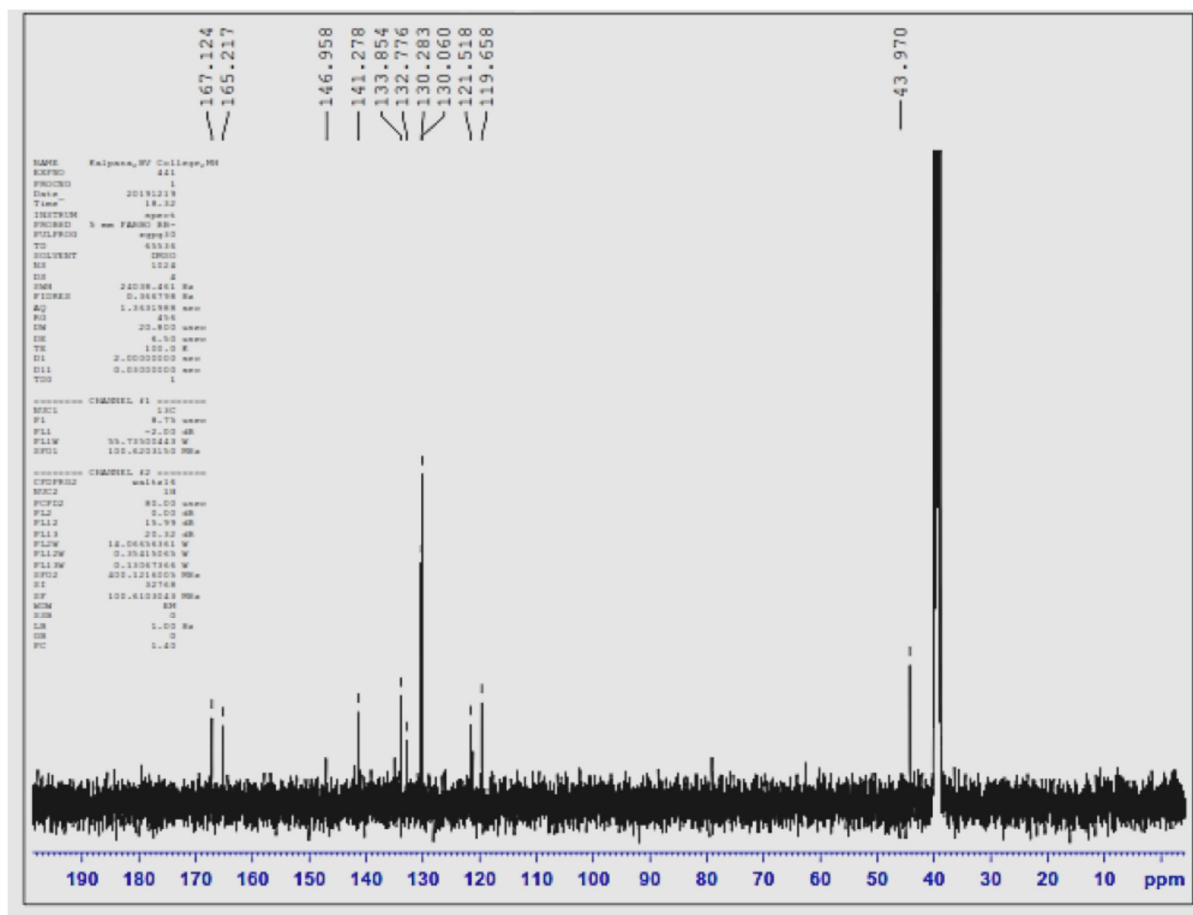
1. FTIR



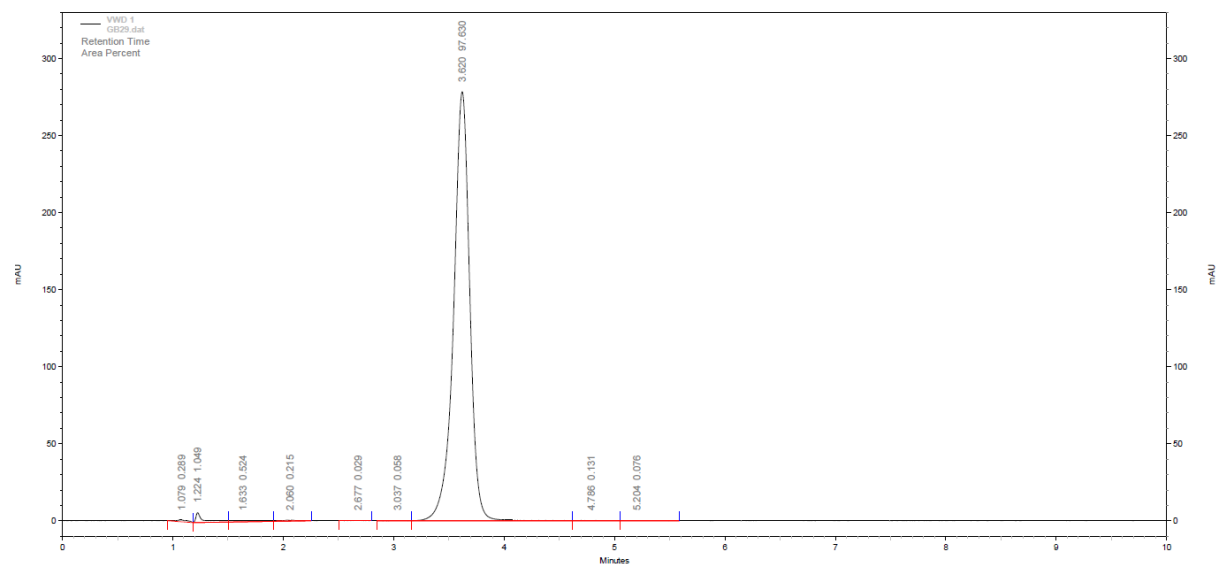
2. ^1H NMR



3. ^{13}C NMR

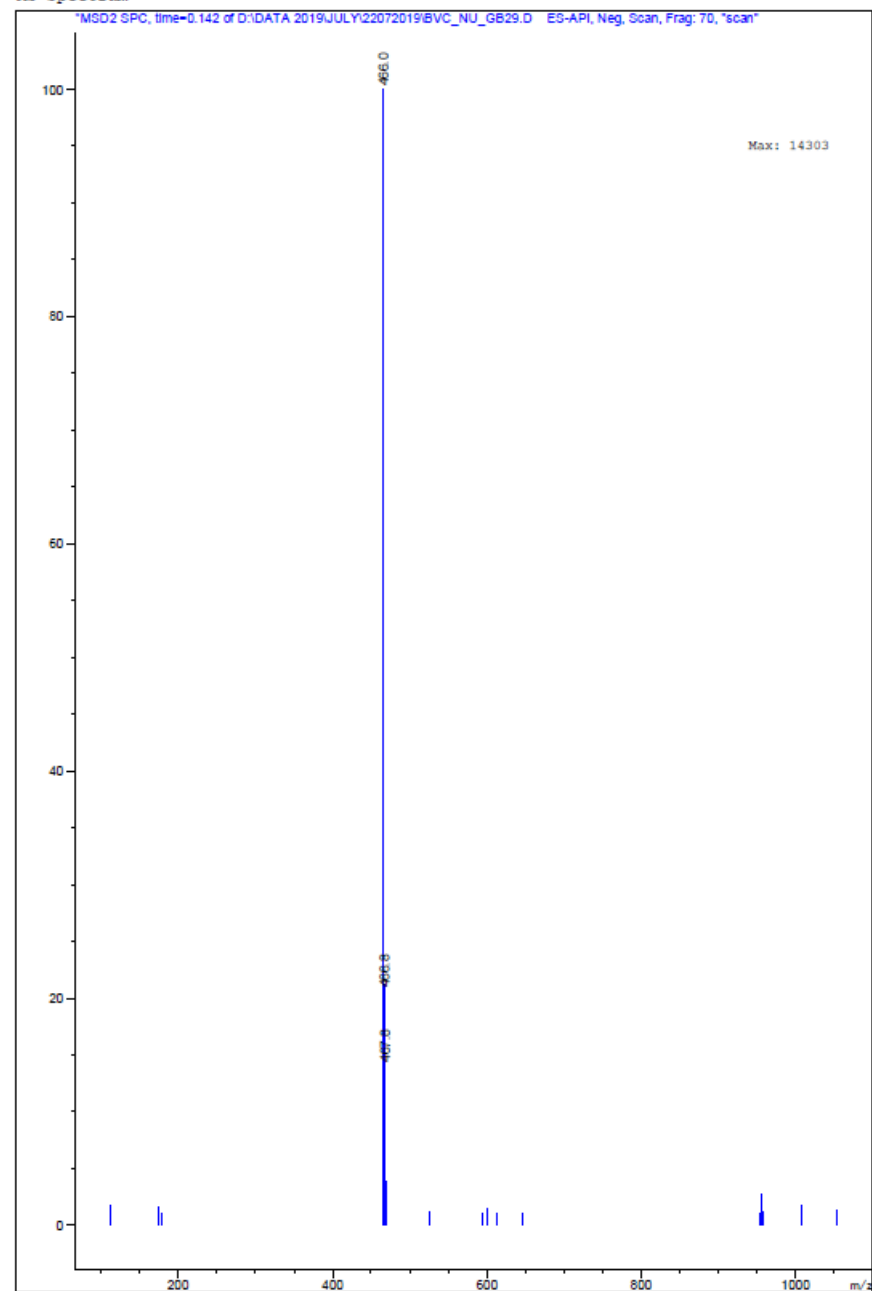


4. HPLC



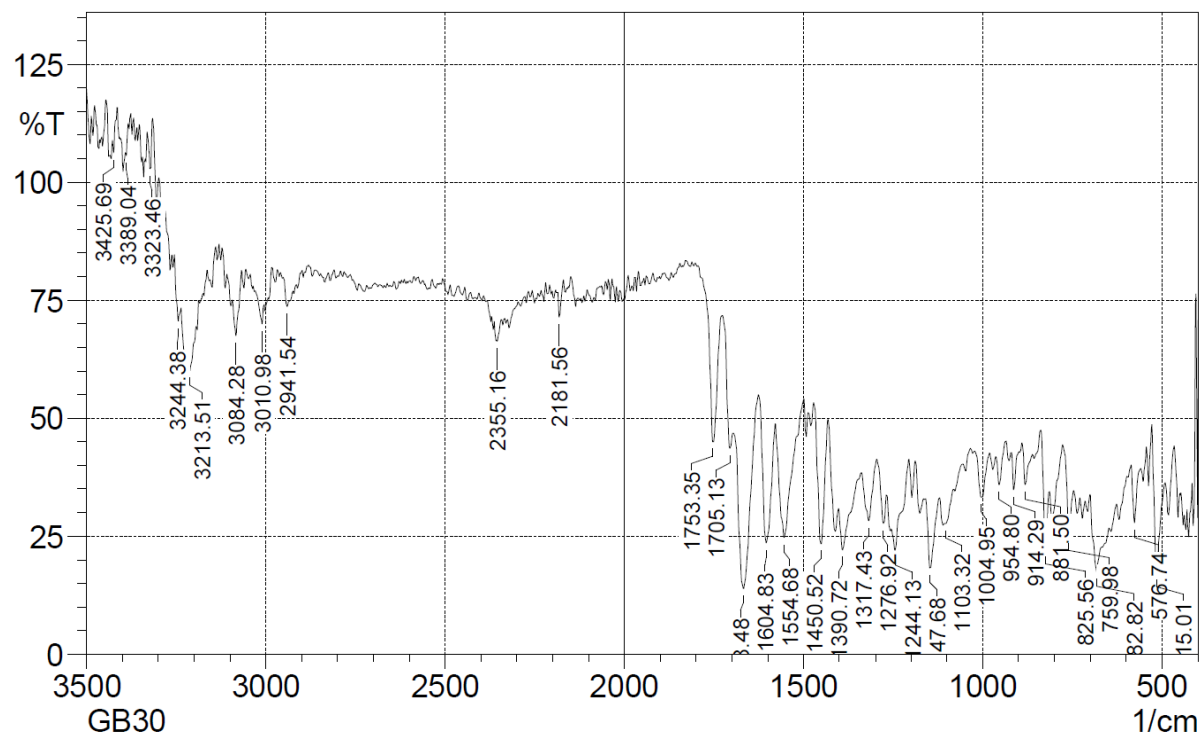
5. Mass

MS Spectrum

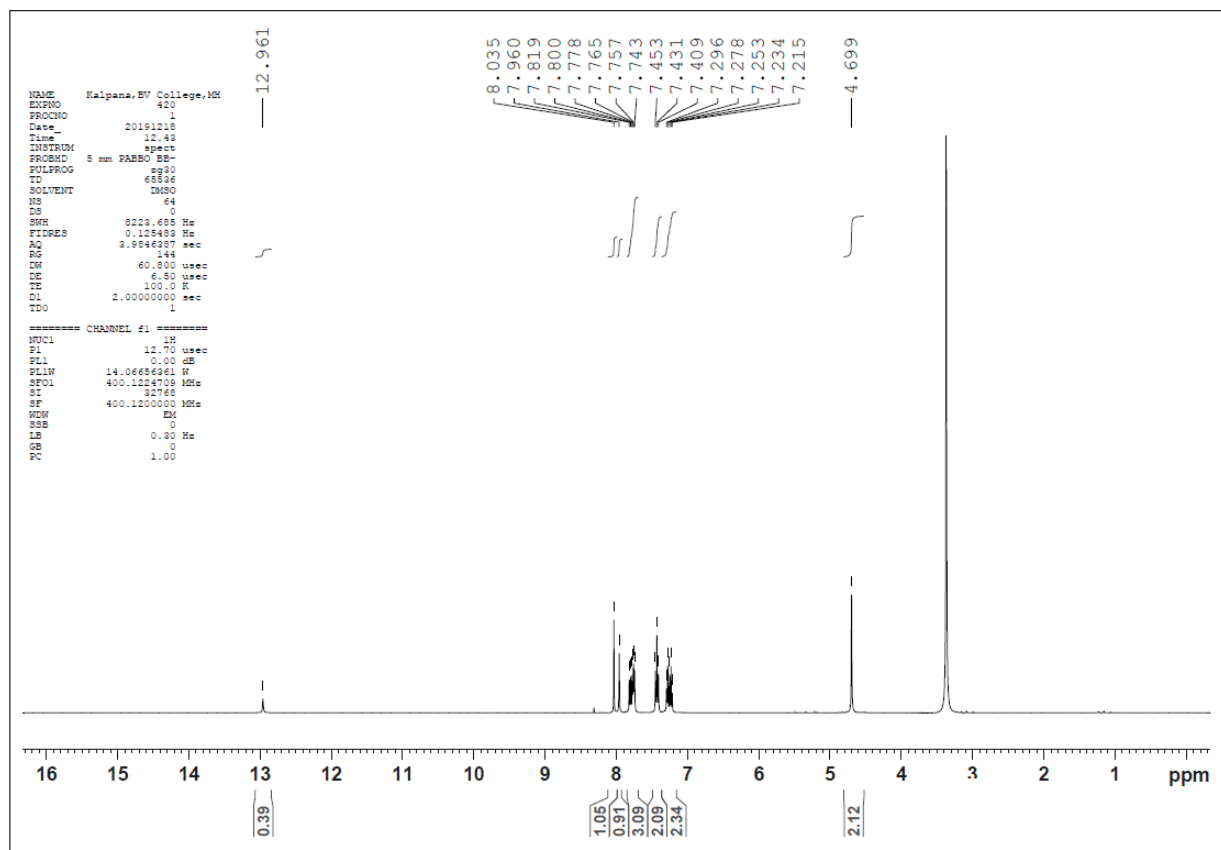


2-(5-benzylidene-2,4-dioxothiazolidin-3-yl)-N-(4-fluorobenzo[d]thiazol-2-yl)acetamide (GB30)

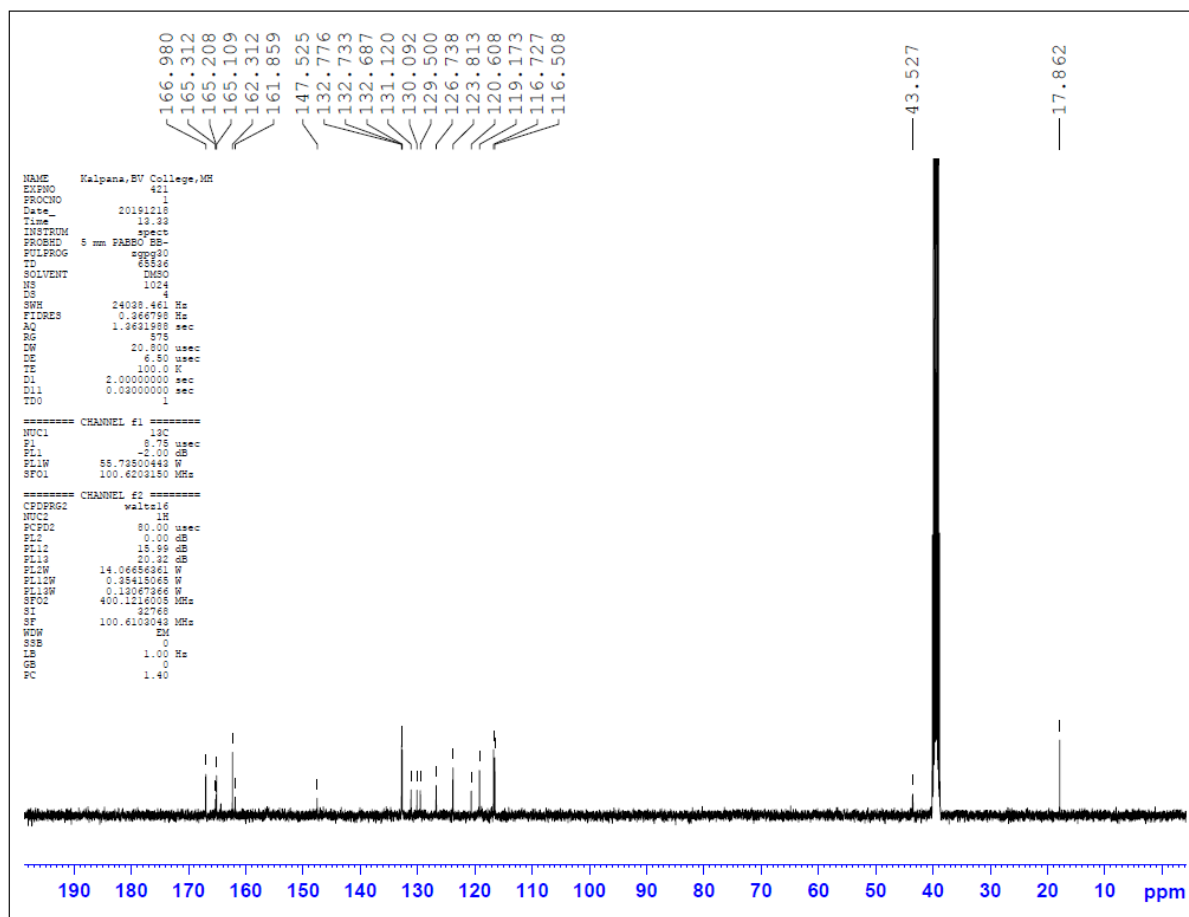
1. FTIR



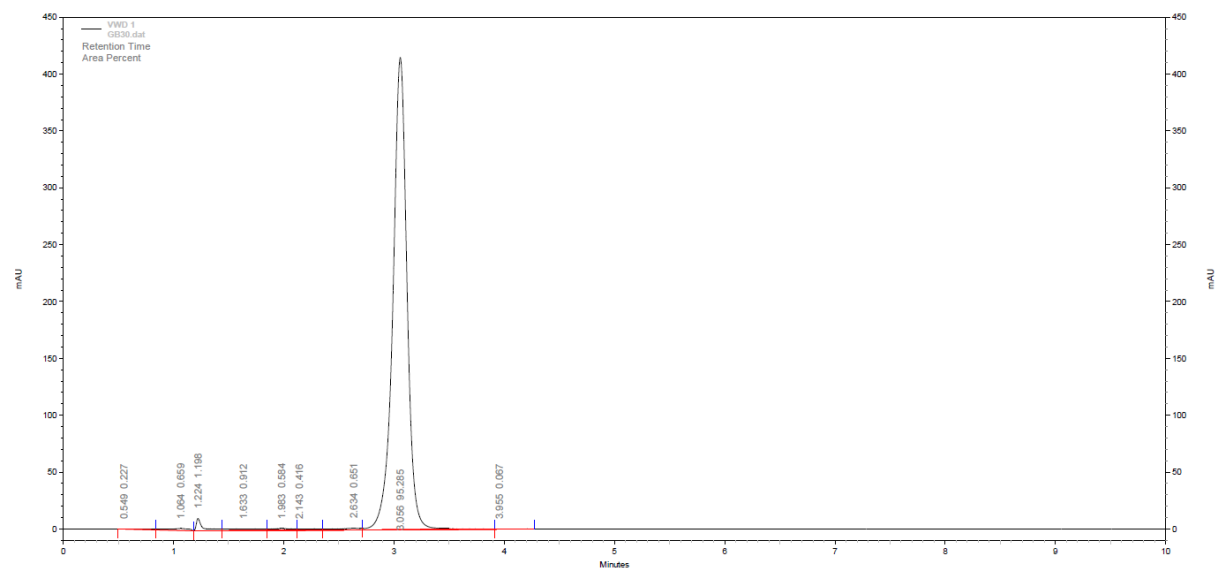
2. 1H-NMR



3. ¹³C-NMR

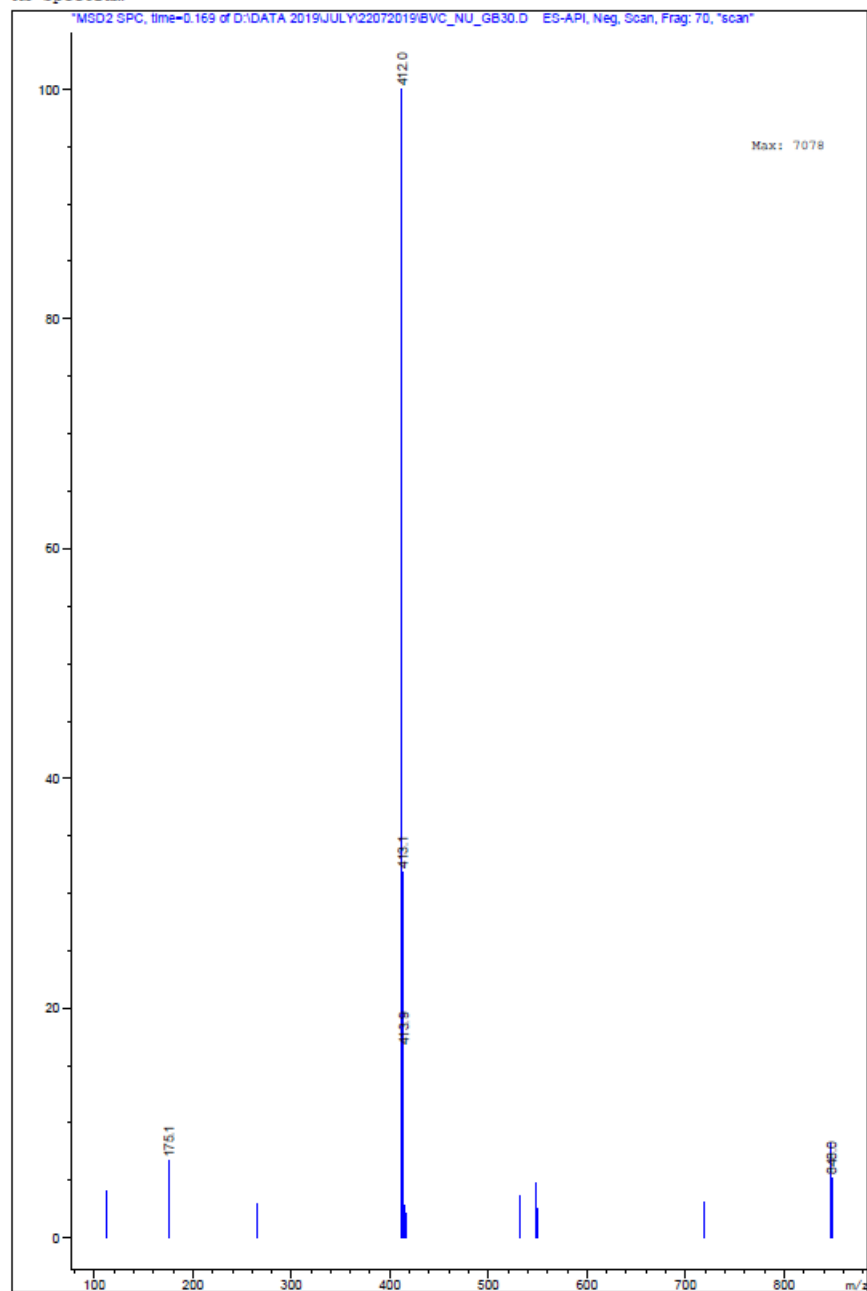


4. HPLC



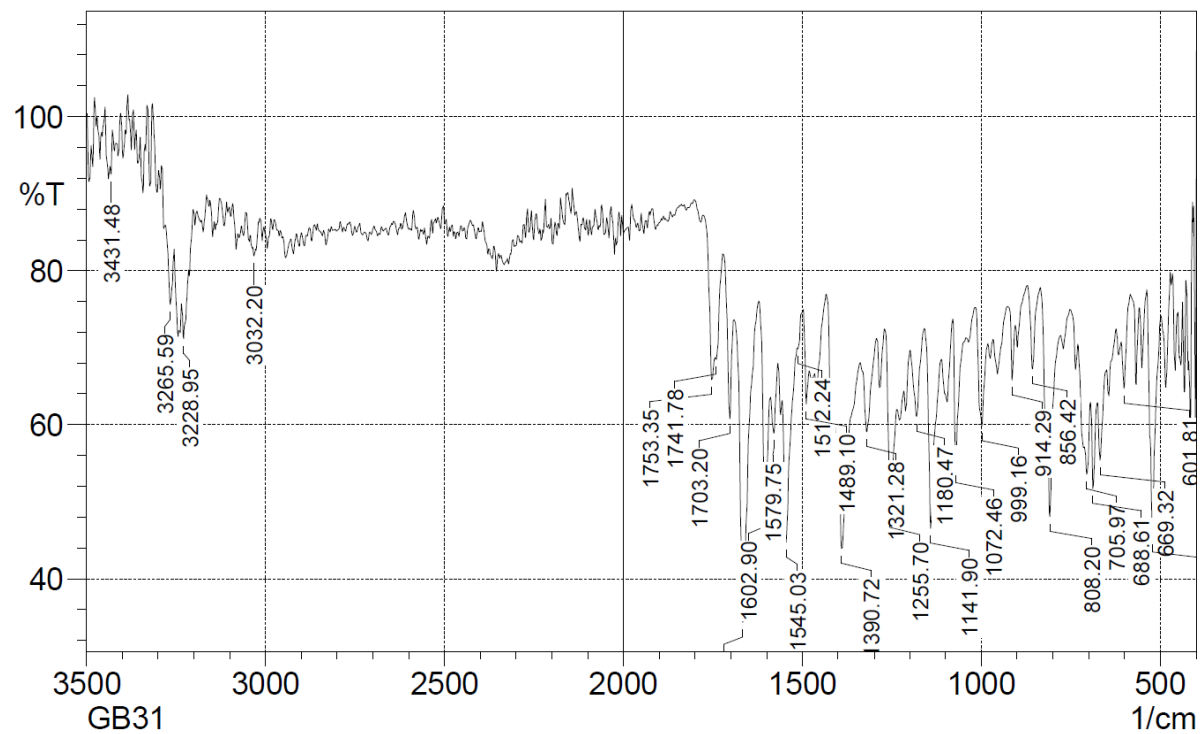
5. Mass

MS Spectrum

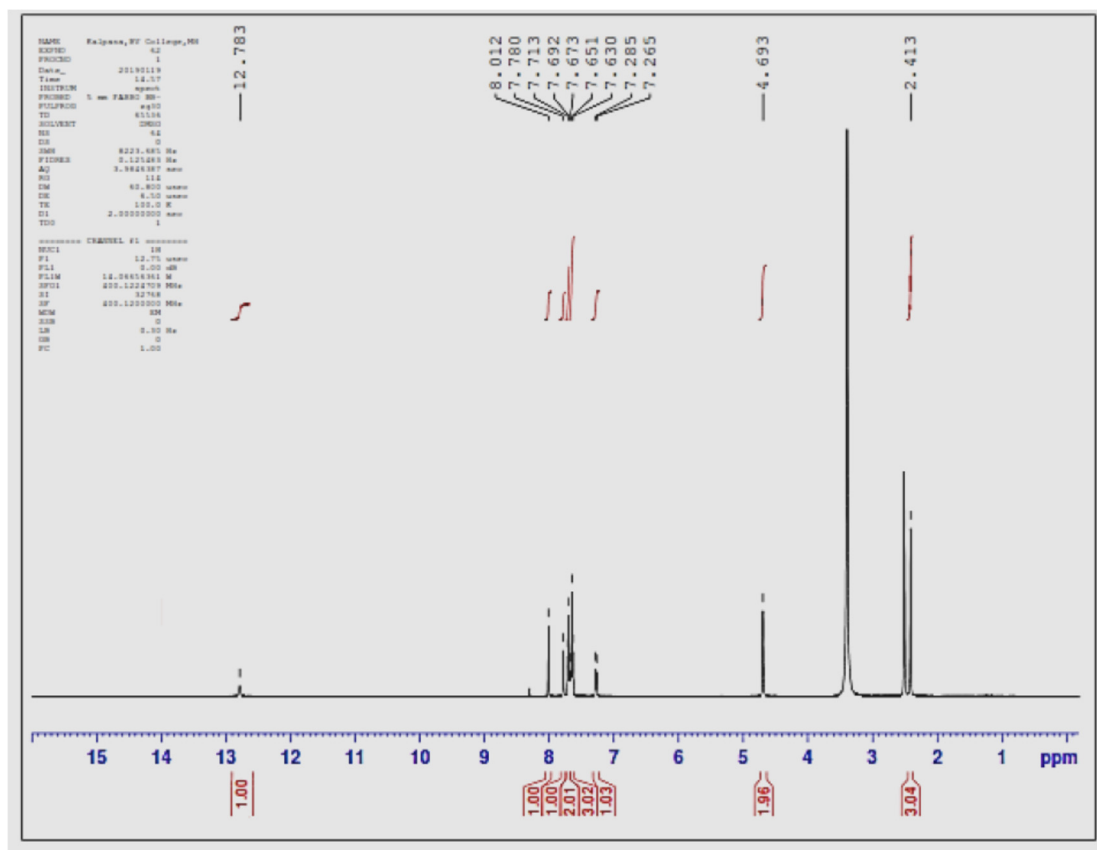


2-(5-(4-bromobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-(6-methylbenzo[d]thiazol-2-yl)acetamide (GB31)

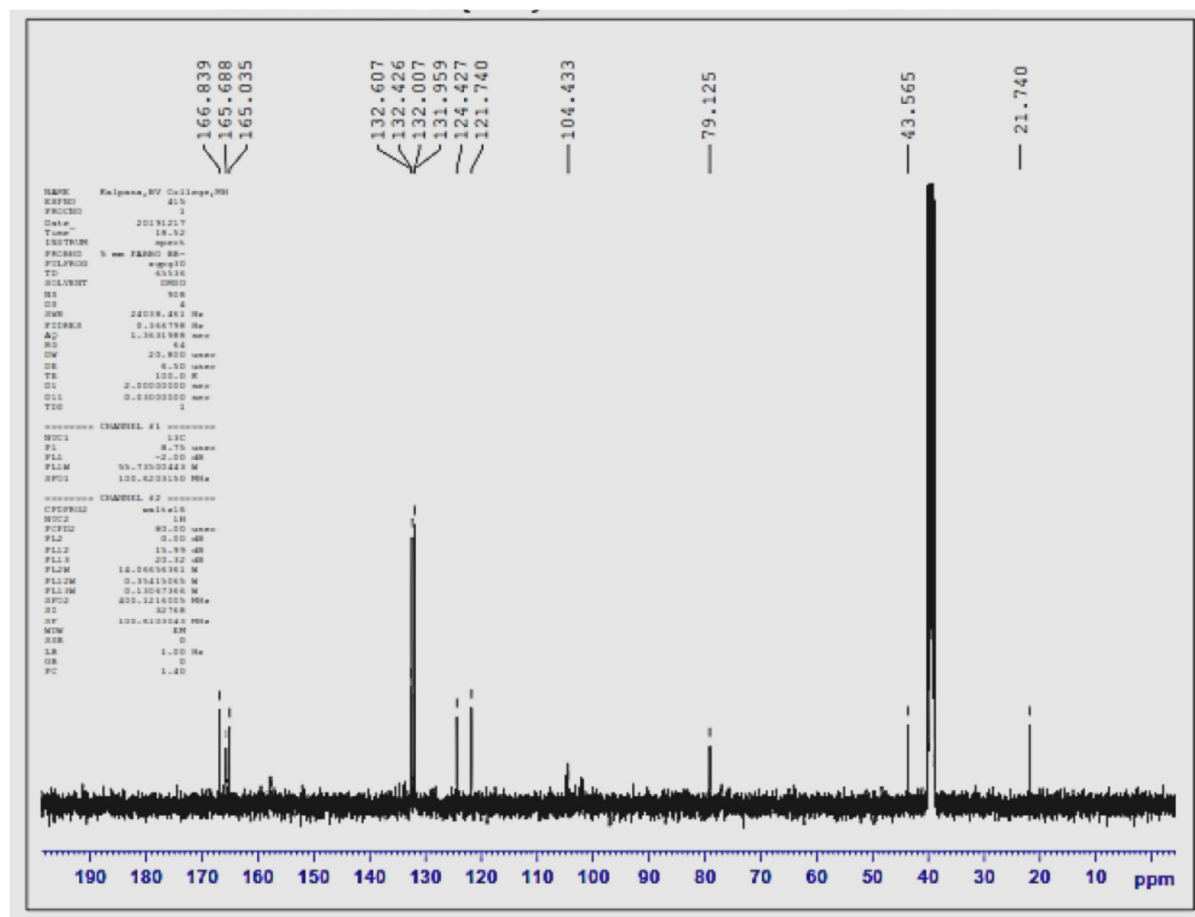
1. FTIR



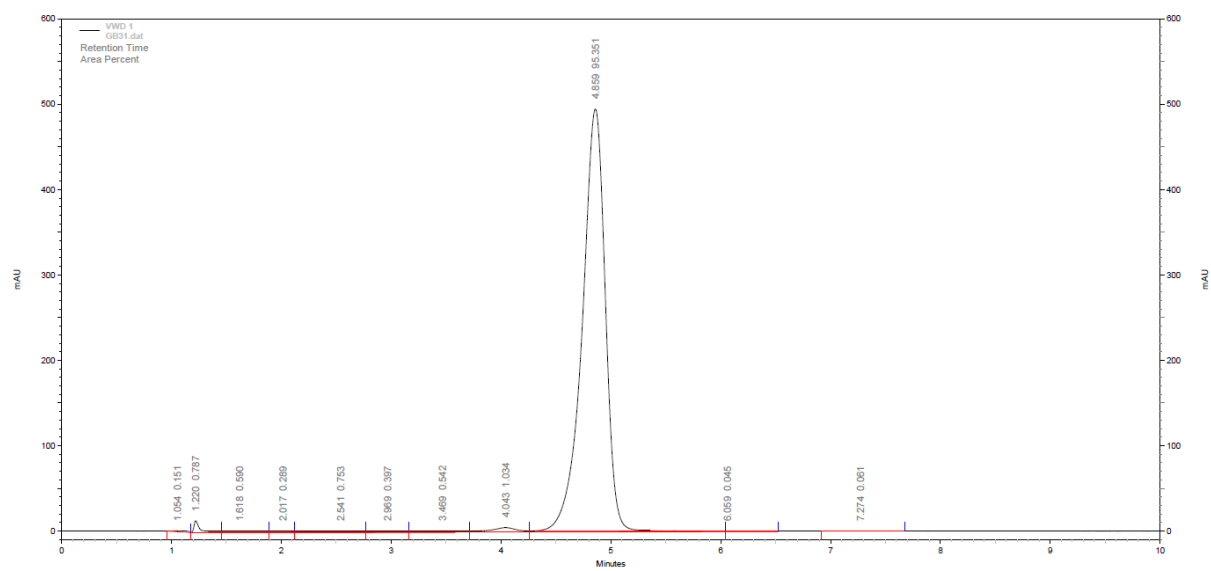
2. ^1H NMR



3. ¹³CNMR

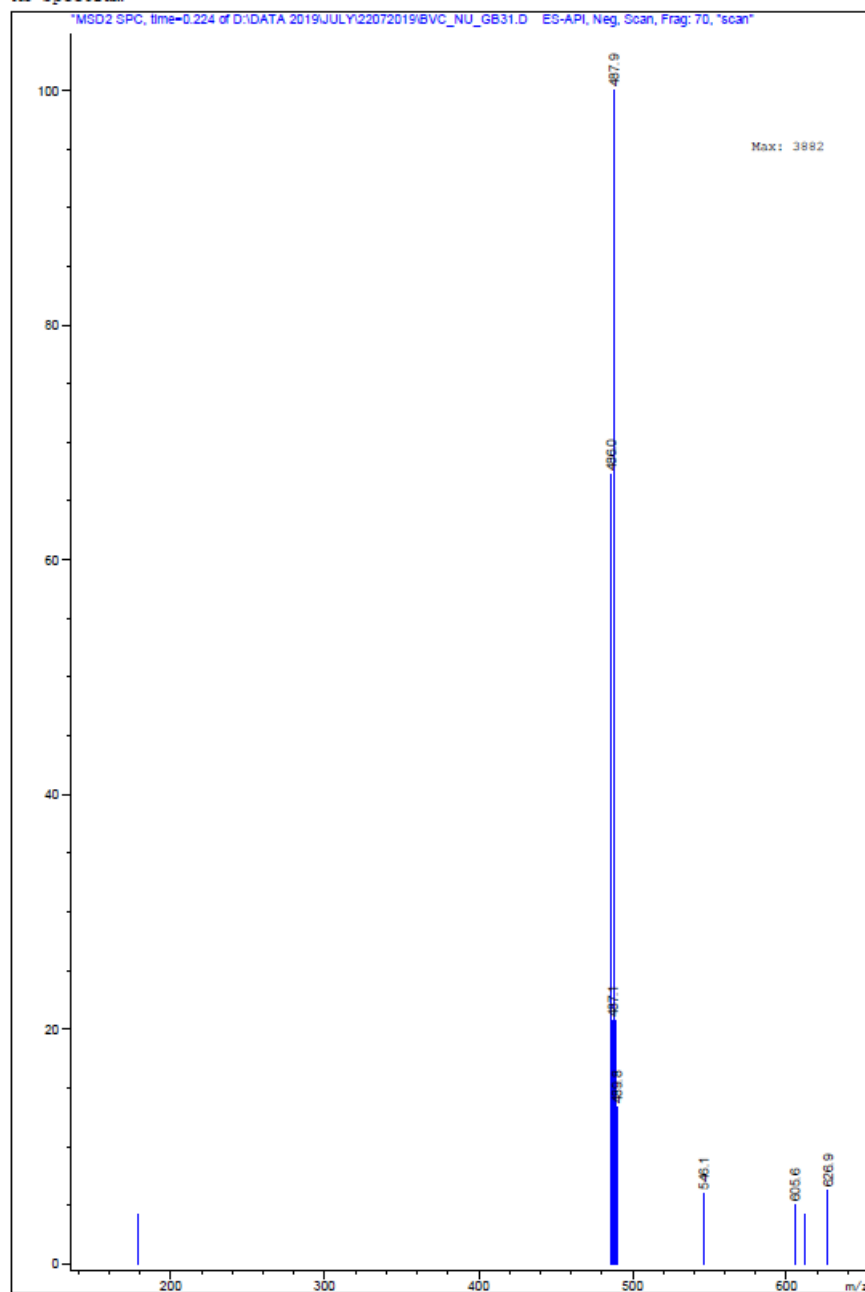


4. HPLC



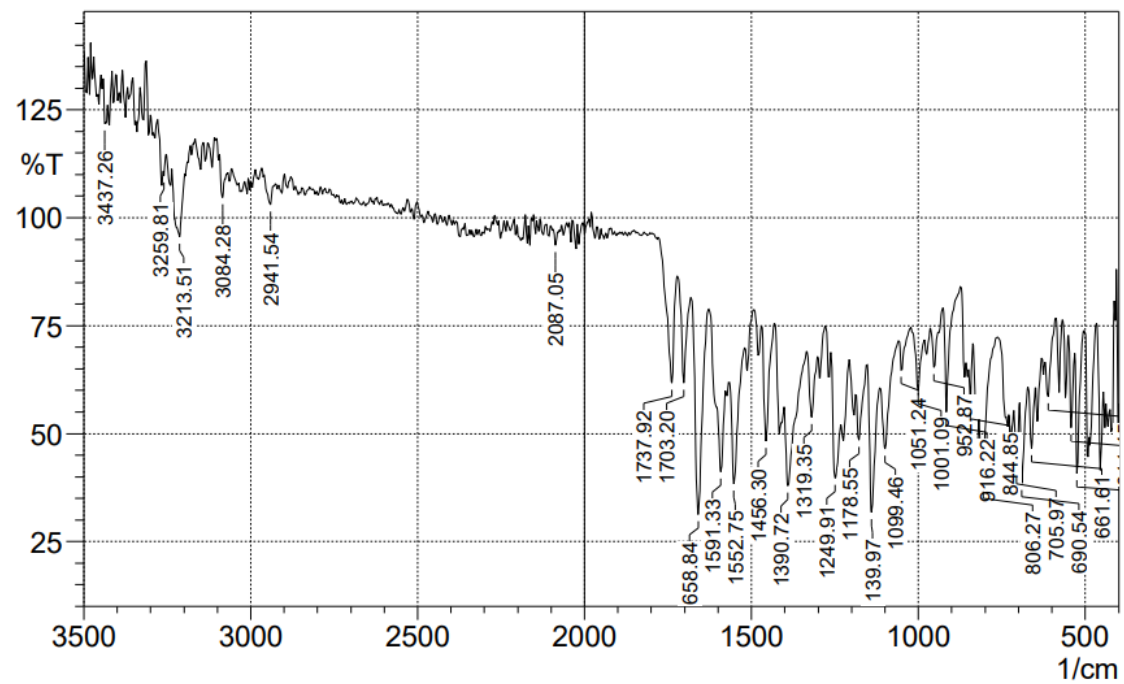
5. Mass

MS Spectrum

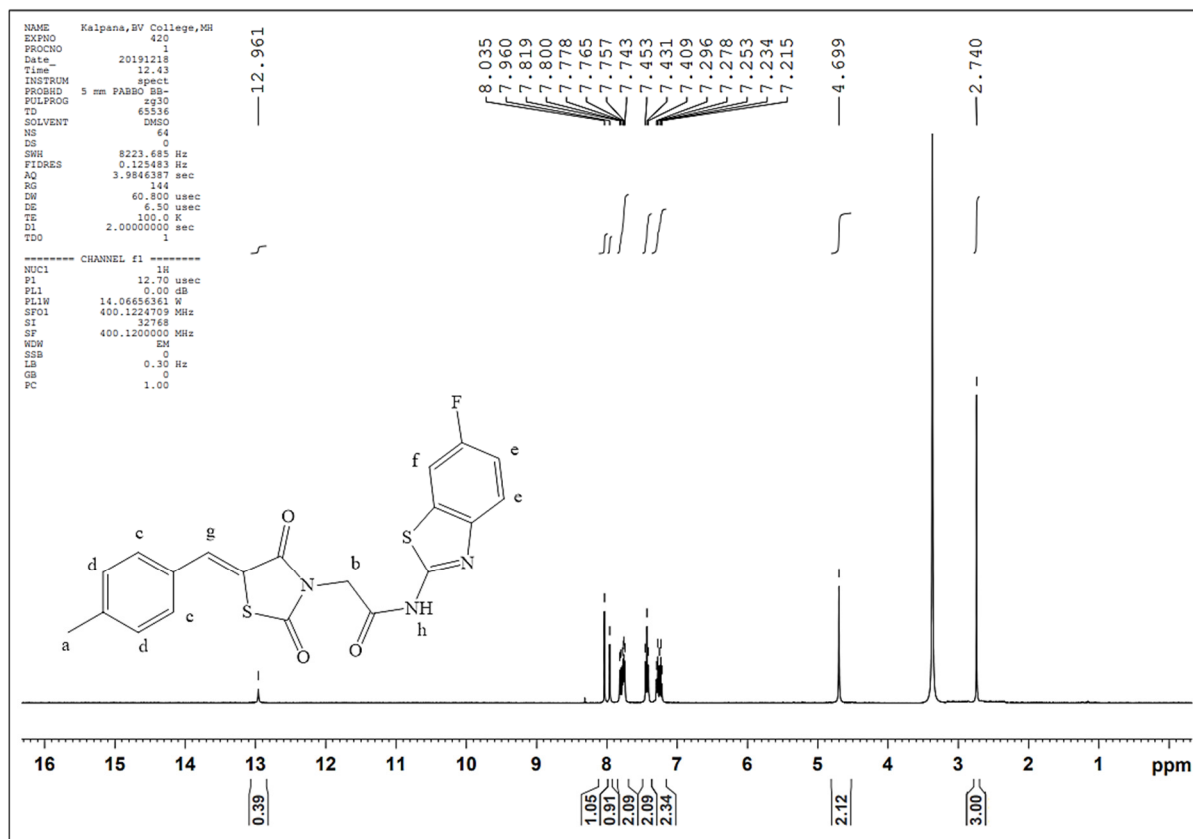


N-(6-fluorobenzo[d]thiazol-2-yl)-2-(5-(4-methylbenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB32)

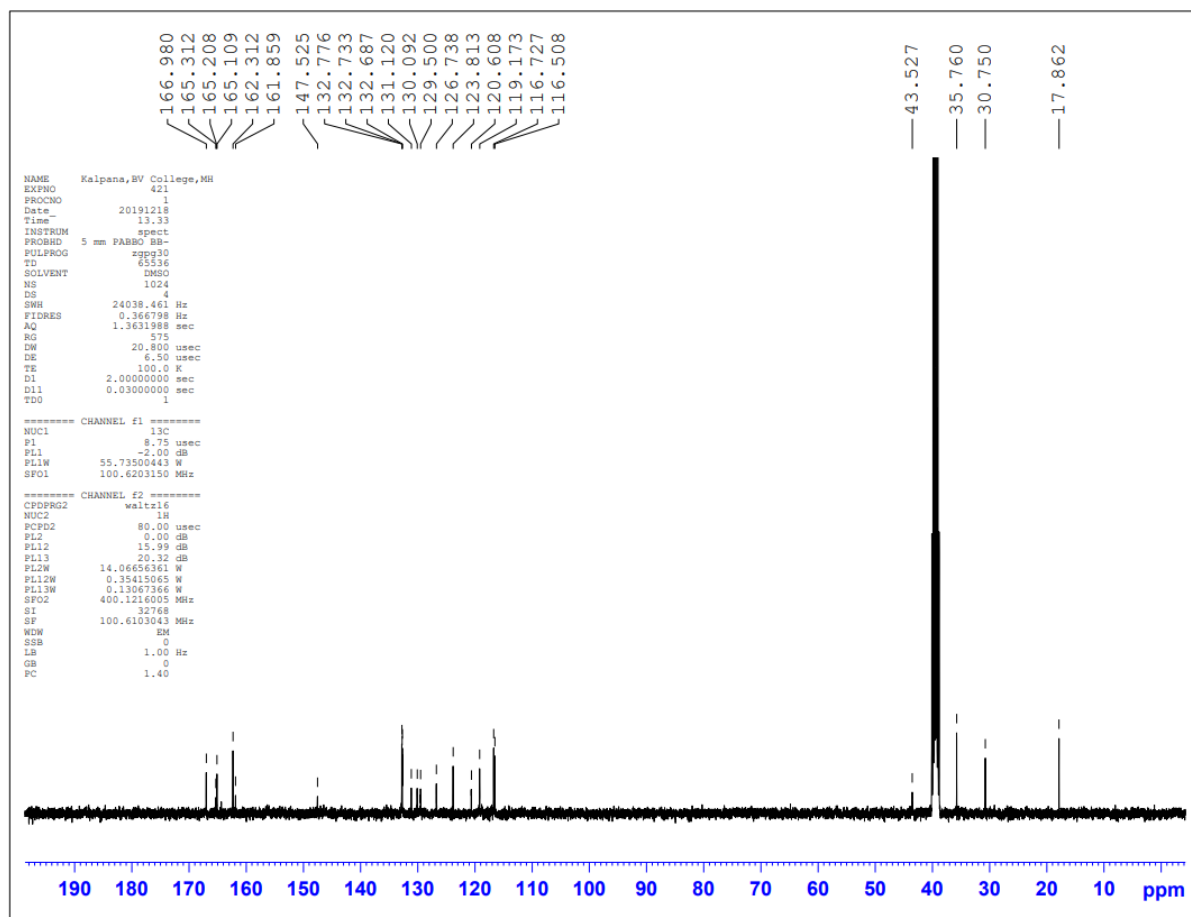
1. FTIR



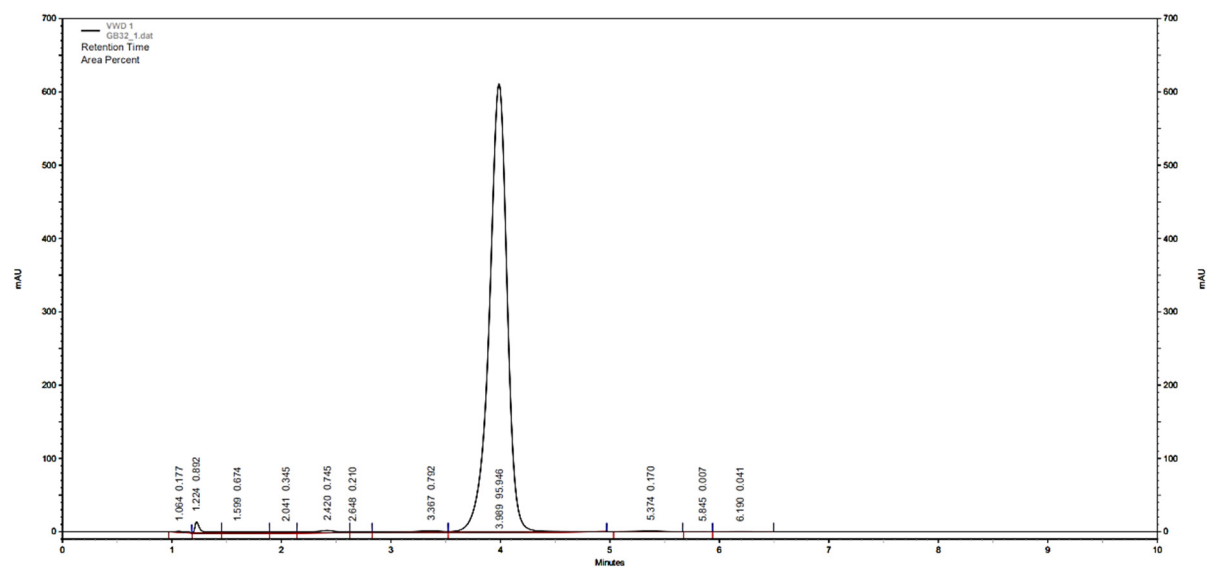
2. ¹H-NMR



3. ¹³C-NMR

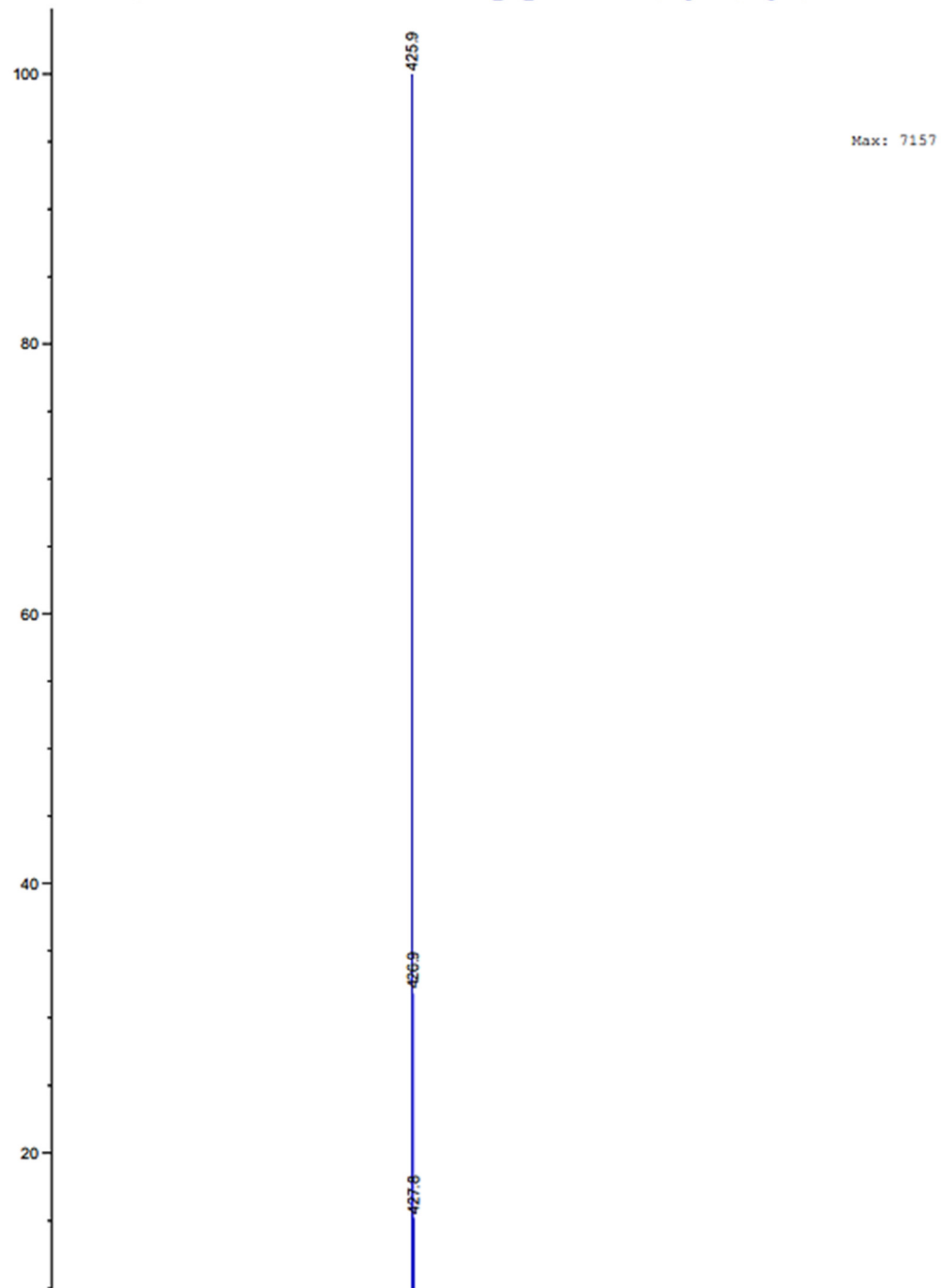


4. HPLC Analysis

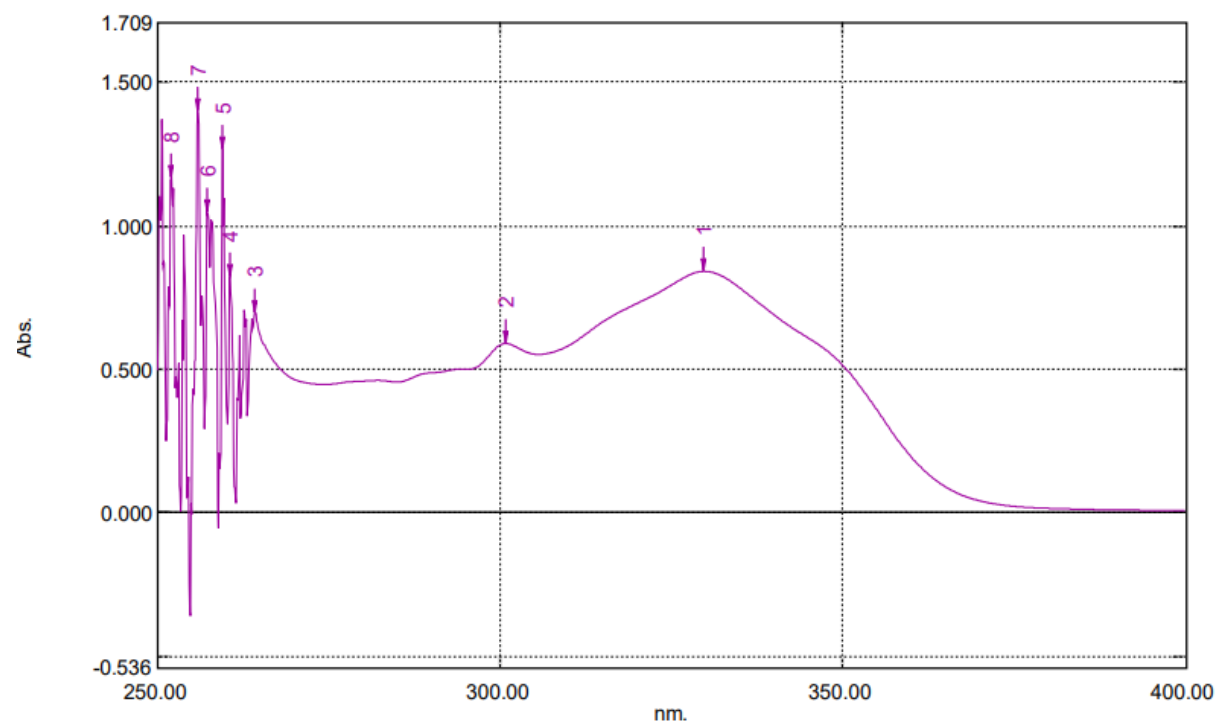


5. Mass Spectrometry

*MSD2 SPC, time=0.224 of D:\DATA 2019\JULY22072019\BVC_NU_GB32.D ES-API, Neg. Scan, Frag: 70, "scan"

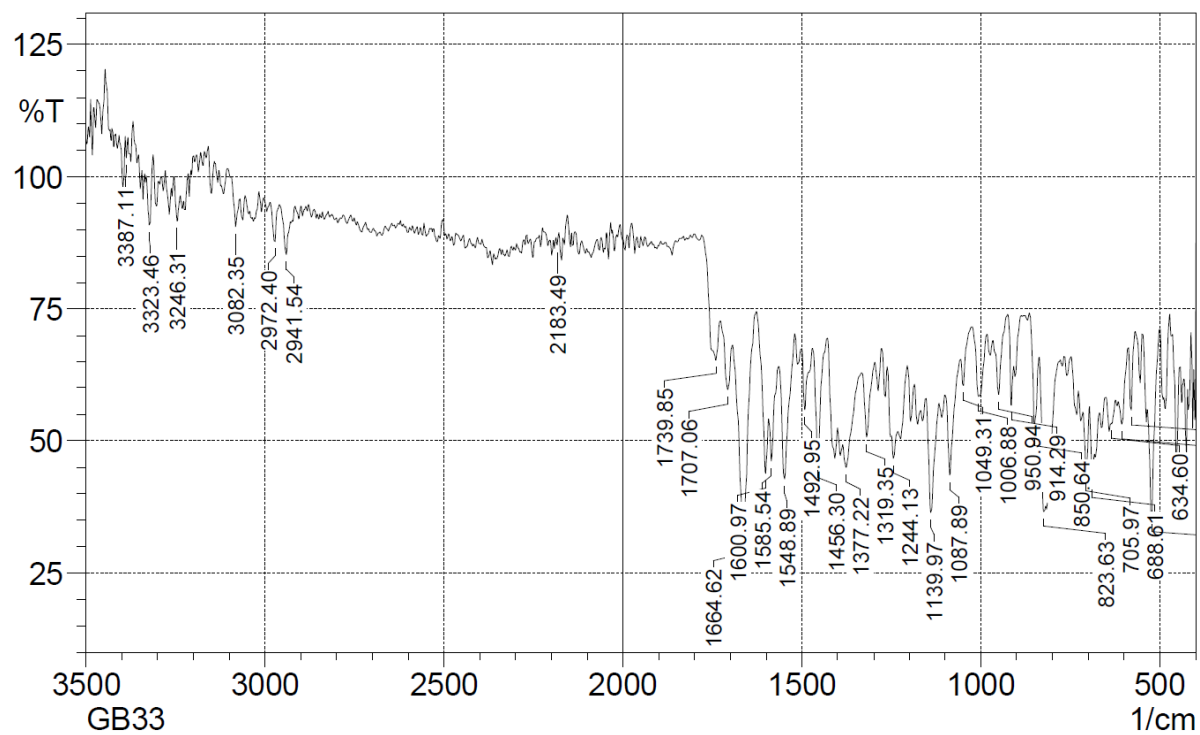


6. UV

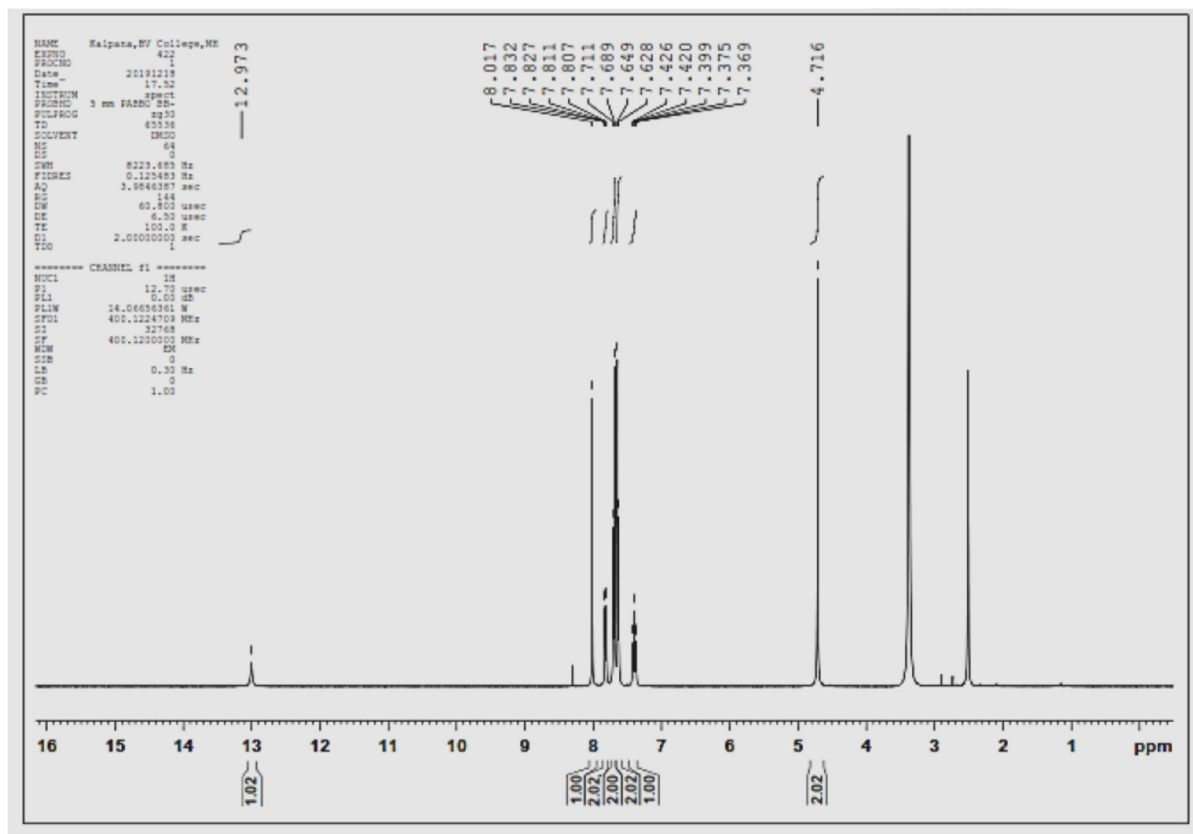


2-(5-(4-chlorobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-(6-fluorobenzo[d]thiazol-2-yl)acetamide (GB33)

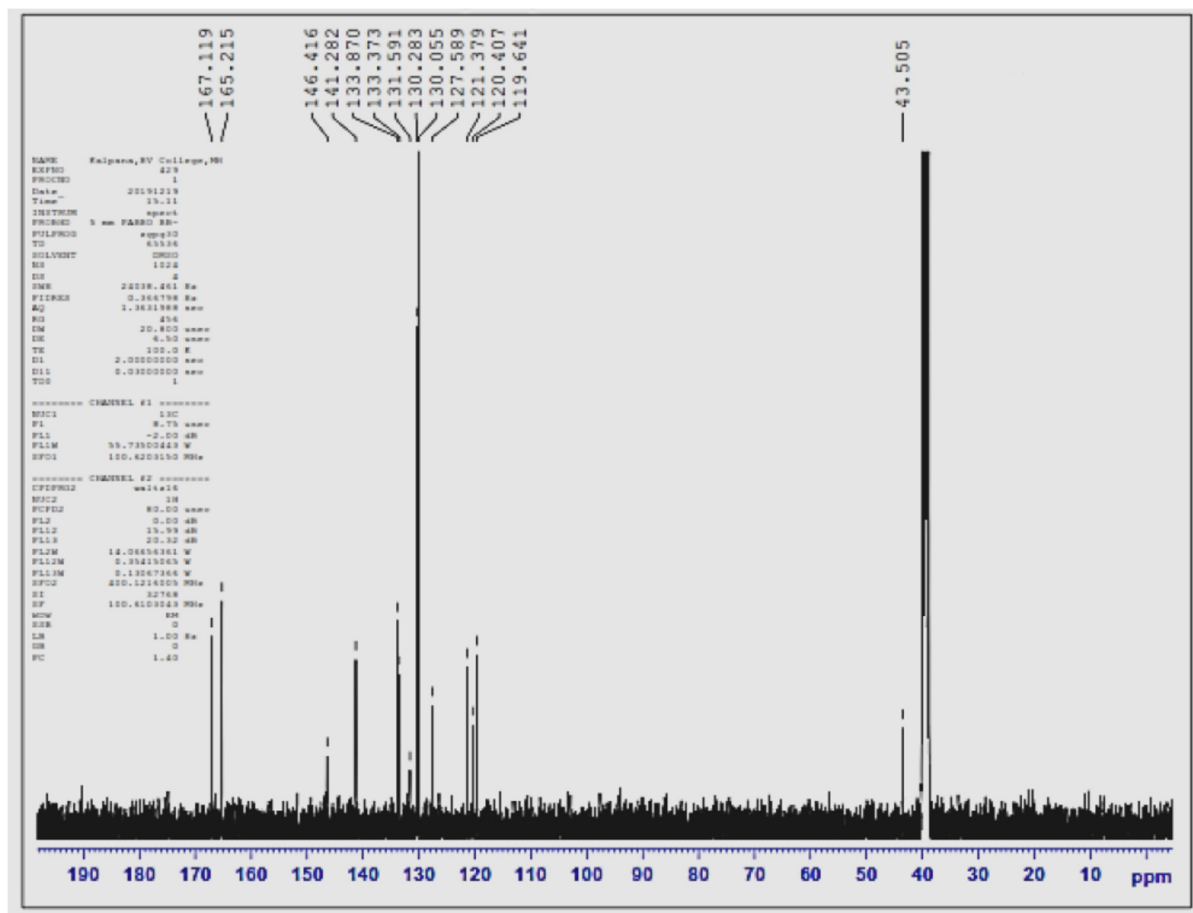
1. FTIR



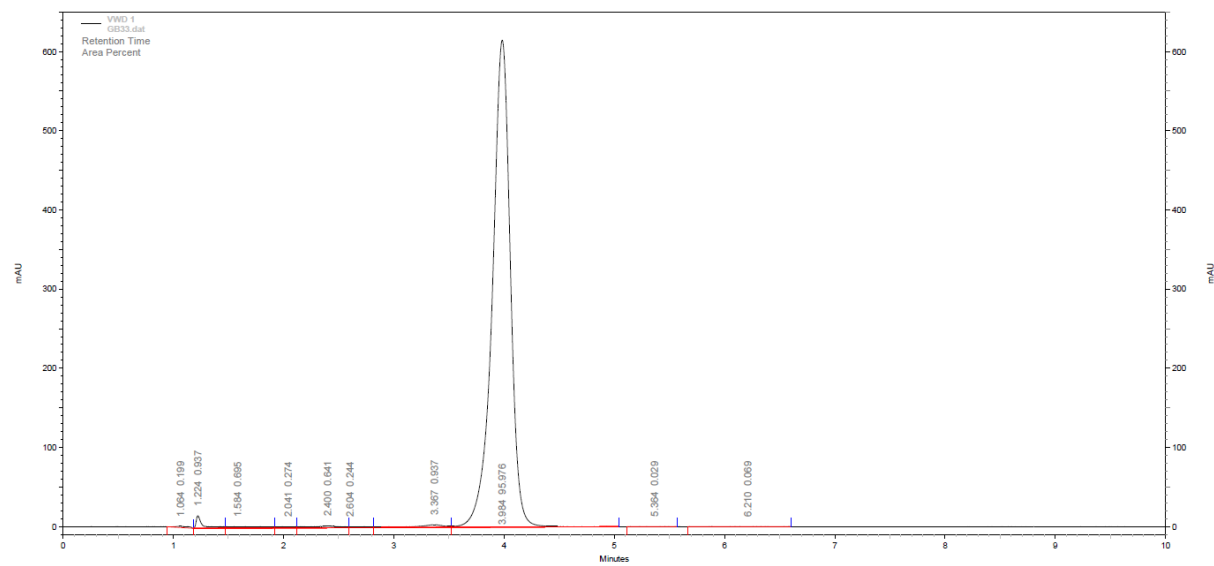
2. ¹HNMR



3. ^{13}C NMR

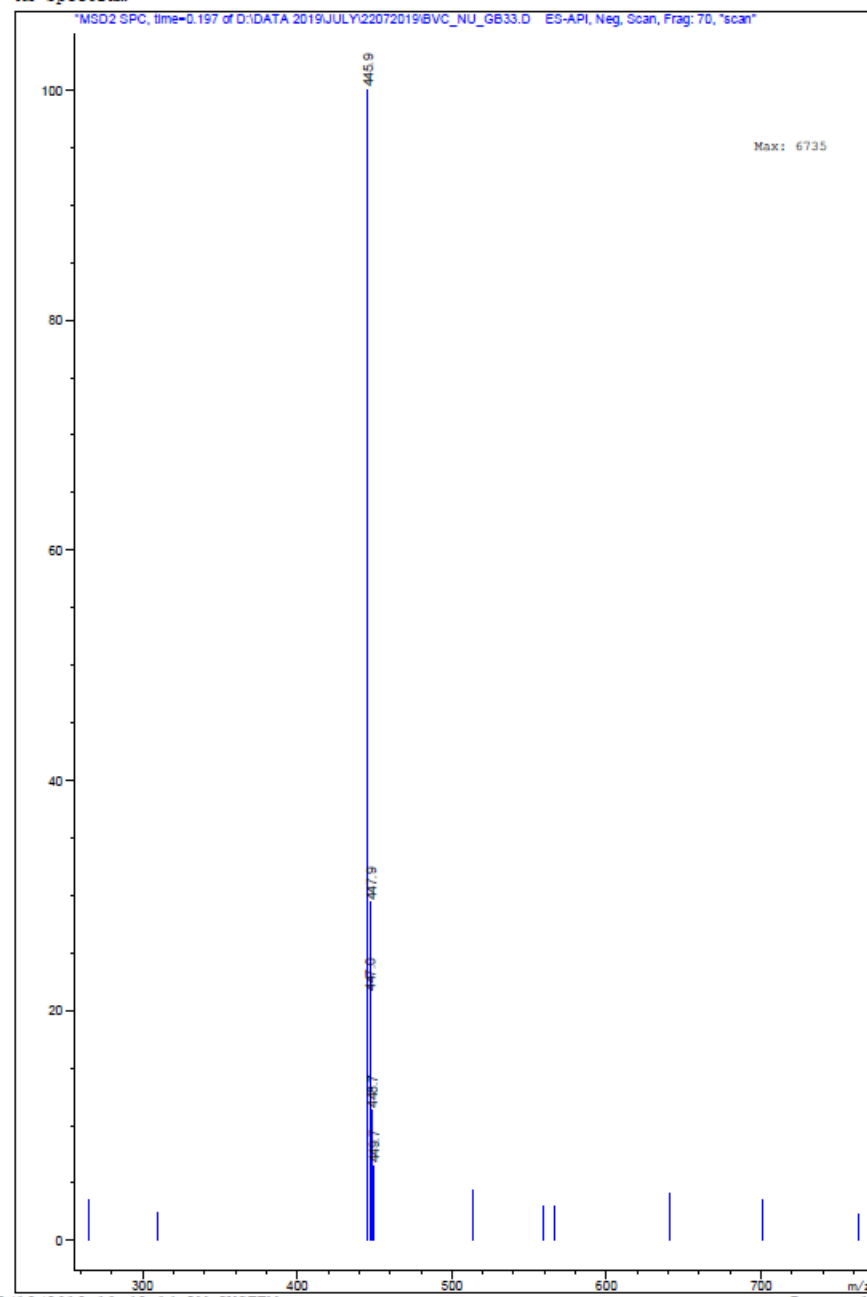


2. HPLC



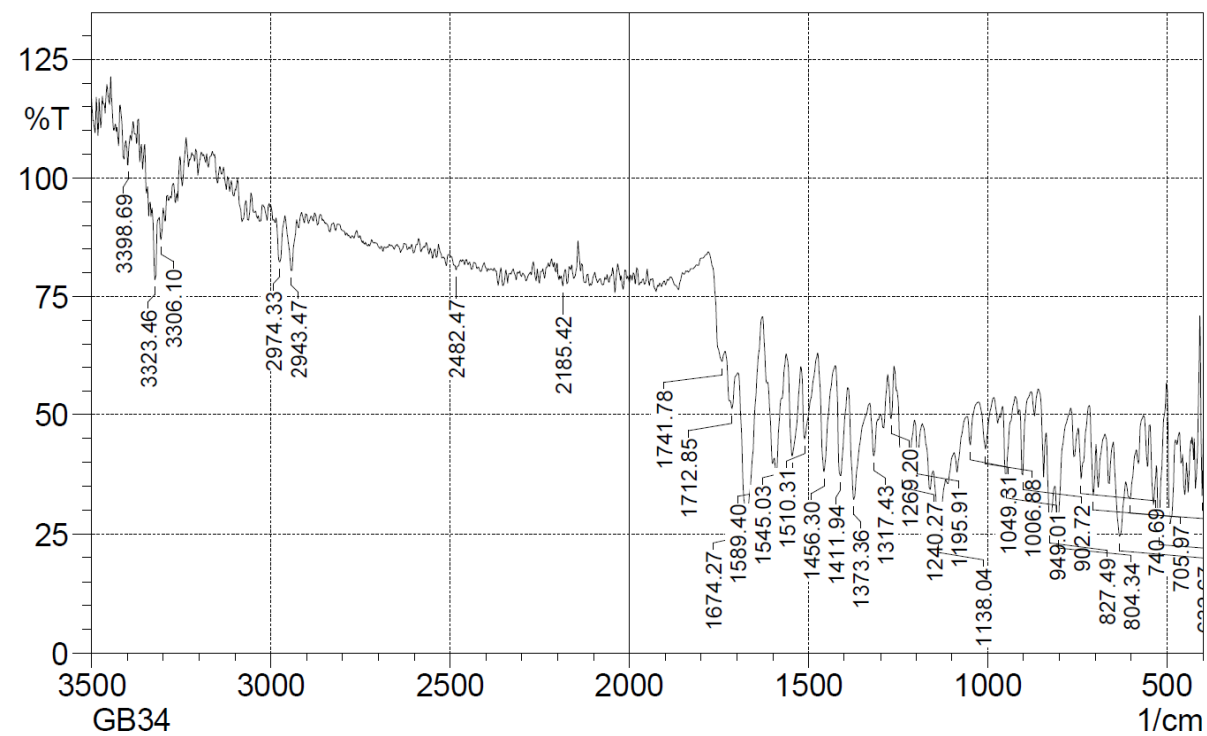
3. Mass

MS Spectrum

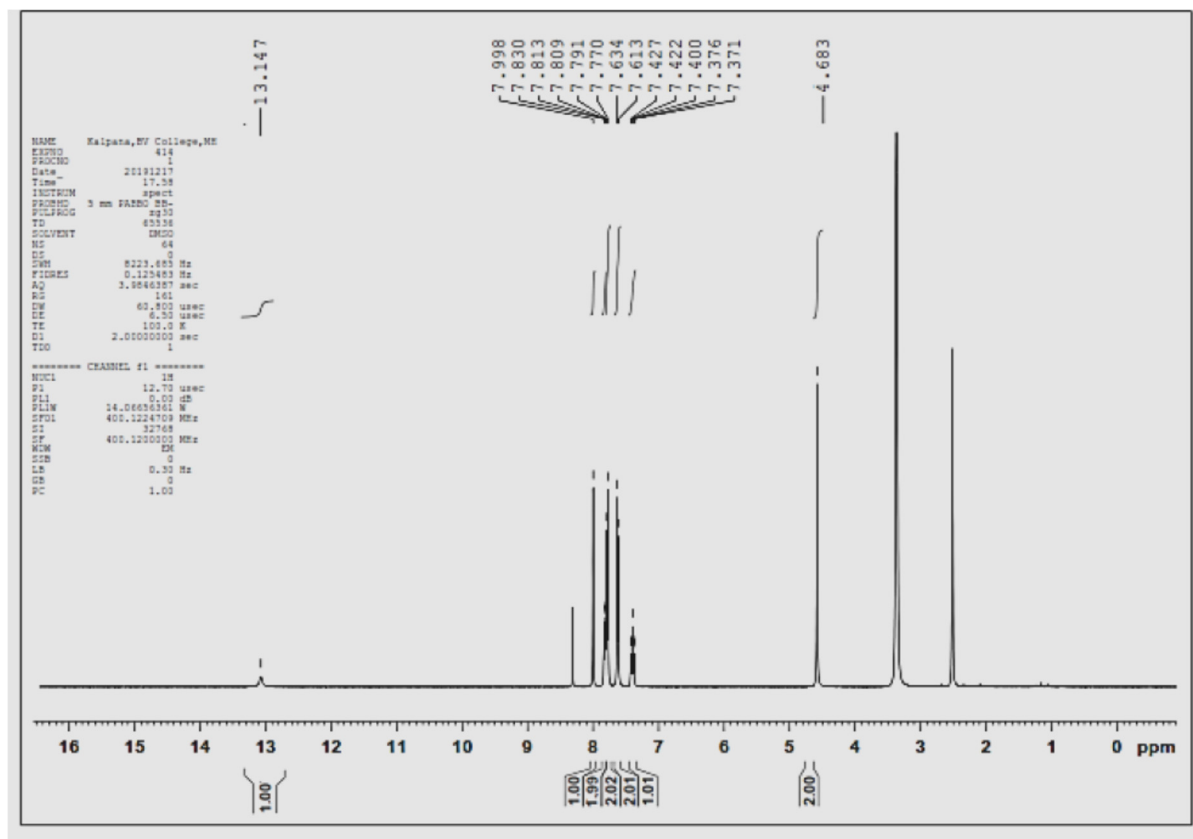


N-(6-fluorobenzo[d]thiazol-2-yl)-2-(5-(4-fluorobenzylidene)-2,4-dioxothiazolidin-3-yl)acetamide (GB34)

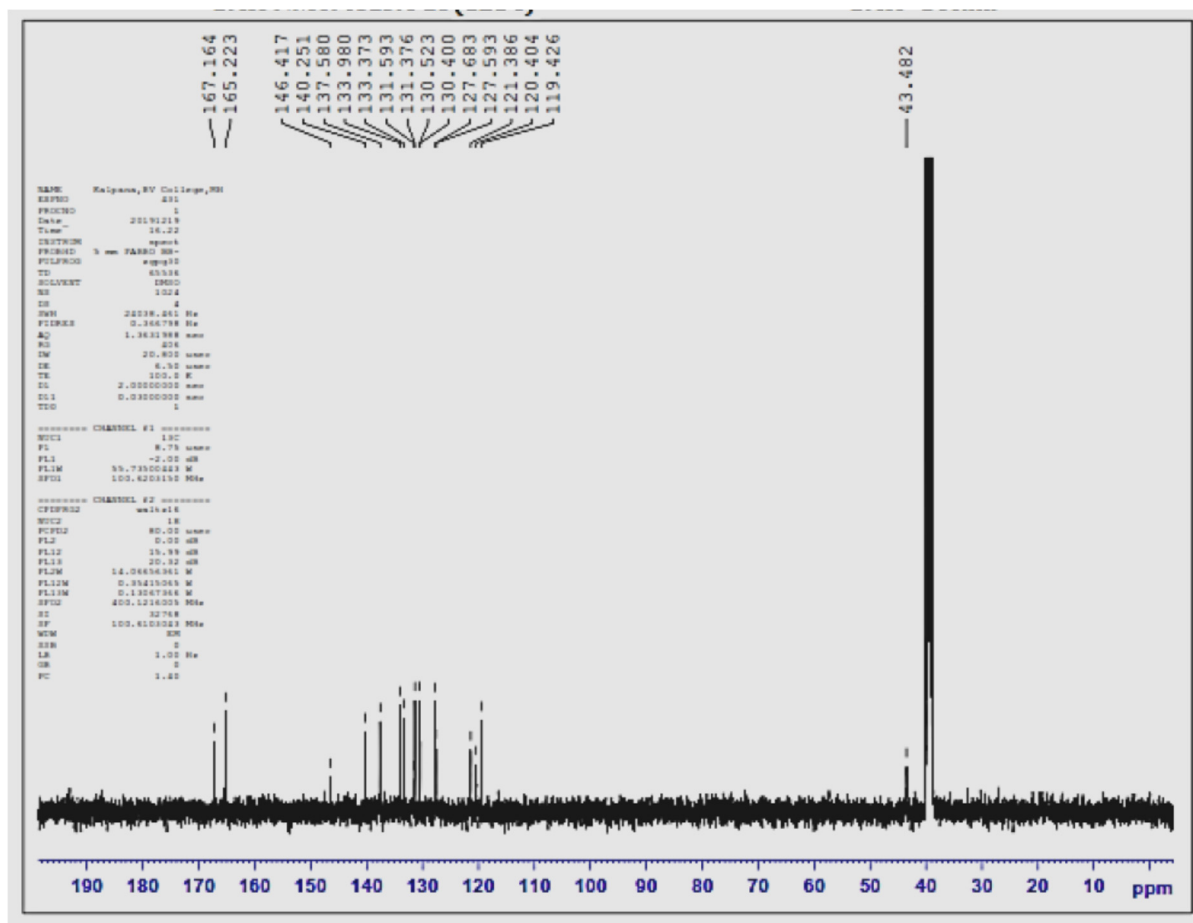
1. FTIR



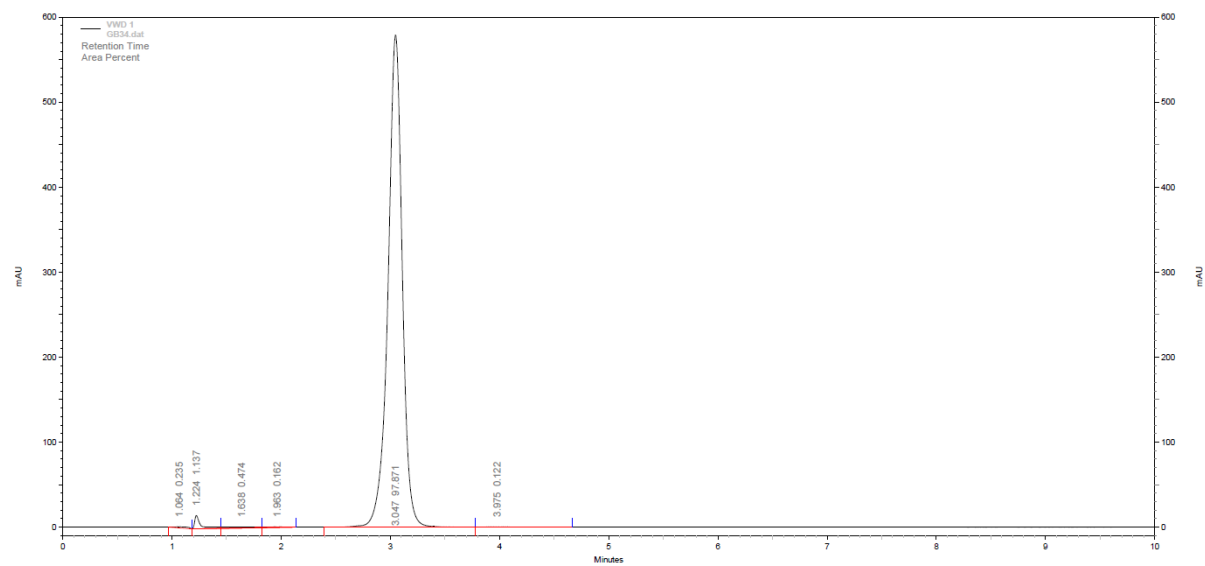
2. ¹H NMR



3. ¹³CNMR

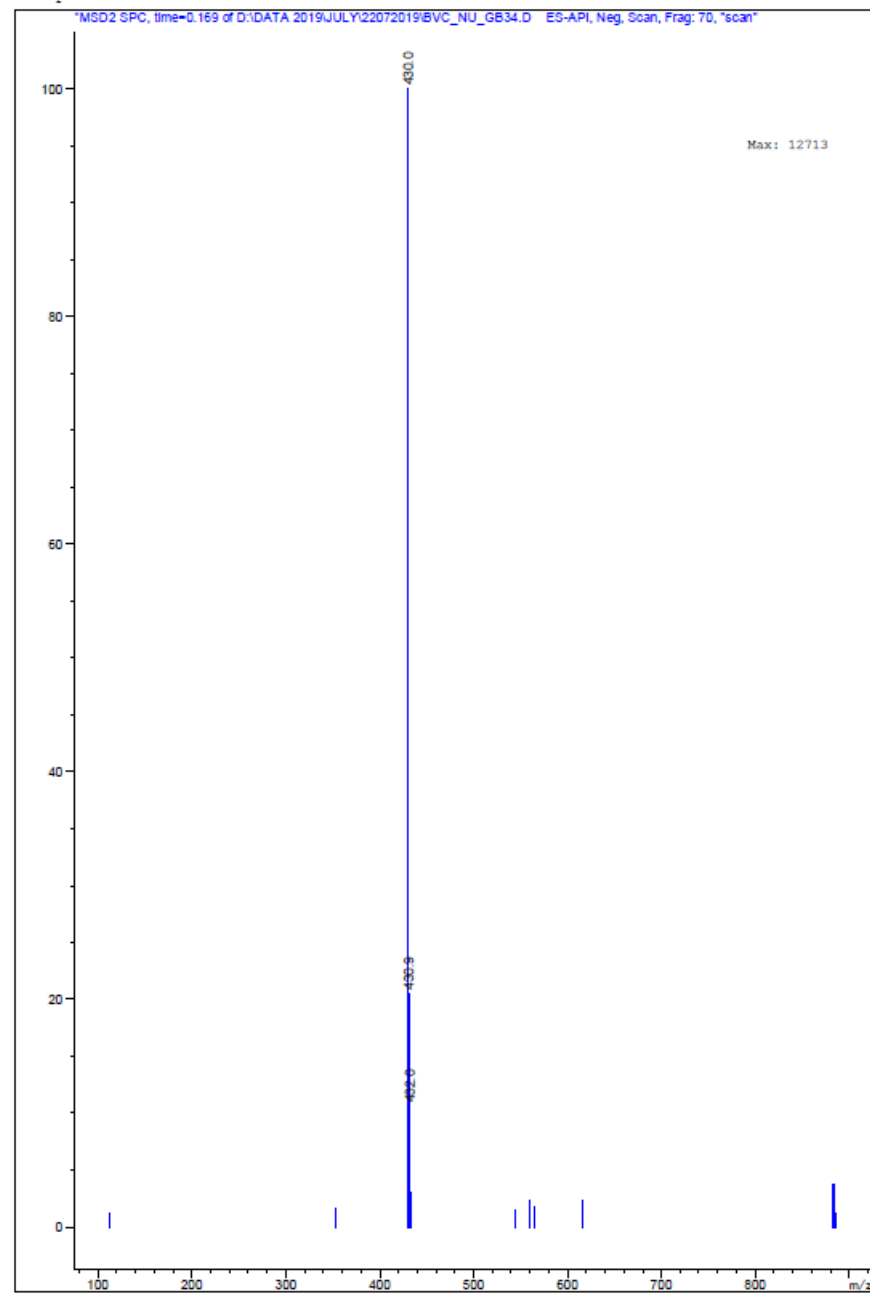


4. HPLC



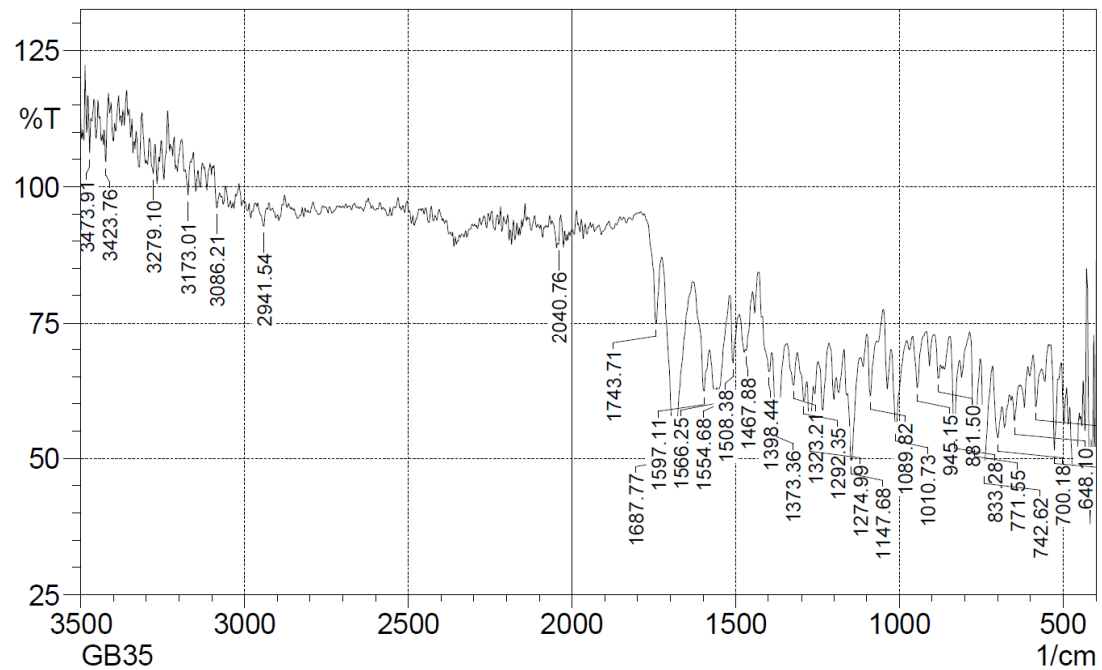
5. Mass

MS Spectrum



2-(5-(4-fluorobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-(4-methoxybenzo[d]thiazol-2-yl)acetamide (GB35)

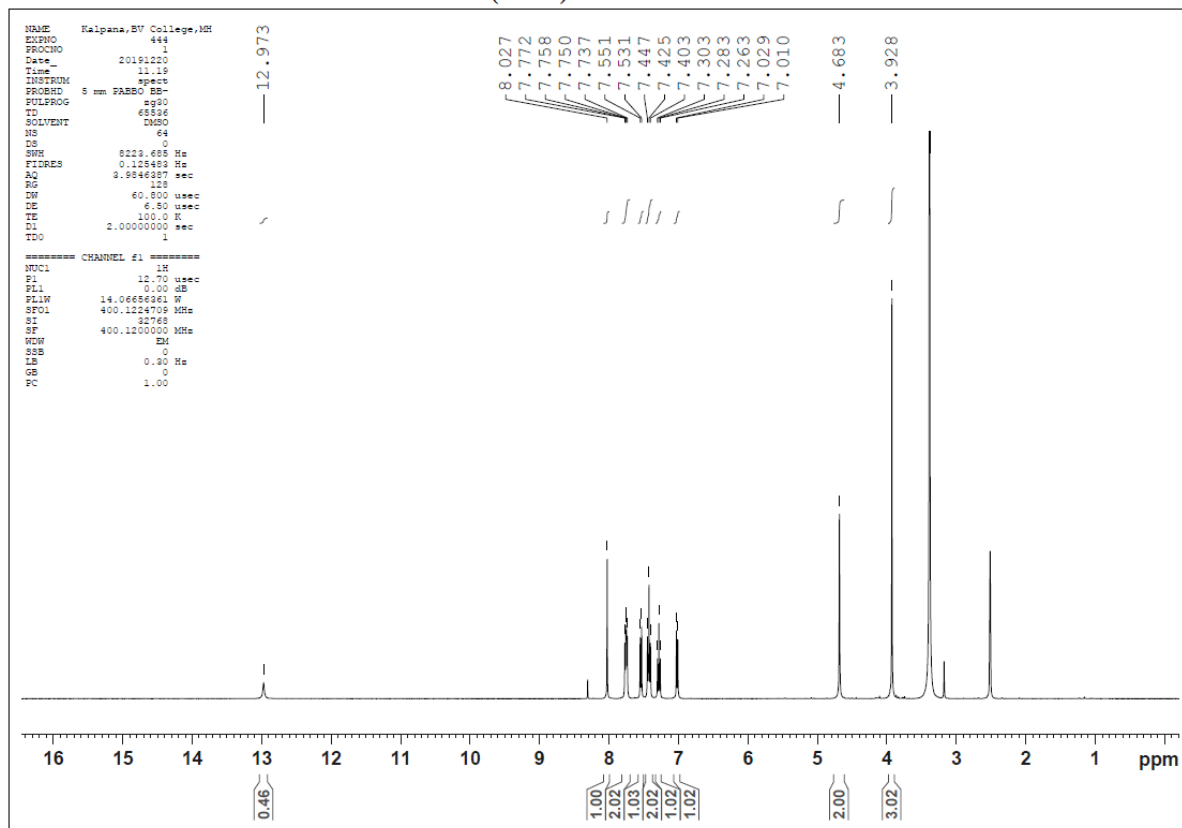
1. FTIR



2. 1H-NMR

SAIFNM190323A-41(GB35)

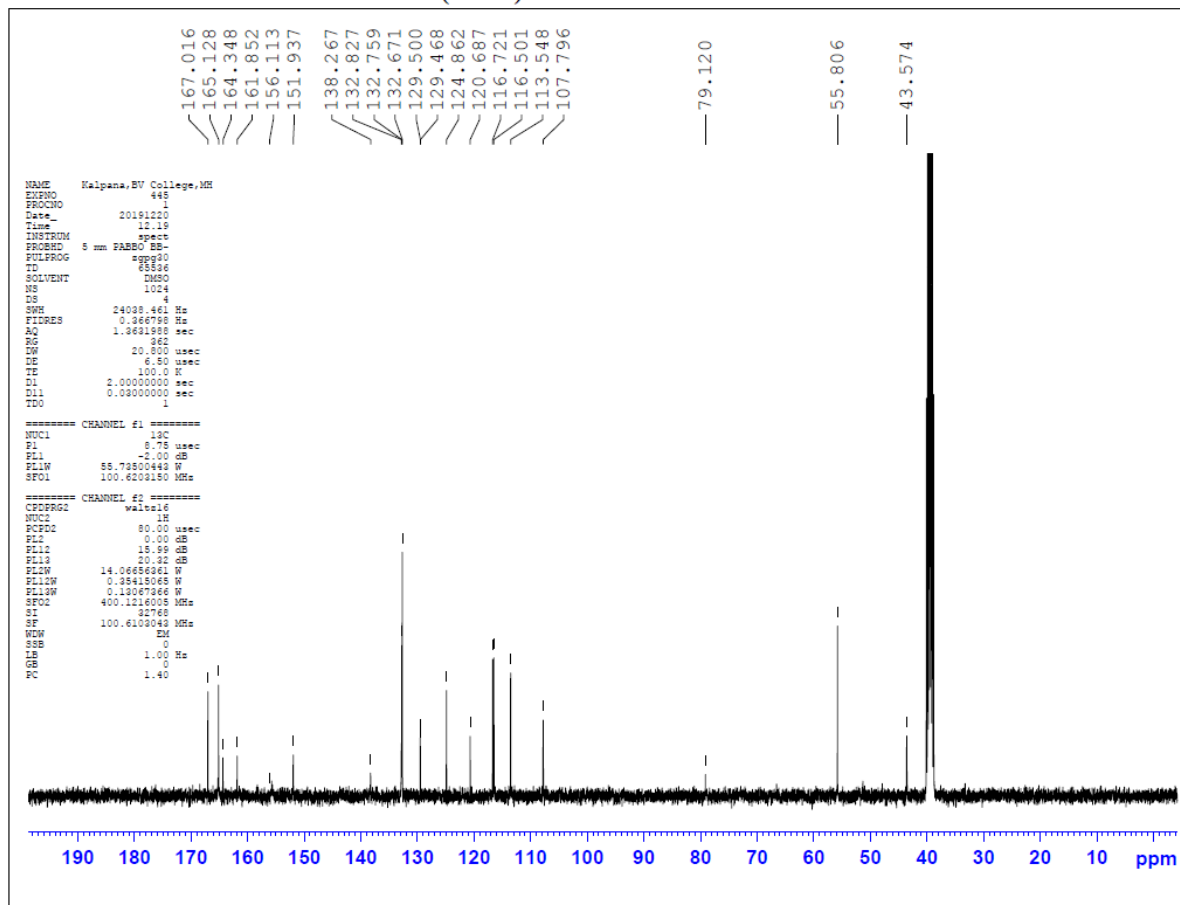
SAIF Cochin



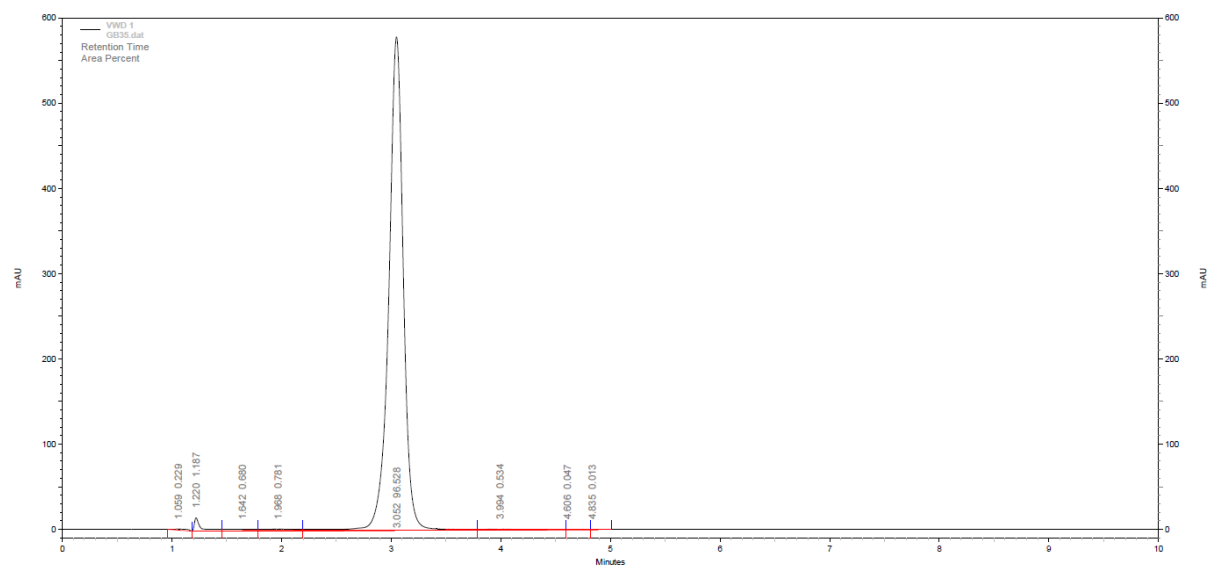
3. 13C-NMR

SAIFNM190323A-42(GB35)

SAIF Cochin

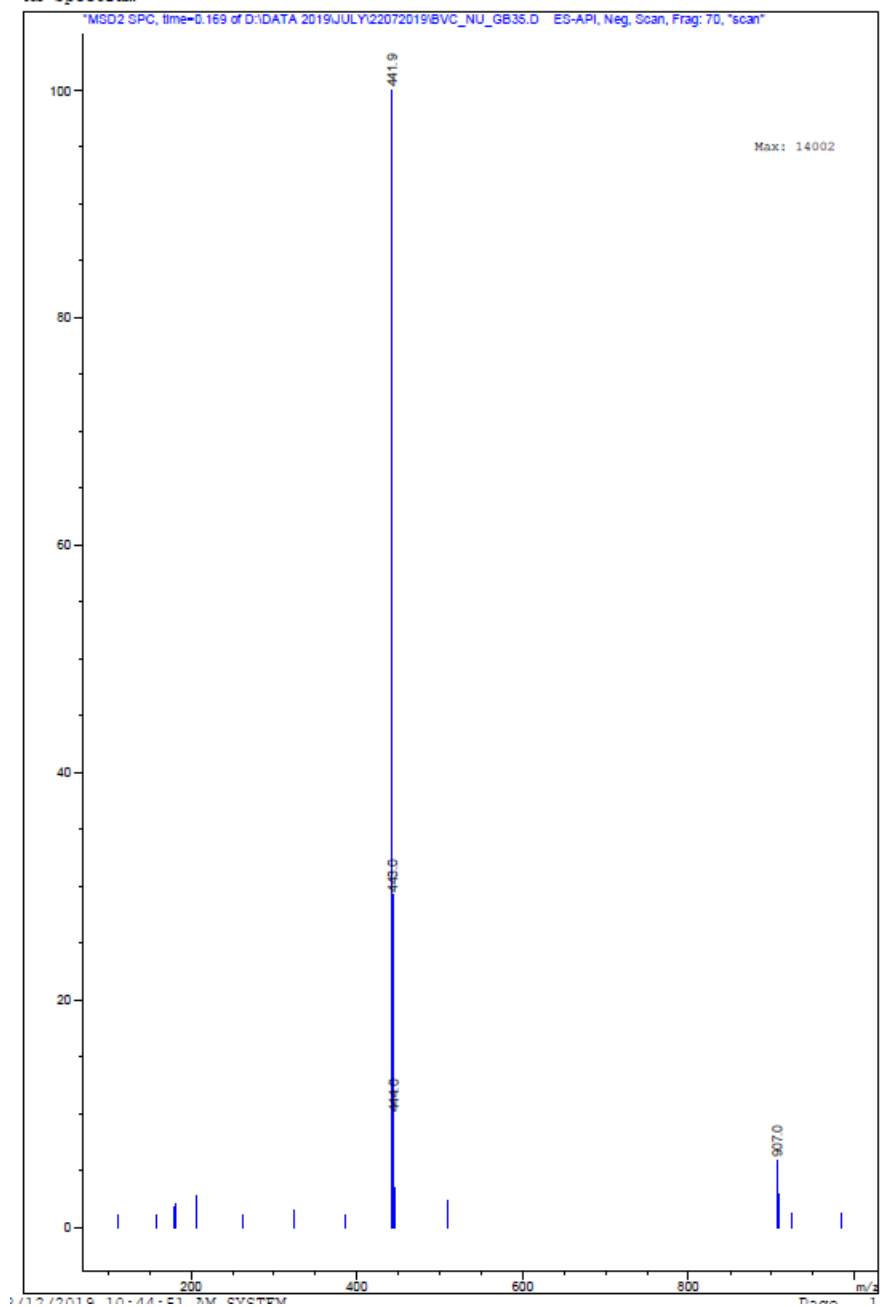


4. HPLC



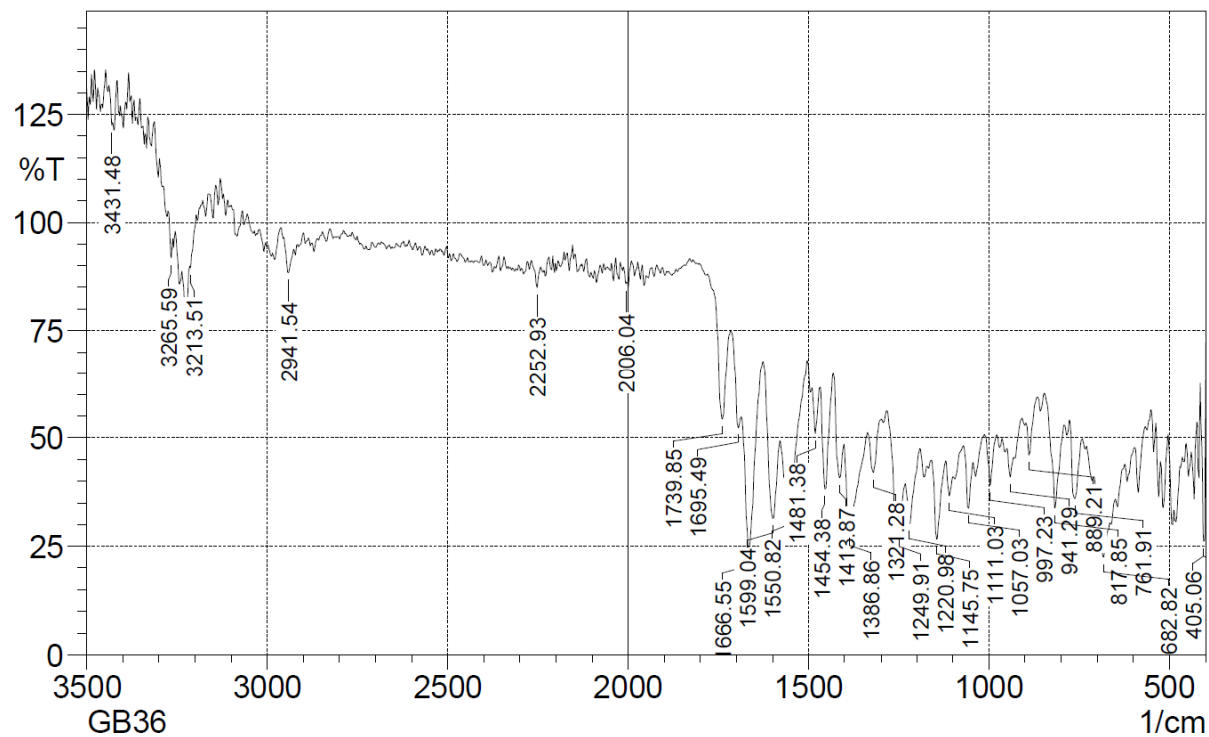
5. Mass

MS Spectrum

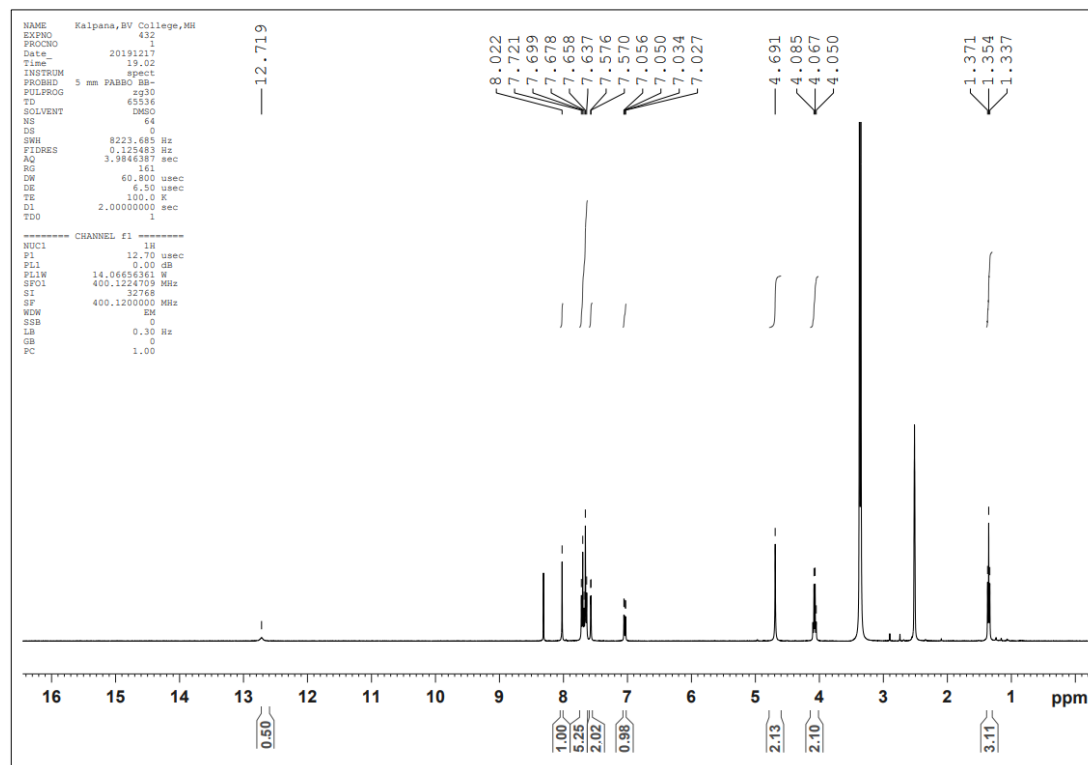


2-(5-benzylidene-2,4-dioxothiazolidin-3-yl)-N-(6-ethoxybenzo[d]thiazol-2-yl)acetamide (GB36)

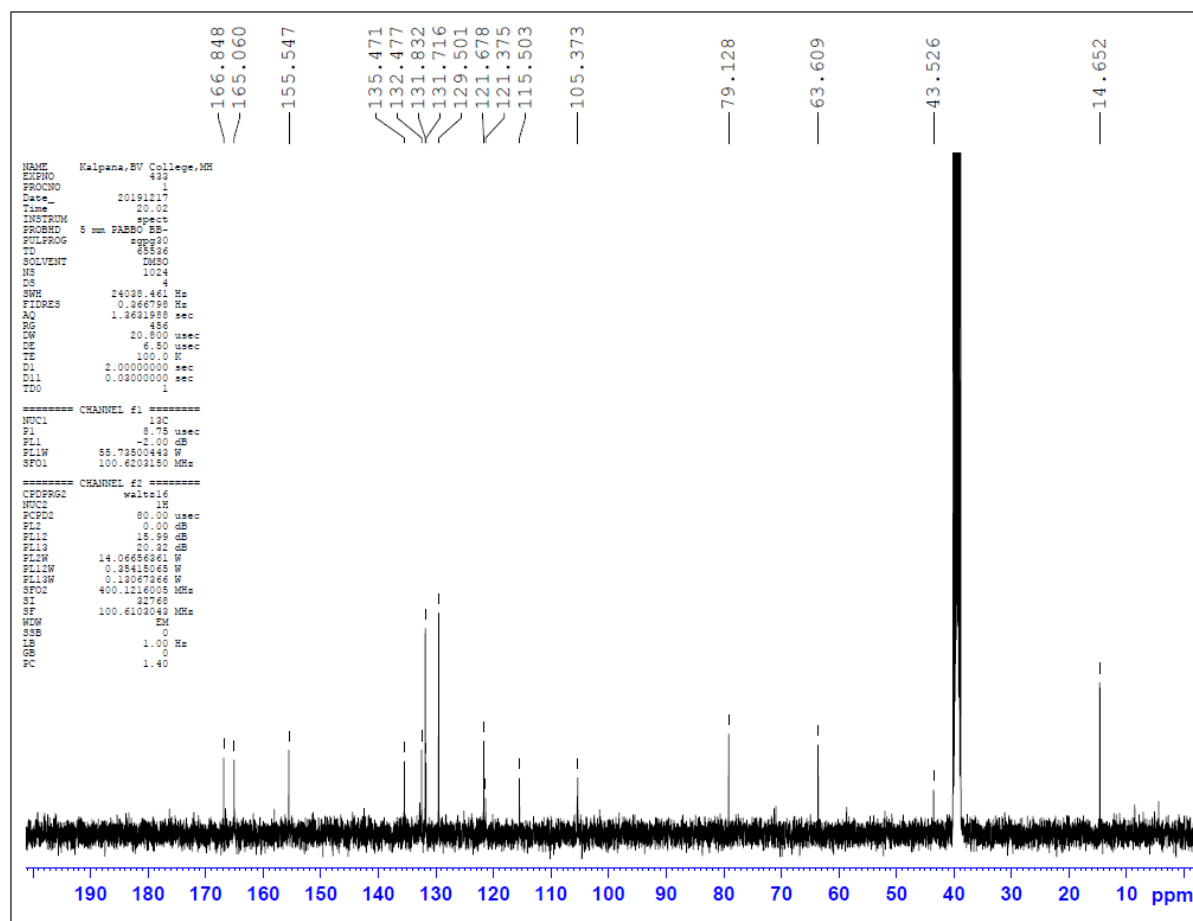
1. FTIR



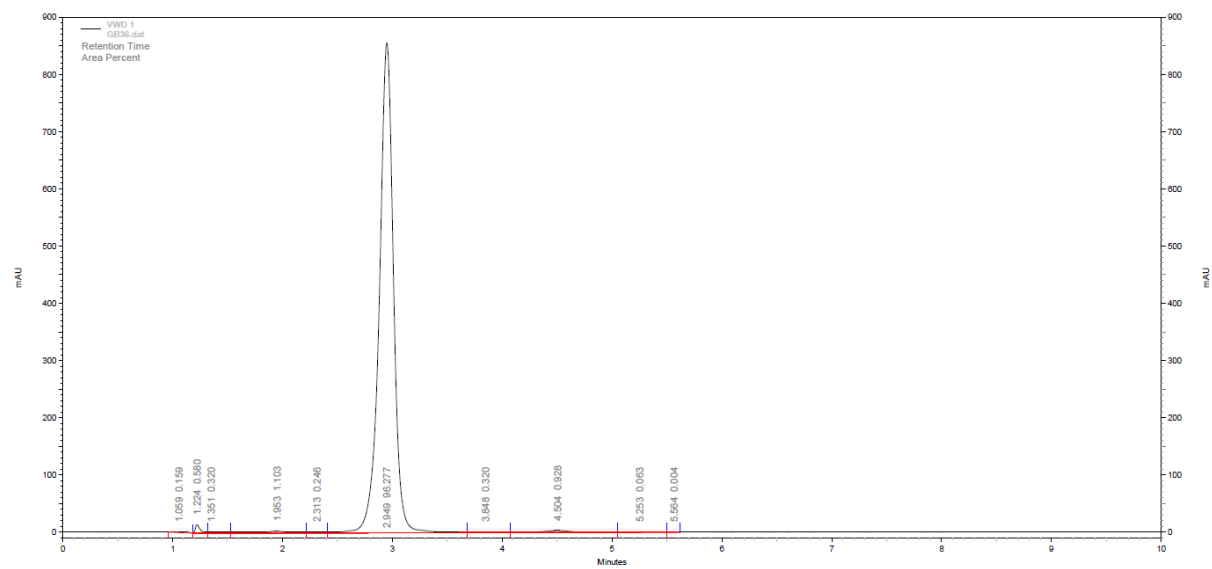
2. ^1H -NMR



3. ¹³C-NMR



4. HPLC



3. Mass

MS Spectrum

