

Selective *in vitro* anti-cancer activity of non-alkylating minor groove binders

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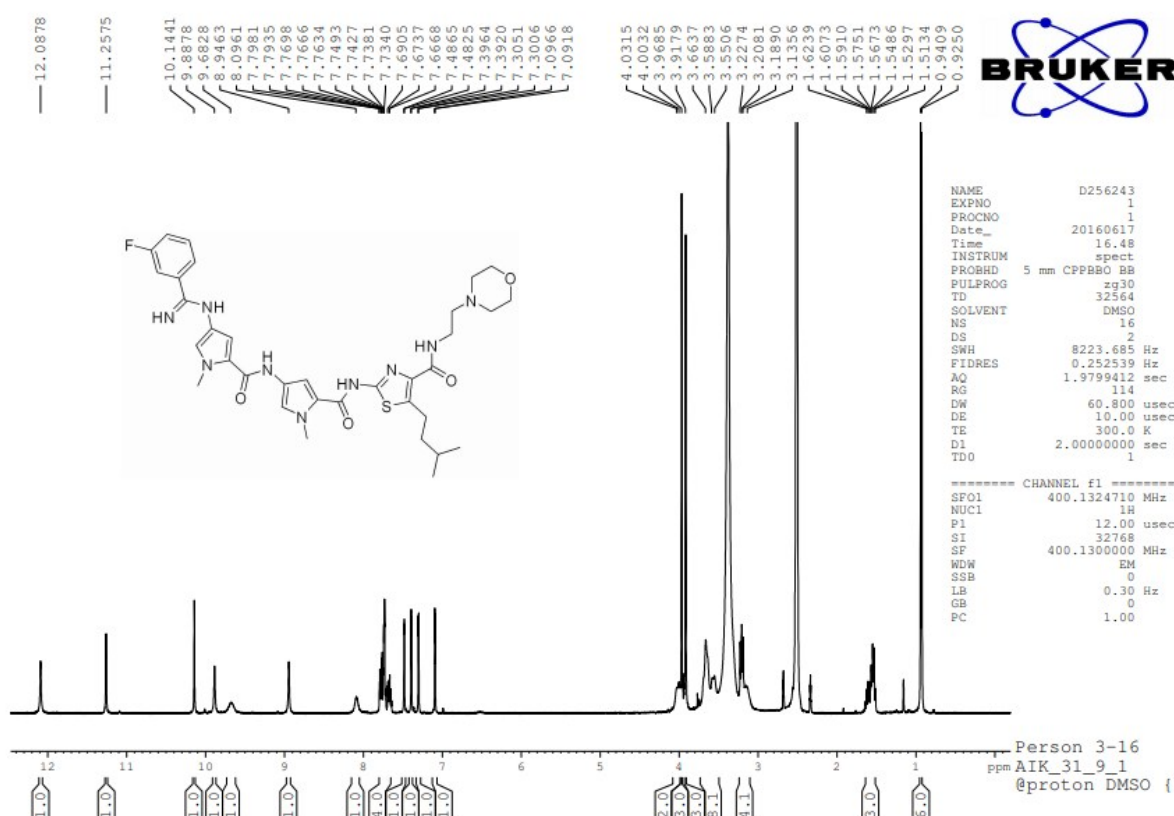
³Department of Pharmacy, School of Applied Sciences, University of Huddersfield, Huddersfield, UK.

Supplementary Information

Below is presented the ¹H NMR, HR-MS and IR data for each of the novel MGBs.

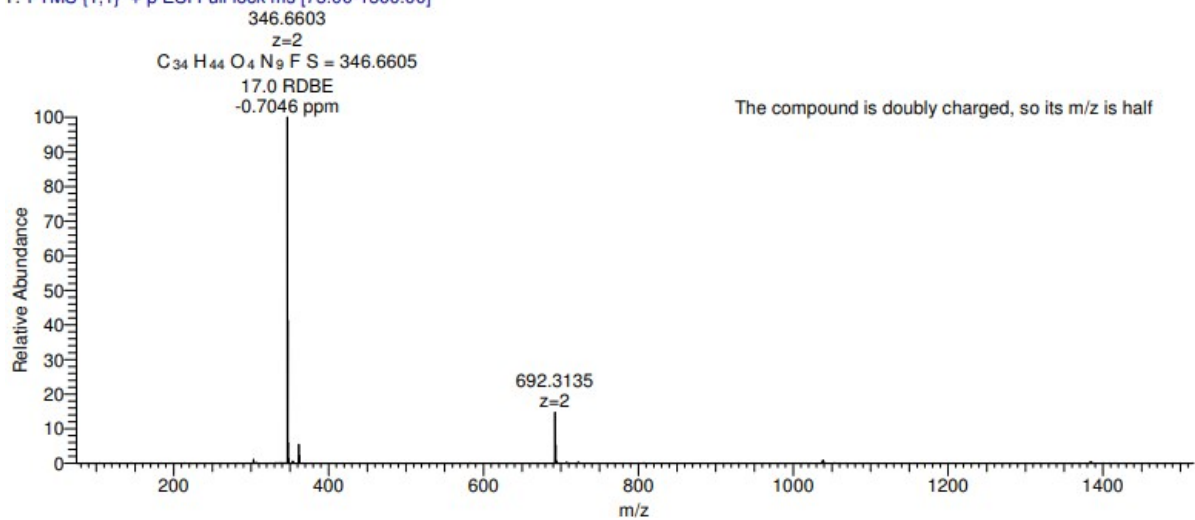
MGB-371

¹H NMR (*d*₆-DMSO)



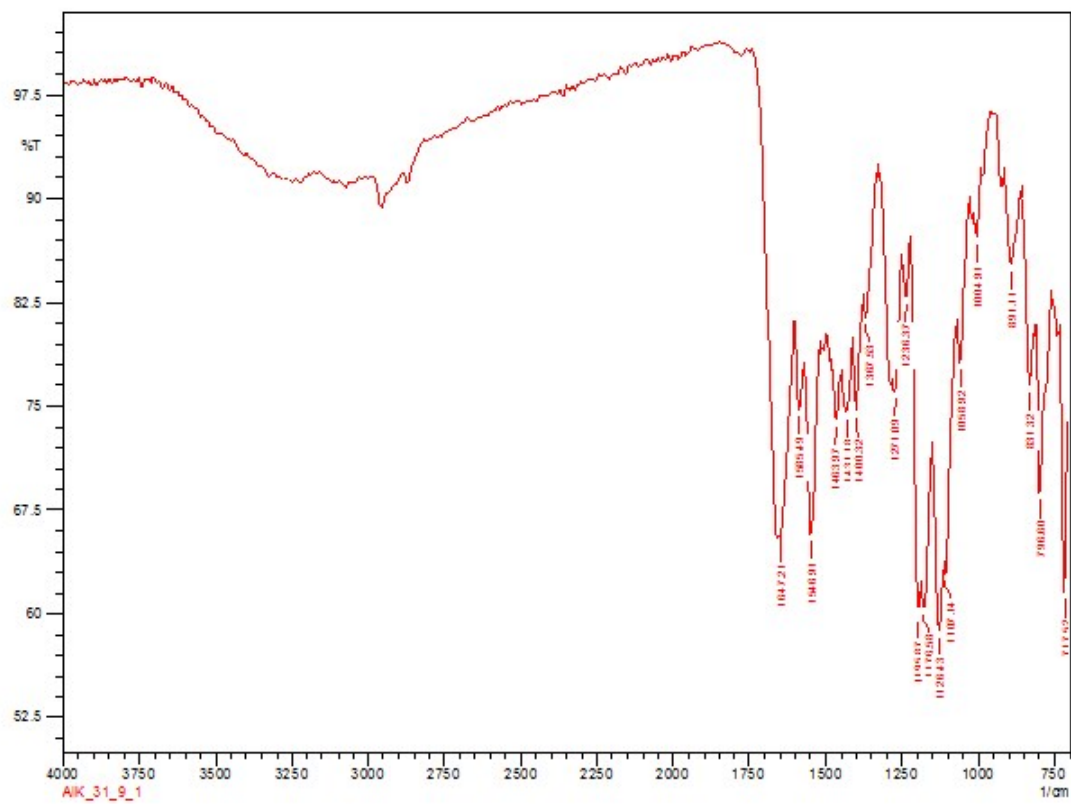
HRMS

AIK-31-9-1 #105 RT: 1.24 AV: 1 SB: 11 0.95-1.07, 1.60-1.71 NL: 8.20E8
T: FTMS (1,1) + p ESI Full lock ms [75.00-1500.00]



IR

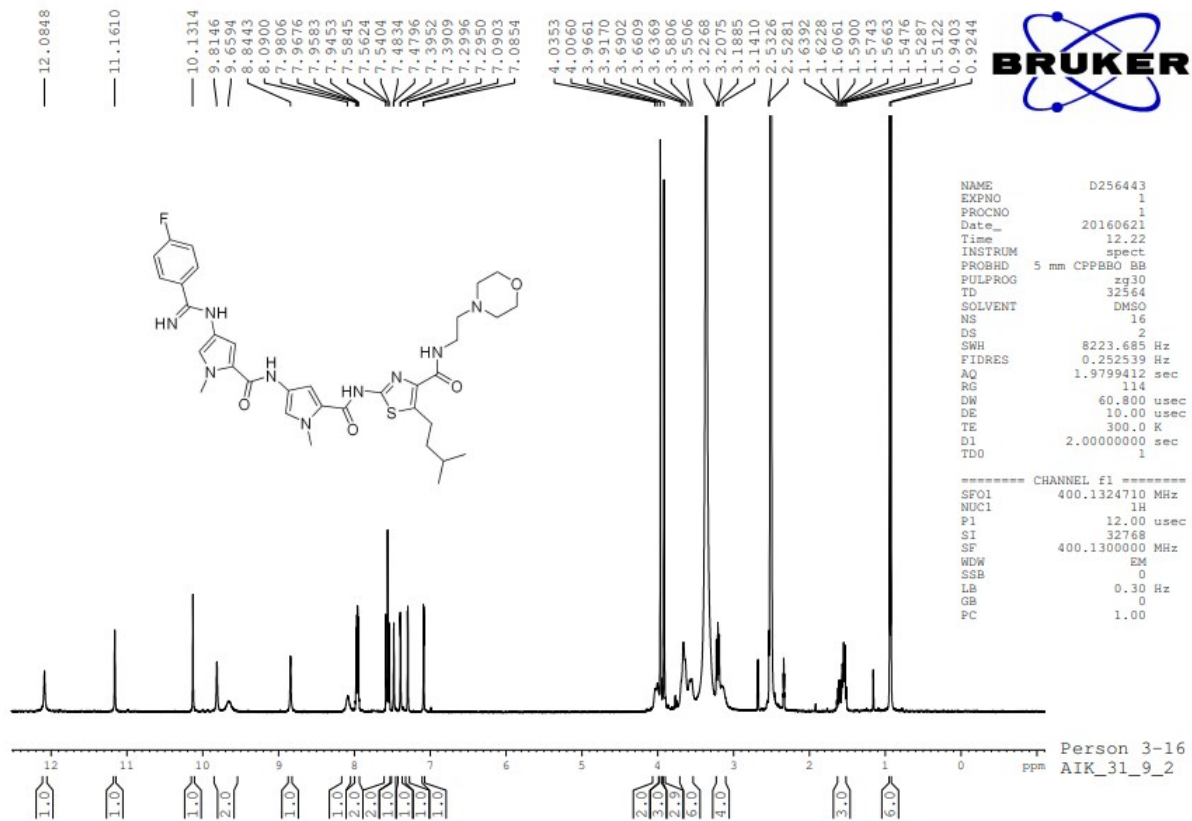
AIK_31_9_1



Peaks: 718, 797, 831, 891, 1005, 1059, 1107, 1126, 1177, 1196, 1236, 1271, 1368, 1400, 1431, 1464, 1547, 1586, 1647 cm⁻¹

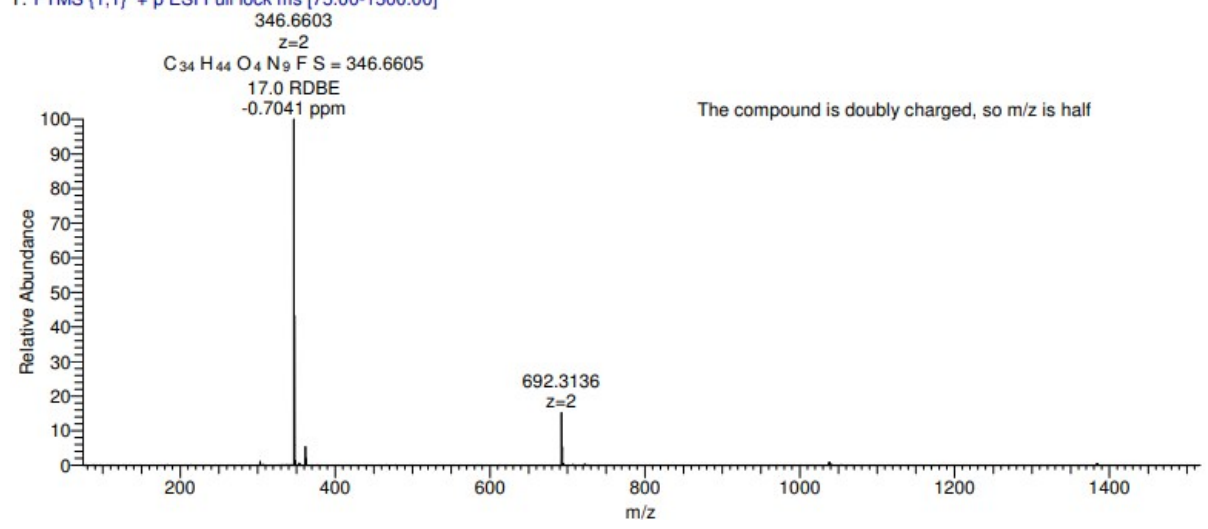
MGB-372

^1H NMR (d_6 -DMSO)



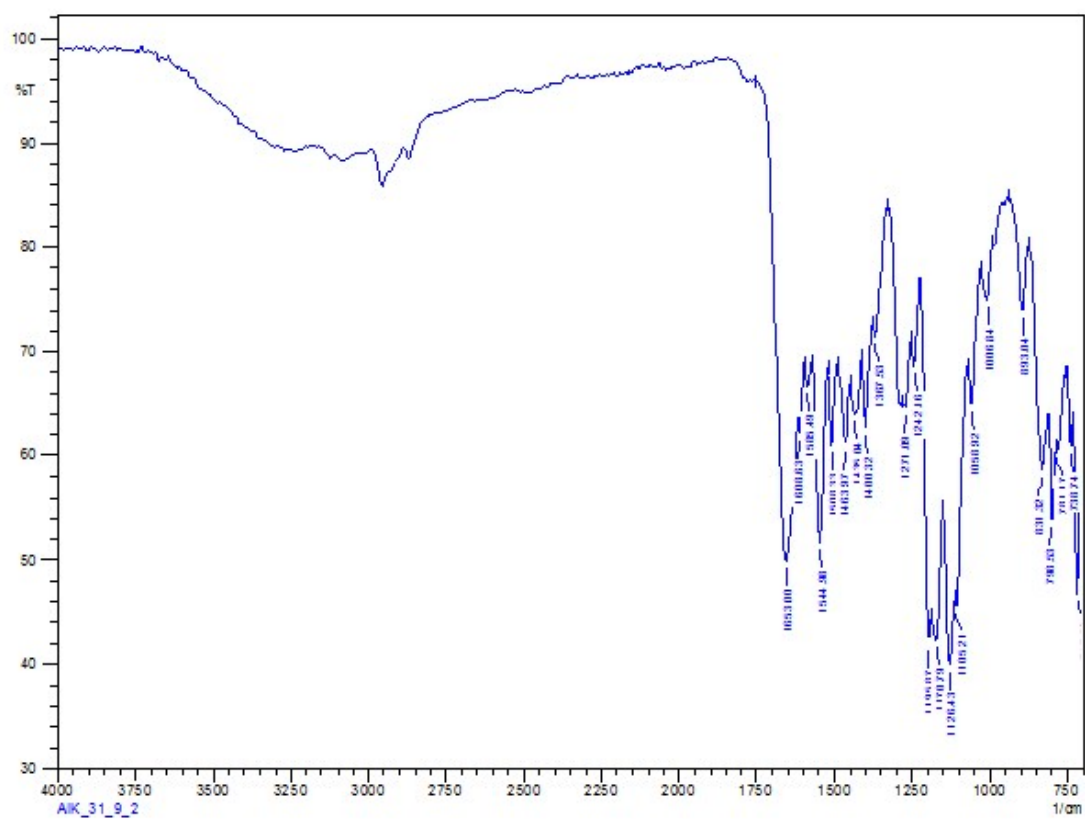
HRMS

AIK-31-9-2 #95 RT: 1.23 AV: 1 SB: 11 0.96-1.08 , 1.59-1.72 NL: 7.99E8
T: FTMS (1,1) + p ESI Full lock ms [75.00-1500.00]



IR

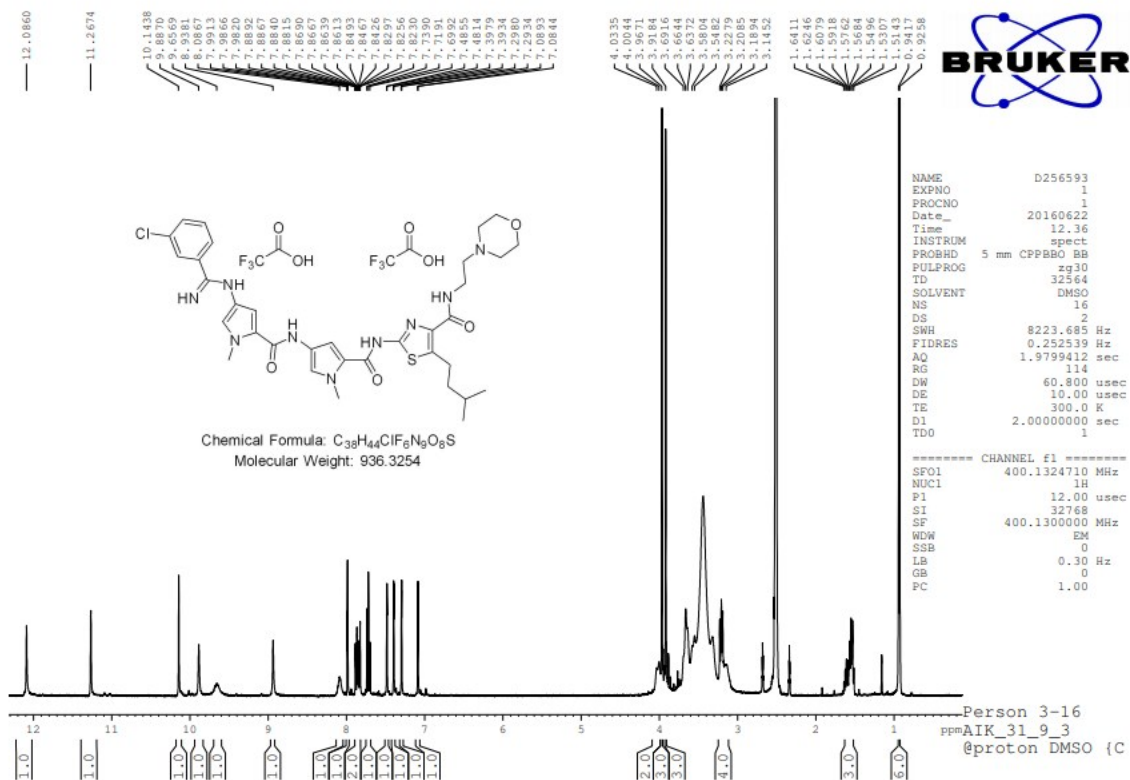
AIK_31_9_2



Peaks: 718, 739, 781, 799, 831, 893, 1007, 1059, 1105, 1126, 1171, 1196, 1242, 1271, 1368, 1400, 1435, 1464, 1508, 1545, 1586, 1609, 1653 cm⁻¹

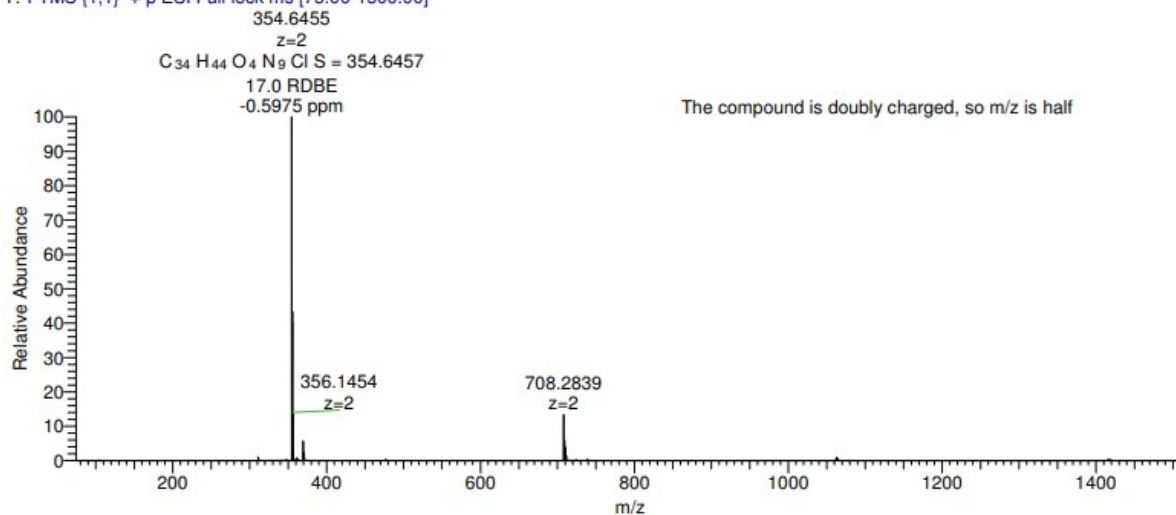
MGB-373

¹H NMR (d₆-DMSO)



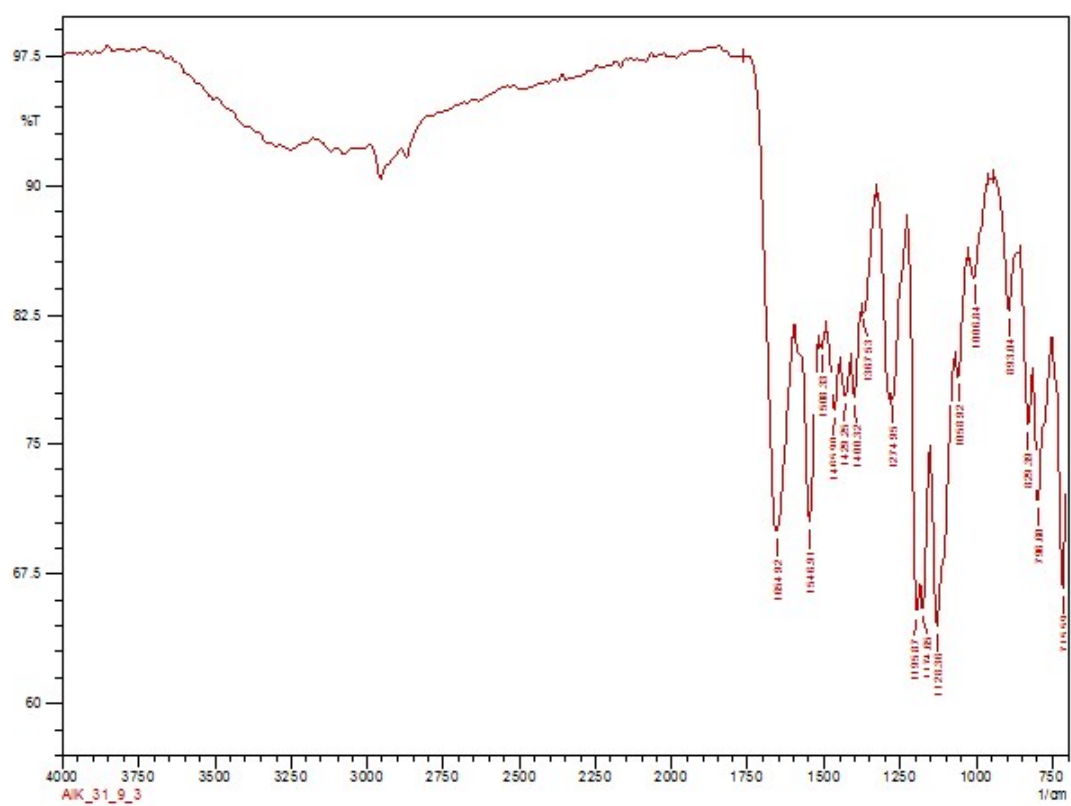
HRMS

AIK-31-9-3 #99 RT: 1.24 AV: 1 SB: 10 0.95-1.08 , 1.59-1.72 NL: 6.03E8
T: FTMS {1,1} + p ESI Full lock ms [75.00-1500.00]



IR

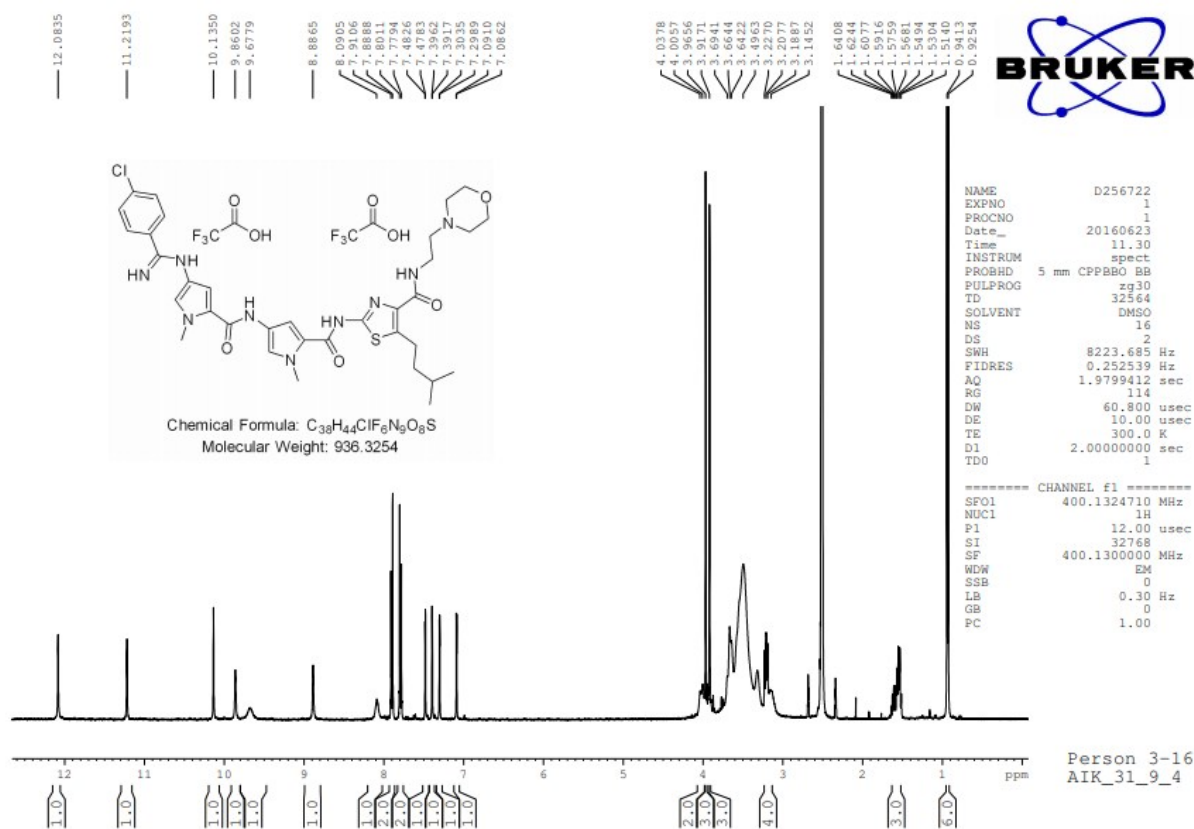
AIK_31_9_3



Peaks: 716, 797, 829, 893, 1007, 1059, 1128, 1175, 1196, 1275, 1368, 1400, 1429, 1466, 1508, 1547, 1655 cm⁻¹

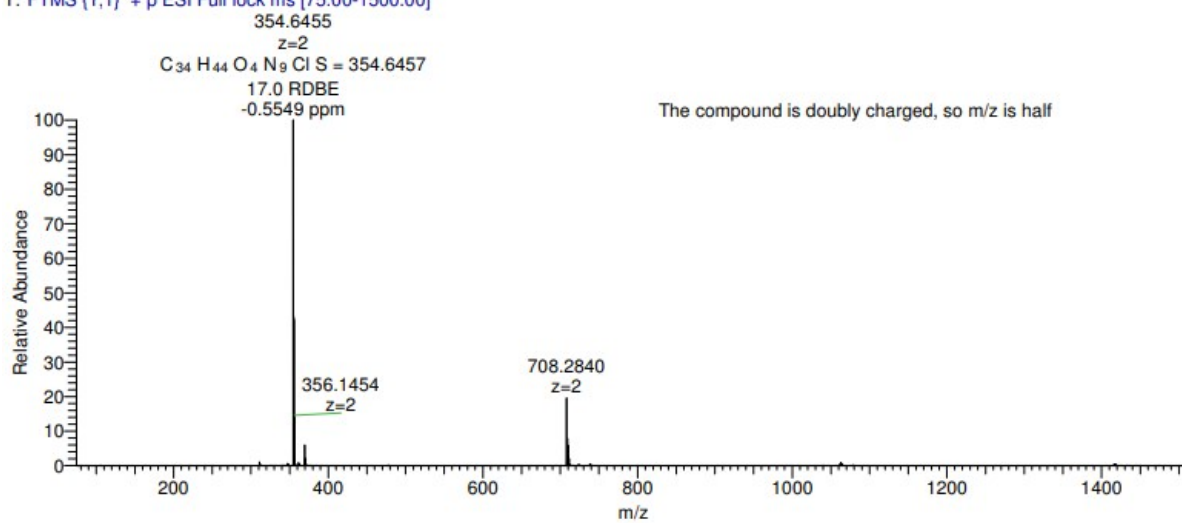
MGB-374

^1H NMR (d_6 -DMSO)



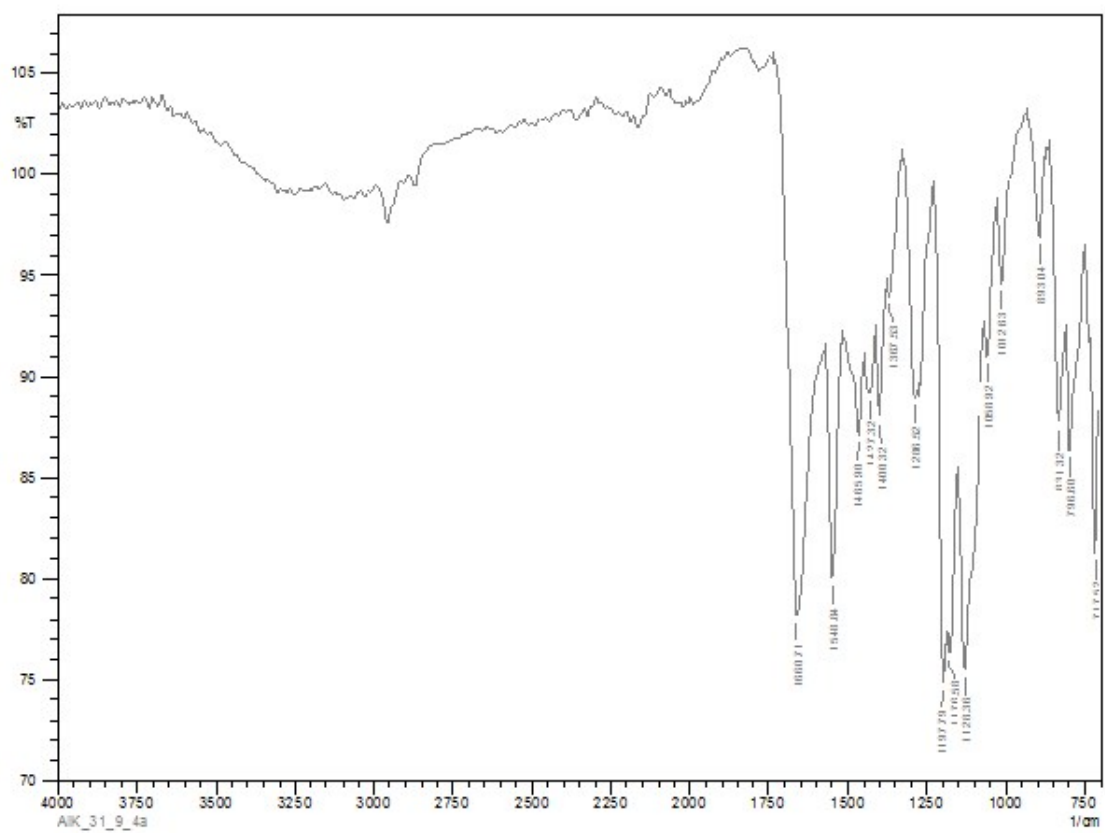
HRMS

AIK-31-9-4 #99 RT: 1.24 AV: 1 SB: 10 0.96-1.07, 1.60-1.72 NL: 6.51E8
T: FTMS (1,1) + p ESI Full lock ms [75.00-1500.00]



IR

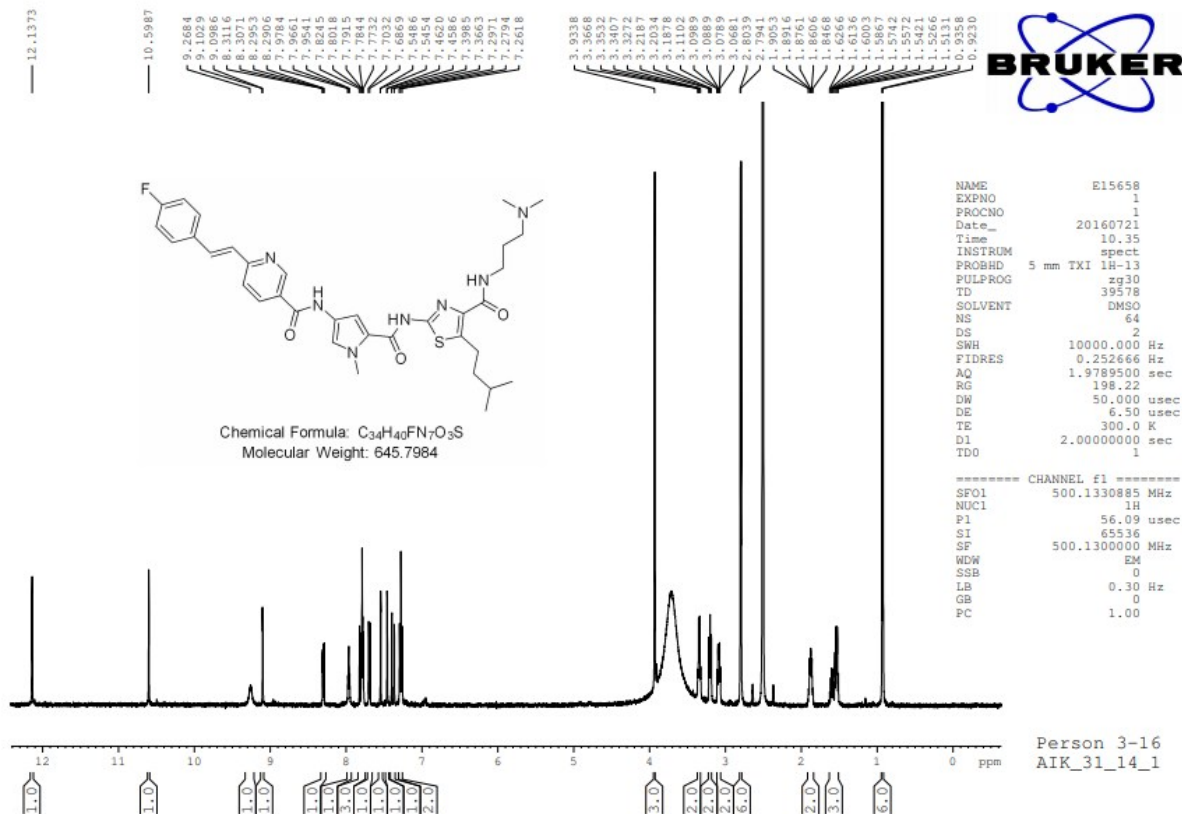
AIK_31_9_4



Peaks: 718, 797, 831, 893, 1013, 1059, 1128, 1177, 1198, 1287, 1368, 1400, 1427, 1466, 1549, 1661 cm^{-1}

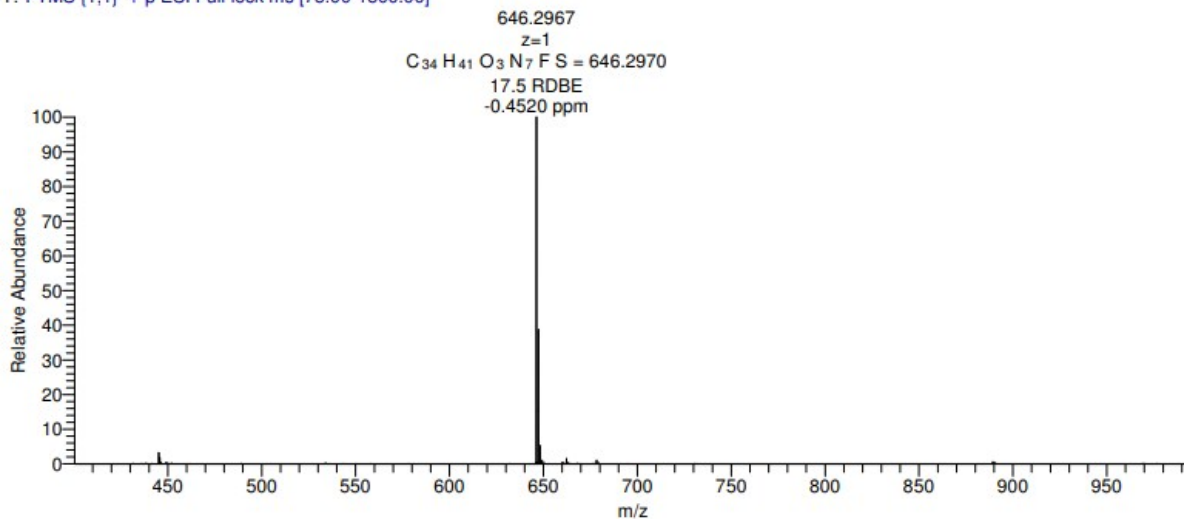
MGB-376

^1H NMR (d_6 -DMSO)



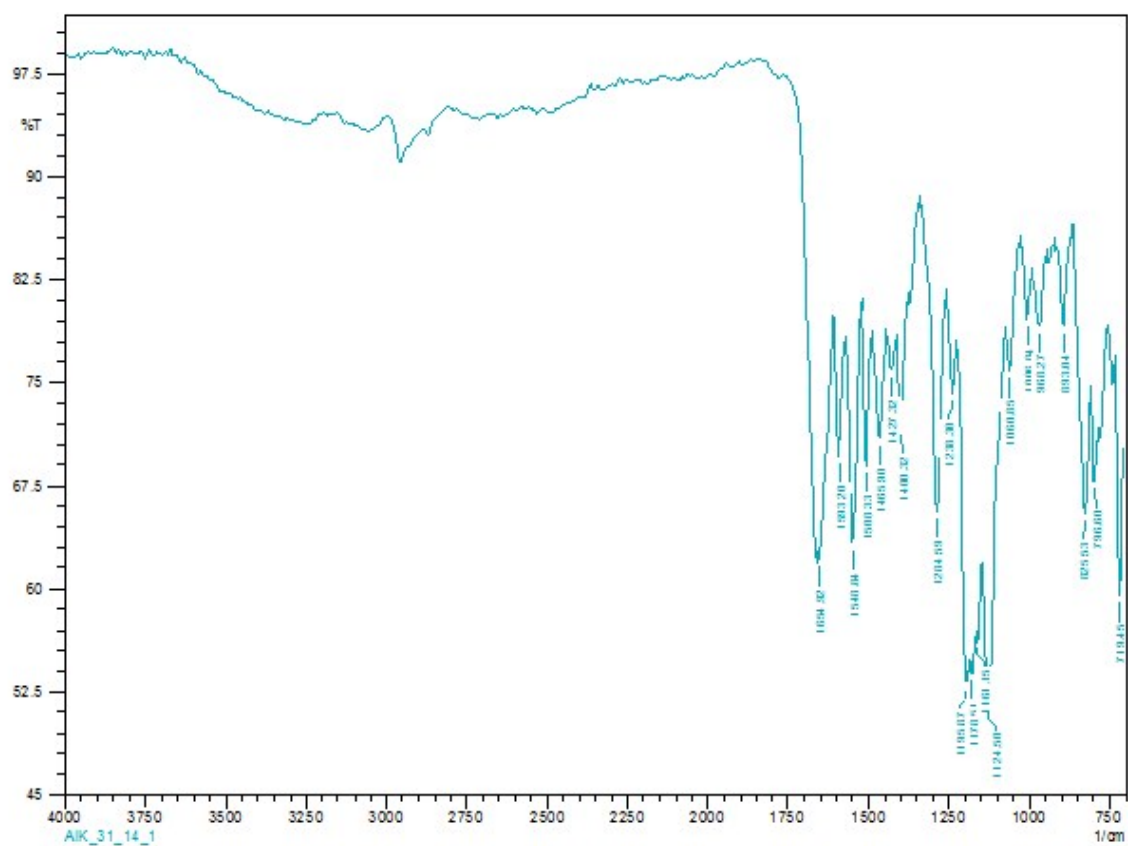
HRMS

AIK-31-14-1 #119 RT: 1.41 AV: 1 SB: 12 0.95-1.08, 1.59-1.71 NL: 2.38E8
T: FTMS (1,1) + p ESI Full lock ms [75.00-1500.00]



IR

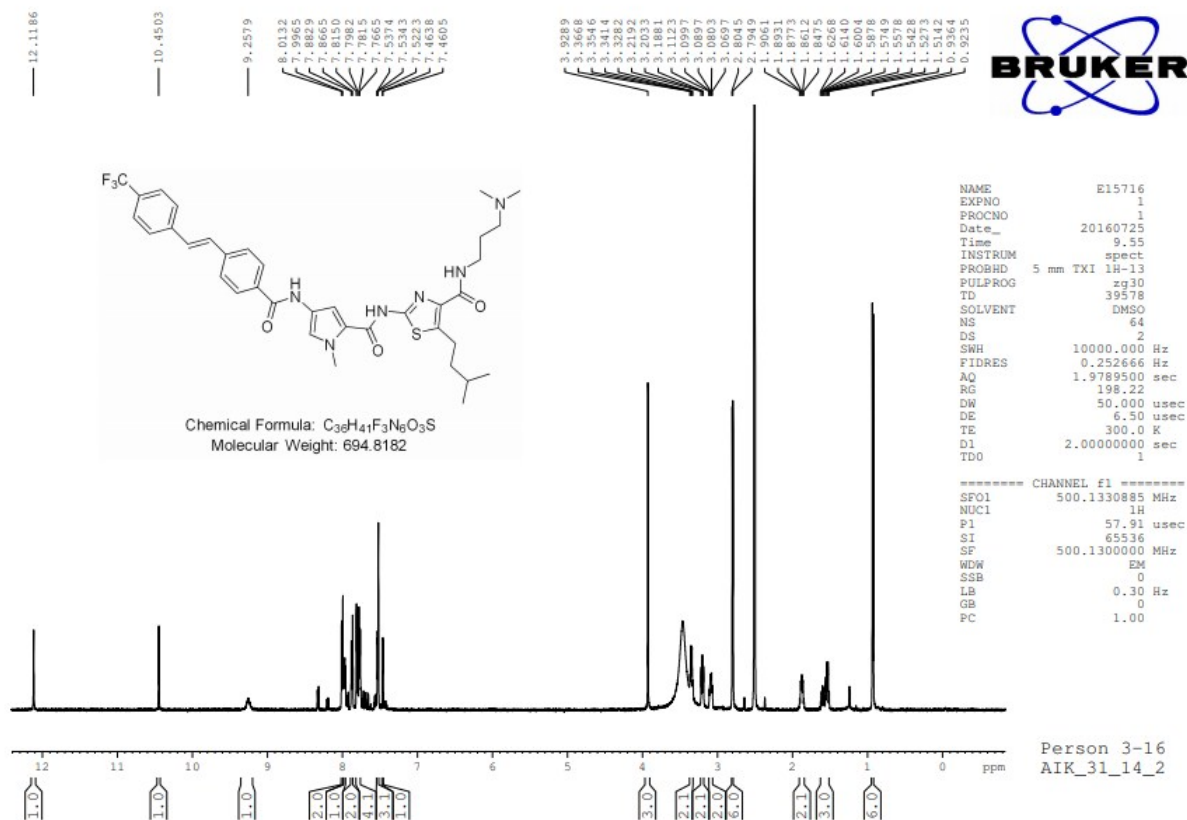
AIK_31_14_1



Peaks: 720, 797, 826, 893968, 1007, 1061, 1125, 1161, 1179, 1196, 1238, 1285, 1400, 1427, 1466, 1508, 1549, 1593, 1655 cm⁻¹

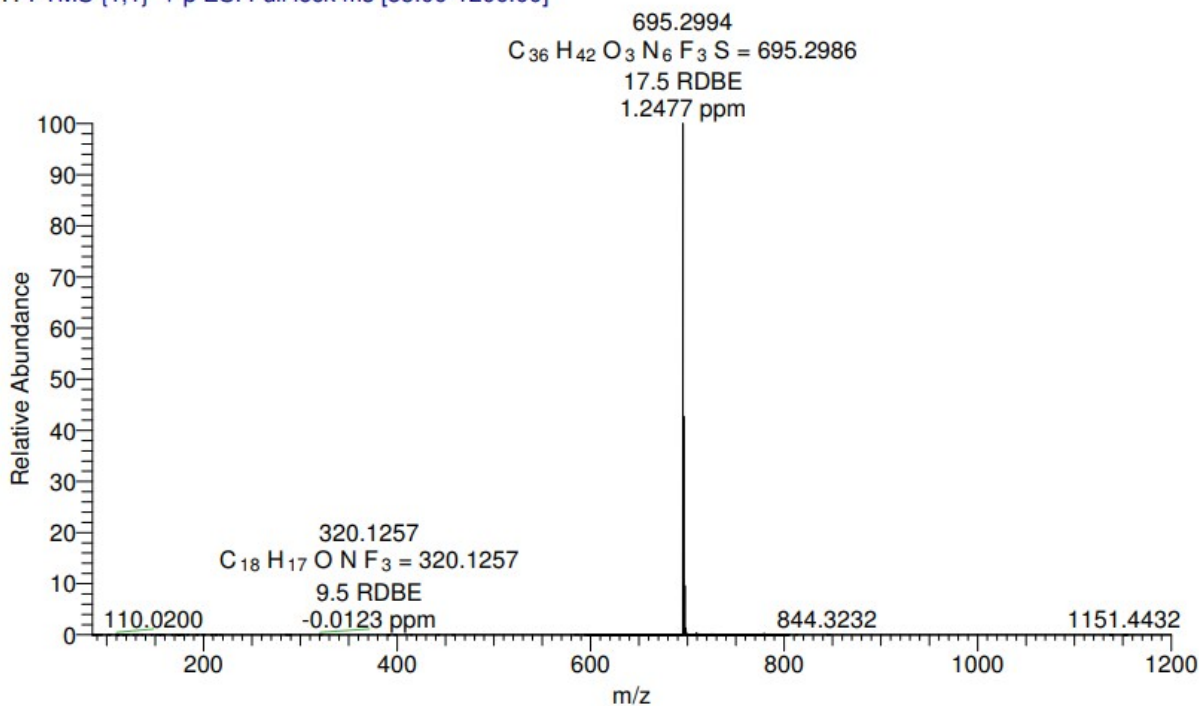
MGB-377

¹H NMR (d₆-DMSO)



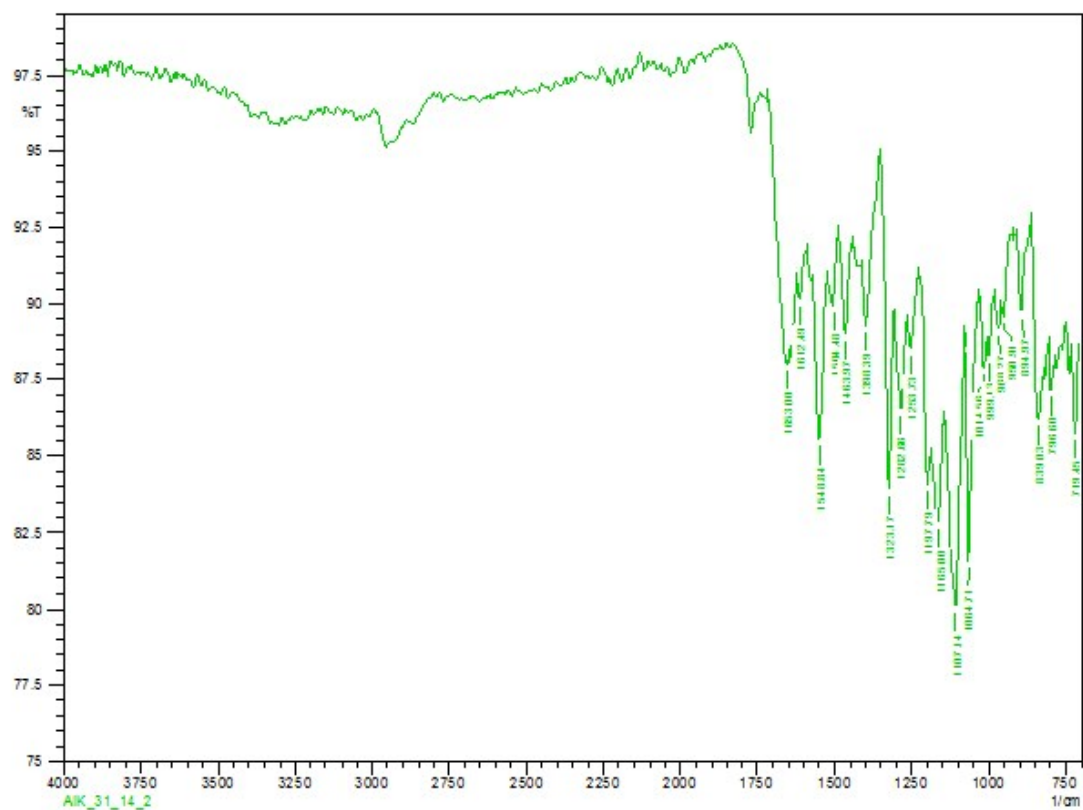
HRMS

AIK-31-14-2 #85 RT: 2.37 AV: 1 NL: 7.79E8
T: FTMS {1,1} + p ESI Full lock ms [85.00-1200.00]



IR

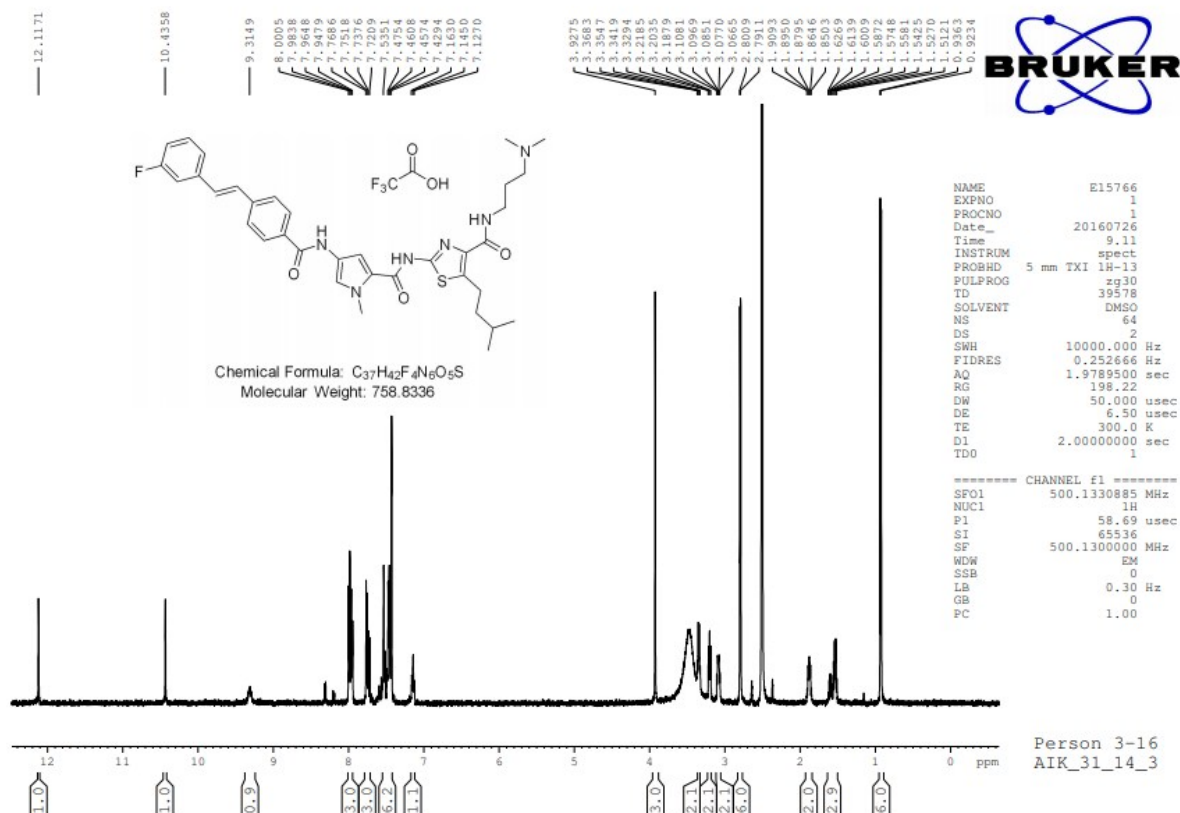
AIK-31_14_2



Peaks: 720, 797, 839, 895, 951, 968, 999, 1015, 1065, 1107, 1165, 1198, 1254, 1283, 1323, 1398, 1464, 1505, 1549, 1613, 1653 cm^{-1}

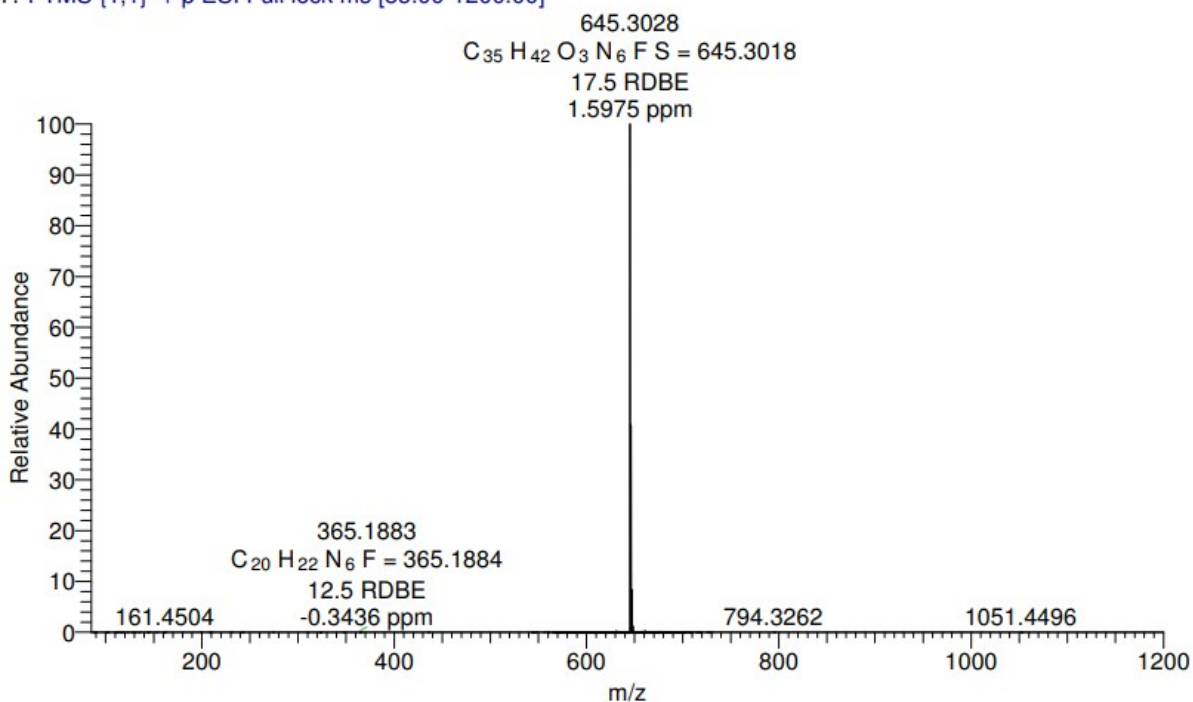
MGB-378

¹H NMR (d₆-DMSO)



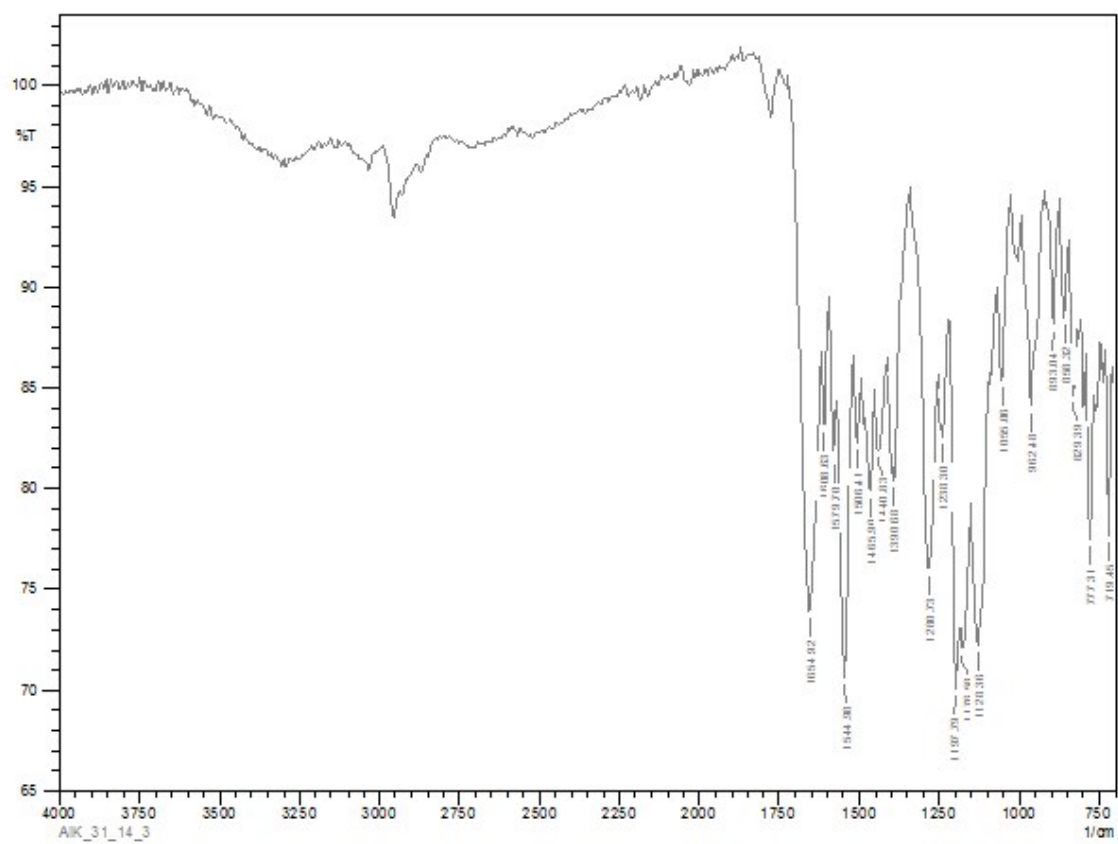
HRMS

AIK-31-14-3 #61 RT: 1.74 AV: 1 NL: 1.08E9
T: FTMS {1,1} + p ESI Full lock ms [85.00-1200.00]



IR

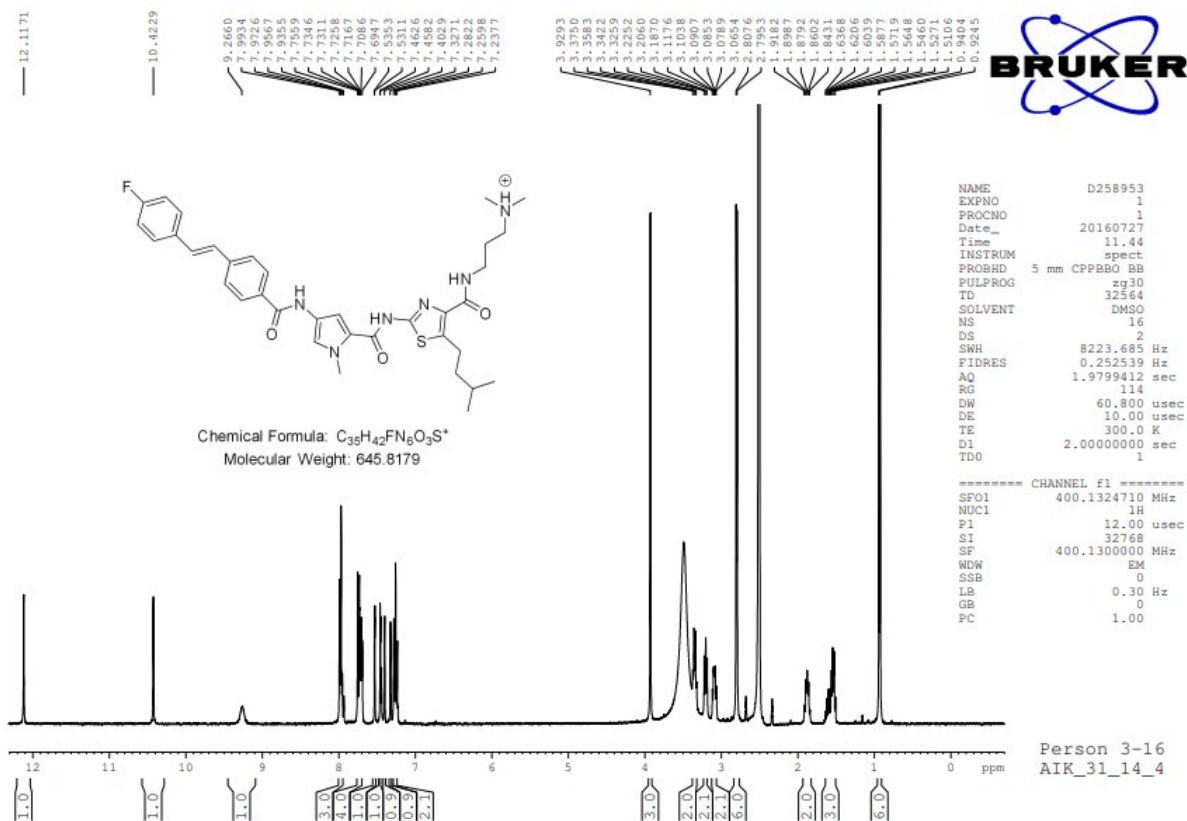
AIK_31_14_3



Peaks: 7120, 777, 829, 858, 893, 963, 1055, 1128, 1177, 1198, 1238, 1281, 1391, 1441, 1466, 1506, 1545, 1580, 1609, 1655 cm^{-1}

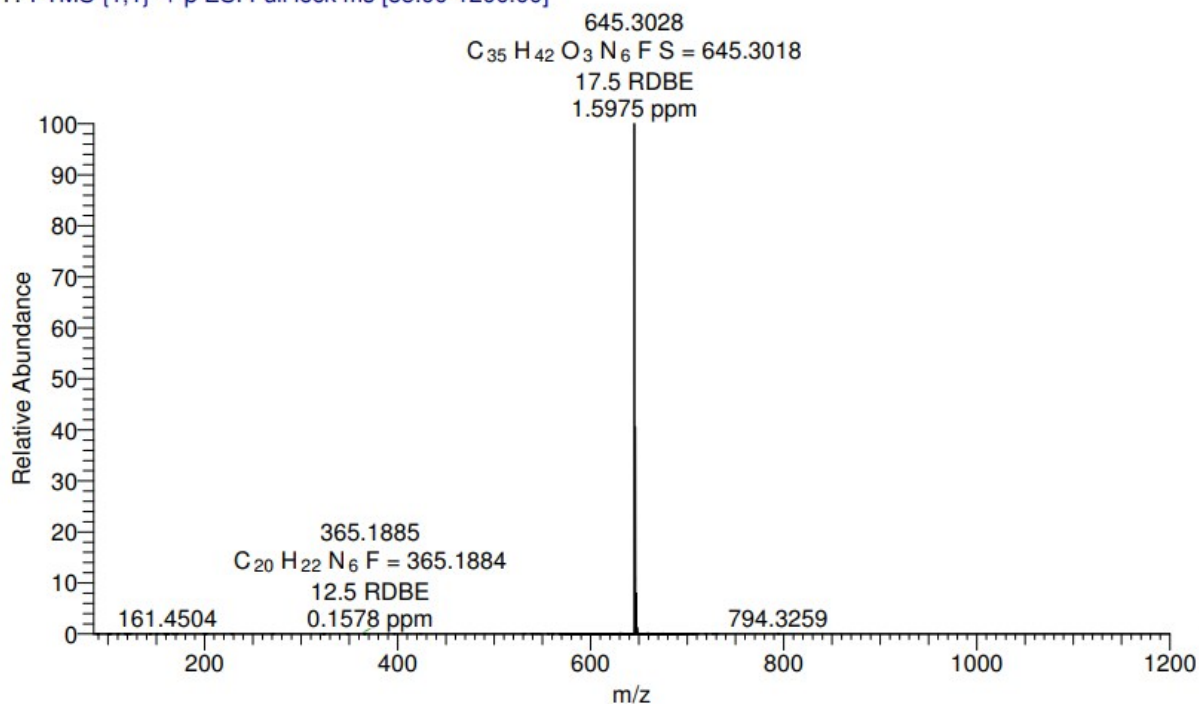
MGB-376

¹H NMR (d₆-DMSO)



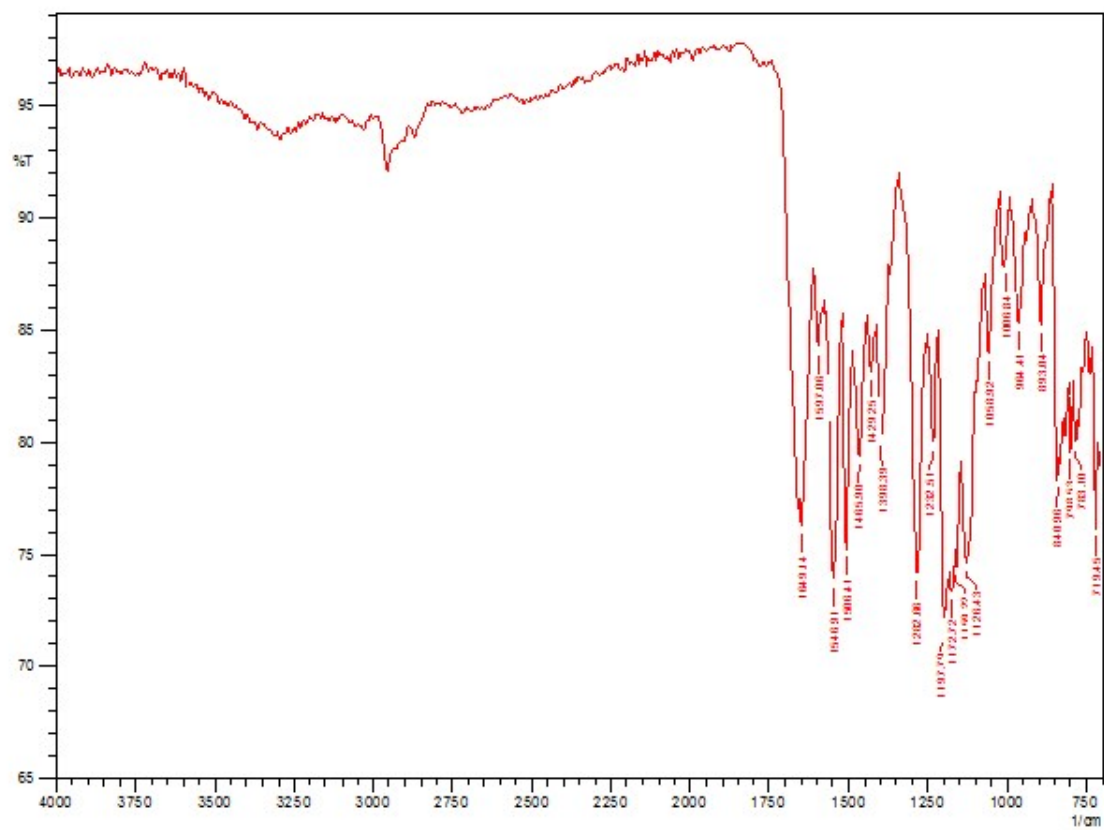
HRMS

AIK-31-14-4 #61 RT: 1.73 AV: 1 NL: 1.05E9
T: FTMS {1,1} + p ESI Full lock ms [85.00-1200.00]



IR

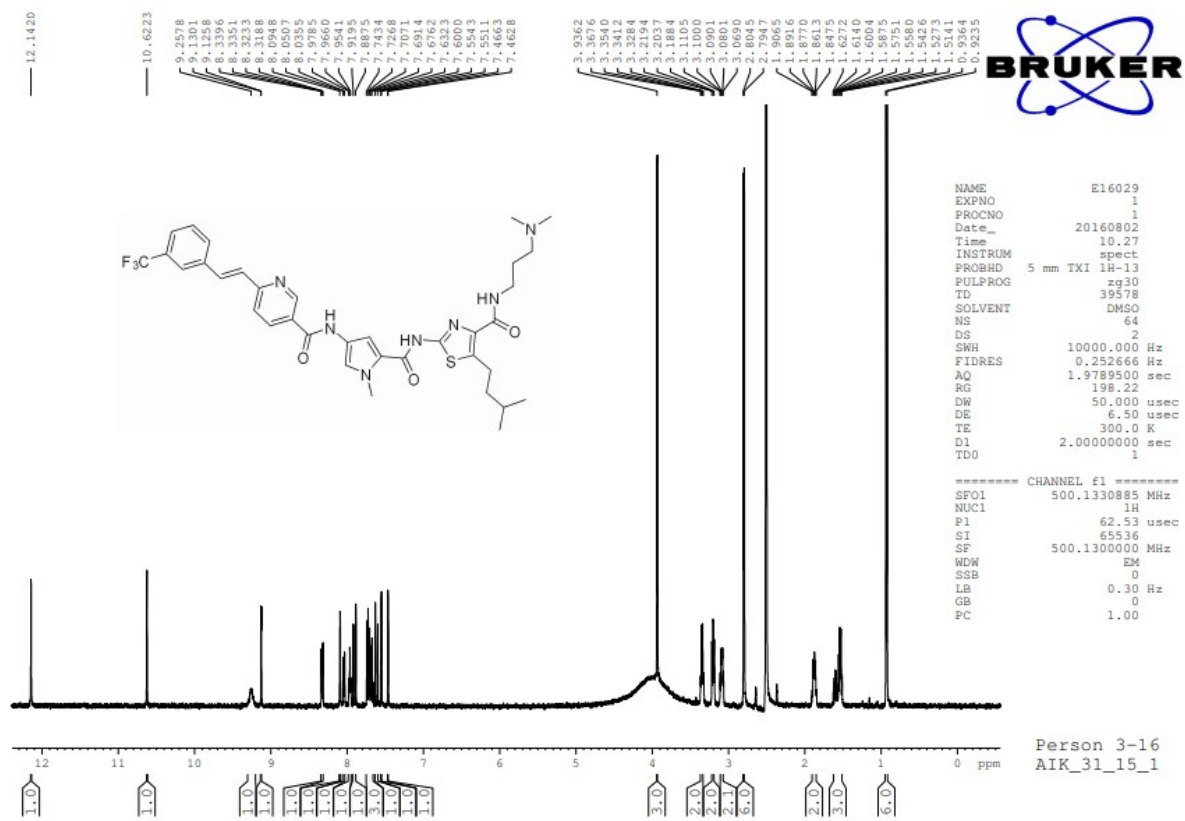
AIK_31_14_4



Peaks: 720, 783, 799, 841, 893, 964, 1007, 1059, 1126, 1159, 1173, 1198, 1233, 1283, 1398, 1429, 1466, 1506, 1547, 1597, 1649 cm^{-1}

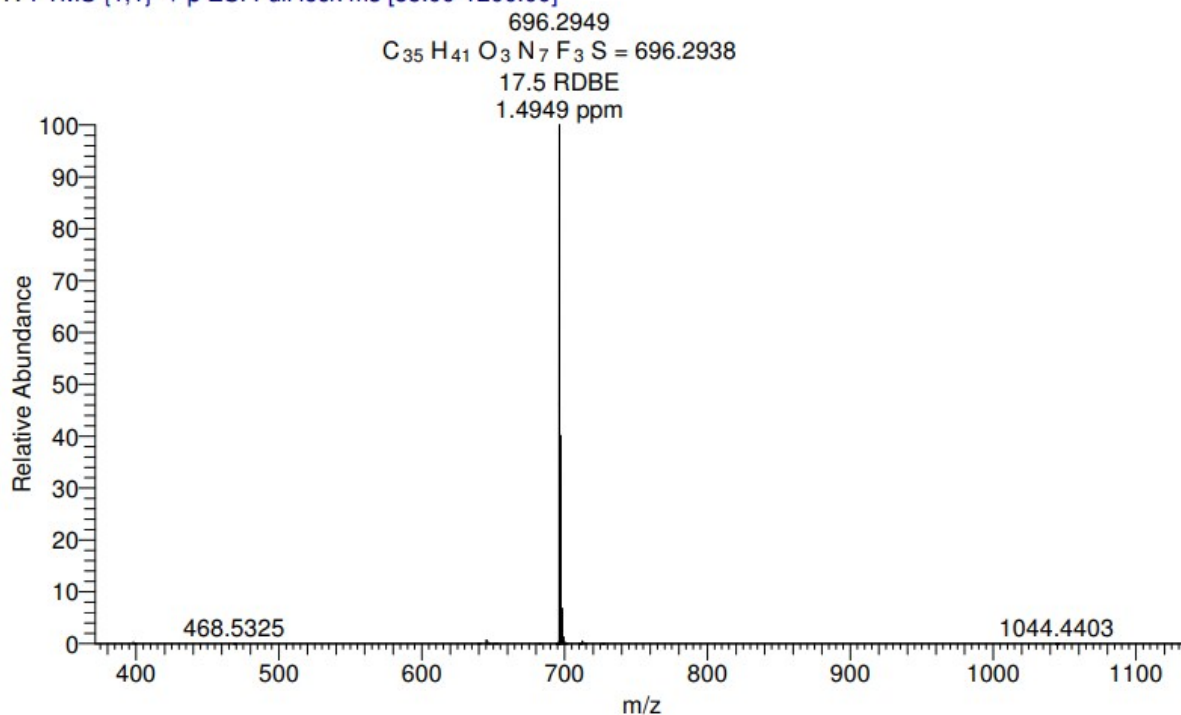
MGB-380

¹H NMR (d₆-DMSO)



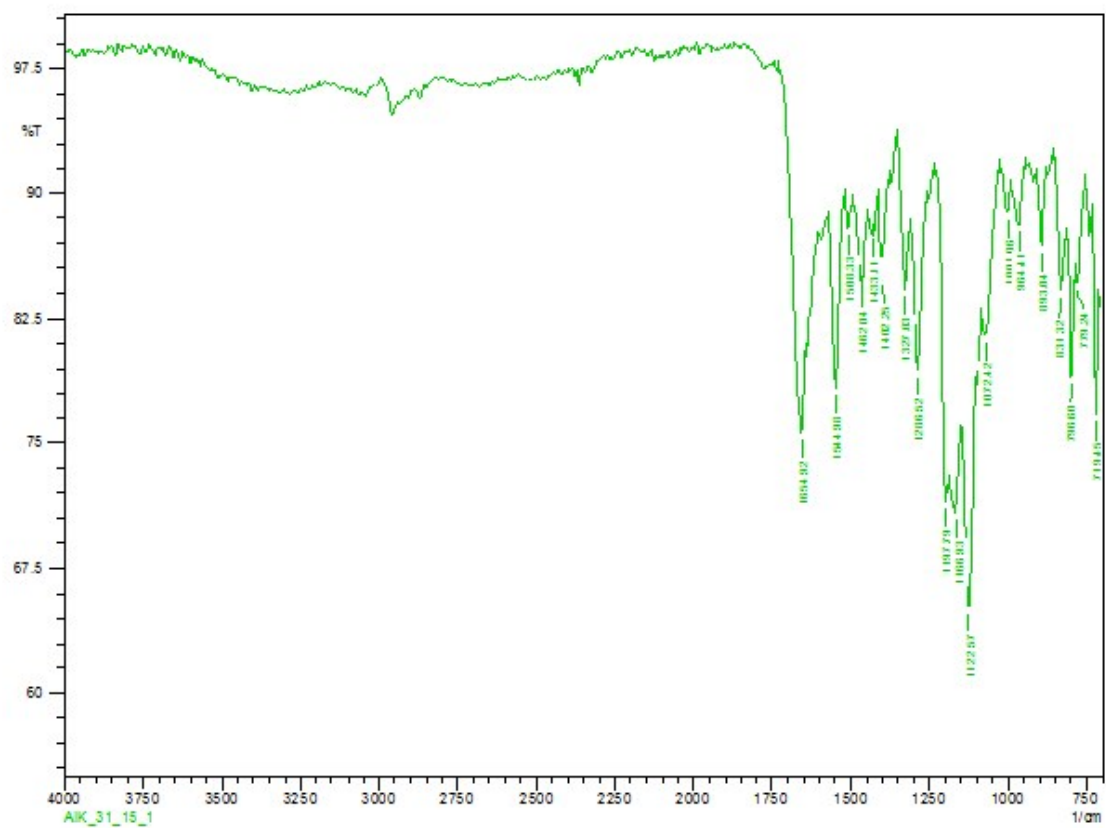
HRMS

AIK-31-15-1 #59 RT: 1.69 AV: 1 NL: 7.47E8
 T: FTMS {1,1} + p ESI Full lock ms [85.00-1200.00]



IR

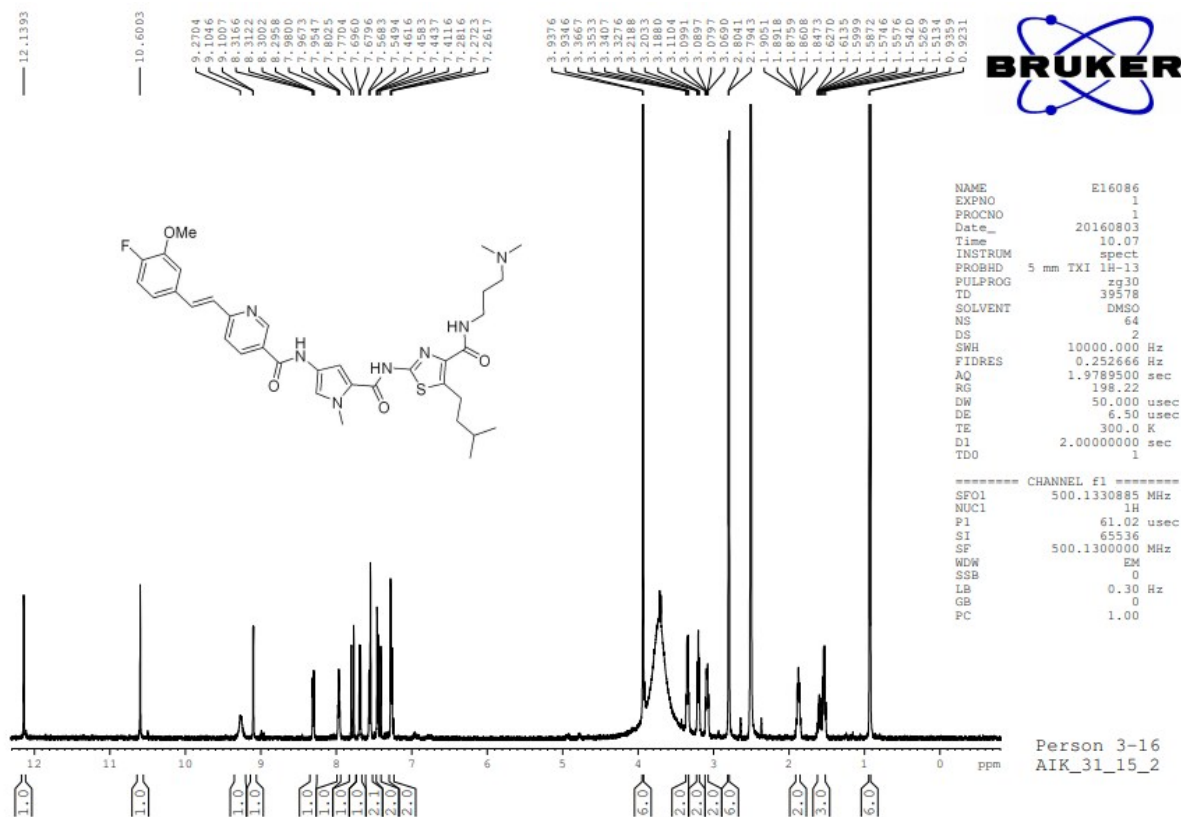
AIK_31_15_1



Peaks: 698, 698, 698, 698, 720, 779, 797, 831, 893, 964, 1001, 1072, 1123, 1167, 1198, 1287, 1327, 1402, 1433, 1462, 1508, 1545, 1655 cm^{-1}

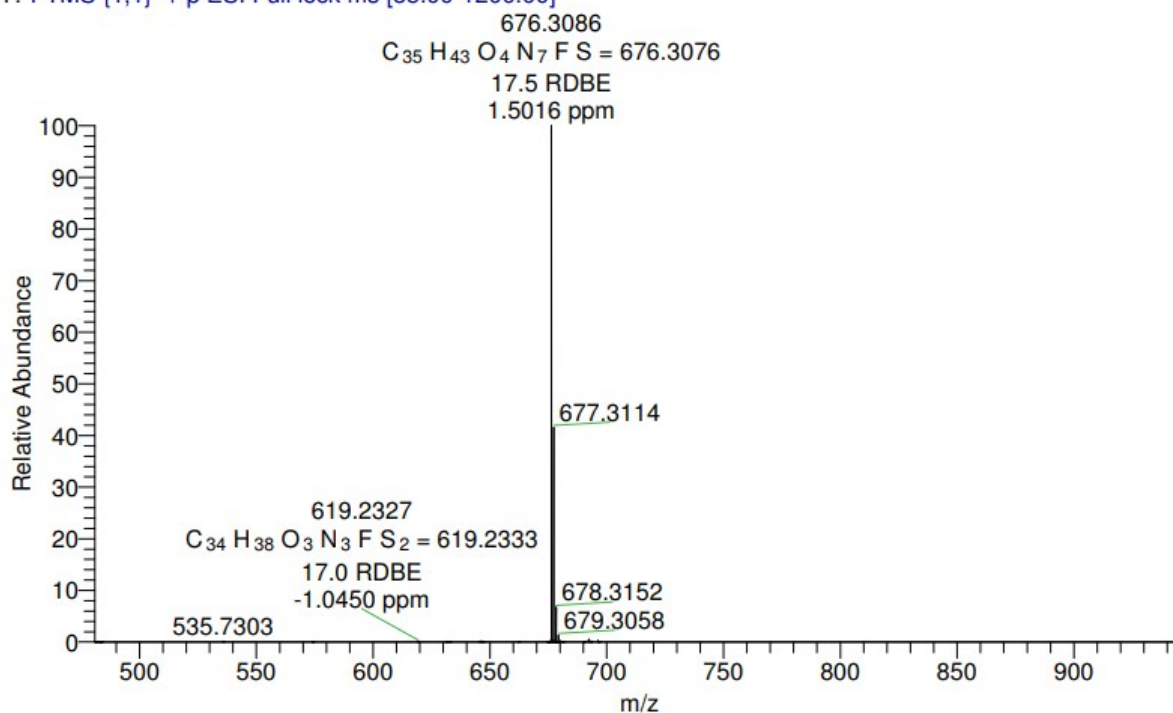
MGB-381

¹H NMR (d₆-DMSO)



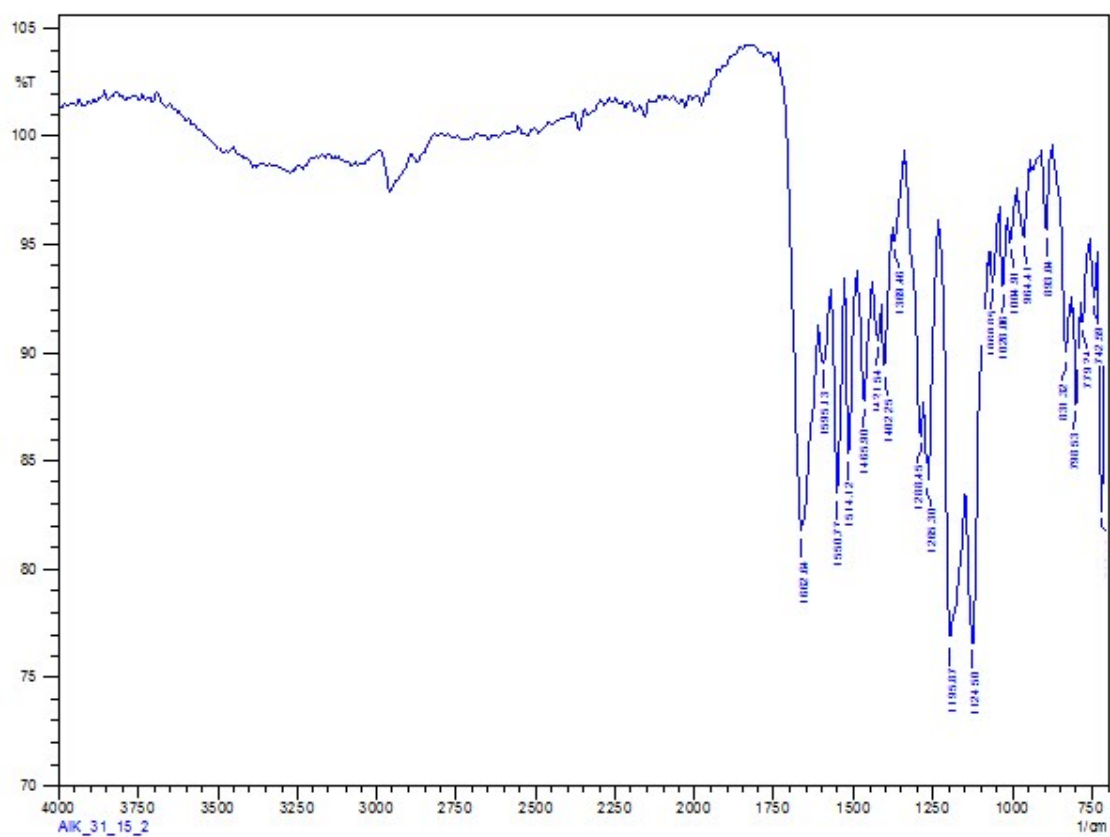
HRMS

AIK-31-15-2 #49 RT: 1.43 AV: 1 NL: 4.86E8
 T: FTMS {1,1} + p ESI Full lock ms [85.00-1200.00]



IR

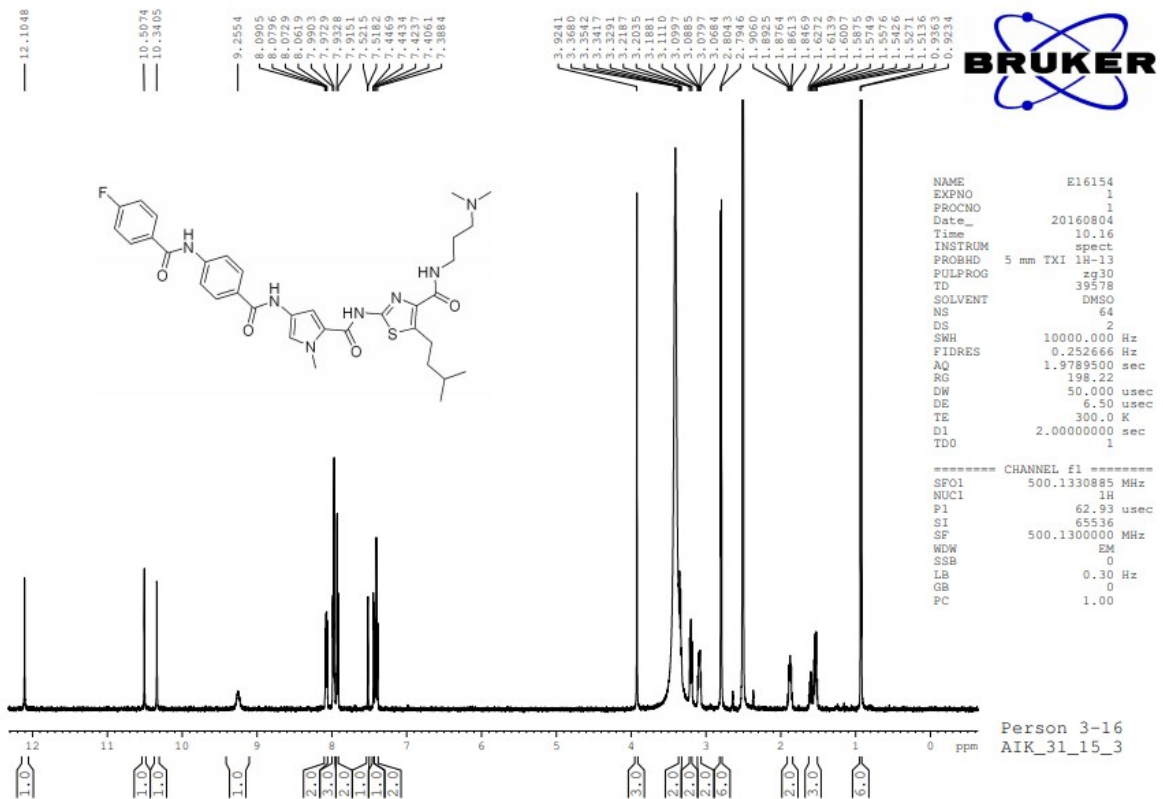
AIK_31_15_2



Peaks: 720, 743, 779, 799, 831, 893, 964, 1005, 1028, 1061, 1125, 1196, 1265, 1289, 1370, 1402, 1422, 1466, 1514, 1551, 1595, 1663 cm^{-1}

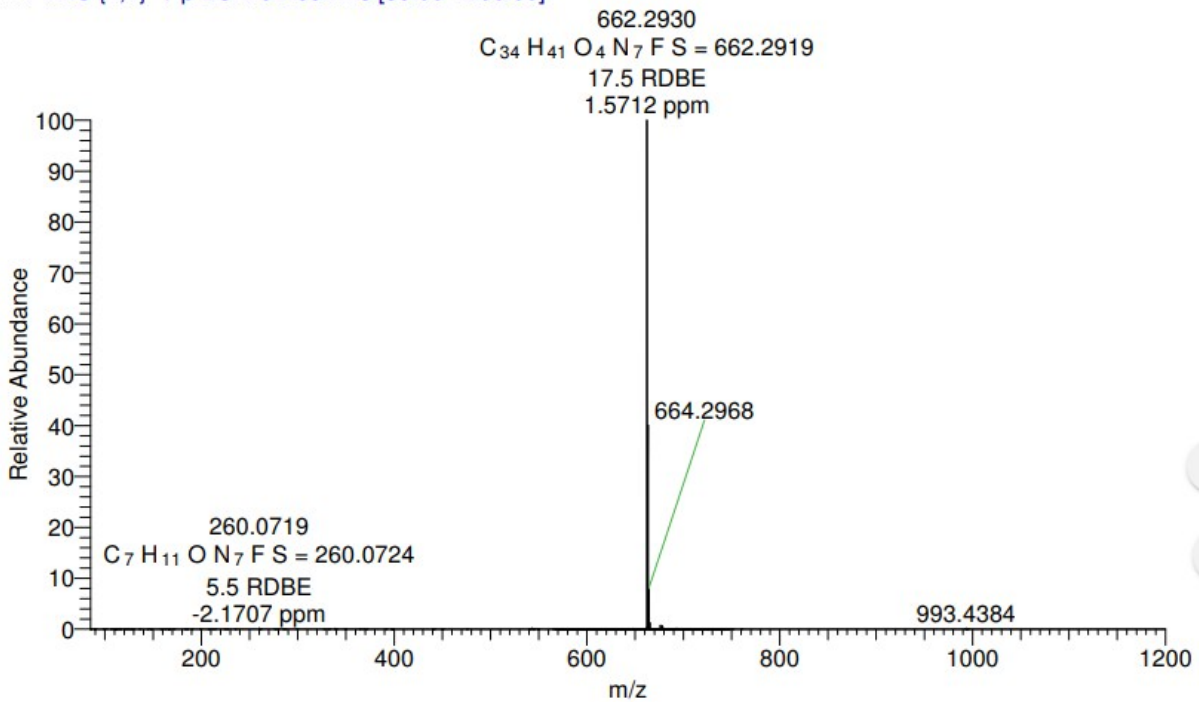
MGB-382

^1H NMR (d_6 -DMSO)



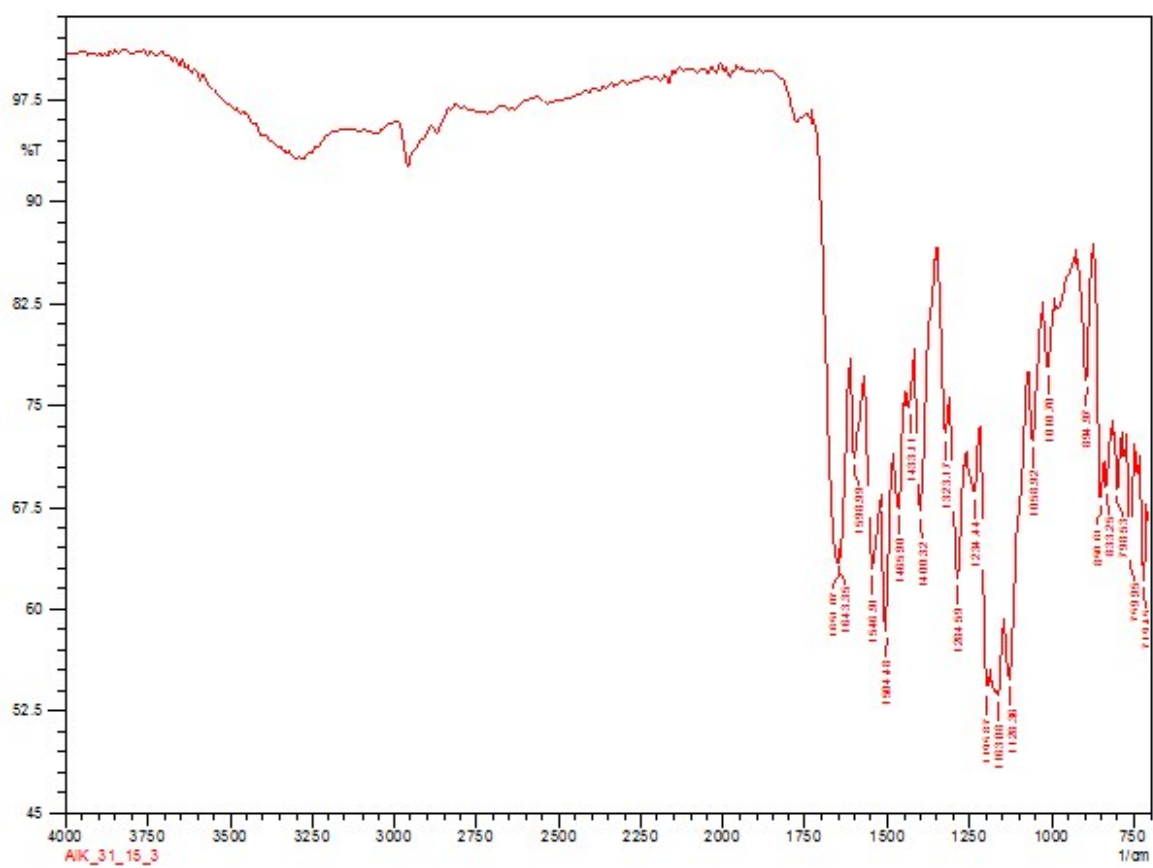
HRMS

AIK-31-15-3 #43 RT: 1.27 AV: 1 NL: 6.54E8
 T: FTMS {1,1} + p ESI Full lock ms [85.00-1200.00]



IR

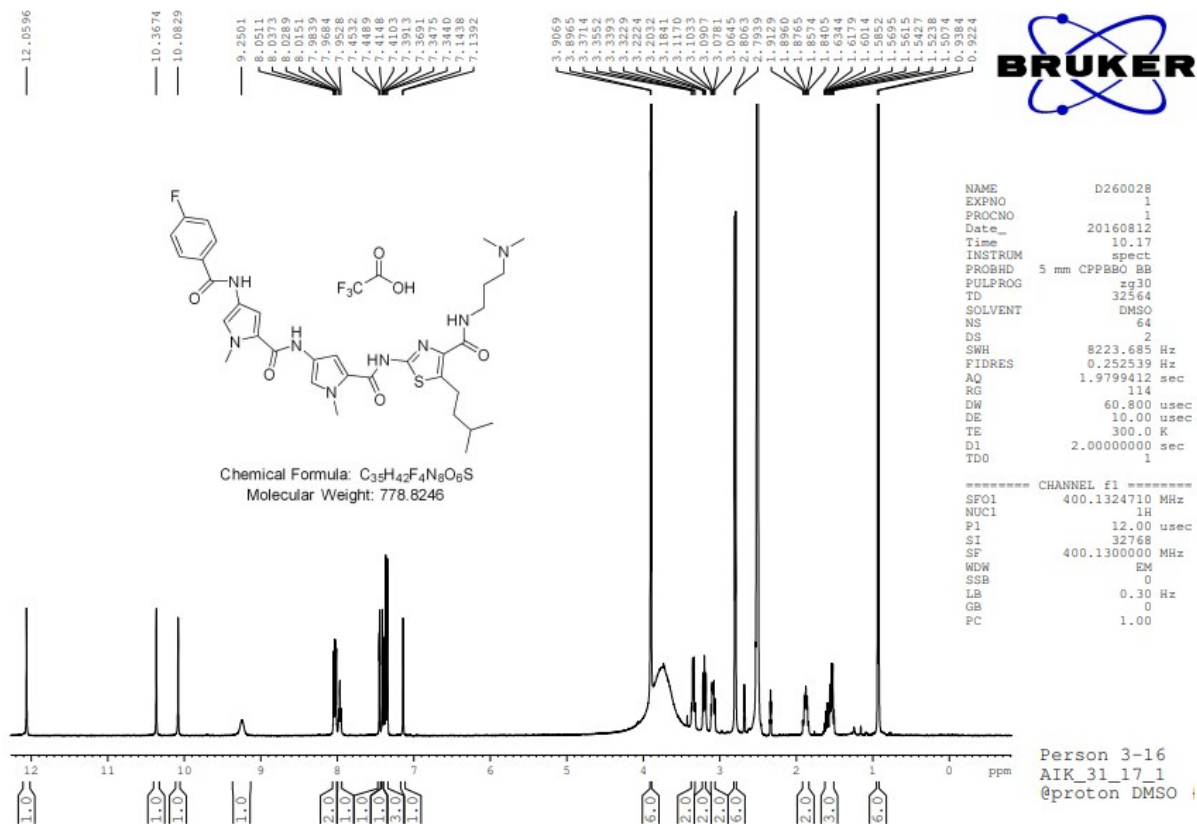
AIK_31_15_3



Peaks: 720, 760, 799, 833, 851, 895, 1011, 1059, 1128, 1163, 1196, 1234, 1285, 1323, 1400, 1433, 1466, 1505, 1547, 1599, 1643, 1651 cm⁻¹

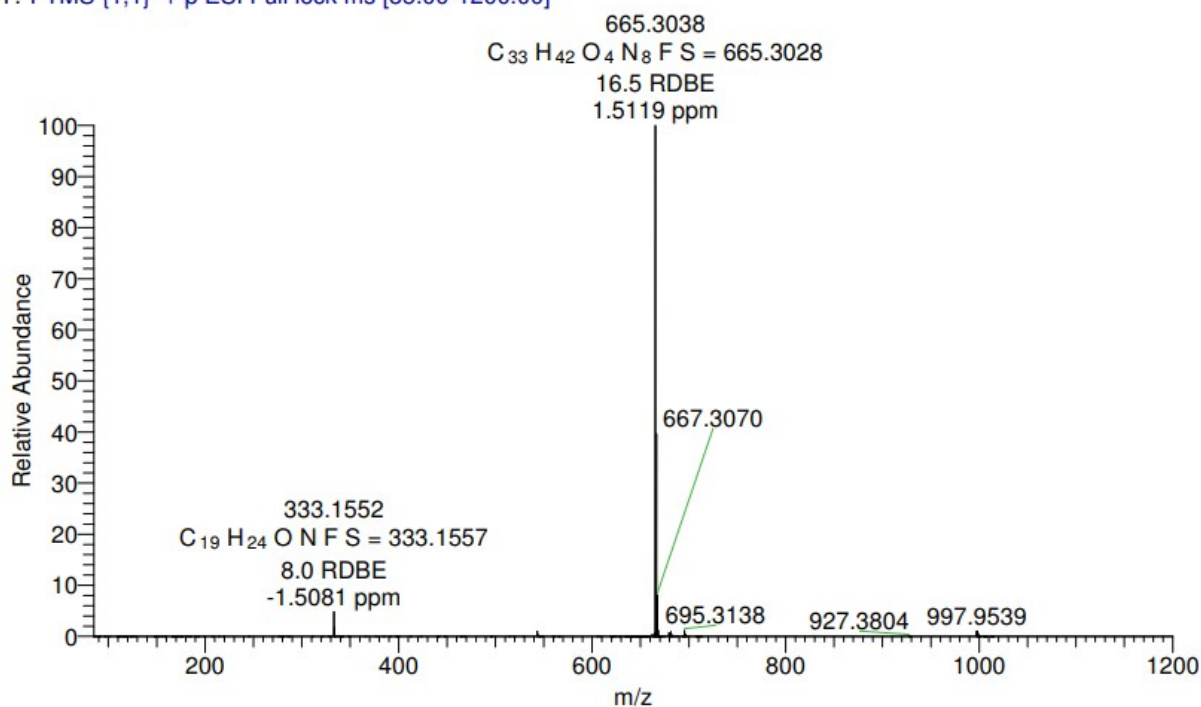
MGB-385

¹H NMR (d₆-DMSO)



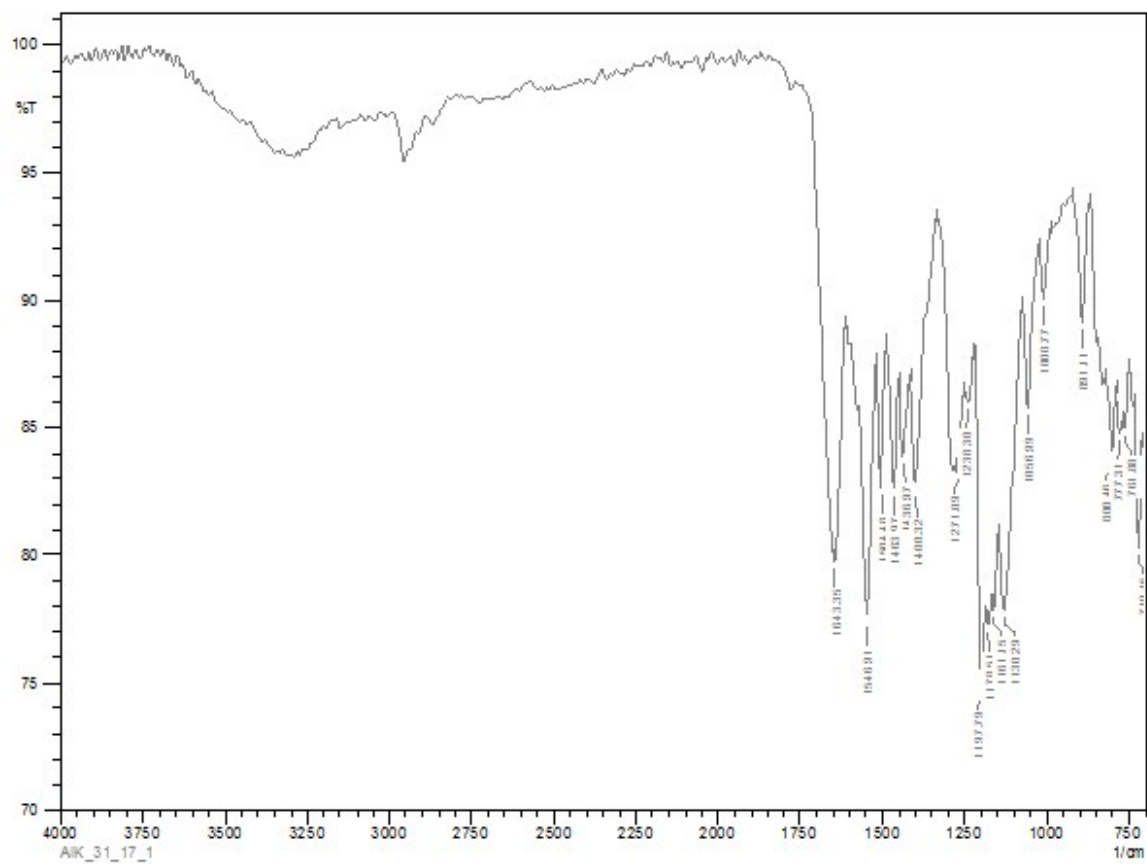
HRMS

AIK-31-17-1 #43 RT: 1.27 AV: 1 NL: 4.85E8
T: FTMS {1,1} + p ESI Full lock ms [85.00-1200.00]



IR

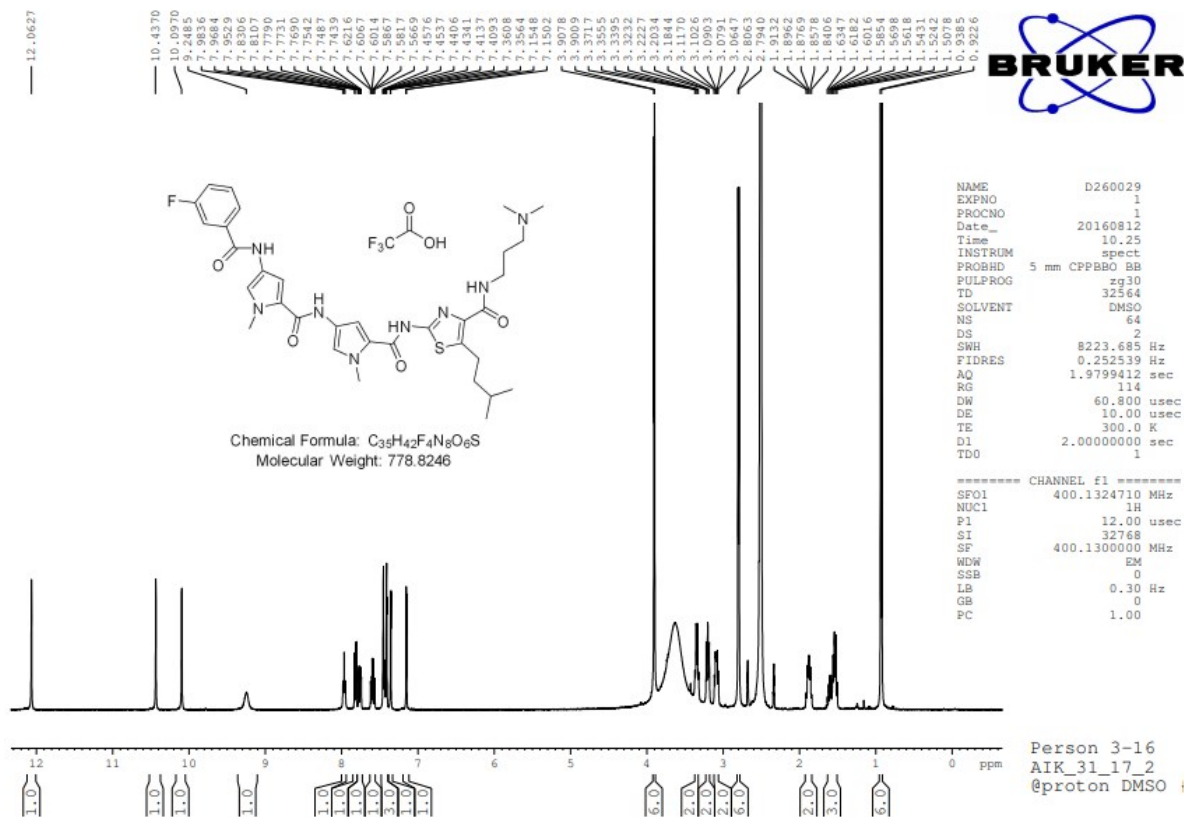
AIK_31_17_1



Peaks: 720, 762, 777, 801, 891, 1009, 1057, 1130, 1161, 1179, 1198, 1238, 1271, 1400, 1437, 1464, 1505, 1547, 1643 cm⁻¹

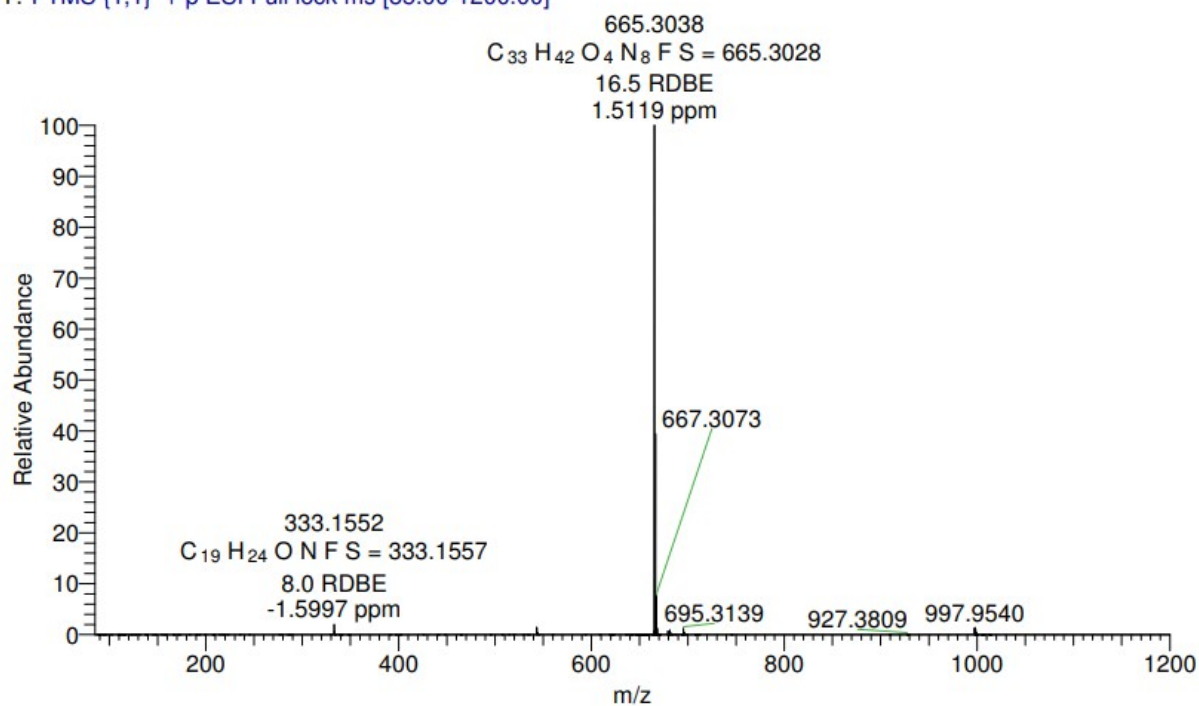
MGB-386

¹H NMR (d₆-DMSO)



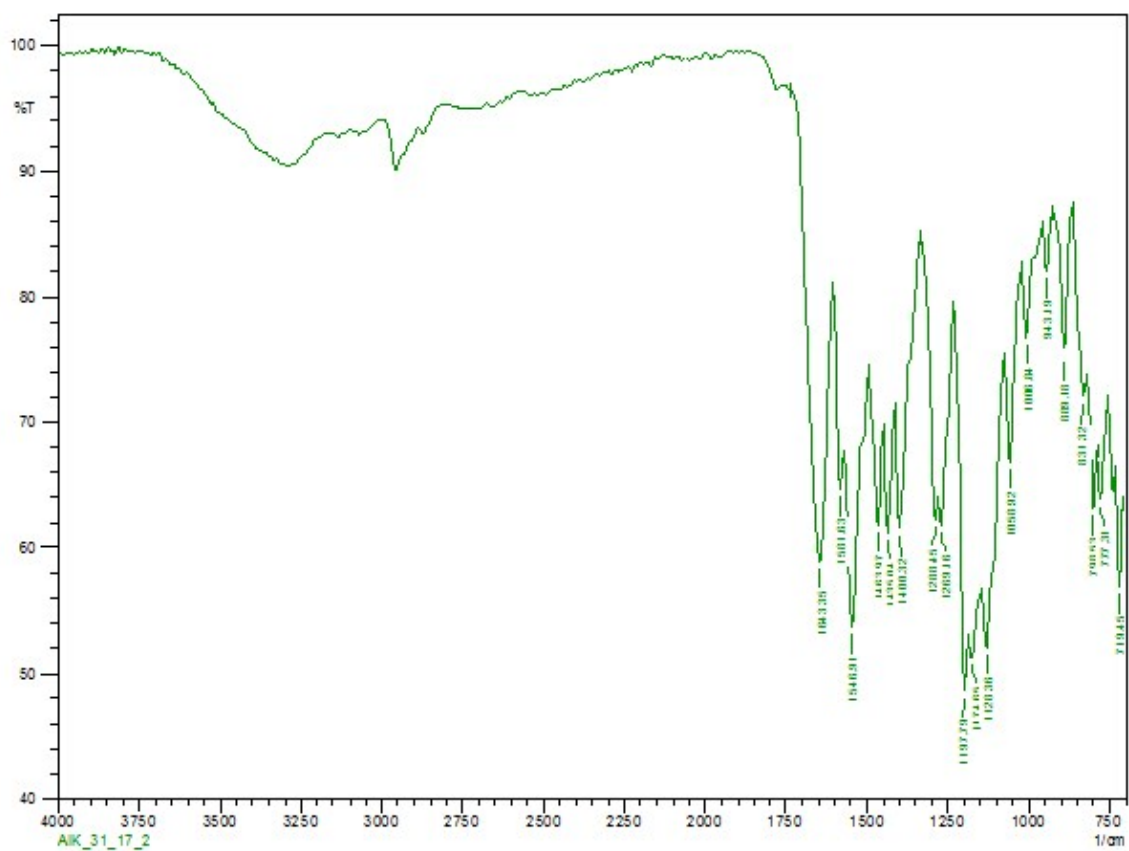
HRMS

AIK-31-17-2 #43 RT: 1.28 AV: 1 NL: 4.47E8
T: FTMS {1,1} + p ESI Full lock ms [85.00-1200.00]



IR

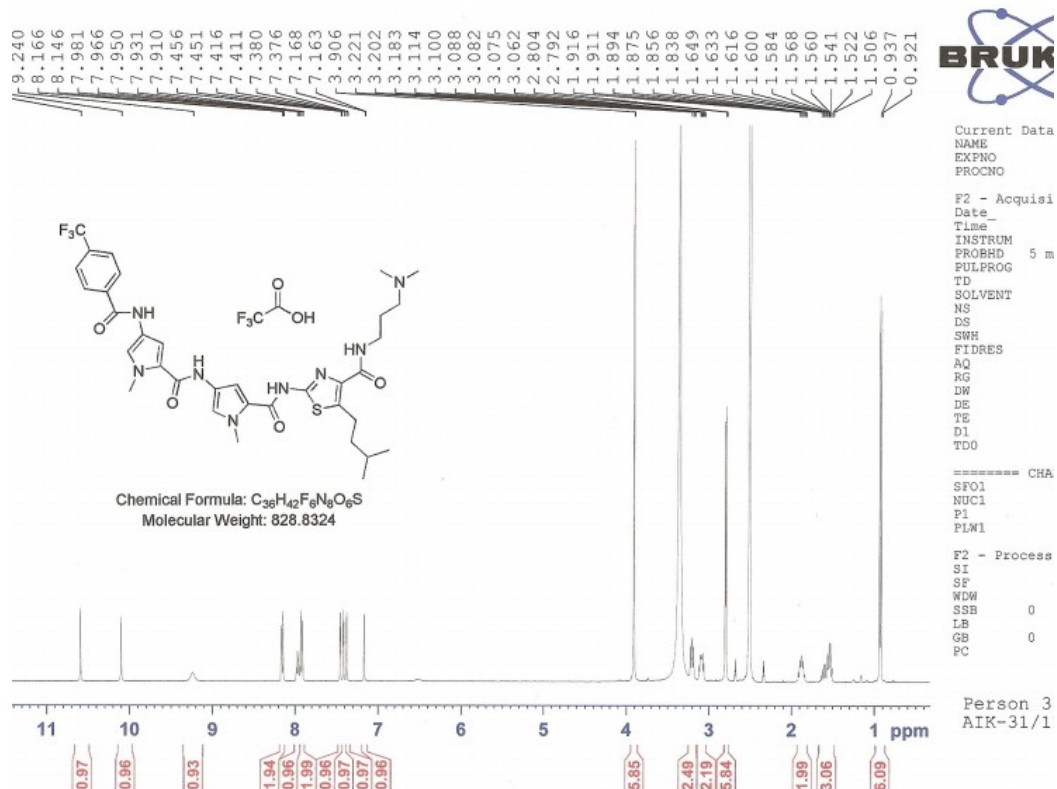
AIK_31_17_2



Peaks: 720, 777, 799, 831, 889, 943, 1007, 1059, 1128, 1175, 1198, 1269, 1289, 1400, 1435, 1464, 1547, 1582, 1643 cm^{-1}

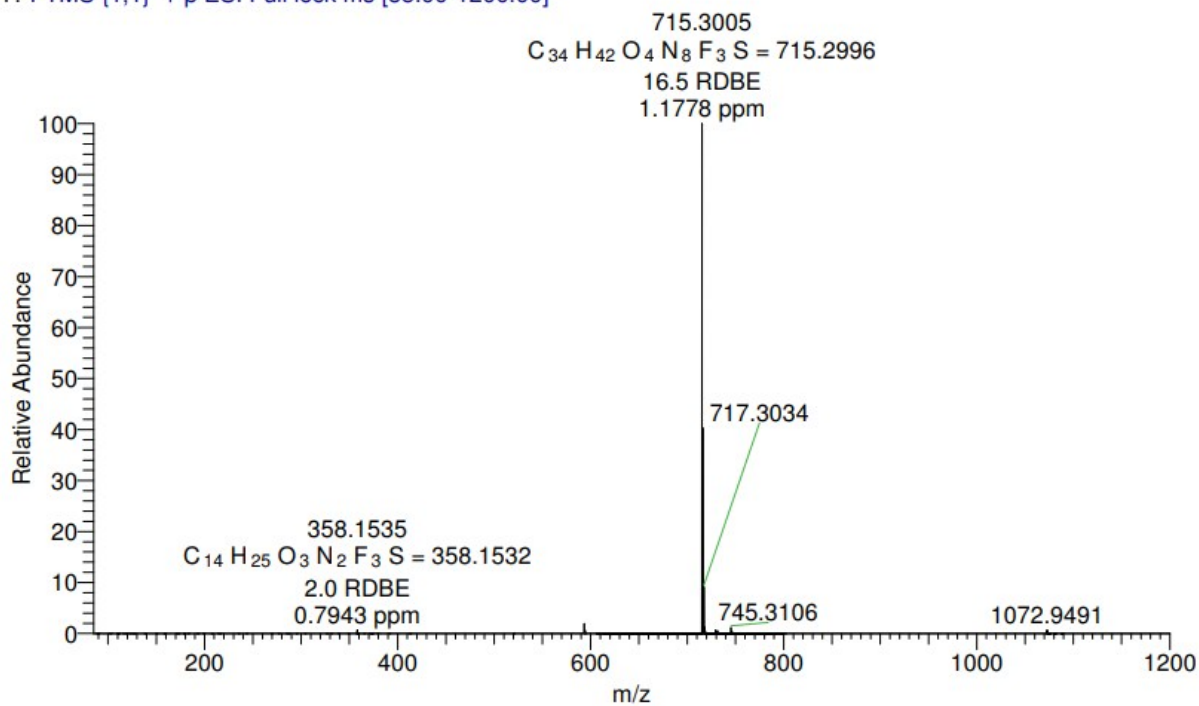
MGB-387

^1H NMR (d_6 -DMSO)



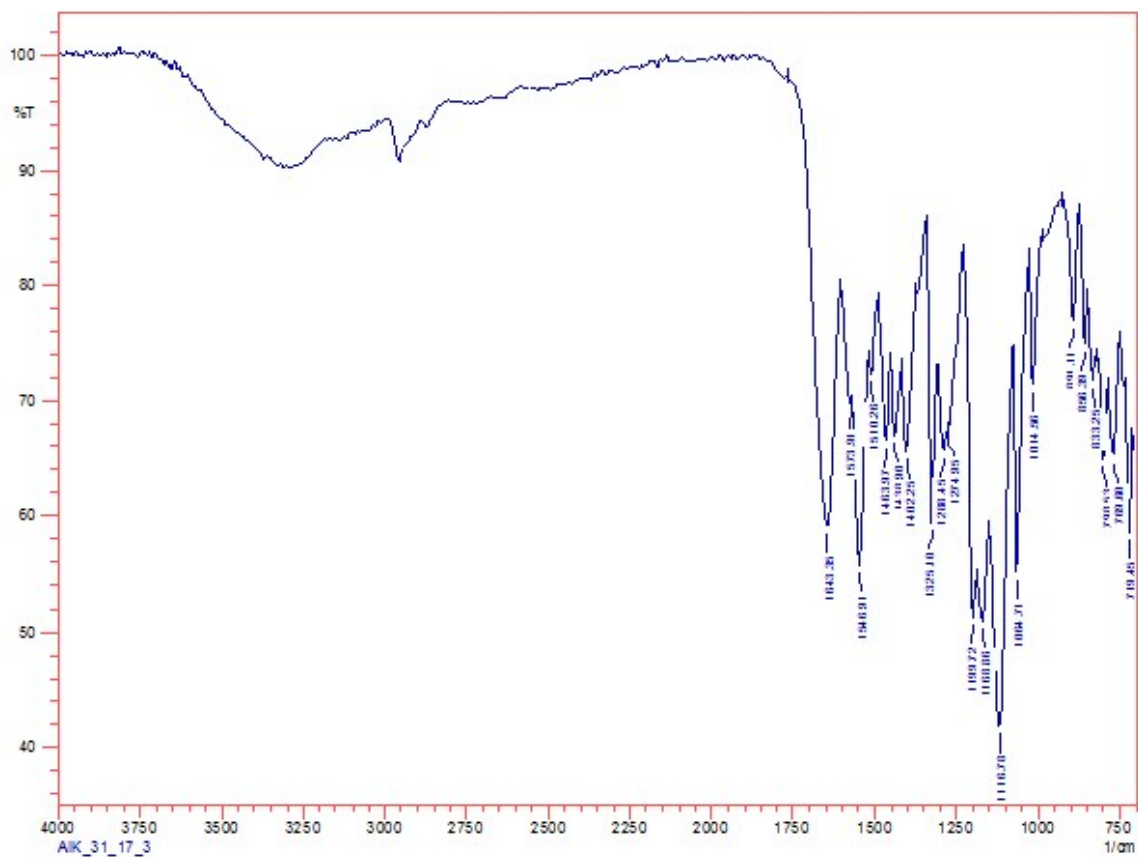
HRMS

AIK-31-17-3 #49 RT: 1.43 AV: 1 NL: 6.81E8
T: FTMS {1,1} + p ESI Full lock ms [85.00-1200.00]



IR

AIK_31_17_3



Peaks: 720, 770, 799, 833, 856, 891, 1015, 1065, 1117, 1169, 1200, 1275, 1289, 1325, 1402, 1439, 1464, 1510, 1547, 1574, 1643 cm^{-1}