Supporting Material

Table S1. Properties of novel compounds calculated with Chemicalize.org program[1]. The Lipinski's and Gelovani's parameters.

Compd.	Molecular formula	Number of atoms	MW	log *P*	H-bond donor	H-bond acceptor	Lipinski score[2]	MR[3] (cm3/mol)	TPSA[4] (Å²)
4a	$C_{25}H_{27}FN_4O_3$	60	450.514	3.22	3	5	4	128.42	92.35
4b	$C_{25}H_{27}FN_4O_3$	60	450.514	3.22	3	5	4	128.42	92.35
4c	$C_{25}H_{27}ClN_4O_3$	60	466.970	3.68	3	5	4	133.00	92.35
4d	$C_{25}H_{27}ClN_4O_3$	60	466.970	3.68	3	5	4	133.00	92.35
4e	$C_{26}H_{27}F_3N_4O_3$	63	500.522	3.96	3	5	4	134.17	92.35
4f	$C_{26}H_{27}F_3N_4O_3$	63	500.522	3.96	3	5	4	134.17	92.35
5a	$C_{25}H_{29}FN_4O_3$	62	452.530	2.86	3	5	4	127.35	92.35
5b	$C_{25}H_{29}FN_4O_3$	62	452.530	2.86	3	5	4	127.35	92.35
5c	$C_{25}H_{29}ClN_4O_3$	62	468.980	3.32	3	5	4	131.93	92.35
5d	$C_{25}H_{29}ClN_4O_3$	62	468.980	3.32	3	5	4	131.93	92.35
5e	$C_{26}H_{29}F_3N_4O_3$	65	502.538	3.60	3	5	4	133.10	92.35
5f	$C_{26}H_{29}F_3N_4O_3$	65	502.538	3.60	3	5	4	133.10	92.35

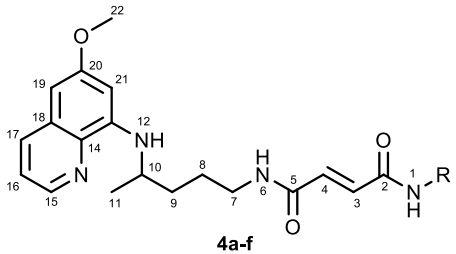
[1] Chemicalize, 2017, ChemAxon Ltd. Available from: http://www.chemicalize.org; [2] Out of four; [3] MR – molar refractivity; [4] TPSA – topological polar surface area.

Table S2. Analytical and spectral data of compounds **4a-f** and **5a-f.**

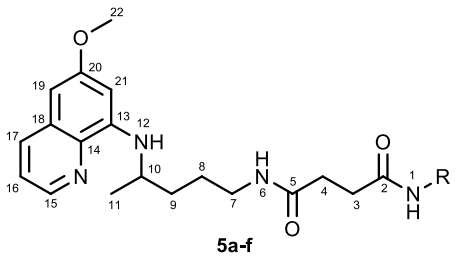
Compd.	Yield (%)	m.p. (°C)	IR (ATR): ν_{max} (cm^{-1})	MS (*m*/*z*)	Molecular formula (M_r)	CHN analysis calcd./found (%)		
4a	34	203–204	3388, 3319, 3269, 3080, 2961, 2935, 2866, 1630, 1554, 1520, 1452, 1387, 1334, 1201, 1158, 782, 680	451.1 (M+1)	$C_{25}H_{27}FN_4O_3$ (450.514)	66.65 66.32	6.04 6.30	12.44 12.49
4b	58	226–227	3386, 3294, 3072, 2963, 2928, 2863, 1635, 1548, 1513, 1452, 1391, 1330, 1212, 1160, 1051, 973, 829, 673	451.1 (M+1)	$C_{25}H_{27}FN_4O_3$ (450.514)	66.65 66.47	6.04 6.38	12.44 12.35
4c	42	187–188	3381, 3298, 3068, 2959, 2928, 2863, 1635, 1591, 1521, 1465, 1419, 1386, 1331, 1210, 1163, 976, 821, 783, 670	467.0 (M+1)	$C_{25}H_{27}ClN_4O_3$ (466.970)	64.30 64.21	5.83 6.05	12.00 11.78

4d	49	223–226	3381, 3289, 3071, 2959, 2931, 2864, 1640, 1526, 1452, 1388, 1331, 1210, 1163, 1094, 1049, 973, 822, 787, 686, 631, 507	467.0 (M+1)	$C_{25}H_{27}ClN_4O_3$ (466.970)	64.30 64.21	5.83 5.56	12.00 11.83
4e	31	149–150	3399, 3357, 3282, 3094, 2960, 2935, 2867, 1651, 1621, 1563, 1526, 1452, 1388, 1331, 1168, 1122, 973, 893, 788, 694	501.1 (M+1)	$C_{26}H_{27}F_3N_4O_3$ (500.522)	62.39 62.25	5.44 5.76	11.19 11.08
4f	34	189–191	3387, 3309, 3071, 2963, 2932, 1636, 1527, 1457, 1417, 1390, 1328, 1213, 1166, 1122, 1065, 970, 832, 681	501.1 (M+1)	$C_{26}H_{27}F_3N_4O_3$ (500.522)	62.39 62.17	5.44 5.61	11.19 11.40
5a	63	140–142	3391, 3283, 3145, 3080, 2959, 2926, 1744, 1646, 1615, 1555, 1507, 1387, 1224, 1202, 1167, 1157, 838, 815, 786, 681	453.3 (M+1)	$C_{25}H_{29}FN_4O_3$ (452.530)	66.35 66.25	6.46 6.50	12.38 12.20
5b	80	118–120	3391, 3283, 3145, 3080, 2959, 2926, 1744, 1646, 1615, 1555, 1507, 1387, 1224, 1202, 1167, 1157, 838, 815, 786, 681	453.4 (M+1)	$C_{25}H_{29}FN_4O_3$ (452.530)	66.35 66.53	6.46 6.29	12.38 12.55
5c	49	156–158	3390, 3287, 3242, 3180, 3102, 3074, 2962, 2922, 2856, 1738, 1650, 1612, 1591, 1572, 1539, 1516, 1422, 1388, 1202, 1066, 816, 787, 698, 682	469.2 (M+1)	$C_{25}H_{29}ClN_4O_3$ (468.980)	64.03 63.91	6.23 6.33	11.95 11.70
5d	60	152–153	3390, 3287, 3242, 3180, 3102, 3074, 2962, 2922, 2856, 1738, 1650, 1612, 1591, 1572, 1539, 1516, 1422, 1388, 1202, 1066, 816, 787, 698, 682	469.3 (M+1)	$C_{25}H_{29}ClN_4O_3$ (468.980)	64.03 64.35	6.23 6.57	11.95 12.13
5e	90	146–149	3394, 3302, 3263, 3216, 3164, 3097, 2963, 2928, 2859, 1651, 1617, 1562, 1518, 1450, 1389, 1331, 1265, 1173, 1127, 1064, 894, 816	503.3 (M+1)	$C_{26}H_{29}F_3N_4O_3$ (502.538)	62.14 62.25	5.82 5.99	11.15 11.08
5f	50	163–165	3387, 3287, 3256, 3198, 3123, 3071, 2963, 2925, 2859, 1652, 1614, 1547, 1515, 1452, 1419, 1389, 1327, 1264, 1169, 1124, 1064, 846, 784	503.3 (M+1)	$C_{26}H_{29}F_3N_4O_3$ (502.538)	62.14 62.39	5.82 5.76	11.15 11.41

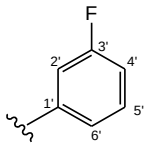
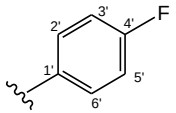
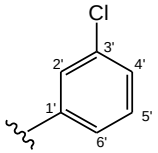
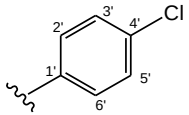
Table S3. ^{1}H and ^{13}C NMR spectra of amides **4a-f** and **5a-f**

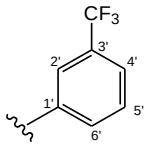
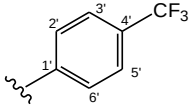
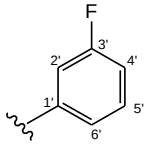
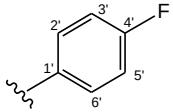
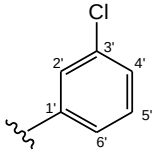
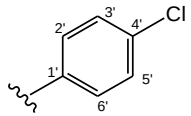


4a-f



5a-f

Compd.	R	^{1}H NMR (DMSO-d_6, δ ppm, J/Hz)	^{13}C NMR (DMSO-d_6, δ ppm, J/Hz)
4a		10.63 (s, 1H, 1), 8.55-8.53 (dd, 1H, 15, J = 1.6, 4.2), 8.52 (t, 1H, 6, J = 5.4), 8.09-8.06 (dd, 1H, 17, J = 1.5, 8.3), 7.69 (d, 2H, 6', J = 11.7), 7.45-7.41 (m, 1H, 16), 7.39-7.36 (m, 2H, 2', 4'), 7.06-7.96 (m, 2H, 3, 4), 6.96-6.92 (m, 1H, 5'), 6.47 (d, 1H, 21, J = 2.4), 6.28 (d, 1H, 19, J = 2.4), 6.15 (d, 1H, 12, J = 8.8), 3.82 (s, 3H, 22), 3.70-3.61 (m, 1H, 10), 3.24-3.18 (m, 2H, 7), 1.74-1.64, 1.63-1.52 (2m, 4H, 8, 9), 1.22 (d, 3H, 11, J = 6.3)	163.25 (5), 162.62 (2), 162.09 (3', J = 242.0), 159.00 (20), 144.63 (13), 144.23 (15), 140.50 (1', d, J = 11.5), 134.79 (17), 134.52 (14), 134.40 (3), 132.28 (4), 130.50 (5', d, J = 9.5), 129.57 (18), 122.09 (16), 115.14 (6'), 110.28 (2', d, J = 18.8), 106.13 (4', d, J = 27.2), 96.14 (21), 91.62 (19), 54.96 (22), 46.97 (10), 38.95 (7), 33.45 (9), 25.77 (8), 20.21 (11)
4b		10.49 (s, 1H, 1), 8.55-8.53 (dd, 1H, 15, J = 1.6, 4.2), 8.52 (t, 1H, 6, J = 5.4), 8.09-8.06 (dd, 1H, 17, J = 1.5, 8.3), 7.72-7.68 (dd, 2H, 2', 6', J = 5.0, J = 8.9), 7.45-7.41 (m, 1H, 16), 7.18 (t, 2H, 3', 5', J = 8.8), 7.05-6.93 (m, 2H, 3, 4), 6.47 (d, 1H, 21, J = 2.1), 6.28 (d, 1H, 19, J = 2.1), 6.15 (d, 1H, 12, J = 8.8), 3.82 (s, 3H, 22), 3.69-3.61 (m, 1H, 10), 3.24-3.18 (m, 2H, 7), 1.74-1.64, 1.63-1.52 (2m, 4H, 8, 9), 1.22 (d, 3H, 11, J = 6.3)	163.34 (5), 162.21 (2), 159.00 (20), 158.26 (4', d, J = 239.99), 144.63 (13), 144.23 (15), 135.22 (1'), 134.79 (17), 134.53 (14), 133.98 (3), 132.52 (4), 129.58 (18), 122.09 (16), 121.05 (2', 6', d, J = 7.6), 115.44 (3', 5', d, J = 21.89), 96.14 (21), 91.62 (19), 54.96 (22), 46.97 (10), 38.95 (7), 33.45 (9), 25.79 (8), 20.21 (11)
4c		10.59 (s, 1H, 1), 8.54-8.53 (dd, 1H, 15, J = 1.5, 4.1), 8.50 (t, 1H, 6, J = 5.5), 8.08-8.06 (dd, 1H, 17, J = 1.4, 8.2), 7.90 (s, 1H, 2'), 7.51 (d, 1H, 6', J = 8.1), 7.43-7.41 (m, 1H, 16), 7.37 (t, H, 5', J = 8.1), 7.16-7.14 (dd, 1H, 4', J = 1.2, J = 8.0), 7.00 (q, 2H, 3, 4, J = 15.1), 6.47 (d, 1H, 21, J = 2.4), 6.28 (d, 1H, 19, J = 2.3), 6.14 (d, 1H, 12, J = 8.8), 3.82 (s, 3H, 22), 3.67-3.63 (m, 1H, 10), 3.23-3.20 (m, 2H, 7), 1.73-1.67, 1.63-1.53 (2m, 4H, 8, 9), 1.22 (d, 3H, 11, J = 6.3)	163.21 (5), 162.60 (2), 158.97 (20), 144.60 (13), 144.19 (15), 140.19 (1'), 134.74 (17), 134.50 (14), 134.41 (3), 133.10 (3'), 132.19 (4), 130.48 (5'), 129.54 (18), 123.45 (6'), 122.03 (16), 118.74 (2'), 117.72 (4'), 96.11 (21), 91.63 (19), 54.93 (22), 46.98 (10), 39.23 (7), 33.44 (9), 25.72 (8), 20.18 (11)
4d		10.56 (s, 1H, 1), 8.55-8.53 (dd, 1H, 15, J = 1.7, 4.2), 8.50 (t, 1H, 6, J = 5.6), 8.09-8.06 (dd, 1H, 17, J = 1.6, 8.3), 7.72-7.68 (m, 2H, 2', 6'), 7.45-7.37 (m, 3H, 16, 3', 5'), 7.06-6.94 (m, 2H, 3, 4), 6.47 (d, 1H, 21, J = 2.5), 6.27 (d, 1H, 19, J = 2.4), 6.14 (d, 1H, 12, J = 8.8), 3.82 (s, 3H, 22), 3.69-3.60 (m, 1H, 10), 3.24-3.18 (m, 2H, 7), 1.74-1.64, 1.63-1.51 (2m, 4H, 8, 9), 1.22 (d, 3H, 11, J = 6.3)	163.29 (5), 162.43 (2), 159.00 (20), 144.63 (13), 144.23 (15), 137.76 (1'), 134.79 (17), 134.52 (14), 134.21 (3), 132.38 (4), 129.57 (18), 128.75 (3', 5'), 127.36 (4'), 122.09 (16), 120.84 (2', 6'), 96.14 (21), 91.61 (19), 54.96 (22), 46.97 (10), 38.82 (7), 33.44 (9), 25.77 (8), 20.21 (11)

4e		10.75 (s, 1H, 1), 8.55-8.52 (m, 2H, 6, 15), 8.18 (s, 1H, 2'), 8.08-8.06 (dd, 1H, 17, *J* = 1.1, 8.2), 7.83 (d, 1H, 6'), 7.59 (t, 1H, 5', *J* = 7.9), 7.45-7.42 (m, 2H, 16, 4'), 7.00-6.98 (q, 2H, 3, 4, *J* = 15.1), 6.47 (d, 1H, 21, *J* = 2.4), 6.28 (d, 1H, 19, *J* = 2.0), 6.15 (d, 1H, 12, *J* = 8.7), 3.82 (s, 3H, 22), 3.67-3.63 (m, 1H, 10), 3.23-3.20 (m, 2H, 7), 1.73-1.67, 1.63-1.53 (2m, 4H, 8, 9), 1.22 (d, 3H, 11, *J* = 6.3)	163.19 (5), 162.81 (2), 158.99 (20), 144.62 (13), 144.21 (15), 139.54 (1'), 134.77 (17), 134.55 (14), 134.52 (3), 132.15 (4), 130.09 (5'), 129.56 (18), 129.82-129.19 (3', q, *J* = 31.7), 126.73-121.32 (7', q, *J* = 273.1), 122.88 (6'), 122.07 (16), 120.09 (4'), 115.33 (2'), 96.13 (21), 91.62 (19), 54.95 (22), 46.19 (10), 39.23 (7), 33.45 (9), 25.76 (8), 20.20 (11)
4f		10.75 (s, 1H, 1), 8.54-8.53 (m, 1H, 15), 8.51 (t, 1H, 6, *J* = 5.3), 8.07 (d, 1H, 17, *J* = 8.2), 7.88 (d, 2H, 3', 5', *J* = 8.5), 7.71 (d, 2H, 2', 6', *J* = 8.5), 7.43-7.41 (m, 1H, 16), 7.07-6.99 (q, 2H, 3, 4, *J* = 15.1), 6.47 (d, 1H, 21, *J* = 2.2), 6.28 (d, 1H, 19, *J* = 2.2), 6.14 (d, 1H, 12, *J* = 8.7), 3.82 (s, 3H, 22), 3.67-3.63 (m, 1H, 10), 3.23-3.20 (dd, 2H, 7, *J* = 6.1, 12.1,), 2.59 (t, 2H, 3, *J* = 7.0), 1.73-1.67, 1.61-1.53 (2m, 4H, 8, 9), 1.22 (d, 3H, 1, *J* = 6.3)	161.17 (5), 162.83 (2), 158.97 (20), 144.60 (13), 144.17 (15), 142.28 (1'), 134.72 (17), 134.66 (3), 134.50 (14), 132.11 (4), 129.53 (18), 126.95-121.55 (7', q, *J* = 271.6), 126.11-126.04 (3', 5', q, *J* = 3.0), 124.02-123.39 (4', q, *J* = 31.7), 122.02 (16), 119.26 (2', 6'), 96.10 (21), 91.63 (19), 54.92 (22), 46.96 (10), 38.80 (7), 33.43 (9), 25.70 (8), 20.17 (11)
5a		10.13 (s, 1H, 1), 8.54-8.53 (dd, 1H, 15, *J* = 1.7, 4.2), 8.08-8.06 (dd, 1H, 17, *J* = 1.6, 8.3), 7.86 (t, 1H, 6, *J* = 5.6), 7.60-7.58 (m, 1H, 6'), 7.43-7.41 (m, 1H, 16), 7.31-7.27 (m, 2H, 2', 5'), 6.85-6.81 (m, 1H, 4'), 6.47 (d, 1H, 21, *J* = 2.5), 6.26 (d, 1H, 19, *J* = 2.5), 6.11 (d, 1H, 12, *J* = 8.7), 3.82 (s, 3H, 22), 3.64-3.59 (m, 1H, 10), 3.10-3.03 (m, 2H, 7), 2.55 (t, 2H, 3, *J* = 7.2), 2.37 (t, 2H, 4, *J* = 7.2), 1.67-1.63, 1.55-1.45 (2m, 4H, 8, 9), 1.19 (d, 3H, 11, *J* = 6.3)	170.86 (5, 2), 162.10 (3', d, *J* = 240.06), 158.98 (20), 144.61 (13), 144.19 (15), 141.03 (1', d, *J* = 13.1), 134.75 (17), 134.51 (14), 130.19 (5', d, *J* = 9.0), 129.55 (18), 122.05 (16), 114.55 (6'), 109.22 (2', d, *J* = 20.1), 105.61 (4', d, *J* = 23.5), 96.07 (21), 91.59 (19), 54.94 (22), 46.99 (10), 38.46 (7), 33.38 (9), 31.75 (3), 30.16 (4), 25.95 (8), 20.15 (11)
5b		9.98 (s, 1H, 1), 8.55-8.53 (dd, 1H, 15, *J* = 1.6, 4.2), 8.09-8.06 (dd, 1H, 17, *J* = 1.5, 8.3), 7.87 (t, 1H, 6, *J* = 5.5), 7.62-7.57 (m, 2H, 2', 6'), 7.45-7.40 (m, 1H, 16), 7.14-7.08 (m, 2H, 3', 5'), 6.47 (d, 1H, 21, *J* = 2.4), 6.26 (d, 1H, 19, *J* = 2.4), 6.12 (d, 1H, 12, *J* = 8.8), 3.82 (s, 3H, 22), 3.65-3.57 (m, 1H, 10), 3.10-3.04 (m, 2H, 7), 2.54 (t, 2H, 3, *J* = 7.1), 2.37 (t, 2H, 4, *J* = 7.0), 1.69-1.59, 1.58-1.43 (2m, 4H, 8, 9), 1.19 (d, 3H, 11, *J* = 6.3)	170.96 (5), 170.35 (2), 159.00 (20), 157.72 (4', d, *J* = 246.3), 144.63 (13), 144.22 (15), 135.76 (1'), 134.79 (17), 134.52 (14), 129.57 (18), 122.09 (16), 120.53 (2', 6', d, *J* = 7.8), 115.14 (3', 5', d, *J* = 22.1), 96.09 (21), 91.58 (19), 54.97 (22), 47.00 (10), 38.48 (7), 33.39 (9), 31.66 (3), 30.34 (4), 25.99 (8), 20.17 (11)
5c		10.11 (s, 1H, 1), 8.54-8.53 (dd, 1H, 15, *J* = 1.6, 4.2), 8.08-8.06 (dd, 1H, 17, *J* = 1.6, 8.3), 7.86 (t, 1H, 6, *J* = 5.5), 7.81 (t, 1H, 2', *J* = 2.0), 7.43-7.41 (m, 2H, 16, 6'), 7.31-7.28 (m, 1H, 5'), 7.07-7.05 (m, 1H, 4'), 6.47 (d, 1H, 21, *J* = 2.5), 6.25 (d, 1H, 19, *J* = 2.5), 6.11 (d, 1H, 12, *J* = 8.2), 3.82 (s, 3H, 22), 3.63-3.59 (m, 1H, 10), 3.10-3.03 (m, 2H, 7), 2.55 (t, 2H, 3, *J* = 7.1), 2.37 (t, 2H, 4, *J* = 7.2), 1.67-1.63, 1.56-1.44 (2m, 4H, 8, 9), 1.19 (d, 3H, 11, *J* = 6.3)	170.89 (5), 170.85 (2), 158.98 (20), 144.60 (13), 144.19 (15), 140.73 (1'), 134.77 (17), 134.49 (14), 132.97 (3'), 130.29 (5'), 129.55 (18), 122.51 (4'), 122.06 (16), 118.31 (6'), 117.19 (2'), 96.08 (21), 91.59 (19), 54.95 (22), 46.99 (10), 38.46 (7), 33.38 (9), 31.74 (3), 30.16 (4), 25.96 (8), 20.16 (11)
5d		10.07 (s, 1H, 1), 8.55-8.53 (dd, 1H, 15, *J* = 1.5, 4.2), 8.10-8.07 (dd, 1H, 17, *J* = 1.4, 8.3), 7.88 (t, 1H, 6, *J* = 5.4), 7.61 (d, 2H, 2', 6', *J* = 8.9), 7.45-7.41 (m, 1H, 16), 7.32 (d, 2H, 3', 5', *J* = 8.9), 6.48 (d, 1H, 21, *J* = 2.3), 6.26 (d, 1H, 19, *J* = 2.3), 6.13 (bs, 1H, 12), 3.81 (s, 3H, 22), 3.63-3.57 (m, 1H, 10), 3.09-3.03 (m, 2H, 7), 2.55 (t, 2H, 3, *J* = 7.4), 2.39 (t, 2H, 4, *J* = 7.0), 1.70-1.59, 1.58-1.43 (2m, 4H, 8, 9), 1.19 (d, 3H, 11, *J* = 6.3)	170.92 (5), 170.64 (2), 159.01 (20), 144.55 (13), 144.18 (15), 138.28 (1'), 134.89 (17), 134.42 (14), 129.59 (18), 128.51 (3', 5'), 126.33 (4'), 122.09 (16), 120.37 (2', 6'), 96.19 (21), 91.63 (19), 54.98 (22), 47.02 (10), 38.47 (7), 33.37 (9), 31.73 (3), 30.23 (4), 25.98 (8), 20.15 (11)

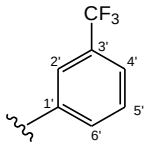
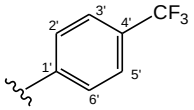
5e		10.26 (s, 1H, 1), 8.54-8.53 (dd, 1H, 15, *J* = 1.6, 4.2), 8.11 (s, 1H, 2'), 8.08-8.06 (dd, 1H, 17, *J* = 1.6, 8.3), 7.88 (t, 1H, 6, *J* = 5.5), 7.74 (d, 1H, 6', *J* = 8.1), 7.52 (t, 1H, 4', *J* = 8.0), 7.43-7.41 (m, 1H, 16), 7.36 (d, 1H, 5', *J* = 7.8), 6.47 (d, 1H, 21, *J* = 2.5), 6.25 (d, 1H, 19, *J* = 2.5), 6.11 (d, 1H, 12, *J* = 8.7), 3.82 (s, 3H, 22), 3.63-3.58 (m, 1H, 10), 3.10-3.04 (m, 2H, 7), 2.57 (t, 2H, 3, *J* = 7.2), 2.41 (t, 2H, 4, *J* = 7.2), 1.67-1.63, 1.56-1.44 (2m, 4H, 8, 9), 1.19 (d, 3H, 11, *J* = 6.3)	171.11 (5), 170.84 (2), 158.98 (20), 144.61 (13), 144.19 (15), 140.03 (1'), 134.75 (17), 134.50 (14), 129.83 (5'), 129.55 (18), 129.67-129.04 (3', q, *J* = 31.9), 126.81-121.40 (7', q, *J* = 269.8), 122.33 (6'), 122.05 (16), 119.14 (4'), 114.88 (2'), 96.06 (21), 91.58 (19), 54.94 (22), 46.98 (10), 38.46 (7), 33.38 (9), 31.72 (3), 30.11 (4), 25.96 (8), 20.14 (11)
5f		10.31 (s, 1H, 1), 8.54-8.52 (dd, 1H, 15, *J* = 1.5, 4.2), 8.09-8.06 (dd, 1H, 17, *J* = 1.5, 8.3), 7.89 (t, 1H, 6, *J* = 5.3), 7.79 (d, 2H, 2', 6', *J* = 8.5), 7.63 (d, 2H, 3', 5', *J* = 8.7), 7.44-7.40 (m, 1H, 16), 6.47 (d, 1H, 21, *J* = 2.4), 6.25 (d, 1H, 19, *J* = 2.4), 6.11 (d, 1H, 12, *J* = 8.7), 3.82 (s, 3H, 22), 3.65-3.57 (m, 1H, 10), 3.09-3.04 (m, 2H, 7), 2.59 (t, 2H, 3, *J* = 7.0), 2.40 (t, 2H, 4, *J* = 7.0), 1.71-1.58, 1.57-1.43 (2m, 4H, 8, 9), 1.19 (d, 3H, 11, *J* = 6.2)	171.18 (5), 170.86 (2), 158.99 (20), 144.61 (13), 144.20 (15), 142.83 (1'), 134.77 (17), 134.51 (14), 129.55 (18), 125.95 (3', 5'), 127.05-121.68 (7', q, *J* = 274.2), 123.15-122.52 (4', q, *J* = 28.2), 122.06 (16), 118.69 (2', 6'), 96.08 (21), 91.59 (19), 54.95 (22), 46.99 (10), 38.47 (7), 33.38 (9), 31.79 (3), 30.10 (4), 25.96 (8), 20.14 (11)

Table S4. Interaction of fumardiamide **4b** with GSH

Time (h)	Reaction			Control		
	4b	**standard**	**4b/standard**	**4b**	**standard**	**4b/standard**
0	1.09E+09	1.49E+09	0.732	6.05E+08	1.26E+09	0.479
5	8.64E+08	1.21E+09	0.715	5.51E+08	1.07E+09	0.516
26	7.65E+08	1.09E+09	0.704	5.27E+08	1.03E+09	0.509
52	5.80E+08	8.71E+08	0.665	5.06E+08	1.02E+09	0.498
124	5.96E+08	9.29E+08	0.642	5.64E+08	1.16E+09	0.488
216	6.64E+08	1.11E+09	0.598	6.06E+08	1.21E+09	0.500

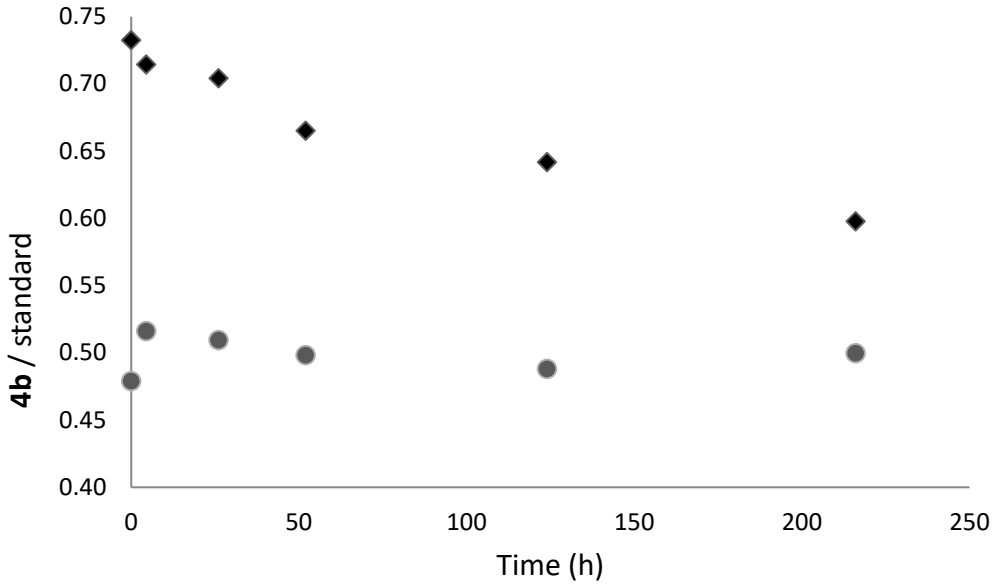
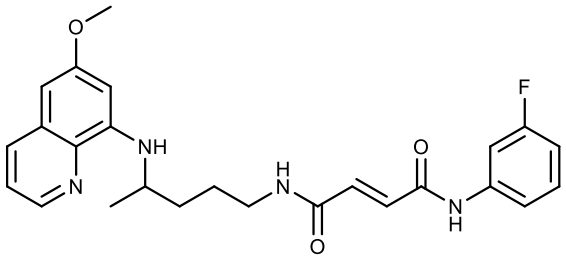
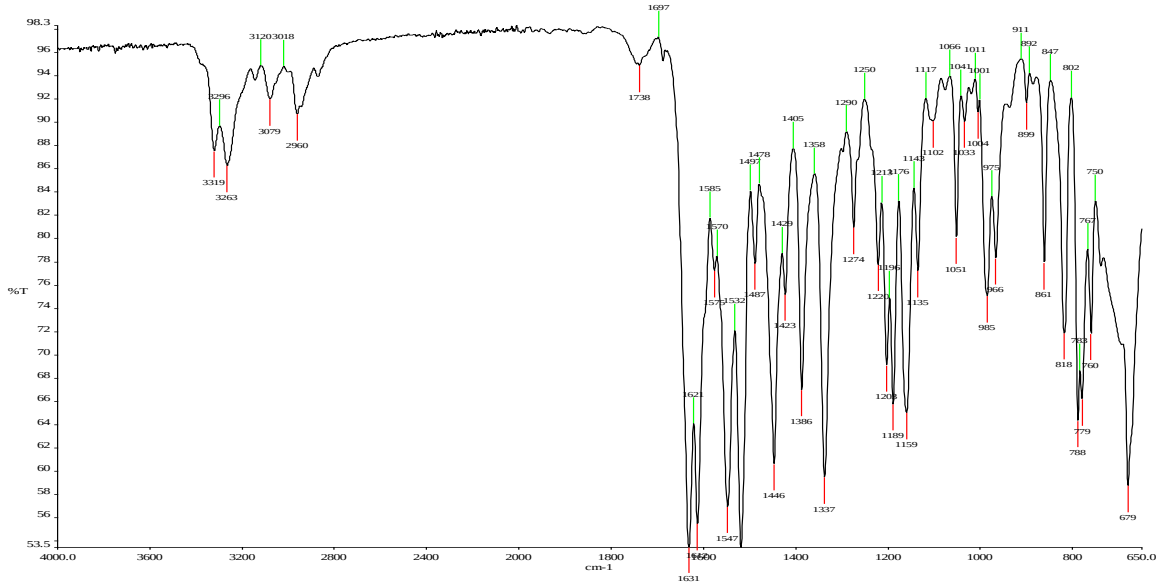


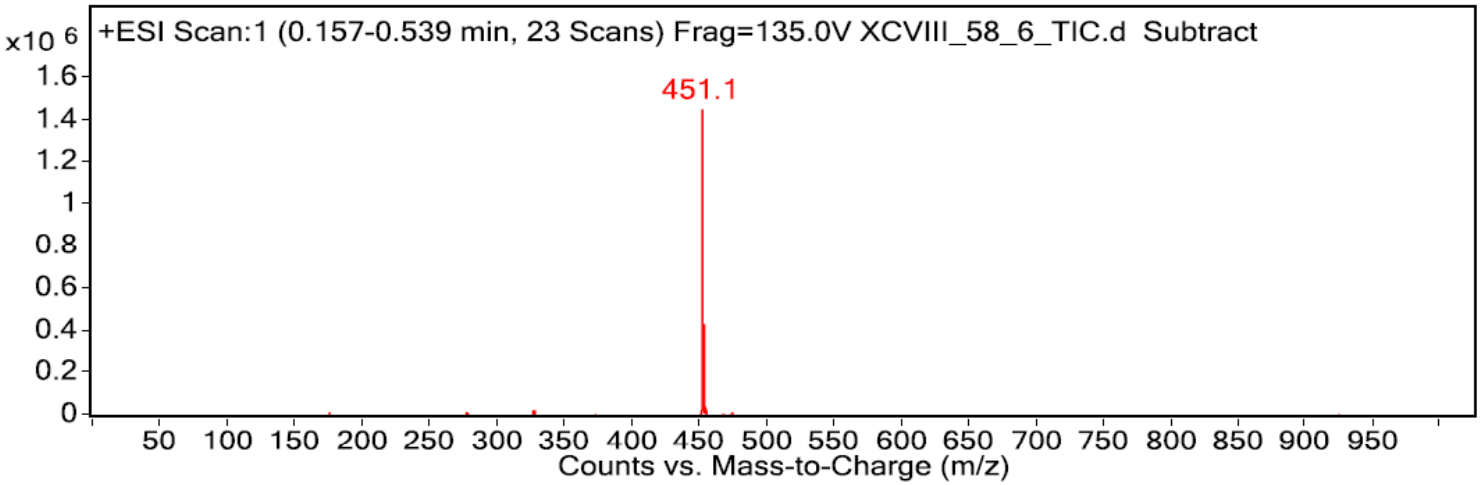
Figure S1. Interaction of fumardiamide **4b** with GSH (♦). Control: (*N*-(benzyloxy)-*N*'-{4-[(6-methoxyquinolin-8-yl)amino]pentyl}butanediamide) (●).

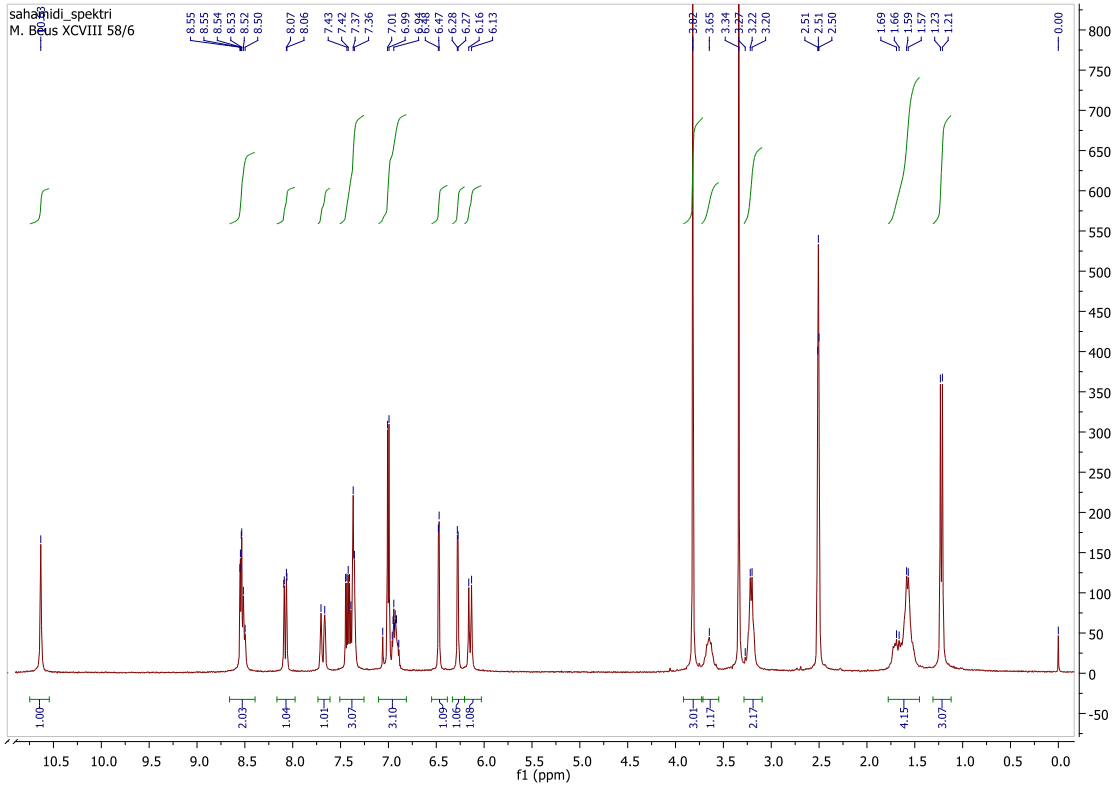
Spectra:

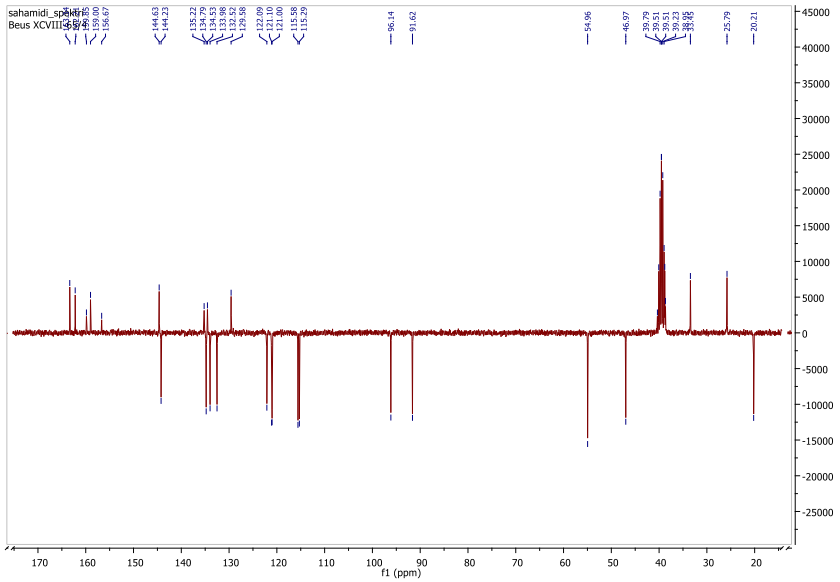

O
NH
N
H
N
O
O
N
H
F

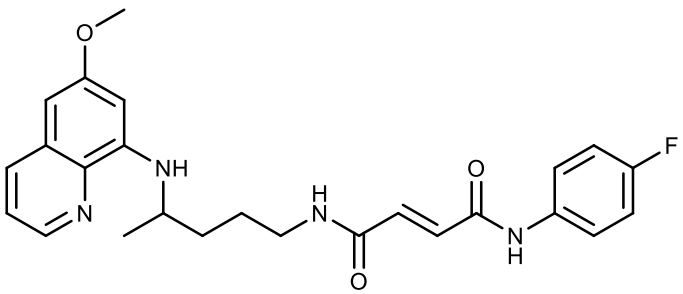
4a


%T
cm-1
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
98.3
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
58
56
53.5
3319
3263
3296
3120
3018
3079
2960
1738
1697
1631
1621
1585
1570
1547
1532
1497
1487
1478
1446
1429
1423
1405
1386
1358
1337
1290
1274
1250
1223
1213
1196
1189
1176
1159
1143
1135
1117
1102
1066
1051
1041
1033
1011
1004
1001
985
975
966
911
899
892
861
847
818
802
788
779
768
760
750
679

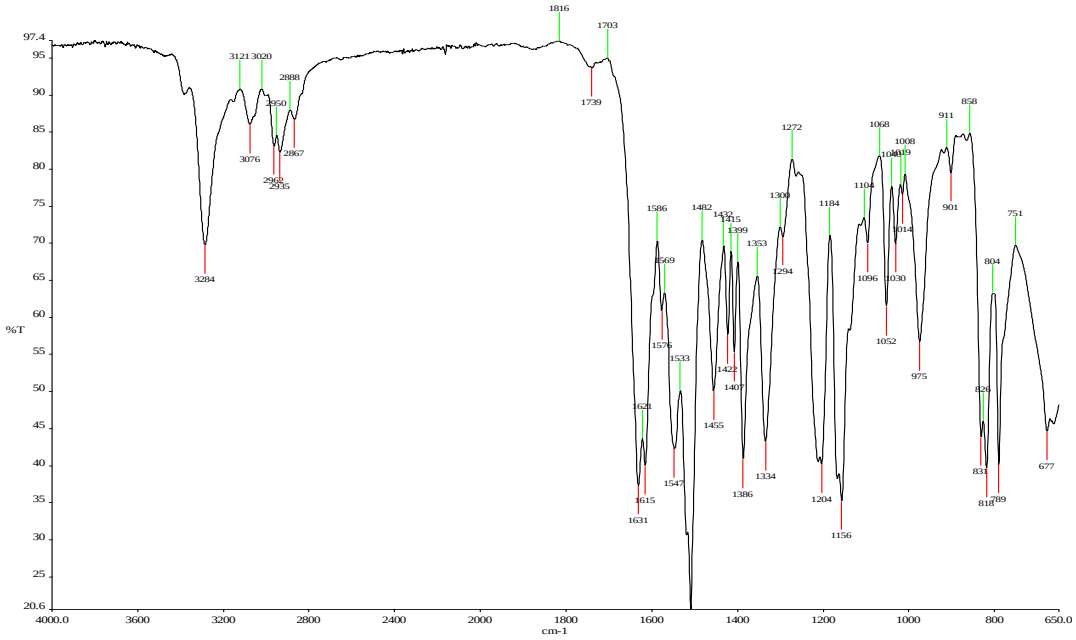

+ESI Scan:1 (0.157-0.539 min, 23 Scans) Frag=135.0V XCVIII_58_6_TIC.d Subtract
x10 6
451.1
Counts vs. Mass-to-Charge (m/z)


sahamidi_spektri
M. Beus XCVIII 58/6
f1 (ppm)

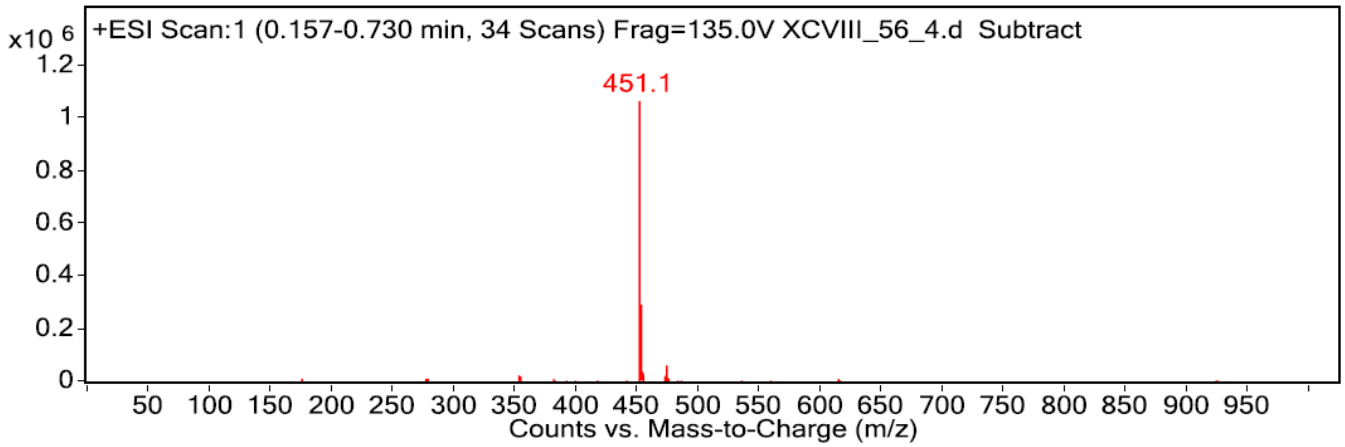

sahamidi_sp4d1
Beus XCVIII-C-1 1H
165.85
159.40
156.07
144.63
144.23
135.22
134.29
134.53
133.98
133.32
129.58
122.09
121.10
121.00
115.58
115.29
96.14
91.62
54.96
46.97
39.79
39.51
39.23
25.79
20.21
f1 (ppm)

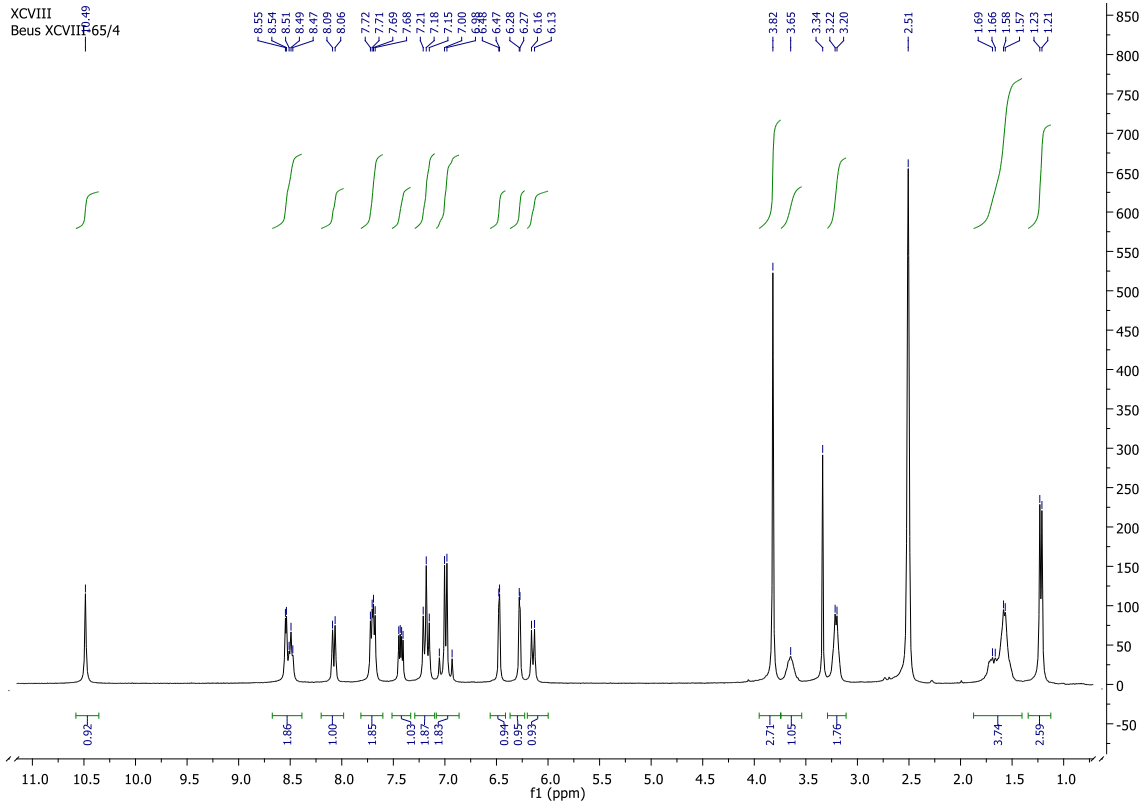

O
NH
N
H
N
O
O
N
H
F

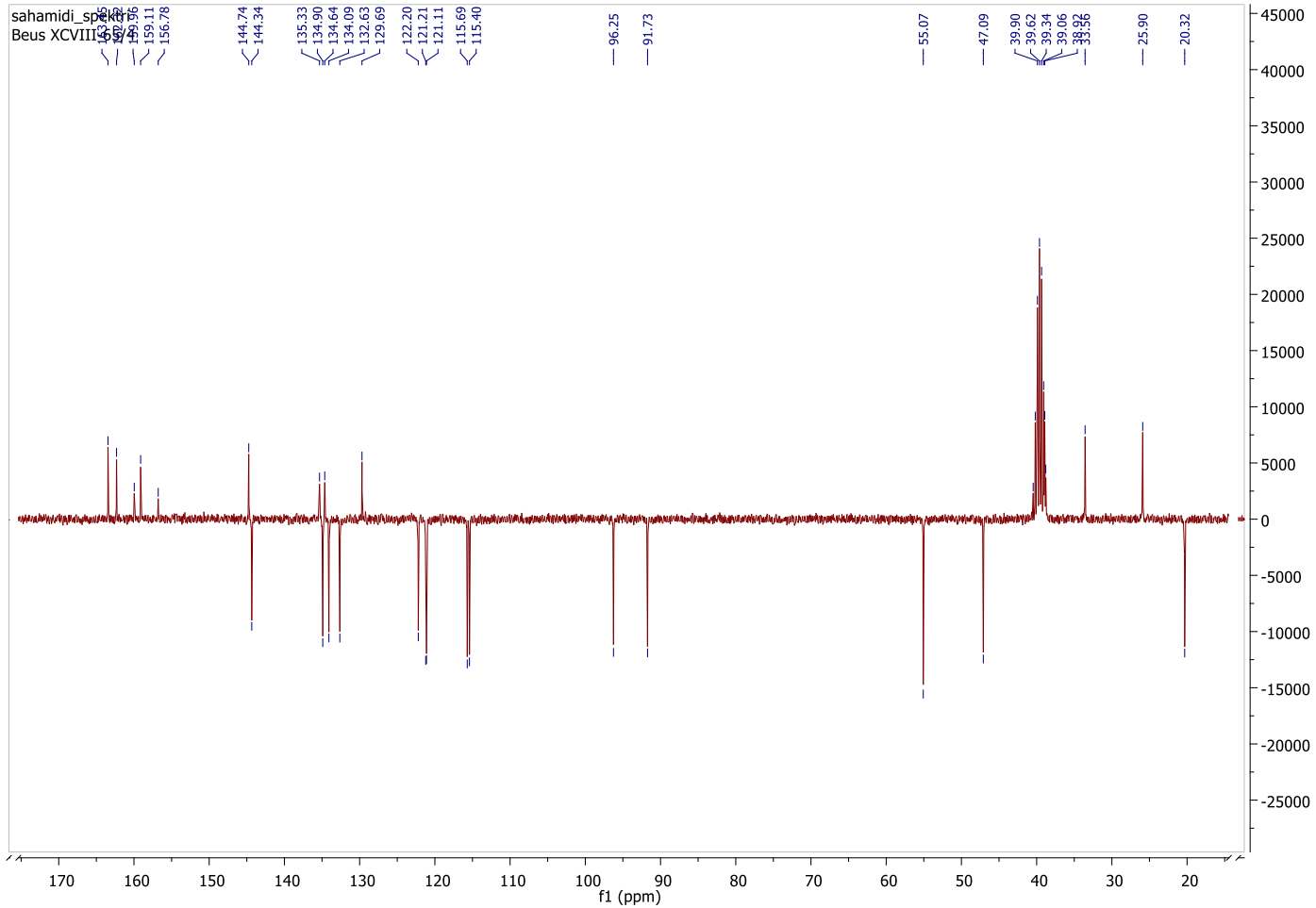
4b

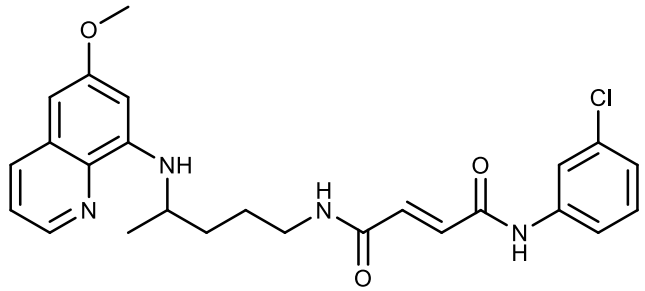

%T
cm-1
97.4
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20.6
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
3284
3076
3121
3020
2960
2935
2888
2867
1739
1816
1703
1631
1621
1615
1586
1569
1576
1547
1533
1482
1455
1432
1422
1415
1407
1399
1386
1353
1334
1300
1294
1272
1204
1184
1156
1104
1096
1068
1052
1040
1030
1014
1008
1000
975
911
901
858
804
751
831
826
818
789
677

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
Peak (1) in "+/- TIC Scan"	135	0	ESI

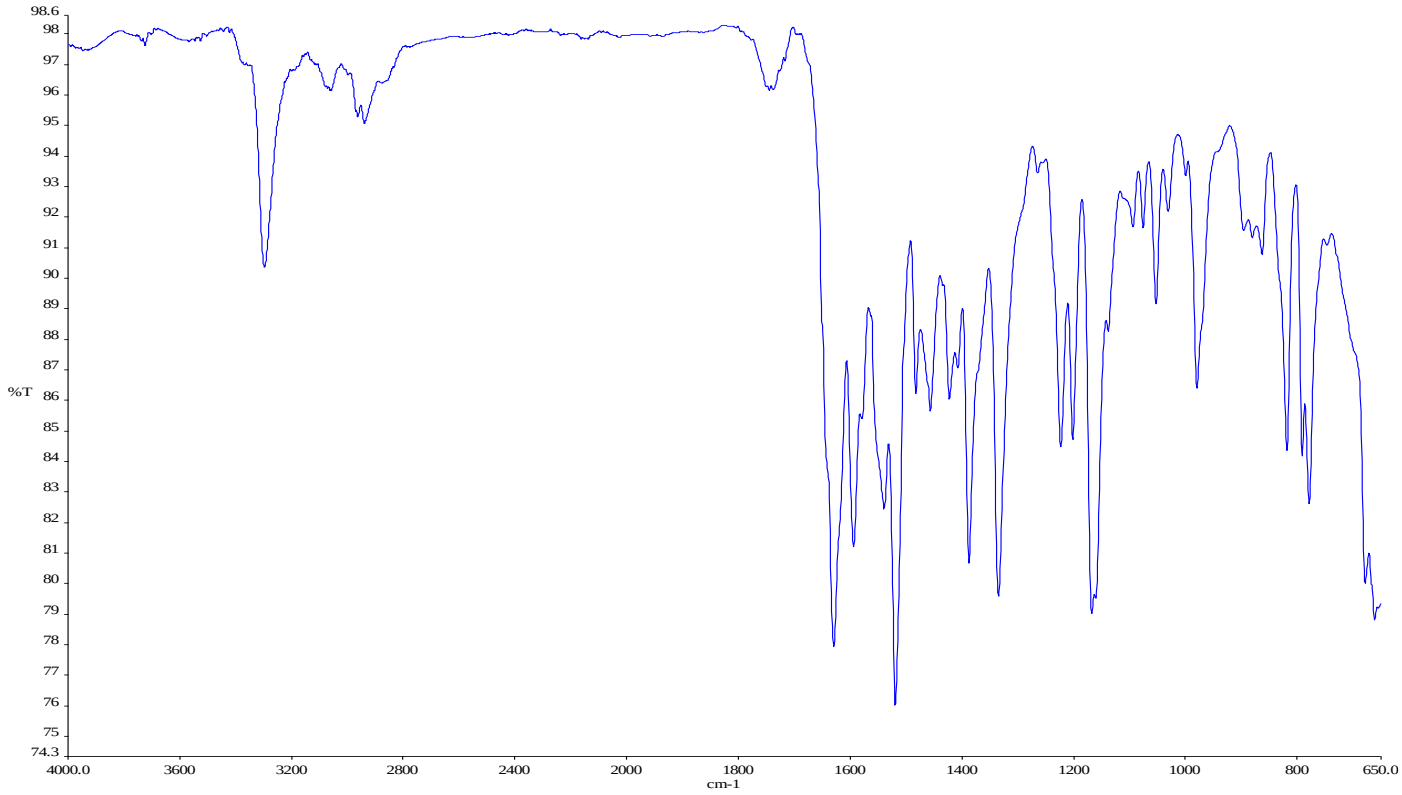


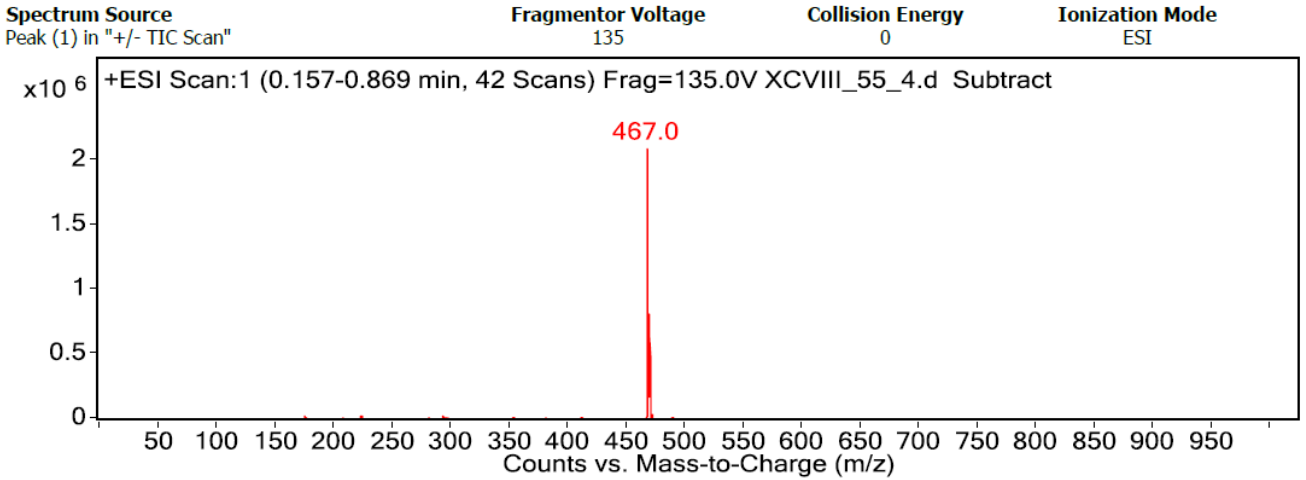



sahamidi_spekki
Beus XCVIII-65/1
163.45
162.28
159.96
159.11
156.78
144.74
144.34
135.33
134.90
134.64
134.09
132.63
129.69
122.20
121.21
121.11
115.69
115.40
96.25
91.73
55.07
47.09
39.90
39.62
39.34
39.06
38.92
33.56
25.90
20.32
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
-10000
-15000
-20000
-25000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

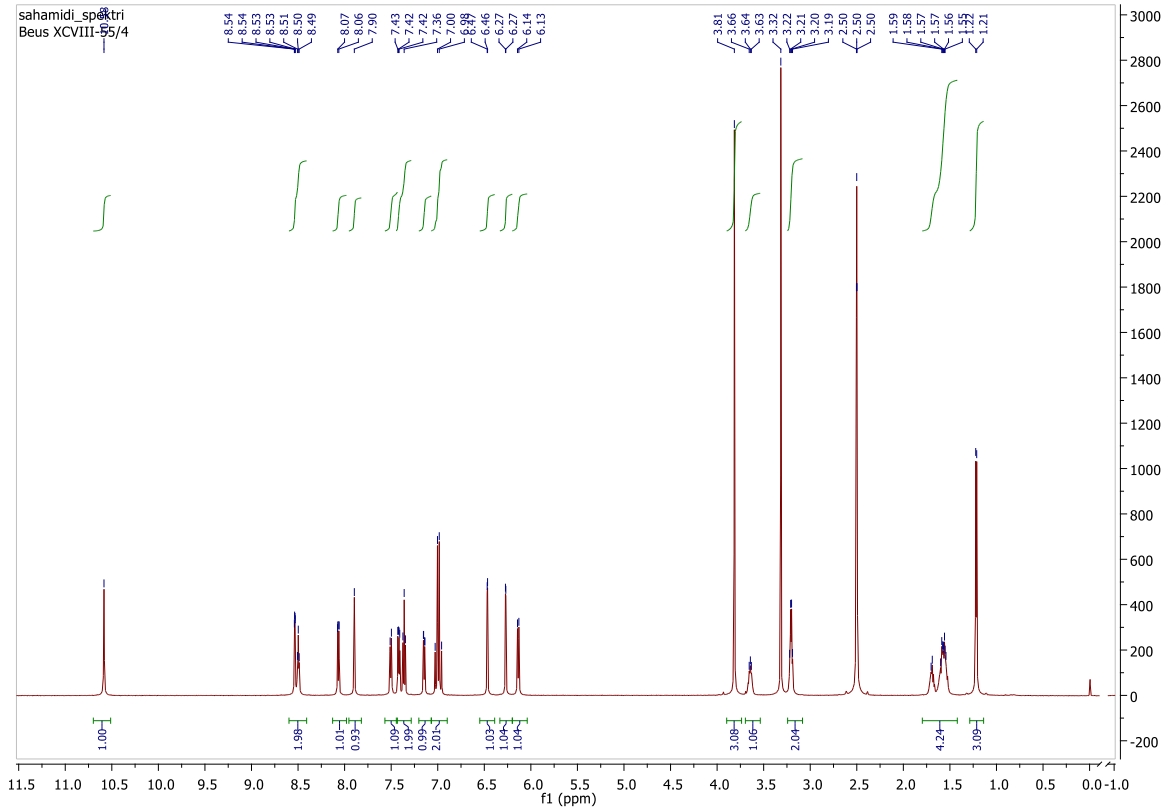

O
NH
N
H
N
O
O
N
H
Cl

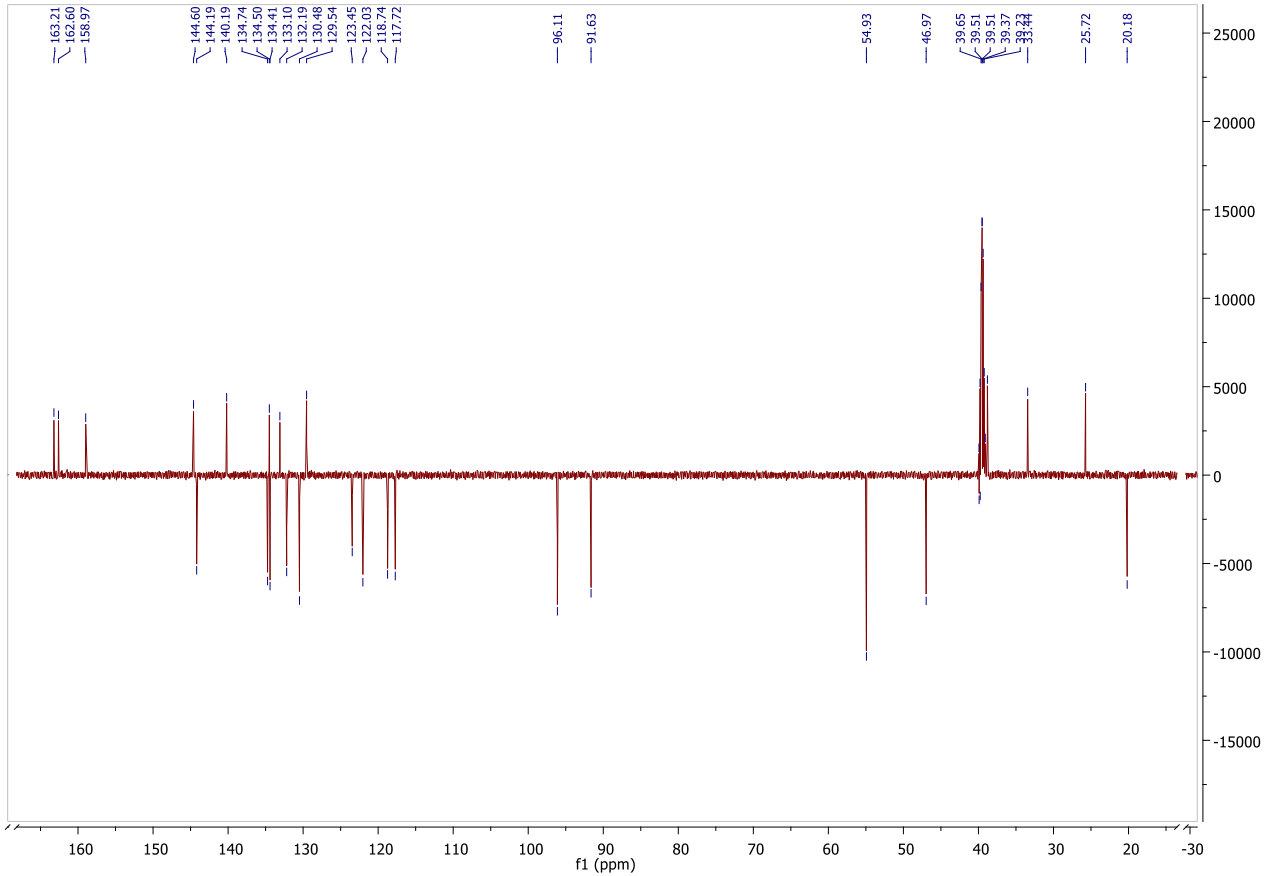
4c

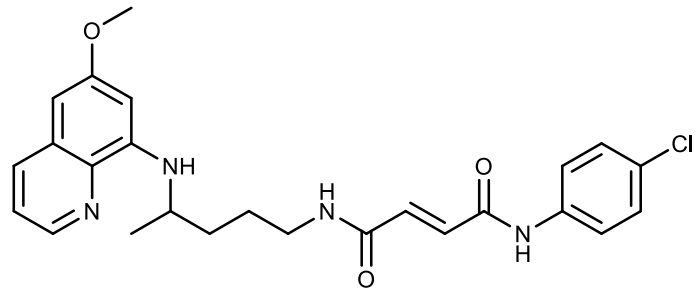

98.6
98
97
96
95
94
93
92
91
90
89
88
87
%T
86
85
84
83
82
81
80
79
78
77
76
75
74.3
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
cm-1


Spectrum Source
Peak (1) in "+/- TIC Scan"
Fragmentor Voltage
135
Collision Energy
0
Ionization Mode
ESI
+ESI Scan:1 (0.157-0.869 min, 42 Scans) Frag=135.0V XCVIII_55_4.d Subtract
x10 6
467.0
Counts vs. Mass-to-Charge (m/z)

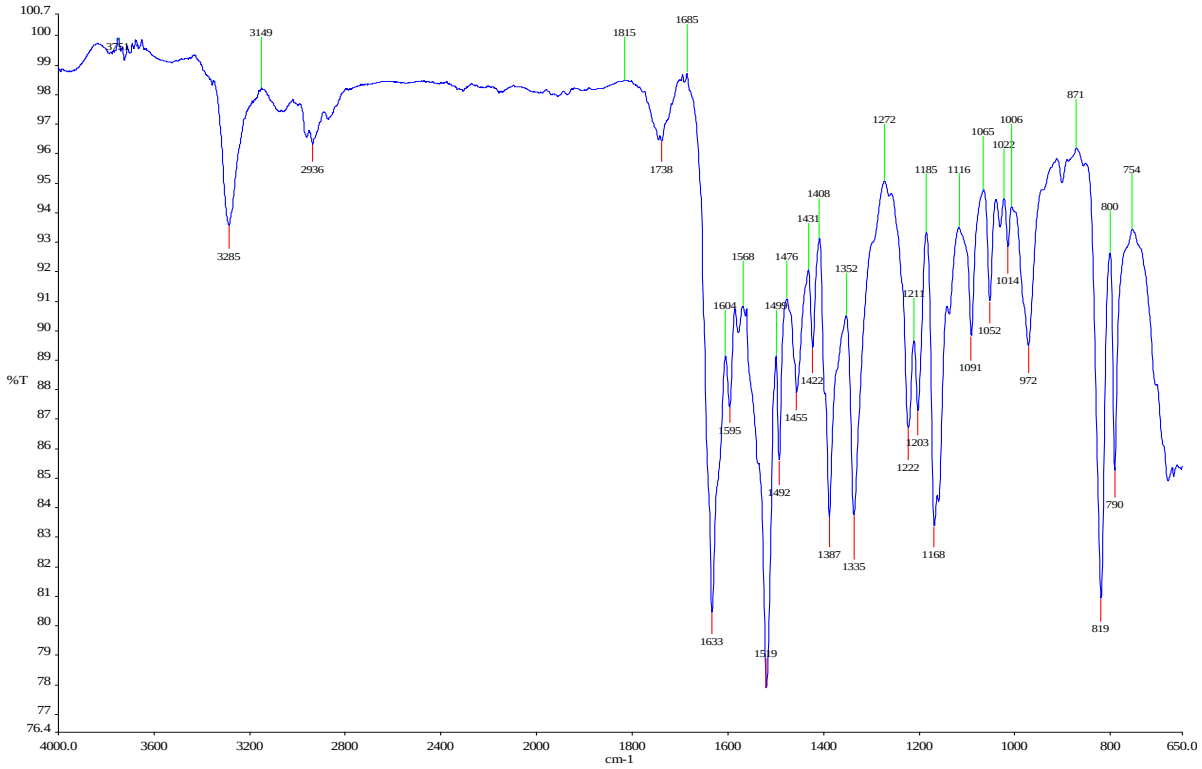
S


sahamidi_spektri
Beus XCVIII-55/4
f1 (ppm)

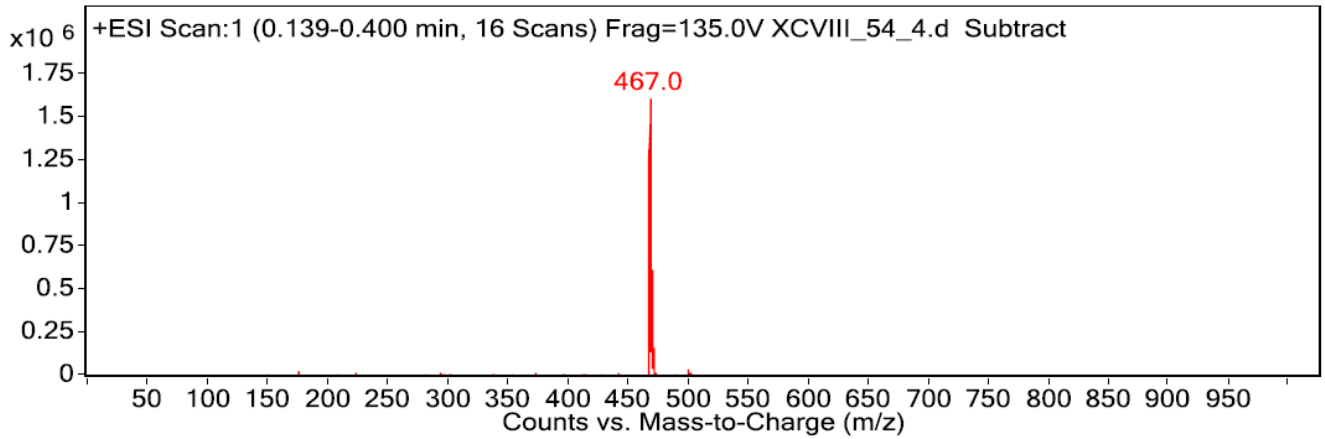

163.21
162.60
158.97
144.60
144.19
140.19
134.74
134.50
134.41
133.10
132.19
130.48
129.54
123.45
122.03
118.74
117.72
96.11
91.63
54.93
46.97
39.65
39.51
39.51
39.37
33.44
25.72
20.18
25000
20000
15000
10000
5000
0
-5000
-10000
-15000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
-30
f1 (ppm)

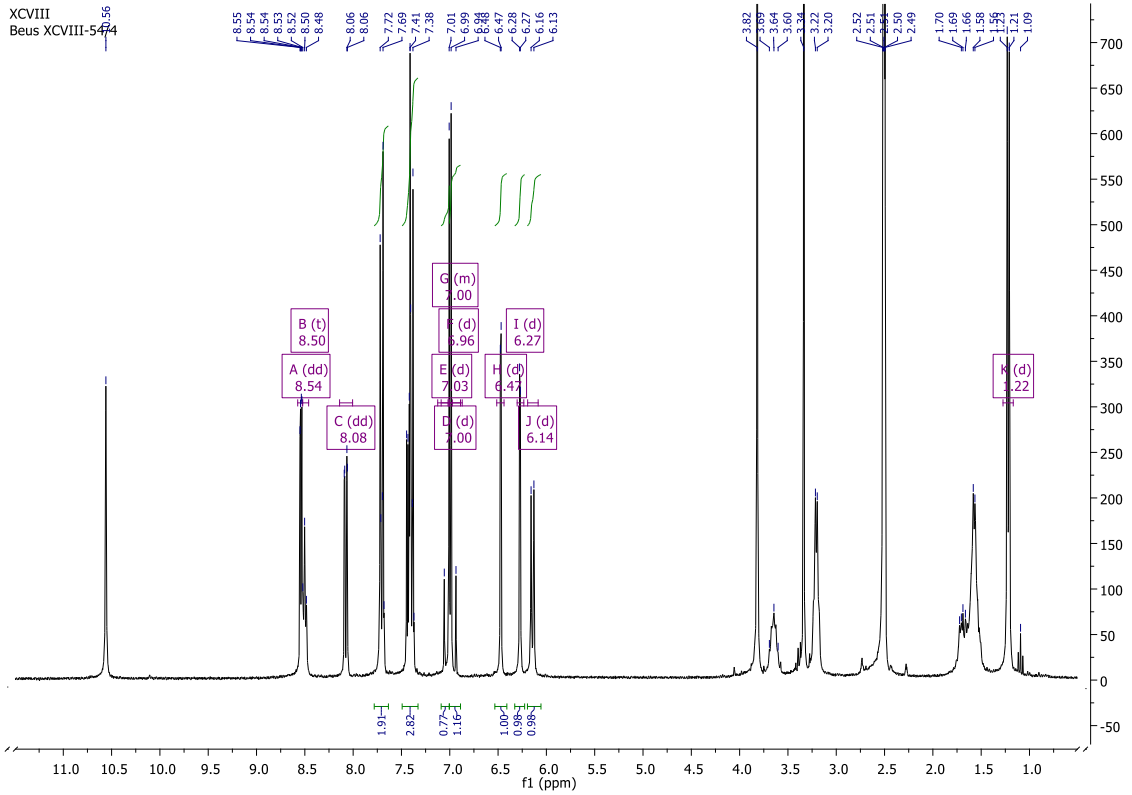

O
NH
N
H
N
O
O
N
H
Cl

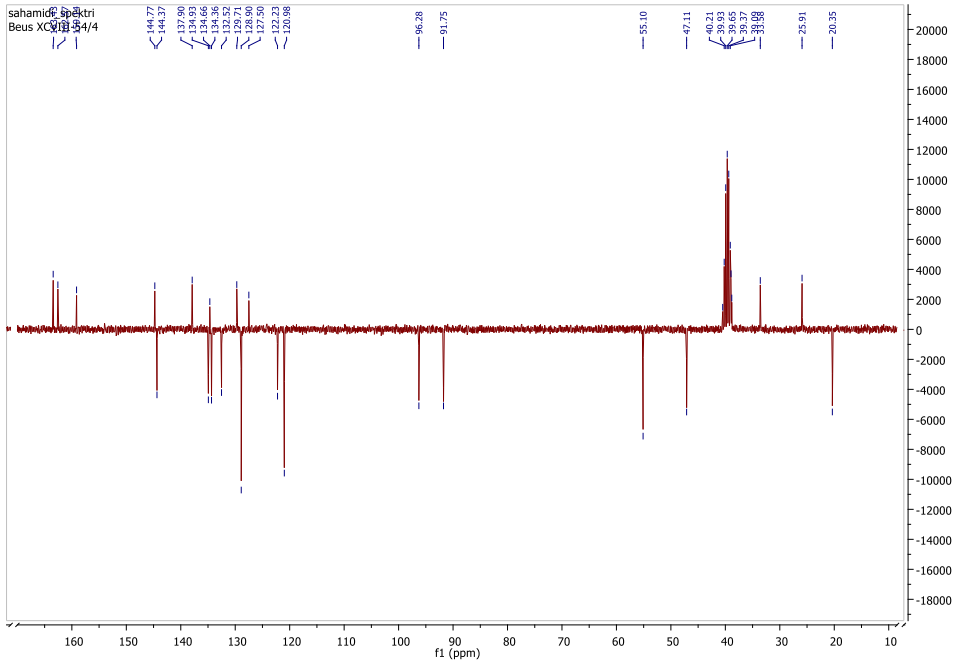
4d

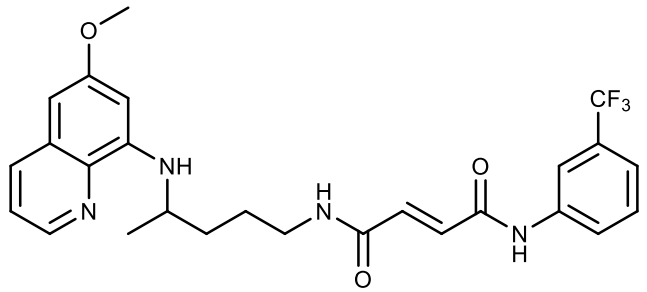

%T
cm-1
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
3149
3285
2936
1815
1738
1685
1633
1604
1595
1568
1519
1499
1492
1476
1455
1431
1422
1408
1387
1352
1335
1272
1222
1211
1203
1185
1168
1116
1091
1065
1052
1022
1014
1006
972
871
819
800
790
754

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
Peak (1) in "+/- TIC Scan"	135	0	ESI



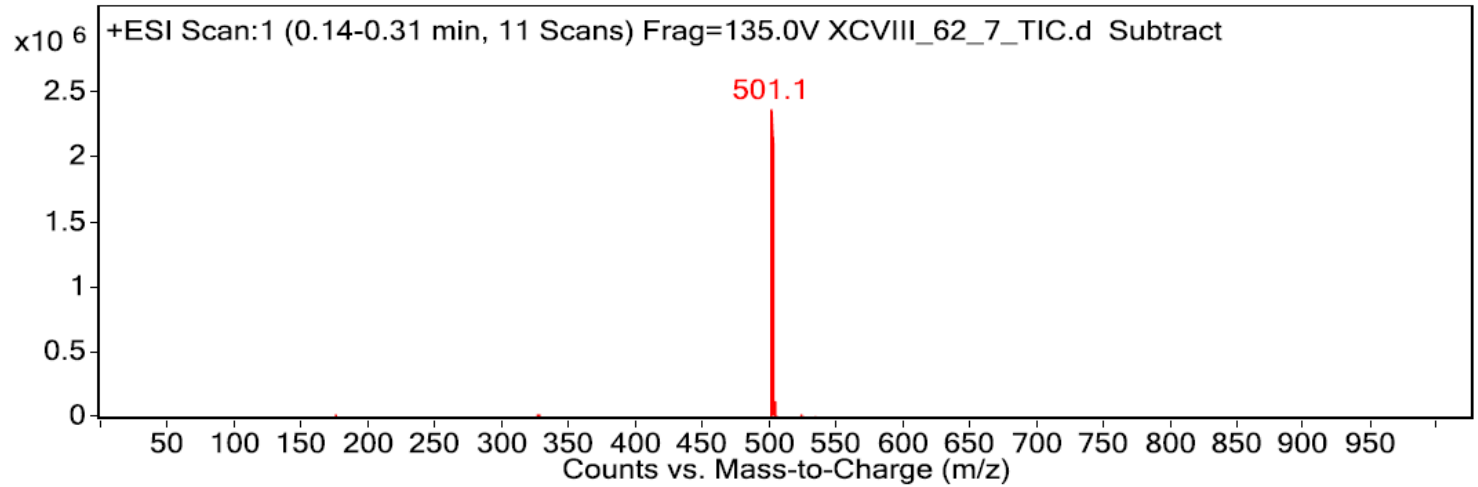


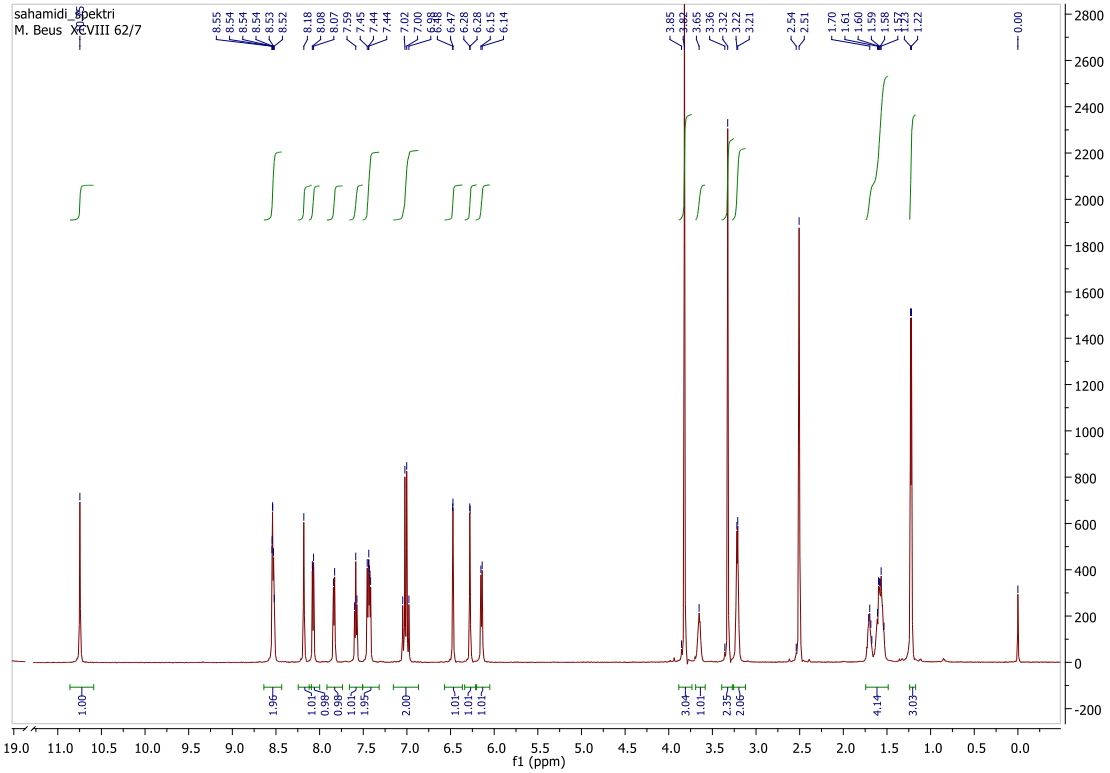

sahamidr spektri
Beus XC-54/4
144.77
144.37
137.90
134.93
134.66
134.36
130.52
129.71
128.90
127.50
122.23
120.98
96.28
91.75
55.10
47.11
40.21
39.93
39.65
39.37
39.09
33.58
25.91
20.35
f1 (ppm)

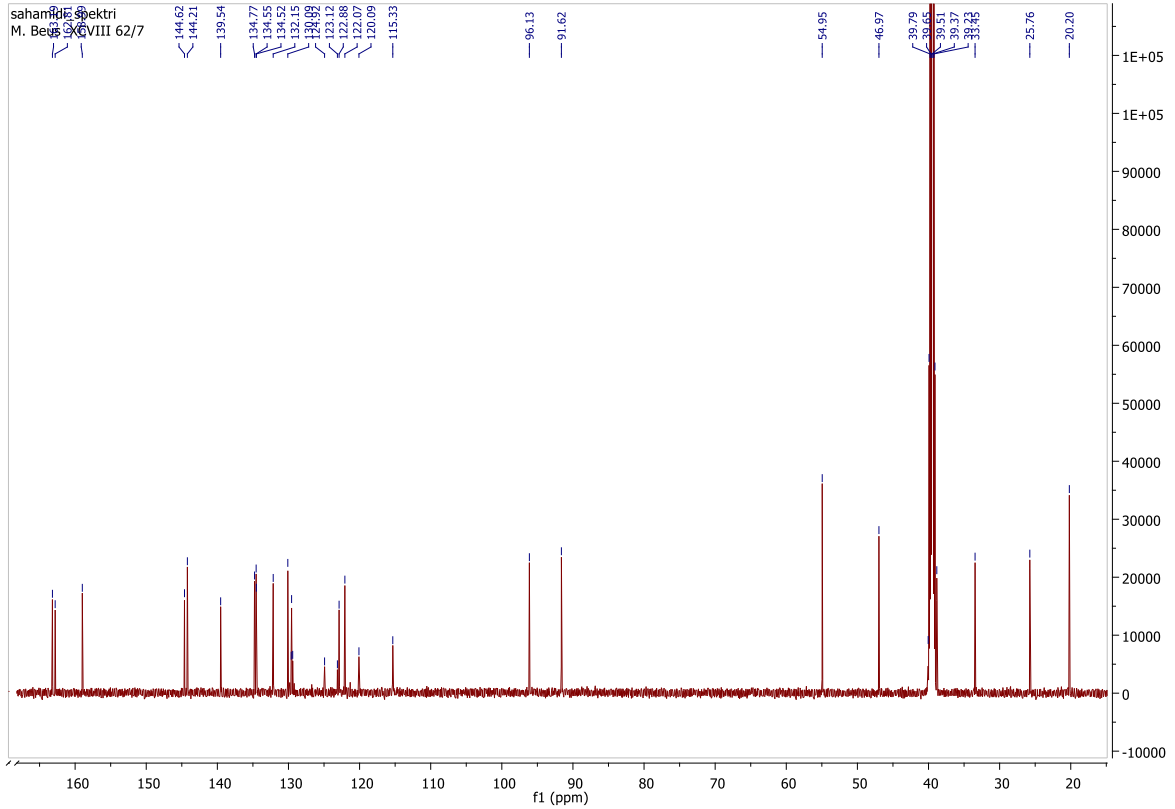


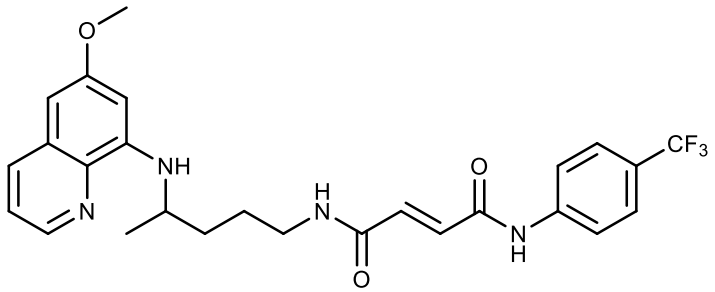
4e

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
Peak (1) in "+/- TIC Scan"	135	0	ESI

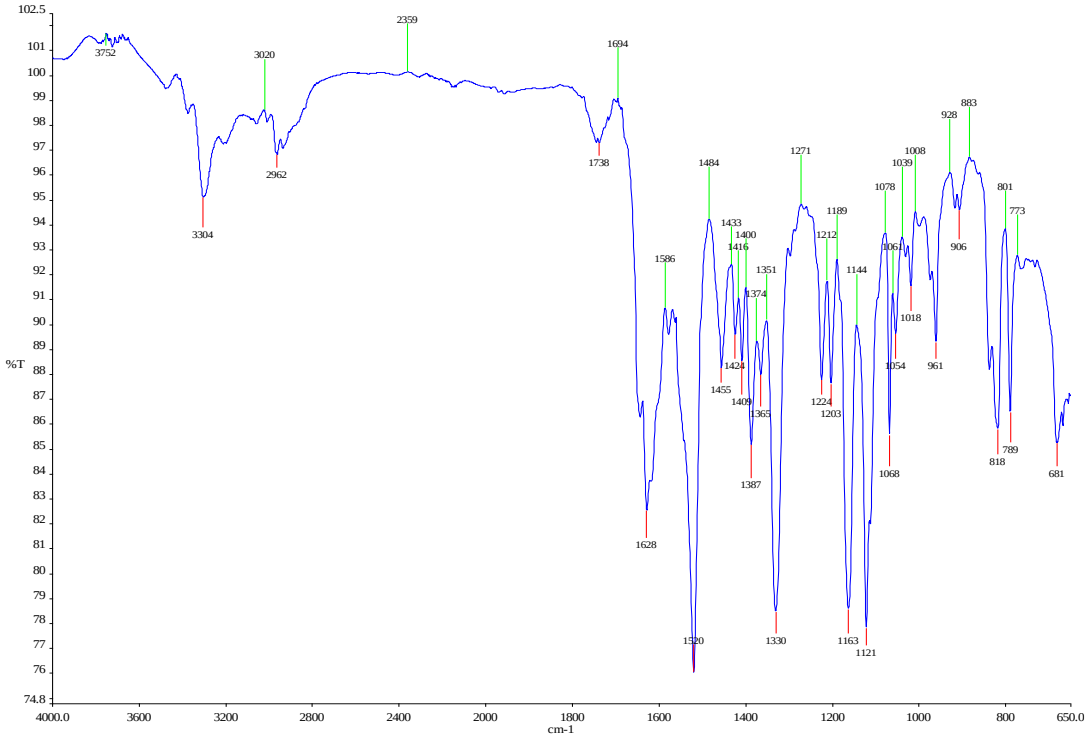


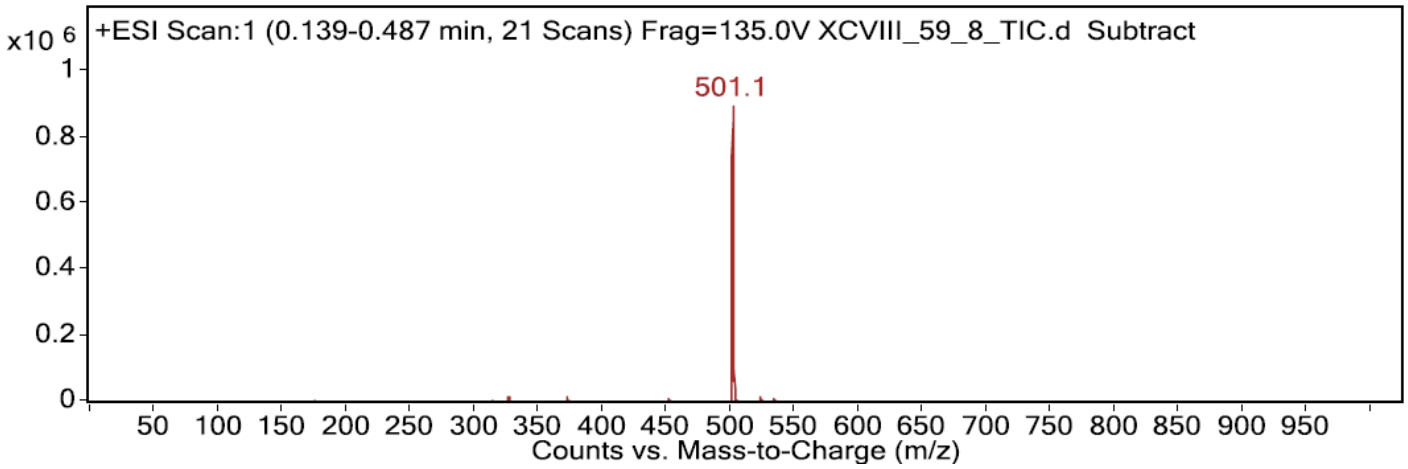

sahamidi_spektri
M. Beus XCVIII 62/7
8.55
8.54
8.54
8.54
8.53
8.52
8.18
8.08
8.07
7.59
7.45
7.44
7.44
7.02
7.00
6.98
6.48
6.47
6.28
6.28
6.15
6.14
3.85
3.82
3.65
3.36
3.32
3.22
3.21
2.54
2.51
1.70
1.61
1.60
1.59
1.58
1.57
1.52
1.22
0.00
1.00
1.96
1.01
0.98
0.99
1.01
1.95
2.00
1.01
1.01
1.01
3.04
1.01
2.35
2.06
4.14
3.03
f1 (ppm)

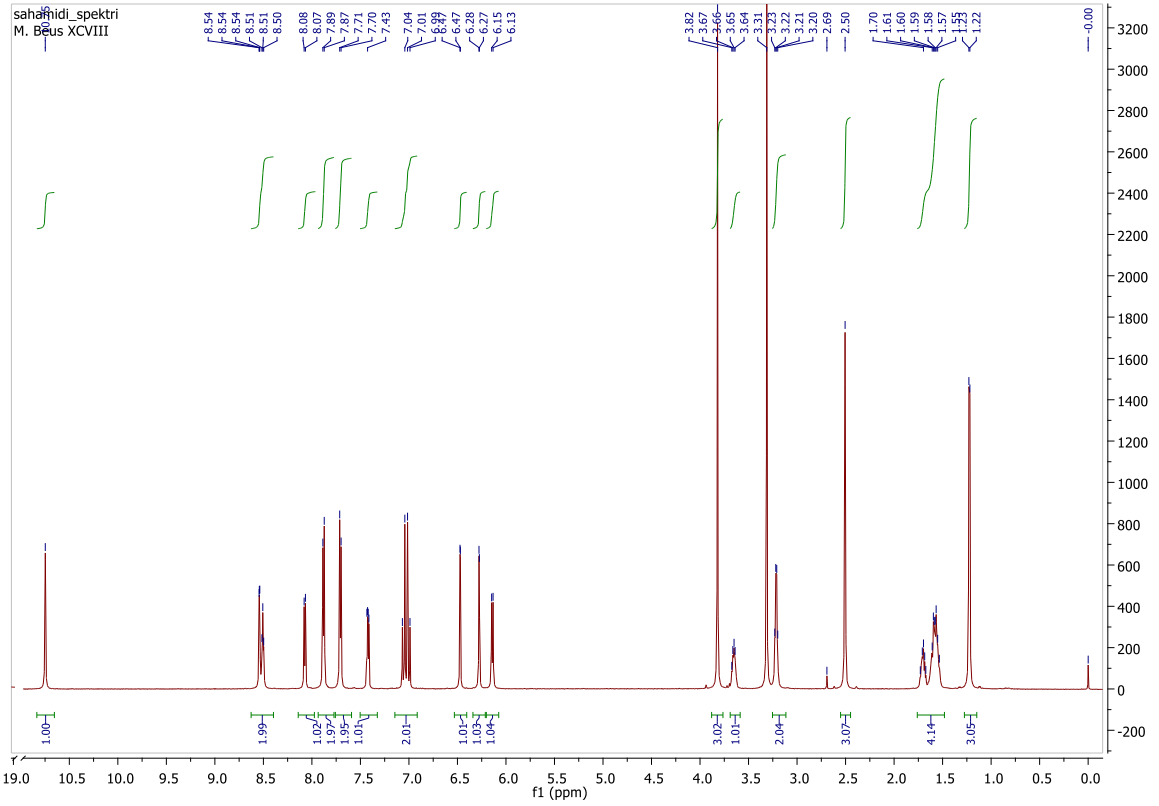

sahamidin spektri
M. Beus SCVIII 62/7
144.62
144.21
139.54
134.77
134.55
134.52
132.15
123.12
122.88
122.07
120.09
115.33
96.13
91.62
54.95
46.97
39.79
39.65
39.51
39.37
39.23
33.43
25.76
20.20
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

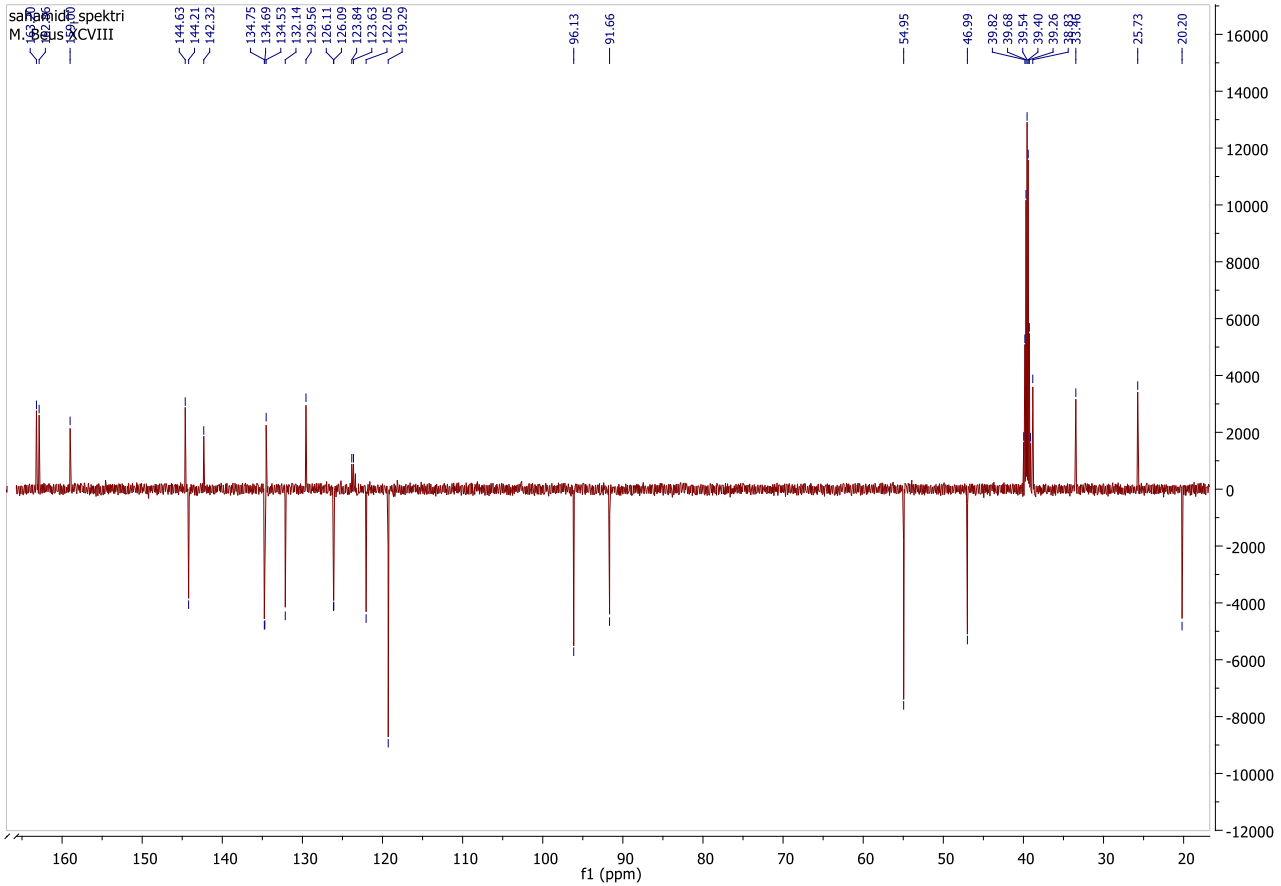

O
NH
N
H
N
O
O
N
H
CF3

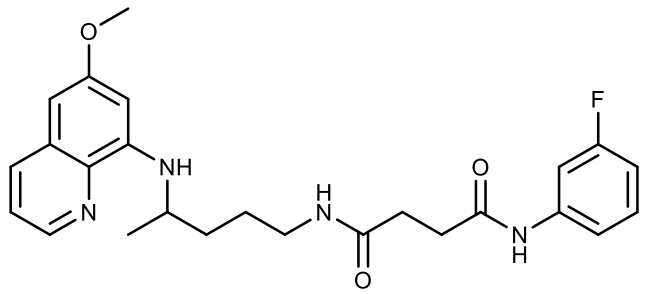
4f


%T
cm-1
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
102.5
101
100
99
98
97
96
95
94
93
92
91
90
89
88
87
86
85
84
83
82
81
80
79
78
77
76
74.8
3752
3304
3020
2962
2359
1738
1694
1628
1586
1520
1484
1455
1433
1424
1416
1409
1400
1387
1374
1365
1351
1330
1271
1224
1212
1203
1189
1163
1144
1121
1078
1068
1064
1054
1039
1018
1008
961
928
906
883
818
801
789
773
681

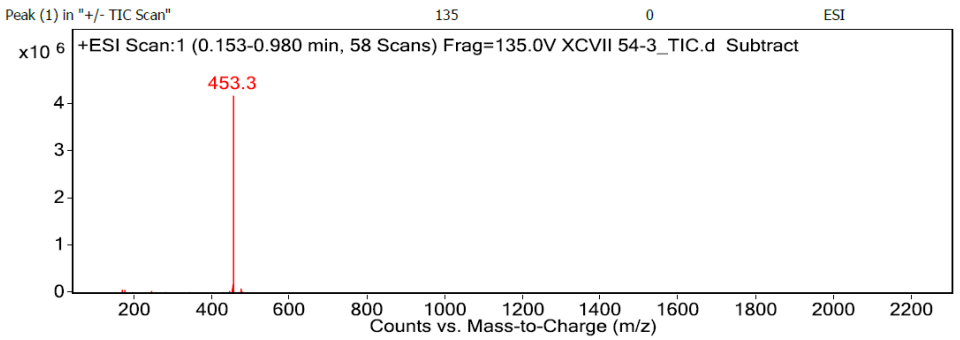

+ESI Scan:1 (0.139-0.487 min, 21 Scans) Frag=135.0V XCVIII_59_8_TIC.d Subtract
x10 6
501.1
Counts vs. Mass-to-Charge (m/z)

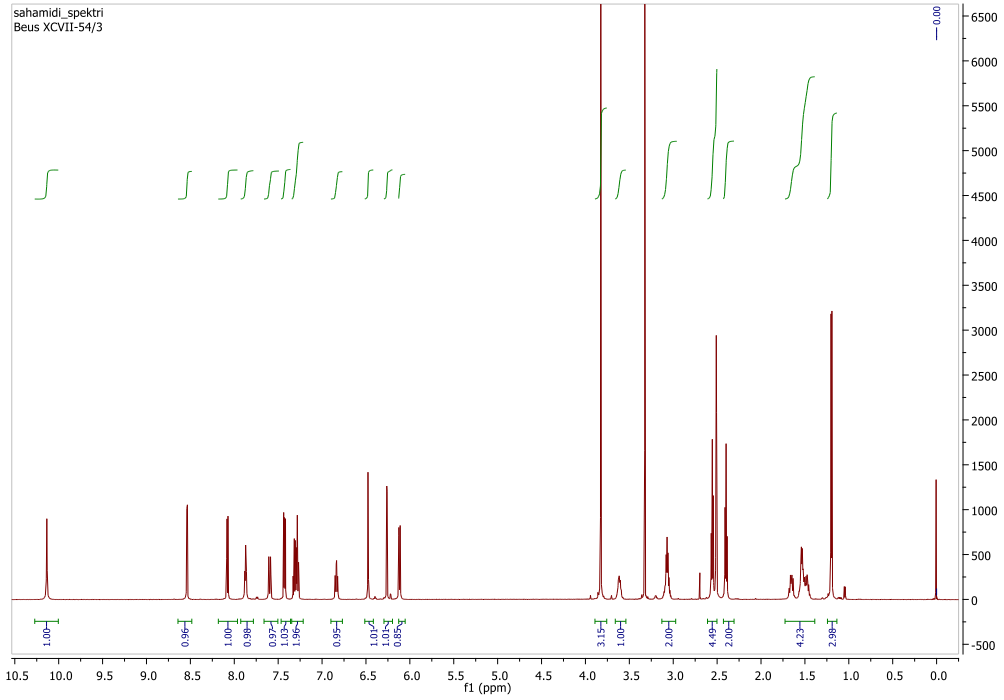

sahamidi_spektri
M. Beus XCVIII
f1 (ppm)

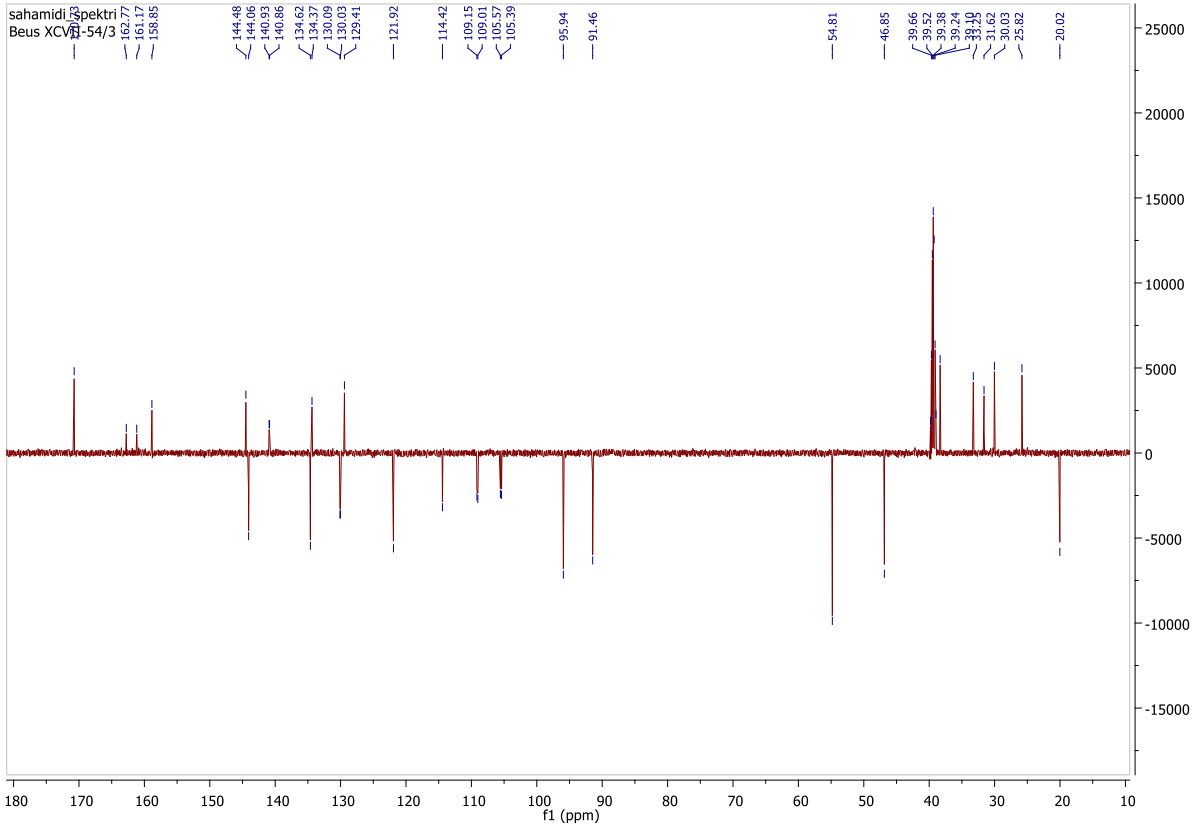

sahamidin spektri
M.faus XCVIII
144.63
144.21
142.32
134.75
134.69
134.53
132.14
129.56
126.11
126.09
123.84
123.63
122.05
119.29
96.13
91.66
54.95
46.99
39.82
39.68
39.54
39.40
39.26
25.73
20.20
f1 (ppm)

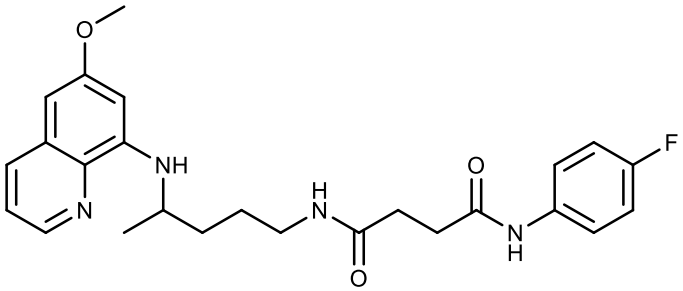


5a

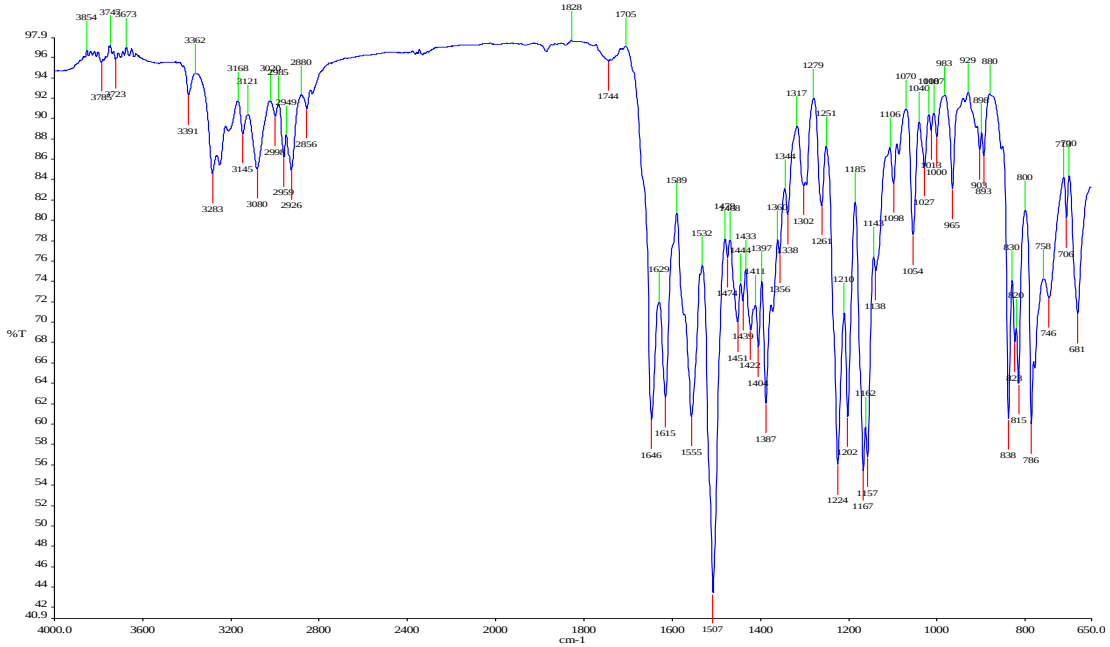

Peak (1) in "+/- TIC Scan"
135
0
ESI
+ESI Scan:1 (0.153-0.980 min, 58 Scans) Frag=135.0V XCVII 54-3_TIC.d Subtract
x10 6
453.3
Counts vs. Mass-to-Charge (m/z)

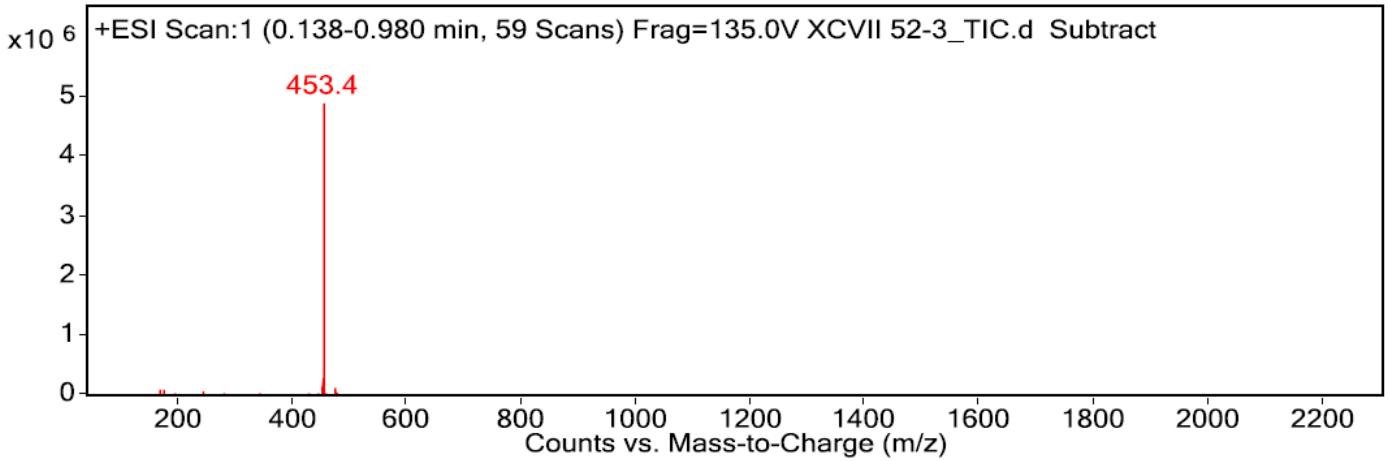

sahamidi_spektri
Beus XCVII-54/3
f1 (ppm)

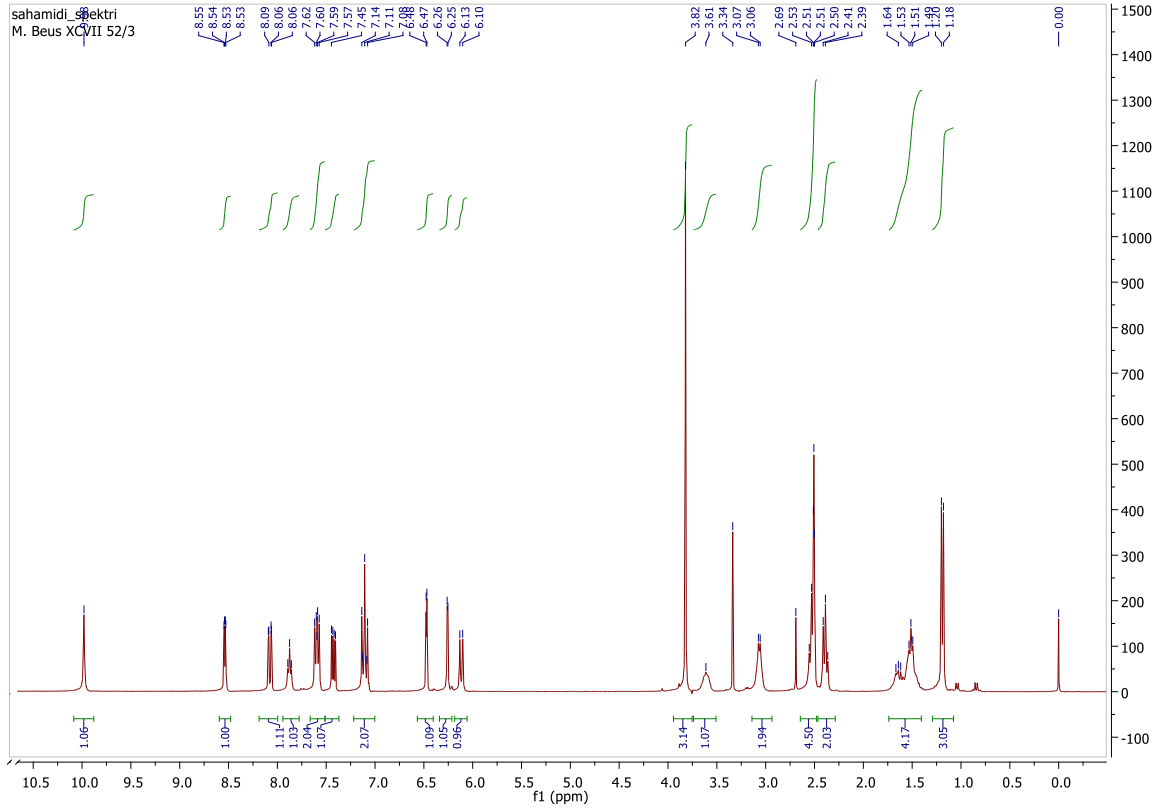

sahamidi spektri
Beus XCVII-54/3
169.63
162.77
161.17
158.85
144.48
144.06
140.93
140.86
134.62
134.37
130.09
130.03
129.41
121.92
114.42
109.15
109.01
105.57
105.39
95.94
91.46
54.81
46.85
39.66
39.52
39.38
39.24
39.10
33.25
31.62
30.03
25.82
20.02
25000
20000
15000
10000
5000
0
-5000
-10000
-15000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

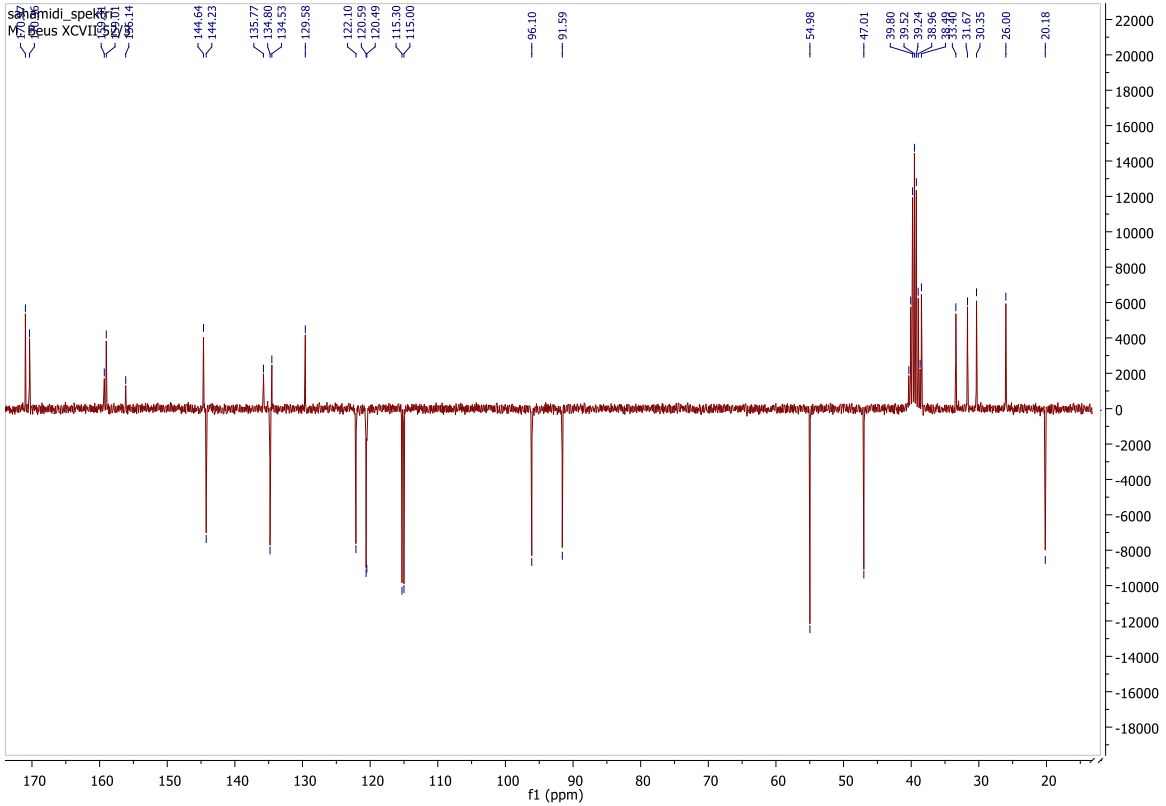

O
NH
N
H
N
O
O
N
H
F

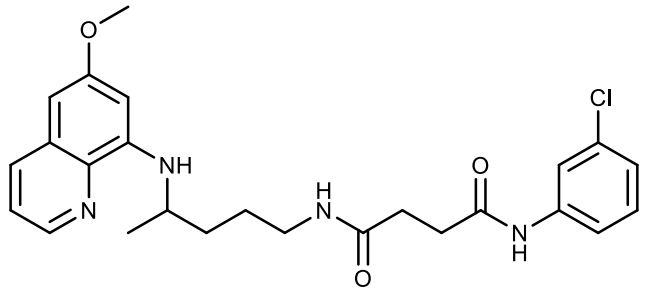
5b


%T
cm-1
4000.0
3600
3200
2800
2400
2000
1800
1600
1507
1400
1200
1000
800
650.0
97.9
40.9
3854
3745
3673
3765
3723
3362
3391
3283
3168
3121
3145
3080
3029
2985
2998
2949
2959
2926
2880
2856
1828
1705
1744
1589
1629
1646
1615
1555
1532
1474
1488
1478
1433
1444
1439
1411
1397
1451
1422
1404
1387
1369
1344
1338
1356
1317
1279
1302
1261
1251
1210
1202
1224
1185
1162
1143
1138
1157
1167
1106
1098
1070
1054
1040
1027
1013
1000
983
965
929
903
893
890
880
800
830
820
815
838
786
758
746
706
700
681

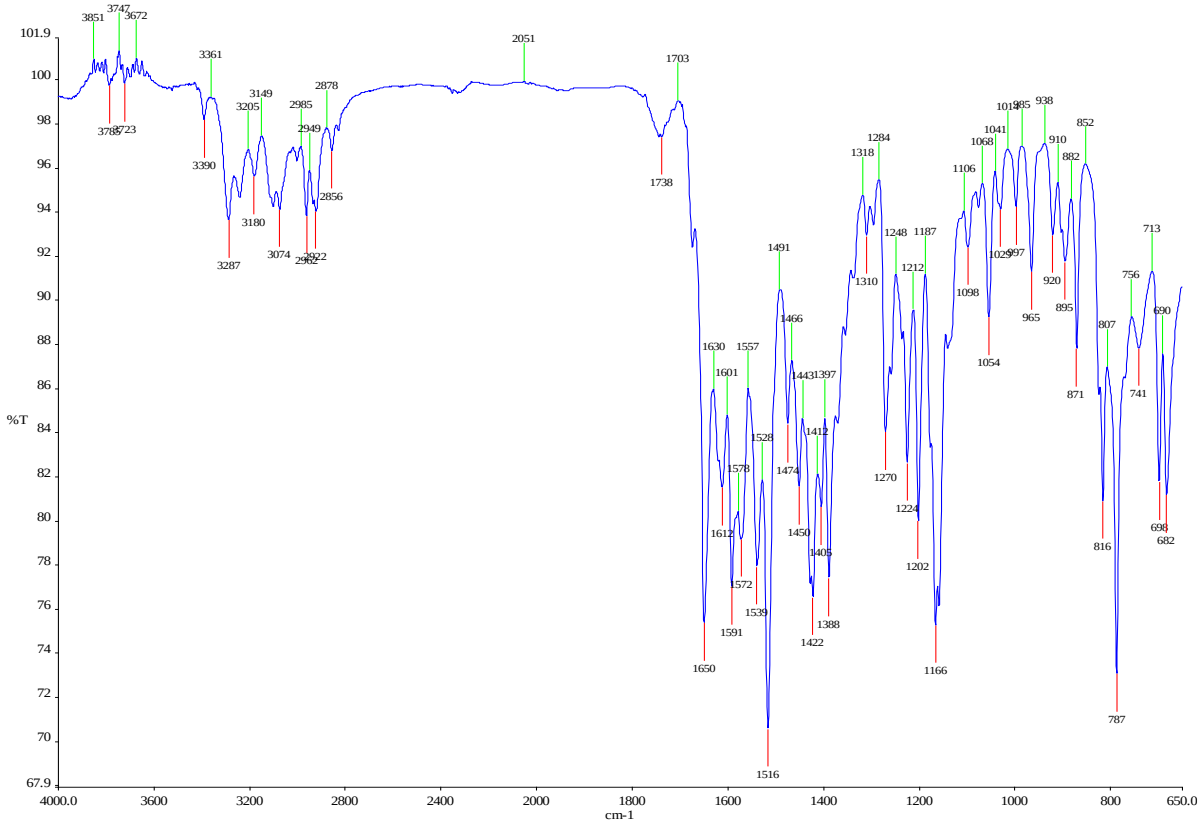

x10 6
+ESI Scan:1 (0.138-0.980 min, 59 Scans) Frag=135.0V XCVII 52-3_TIC.d Subtract
453.4
Counts vs. Mass-to-Charge (m/z)


sahamidi_spektri
M. Beus XCVII 52/3
f1 (ppm)

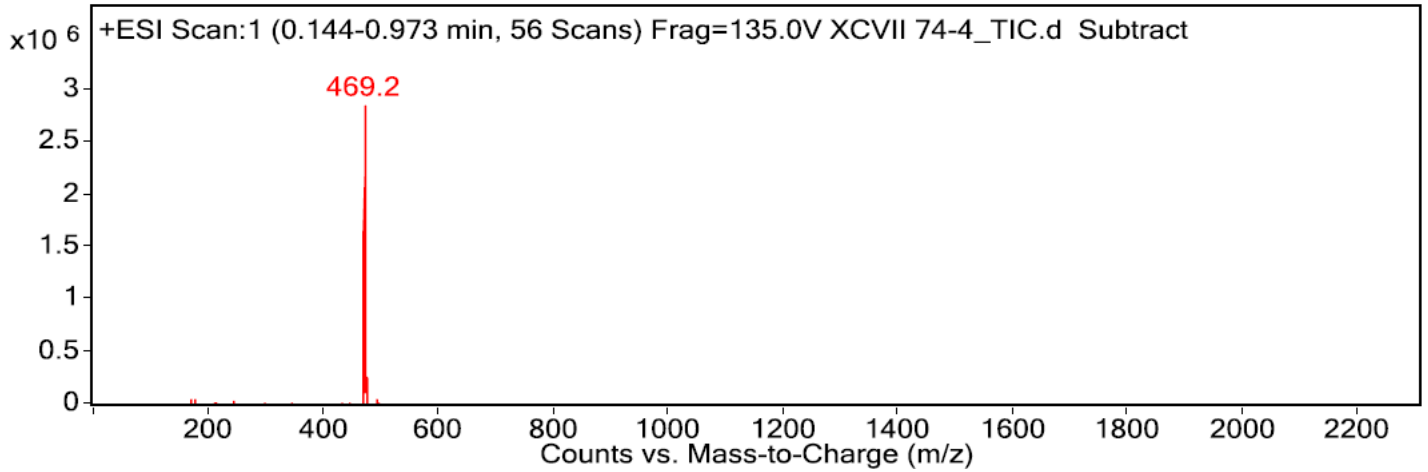

sanamidi_spektri
Mr Bleus XCVII-52-2-s
170.06
169.71
156.14
144.64
144.23
135.77
134.80
134.53
129.58
122.10
120.59
120.49
115.30
115.00
96.10
91.59
54.98
47.01
39.80
39.52
39.24
38.96
31.67
30.35
26.00
20.18
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
-4000
-6000
-8000
-10000
-12000
-14000
-16000
-18000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

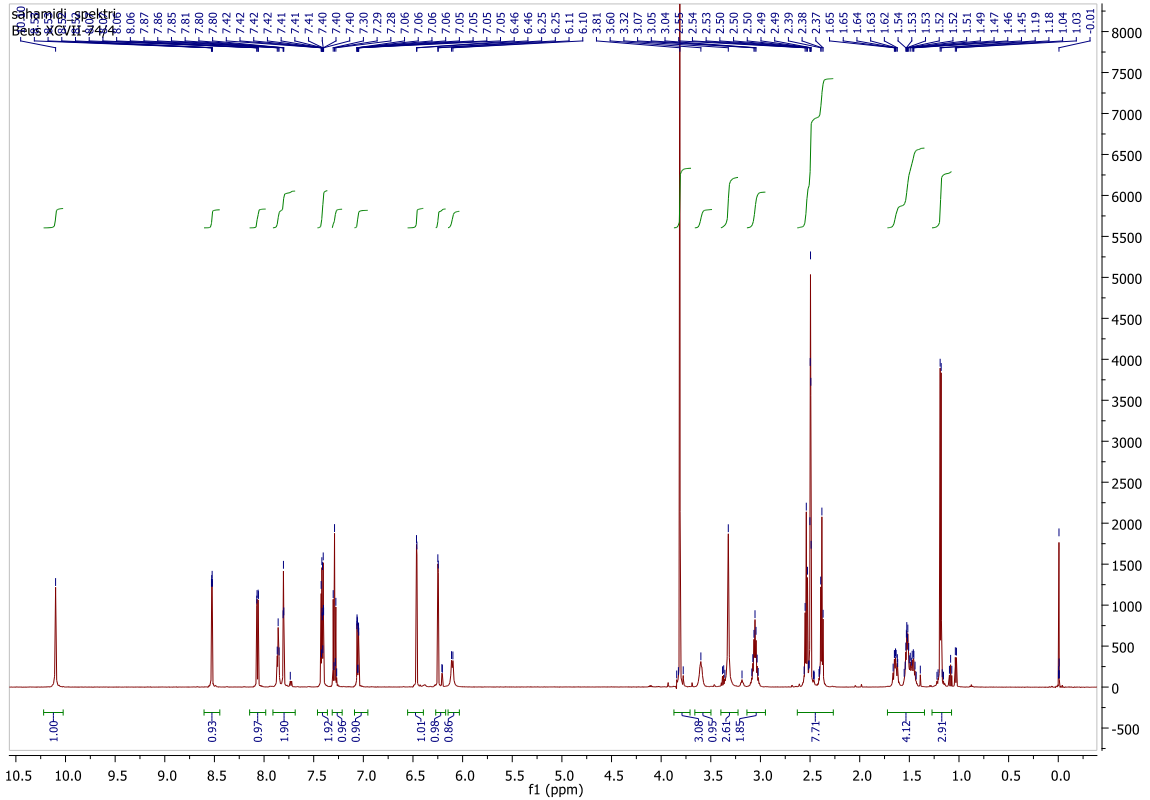

O
NH
N
H
N
O
O
N
H
Cl

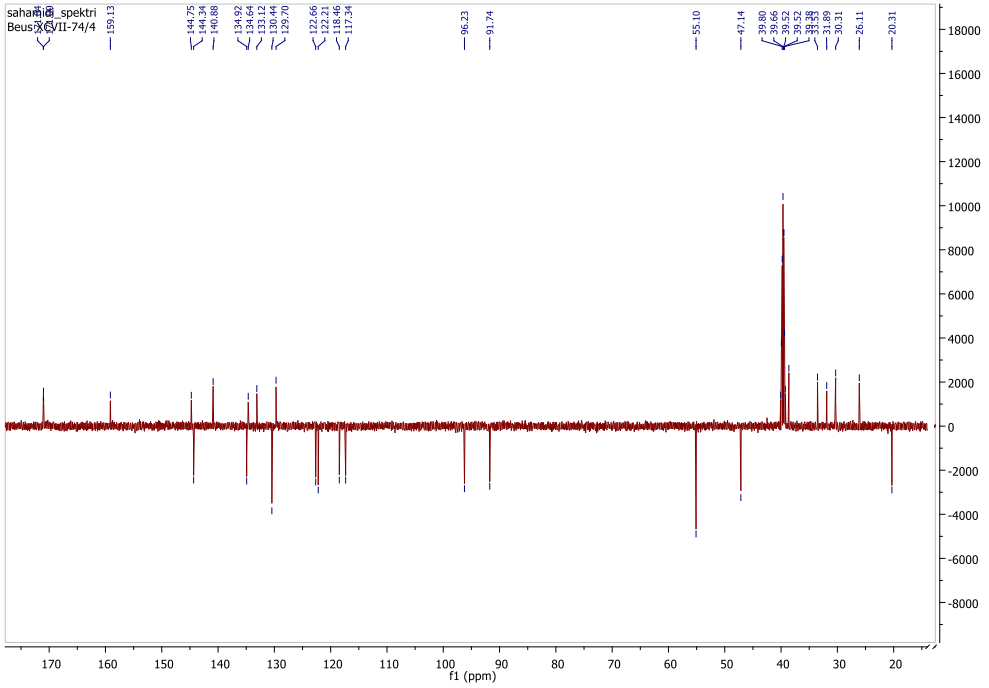
5c

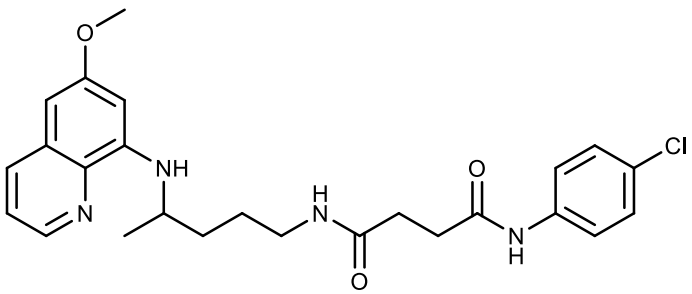

%T
cm-1
101.9
100
98
96
94
92
90
88
86
84
82
80
78
76
74
72
70
67.9
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
3851
3747
3672
3788
3723
3361
3390
3287
3205
3149
3180
3074
2985
2949
2878
2962
2922
2856
2051
1738
1703
1650
1630
1601
1591
1578
1572
1557
1539
1528
1516
1491
1474
1466
1450
1443
1422
1412
1405
1397
1388
1318
1310
1284
1270
1248
1224
1212
1202
1187
1166
1106
1098
1068
1054
1041
1029
1019
997
985
965
938
920
910
895
882
871
852
816
807
787
756
741
713
698
690
682

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
Peak (1) in "+/- TIC Scan"	135	0	ESI

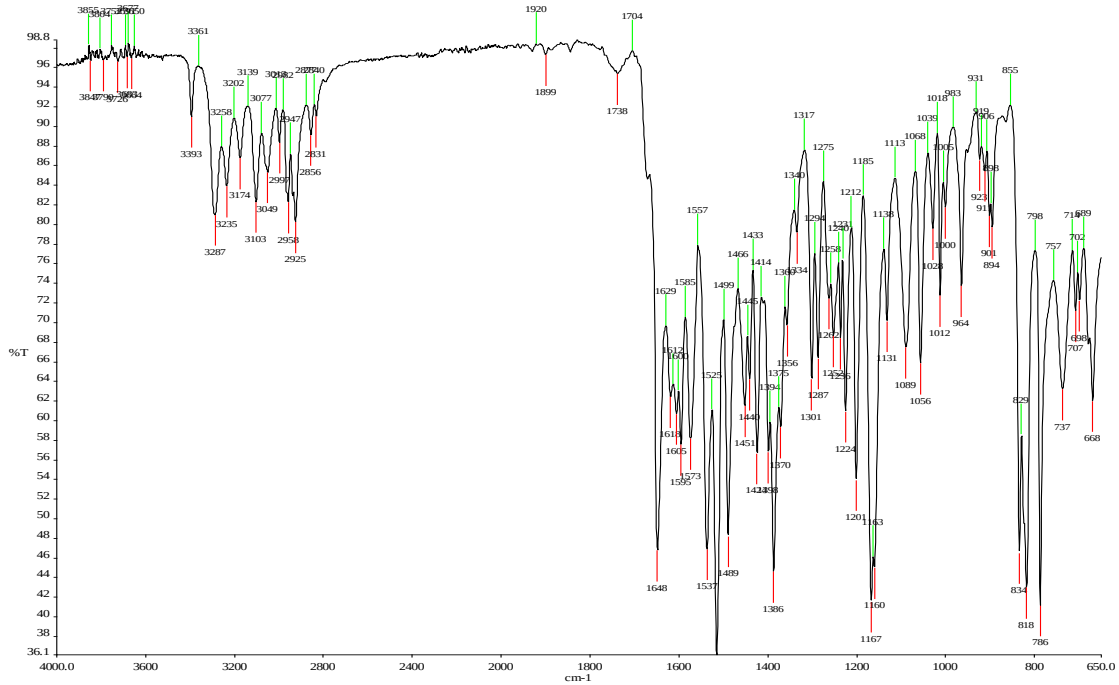


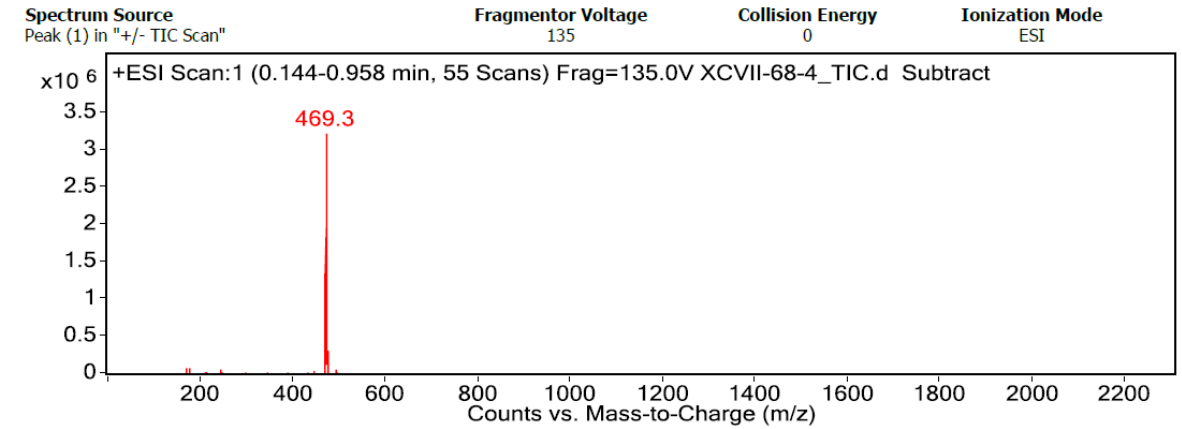


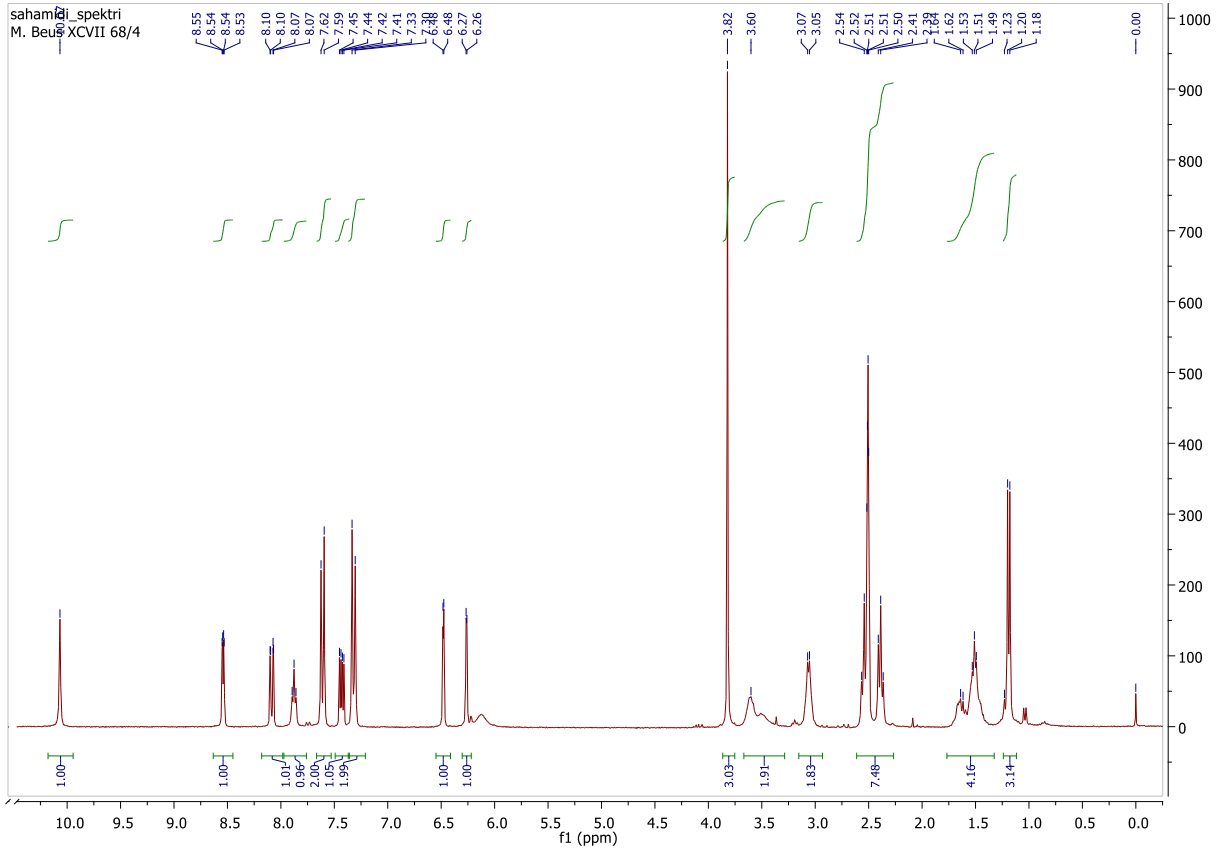

sahamidi_spektri
Beus XCVII-74/4
159.13
144.75
144.34
140.88
134.92
134.64
133.12
130.44
129.70
122.66
122.21
119.46
117.34
96.23
91.74
55.10
47.14
39.80
39.66
39.52
39.52
33.38
31.89
30.31
26.11
20.31
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
-4000
-6000
-8000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

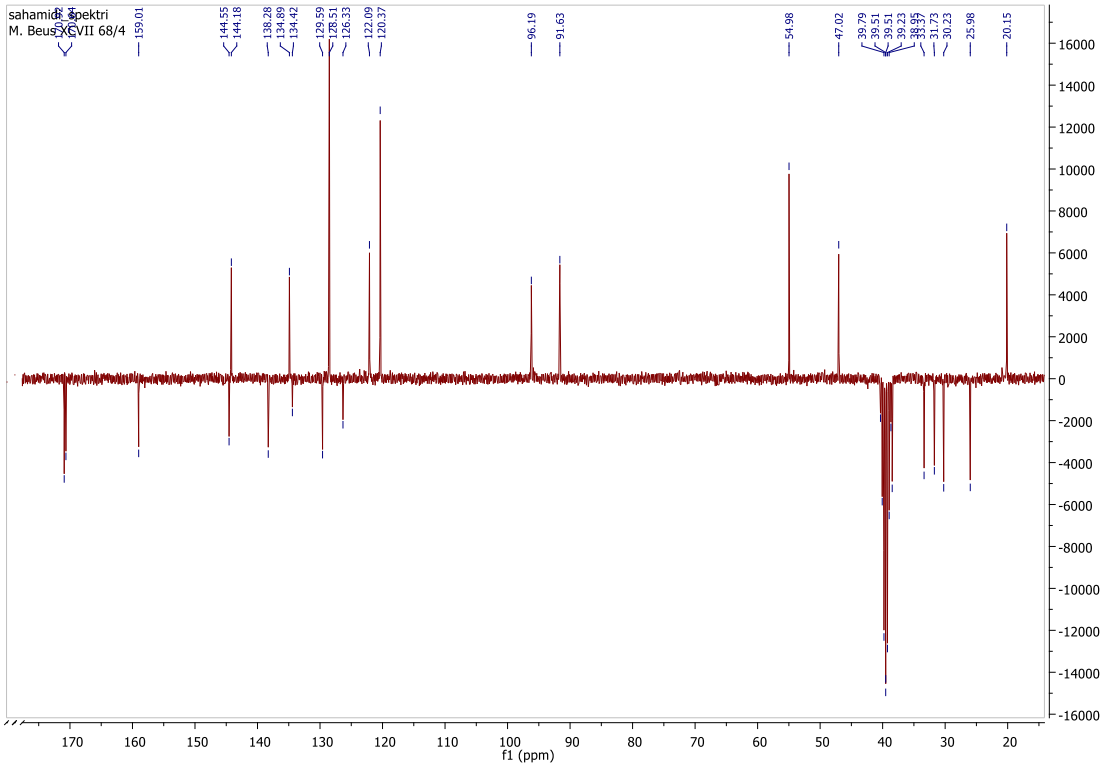

O
NH
N
H
N
O
O
N
H
Cl

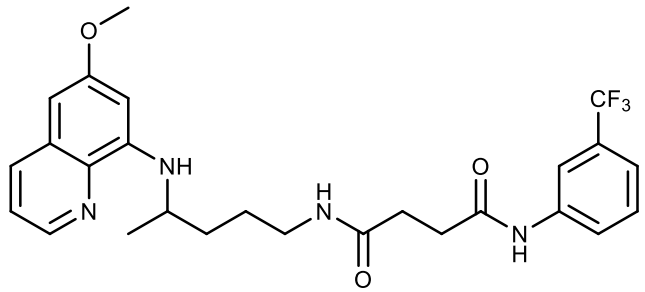
5d


%T
cm-1
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
98.8
36.1
3361
3393
3258
3202
3139
3077
3235
3287
3174
3103
3049
2958
2925
2856
2831
1920
1899
1738
1704
1648
1629
1585
1557
1537
1499
1489
1466
1451
1433
1414
1386
1370
1340
1317
1275
1212
1185
1160
1167
1138
1131
1113
1089
1068
1056
1039
1028
1018
1012
1000
983
964
931
923
911
901
894
855
834
818
798
786
757
737
714
702
689
668
707
698
829
525
1605
1595
1573
1612
1618
1356
1375
1394
1301
1287
1262
1224
1201
1163
1056

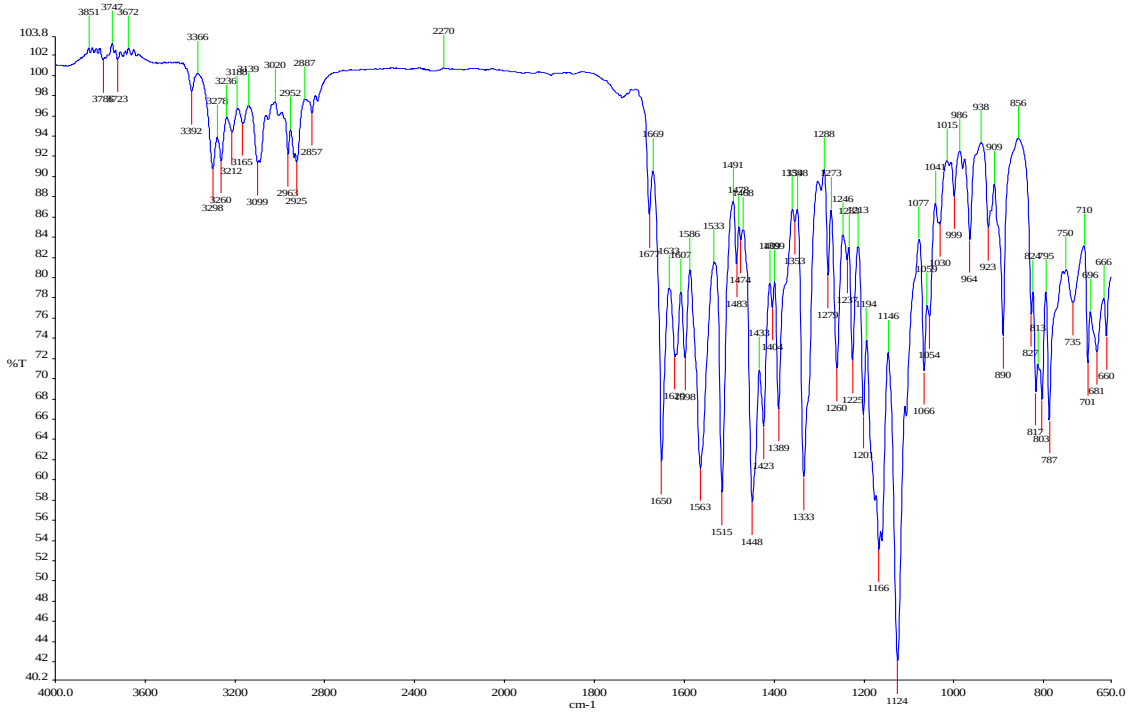

Spectrum Source
Peak (1) in "+/- TIC Scan"
Fragmentor Voltage
135
Collision Energy
0
Ionization Mode
ESI
+ESI Scan:1 (0.144-0.958 min, 55 Scans) Frag=135.0V XCVII-68-4_TIC.d Subtract
x10 6
469.3
Counts vs. Mass-to-Charge (m/z)

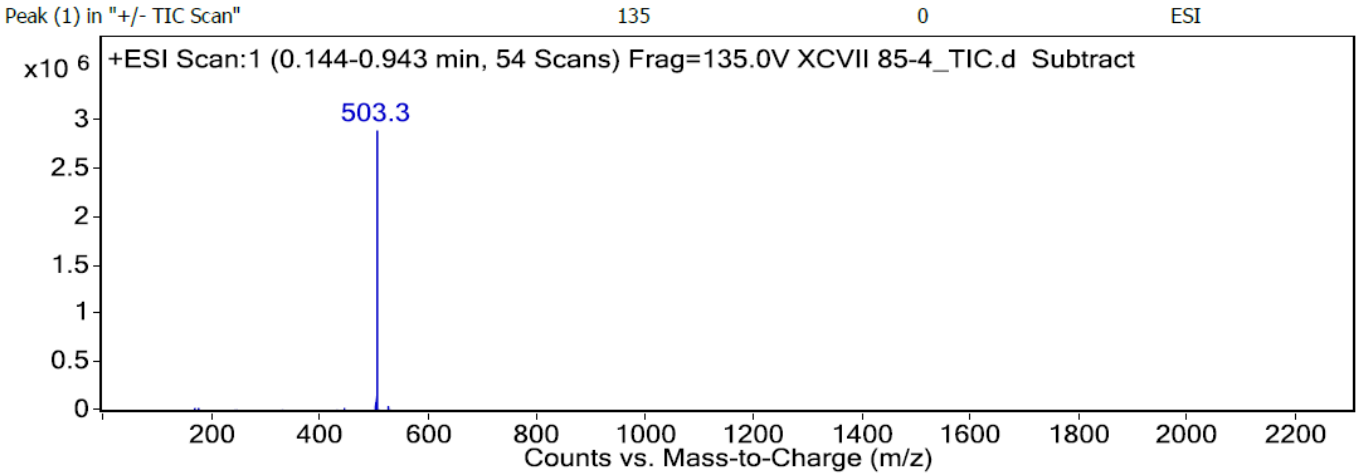

sahamidi_spektri
M. Beus XCVII 68/4
f1 (ppm)

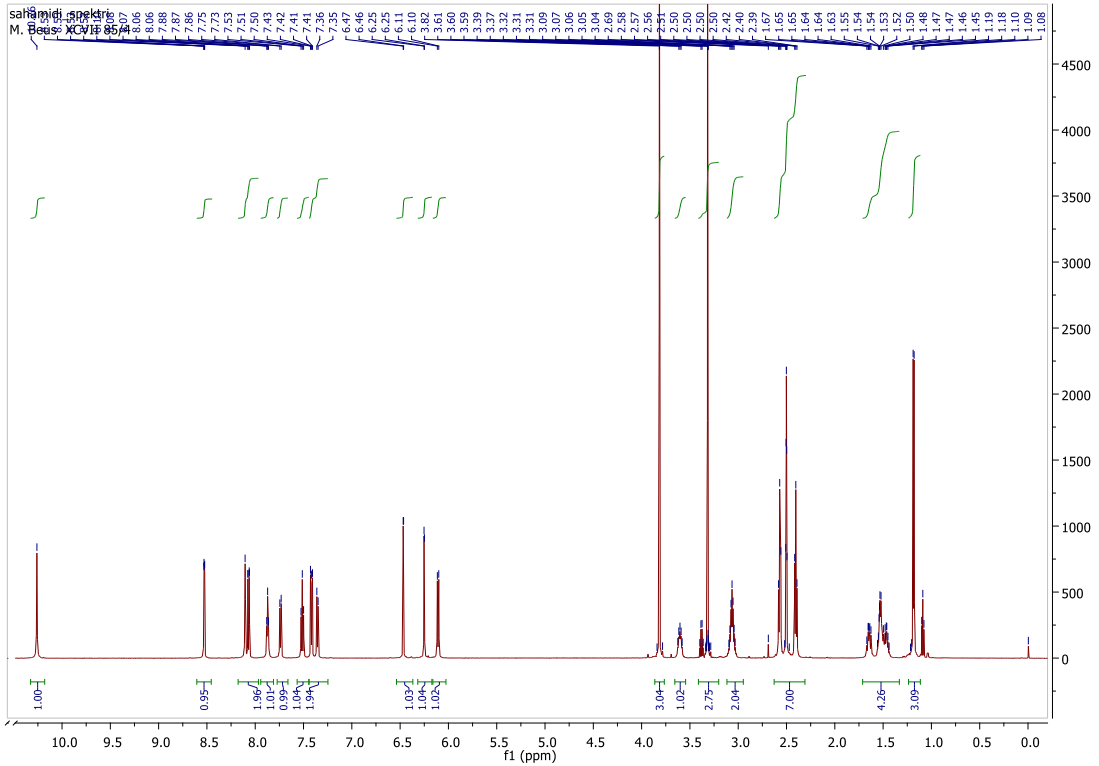

sahamida spektri
M. Beus XCVII 68/4
169.74
159.01
144.55
144.18
138.28
134.89
134.42
129.59
128.51
126.33
122.09
120.37
96.19
91.63
54.98
47.02
39.79
39.51
39.51
39.23
33.37
31.73
30.23
25.98
20.15
f1 (ppm)

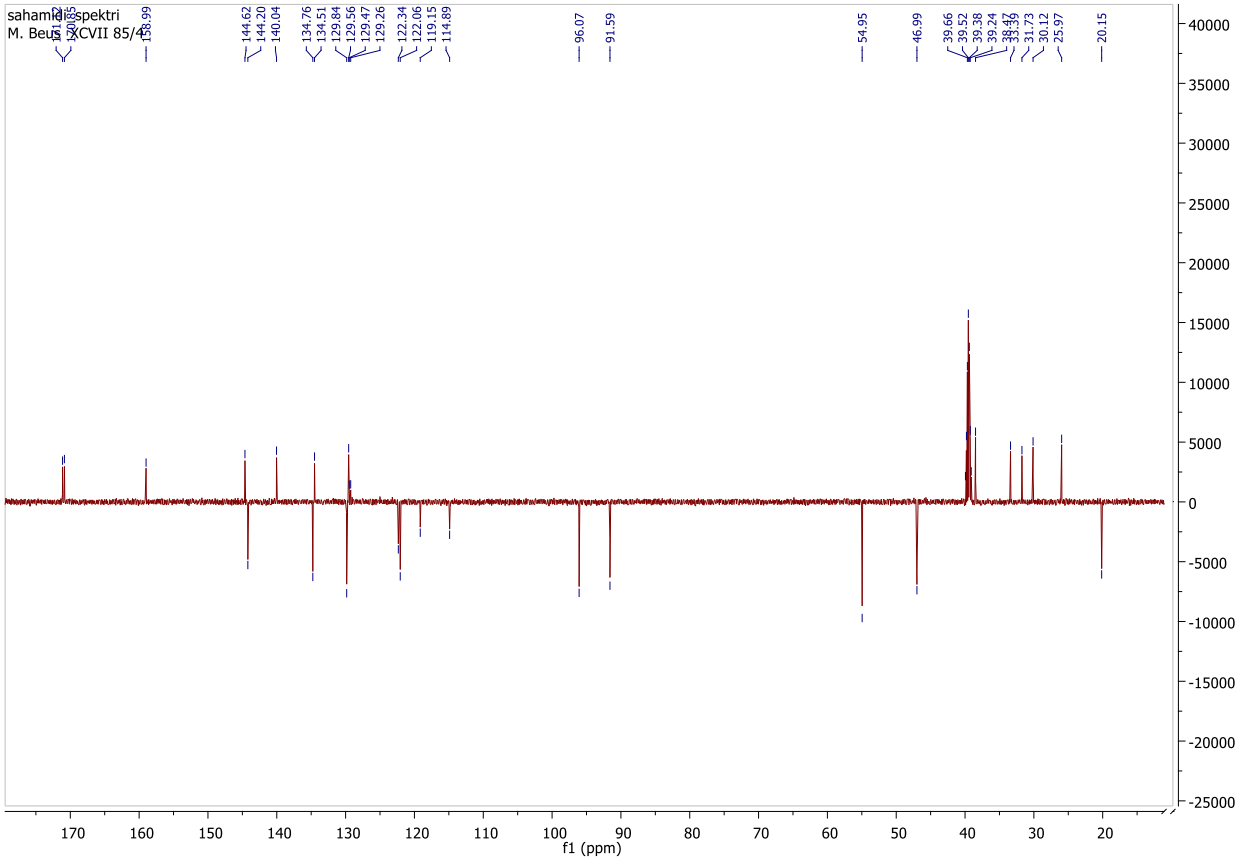

O
NH
N
H
N
O
O
N
H
CF3

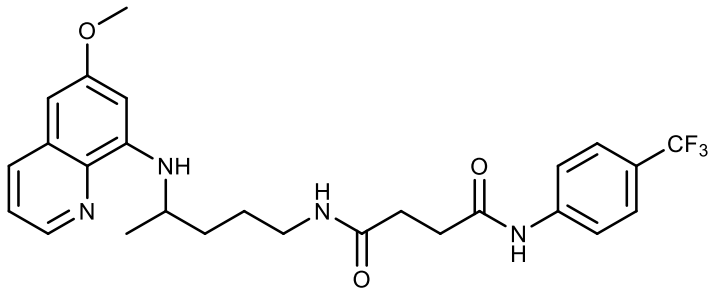
5e


%T
cm-1
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
3851
3747
3672
3366
2270
3392
3278
3236
3212
3165
3139
3099
3020
2952
2925
2887
2857
1669
1650
1586
1563
1533
1515
1491
1474
1448
1433
1404
1389
1353
1333
1288
1273
1246
1201
1166
1146
1124
1077
1054
1041
1030
1015
999
986
964
938
923
909
890
856
824
813
795
787
750
735
710
701
696
681
666
660

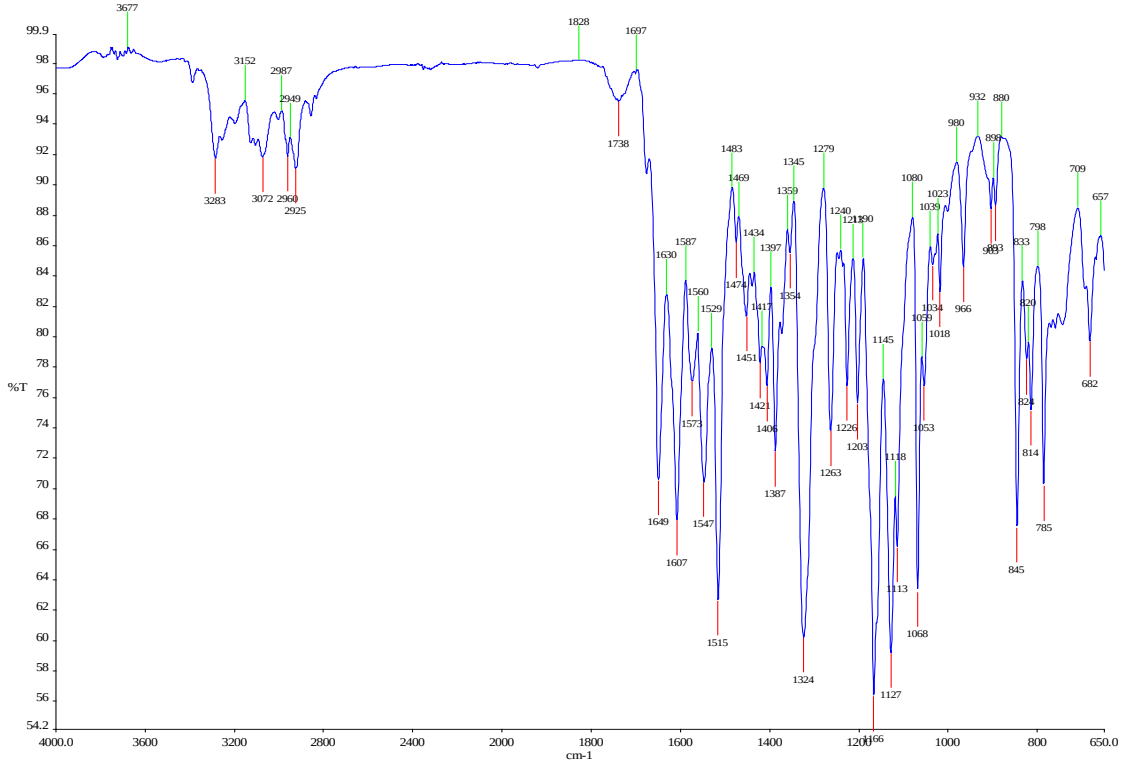

Peak (1) in "+/- TIC Scan"
135
0
ESI
+ESI Scan:1 (0.144-0.943 min, 54 Scans) Frag=135.0V XCVII 85-4_TIC.d Subtract
x10 6
503.3
Counts vs. Mass-to-Charge (m/z)


f1 (ppm)

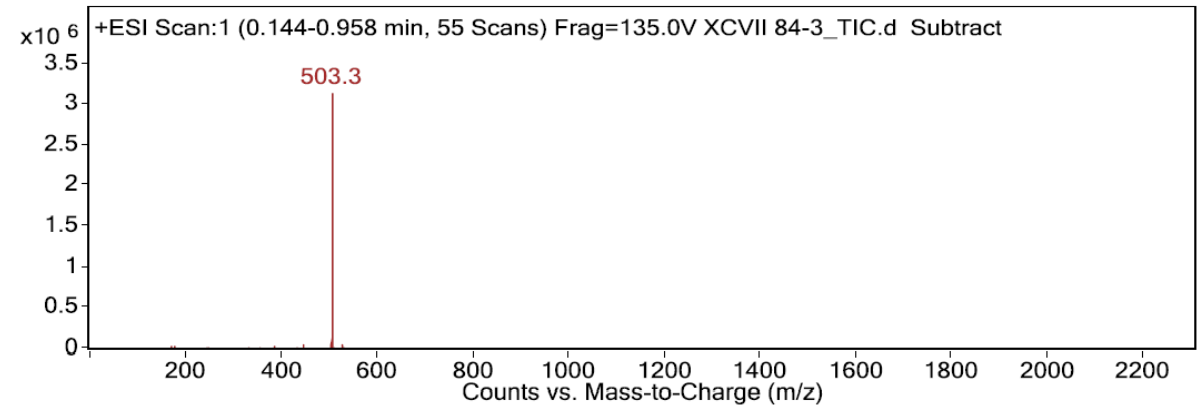

sahamidi-spektri
M. Beus XCVII 85/4
170.05
170.05
158.99
144.62
144.20
140.04
134.76
134.51
129.84
129.56
129.47
129.26
122.34
122.06
119.15
114.89
96.07
91.59
54.95
46.99
39.66
39.52
39.38
39.24
38.47
33.39
31.73
30.12
25.97
20.15
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
-10000
-15000
-20000
-25000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

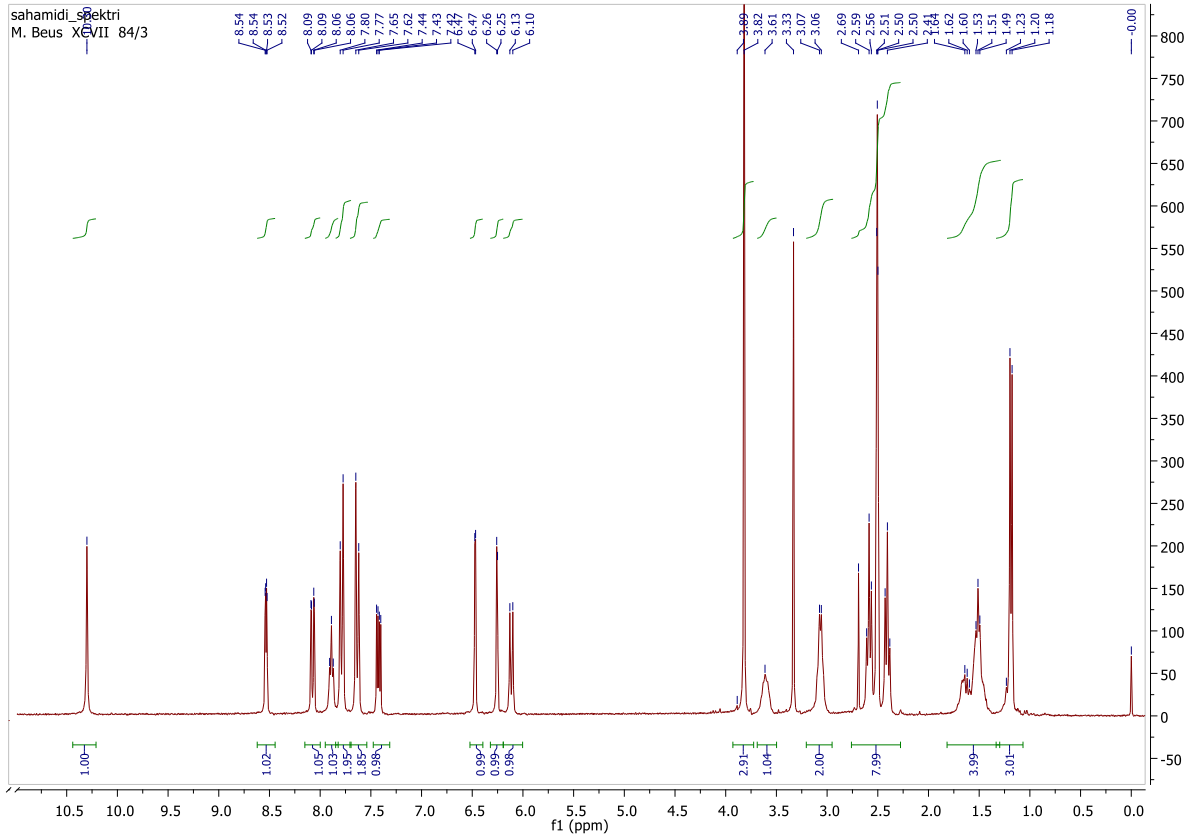

O
NH
N
H
N
O
O
N
H
CF3

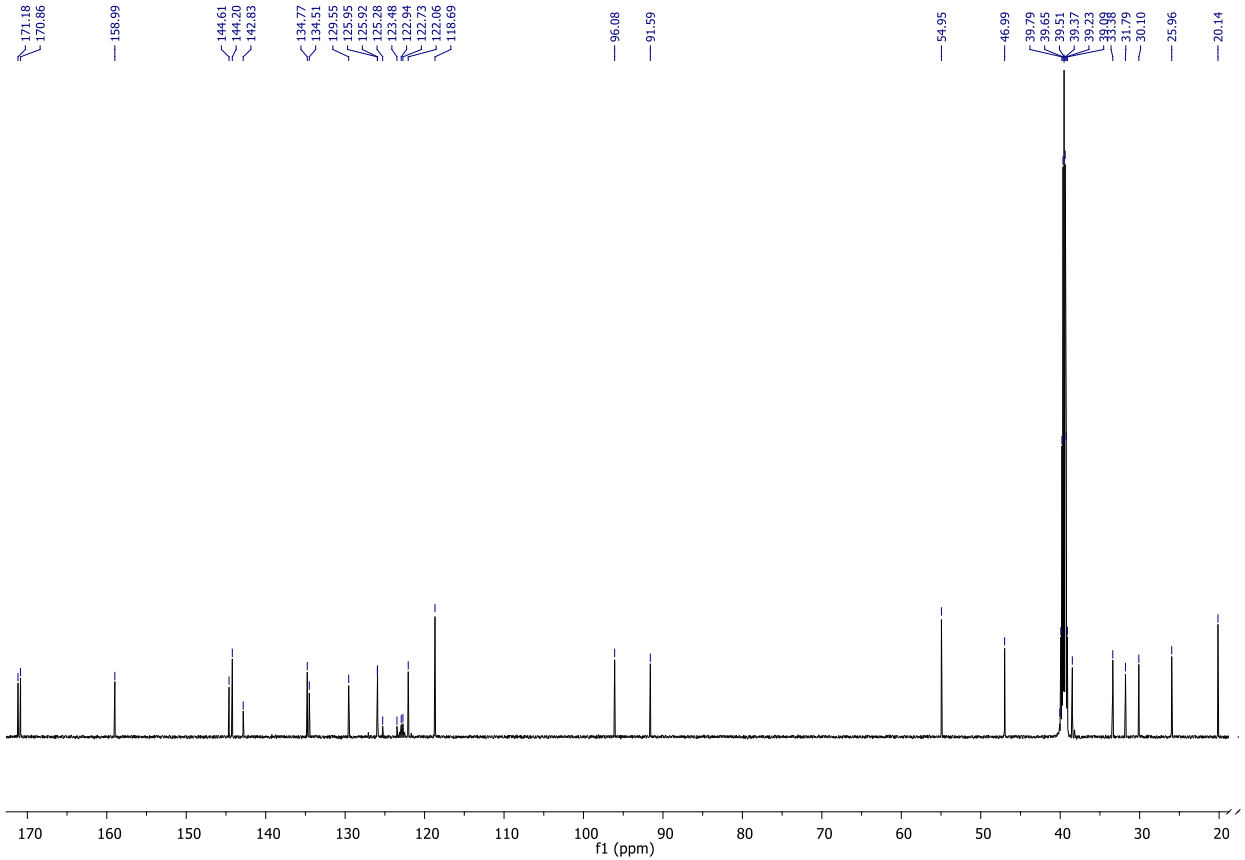
5f


%T
cm-1
4000.0
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
650.0
99.9
98
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
58
56
54.2
3677
3283
3152
3072
2987
2949
2960
2925
1828
1738
1697
1649
1630
1607
1587
1573
1560
1547
1529
1515
1483
1469
1474
1451
1434
1421
1417
1406
1397
1387
1359
1354
1345
1324
1279
1263
1240
1226
1203
1145
1127
1118
1113
1080
1068
1053
1039
1034
1029
1023
1018
980
966
932
880
845
833
824
820
814
798
785
709
682
657

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
Peak (1) in "+/- TIC Scan"	135	0	ESI






171.18
170.86
158.99
144.61
144.20
142.83
134.77
134.51
129.55
125.95
125.92
125.28
123.48
122.94
122.73
122.06
118.69
96.08
91.59
54.95
46.99
39.79
39.65
39.51
39.37
39.23
33.38
31.79
30.10
25.96
20.14
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)