

Electronic Supplementary Material (ESI) for RSC Adv.

Supporting Information to

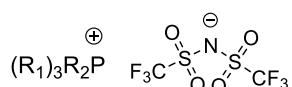
Rapid, effective deprotection of *tert*-butoxycarbonyl (Boc) amino acids and peptides at high temperatures using a thermally stable Ionic Liquid.

Sumit S. Bhawal,^a Rahul A. Patil^a and Daniel W. Armstrong* ^a

^a*Department of Chemistry and Biochemistry, The University of Texas at Arlington, 700 Planetarium Place, Arlington, Texas 76019-0065, USA. E-mail: sec4dwa@uta.edu*

General.....	S2
General Procedure for Experiments.....	S2
NMR Spectra.....	S5-S90

General: Compounds were purchased in their purest commercial quality. All materials were used as obtained, unless and otherwise indicated. Column chromatography for recovery of Ionic Liquid was performed using silica gel (300-400 mesh) with Hexane/EtOAc as eluent. ^1H NMR, ^{13}C NMR, ^{19}F NMR and ^{31}P NMR experiments were performed on 500 MHz a JEOL Eclipse Plus 500 instrument. Chemical shifts were recorded with reference to residual solvent peaks (D_2O residue = 4.79 ppm, CDCl_3 residue = 7.26 ppm). ESI Mass spectroscopy was performed with Thermo Finnigan LXQ linear Ion Trap mass spectrometer, when required.

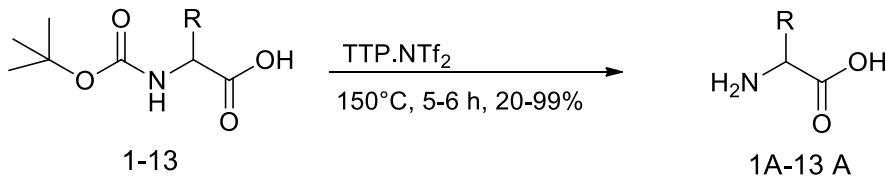


R_1 = Hexyl, R_2 = Tetradecyl

Trihexyl tetradecyl phosphonium
bis(trifluoromethane)sulfonimide
(TTP.NTf₂)

General Procedures for Experiments

Preparation of TTP-NTf₂: To a solution of (40 g, 77 mmol) trihexyl tetradecylphosphonium chloride, (graciously donated by CYTEC, West Paterson, NJ, USA) in methanol (20 mL) was added (24.32 g, 84.71 mmol) LiNTf₂. Additional methanol was added to obtain a clear solution. The solution was slightly warm at the beginning and was stirred overnight. Methanol was removed under reduced pressure and ~200 mL CH₂Cl₂ was added to the round bottom flask. The organic layer containing the ionic liquid was transferred to the separating funnel and LiCl was extracted with (3x100 mL) deionized water. The organic layer was concentrated under reduced pressure at and dried in vacuum oven (maintained at 40 °C) over P₂O₅ for at least 36 h before use. The products were characterized by ^1H NMR, ^{13}C NMR, ^{19}F and ^{31}P NMR.

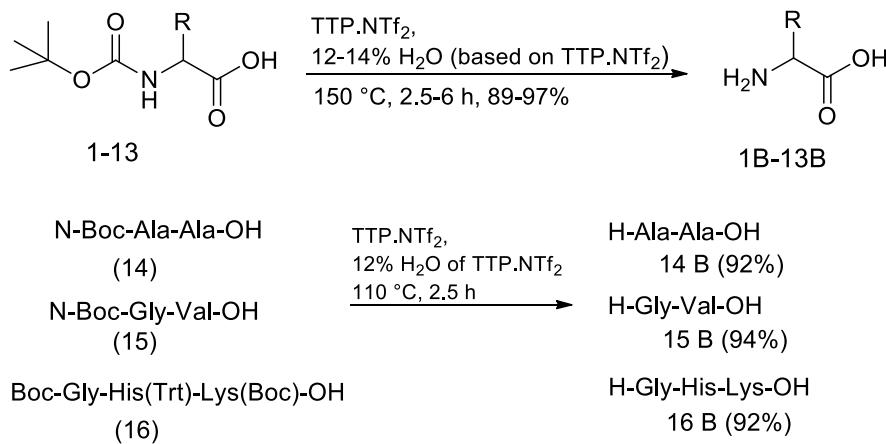


R = H, Me, iPr, iso-Bu, s-Bu, Bzl, pyrrolidine, thiomethylethyl, 1-hydroxyethyl, 3-(1H-imidazol-4-yl), 4-amino-butyl, carboxymethyl, carboxyethyl.

Method A (Neat Reaction in TTP-NTf₂) A mixture of (0.25 g, 0.32-1.43 mmol) N-Boc protected amino acid/peptides and TTP-NTf₂ (7 g, 9.16 mmol) was stirred (~150 rpm) for 5-6 h at 150 °C in a round bottom flask (50 mL) equipped with a reflux condenser. Completion of reaction was monitored by TLC using ethyl acetate/methanol (95:5) and ninhydrin as staining agent. On cooling, the reaction mixture was

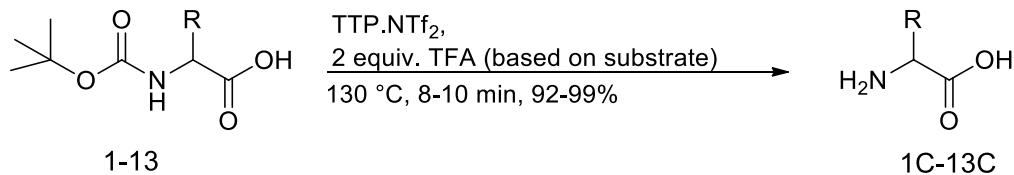
transferred into separating funnel with 3x10 mL (CH₂Cl₂/water 1:1). In addition, CH₂Cl₂ (100 mL) and water (50 – 80 mL, depending on the substrate) was added to the separating funnel. The layers were allowed to separate after shaking and the organic layer (containing the ionic liquid) was removed. To the aqueous layer (containing the amino acids) fresh CH₂Cl₂ (2x 75mL) was added to ensure removal of any trace of ionic liquid remaining. The aqueous layer was evaporated to dryness to obtain the product. In most of the cases, this gave us the purified amino acid, but otherwise a final washing with ~ 5 mL isopropanol (using centrifuge) proved very effective. All the products were characterized by ¹H NMR, ¹³C NMR. ESI-MS was done in some cases.

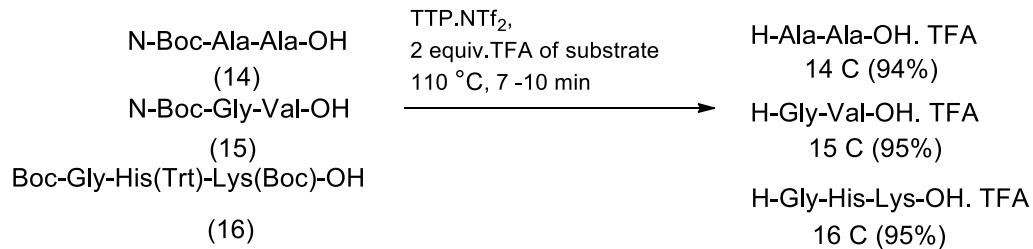
The peptides were added to TTP-NTf₂ and heated at 120 °C for 3 h (Scheme not shown). However, incomplete conversions and product decompositions were observed (14A-16A).



Method B (TTP-NTf₂ and water) To a mixture of (0.25 g, 0.32-1.43 mmol) N-Boc protected amino acid/peptides and TTP-NTf₂ (7 g, 9.16 mmol) was added deionized water 12-14% (based on TTP-NTf₂). The resulting mixture was stirred (~200 rpm) for 2.5-6 h at 150 °C (for amino acids) and 2.5 h at 110 °C (for peptides). The remaining work-up is similar to method A. All the products were characterized by ¹H NMR, ¹³C NMR. ESI-MS was done in some cases.

L-Histidine and L-Lysine tends to form emulsions especially for method B. They were centrifuged for 5 min at around 5000 rpm (The Drucker Co., Model 614 B) to obtain the purified compound. For peptides, the water was generally removed at ~ 40-45 °C under reduced pressure.



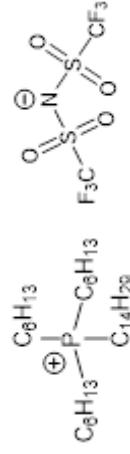


Method C (TTP-NTf₂ and TFA) To a stirring mixture of (0.25 g, 0.32-1.43 mmol) N-Boc protected amino acid/peptides and TTP-NTf₂ (7 g, 9.16 mmol) was added TFA (2 equiv, based on substrate). The resulting mixture was stirred (~150 rpm) for 7-10 min at 100 °C (for peptides) and 130 °C (for amino acids). The remaining procedure is similar to method A.

For peptides, the water was removed by either freeze drying or simply air drying at higher flow using an inverted funnel at room temperature. All the products were characterized by ¹H NMR, ¹³ C NMR. ESI-MS was done in some cases.

SBIII.16H-3.idf

TTP-N⁺Tf₂



TTP-NTT₂

Trihexyl tetradecyl phosphonium bis(trifluoromethane)sulfonimide

4.02

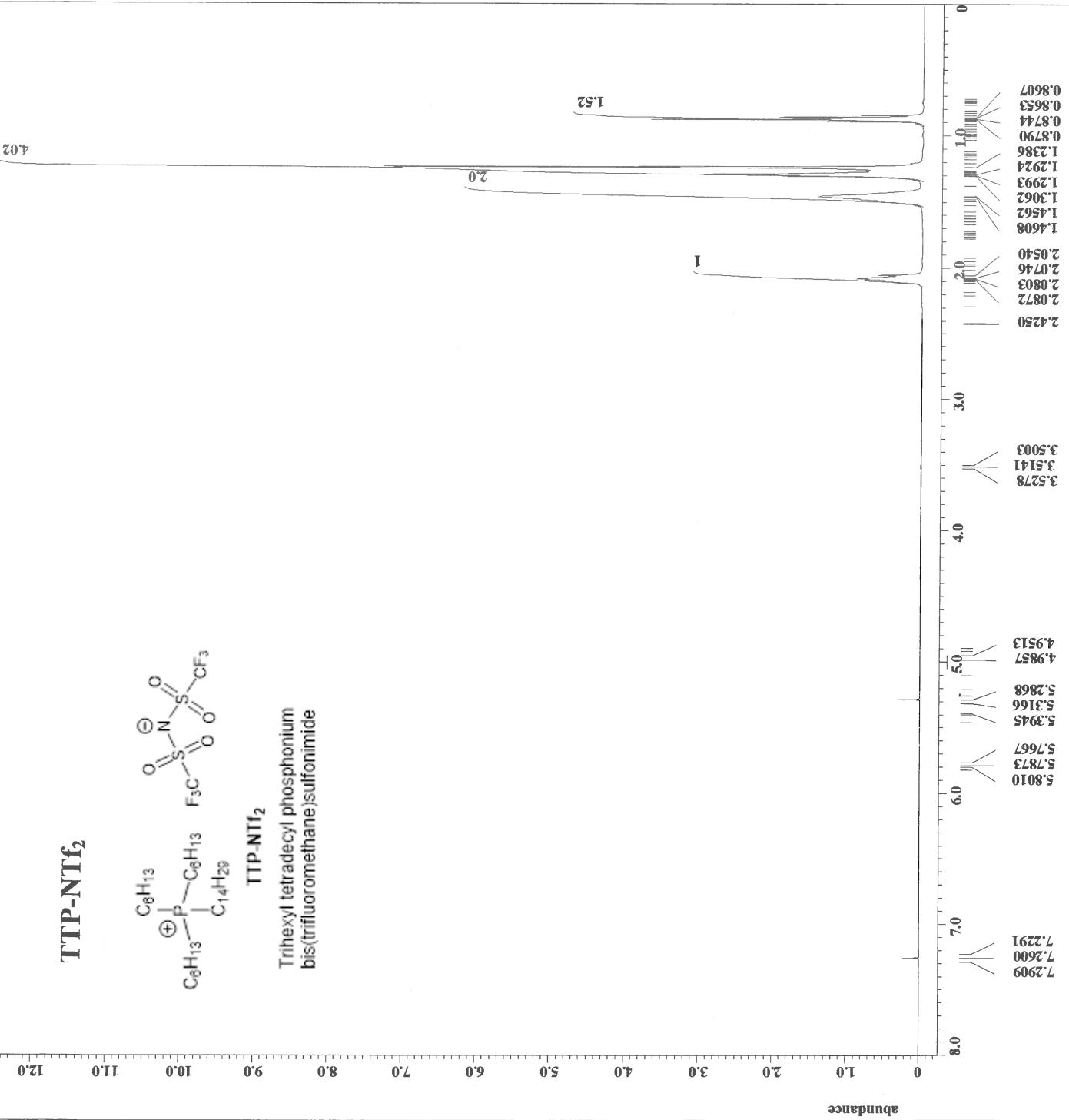
卷之三

```

Filename = SBIL16H-3-jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#326644
Solvent = CHLOROFORM-D
Creation_time = 27--SEP--2015 21:15:31
Revision_time = 27--SEP--2015 09:19:16
Current_time = 27--SEP--2015 09:20:11

```

Comment	= single_pulse
Data_format	= 1D_COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [PPM]
Dimensions	= X
Site	= ECR_500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MHz])
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[PPM]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[MHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[PPM]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[PPM]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.21[us]
Irr_mode	= OFF
Tri_mode	= OFF
Dante_Presat	= FALSE
Initial_wait	= 1[s]
Recv_gain	= 22
Relaxation_delay	= 10[s]
Repetition_time	= 11.4587904[s]
Temp_get	= 21.5[dc]



```

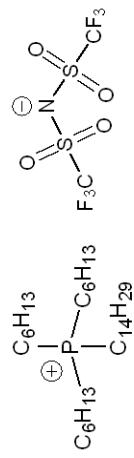
filename = SBIL16C-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#32980
Solvent = CHLOROFORM-D
Creation_time = 27-SEP-2015 22:20:40
Revision_time = 27-SEP-2015 09:37:53
Current_time = 27-SEP-2015 09:38:16
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MHz])
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 125.76529768 [MHz]
X_offset = 100.0 [ppm]
X_points = 32768
X_prescans = 4
X_sweep = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 10
Scans = 1280
Total_scans = 1280

X_90_width = 10.73 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_attn = 9 [dB]
X_pulse = 3.57666667 [us]
Irr_attn_dec = 20 [dB]
Irr_attn_noe = 20 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
0.4 [s]
Reovr_gain = 50
Relaxation_delay = 0.4 [s]
Repetition_time = 1.23361792 [s]
Temp_get = 22.1 [dC]

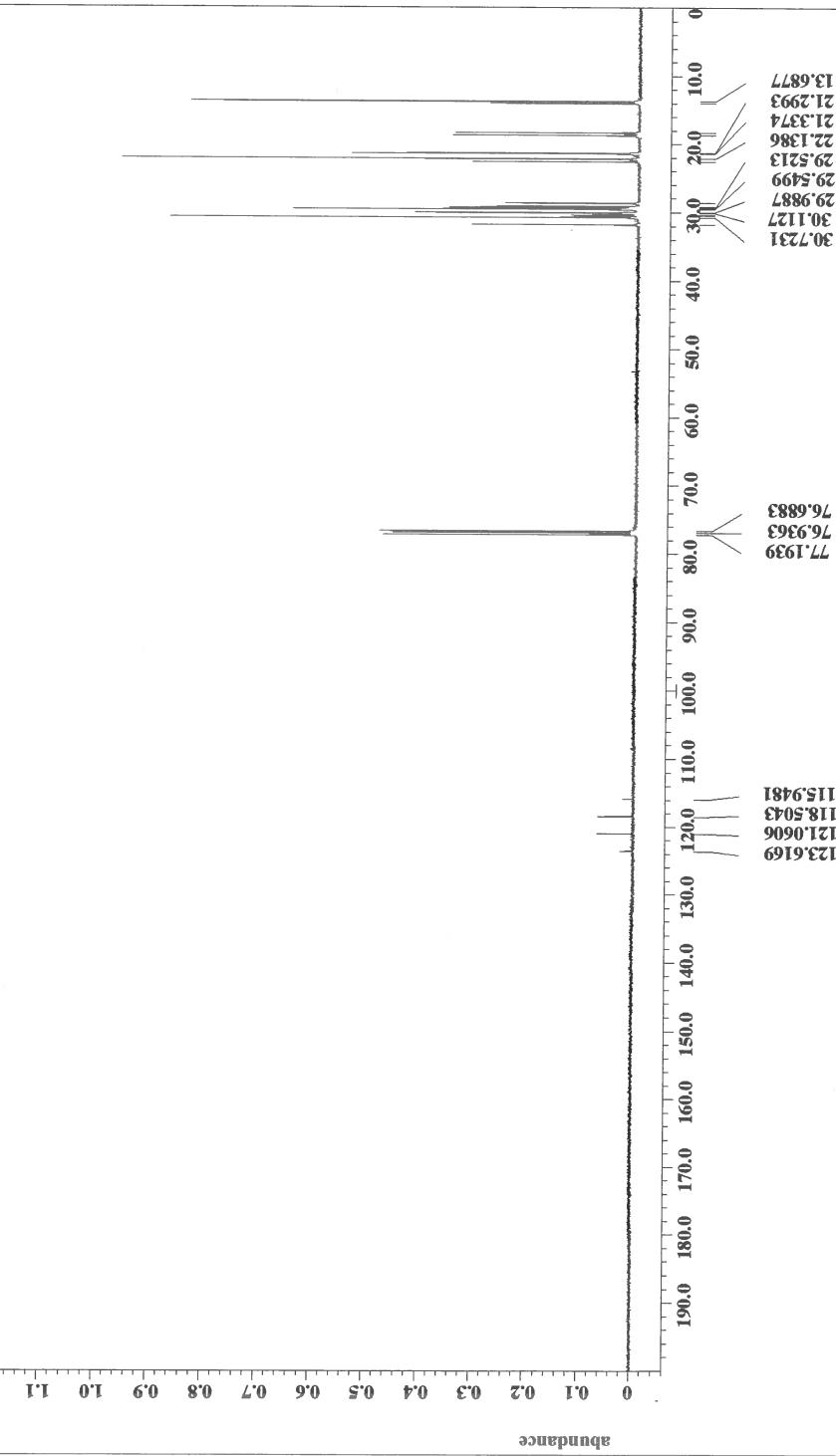
```

TTP-NTf₂ carbon



TTP-NTf₂

Trihexyl tetradecyl phosphonium
bis(trifluoromethane)sulfonylimide



X : parts per Million : 13C

77.1939
76.9363
76.6883

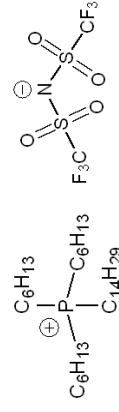
123.6169
118.5043
112.0606
115.9481

30.7231
30.1127
29.9887
29.5213
21.1386
21.3374
21.2993
21.2980
20.5499
13.6877

SB11L16P-2.pdf

卷之三

TTP-NTf₂ ³¹P

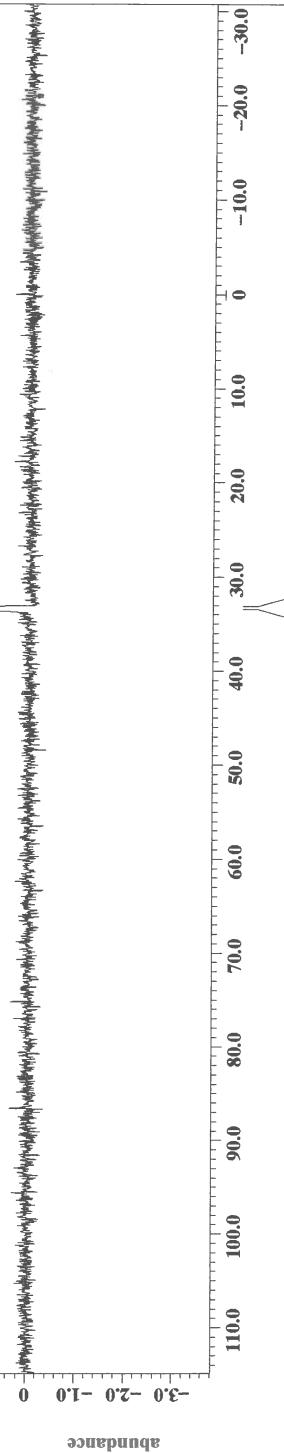


TTP-NTf₂

Trihexyl tetradecyl phosphonium bis(trifluoromethane)sulfonimide

```

A_points = 16384
X_prescans = 0
X_resolution = 10.89913504 [Hz]
X_sweep = 178.57142857 [kHz]
X_domain = 31P
Irr_freq = 202.46831075 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 31P
Tri_freq = 202.46831075 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 9
Total_scans = 9
X_90_width = 11.9 [us]
X_acq_time = 91.7504 [ms]
X_angle = 45 [deg]
X_atan = 9 [dB]
X_pulse = 5.95 [us]
Irr_mode = Off
Tri_mode = Off
Dante_Presat = FALSE
Initial_wait = 1 [s]
Recur_Gain = 50
Relaxation_delay = 10 [s]
Relaxation_time = 10.1917504 [s]
Team_Set = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204, 205, 206, 207, 208, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225, 226, 227, 228, 229, 230, 231, 232, 233, 234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246, 247, 248, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258, 259, 259, 260, 261, 262, 263, 264, 265, 266, 267, 268, 269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282, 283, 284, 285, 286, 287, 288, 289, 290, 291, 292, 293, 294, 295, 296, 297, 298, 299, 299, 300, 301, 302, 303, 304, 305, 306, 307, 308, 309, 309, 310, 311, 312, 313, 314, 315, 316, 317, 318, 319, 319, 320, 321, 322, 323, 324, 325, 326, 327, 328, 329, 329, 330, 331, 332, 333, 334, 335, 336, 337, 338, 339, 339, 340, 341, 342, 343, 344, 345, 346, 347, 348, 349, 349, 350, 351, 352, 353, 354, 355, 356, 357, 358, 359, 359, 360, 361, 362, 363, 364, 365, 366, 367, 368, 369, 369, 370, 371, 372, 373, 374, 375, 376, 377, 378, 379, 379, 380, 381, 382, 383, 384, 385, 386, 387, 388, 389, 389, 390, 391, 392, 393, 394, 395, 396, 397, 398, 399, 399, 400, 401, 402, 403, 404, 405, 406, 407, 408, 409, 409, 410, 411, 412, 413, 414, 415, 416, 417, 418, 419, 419, 420, 421, 422, 423, 424, 425, 426, 427, 428, 429, 429, 430, 431, 432, 433, 434, 435, 436, 437, 438, 439, 439, 440, 441, 442, 443, 444, 445, 446, 447, 448, 449, 449, 450, 451, 452, 453, 454, 455, 456, 457, 458, 459, 459, 460, 461, 462, 463, 464, 465, 466, 467, 468, 469, 469, 470, 471, 472, 473, 474, 475, 476, 477, 478, 479, 479, 480, 481, 482, 483, 484, 485, 486, 487, 488, 489, 489, 490, 491, 492, 493, 494, 495, 496, 497, 498, 499, 499, 500, 501, 502, 503, 504, 505, 506, 507, 508, 509, 509, 510, 511, 512, 513, 514, 515, 516, 517, 518, 519, 519, 520, 521, 522, 523, 524, 525, 526, 527, 528, 529, 529, 530, 531, 532, 533, 534, 535, 536, 537, 538, 539, 539, 540, 541, 542, 543, 544, 545, 546, 547, 548, 549, 549, 550, 551, 552, 553, 554, 555, 556, 557, 558, 559, 559, 560, 561, 562, 563, 564, 565, 566, 567, 568, 569, 569, 570, 571, 572, 573, 574, 575, 576, 577, 578, 579, 579, 580, 581, 582, 583, 584, 585, 586, 587, 588, 589, 589, 590, 591, 592, 593, 594, 595, 596, 597, 598, 599, 599, 600, 601, 602, 603, 604, 605, 606, 607, 608, 609, 609, 610, 611, 612, 613, 614, 615, 616, 617, 618, 619, 619, 620, 621, 622, 623, 624, 625, 626, 627, 628, 629, 629, 630, 631, 632, 633, 634, 635, 636, 637, 638, 639, 639, 640, 641, 642, 643, 644, 645, 646, 647, 648, 649, 649, 650, 651, 652, 653, 654, 655, 656, 657, 658, 659, 659, 660, 661, 662, 663, 664, 665, 666, 667, 668, 669, 669, 670, 671, 672, 673, 674, 675, 676, 677, 678, 679, 679, 680, 681, 682, 683, 684, 685, 686, 687, 688, 689, 689, 690, 691, 692, 693, 694, 695, 696, 697, 698, 699, 699, 700, 701, 702, 703, 704, 705, 706, 707, 708, 709, 709, 710, 711, 712, 713, 714, 715, 716, 717, 718, 719, 719, 720, 721, 722, 723, 724, 725, 726, 727, 728, 729, 729, 730, 731, 732, 733, 734, 735, 736, 737, 738, 739, 739, 740, 741, 742, 743, 744, 745, 746, 747, 748, 749, 749, 750, 751, 752, 753, 754, 755, 756, 757, 758, 759, 759, 760, 761, 762, 763, 764, 765, 766, 767, 768, 769, 769, 770, 771, 772, 773, 774, 775, 776, 777, 778, 779, 779, 780, 781, 782, 783, 784, 785, 786, 787, 788, 789, 789, 790, 791, 792, 793, 794, 795, 796, 797, 798, 799, 799, 800, 801, 802, 803, 804, 805, 806, 807, 808, 809, 809, 810, 811, 812, 813, 814, 815, 816, 817, 818, 819, 819, 820, 821, 822, 823, 824, 825, 826, 827, 828, 829, 829, 830, 831, 832, 833, 834, 835, 836, 837, 838, 839, 839, 840, 841, 842, 843, 844, 845, 846, 847, 848, 849, 849, 850, 851, 852, 853, 854, 855, 856, 857, 858, 859, 859, 860, 861, 862, 863, 864, 865, 866, 867, 868, 869, 869, 870, 871, 872, 873, 874, 875, 876, 877, 878, 879, 879, 880, 881, 882, 883, 884, 885, 886, 887, 888, 889, 889, 890, 891, 892, 893, 894, 895, 896, 897, 898, 899, 899, 900, 901, 902, 903, 904, 905, 906, 907, 908, 909, 909, 910, 911, 912, 913, 914, 915, 916, 917, 918, 919, 919, 920, 921, 922, 923, 924, 925, 926, 927, 928, 929, 929, 930, 931, 932, 933, 934, 935, 936, 937, 938, 939, 939, 940, 941, 942, 943, 944, 945, 946, 947, 948, 949, 949, 950, 951, 952, 953, 954, 955, 956, 957, 958, 959, 959, 960, 961, 962, 963, 964, 965, 966, 967, 968, 969, 969, 970, 971, 972, 973, 974, 975, 976, 977, 978, 979, 979, 980, 981, 982, 983, 984, 985, 986, 987, 988, 989, 989, 990, 991, 992, 993, 994, 995, 996, 997, 997, 998, 999, 999, 1000, 1001, 1002, 1003, 1004, 1005, 1006, 1007, 1008, 1009, 1009, 1010, 1011, 1012, 1013, 1014, 1015, 1016, 1017, 1018, 1019, 1019, 1020, 1021, 1022, 1023, 1024, 1025, 1026, 1027, 1028, 1029, 1029, 1030, 1031, 1032, 1033, 1034, 1035, 1036, 1037, 1038, 1039, 1039, 1040, 1041, 1042, 1043, 1044, 1045, 1046, 1047, 1048, 1049, 1049, 1050, 1051, 1052, 1053, 1054, 1055, 1056, 1057, 1058, 1059, 1059, 1060, 1061, 1062, 1063, 1064, 1065, 1066, 1067, 1068, 1069, 1069, 1070, 1071, 1072, 1073, 1074, 1075, 1076, 1077, 1078, 1079, 1079, 1080, 1081, 1082, 1083, 1084, 1085, 1086, 1087, 1088, 1089, 1089, 1090, 1091, 1092, 1093, 1094, 1095, 1096, 1097, 1098, 1098, 1099, 1100, 1101, 1102, 1103, 1104, 1105, 1106, 1107, 1108, 1109, 1109, 1110, 1111, 1112, 1113, 1114, 1115, 1116, 1117, 1118, 1119, 1119, 1120, 1121, 1122, 1123, 1124, 1125, 1126, 1127, 1128, 1129, 1129, 1130, 1131, 1132, 1133, 1134, 1135, 1136, 1137, 1138, 1139, 1139, 1140, 1141, 1142, 1143, 1144, 1145, 1146, 1147, 1148, 1149, 1149, 1150, 1151, 1152, 1153, 1154, 1155, 1156, 1157, 1158, 1159, 1159, 1160, 1161, 1162, 1163, 1164, 1165, 1166, 1167, 1168, 1169, 1169, 1170, 1171, 1172, 1173, 1174, 1175, 1176, 1177, 1178, 1179, 1179, 1180, 1181, 1182, 1183, 1184, 1185, 1186, 1187, 1188, 1189, 1189, 1190, 1191, 1192, 1193, 1194, 1195, 1196, 1197, 1198, 1198, 1199, 1200, 1201, 1202, 1203, 1204, 1205, 1206, 1207, 1208, 1209, 1209, 1210, 1211, 1212, 1213, 1214, 1215, 1216, 1217, 1218, 1219, 1219, 1220, 1221, 1222, 1223, 1224, 1225, 1226, 1227, 1228, 1229, 1229, 1230, 1231, 1232, 1233, 1234, 1235, 1236, 1237, 1238, 1239, 1239, 1240, 1241, 1242, 1243, 1244, 1245, 1246, 1247, 1248, 1249, 1249, 1250, 1251, 1252, 1253, 1254, 1255, 1256, 1257, 1258, 1259, 1259, 1260, 1261, 1262, 1263, 1264, 1265, 1266, 1267, 1268, 1269, 1269, 1270, 1271, 1272, 1273, 1274, 1275, 1276, 1277, 1278, 1279, 1279, 1280, 1281, 1282, 1283, 1284, 1285, 1286, 1287, 1288, 1289, 1289, 1290, 1291, 1292, 1293, 1294, 1295, 1296, 1297, 1298, 1298, 1299, 1300, 1301, 1302, 1303, 1304, 1305, 1306, 1307, 1308, 1309, 1309, 1310, 1311, 1312, 1313, 1314, 1315, 1316, 1317, 1318, 1319, 1319, 1320, 1321, 1322, 1323, 1324, 1325, 1326, 1327, 1328, 1329, 1329, 1330, 1331, 1332, 1333, 1334, 1335, 1336, 1337, 1338, 1339, 1339, 1340, 1341, 1342, 1343, 1344, 1345, 1346, 1347, 1348, 1349, 1349, 1350, 1351, 1352, 1353, 1354, 1355, 1356, 1357, 1358, 1359, 1359, 1360, 1361, 1362, 1363, 1364, 1365, 1366, 1367, 1368, 1369, 1369, 1370, 1371, 1372, 1373, 1374, 1375, 1376, 1377, 1378, 1379, 1379, 1380, 1381, 1382, 1383, 1384, 1385, 1386, 1387, 1388, 1389, 1389, 1390, 1391, 1392, 1393, 1394, 1395, 1396, 1397, 1398, 1398, 1399, 1400, 1401, 1402, 1403, 1404, 1405, 1406, 1407, 1408, 1409, 1409, 1410, 1411, 1412, 1413, 1414, 1415, 1416, 1417, 1418, 1419, 1419, 1420, 1421, 1422, 1423, 1424, 1425, 1426, 1427, 1428, 1429, 1429, 1430, 1431, 1432, 1433, 1434, 1435, 1436, 1437, 1438, 1439, 1439, 1440, 1441, 1442, 1443, 1444, 1445, 1446, 1447, 1448, 1449, 1449, 1450, 1451, 1452, 1453, 1454, 1455, 1456, 1457, 1458, 1459, 1459, 1460, 1461, 1462, 1463, 1464, 1465, 1466, 1467, 1468, 1469, 1469, 1470, 1471, 1472, 1473, 1474, 1475, 1476, 1477, 1478, 1479, 1479, 1480, 1481, 1482, 1483, 1484, 1485, 1486, 1487, 1488, 1489, 1489, 1490, 1491, 1492, 1493, 1494, 1495, 1496, 1497, 1498, 1498, 1499, 1500, 1501, 1502, 1503, 1504, 1505, 1506, 1507, 1508, 1509, 1509, 1510, 1511, 1512, 1513, 1514, 1515, 1516, 1517, 1518, 1519, 1519, 1520, 1521, 1522, 1523, 1524, 1525, 1526, 1527, 1528, 1529, 1529, 1530, 1531, 1532, 1533, 1534, 1535, 1536, 1537, 1538, 1539, 1539, 1540, 1541, 1542, 1543, 1544, 1545, 1546, 1547, 1548, 1549, 1549, 1550, 1551, 1552, 1553, 1554, 1555, 1556, 1557, 1558, 1559, 1559, 1560, 1561, 1562, 1563, 1564, 1565, 1566, 1567, 1568, 1569, 1569, 1570, 1571, 1572, 1573, 1574, 1575, 1576, 1577, 1578, 1579, 1579, 1580, 1581, 1582, 1583, 1584, 1585, 1586, 1587, 1588, 1589, 1589, 1590, 1591, 1592, 1593, 1594, 1595, 1596, 1597, 1598, 1598, 1599, 1600, 1601, 1602, 1603, 1604, 1605, 1606, 1607, 1608, 1609, 1609, 1610, 1611, 1612, 1613, 1614, 1615, 1616, 1617, 1618, 1619, 1619, 1620, 1621, 1622, 1623, 1624, 1625, 1626, 1627, 1628, 1629, 1629, 1630, 1631, 1632, 1633, 1634, 1635, 1636, 1637, 1638, 1639, 1639, 1640, 1641, 1642, 1643, 1644, 1645, 1646, 1647, 1648, 1649, 1649, 1650, 1651, 1652, 1653, 1654, 1655, 1656, 1657, 1658, 1659, 1659, 1660, 1661, 1662, 1663, 1664, 1665, 1666, 1667, 1668, 1669, 1669, 1670, 1671, 1672, 1673, 1674, 1675, 1676, 1677, 1678, 1679, 1679, 1680, 1681, 1682, 1683, 1684, 1685, 1686, 1687, 1688, 1689, 1689, 1690, 1691, 1692, 1693, 1694, 1695, 1696, 1697, 1698, 1698, 1699, 1700, 1701, 1702, 1703, 1704, 1705, 1706, 1707, 1708, 1709, 1709, 1710, 1711, 1712, 1713, 1714, 1715, 1716, 1717, 1718, 1719, 1719, 1720, 1721, 1722, 1723, 1724, 1725, 1726, 1727, 1728, 1729, 1729, 1730, 1731, 1732, 1733, 1734, 1735, 1736, 1737, 1738, 1739, 1739, 1740, 1741, 1742, 1743, 1744, 1745, 1746, 1747, 1748, 1749, 1749, 1750, 1751, 1752, 1753, 1754, 1755, 1756, 1757, 1758, 1759, 1759, 1760, 1761, 1762, 1763, 1764, 1765, 1766, 1767, 1768, 1769, 1769, 1770, 1771, 1772, 1773, 1774, 1775, 1776, 1777, 1778, 1779, 1779, 1780, 1781, 1782, 1783, 1784, 1785, 1786, 1787, 1788, 1789, 1789, 1790, 1791, 1792, 1793, 1794, 1795, 1796, 1797, 1798, 1798, 1799, 1800, 1801, 1802, 1803, 1804, 1805, 1806, 1807, 1808, 1809, 1809, 1810, 1811, 1812, 1813, 1814, 1815, 1816, 1817, 1818, 1819, 1819, 1820, 1821, 1822, 1823, 1824, 1825, 1826, 1827, 1828, 1829, 1829, 1830, 1831, 1832, 1833, 1834, 1835, 1836, 1837, 1838, 1839, 1839, 1840, 1841, 1842, 1843, 1844, 1845, 1846, 1847, 1848, 1849, 1849, 1850, 1851, 1852, 1853, 1854, 1855, 1856, 1857, 1858, 1859, 1859, 1860, 1861, 1862, 1863, 1864, 1865, 1866, 1867, 1868, 1869, 1869, 1870, 1871, 1872, 1873, 1874, 1875, 1876, 1877, 1878, 1878, 1879, 1880, 1881, 1882, 1883, 1884, 1885, 1886, 1887, 1888, 1889, 1889, 1890, 1891, 1892, 1893, 1894, 1895, 1896, 1897, 1898, 1898, 1899, 1900, 1901, 1902, 1903, 1904, 1905, 1906, 1907, 1908, 1909, 1909, 1910, 1911, 1912, 1913, 1914, 1915, 1916, 1917, 1918, 1919, 1919, 1920, 1921, 1922, 1923, 1924, 1925, 1926, 1927, 1928, 1929, 1929, 1930, 1931, 1932, 1933, 1934, 1935, 1936, 1937, 1938, 1939, 1939, 1940, 1941, 1942, 1943, 1944, 1945, 1946, 1947, 1948, 1949, 1949, 1950, 1951, 1952, 1953, 1954, 1955, 1956, 1957, 1958, 1959, 1959, 1960, 1961, 1962, 1963, 1964, 1965, 1966, 1967, 1968, 1969, 1969, 1970, 1971, 1972, 1973, 1974, 1975, 1976, 1977, 1978, 1978, 1979, 1980, 1981, 1982, 1983, 1984, 1985, 1986, 1987, 1988, 1989, 1989, 1990, 1991, 1992, 1993, 1994, 1995, 1996, 1997, 1998, 1998, 1999, 2000, 2001, 2002, 2003, 2004, 2005, 2006, 2007, 2008, 2009, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019, 2019, 2020, 2021, 2022, 2023, 2024, 2025, 2026, 2027, 2028, 2029, 2029, 2030, 2031, 2032, 203
```

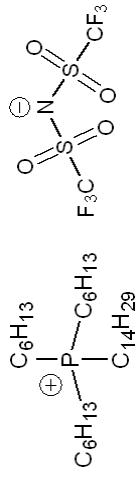


33.4292
33.1063

X: parts per Million : 31P

SBIL 16-3.1df

TTP-NTf2-¹⁹F



TTP-NTf₂

Trihexyl tetradecyl phosphonium bis(trifluoromethane)sulfonimide

```

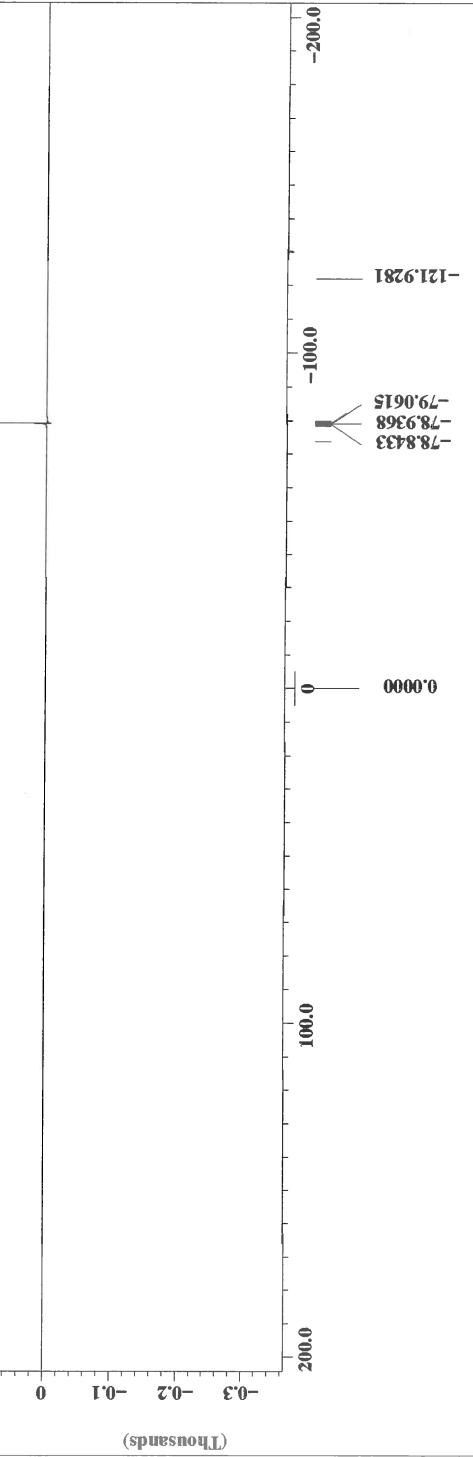
filename = SBIL16-3.jdf
Author = delta
Experiment = single_pulse.e
Sample_id = S#346613
Solvent = CHLOROFORM-D
Creation_time = 27-SEP-2015 09
Revision_time = 27-SEP-2015 09
Current_Time = 27-SEP-2015 09

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECX500

Field_strength = 11.7473579 [T]
X_acq_duration = 68.15744 [ms]
X_domain = 19F
X_freq = 470.62046084 [MHz]
X_offset = 16384
X_points = 0
X_Prescans = 14.67191255 [Hz]
X_resolution = 240.38461535 [kHz]
X_sweep = 19F
Irr_domain = 470.62046084 [MHz]
Irr_freq = 470.62046084 [MHz]
Irr_offset = 19F
Tri_domain = 470.62046084 [MHz]
Tri_freq = 5 [ppm]
Tri_offset = FALSE
Clipped = 1
Mod_return = 10
scans = 10
Total_scans = 10

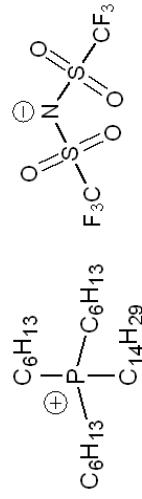
X_90_width = 13.08 [us]
X_acq_time = 68.15744 [ms]
X_angle = 45 [deg]
X_attn = 3 [dB]
X_pulse = 6.54 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recv_gain = 44
Relaxation_delay = 10 [s]
Repetition_time = 10.08815744 [s]
Temp_get = 21.71 [dc]

```



TPRCVD-3.[df]

TTP-NTf₂ (Recovered)



TTP-NTf₂

Trihexyl tetradecyl phosphonium bis(trifluoromethane)sulfonimide

32.56

```

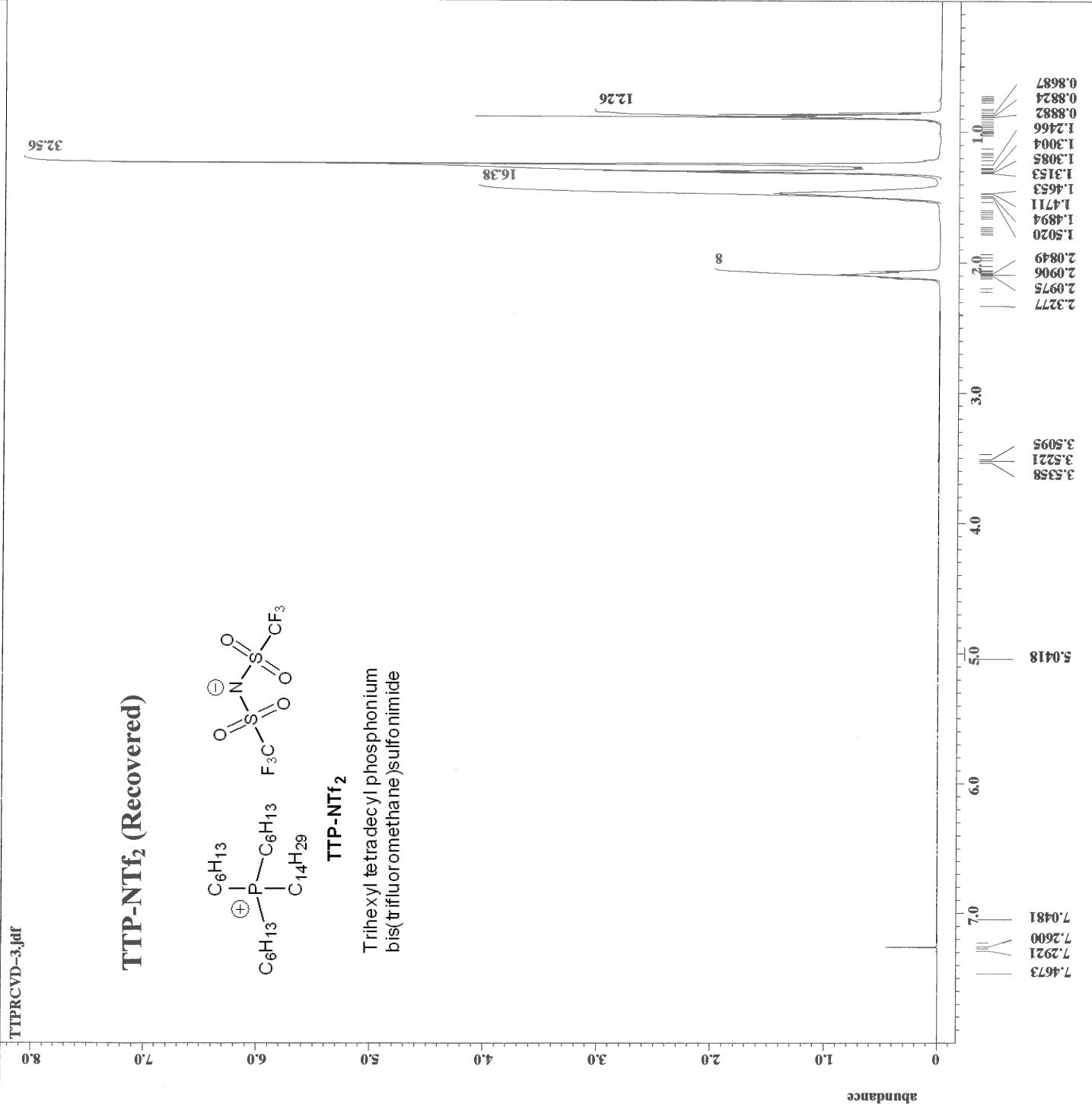
Filename = TTPRCVD-3.jdf
Author = delta
Experiment =
Sample_id = single_pulse.ex2
Solvent = S708075
Creation_time = 1-OCCT-2015 08:28:39
Revision_time = 30-SEP-2015 19:48:35
Current_time = 30-SEP-2015 19:49:11

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 11107
Dim_title = 1H
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
spectrometer = JNM-ECA500

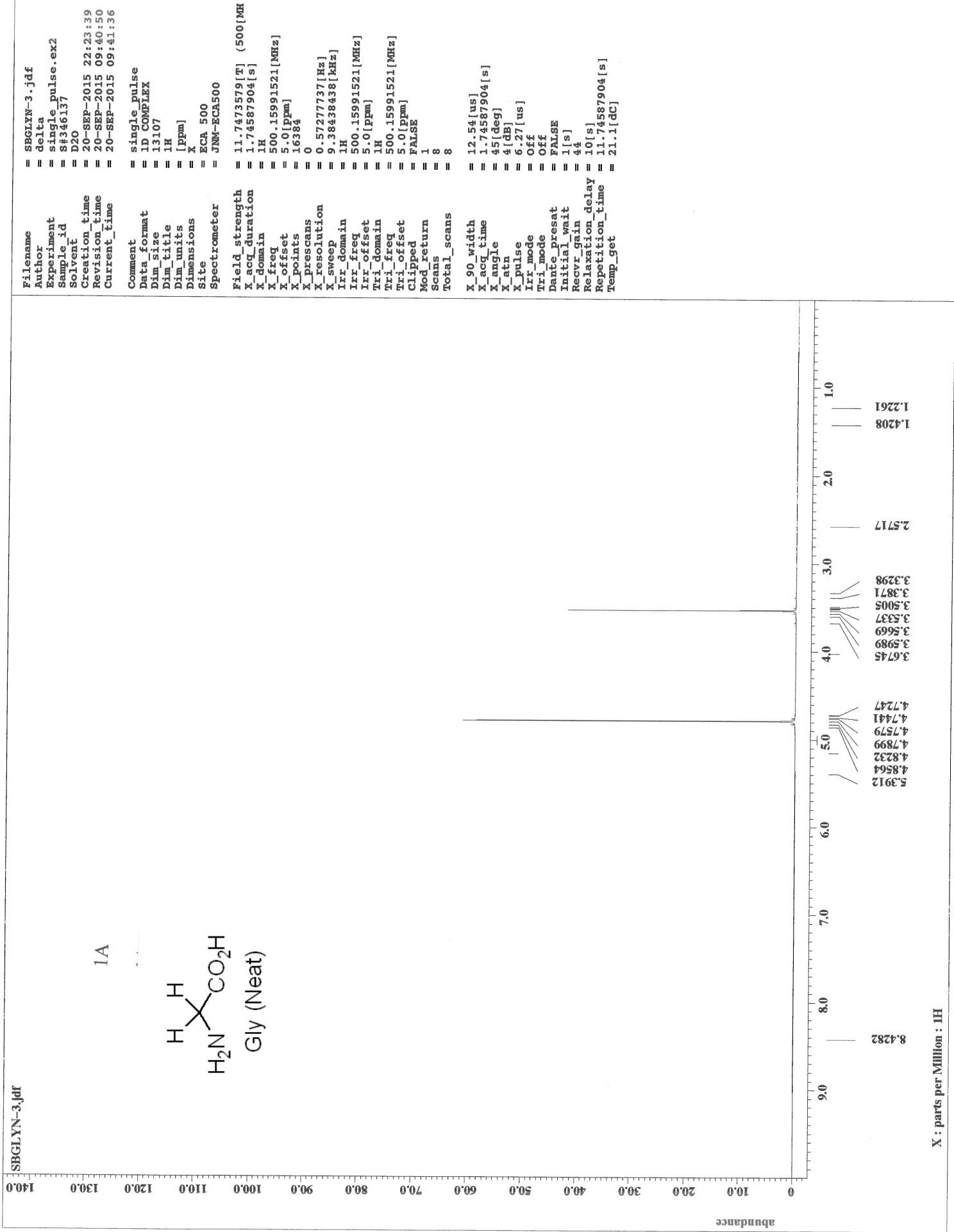
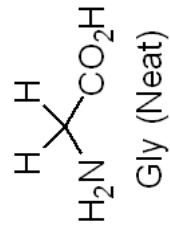
Field_strength = 11.7432579 [T] (500 [MHz])
X_acq_duration = 1.7457904 [s]
X_domain = 1H
X_freq = 500.15991521 [MHz]
X_offset = 5.0 [ppm]
X_pps = 16384
X_resolution = 0
X_sweep = 0.5727737 [Hz]
X_sweep = 9.38438438 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Tri_domain = 1H
Tri_freq = 500.15991521 [MHz]
Tri_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 15
Total_scans = 15

X_90_width = 12.54 [us]
X_acq_time = 1.7457904 [s]
X_angle = 95 [deg]
X_atn = 4 [dB]
X_pulse = 6.27 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recv_gain = 26
Relaxation_delay = 10 [s]
Relaxation_time = 11.74587904 [s]
Temp_Set = 21.6 [dc]

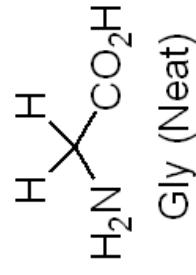
```



1A



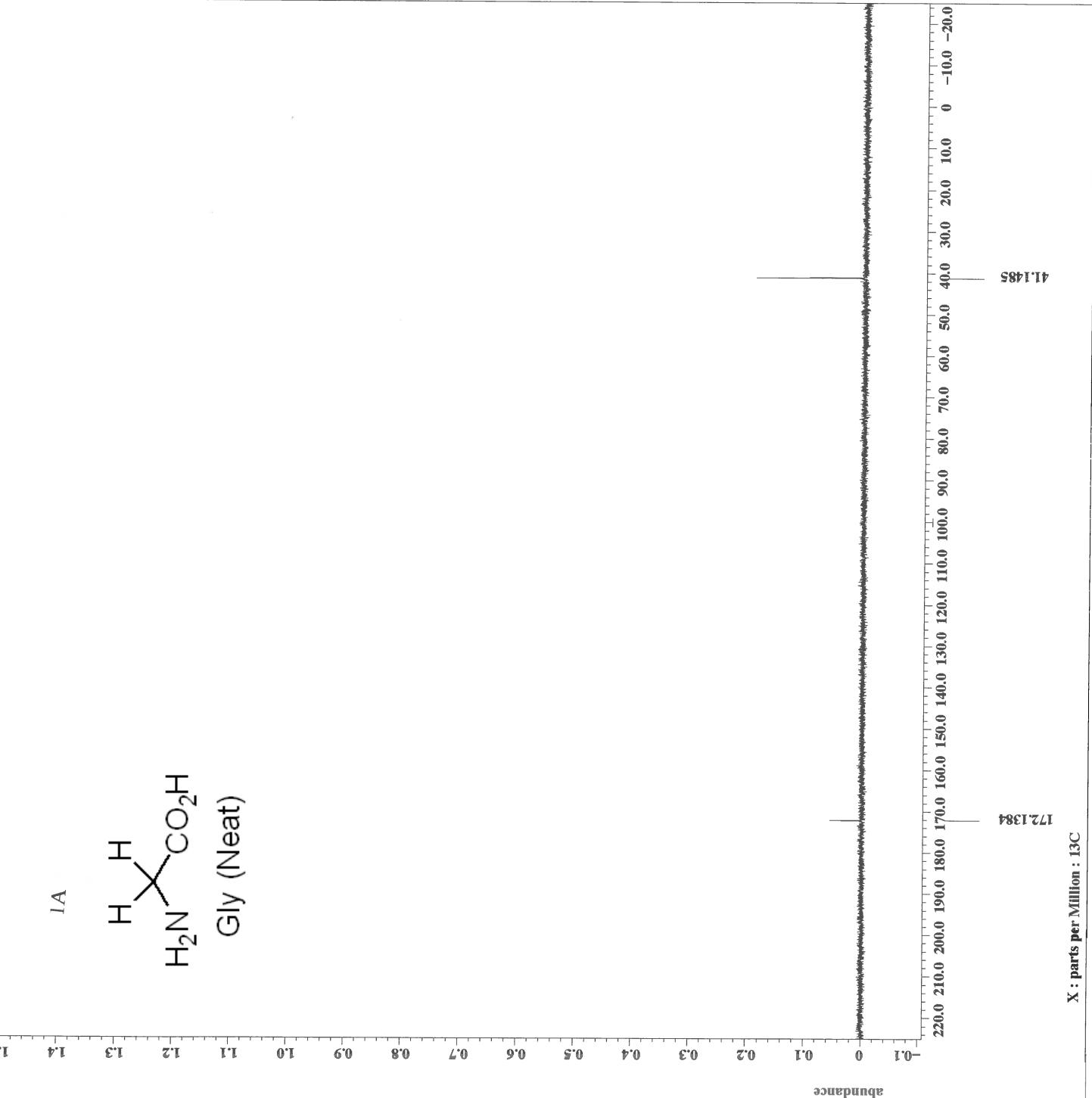
1A



```

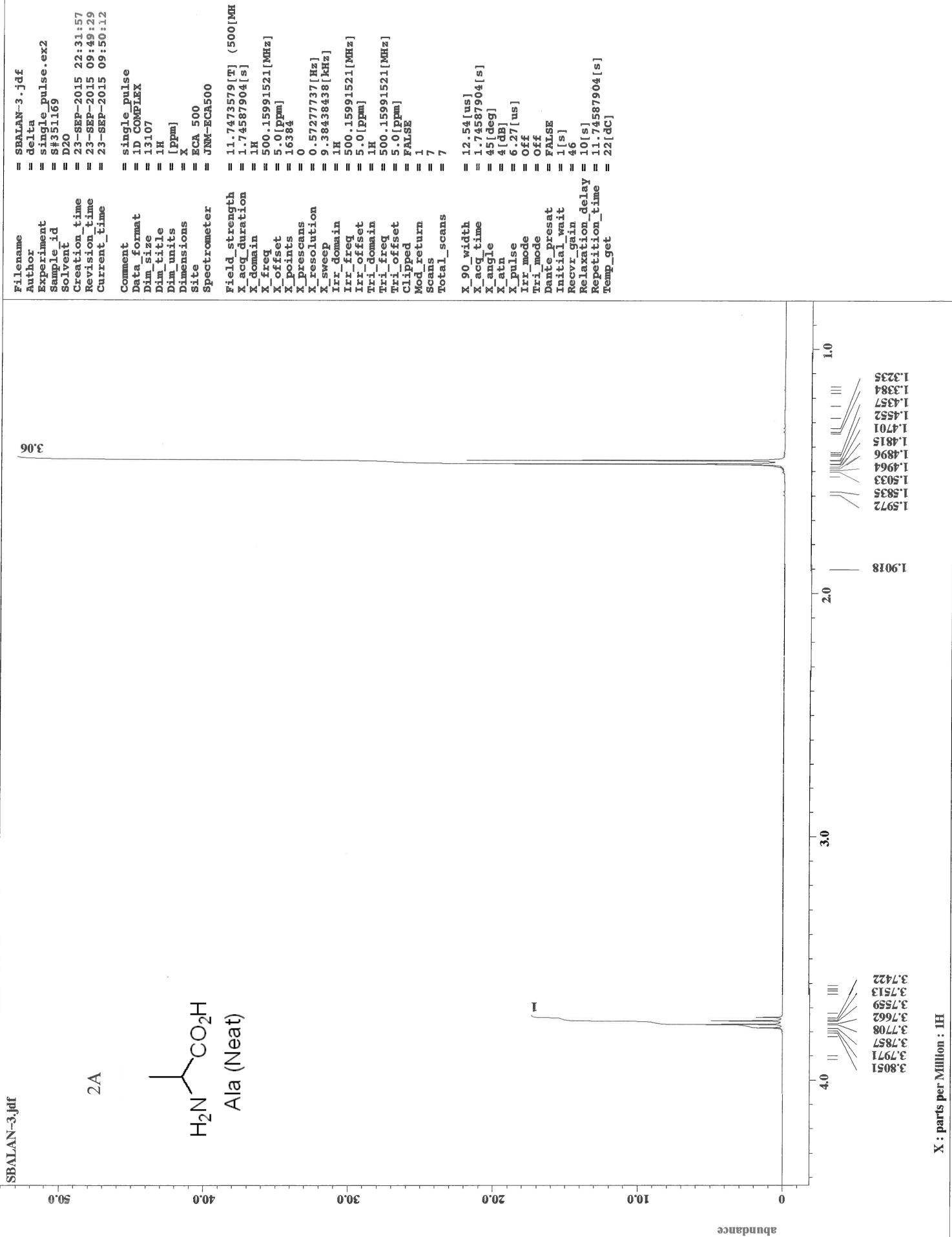
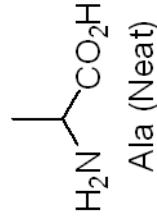
Filename = SBGLYNC-2.jdf
Author = delta
Experiment = single_pulse_decouple
Sample_id = S#48099
Solvent = D2O
Creation_time = 20-SEP-2015 22:29:05
Revision_time = 20-SEP-2015 09:45:19
Current_time = 20-SEP-2015 09:45:35
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500
Field_strength = 11.7473579 [T] (500 [MHz])
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 125.76539768 [MHz]
X_offset = 100 [PPM]
X_points = 32768
X_prescans = 4
X_resolution = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 10
Scans = 270
Total_scans = 270
X_90_width = 10.73 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.576666667 [us]
Irr_atn_dec = 20 [dB]
Irr_atn_noe = 20 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_time = 0.2 [s]
Recvr_gain = 50
Relaxation_delay = 0.2 [s]
Repetition_time = 1.03361792 [s]
Temp_get = 21.6 [deg]

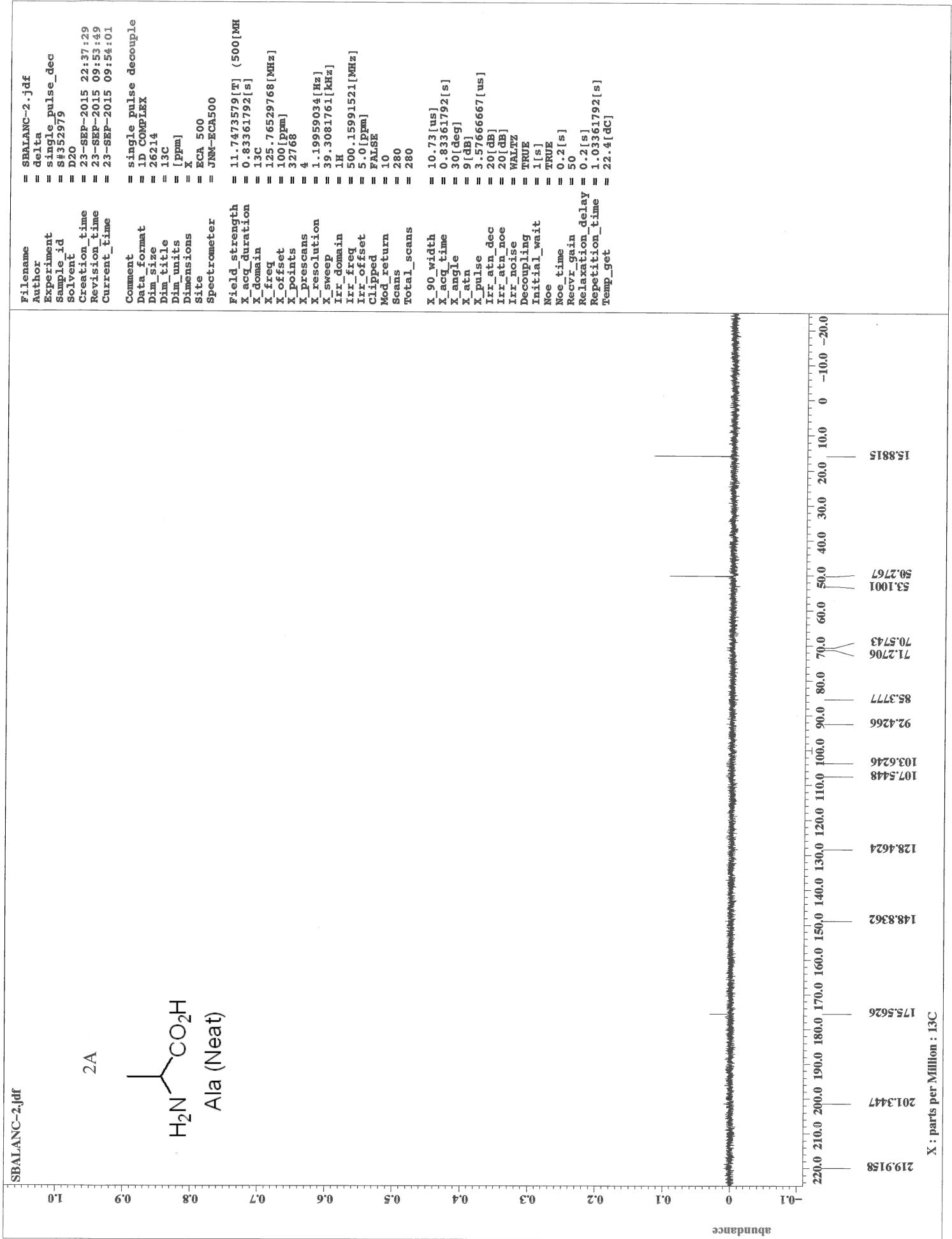
```



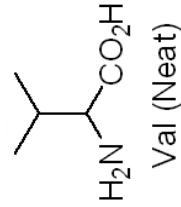
3.06

2A



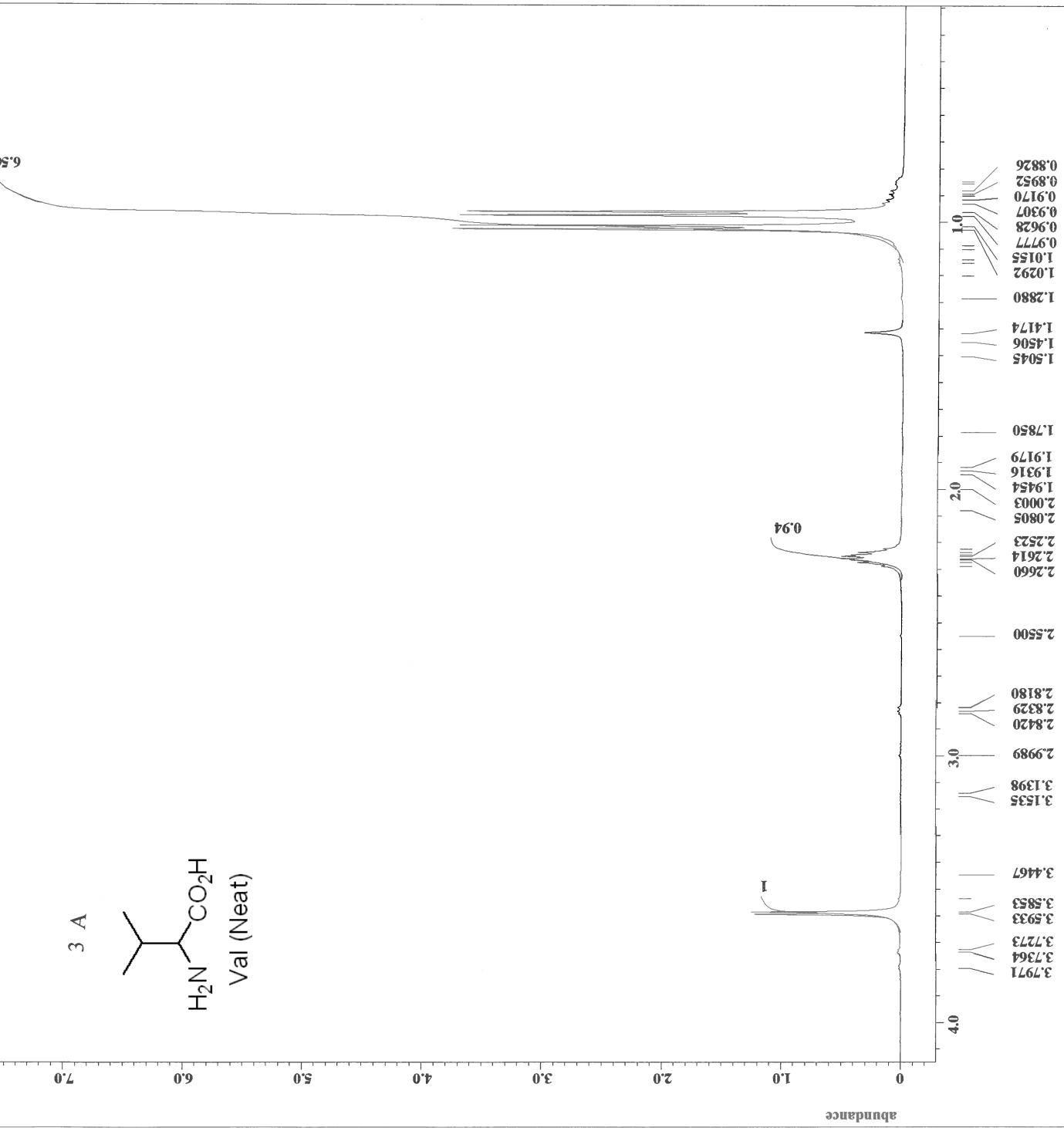


3 A



Val (Neat)

6.36



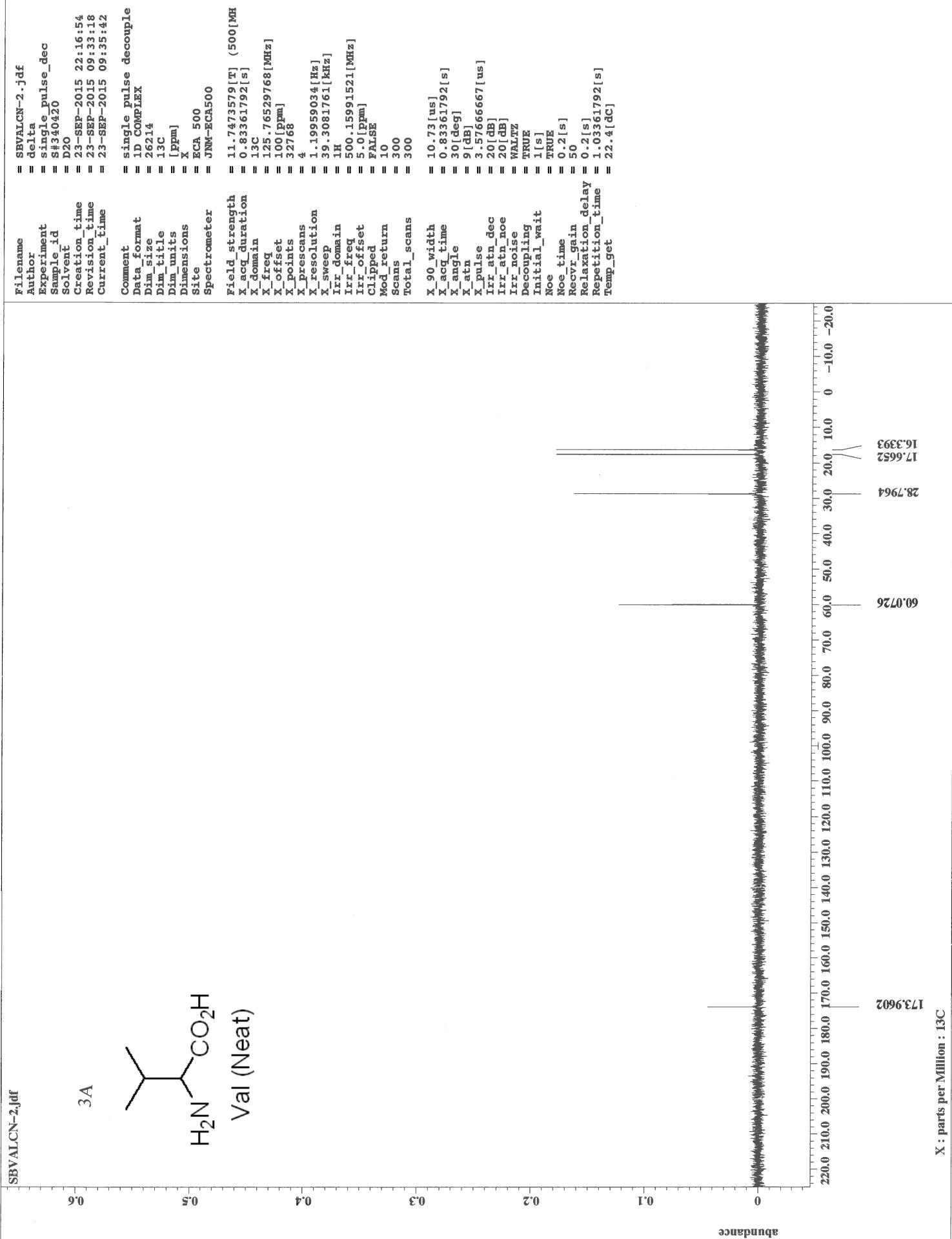
```

Filename = SBVALN-3.jdf
Author = delta
Experiment = single_pulse_ex2
Sample_id = S#138198
Solvent = D2O
Creation_time = 23-SEP-2015 22:10:56
Revision_time = 23-SEP-2015 09:28:38
Current_time = 23-SEP-2015 09:29:28
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] (500[MHz]
X_acq_duration = 1.74587904 [s]
X_domain = 1H
X_freq = 500.15991521 [MHz]
X_offset = 5.0 [PPM]
X_Points = 16384
X_prescans = 0
X_resolution = 0.57277737 [Hz]
X_sweep = 9.38438438 [KHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [PPM]
Tri_domain = 1H
Tri_freq = 500.15991521 [MHz]
Tri_offset = 5.0 [PPM]
Clipped = FALSE
Mod_return = 1
Scans = 10
total_scans = 10

X_90_width = 12.54 [us]
X_acq_time = 1.74587904 [s]
X_angle = 45 [deg]
X_atn = 4 [dB]
X_pulse = 6.27 [us]
Irr_mode = Off
Tri_mode = Off
Pulse_Presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 36
Relaxation_delay = 1.0 [s]
Repetition_time = 1.74587904 [s]
Temp_get = 21.9 [dC]

```



```

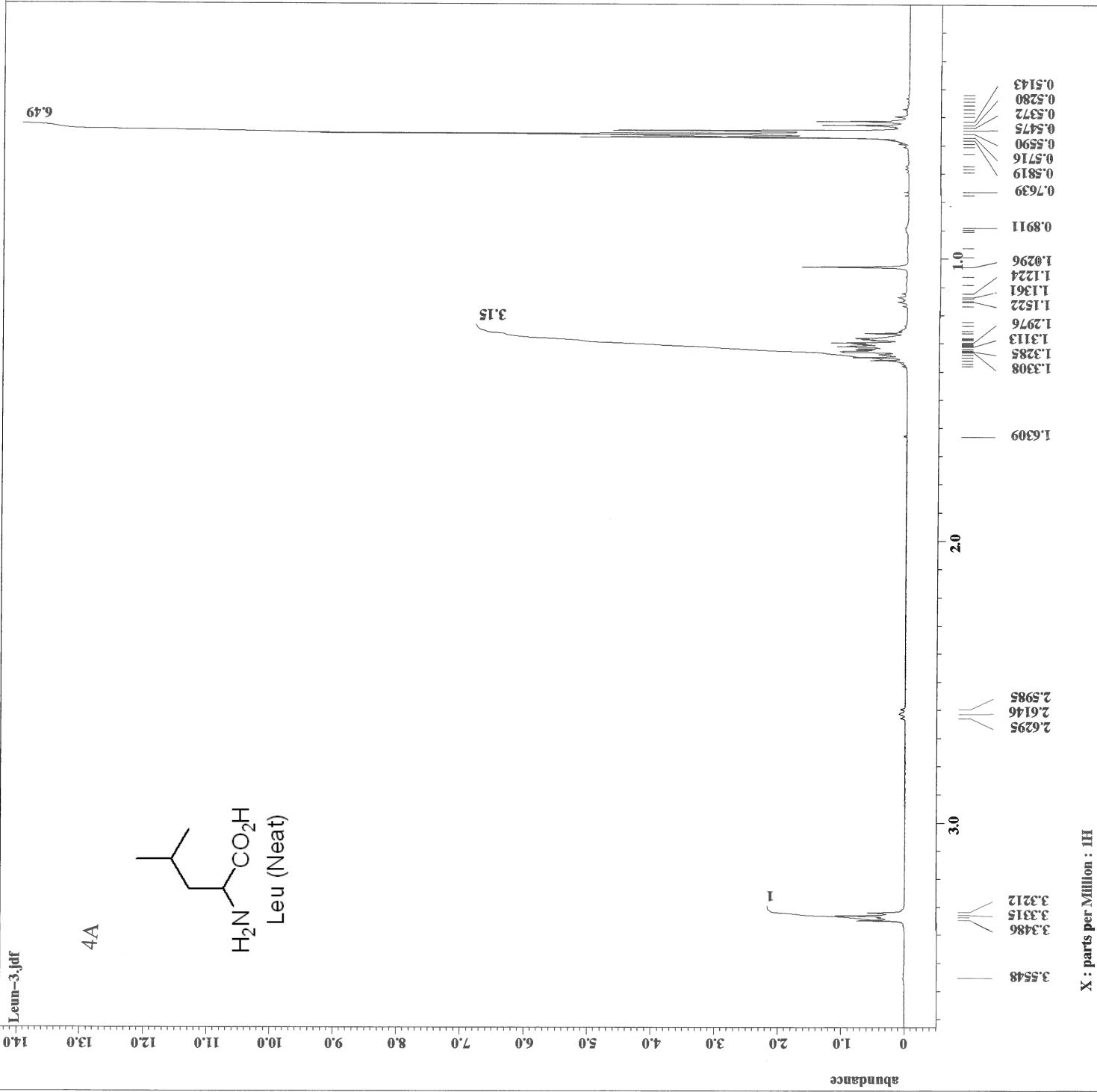
Filename = LeuN-3.jdf
Author = delta
Experiment = single_pulse_ex2
Sample_id = S#728776
Solvent = D2O
Creation_time = 24-SEP-2015 09:03:05
Revision_time = 23-SEP-2015 20:20:02
Current_time = 23-SEP-2015 20:21:18

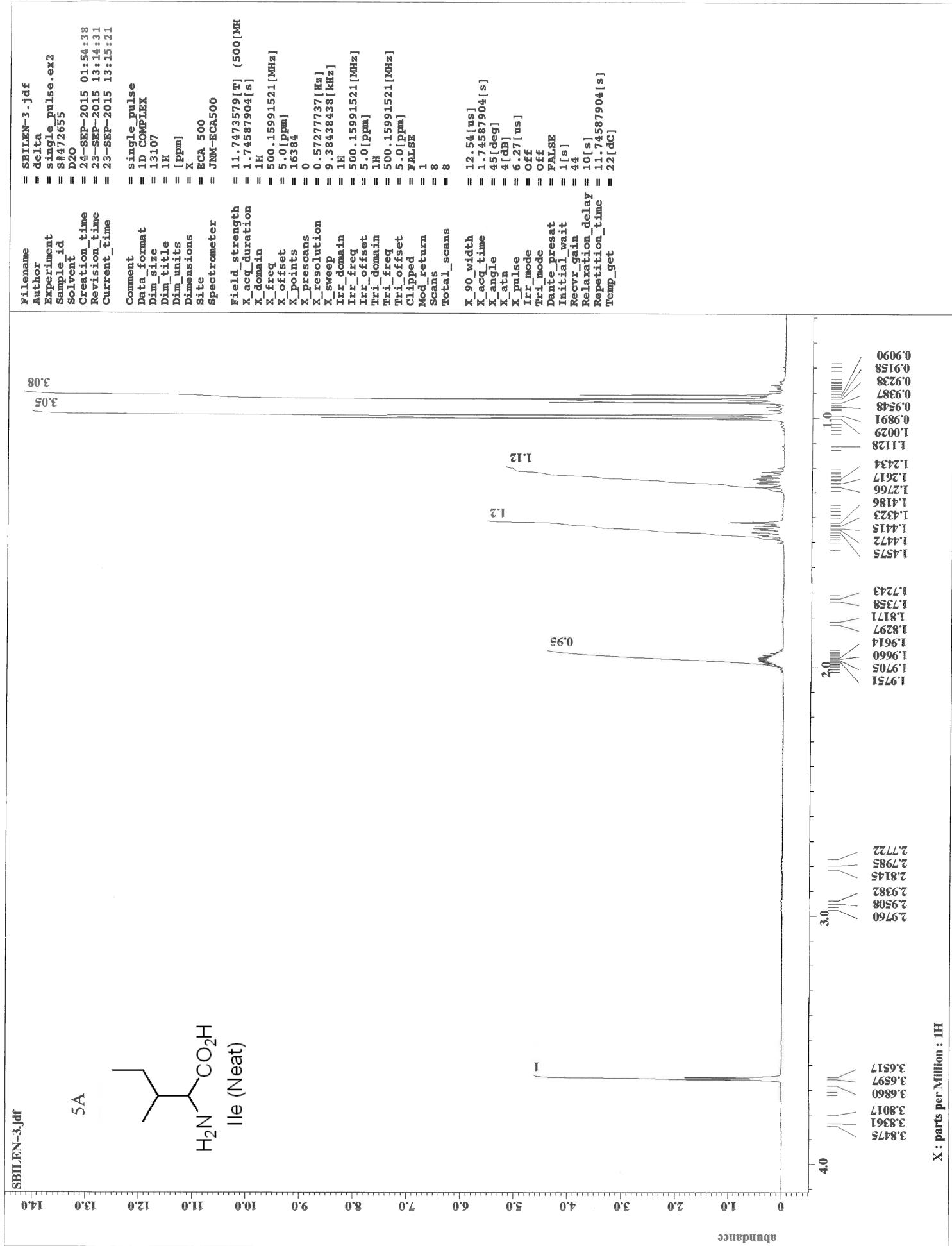
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

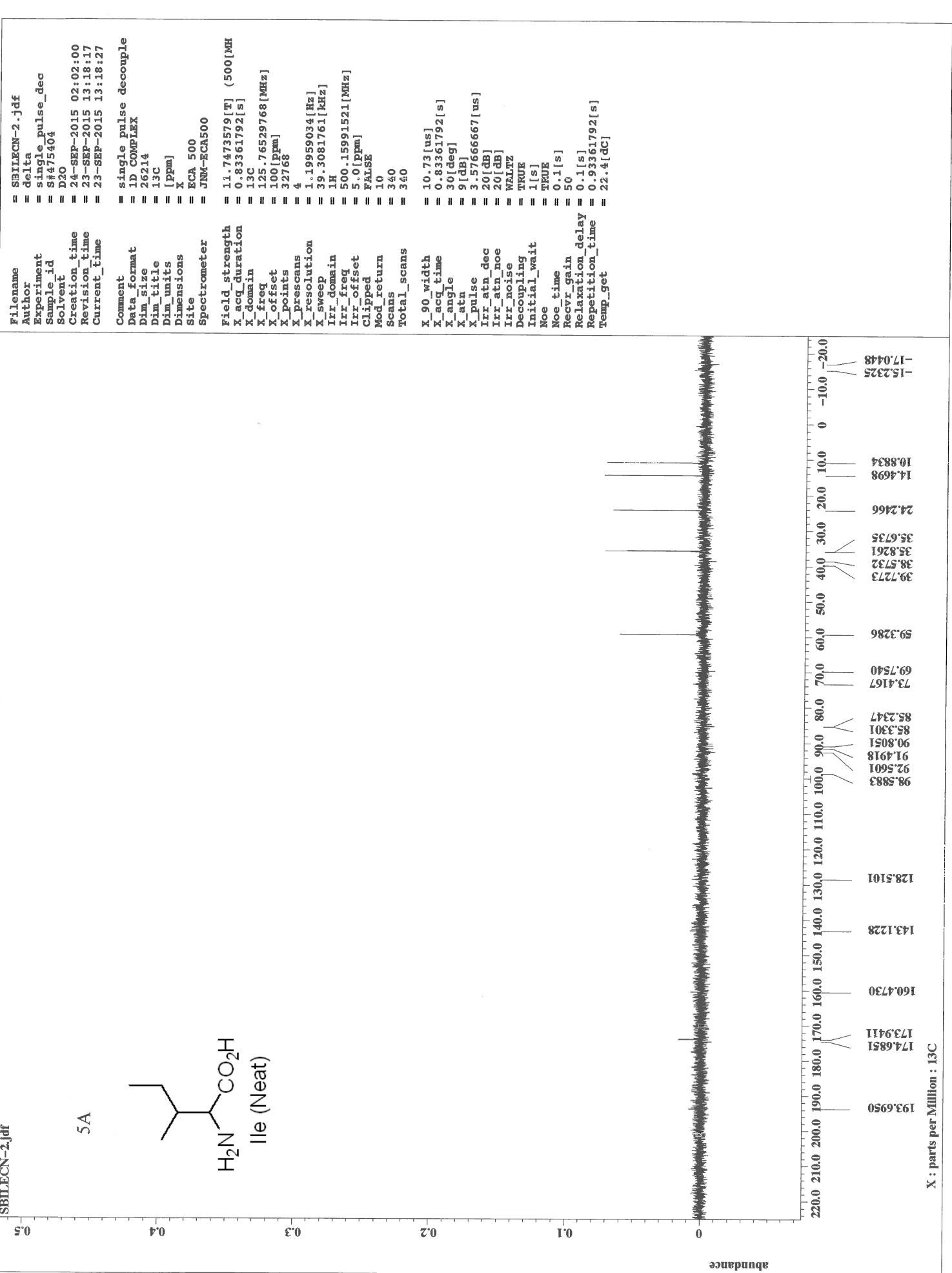
Field_strength = 11.7473579 [T] (500 [MHz])
X_acq_duration = 1.74587904 [s]
X_domain = 1H
X_freq = 500.15991521 [MHz]
X_offset = 5.0 [ppm]
X_points = 16384
X_prescans = 0
X_pulses = 0.57277737 [Hz]
X_sweep = 9.38438438 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Tri_domain = 1H
Tri_freq = 500.15991521 [MHz]
Tri_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 12.54 [us]
X_acq_time = 1.74587904 [s]
X_angle = 45 [deg]
X_atn = 4 [dB]
X_pulse = 6.27 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Revr_gain = 48
Relaxation_delay = 10 [s]
Repetition_time = 11.74587904 [s]
Temp_get = 22 [dC]

```







SBPHAN-3.indd

5.27

```

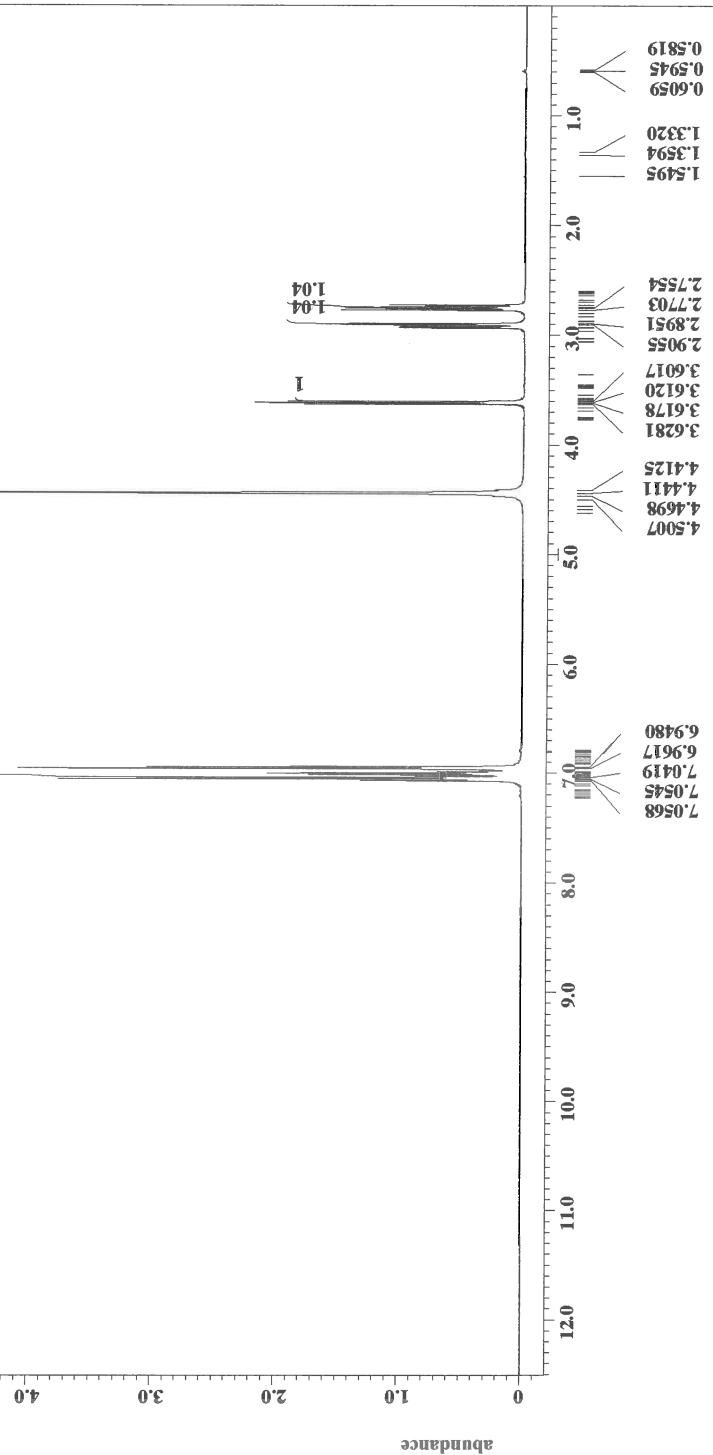
Filename = SBPHAN-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S347797
Solvent = D2O
Creation_time = 24-SEP-2015 22:26:17
Revision_time = 24-SEP-2015 09:44:10
Current_Time = 24-SEP-2015 09:44:46

```

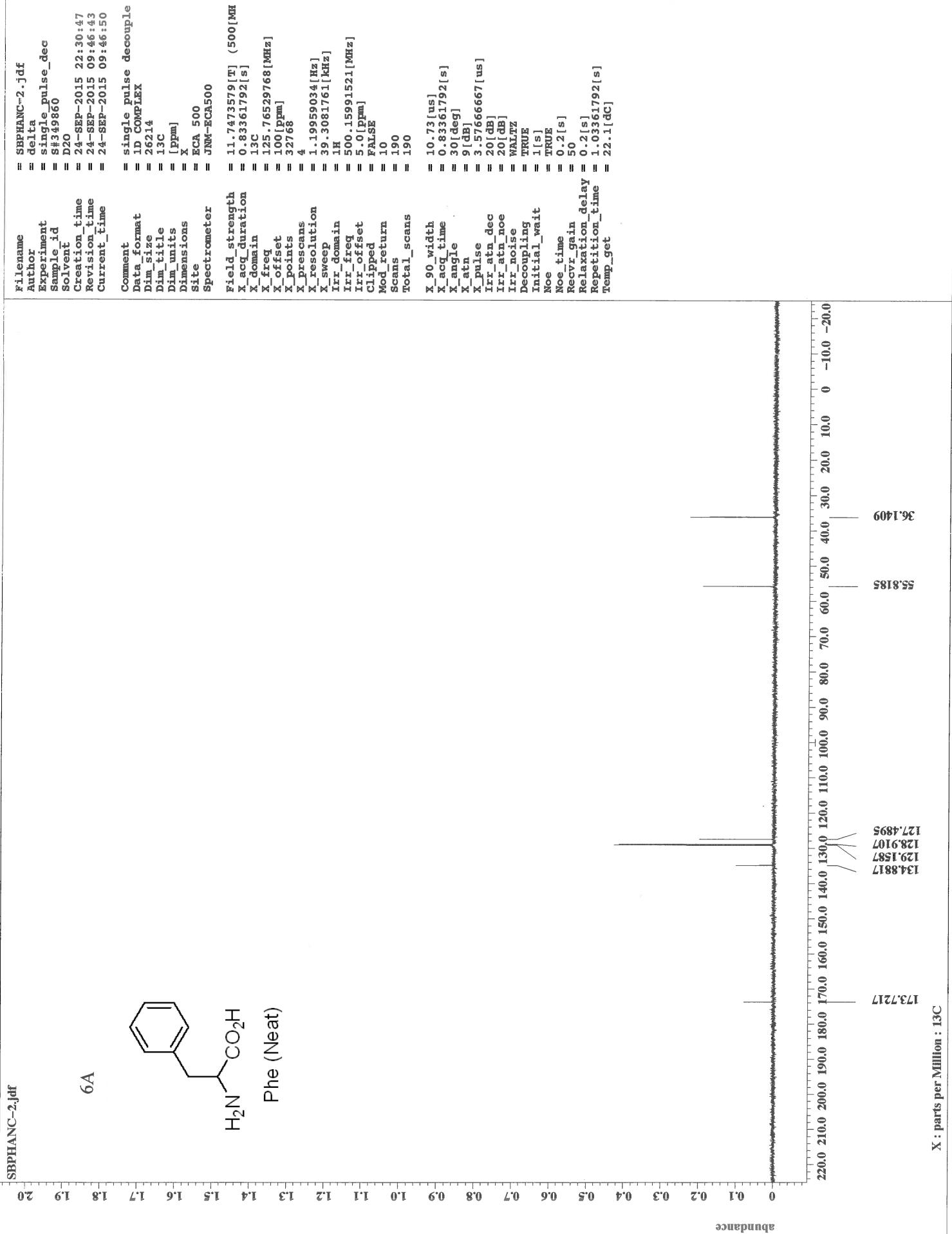
CC(C(=O)N)Cc1ccccc1

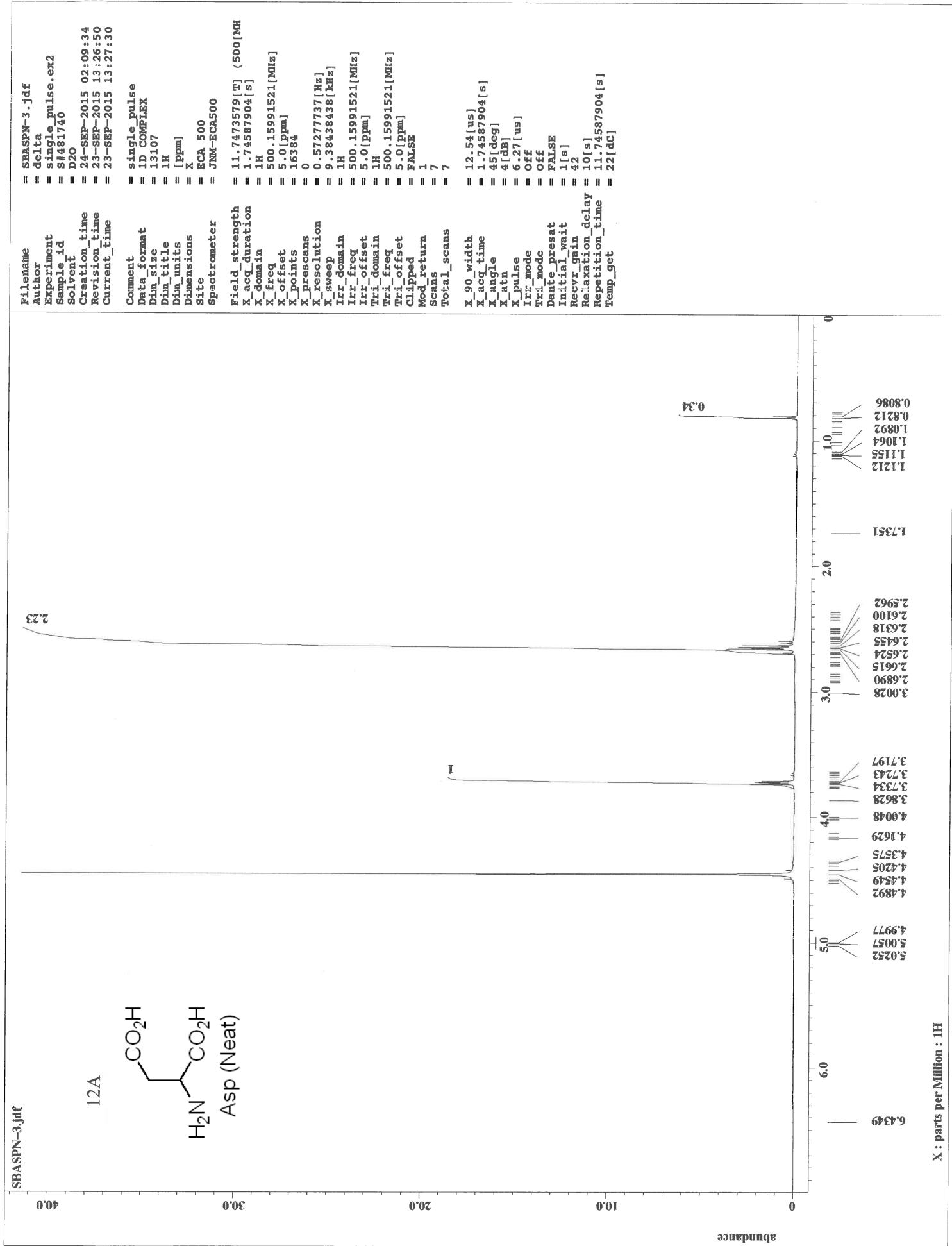
6A

Phe (Neat)

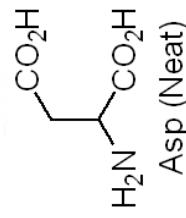


X : parts per Million : 1H





12A



```

Filename      = SBASPCN-2.jdf
Author        = delta
Experiment   = single_pulse_dec
Sample_id    = SH483593
Solvent      = D2O
Creation_time= 24-SEP-2015 02:17:04
Revision_time= 23-SEP-2015 13:33:04
Current_time = 23-SEP-2015 13:33:16

```

```

Comment      = single pulse decouple
Data_format = 1D COMPLEX
Dim_size    = 26214
Dim_title  = 13C
Dim_units  = [PPM]
Dimensions = X
Site        = ECA 500
Spectrometer = JNM-ECA500
Field_strength = 11.7473579[T] (500[MHz])
X_acq_duration = 0.83361792[s]
X_domain    = 13C
X_freq      = 125.76529768[MHz]
X_offset    = 100[ppm]
X_points    = 32768
X_resolution = 4
X_sweep     = 1.19959034[Hz]
Irr_domain = 1H
Irr_freq   = 500.15991521[MHz]
Irr_offset = 5.0[ppm]
Clipped     = FALSE
Mod_return = 10
scans       = 430
Total_scans = 430
X_90_width = 10.73[us]
X_acq_time = 0.83361792[s]
X_angle    = 30[deg]
X_atn     = 9[dB]
X_pulse    = 3.576666671[us]
Irr_atn_dec = 20[dB]
Irr_atn_noe = 20[dB]
Irr_noise  = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe        = TRUE
Noe_time   = 0.1[s]
Recurr_gain = 50
Relaxation_delay = 0.1[s]
Repetition_time = 0.93361792[s]
Temp_get   = 22.5[degC]

```



X : parts per Million : 13C

137.4475

133.3966

82.7642

82.7642

50.4770

12.6957

16.1390

23.4431

24.4472

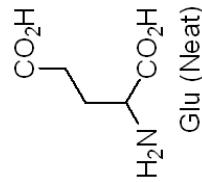
34.2428

34.2428

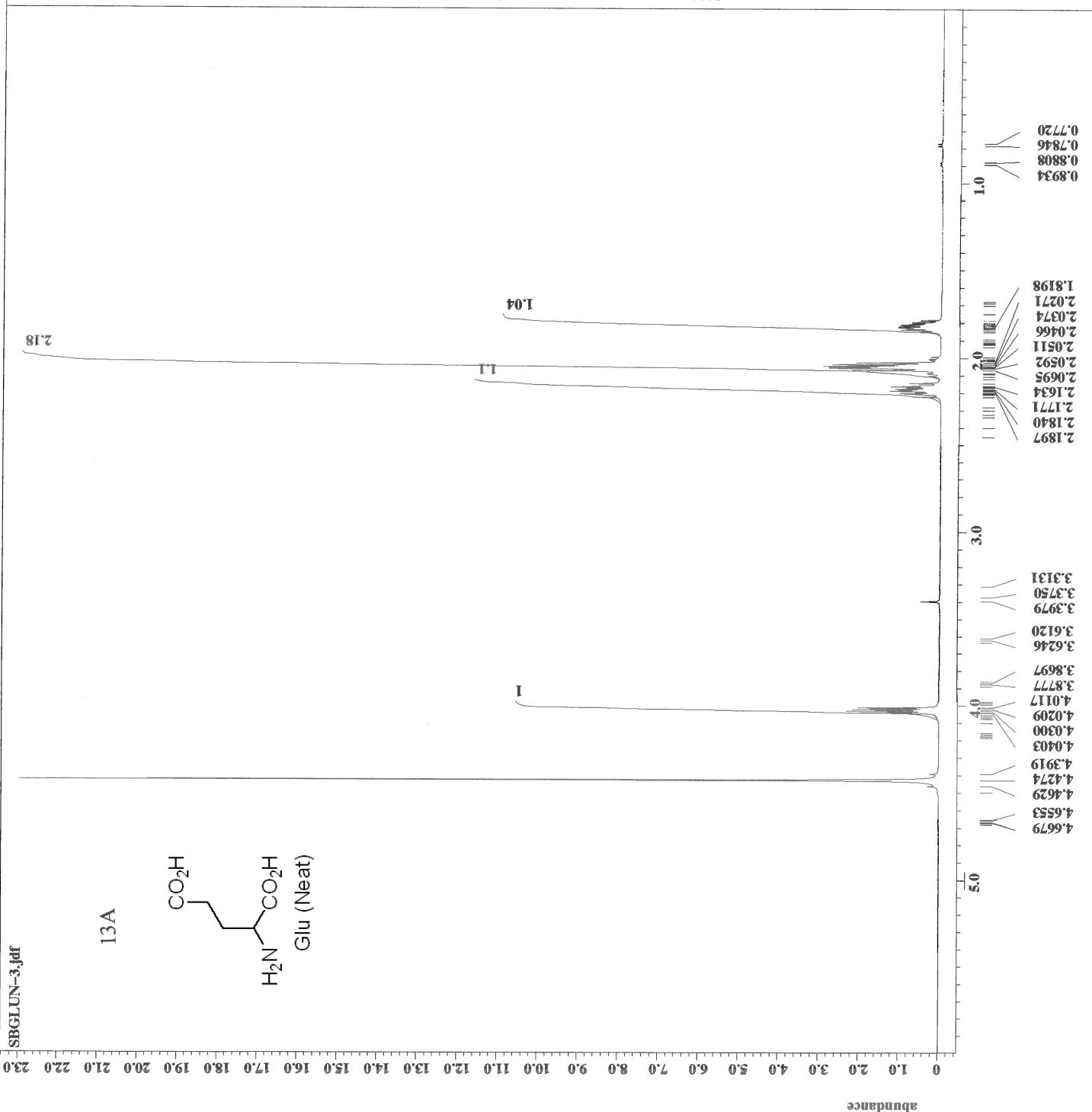
50.4770

abundance

13A



Glu (Neat)



```

= SBGLUN-3.jdf
  filename = delta
  author   = single_pulse.ex2
  sample_id = S#7.5952
  solvent  = D2O
  creation_time = 24-SEP-2015 08:40:44
  revision_time = 23-SEP-2015 19:57:41
  current_time = 23-SEP-2015 19:58:39

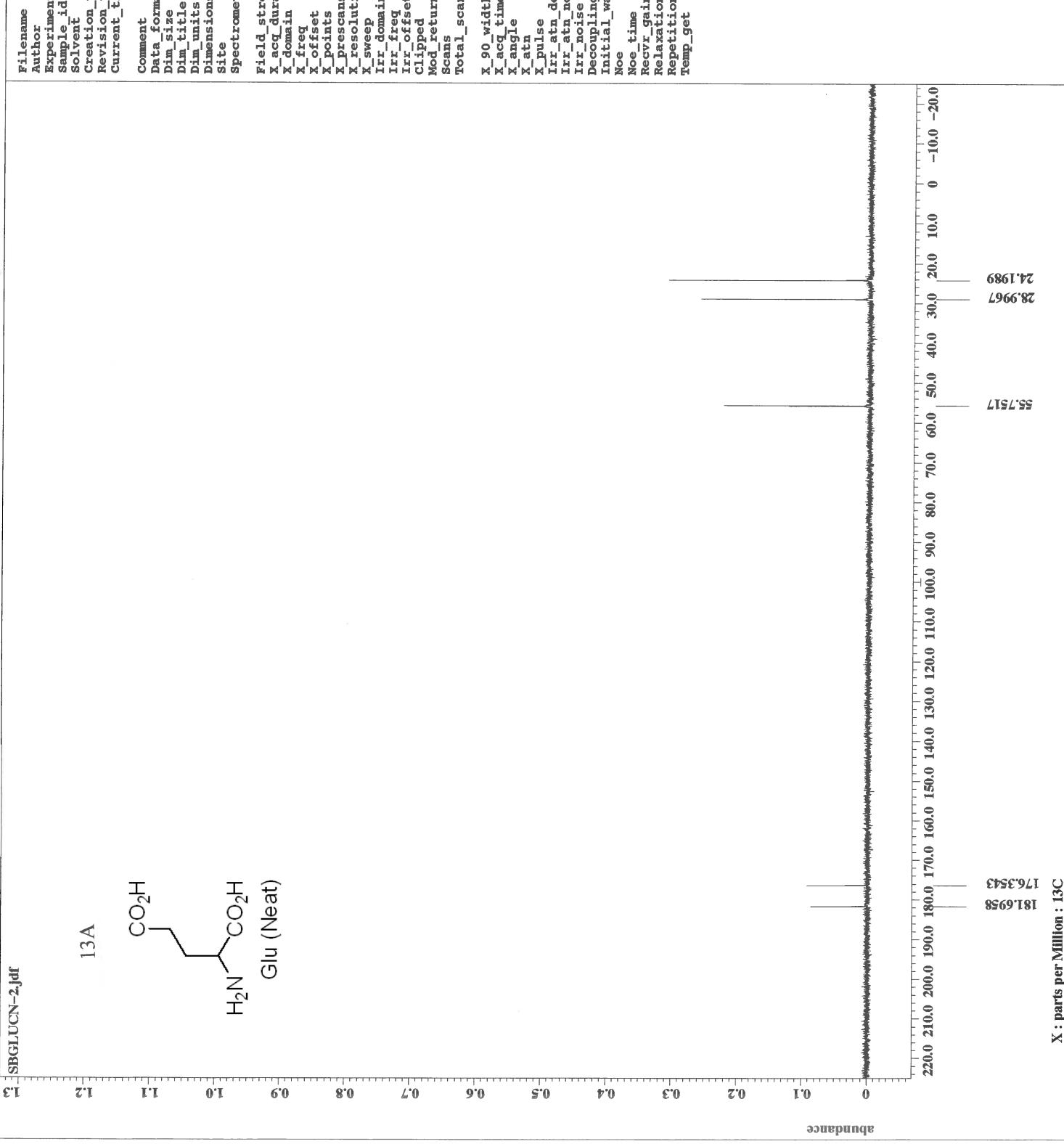
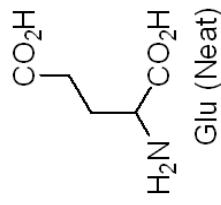
  comment = single_pulse
  data_format = 1D COMPLEX
  dim_size = 13107
  dim_title = 1H
  dim_units = [PPM]
  dimensions = X
  site = ECA 500
  spectrometer = JNM-ECA500

  field_strength = 11.7473579 [T] (500 [MHz])
  x_acq_duration = 1.74587904 [s]
  x_domain = 1H
  x_freq = 500.15991521 [MHz]
  x_offset = 5.0 [ppm]
  x_points = 16384
  x_resolution = 0.57277737 [Hz]
  x_sweep = 9.38438438 [MHz]
  irr_domain = 1H
  irr_freq = 500.15991521 [MHz]
  irr_offset = 5.0 [ppm]
  tri_domain = 1H
  tri_freq = 500.15991521 [MHz]
  tri_offset = 5.0 [ppm]
  clipped = FALSE
  mod_return = 1
  scans = 11
  total_scans = 11

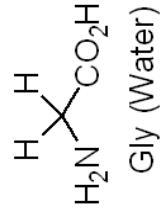
  x90_width = 12.54 [us]
  x_acq_time = 1.74587904 [s]
  x_angle = 45 [deg]
  x_atn = 4 [dB]
  x_pulse = 6.27 [us]
  irr_mode = Off
  tri_mode = Off
  dante_presat = FALSE
  initial_wait = 1 [s]
  recvr_gain = 38
  relaxation_delay = 10 [s]
  repetition_time = 11.74587904 [s]
  temp_get = 21.9 [dC]

```

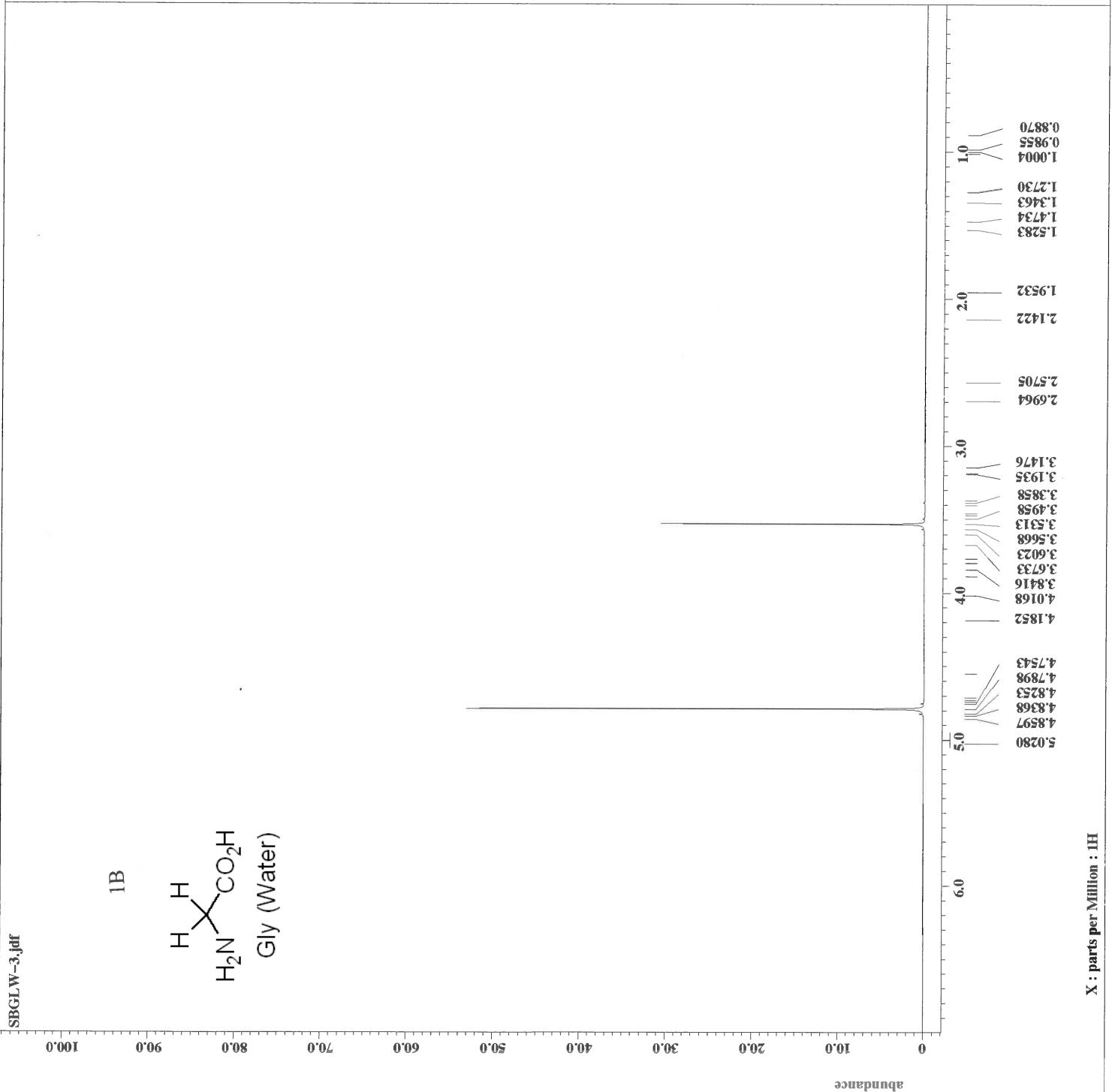
13A



B
1



Gly (Water)



```

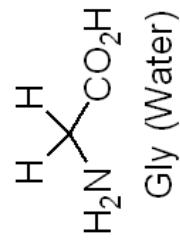
Filename = SBGLW-3-jdf
Author = delta
Experiment = single_pulse.e
Sample_id = S#356998
Solvent = D2O
Creation_time = 5-SEP-2015 22
Revision_time = 5-SEP-2015 10
Current_time = 5-SEP-2015 10

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

Field_strenght = 11.7473579 [T]
X_acq_duration = 1.74587904 [s]
X_domain = 1H
X_freq = 500.15991521 [MHz]
X_offset = 5.0 [ppm]
X_points = 16384
X_presses = 0
X_resolution = 0.57277737 [Hz]
X_sweep = 9.38438438 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Tri_domain = 1H
Tri_freq = 500.15991521 [MHz]
Tri_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 10
Total_scans = 10

X90_width = 1.254 [us]
X_acq_time = 1.74587904 [s]
X_angle = 45 [deg]
X_atm = 4 [dB]
X_pulse = 6.27 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recur_gain = 40
Relaxation_delay = 10 [s]
Repetition_time = 11.7587904 [s]
T1_min = 21.0
T1_max = 21.0

```



Filename

```

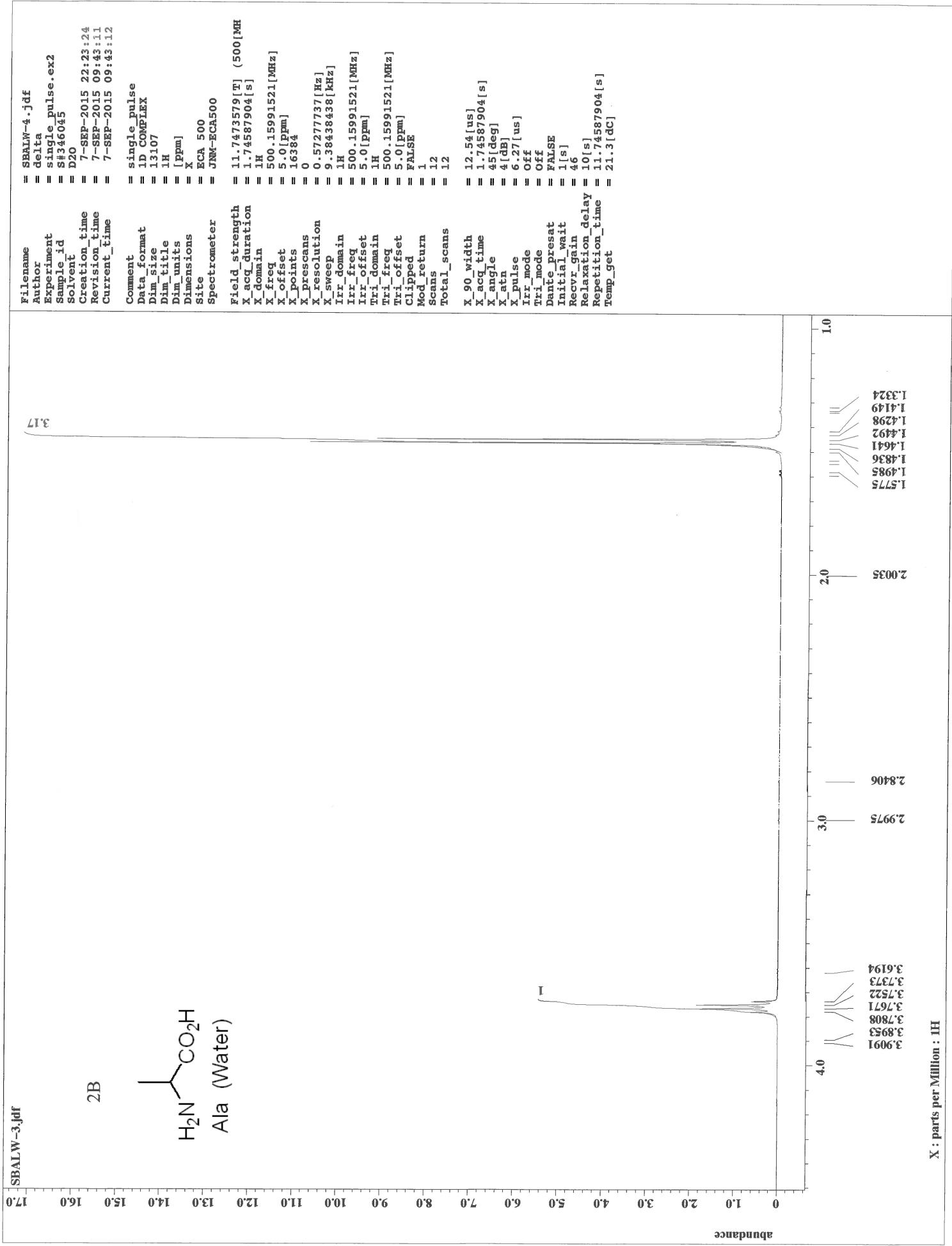
SBGLWC-2.jdf
  = delta
  = single_pulse_dec
Author
Experiment
Sample_id
  = S#339532
Solvent
D2O
Creation_time
  = 5-SEP-2015 22:49:11
Revision_time
  = 5-SEP-2015 10:05:57
Current_time
  = 5-SEP-2015 10:06:07
Comment
  = single pulse decouple
Data_format
  = 1D COMPLEX
Dim_size
  = 26214
Dim_title
  = 13C
Dim_units
  = [ppm]
Dimensions
  = X
Site
  = ECA 500
Spectrometer
  = JNM-ECA500
Field_strength
  = 11.7473579 [T] (500 [MHz])
X_acq_duration
  = 0.83361792 [s]
X_domain
  = 13C
X_freq
  = 125.76529768 [MHz]
X_offset
  = 100 [ppm]
X_points
  = 32768
X_prescans
  = 4
X_resolution
  = 1.19959034 [Hz]
X_sweep
  = 39.3081761 [kHz]
Irr_domain
  = 1H
Irr_freq
  = 500.15991521 [MHz]
Irr_offset
  = 5.0 [ppm]
Clipped
  = FALSE
Mod_return
  = 10
Scans
  = 130
Total_scans
  = 130
X_90_width
  = 10.73 [us]
X_acq_time
  = 0.83361792 [s]
X_angle
  = 30 [deg]
X_atn
  = 9 [dB]
X_pulse
  = 3.57666667 [us]
Irr_atn_dec
  = 20 [dB]
Irr_atn_noe
  = 20 [dB]
Irr_noise
  = WALTZ
Decoupling
  = TRUE
Initial_wait
  = 1 [s]
Noe
  = TRUE
Noe_time
  = 2 [s]
Reovr_gain
  = 50
Relaxation_delay
  = 2 [s]
Repetition_time
  = 2.83361792 [s]
Temp_get
  = 21.5 [dC]

```

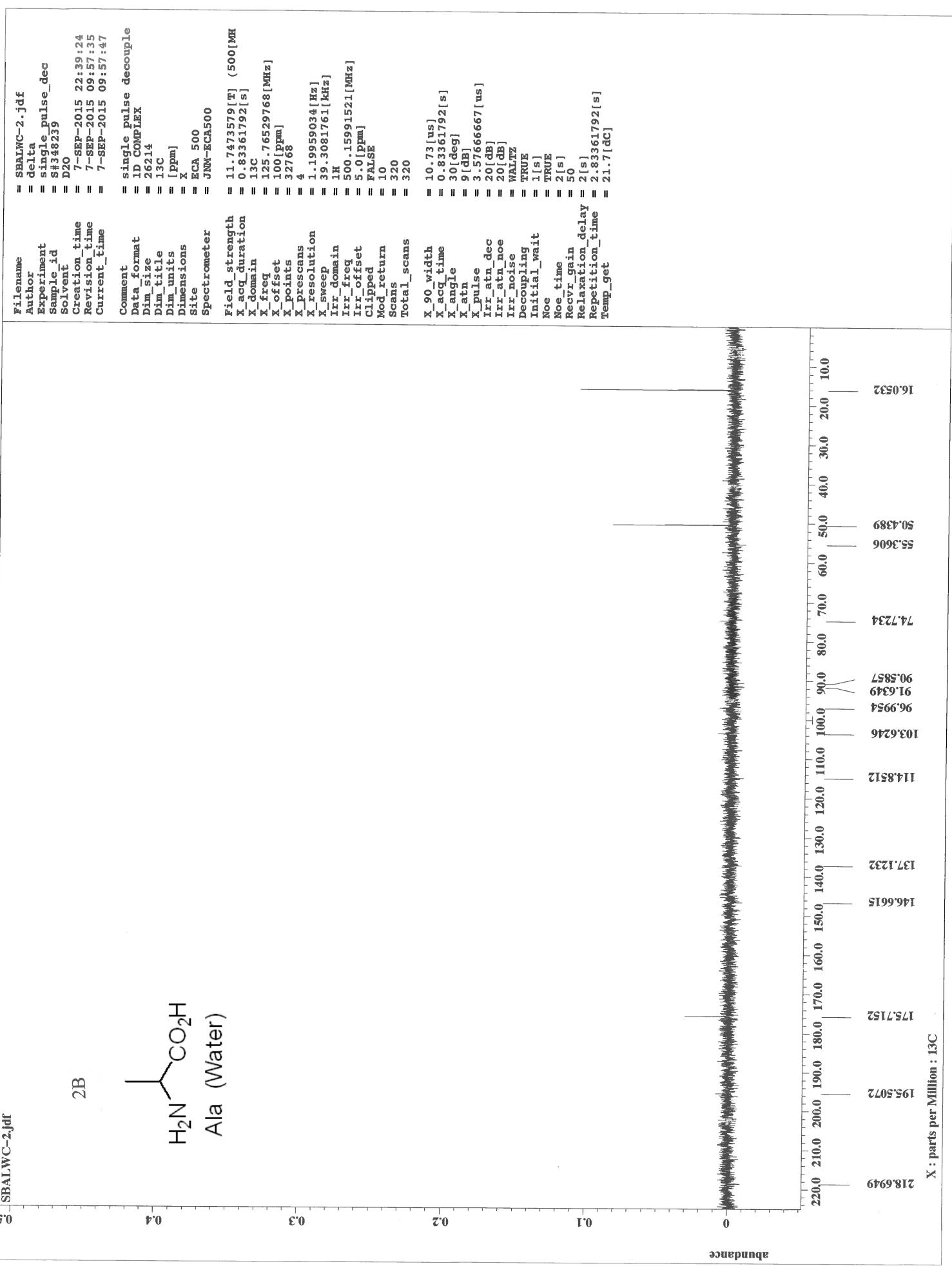
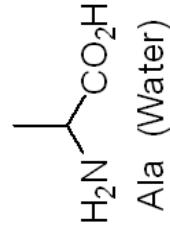


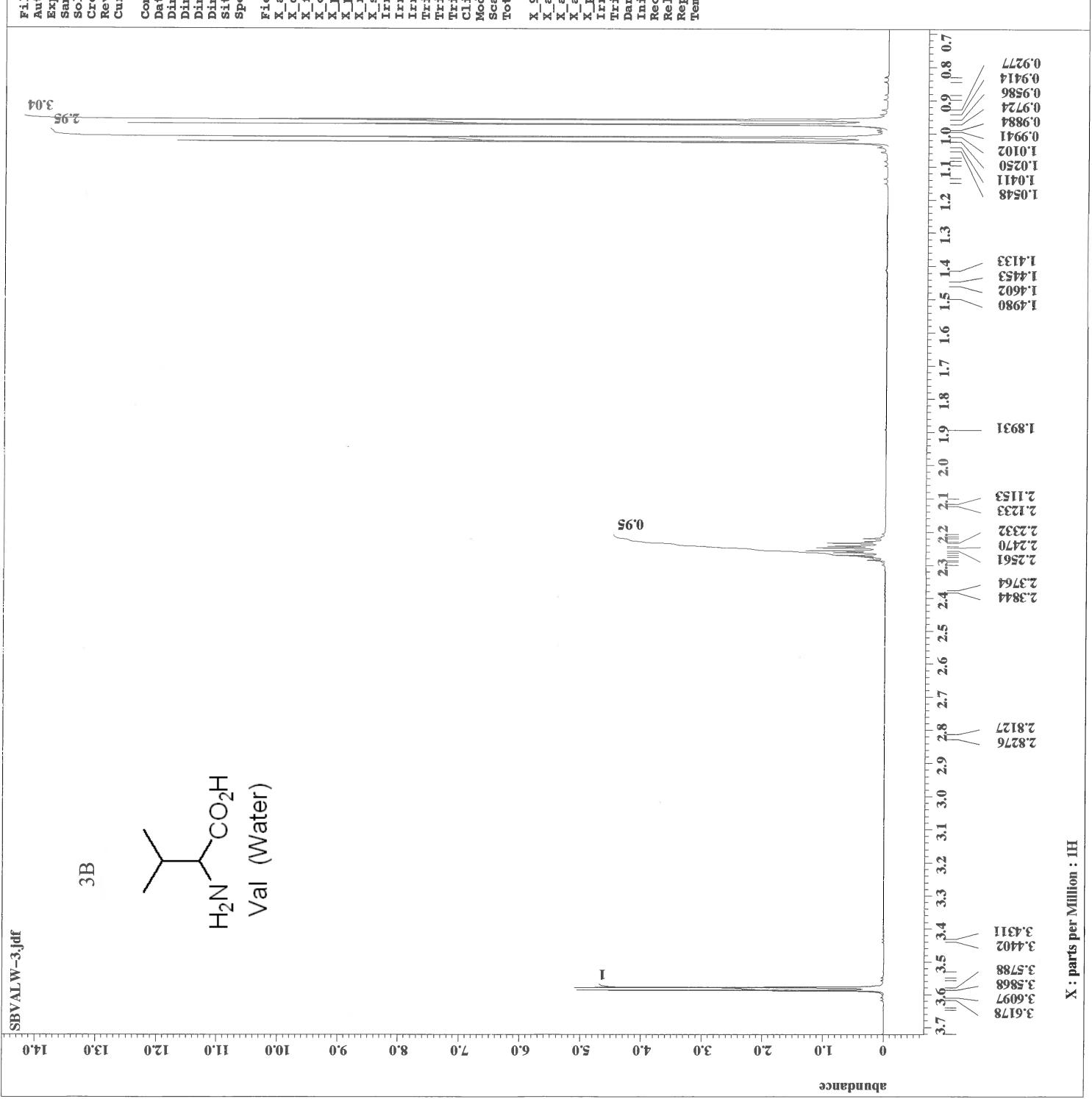
172.1574
X : parts per Million : 13C

41.1581



2B





```

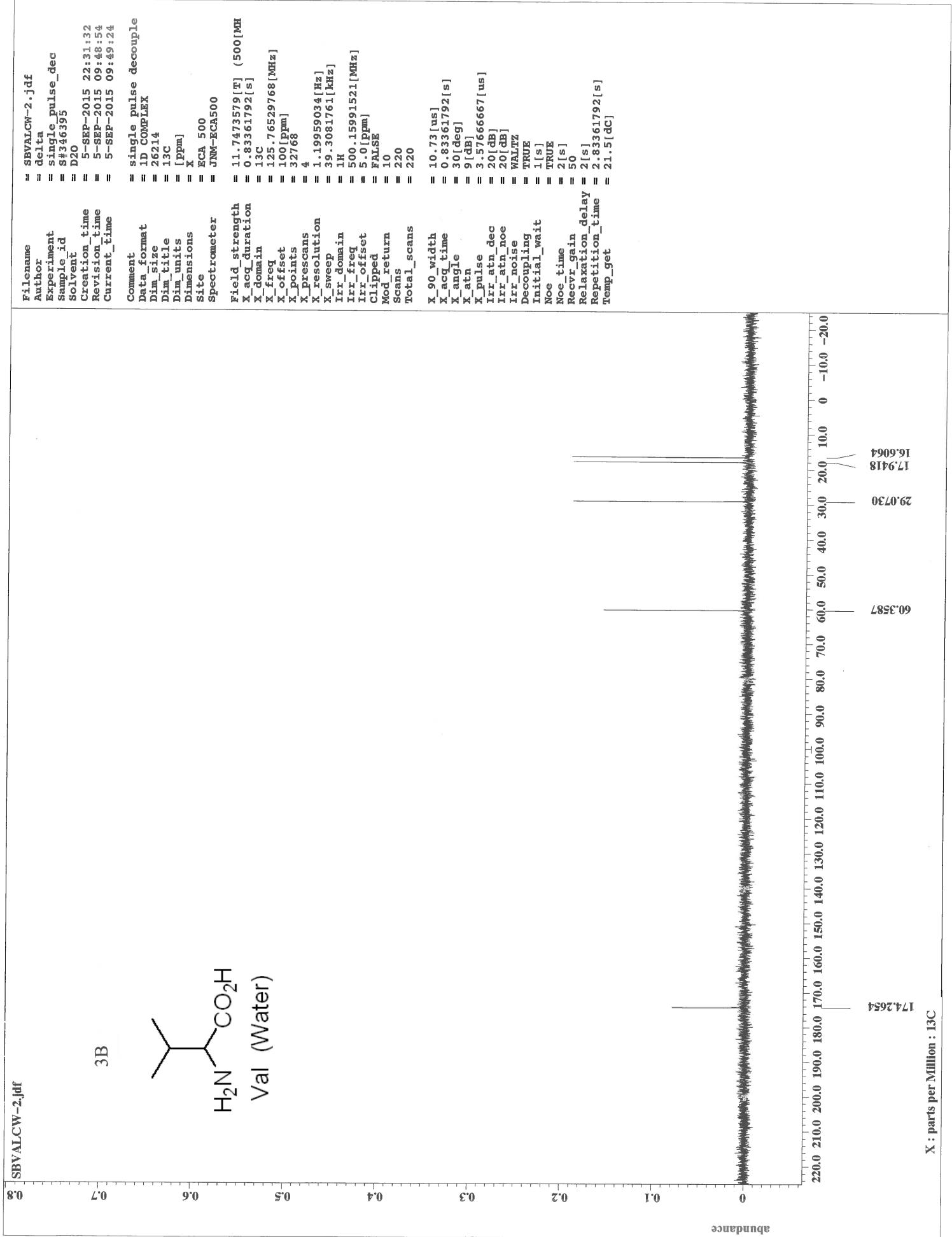
SBVALW-3.jdf
  = SBVALW-3.jdf
  Author      = delta
  Experiment = single_pulse.ex2
  Sample_id   = S1344173
  Solvent     = D2O
  Creation_time = 5-SEP-2015 22:20:08
  Revision_time = 5-SEP-2015 09:43:45
  Current_time  = 5-SEP-2015 09:44:35

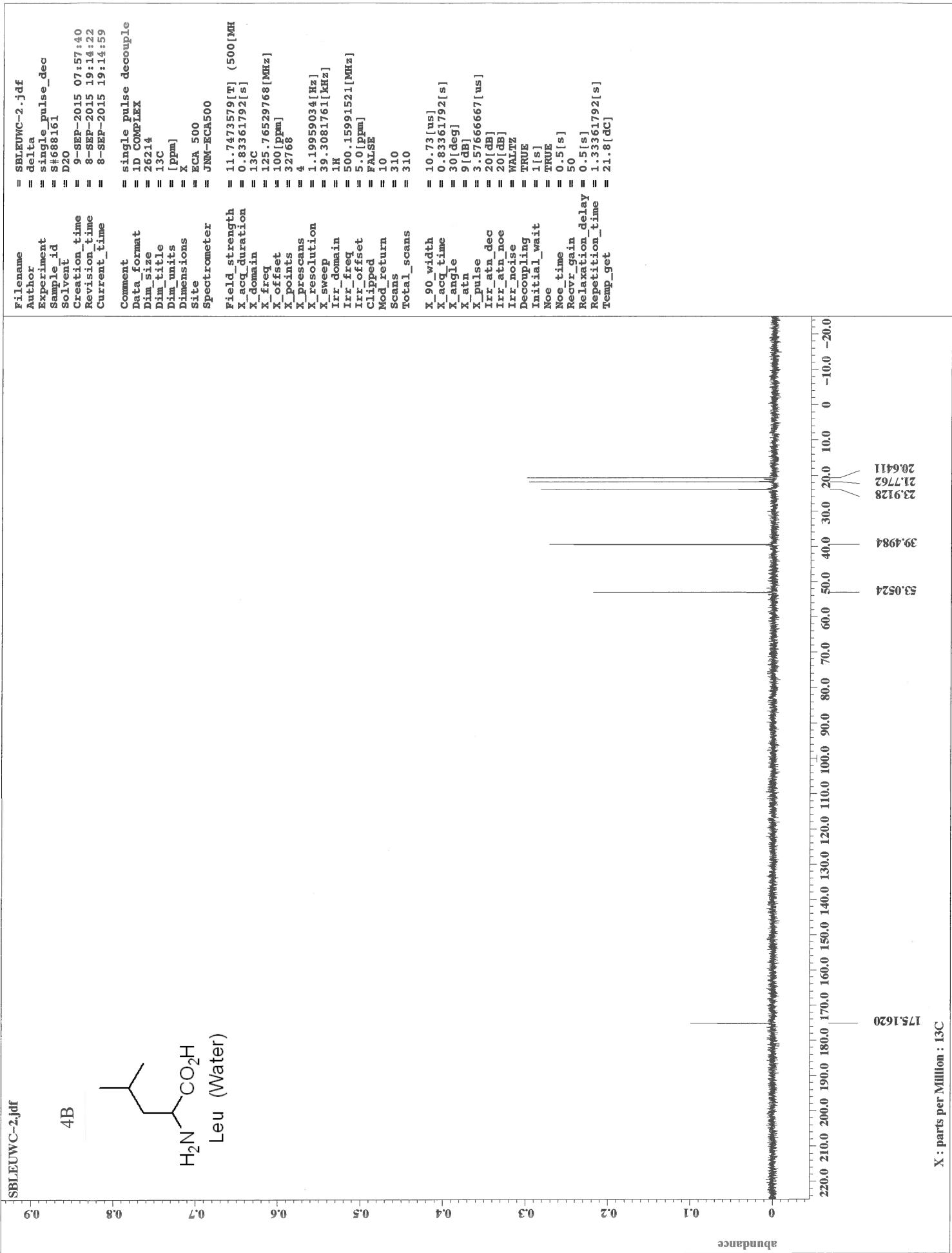
  Comment      = single_pulse
  Data_format = 1D COMPLEX
  Dim_size    = 13107
  Dim_title   = 1H
  Dim_units   = [PPM]
  Dimensions  = X
  Site        = ECR 500
  Spectrometer = JNM-ECR500

  Field_strength = 11.7473579 [T] (500 [MHz])
  X_acq_duration = 1.74581904 [s]
  X_domain     = 1H
  X_freq        = 500.15991521 [MHz]
  X_offset      = 5.0 [ppm]
  X_points      = 16384
  X_prescans   = 0
  X_resolution = 0.5727737 [Hz]
  X_sweep       = 9.38438438 [kHz]
  Irr_domain   = 1H
  Irr_freq     = 500.15991521 [MHz]
  Irr_offset   = 5.0 [ppm]
  Tri_domain   = 1H
  Tri_freq     = 500.15991521 [MHz]
  Tri_offset   = 5.0 [ppm]
  Clipped      = FALSE
  Mod_return   = 1
  Scans        = 10
  Total_scans  = 10

  X_90_width   = 12.54 [us]
  X_acq_time   = 1.74581904 [s]
  X_angle       = 45 [deg]
  X_athn       = 4 [dB]
  X_pulse      = 6.27 [us]
  Irr_mode     = Off
  Tri_mode     = Off
  Dant_Presat = FALSE
  Initial_wait = 1 [s]
  Recvr_gain   = 40
  Relaxation_delay = 1.0 [s]
  Repetition_time = 11.74587904 [s]
  Temp_get     = 21.1 [dC]

```





SB1LW-3.jdf

Filename = ab1rw-2.13c

5B

CC(C)C(C)N(C)C(=O)O lle (Water)

SB112-3.jdr

filename = SB112-3.jdr
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#60441
 Solvent = D2O
 Creation_time = 8-SEP-2015 06:34:04
 Revision_time = 7-SEP-2015 17:58:14
 Current_time = 7-SEP-2015 17:58:59

Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MHz])
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.51277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 12
 Total_scans = 12

X_00_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_itn = 4 [dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Date_preset = FALSE
 Initial_wait = 1[s]
 Recvr_Gain = 46
 Relaxation_delay = 10[s]
 Repetition_time = 11.74587904[s]
 Temp_get = 20.9[dC]

0.296

0.91

0.97

0.97

0.94

3.4922

3.5002

3.6732

3.6888

3.6888

3.6888

3.6888

4.48241

4.47909

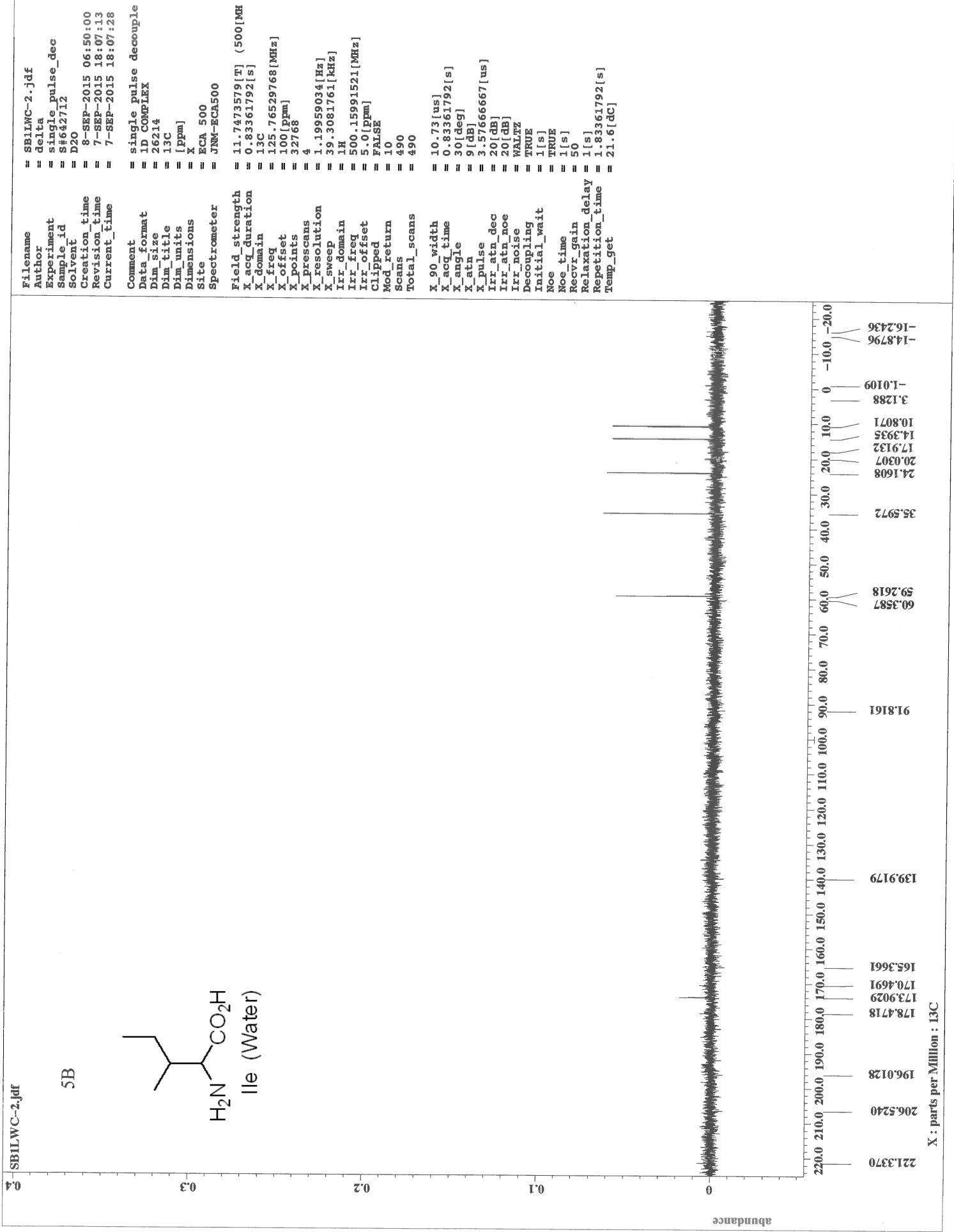
4.47565

5.4104

5.4104

Y

X : parts per Million : 1H



```

Filename = SBPAW-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#95842
Solvent = D2O
Creation_time = 9-SEP-2015 08:06:28
Revision_time = 8-SEP-2015 19:25:33
Current_time = 8-SEP-2015 19:26:16

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] (500[MHz]
X_acq_duration = 1.74587904 [s]
X_domain = 1H
X_freq = 500.15991521 [MHz]
X_offset = 5.0 [PPM]
X_Points = 16384
X_prescans = 0
X_resolution = 0.57277737 [Hz]
X_sweep = 9.38438438 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [PPM]
Tri_domain = 1H
Tri_freq = 500.15991521 [MHz]
Tri_offset = 5.0 [PPM]
Clipped = FALSE
Mod_return = 1
Scans = 10
Total_scans = 10

X_90_width = 12.54 [us]
X_acq_time = 1.74587904 [s]
X_angle = 45 [deg]
X_atn = 4 [dB]
X_pulse = 6.27 [us]
Irr_mode = Off
Tri_mode = Off
Dante_Presat = FALSE
Initial_wait = 1 [s]
Recvr_Gain = 34
Relaxation_delay = 10 [s]
Repetition_time = 1.74587904 [s]
Temp_get = 21.3 [dC]

```

L



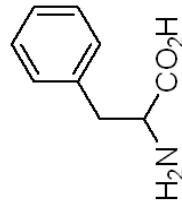
Phe (Water)

6B



X : parts per Million : 1H

6B



Phe (Water)

```

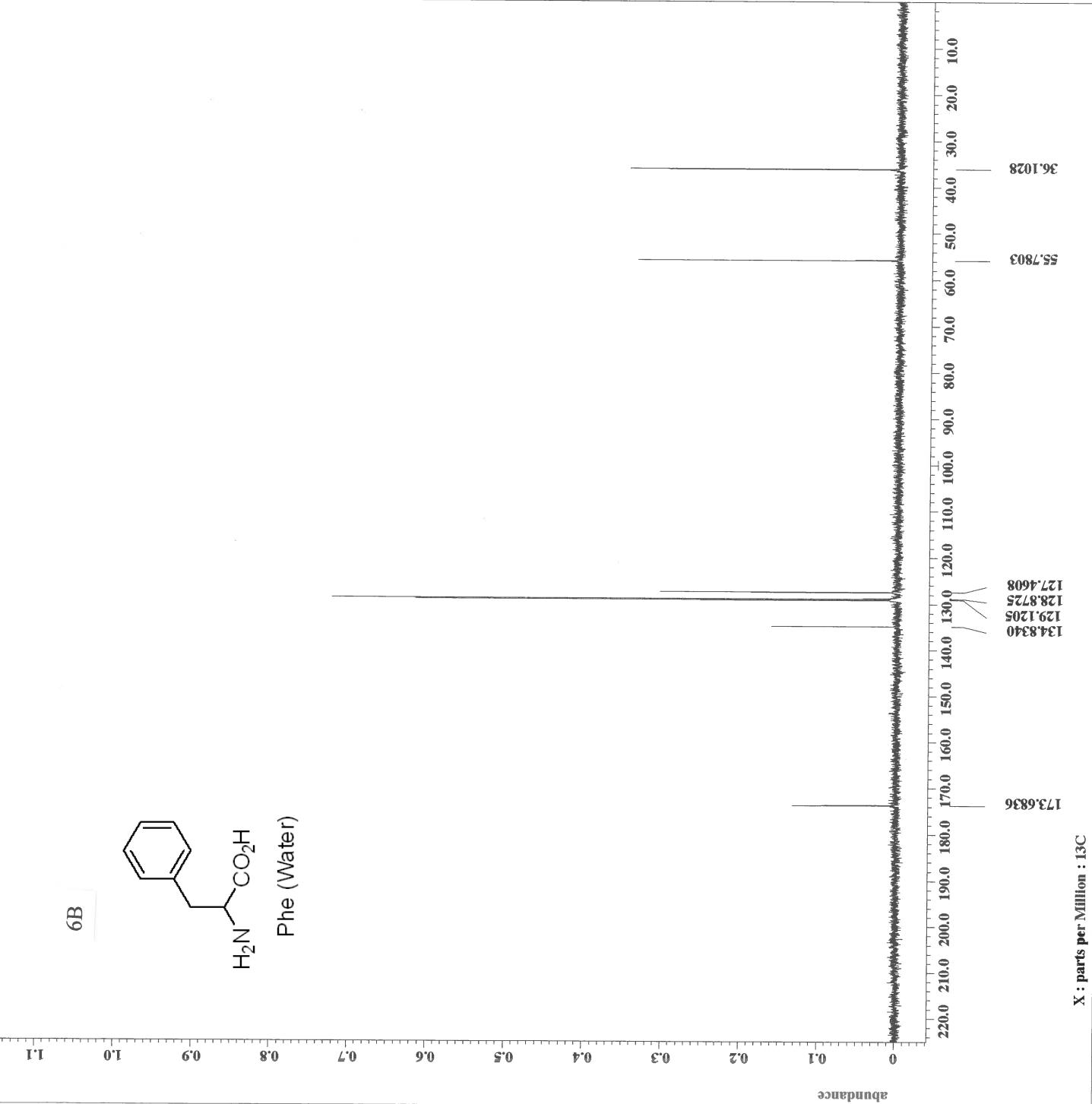
filename = SBPAWC-2.jdf
Author = delta
Sample_id = S#68167
Solvent = D2O
Creation_time = 9-SEP-2015 08:12:34
Revision_time = 8-SEP-2015 19:29:24
Current_time = 8-SEP-2015 19:29:33

Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

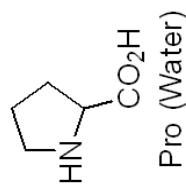
Field_strength = 11.7473579 [T] (500 [MHz])
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 129.76529768 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_Prescans = 4
X_resolution = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 10
Scans = 230.0
Total_scans = 230.0

X_90_width = 10.73 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_attn = 9 [dB]
X_pulse = 3.576666667 [us]
Irr_attn_dec = 20 [dB]
Irr_attn_noe = 20 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 0.5 [s]
Recv_gain = 50
Relaxation_delay = 0.5 [s]
Repetition_time = 1.33361792 [s]
Temp_get = 21.7 [dC]

```



7B



3.05

1.03

1.01

0.99

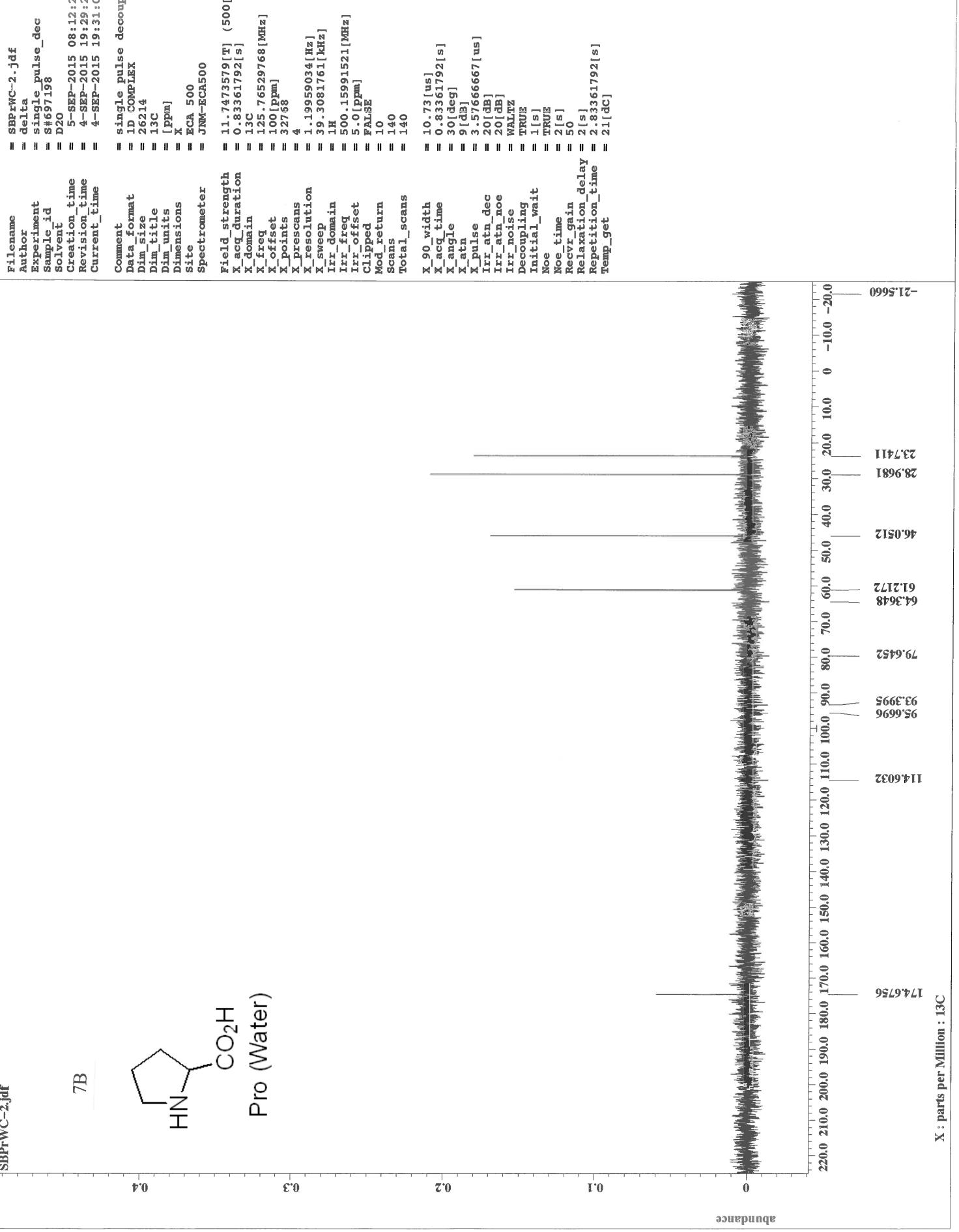
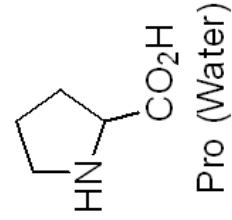


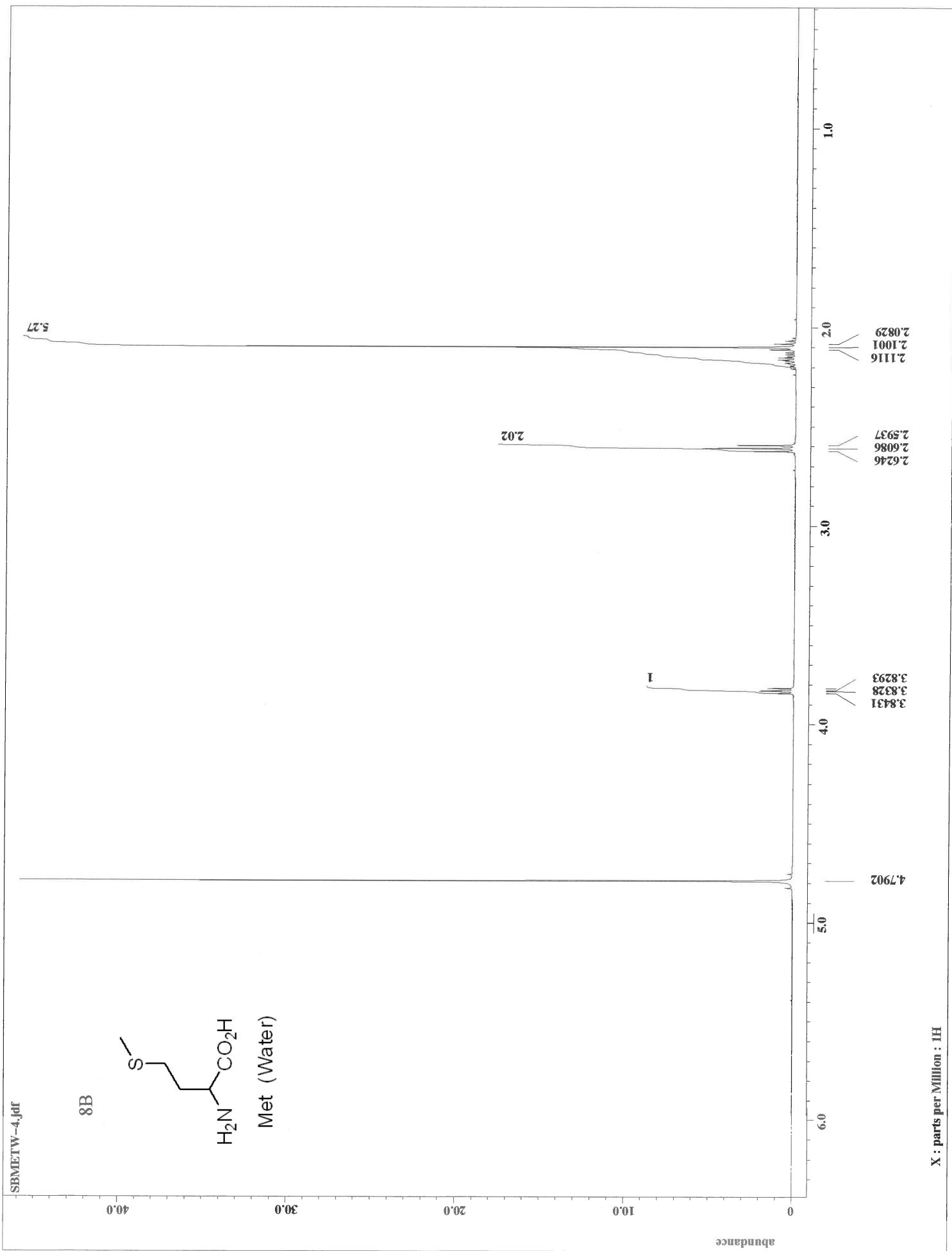
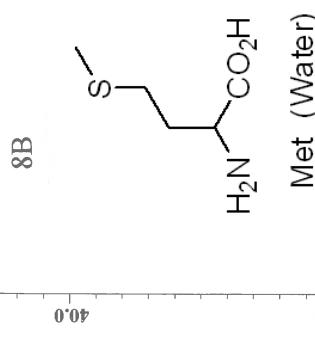
abundance

X : parts per Million : ppm

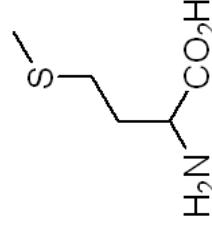
3.3979
3.2765
3.2663
3.2536
3.1982
3.1769
3.1723
3.1620
3.1730
3.1769
3.1780
2.1886
2.1966
2.1912
2.0534
2.0408
1.9206
1.9080
1.8817
1.8679
1.8599
1.8553
1.8313
1.7190
1.7087

4.1148
4.1010
3.9991
3.9854
3.9728
3.9556
3.8182
3.8044
3.0360
3.0162
3.0173
3.0172
3.0169
3.0168
3.0198
3.0236
3.0263
3.0365
2.2138
2.2012
2.1886
2.1851
2.1714
2.1606
2.0534
2.0408
1.9206
1.9080
1.8817
1.8679
1.8599
1.8553
1.8313
1.7190
1.7087

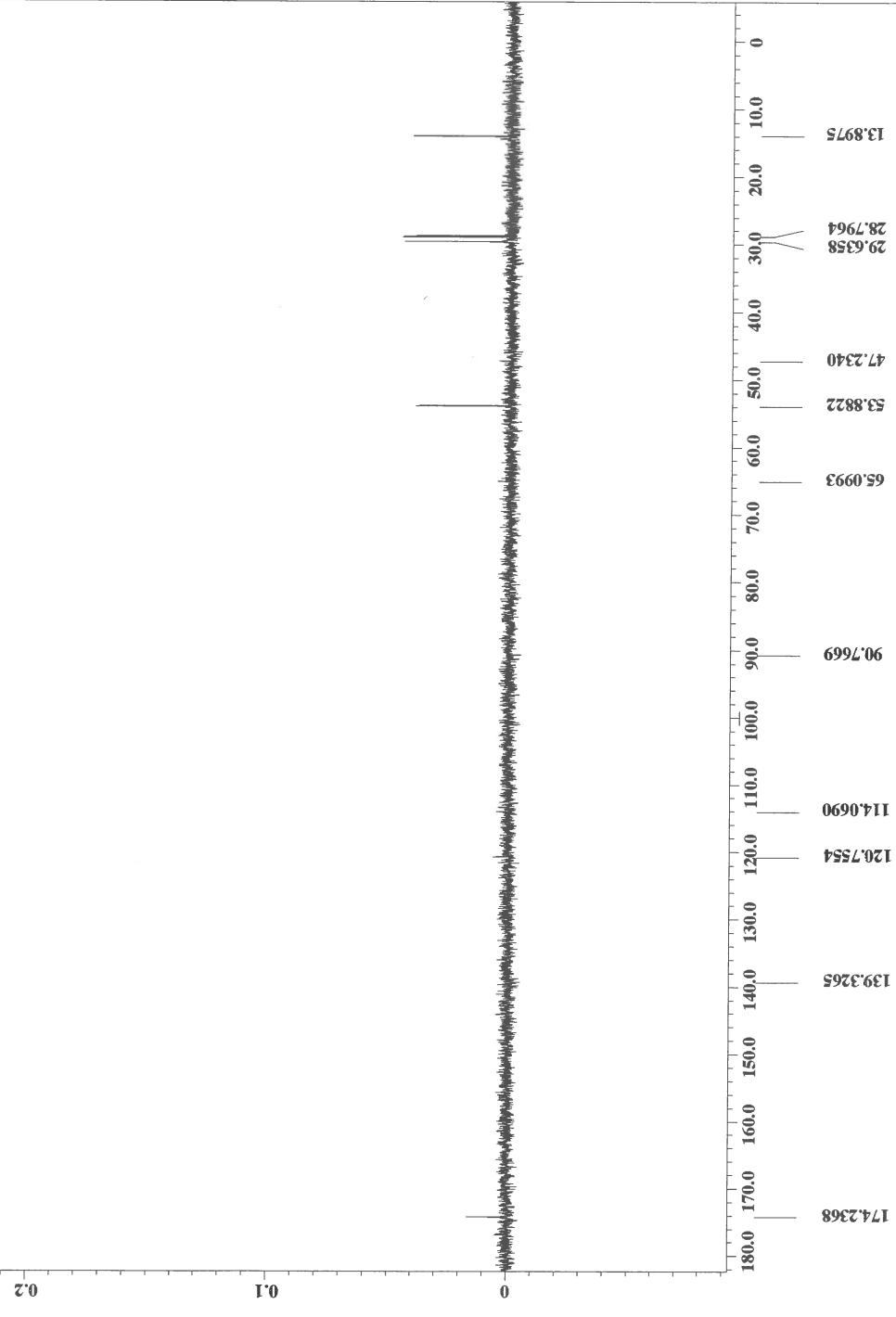




8B



Met (Water)



X : parts per Million : 13C

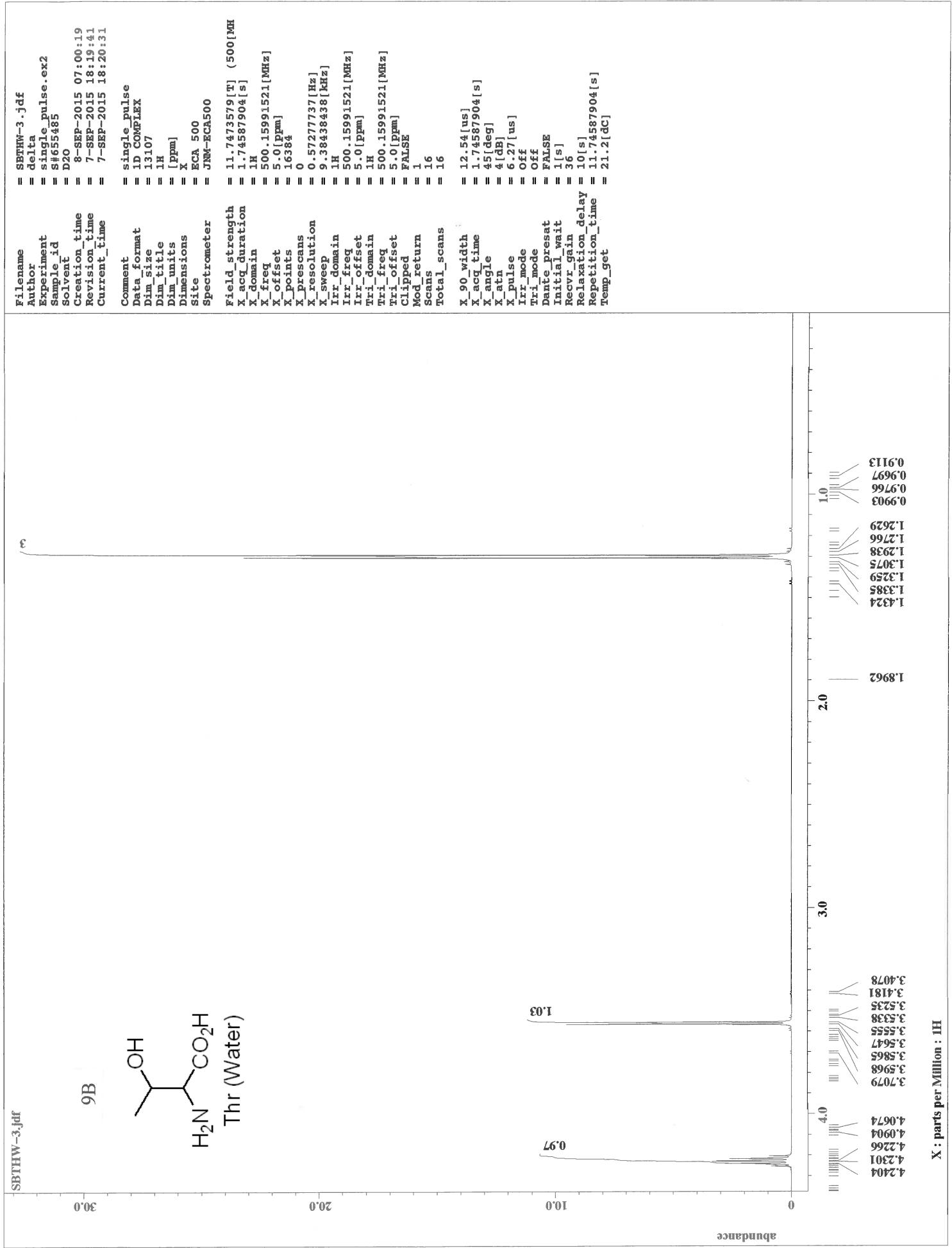
```

= SBMetWC-2.jdf
= delta
= single_pulse_dec
Sample_id = S#703584
Creation_time = 5-SEP-2015 08:56:06
Revision_time = 4-SEP-2015 20:13:30
Current_time = 4-SEP-2015 20:13:59
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] ( 500 [MHz]
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 125.76529768 [MHz]
X_offset = 100 [PPM]
X_points = 32768
X_Prescans = 4
X_presolutions = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [PPM]
Clipped = FALSE
Mod_return = 10
Scans = 840
Total_scans = 840

X_90_width = 10.73 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.576666667 [us]
Irr_atn_dec = 20 [dB]
Irr_atn_noe = 20 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_time = 2 [s]
Recvr_gain = 50
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get = 21.5 [dc]

```



```

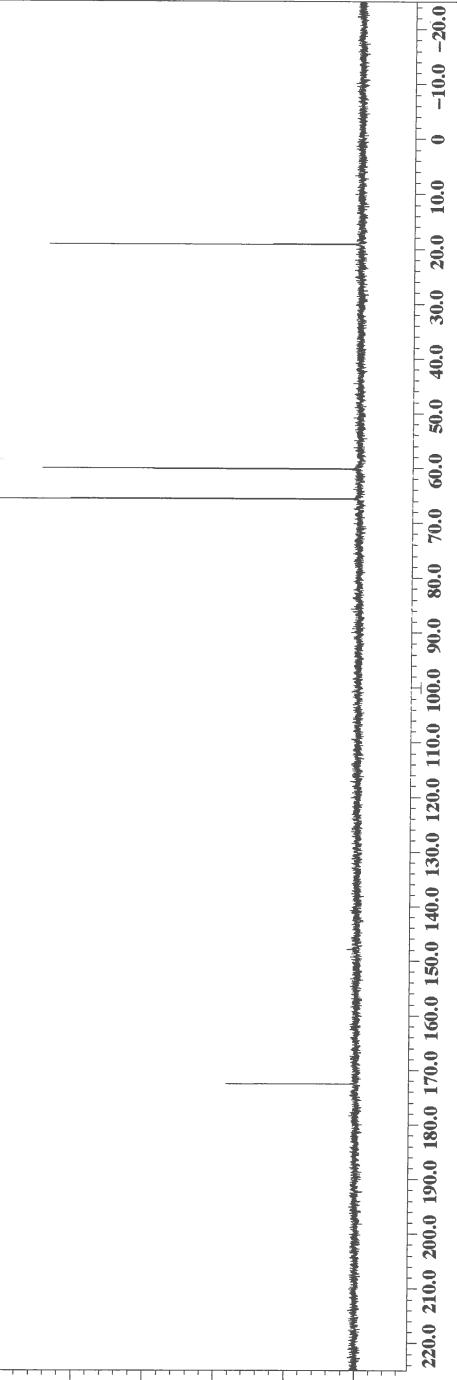
filename = SBTHWC-2.jdf
author = delta
Experiment = single_pulse_dec
sample_id = S#658391
solvent = D2O
creation_time = 8-SEP-2015 07:07:34
revision_time = 7-SEP-2015 18:23:57
current_time = 7-SEP-2015 18:24:24

comment = single pulse decouple
data_format = 1D COMPLEX
dim_size = 26214
dim_title = 13C
dim_units = [ppm]
dimensions = X
site = ECA 500
spectrometer = JNM-ECA500

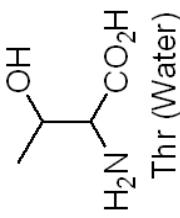
field_strength = 11.7473579 [T] (500 [MHz])
x_acq_duration = 0.83361792 [s]
x_domain = 13C
x_freq = 125.76529768 [MHz]
x_offset = 100 [ppm]
x_points = 32768
x_prcsans = 4
x_resolution = 1.19959034 [Hz]
x_sweep = 39.3081761 [kHz]
irr_domain = 1H
irr_freq = 500.15991521 [MHz]
irr_offset = 5.0 [ppm]
clipped = FALSE
mod_return = 10
scans = 210
total_scans = 210

x_90_width = 10.73 [us]
x_acq_time = 0.83361792 [s]
x_angle = 30 [deg]
x_attn = 9 [dB]
x_pulse = 3.27666667 [us]
irr_attn_dec = 20 [dB]
irr_attn_noe = 20 [dB]
irr_noise = WALTZ
decoupling = TRUE
initial_wait = 1 [s]
noe_time = 1 [s]
recv_gain = 50
relaxation_delay = 1 [s]
repetition_time = 1.83361792 [s]
temp_get = 21.7 [dC]

```



9B



Chemical structure of Thr(Water):
 $\text{H}_2\text{N}-\text{CH}(\text{CO}_2\text{H})-\text{CH}_2\text{OH}$
 Thr (Water)

Filename

Author

Experiment

Sample id

Solvent

Creation_time

Revision_time

Current_time

Comment

Data_format

Dim_size

Dim_title

Dim_units

Dimensions

Site

Spectrometer

Field_strength

X_acq_duration

X_domain

X_freq

X_offset

X_points

X_prescans

X_resolution

X_sweep

Irr_domain

Irr_freq

Irr_offset

Tri_domain

Tri_freq

Tri_offset

Clipped

Mod_return

Scans

Total_scans

X_90_width

X_acq_time

X_angle

X_atn

X_Pulse

Irr_mode

Tri_mode

Off

Dante_Presat

Initial_wait

Reovr_gain

Relaxation_delay

Repetition_time

Temp_get

X

Y

Z

W

V

U

T

S

R

Q

P

O

N

M

L

K

J

I

H

G

F

E

D

C

B

A

Z

Y

X

W

V

U

T

S

R

Q

P

N

M

L

K

J

I

H

G

F

E

D

C

B

A

Z

Y

X

W

V

U

T

S

R

Q

P

N

M

L

K

J

I

H

G

F

E

D

C

B

A

Z

Y

X

W

V

U

T

S

R

Q

P

N

M

L

K

J

I

H

G

F

E

D

C

B

A

Z

Y

X

W

V

U

T

S

R

Q

P

N

M

L

K

J

I

H

G

F

E

D

C

B

A

Z

Y

X

W

V

U

T

S

R

Q

P

N

M

L

K

J

I

H

G

F

E

D

C

B

A

Z

Y

X

W

V

U

T

S

R

Q

P

N

M

L

K

J

I

H

G

F

E

D

C

B

A

Z

Y

X

W

V

U

T

S

R

Q

P

N

M

L

K

J

I

H

G

F

E

D

C

B

A

Z

Y

X

W

V

U

T

S

R

Q

P

N

M

L

K

J

I

H

G

F

E

D

C

B

A

Z

Y

X

W

V

U

T

S

R

Q

P

N

M

L

K

J

I

H

G

F

E

D

C

B

A

Z

Y

X

W

V

U

T

S

R

Q

P

N

M

L

K

J

I

H

G

F

E

D

C

B

A

Z

Y

X

W

V

U

T

S

R

Q

P

N

M

L

K

J

I

H

G

F

E

D

C

B

A

Z

Y

X

W

V

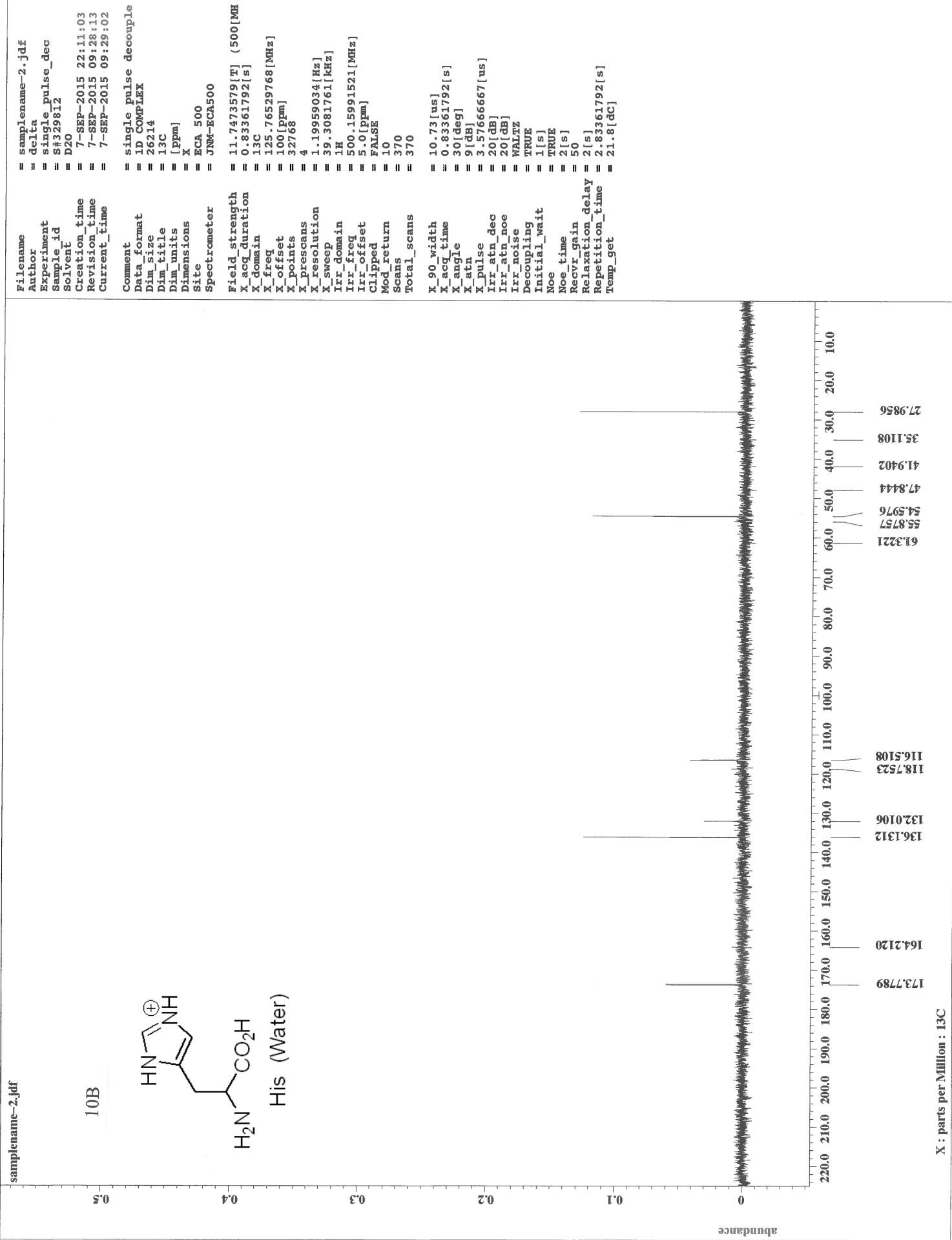
U

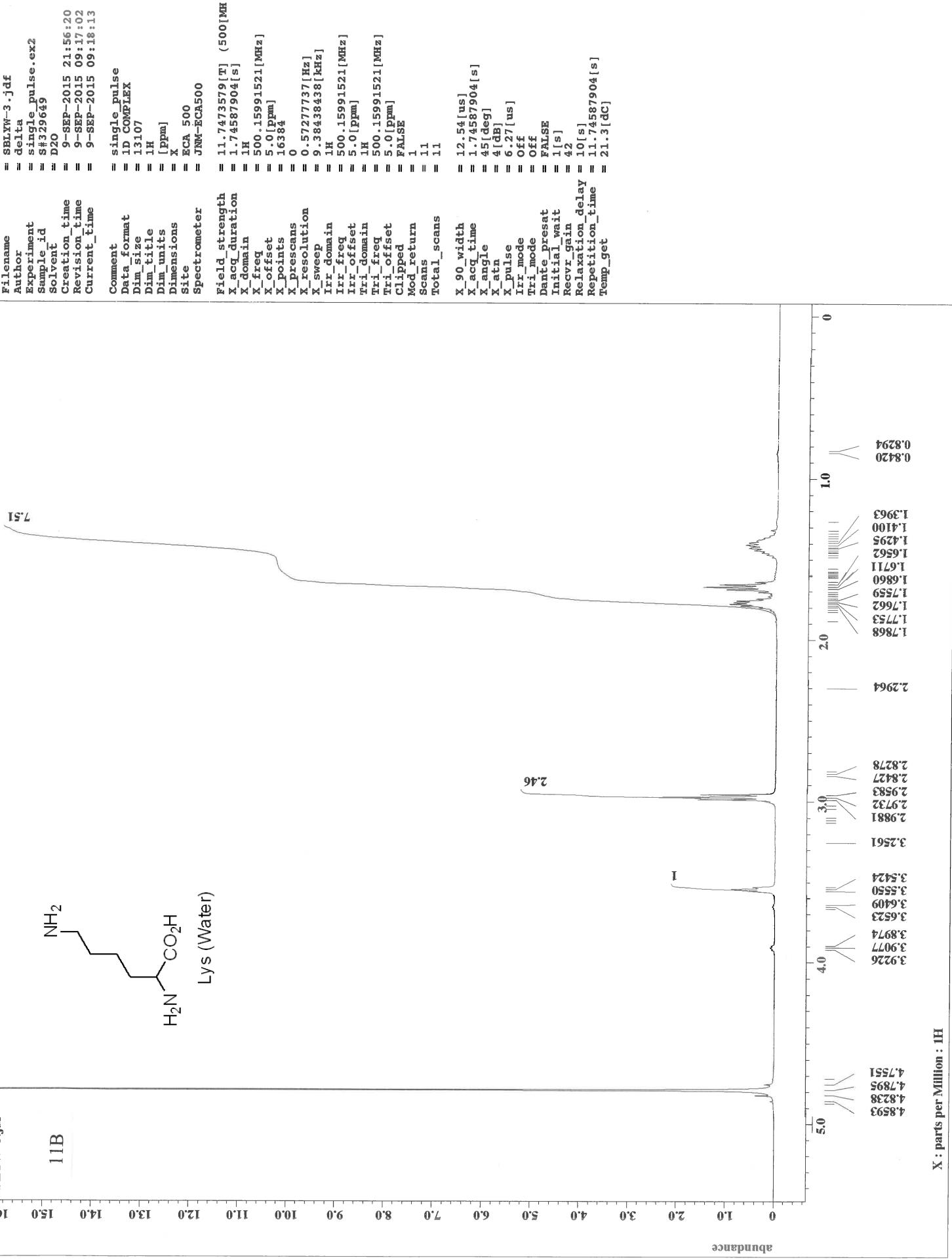
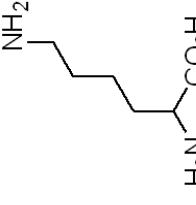
T

S

R

Q





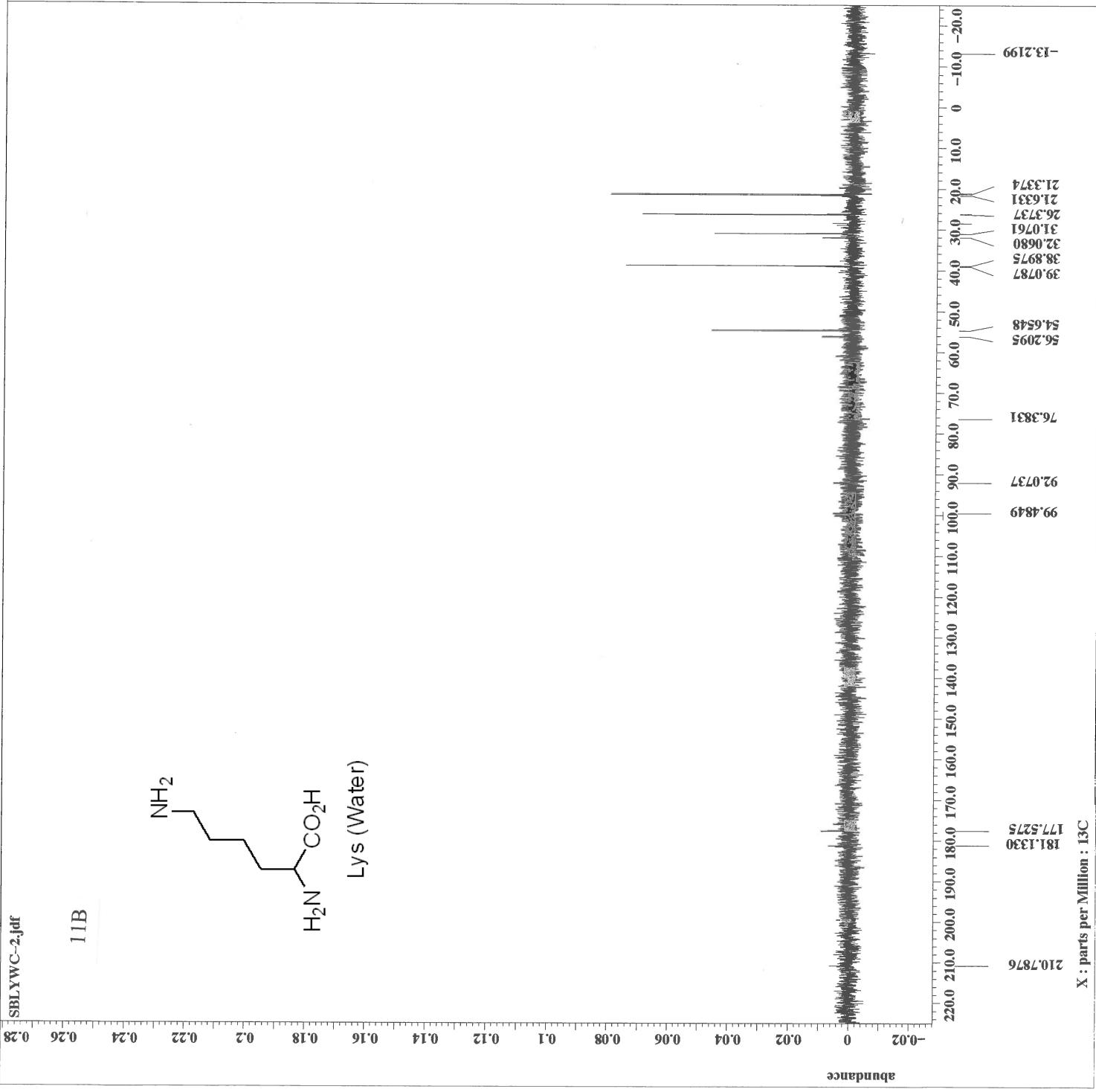
```

Filename = SBLYWC-2.jdf
Author
Experiment
Sample_id = S#331949
Solvent = D2O
Creation_time = 9-SEP-2015 22:12:00
Revision_time = 9-SEP-2015 09:28:36
Current_time = 9-SEP-2015 09:29:30
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] ( 500 [MHz]
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 125.76529768 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prcsams = 4
X_resolution = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 10
Scans = 670
Total_scans = 670

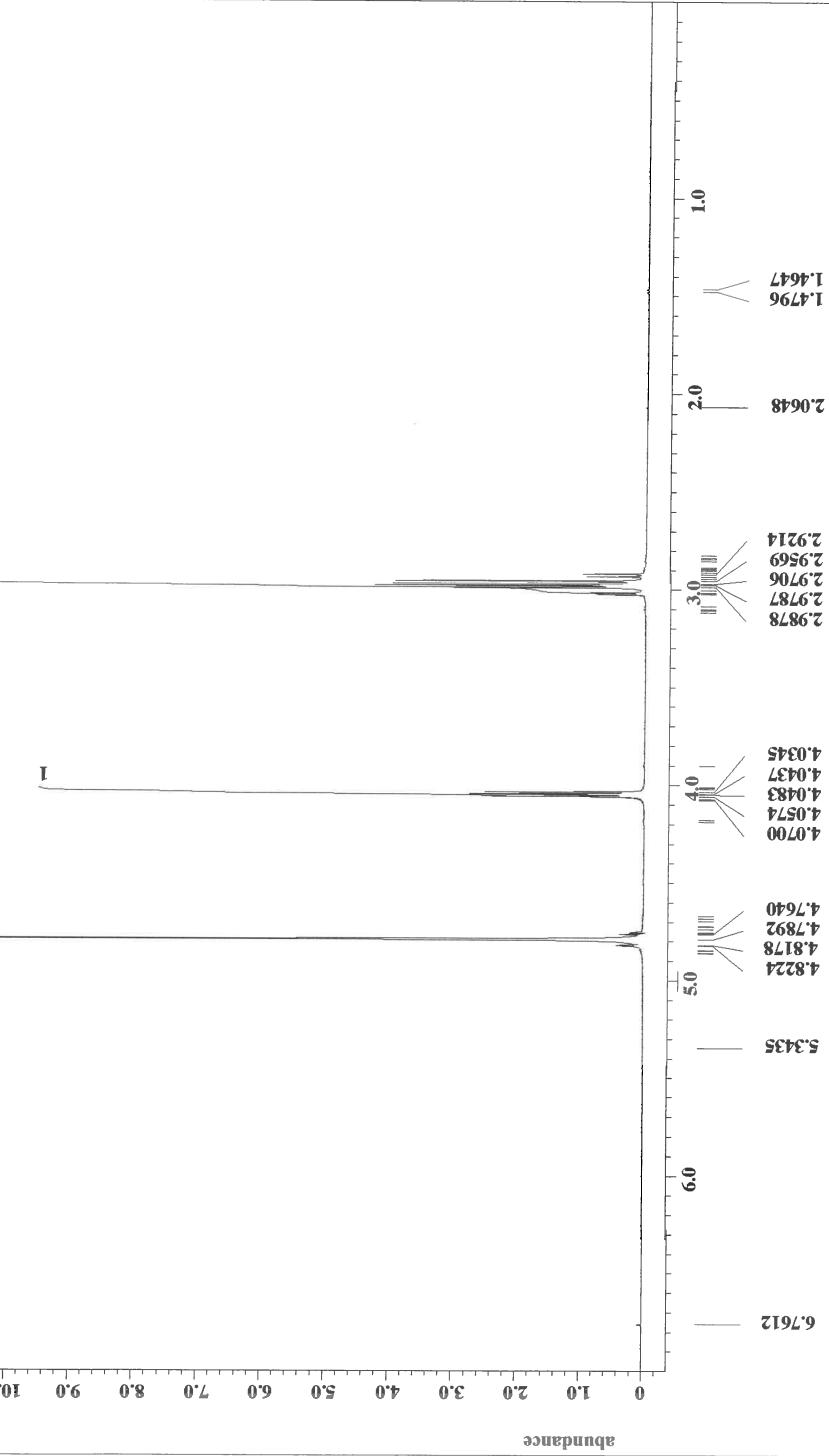
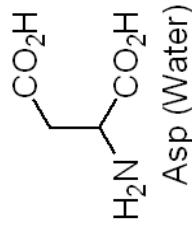
X_90_width = 10.73 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.276666667 [us]
Irr_atn_dec = 20 [dB]
Irr_atn_noe = 20 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = 0.5 [s]
Reovr_gain = 50
Relaxation_delay = 0.5 [s]
Repetition_time = 1.33361792 [s]
Temp_get = 21.7 [dC]

```



1.99

12B



```

Filename = SBASW-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#340075
Solvent = D2O
Creation_time = 8-SEP-2015 22:12:54
Revision_time = 8-SEP-2015 09:31:32
Current_time = 8-SEP-2015 09:32:03

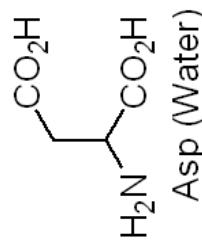
Comment = single_pulse
Data_format = 1D_COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MHz])
X_acq_duration = 1.74587904 [s]
X_domain = 1H
X_freq = 500.15991521 [MHz]
X_offset = 5.0 [ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.57277737 [Hz]
X_sweep = 9.38438438 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Tri_domain = 1H
Tri_freq = 500.15991521 [MHz]
Tri_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
scans = 9
Total_scans = 9

X_90_width = 12.54 [us]
X_acq_time = 1.74587904 [s]
X_angle = 45 [deg]
X_atn = 4 [dB]
X_pulse = 6.27 [us]
Irr_mode = Off
Tri_mode = Off
Dante_Presat = FALSE
Initial_wait = 1 [s]
Reovr_gain = 46
Relaxation_delay = 10 [s]
Repetition_time = 11.74587904 [s]
Temp_Set = 21.4 [dC]

```

12B



```

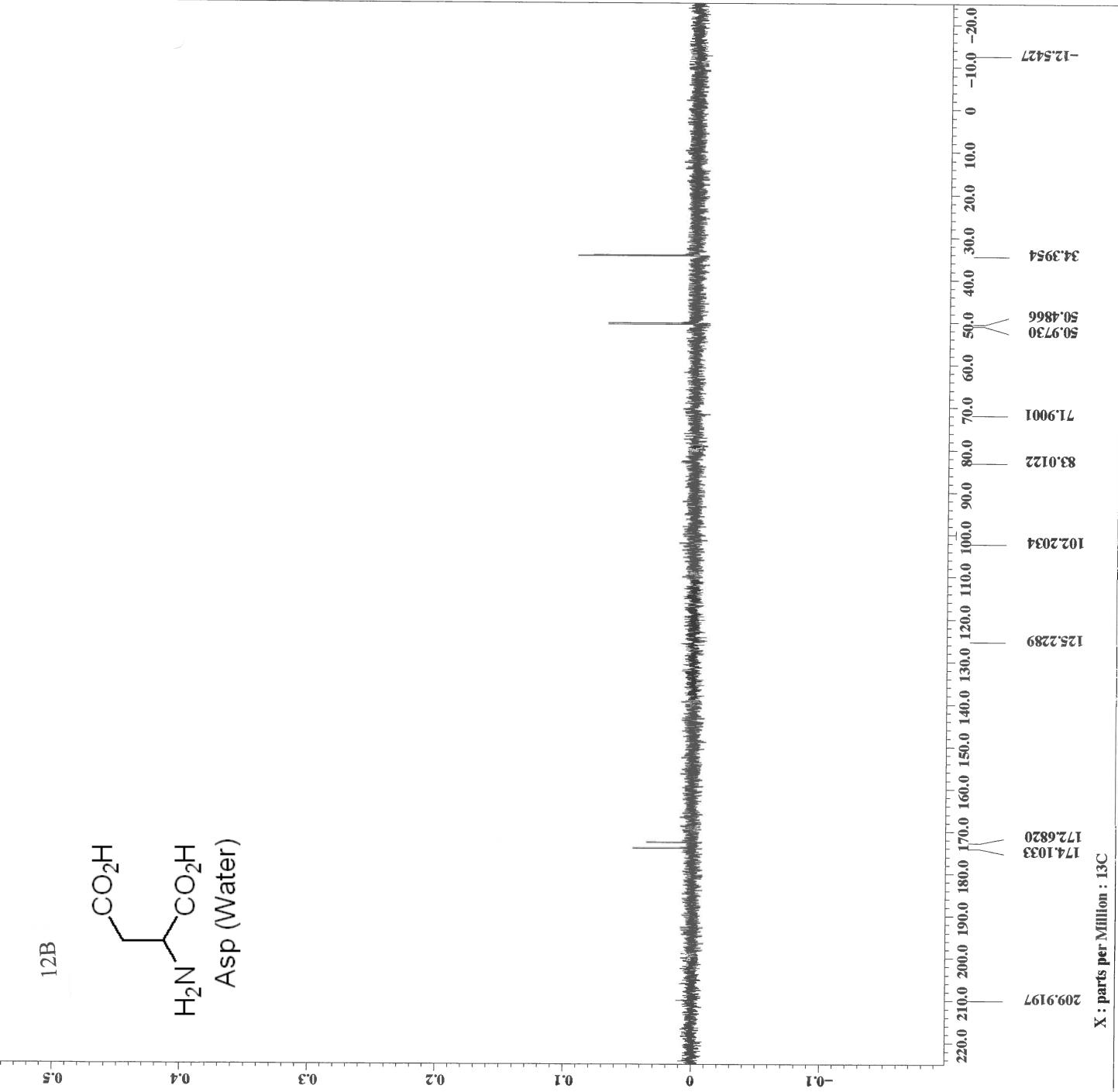
Filename = SBASWC-3.jdf
Author = delta
Sample_id = S#311913
Solvent = D2O
Creation_time = 8-SEP-2015 22:20:09
Revision_time = 8-SEP-2015 09:37:27
Current_time = 8-SEP-2015 09:37:49

Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
Spectrometer = INN-ECAS500

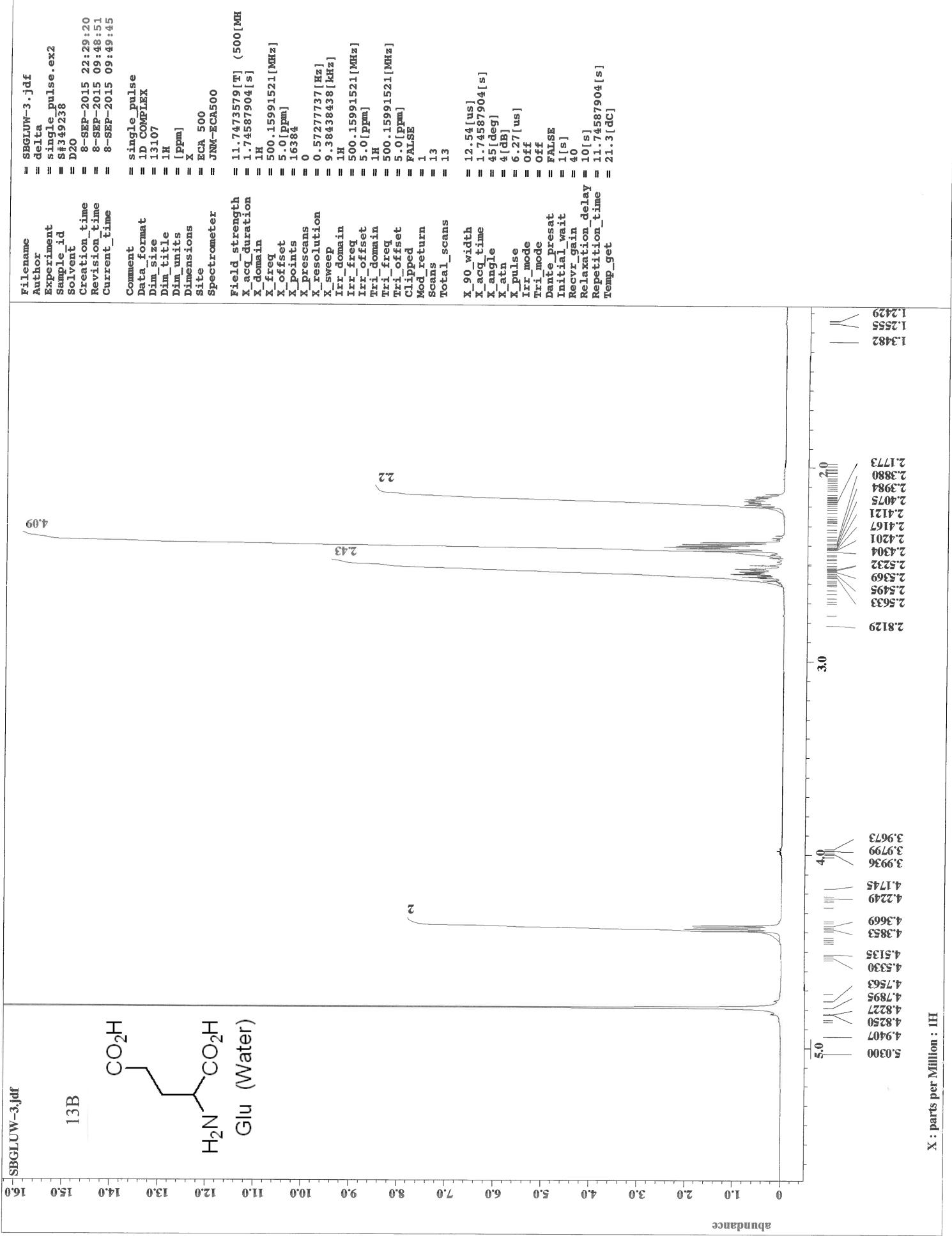
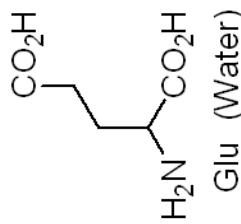
Field_strength = 11.7473579 [T] (500[MHz])
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 125.76529768 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_Prescans = 4
X_sweep = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 10
Scans = 210
Total_scans = 210

X_90_width = 10.73 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 3.57666667 [us]
X_pulse = 20 [dB]
Irr_atn_dec = 20 [dB]
Irr_atn_noe = 20 [dB]
Irr_noe = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 1 [s]
Recvr_gain = 50
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get = 21.8 [dc]

```

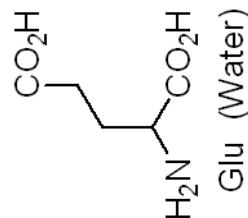


13B



X : parts per Million : 1H

13B

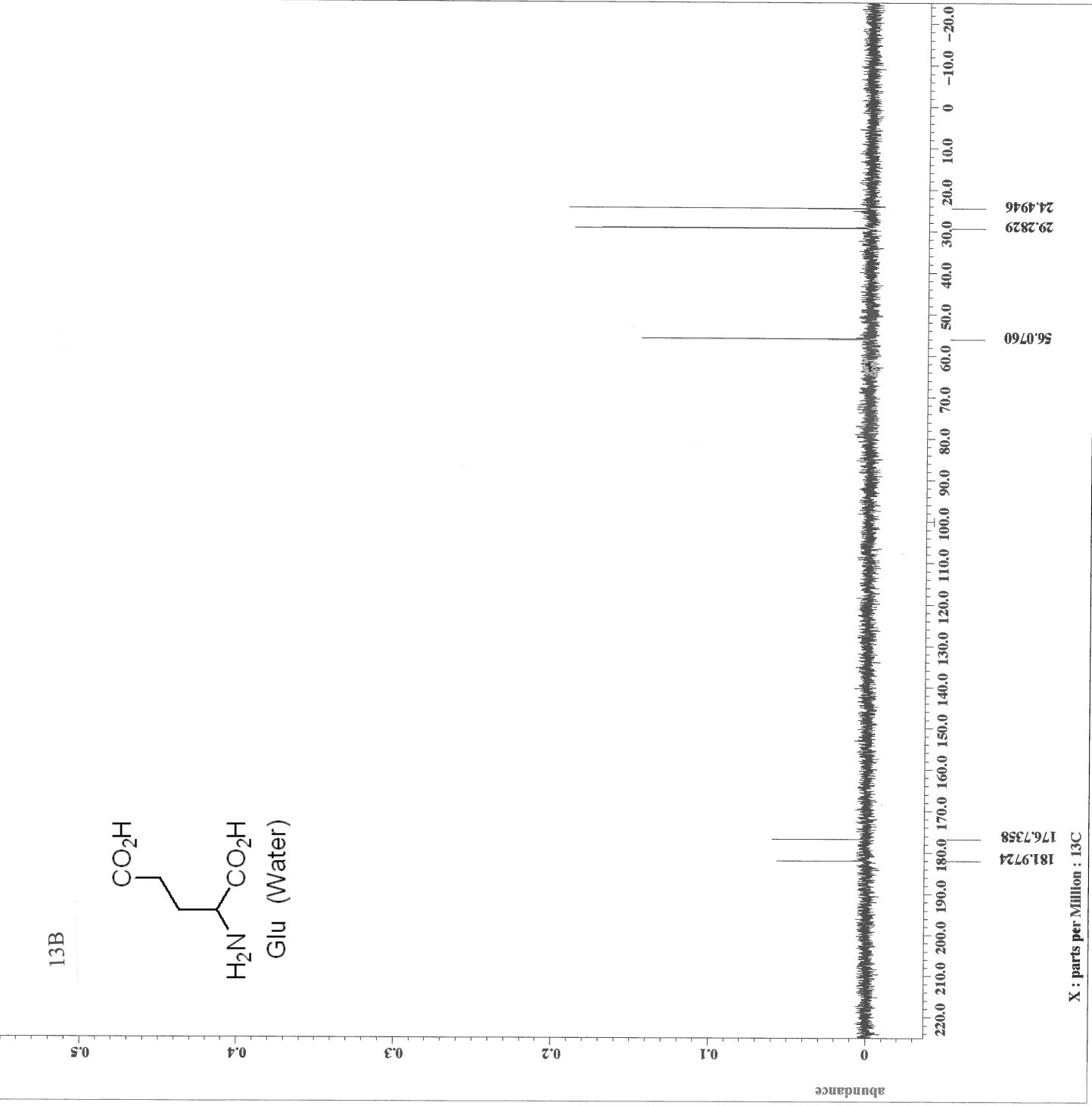


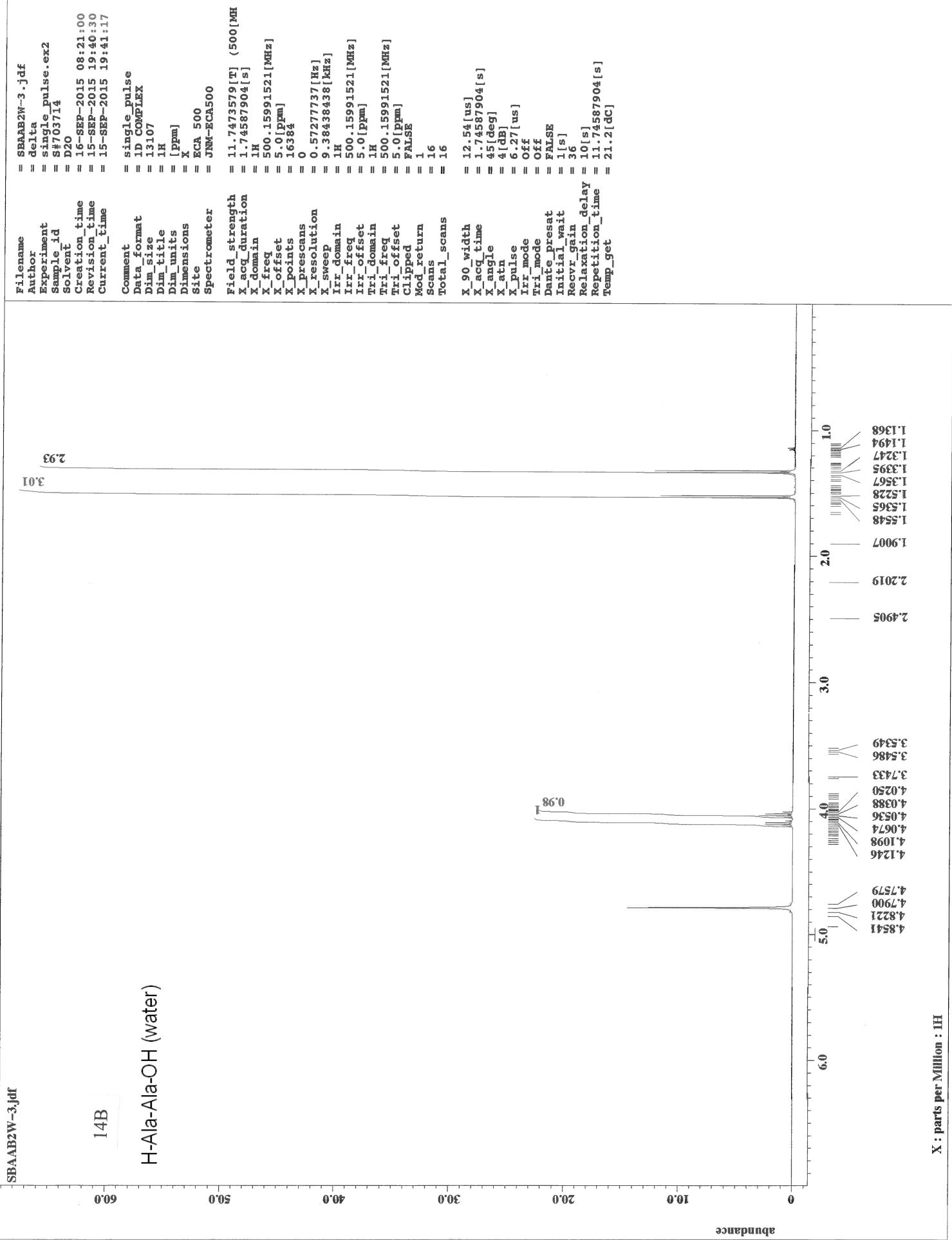
```

Filename = SBGLUWC-2.jdf
Author = delta
Experiment = single_pulse_decouple
Sample_id = S#311786
Solvent = D2O
Creation_time = 8-SEP-2015 22:37:02
Revision_time = 8-SEP-2015 09:53:35
Current_time = 8-SEP-2015 09:53:52

Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

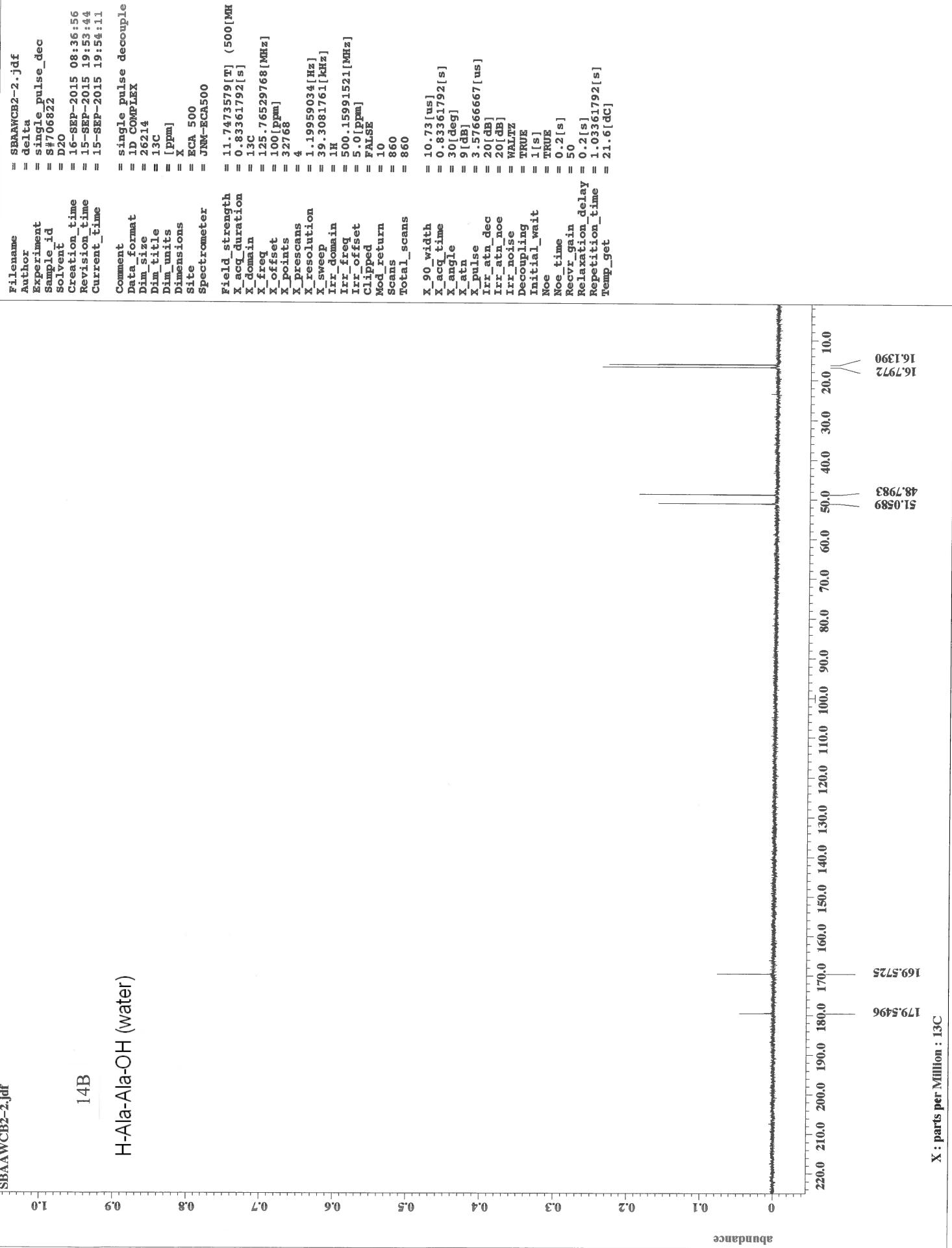
Field_strength = 11.7473579 [MHz] ( 500 [MHz]
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 125.76529768 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_Prescans = 4
X_resolution = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 10
Scans = 310
Total_scans = 310
X_90_width = 10.73 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 3.576666667 [us]
X_pulse = 20 [dB]
Irr_atn_dec = 20 [dB]
Irr_atn_noe = 50
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 0.5 [s]
Recur_gain = 50
Relaxation_delay = 0.5 [s]
Repetition_time = 1.33361792 [s]
Temp_get = 21.7 [deg]
  
```



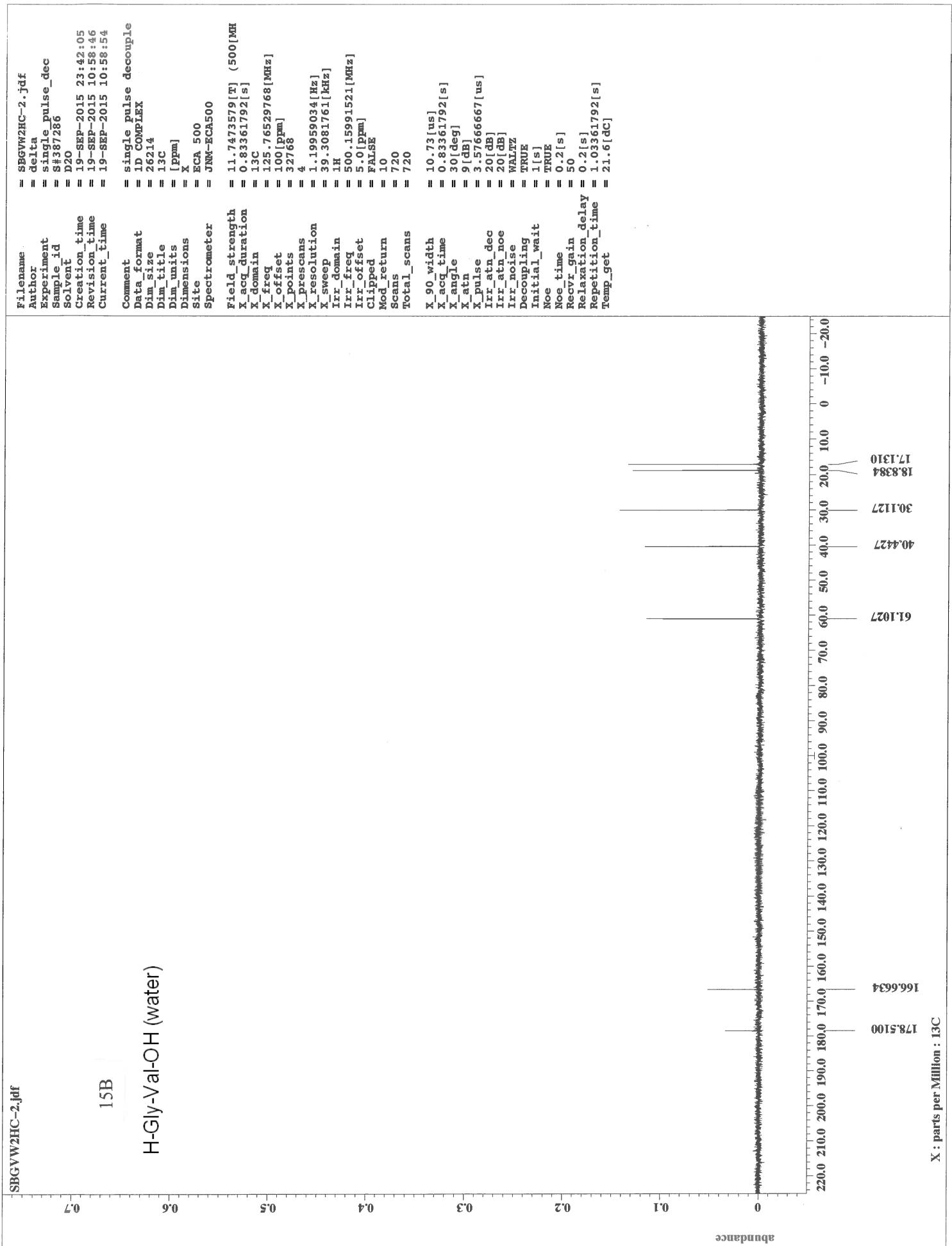


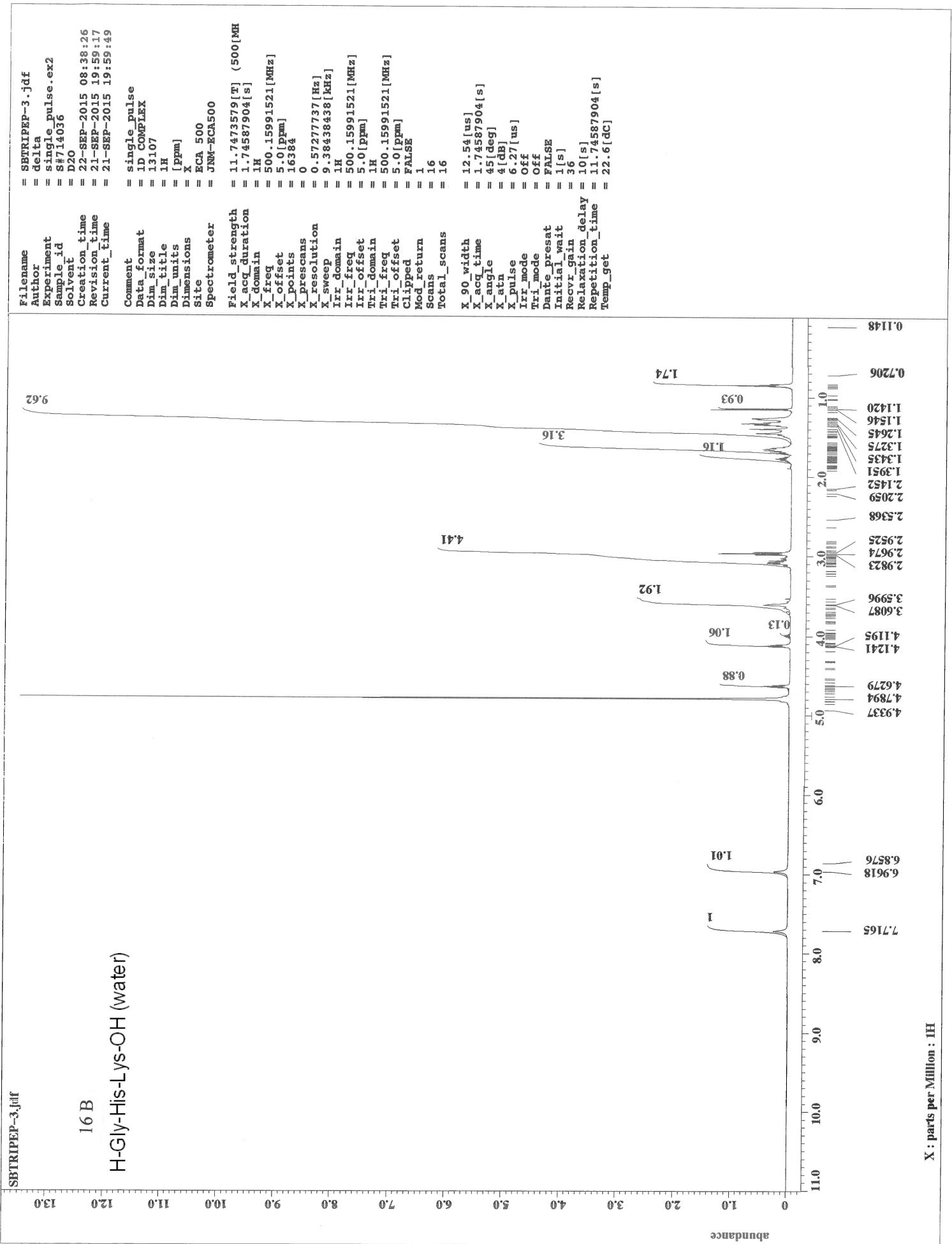
14B

H-Ala-Ala-OH (water)



SBGVW2H-3.jdf





16B

H-Gly-His-Lys-OH (water)

```

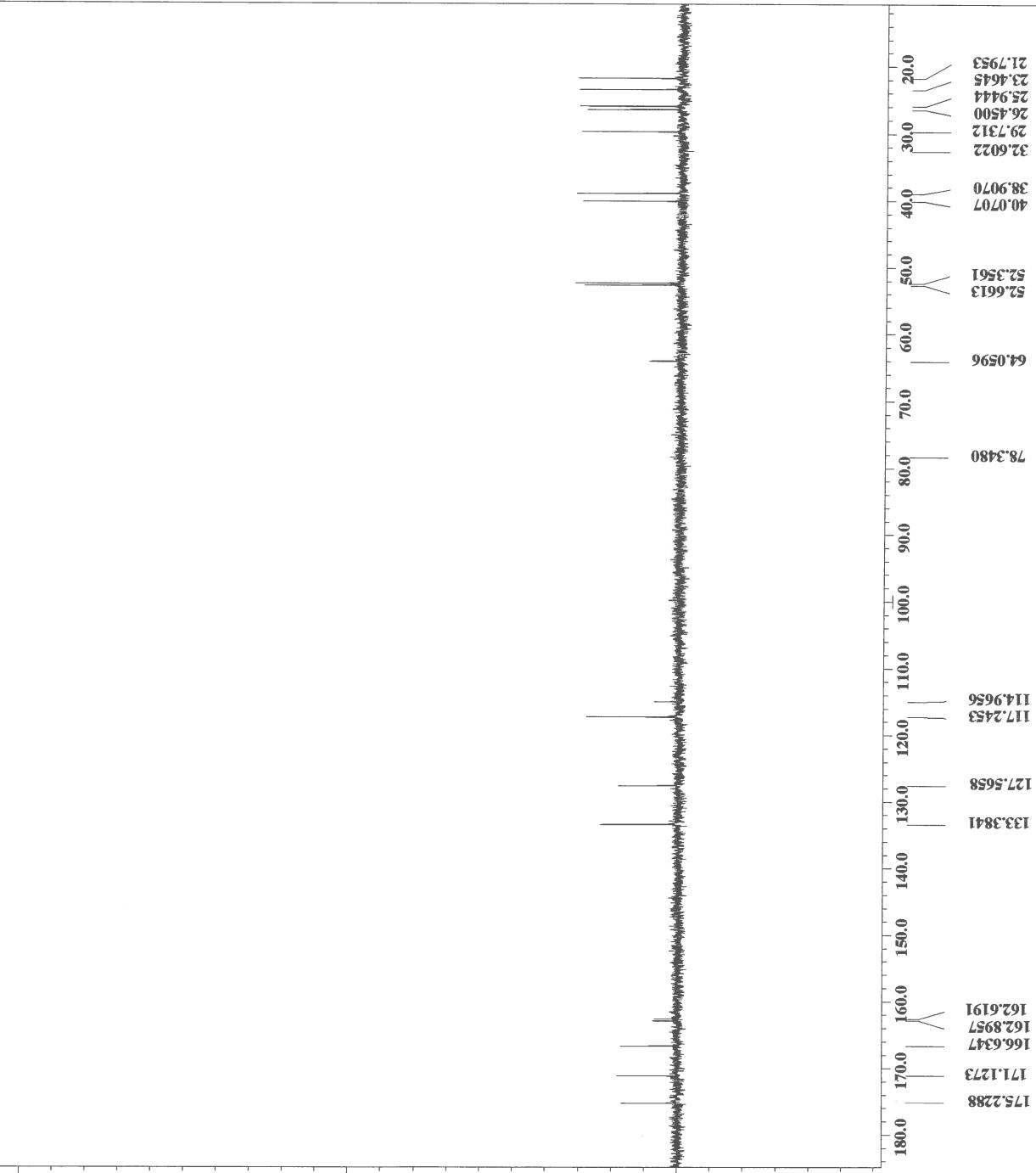
Filename = SBTRIPEPCW-2.jdf
Author = delta
Experiment = single_pulse_decouple
Sample_id = S#559807
Solvent = D2O
Creation_time = 23-SEP-2015 23:21:05
Revision_time = 23-SEP-2015 10:37:13
Current_time = 23-SEP-2015 10:37:39

Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

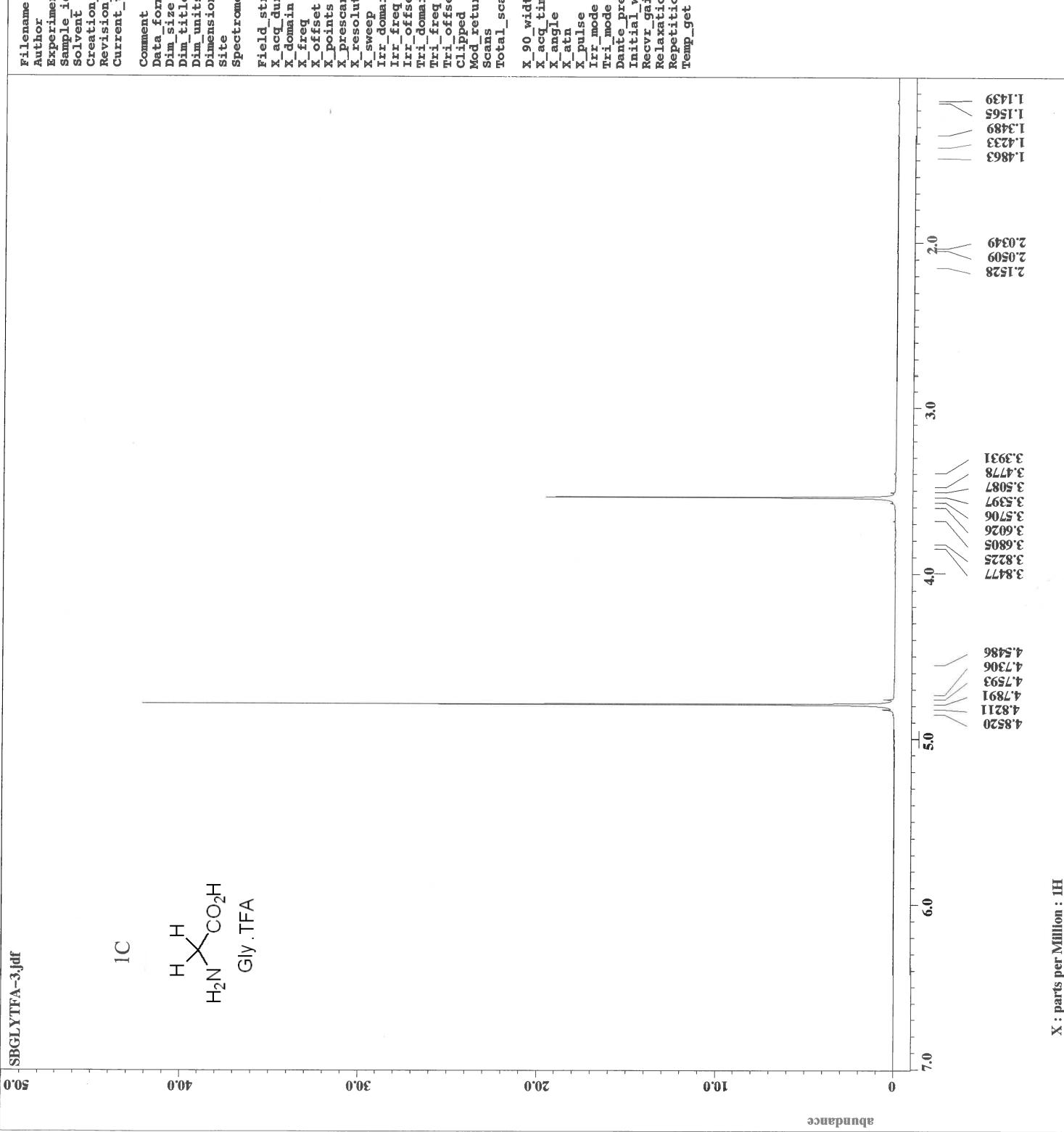
Field_strength = 11.7473579 [T] (500 [MHz])
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 125.76539768 [MHz]
X_offset = 100 [PPM]
X_points = 32768
X_prescans = 4
X_resolution = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [PPM]
Clipped = FALSE
Mod_return = 10
Scans = 2150
Total_scans = 2150

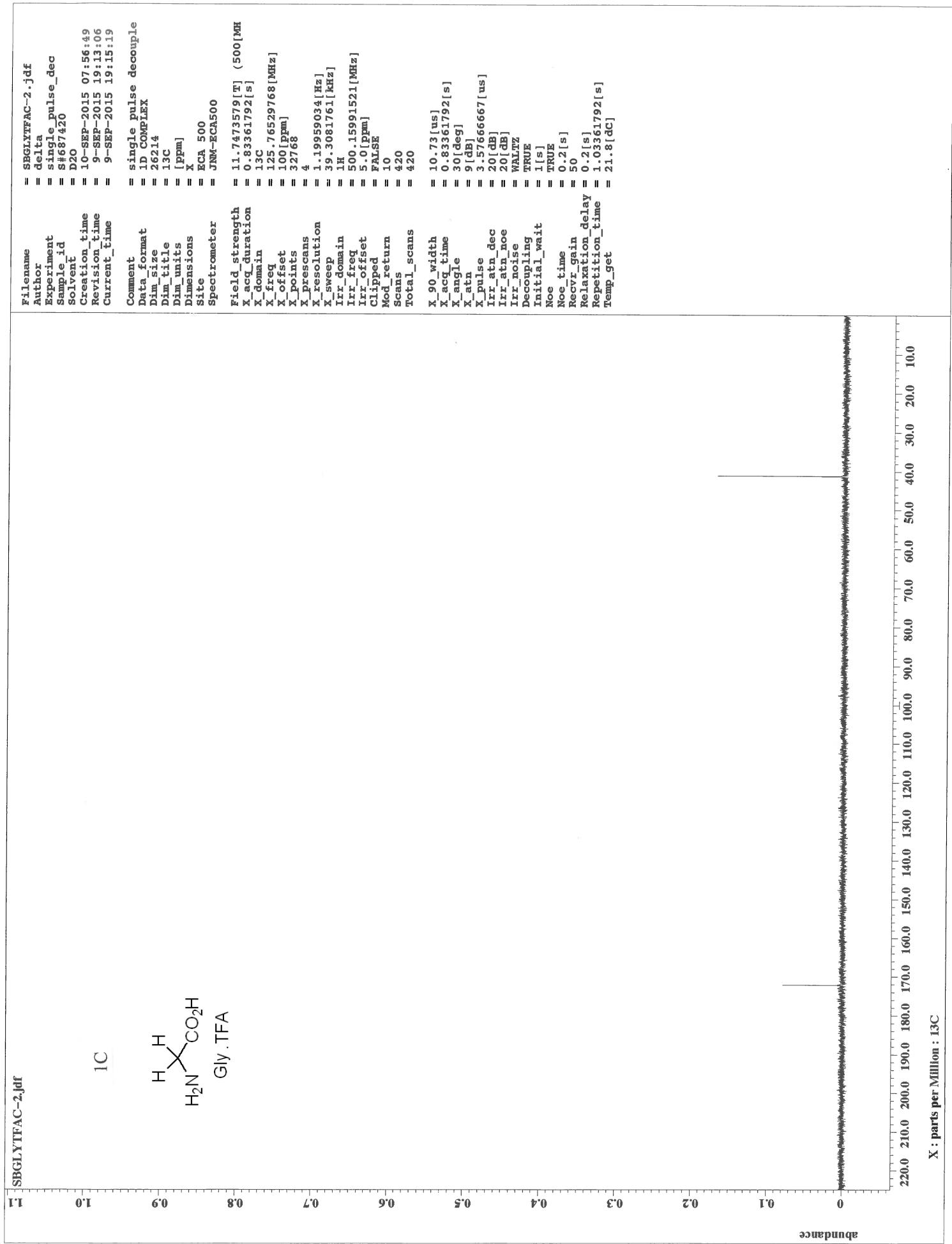
X_90_width = 10.73 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.576666667 [us]
Irr_atn_dec = 20 [dB]
Irr_atn_noe = 20 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_time = 0.2 [s]
Recurr_gain = 50
Relaxation_delay = 0.2 [s]
Repetition_time = 1.03361792 [s]
Temp_get = 22.5 [dC]

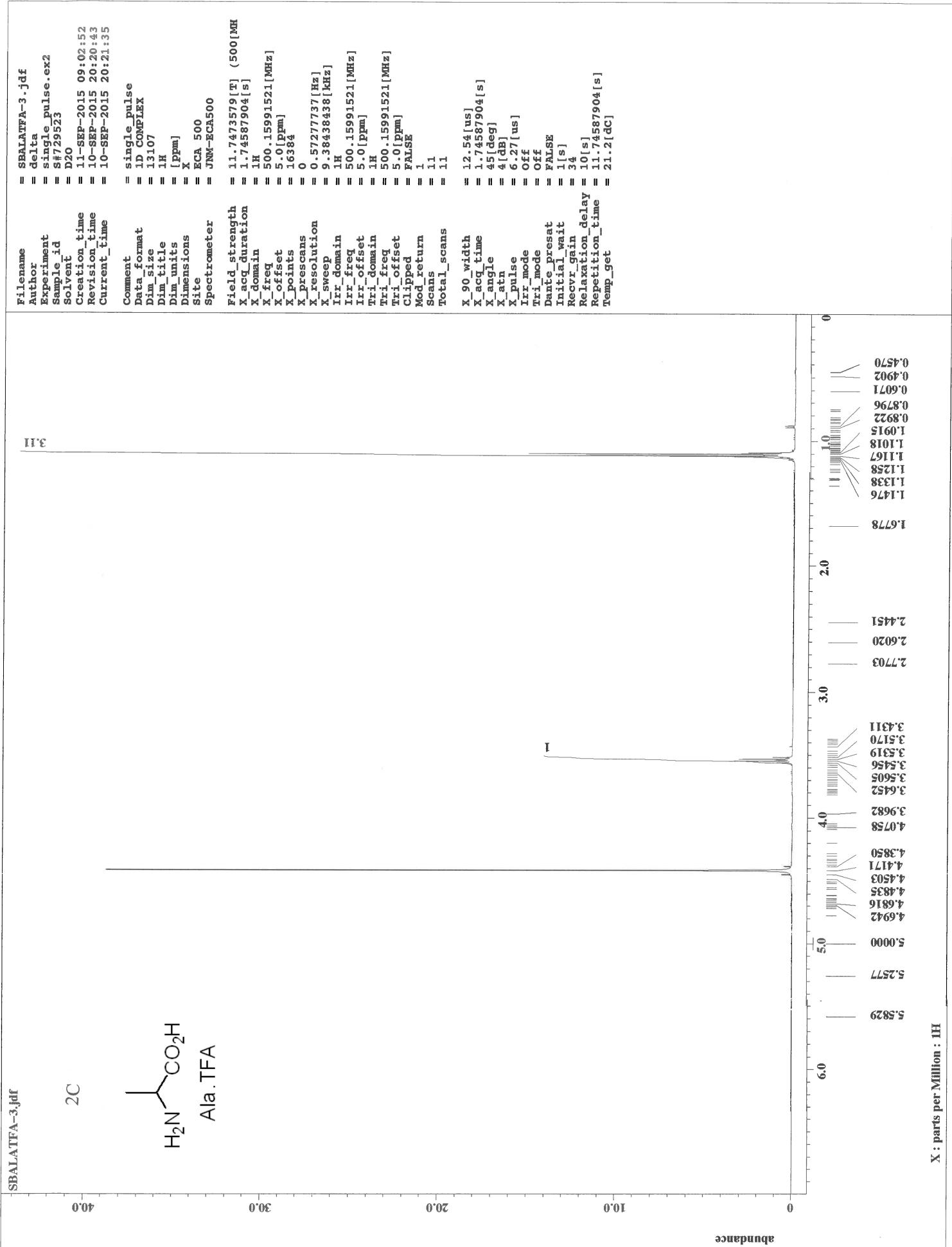
```



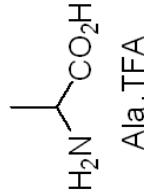
1C







2C



```

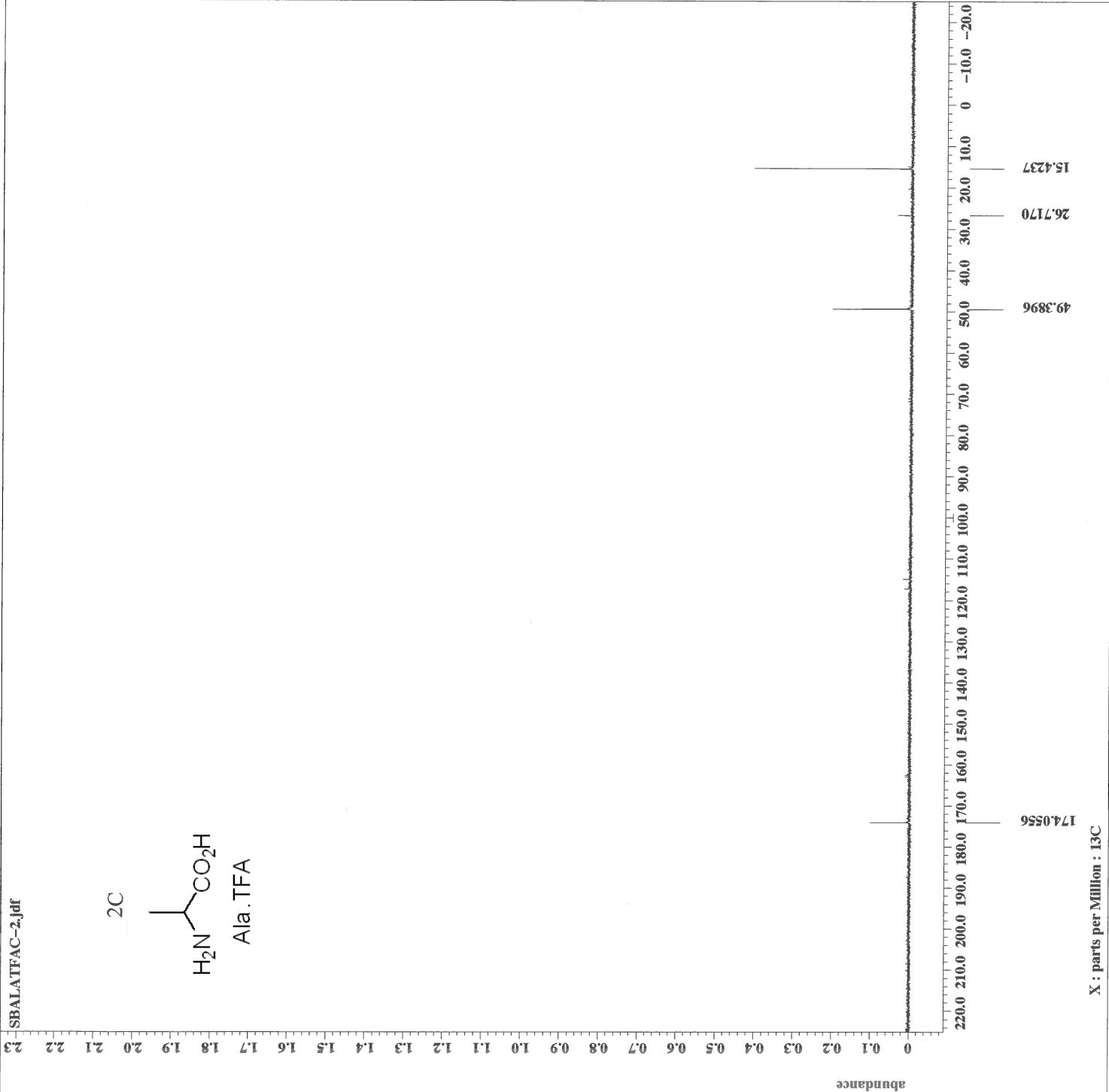
Filename           = SBALATFAC-2.jdf
Author            = delta
Experiment        = single_pulse_decouple
Sample_id         = S#31862
Solvent           = D2O
Creation_time    = 11-SEP-2015 09:10:54
Revision_time    = 10-SEP-2015 20:27:27
Current_time     = 10-SEP-2015 20:28:06

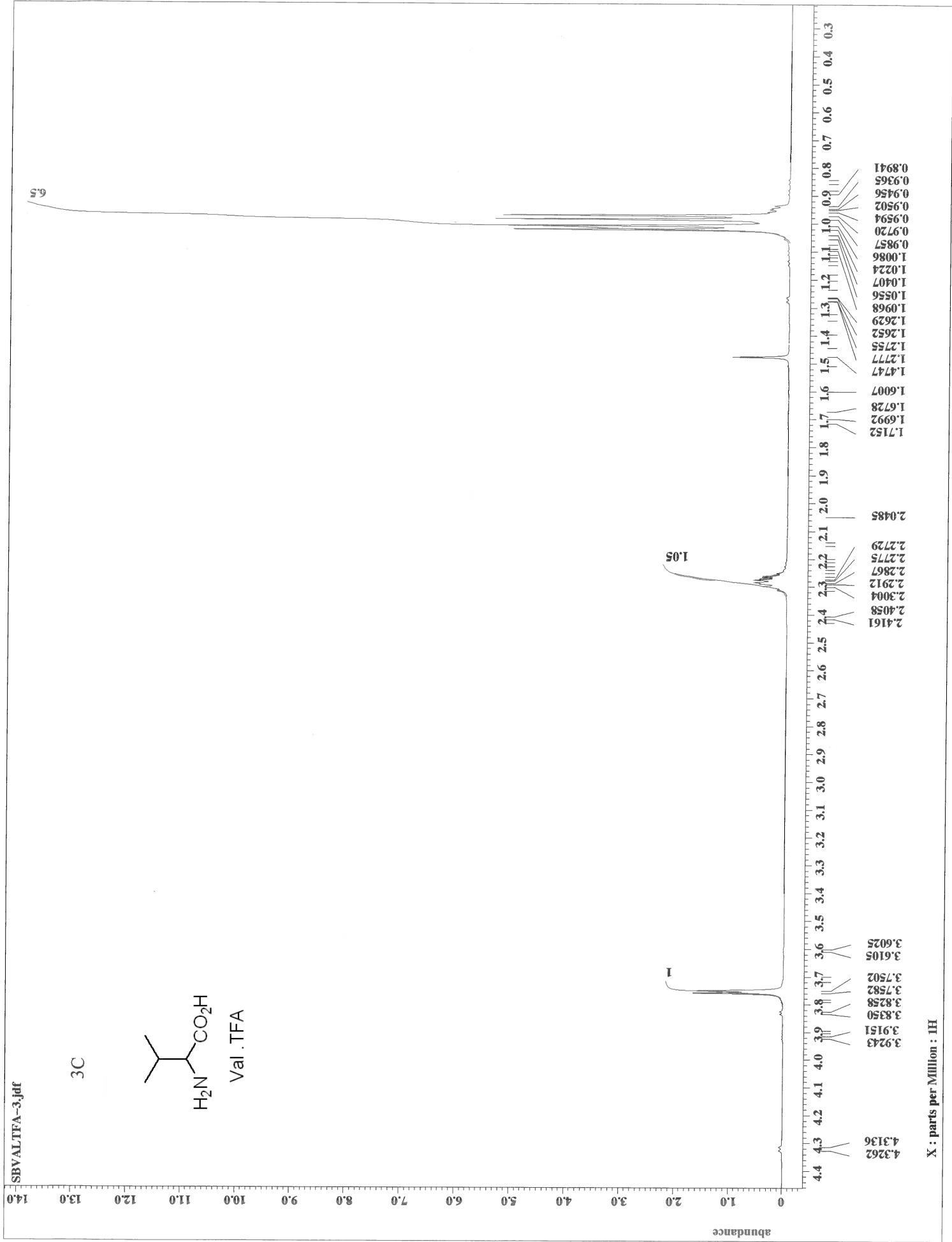
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 2614
Dim_title         = 13C
Dim_units         = [PPM]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

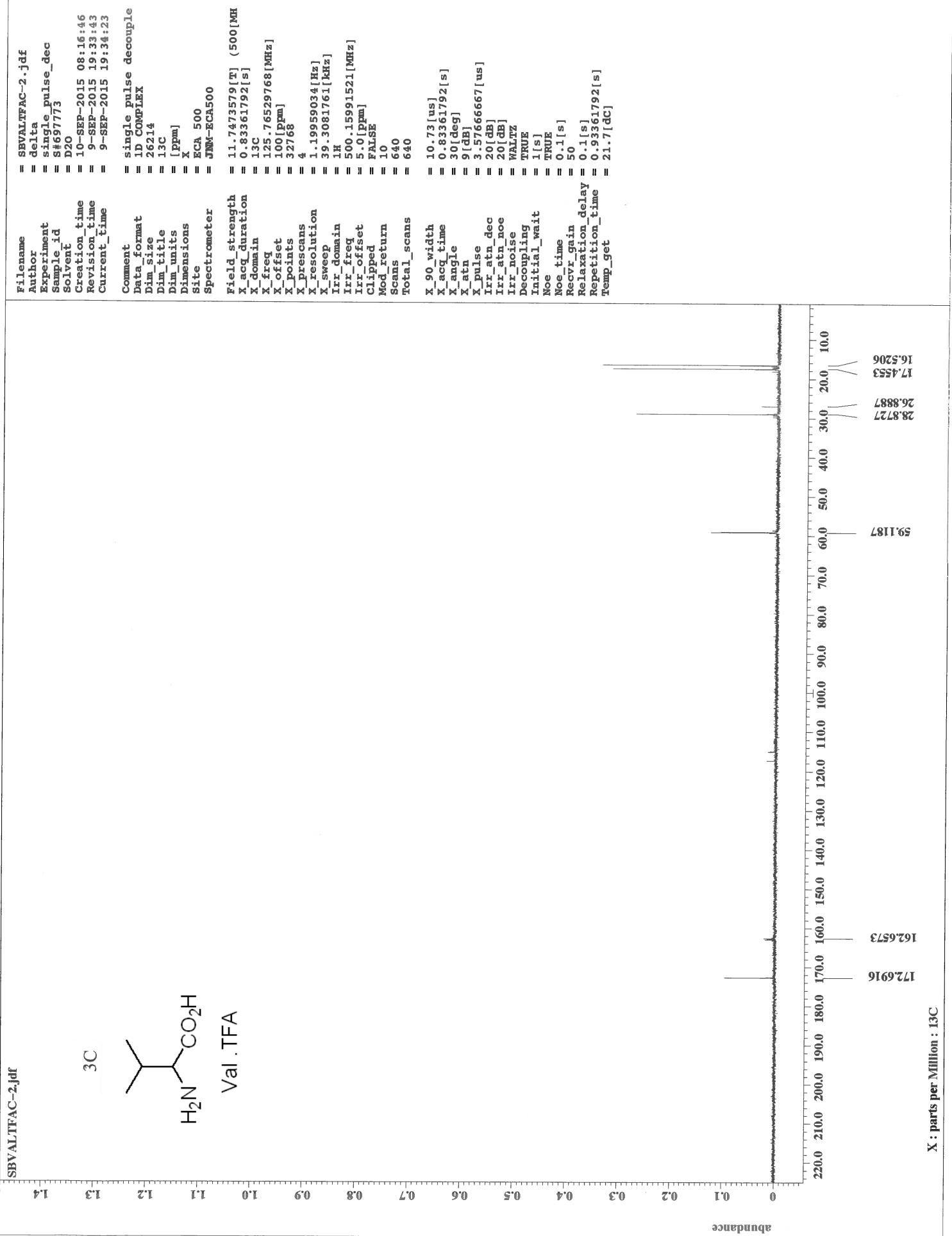
Field_strength   = 11.7473579 [T] ( 500 [MHz]
X_acq_duration  = 0.83361792 [s]
X_domain_in     = 13C
X_freq           = 125.76529768 [MHz]
X_offset          = 100 [ppm]
X_points          = 32768
X_prescans       = 4
X_resolution     = 1.19959034 [Hz]
X_sweep           = 39.3081761 [kHz]
Irr_domain       = 1H
Irr_freq          = 500.15991521 [MHz]
Irr_offset        = 5.0 [ppm]
Clipped           = FALSE
Mod_return        = 1.0
Scans             = 420
Total_scans       = 420

X_90_width       = 10.73 [us]
X_acq_time       = 0.83361792 [s]
X_angle           = 30 [deg]
X_atn             = 9 [dB]
X_pulse           = 3.57666667 [us]
Irr_atn_dec      = 20 [dB]
Irr_atn_noe      = 20 [dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1 [s]
Noe               = TRUE
Noe_time          = 0.2 [s]
Recurr_gain       = 50
Relaxation_delay = 0.2 [s]
Repetition_time   = 1.03361792 [s]
Temp_q_get        = 21.6 [dC]

```

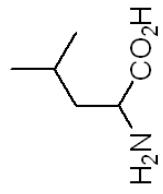






SBLEUTFA-3.idf

4C



Leu.TFA

639

```

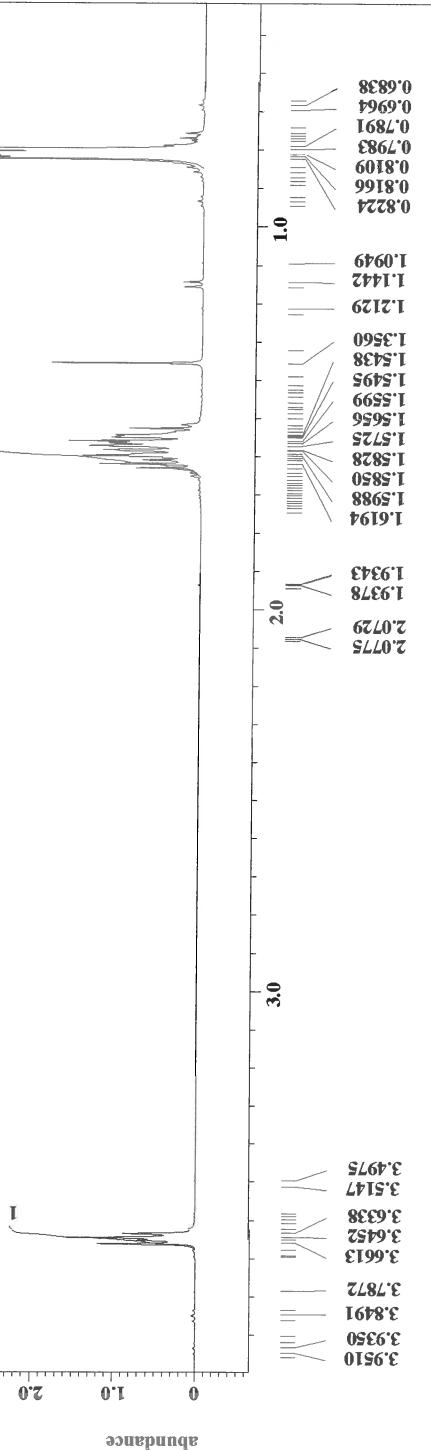
filename = SBLEUTFA-3.jdf
author = delta
experiment = single_pulse.ex2
sample_id = S#720720
solvent = D2O
creation_time = 11-SEP-2015 08:47:15
revision_time = 10-SEP-2015 20:06:22
current_time = 10-SEP-2015 20:08:00

comment = single_pulse
data_format = 1D COMPLEX
dim_size = 13107
dim_title = 1H
dim_units = [ppm]
dimensions = X
site = ECA 500
spectrometer = JNM-ECA500

field_strength = 11.7473579[T] (500[Hz])
acq_duration = 1.74587904[s]
x_domain = 1H
x_freq = 500.15991521[MHz]
x_offset = 5.0[ppm]
x_points = 16384
x_prescans = 0
x_resolution = 0.5727737[Hz]
x_sweep = 9.38238438[kHz]
irr_domain = 1H
irr_freq = 500.15991521[MHz]
irr_offset = 5.0[ppm]
tri_domain = 1H
tri_freq = 500.15991521[MHz]
tri_offset = 5.0[ppm]
clipped = FALSE
mod_return = 1
scans = 10
total_scans = 10

x_90_width = 12.54[us]
x_acq_time = 1.74587904[s]
x_angle = 45[deg]
x_atn = 4[db]
x_pulse = 6.27[us]
irr_mode = Off
tri_mode = Off
dante_preset = FALSE
initial_wait = 1[s]
recvr_gain = 34
relaxation_delay = 10[s]
repetition_time = 11.74587904[s]
temp_get = 21.2[dc]

```

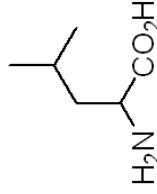


```

filename = SBLEUTFAC-2.jdf
author = delta
single_pulse_dec = single_pulse_dec
sample_id = S#23009
solvent = D2O
creation_time = 11-SEP-2015 08:54:15
revision_time = 10-SEP-2015 20:11:01
current_time = 10-SEP-2015 20:11:43
comment = single pulse decouple
data_format = 1D COMPLEX
dim_size = 2614
dim_title = 13C
dim_units = [ppm]
dimensions = X
site = ECA 500
spectrometer = JNM-ECA500
field_strength = 11.7473579 [T] (500 [MHz])
x_acq_duration = 0.83361792 [s]
x_domain = 13C
x_freq = 125.76529768 [MHz]
x_offset = 100 [ppm]
x_points = 32768
x_pressans = 4
x_resolution = 1.19959034 [Hz]
x_sweep = 39.3081761 [kHz]
irr_domain = 1H
irr_freq = 500.15991521 [MHz]
irr_offset = 5.0 [ppm]
clipped = FALSE
mod_return = 10
scans = 310
total_scans = 310
x_90_width = 10.73 [us]
x_acq_time = 0.83361792 [s]
x_angle = 30 [deg]
x_atn = 3.576666667 [us]
x_pulse = 9 [dB]
irr_atn_dec = 20 [dB]
irr_atn_noe = 20 [dB]
irr_noise = WALTZ
decoupling = TRUE
initial_wait = 1 [s]
noe_time = TRUE
noe_time = 0.2 [s]
recvr_gain = 50
recvr_gain = 50
relaxation_delay = 0.2 [s]
repetition_time = 1.03361792 [s]
temp_get = 21.6 [dc]

```

4C

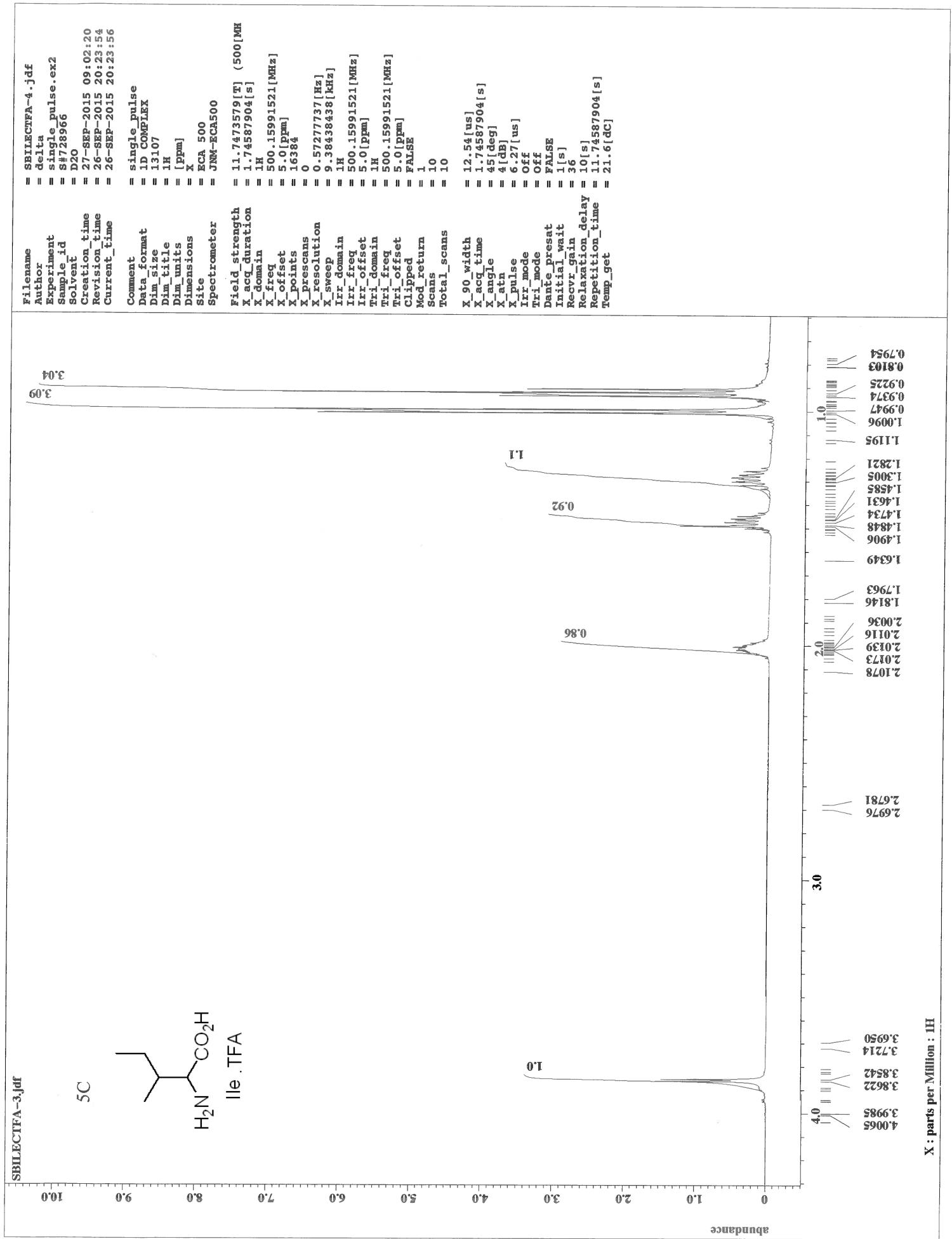


175.0285
X : parts per Million : 13C

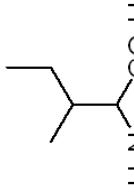


53.0524
39.6224
24.1226
21.9574
20.8701

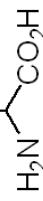
175.0285
X : parts per Million : 13C



5C



Ile .TFA



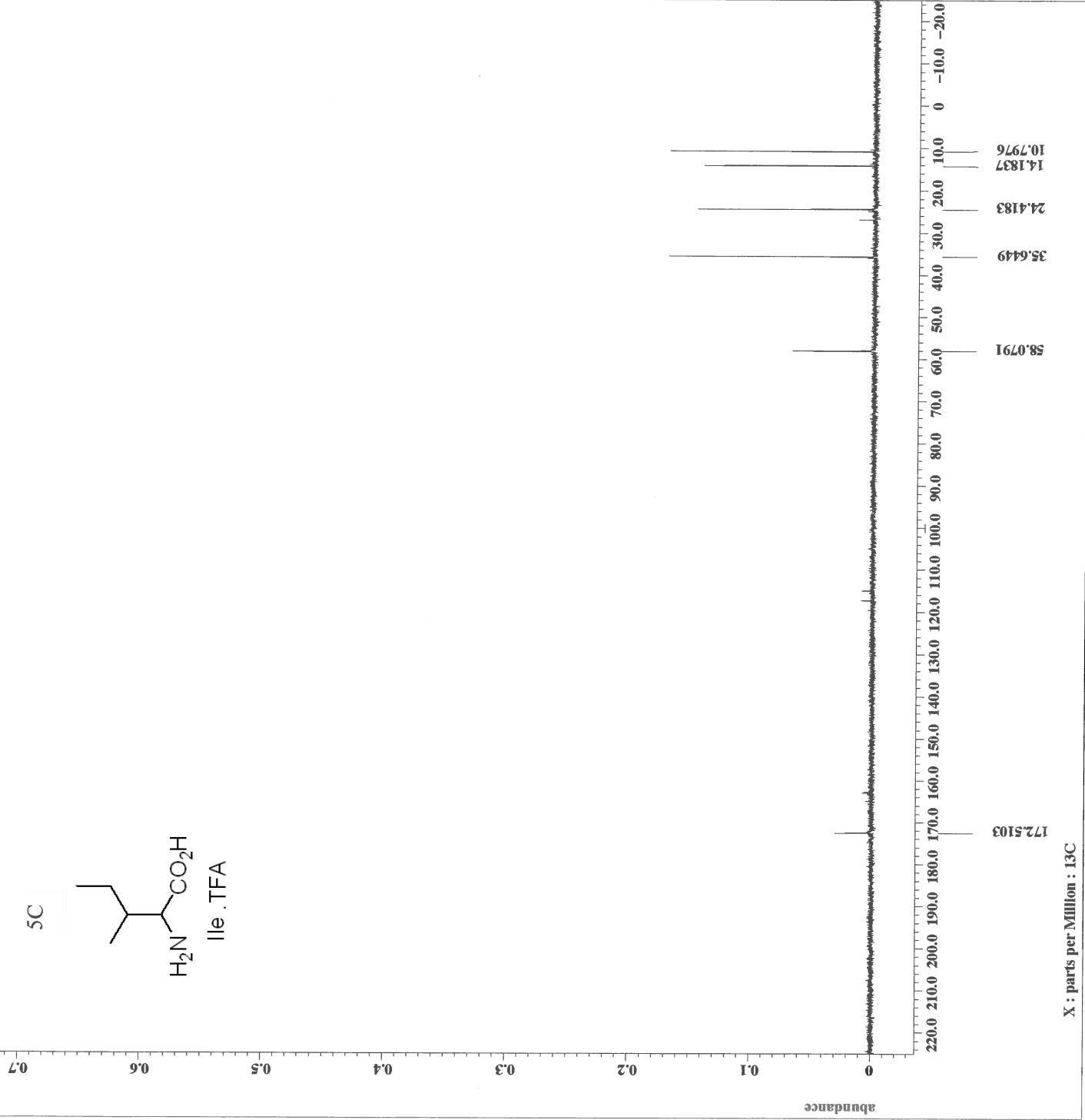
```

Filename = SBILECTFA-2.jdf
Author = delta
Experiment = single_pulse_decouple
Sample_id = S#131232
Solvent = D2O
Creation_time = 27-SEP-2015 09:27:10
Revision_time = 26-SEP-2015 20:43:10
Current_time = 26-SEP-2015 20:45:11
Comment = single_pulse_decouple
Data_format = 1D COMPLEX
Dim_size = 26514
Dim_title = 13C
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MHz])
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 125.76529768 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.19959034 [Hz]
X_sweep = 39-3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 10
Scans = 1390
Total_scans = 1390

X_90_width = 10.73 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.576666667 [us]
Irr_atn_dec = 20 [dB]
Irr_atn_noe = 20 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 0.2 [s]
Recvr_gain = 50
Relaxation_delay = 0.2 [s]
Repetition_time = 1.03361792 [s]
Temp_get = 22.1 [deg]

```

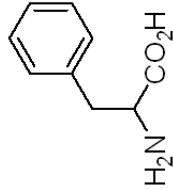


X : parts per Million : 13C

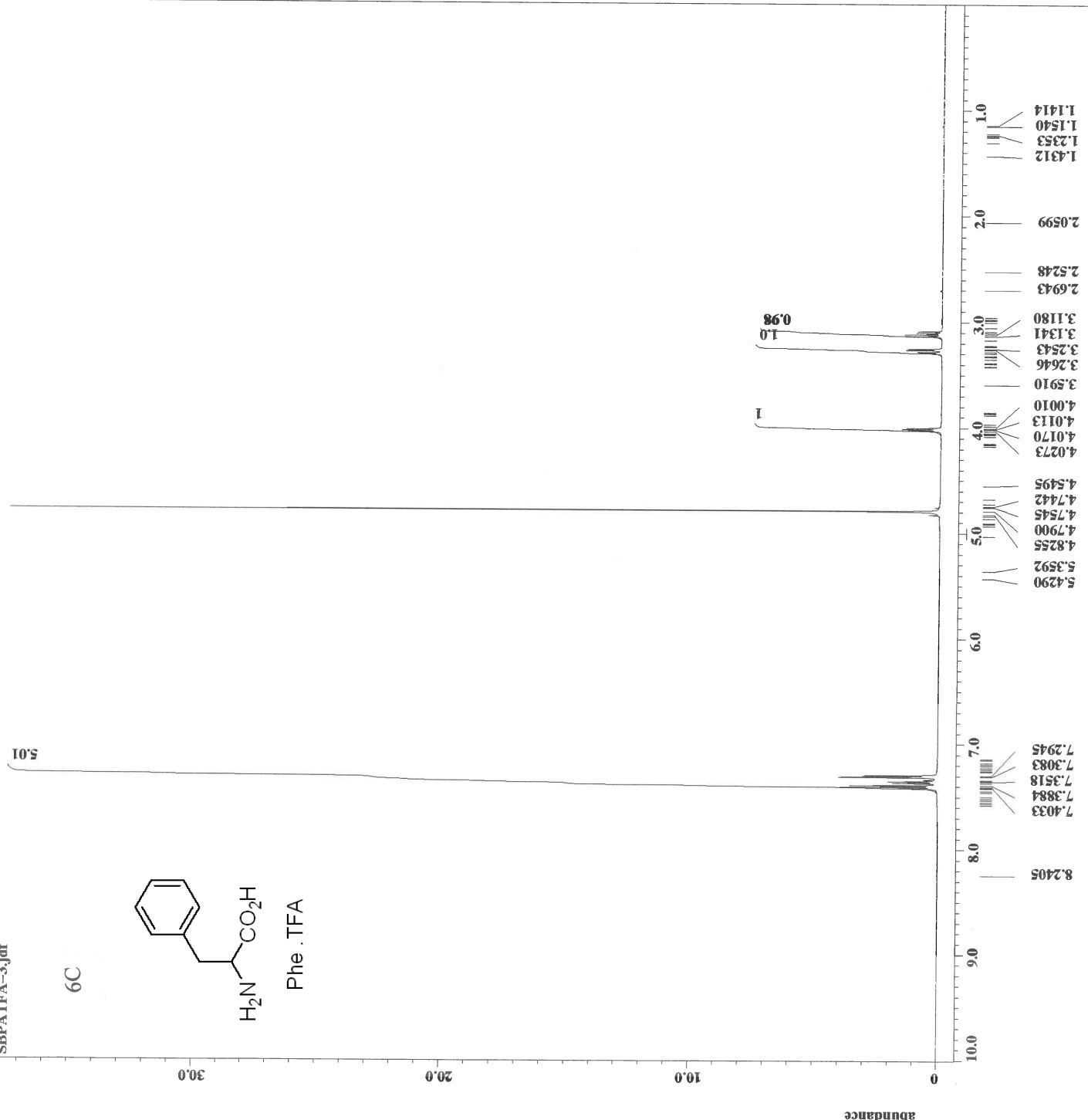
SBPATFA-3.idf

5.01

60



Phe TEA



```

Filename = SBPATFA-3.jdf
Author = delta
Experiment =
Sample id = Single_pulse.ex2
Solvent = #398428
Creation_time = 19-SEP-2015 23:52:20
Revision_time = 19-SEP-2015 11:10:20
Current_time = 19-SEP-2015 11:11:11

Comment = single pulse
Data format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

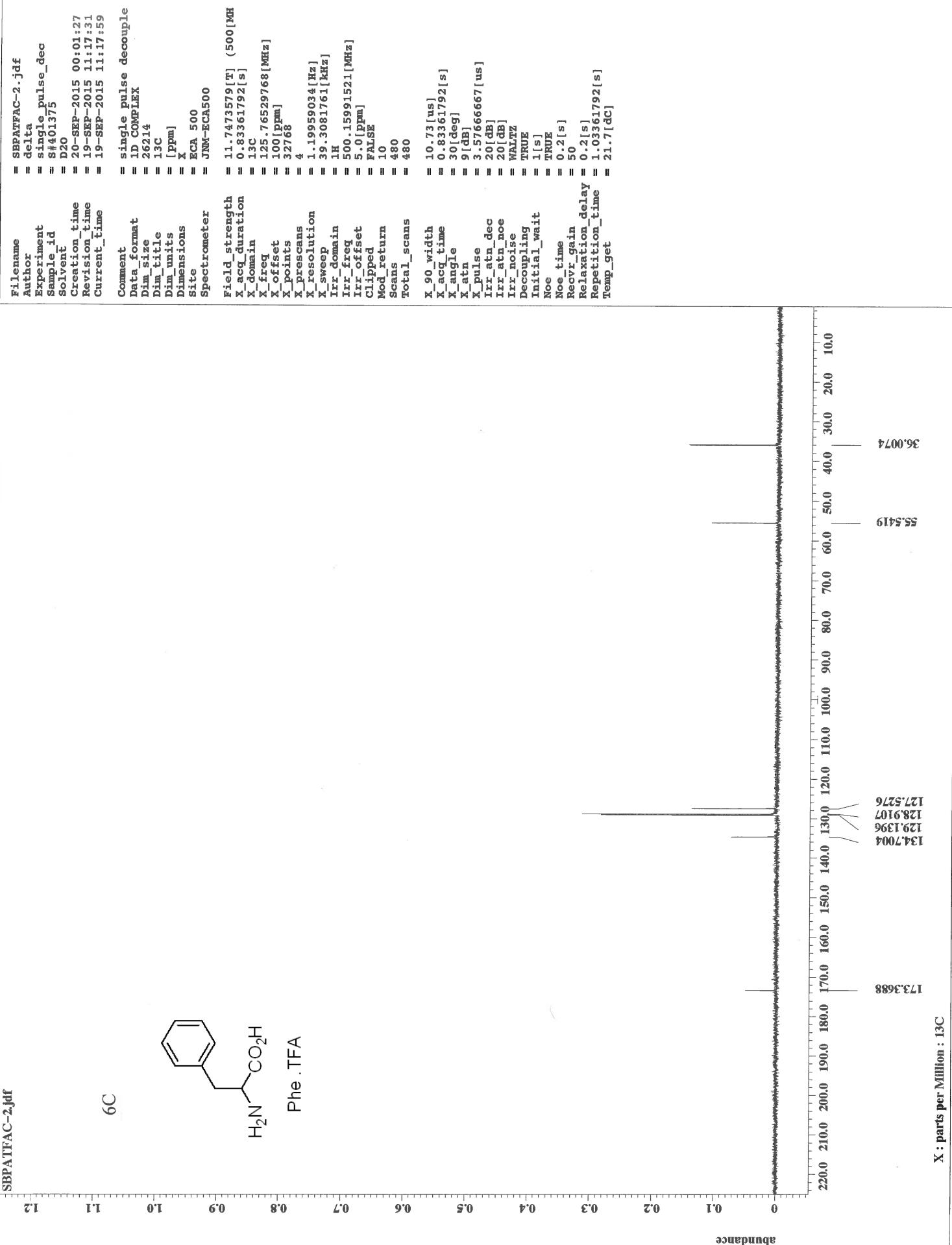
Field_strength = 11.7473579[T] (500 [MHz])
X_acq_duration = 1H 45:58:7904[s]
X_domain = 1H
X_freq = 500.15991521[MHz]
X_offset = 5.01[PPM]
X_points = 16384
X_prescans = 0
X_resolution = 0.577737[Hz]
X_sweep = 9.386338438[kHz]
Irr_domain = 1H
Irr_offset = 500.15991521[MHz]
Irr_offset = 5.01[PPM]
Tri_domain = 1H
Tri_freq = 500.15991521[MHz]
Tri_offset = 5.01[PPM]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

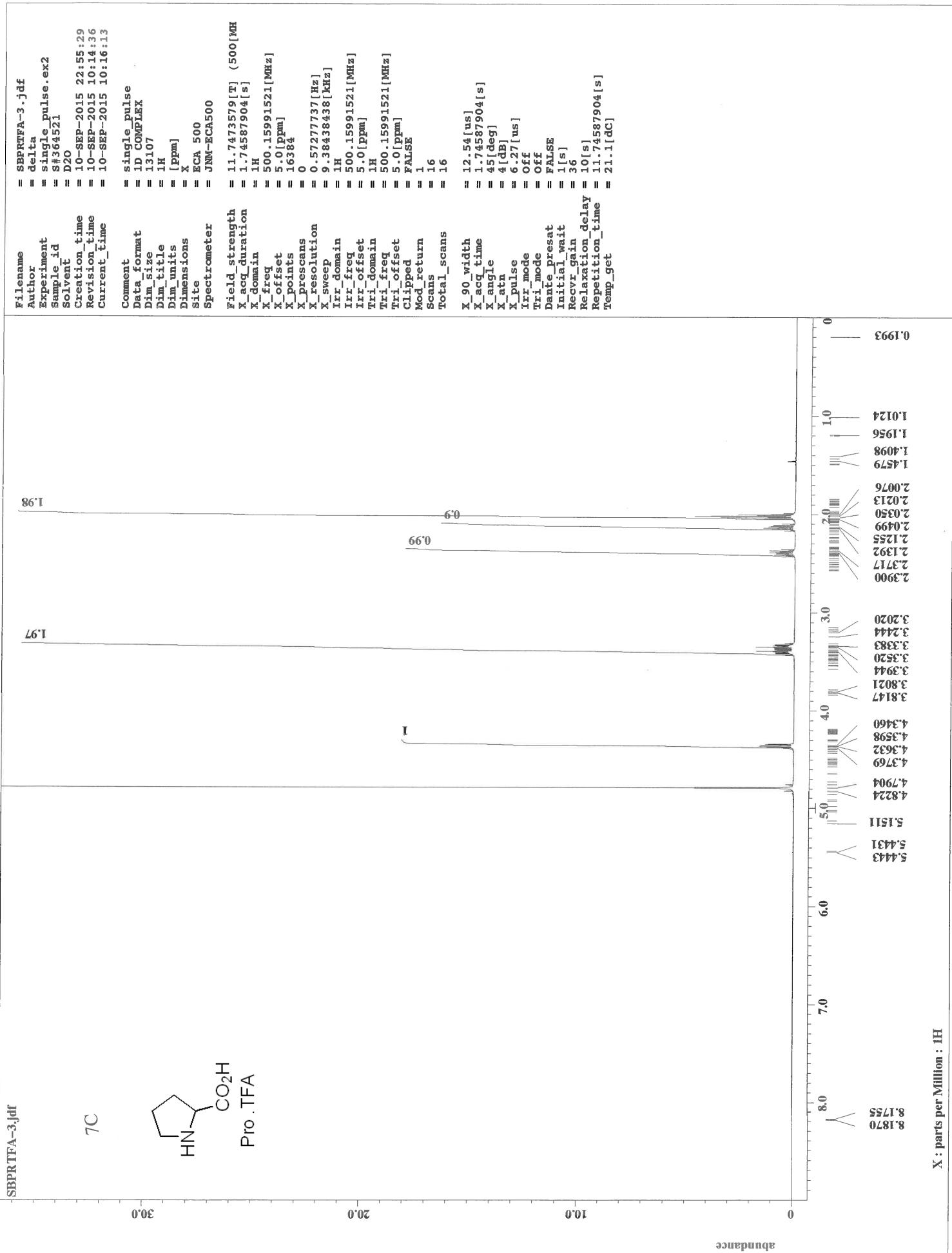
X_90_width = 12.54[us]
X_acq_time = 1.74587904[s]
X_angle =
X_atn =
X_pulse = 6.22[us]
Irr_mode = Off
Tri_mode = Off
Danc_Preset = FALSE
Initial_wait = 1[s]
Recv_gain = 40
Relaxation_delay = 10[s]
Repetition_time = 11.74587904[s]
Temp_get = 21.2[dc]

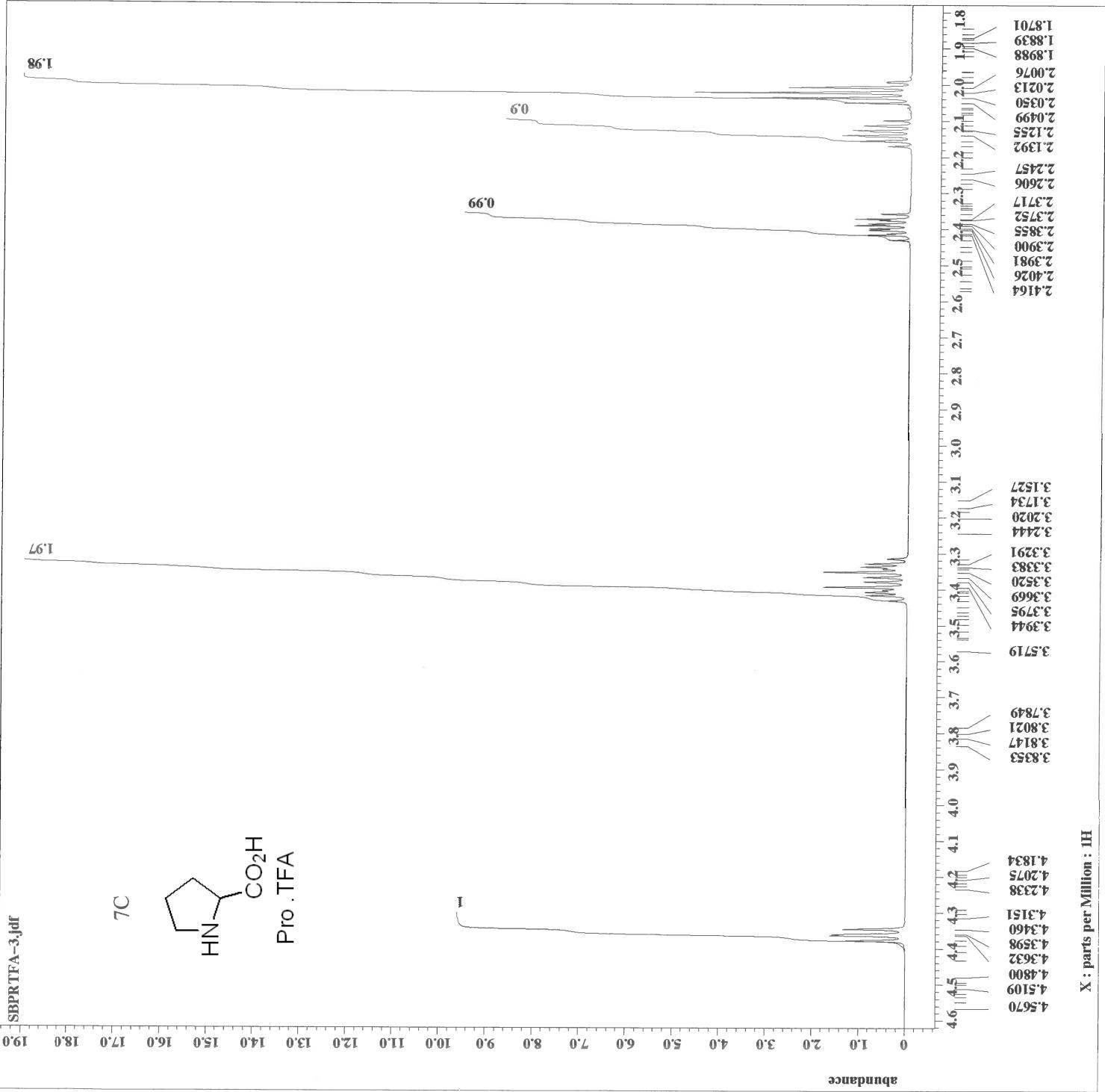
```

1.4312	1.2353	1.1540	1.1414
2.6943	2.5248	2.5248	2.0599
3.5910	3.2643	3.2643	3.1180
4.0010	4.0113	4.0113	4.0113
4.0273	4.0170	4.0170	4.0170
4.8255	4.7900	4.7545	4.7442
5.4290	5.3592	5.3592	4.5495

X : parts per Million : 1H





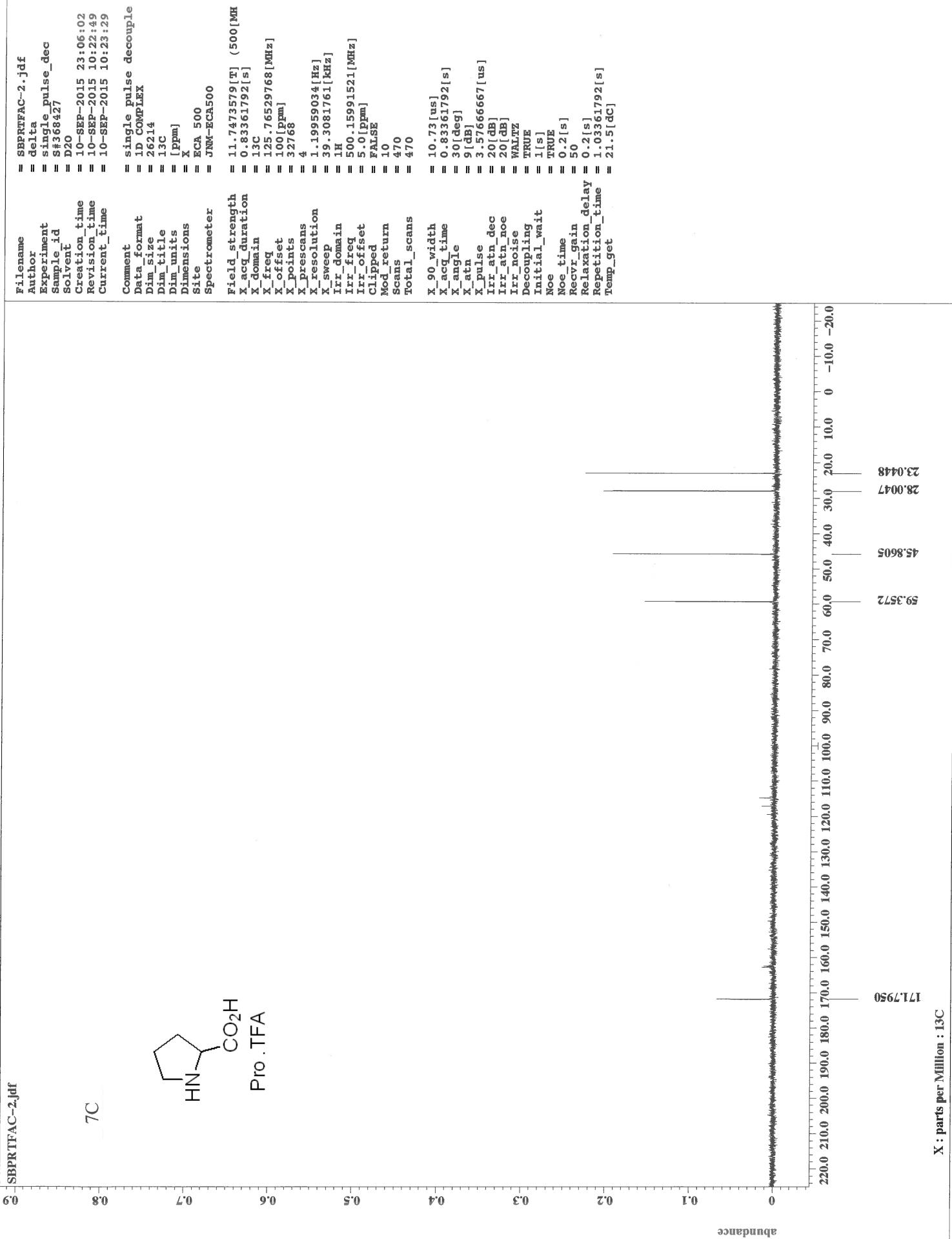


```

filename = SBPRTFA-3.jdf
author = delta
single_pulse.ex2
sample_id = S#364521
D20
creation_time = 10-SEP-2015 22:55:29
revision_time = 10-SEP-2015 10:14:36
current_time = 10-SEP-2015 10:16:47
comment = single_pulse
data_format = 1D COMPLEX
dim_size = 13107
dim_title = 1H
dim_units = [ppm]
dimensions = X
site = ECA 500
spectrometer = JNM-ECA500

field_strength = 1.7473579 [T] (500 [MHz])
x_acq_duration = 1.74587904 [s]
x_domain = 1H
x_freq = 500.15991521 [MHz]
x_offset = 5.0 [ppm]
x_points = 16384
x_prescans = 0
x_resolution = 0.57277737 [Hz]
x_sweep = 9.38438438 [kHz]
irr_domain = 1H
irr_freq = 500.15991521 [MHz]
irr_offset = 5.0 [ppm]
tri_domain = 1H
tri_freq = 500.15991521 [MHz]
tri_offset = 5.0 [ppm]
clipped = FALSE
mod_return = 1
scans = 16
total_scans = 16
x90_width = 12.54 [us]
x_acq_time = 1.74587904 [s]
x_angle = 45 [deg]
x_atn = 4 [dB]
x_pulse = 6.27 [us]
irr_mode = off
tri_mode = off
dante_preset = FALSE
initial_wait = 1 [s]
recvr_grain = 36
relaxation_delay = 10 [s]
repetition_time = 11.74587904 [s]
temp_get = 21.1 [dC]

```



SBMIEITFA-3.rdf

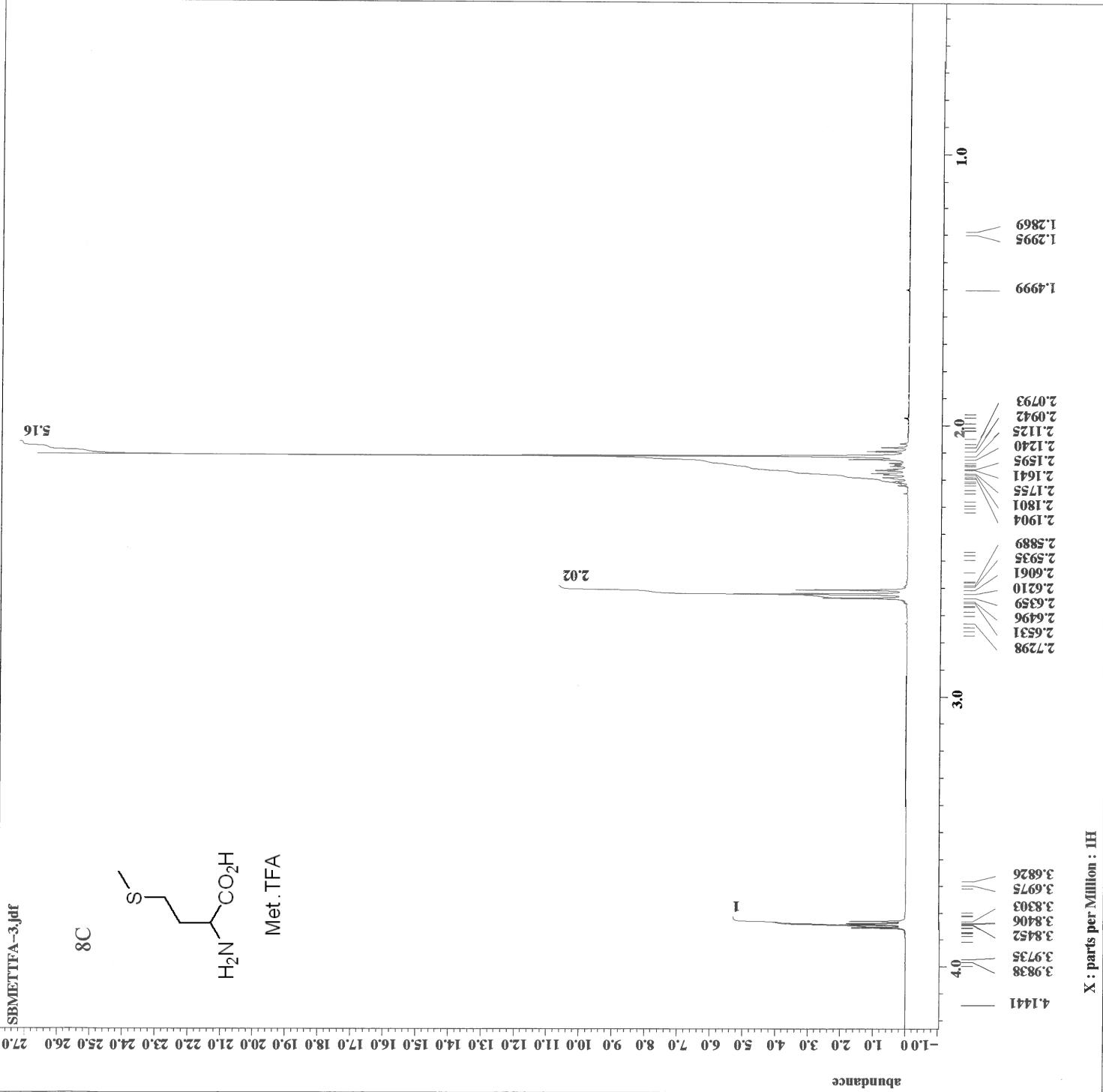
```

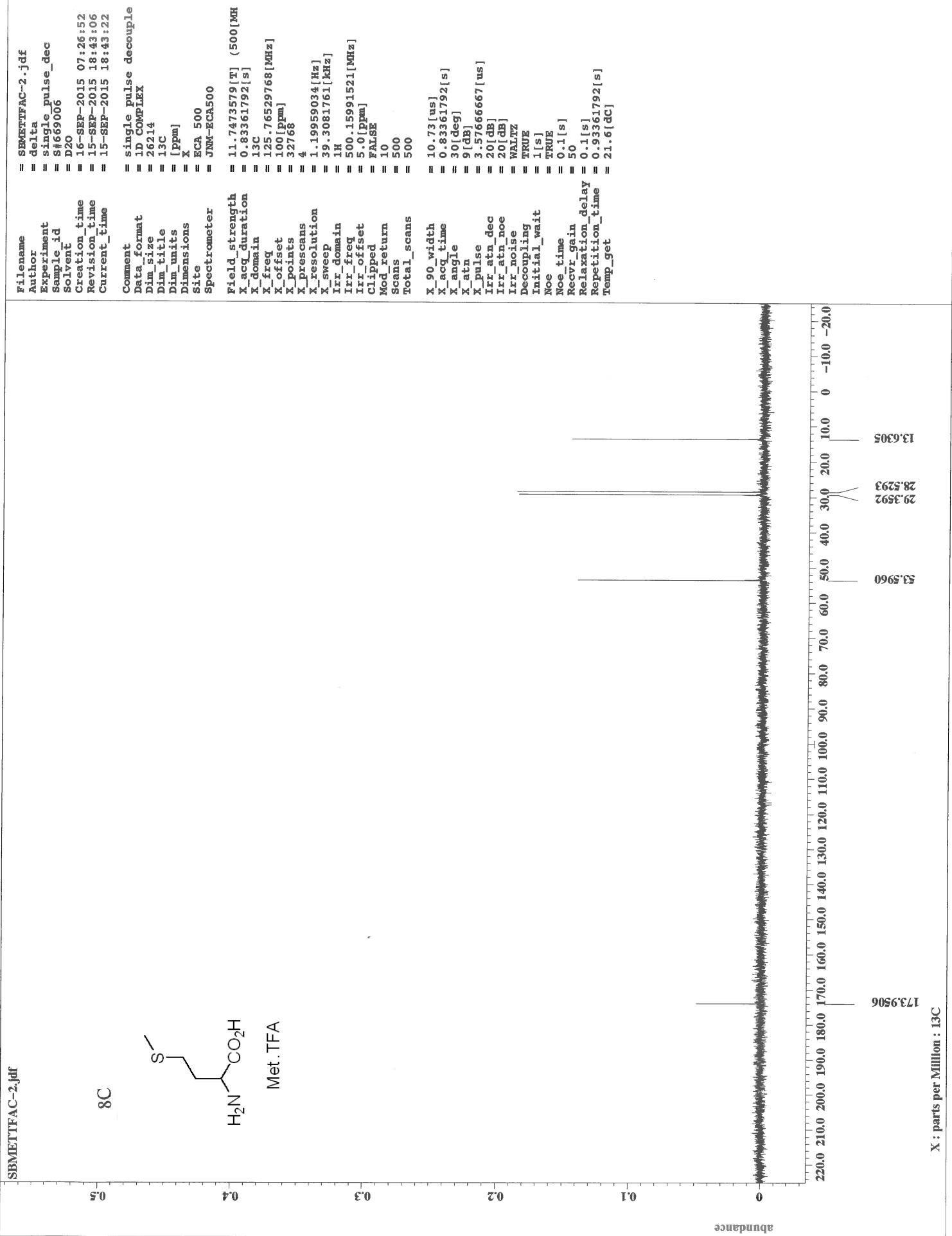
Filename      = SEMETTA-3.jdf
Author        = delta
Experiment   = single_pulse.ex2
Solvent       = S#665759
Data_format  = ID COMPLEX
Comment      = single_pulse
Dim_size     = 13107
Dim_units   = 1H
Dimensions  = [ppm]
Site          = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MHz])
X_acq_duration = 1.74581904 [s]
X_domain     = 1H
X_freq        = 500.15991521 [MHz]
X_offset      = 5.0 [ppm]
X_points      = 16384
X_prescans   = 0
X_resolution = 0.57277737 [Hz]
X_sweep       = 9.38438438 [kHz]
Irr_domain   = 1H
Irr_freq      = 500.15991521 [MHz]
Irr_offset    = 5.0 [ppm]
Tri_domain   = 1H
Tri_freq      = 500.15991521 [MHz]
Tri_offset    = 5.0 [ppm]
Clipped      = FALSE
Mod_return   = 1
Scans         = 11
Total_scans  = 11

X_90_width   = 12.54 [us]
X_acq_time   = 1.74581904 [s]
X_angle      = 45 [deg]
X_atn        = 4 [dB]
X_pulse      = 6.27 [us]
Irr_mode     = Off
Tri_mode     = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain   = 38
Relaxation_delay = 10 [s]
Repetition_time = 11.74581904 [s]
Temp_Get     = 21.2 [dc]

```





```

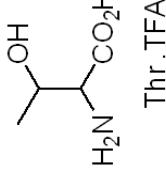
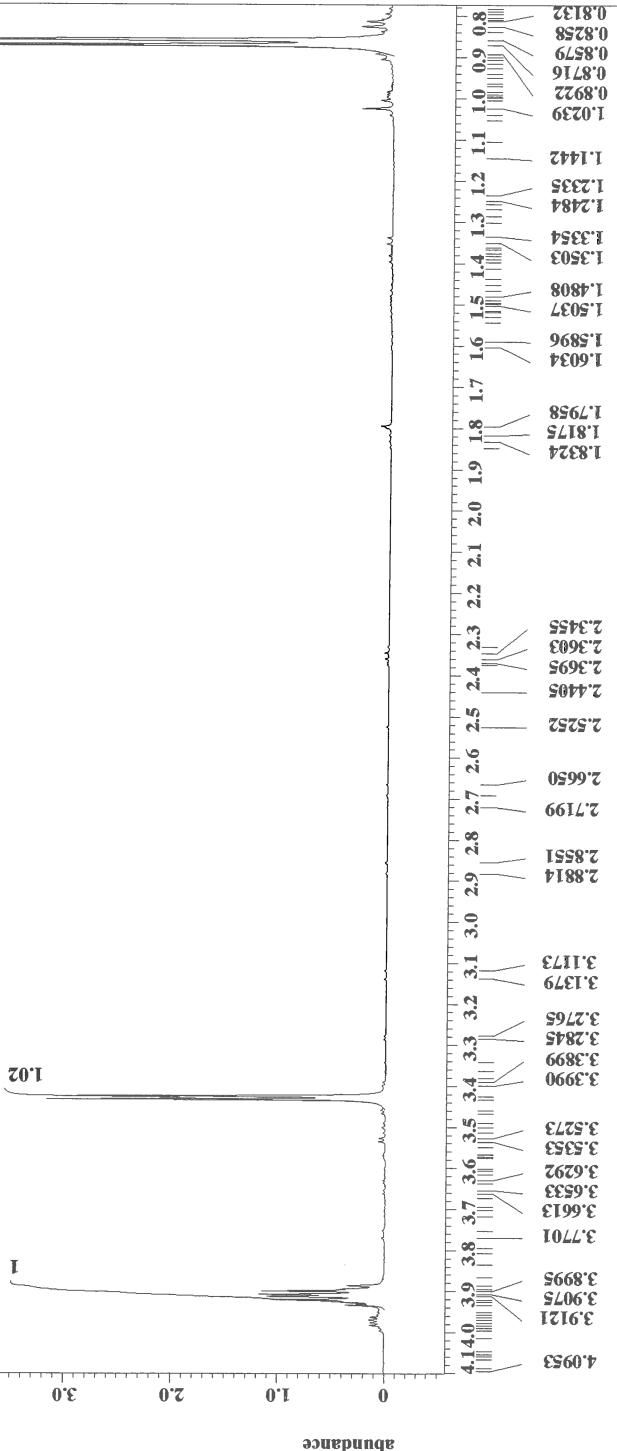
Filename = SBTRHFFA-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#508822
Solvent = D2O
Creation_time = 10-SEP-2015 02:54:48
Revision_time = 9-SEP-2015 14:12:32
Current_time = 9-SEP-2015 14:13:28

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_units = IH
Dimensions = [PPM]
Site = ECA 500
spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MHz])
X_acq_duration = 1.74587904[s]
X_domain = 1H
X_freq = 500.15991521[MHz]
X_offset = 5.0[PPM]
X_Points = 16384
X_Prescans = 0
X_resolution = 0.5777737[Hz]
X_sweep = 9.38438438[Hz]
Inr_domain = 1H
Inr_freq = 500.15991521[MHz]
Inr_offset = 5.0[PPM]
Inr_domain = 1H
Tri_freq = 500.15991521[MHz]
Tri_offset = 5.0[PPM]
Clipped = FALSE
Mod_return = 1
Scans = 10
Total_scans = 10

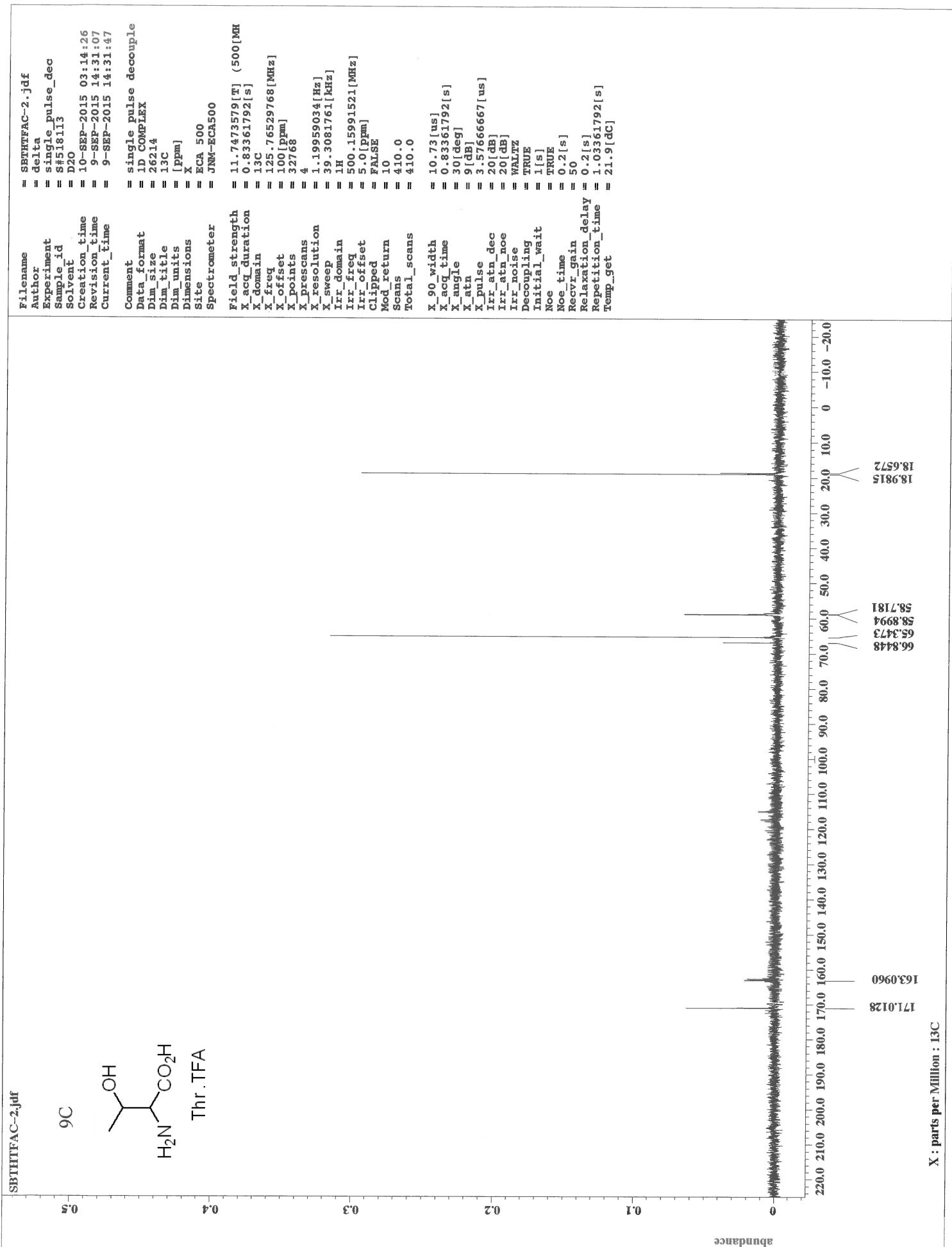
X_90_width = 12.54[us]
X_acq_time = 1.74587904[s]
X_angle = 45[deg]
X_atn = 4[dB]
X_pulse = 6.27[us]
Inr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recurr_gin = 32
Relaxation_delay = 10[s]
Relaxation_time = 11.74587904[s]
Temp_get = 21.5[dc]

```



6

X: parts per Million : 1H



```

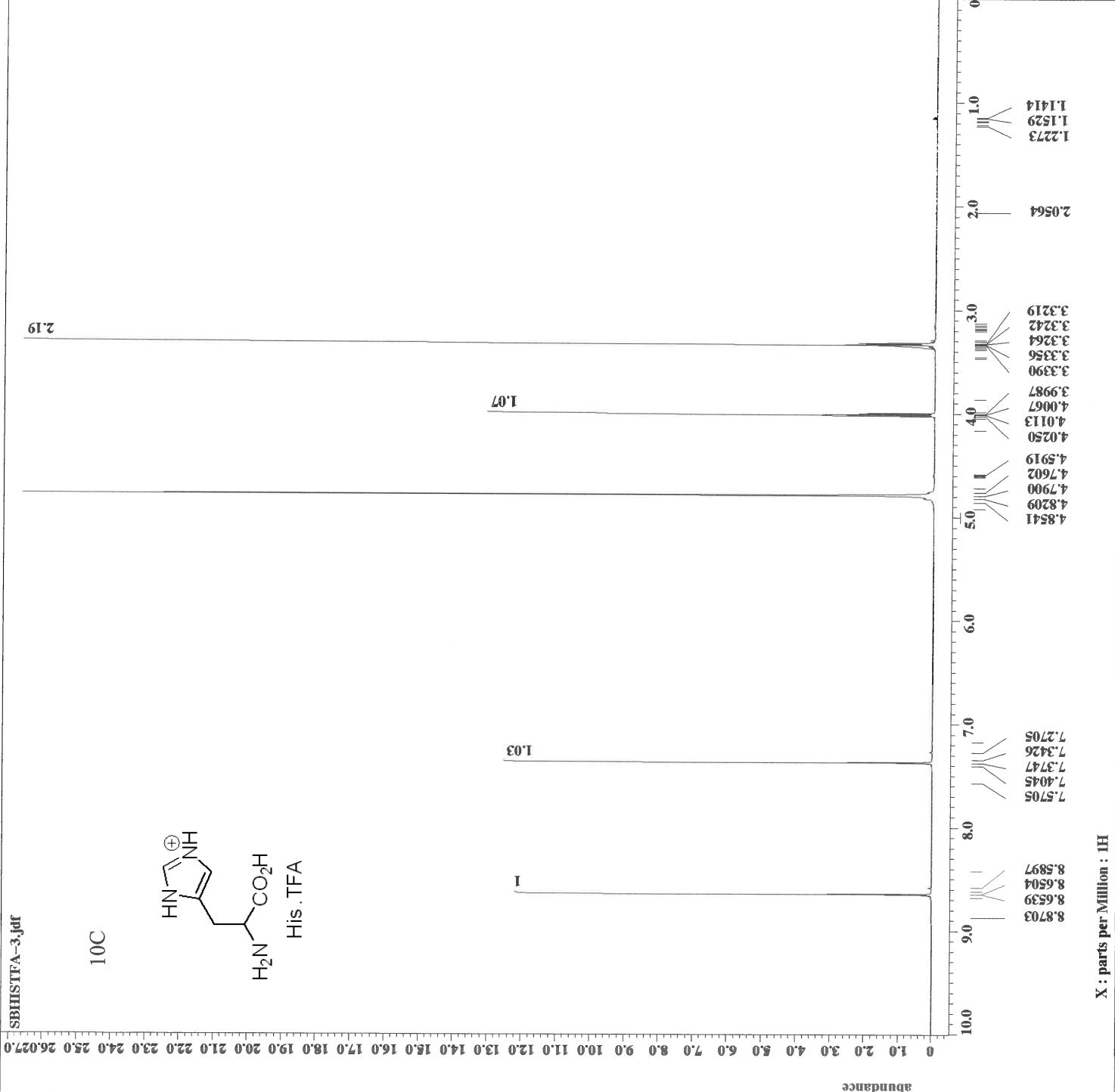
Filename = SEH1715PA-3.jdf
Author = delta
Experiment = single_pulse.ex2
sample_id = S#6153572
Solvent = D2O
Creation_time = 16-SEP-2015 06:55:52
Revision_time = 15-SEP-2015 18:14:40
Current_time = 15-SEP-2015 18:15:28

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_units = 1H
Dimensions = [ppm]
Site = ECA 500
spectrometer = JNM-ECA500

Field_strength = 11.7473579[T]
X_acq_duration = 1.74587904[s]
X_domain = 1H
X_freq = 500.15991521[MHz]
X_offset = 5.0[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.5727737[Hz]
X_sweep = 9.38438438[KHz]
Irr_domain = 1H
Irr_freq = 500.15991521[MHz]
Irr_offset = 5.0[ppm]
Wri_domain = 1H
Tri_freq = 500.15991521[MHz]
Tri_offset = 5.0[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 10
Total_scans = 10

X_90_width = 12.54[us]
X_acq_time = 1.74587904[s]
X_angle = 45[deg]
X_attn = 4[db]
X_pulse = 6.271[us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Reccv_gain = 48
Relaxation_delay = 10[s]
Repetition_time = 11.7587904[s]
Temp_get = 21.1[dc]

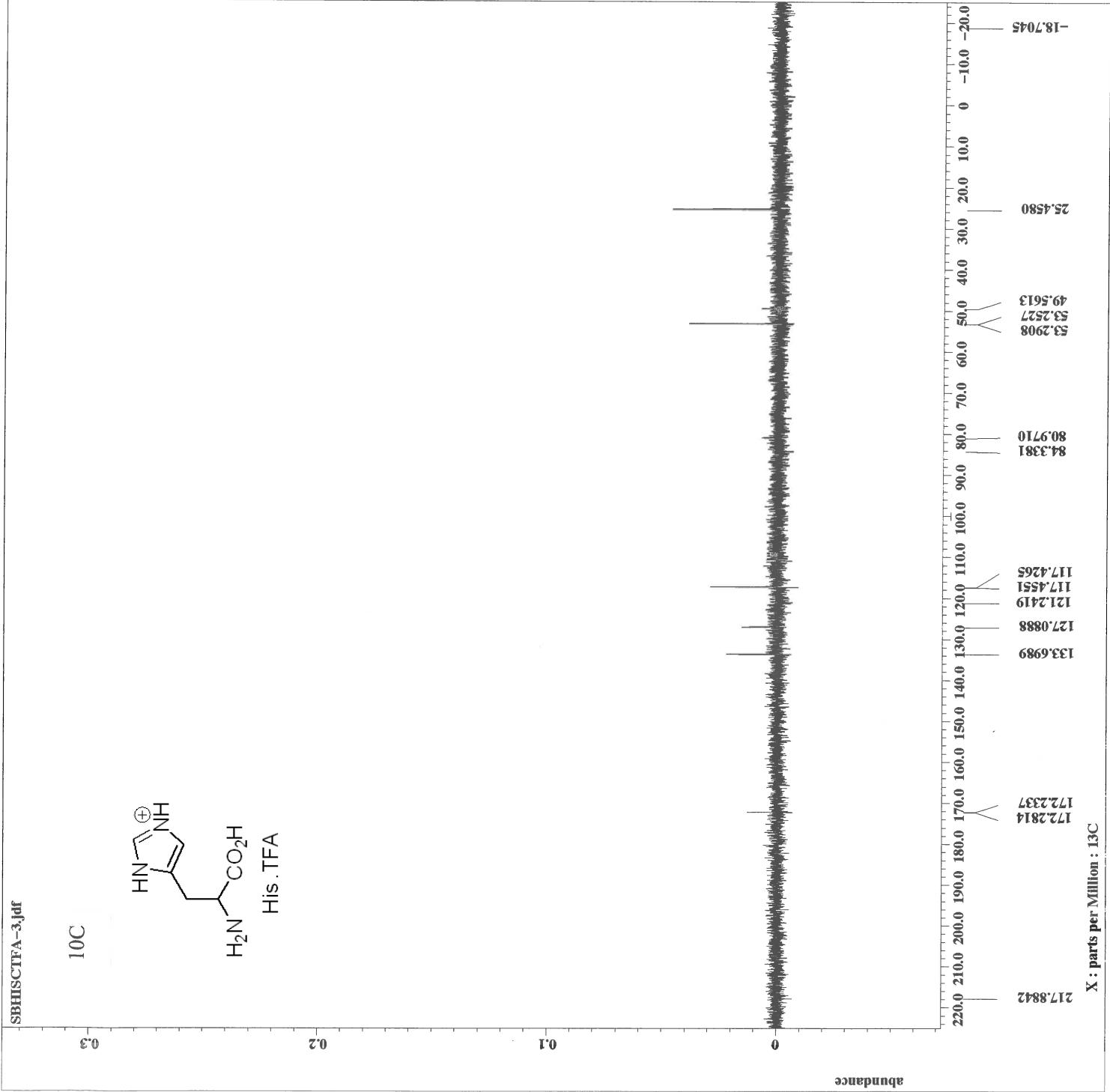
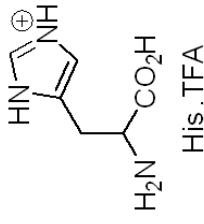
```

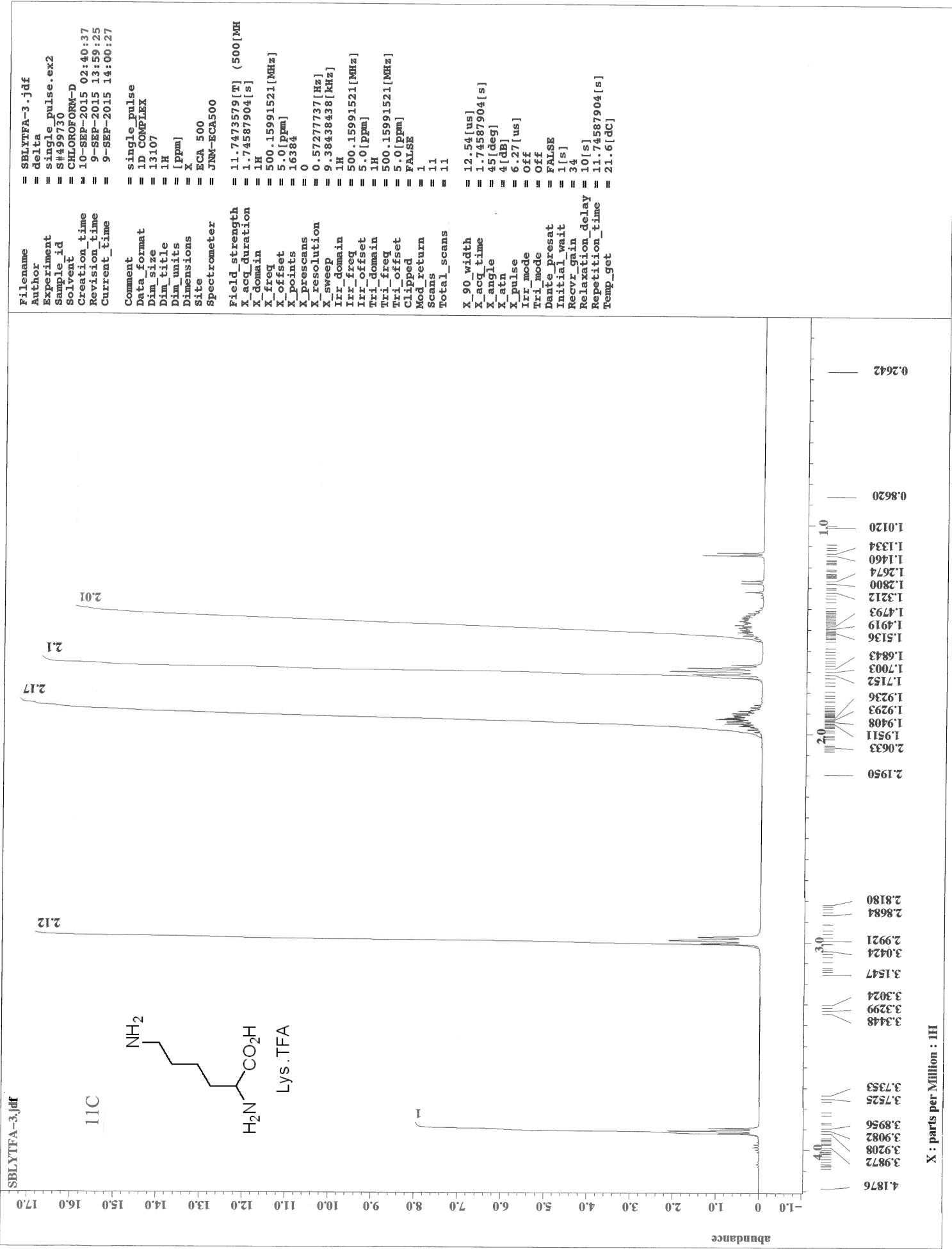


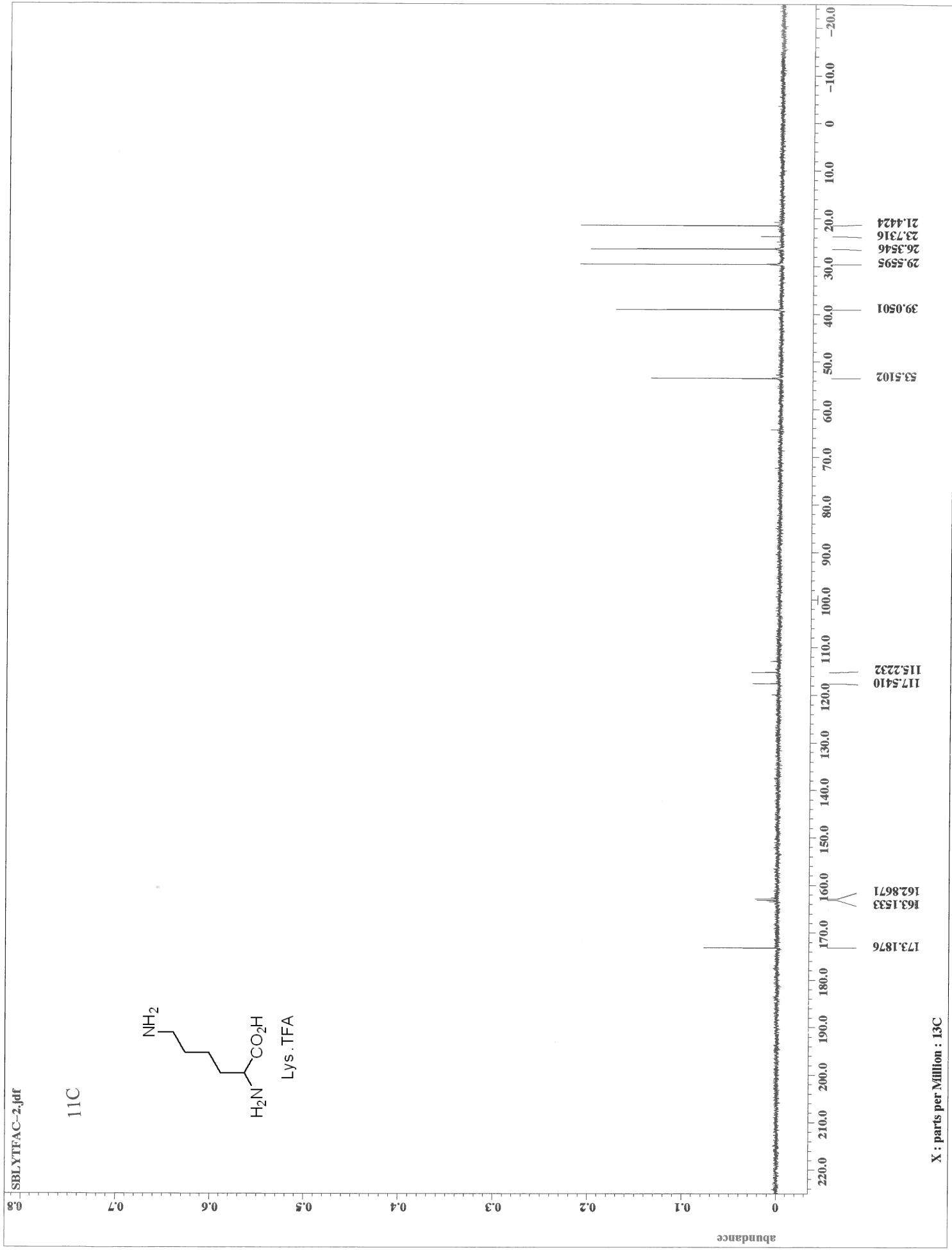
```

Filename = SBHISCTFA-3.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#655640
Solvent = D2O
Creation_time = 16-SEP-2015 07:06:50
Revision_time = 15-SEP-2015 18:23:26
Current_Time = 15-SEP-2015 18:23:42
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500
Field_strength = 11.7473579 [T] ( 500 [MHz]
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 125.76539768 [MHz]
X_offset = 100 [PPM]
X_points = 32768
X_resolution = 4
X_prescans = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15891521 [MHz]
Irr_offset = 5.0 [PPM]
Clipped = FALSE
Mod_return = 10
Scans = 580
Total_scans = 580
X_90_width = 10.73 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.576666667 [us]
Irr_atn_dec = 20 [dB]
Irr_atn_noe = 20 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_time = 0.2 [s]
Recvr_gain = 50
Relaxation_delay = 0.2 [s]
Repetition_time = 1.03361792 [s]
Temp_get = 21.6 [dC]

```







SBASPTFA-3.jdf

```
Filename = SBASPTFA-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#381529
Solvent = D2O
Creation_time = 12-SEP-2015 23:22:32
Revision_time = 12-SEP-2015 10:41:13
Current_Time = 12-SEP-2015 10:41:33
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
site = ECA 500
spectrometer = JNM-ECA500

Field_strength = 11.7473579 [Hz] (500 [MHz])
X_acq_duration = 1.74587904 [s]
X_domain = 1H
X_freq = 500.15991521 [MHz]
X_offset = 5.0 [ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.5727737 [Hz]
X_sweep = 9.38438438 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Tri_domain = 1H
Tri_freq = 500.15991521 [MHz]
Tri_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 9
Total_scans = 9

X_90_width = 12.54 [us]
X_acq_time = 1.74587904 [s]
X_angle = 45 [deg]
X_atn = 4 [dB]
X_pulse = 6.27 [us]
Tri_mode = Off
Dante_presat = Off
Initial_wait = FALSE
Recv_gain = 1 [s]
Relaxation_delay = 10 [s]
Repetition_time = 11.74587904 [s]
Temp_get = 21.3 [dc]
```

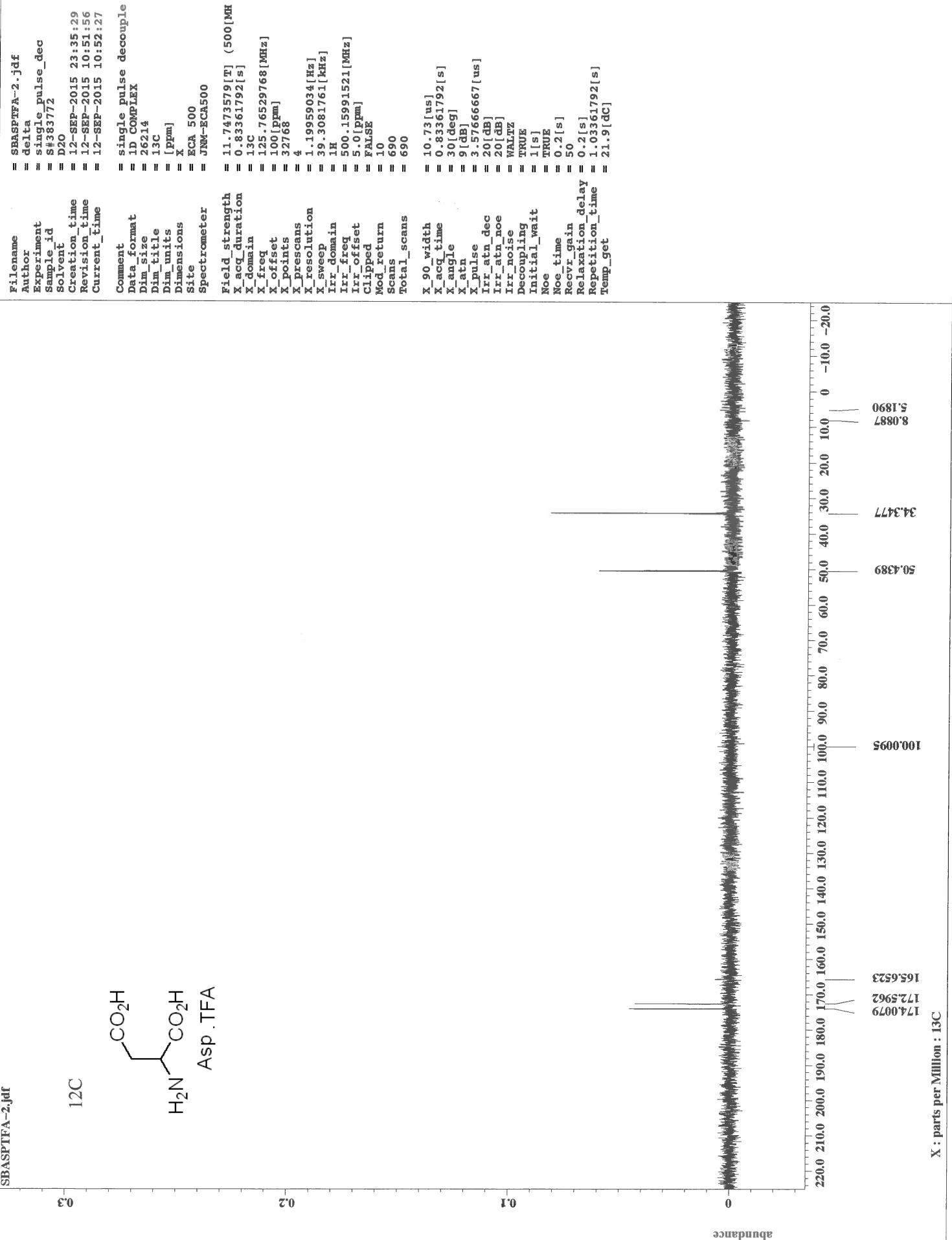
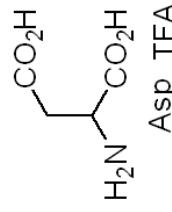
12C

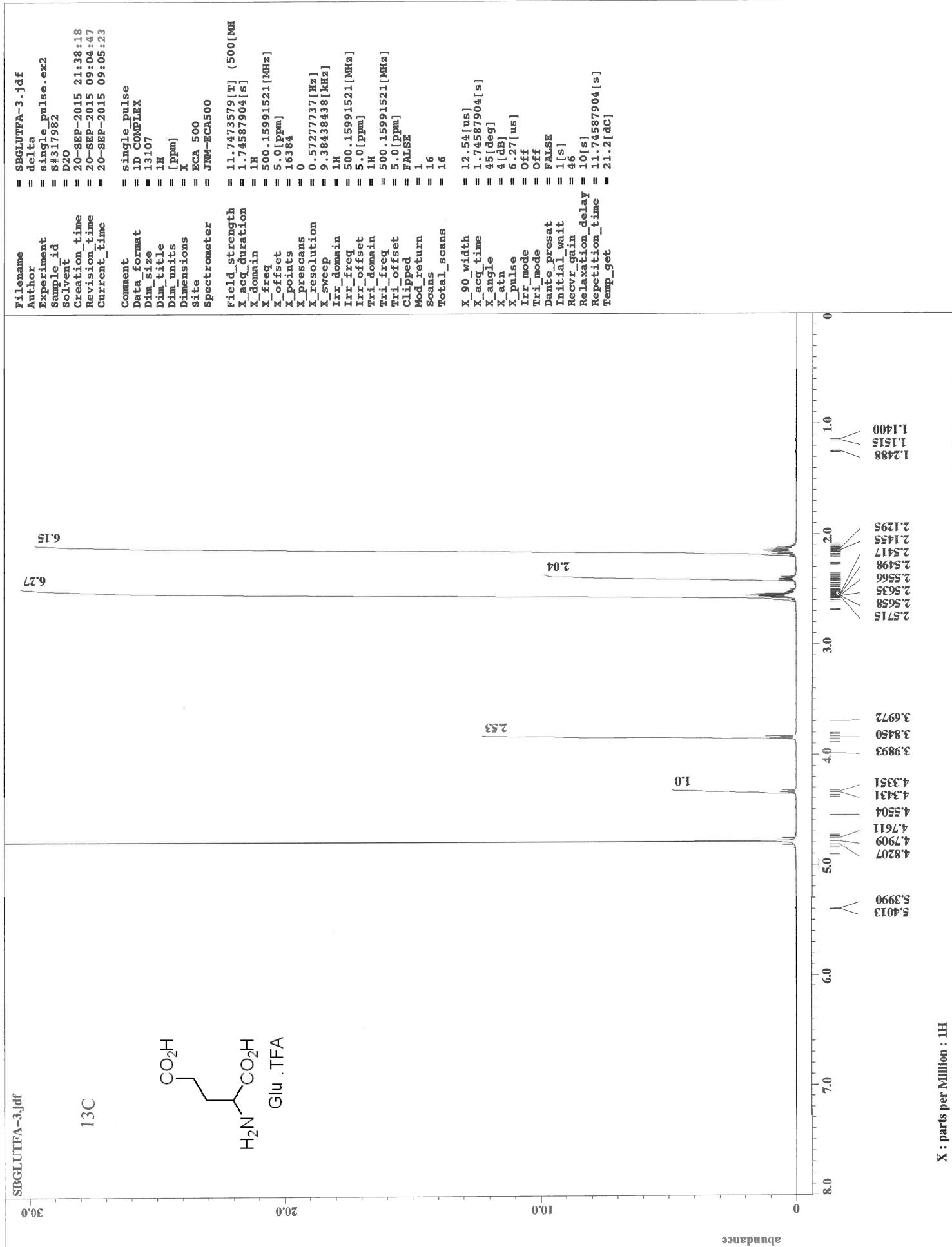
Asp . TFA

CC(C(=O)O)N

abundance

12C





SBGLUTFAC-4.jdf

```

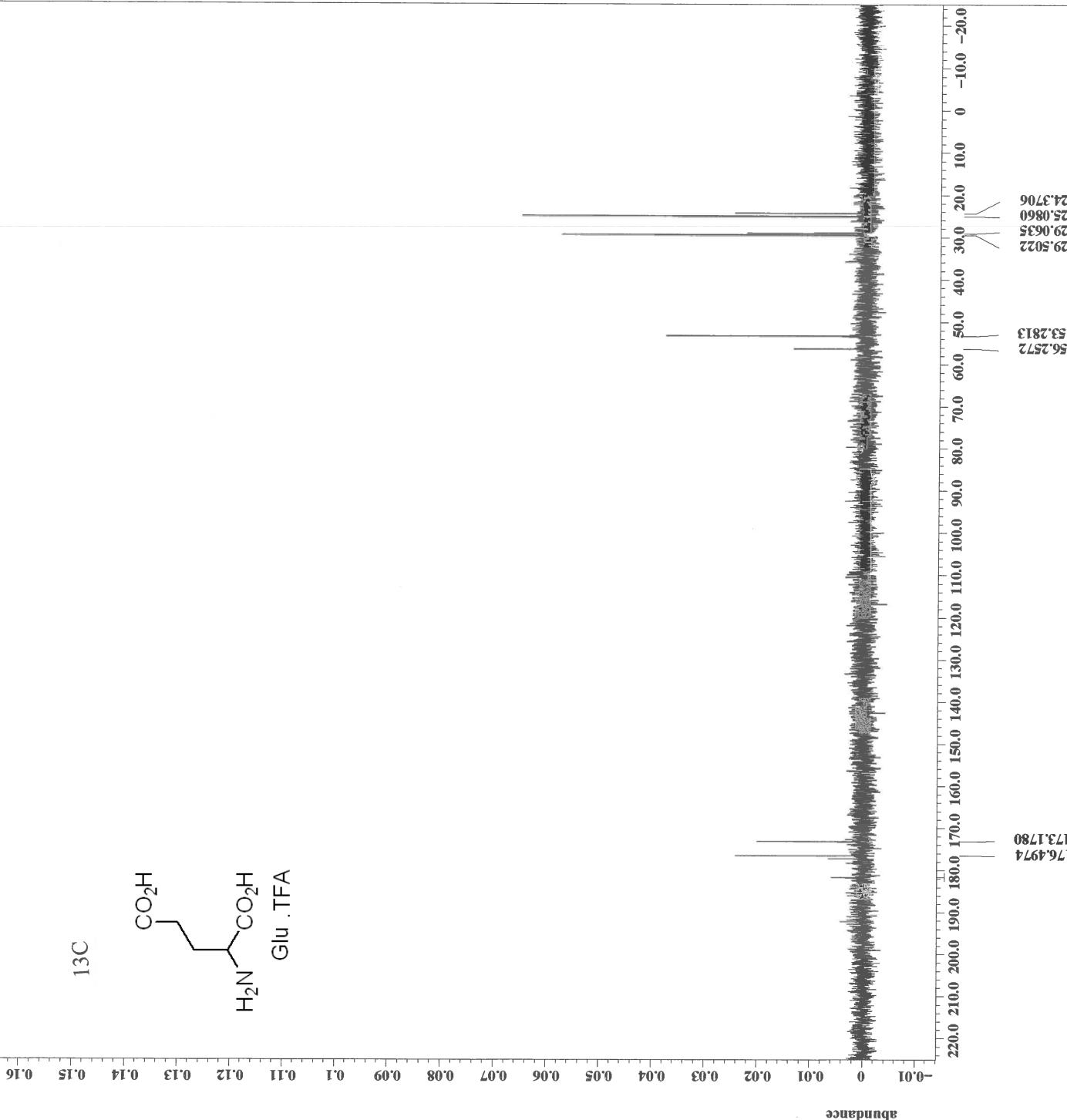
Filename = SBRGJUTFAC-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#321121
Solvent = D2O
Creation_time = 20-SEP-2015 22:07:11
Revision_time = 20-SEP-2015 09:26:16
Current_time = 20-SEP-2015 09:27:11

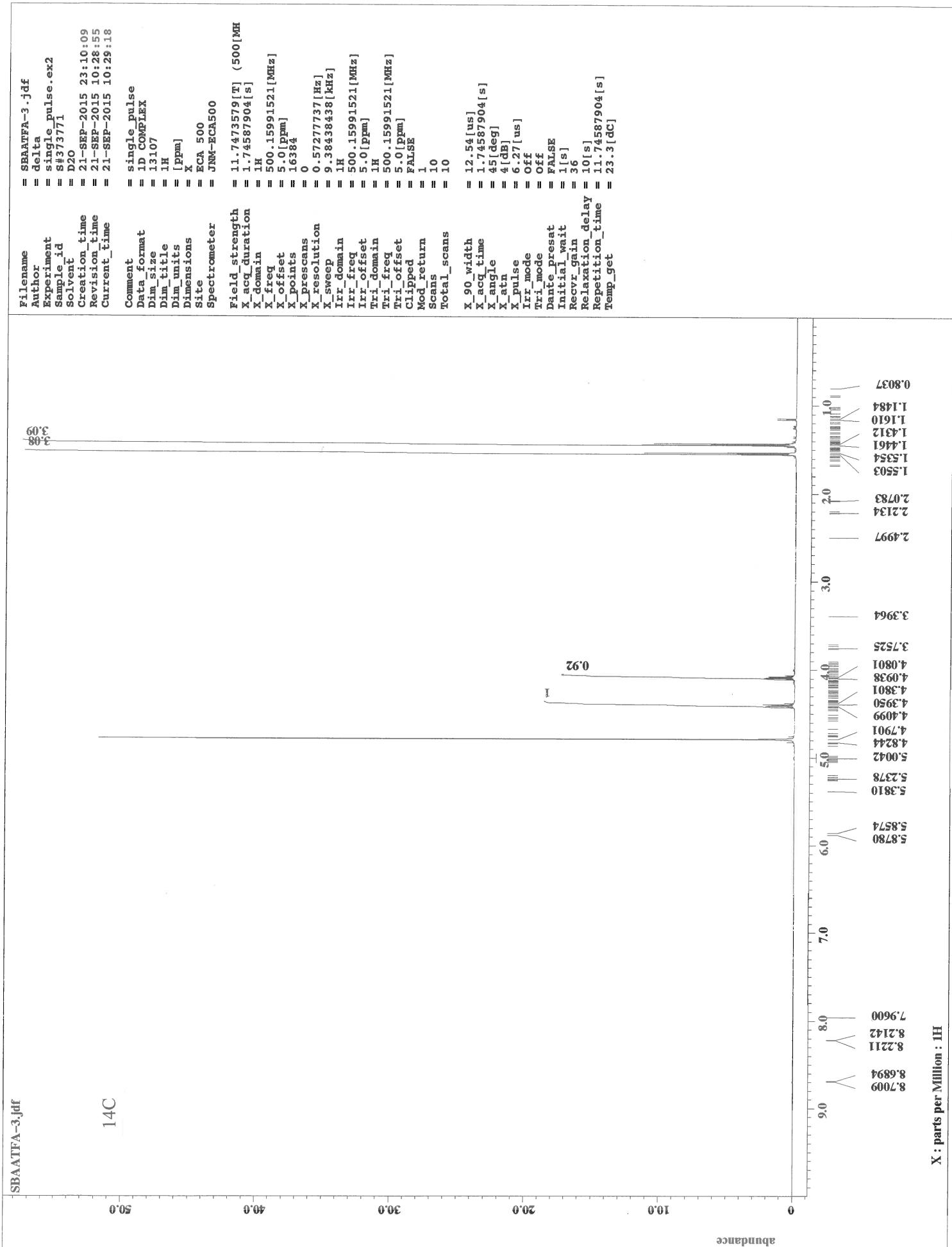
Comment = single pulse decoupling
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_bitfile = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

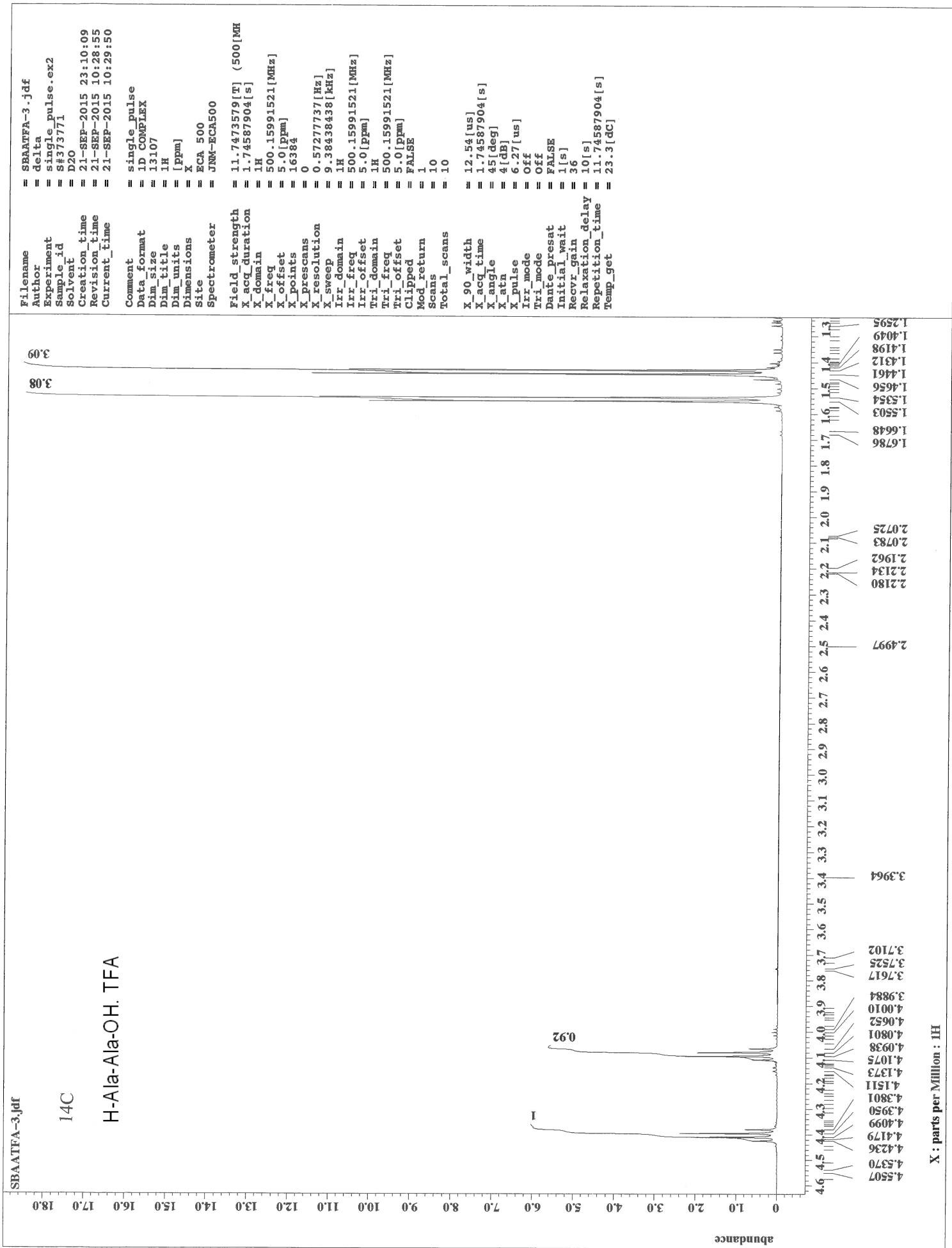
Field_strength = 11.7473579[T] (500)
X_acq_duration = 0.83361792[s]
X_domain = 13C
X_freq = 125.76529768[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.19959034[Hz]
X_sweep = 39.30817101[kHz]
Irr_domain = 1H
Irr_freq = 500.15991521[MHz]
Irr_offset = 5.01[ppm]
Clipped = FALSE
Mod_return = 10
Scans = 1650
Total_scans = 1650

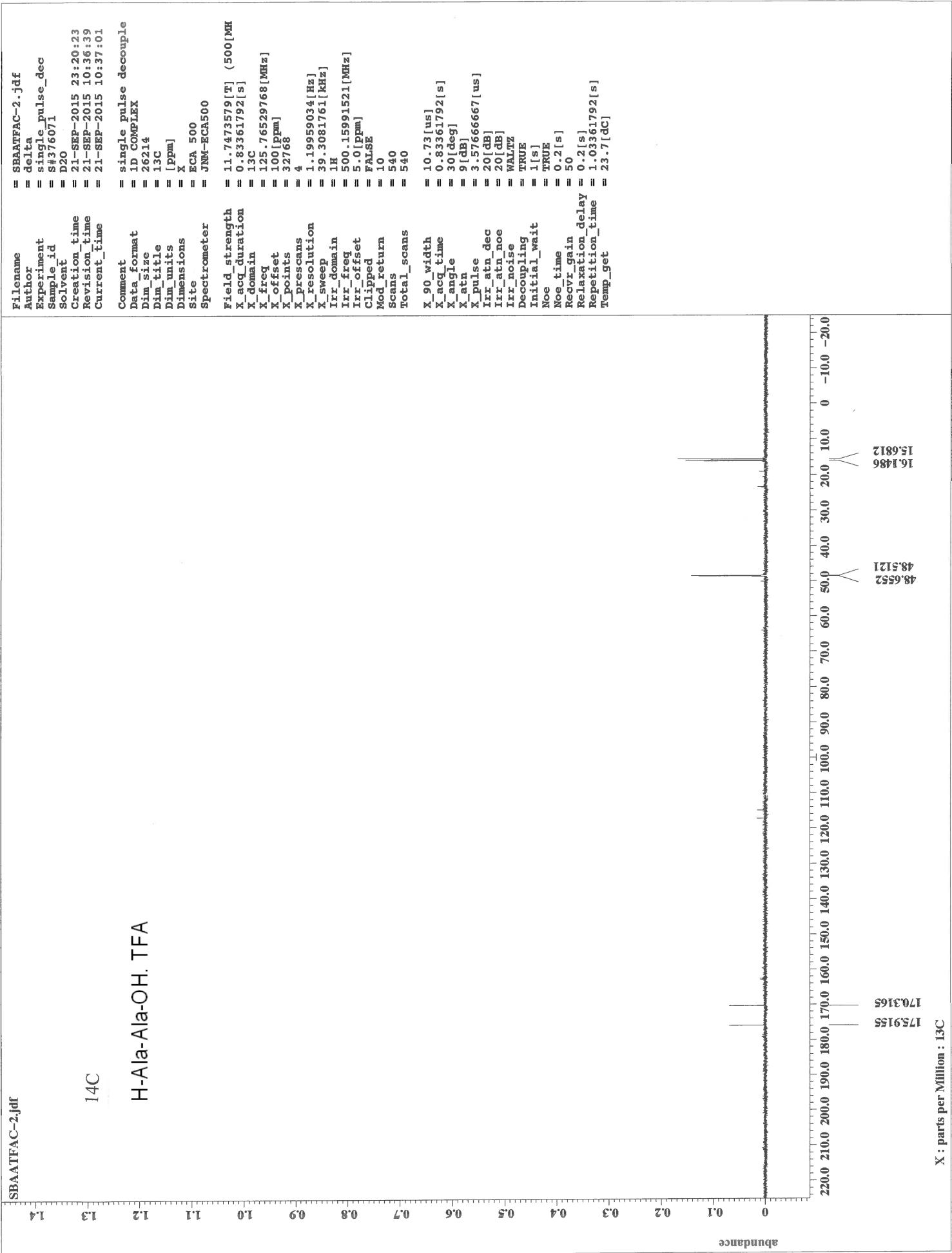
X_90_width = 10.73[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 9[dB]
X_pulse = 3.57666667[us]
Irr_atn_dec = 20[dB]
Irr_atn_noe = 20[dB]
Irr_noise = 1[W]
Decoupling = TRUE
Initial_wait = 1[s]
Nose = TRUE
Noe_time = 0.2[s]
Recv_gain = 50
Relaxation_delay = 0.2[s]
Repetition_time = 1.0361792[s]
Temp_Get = 21.7[dc]

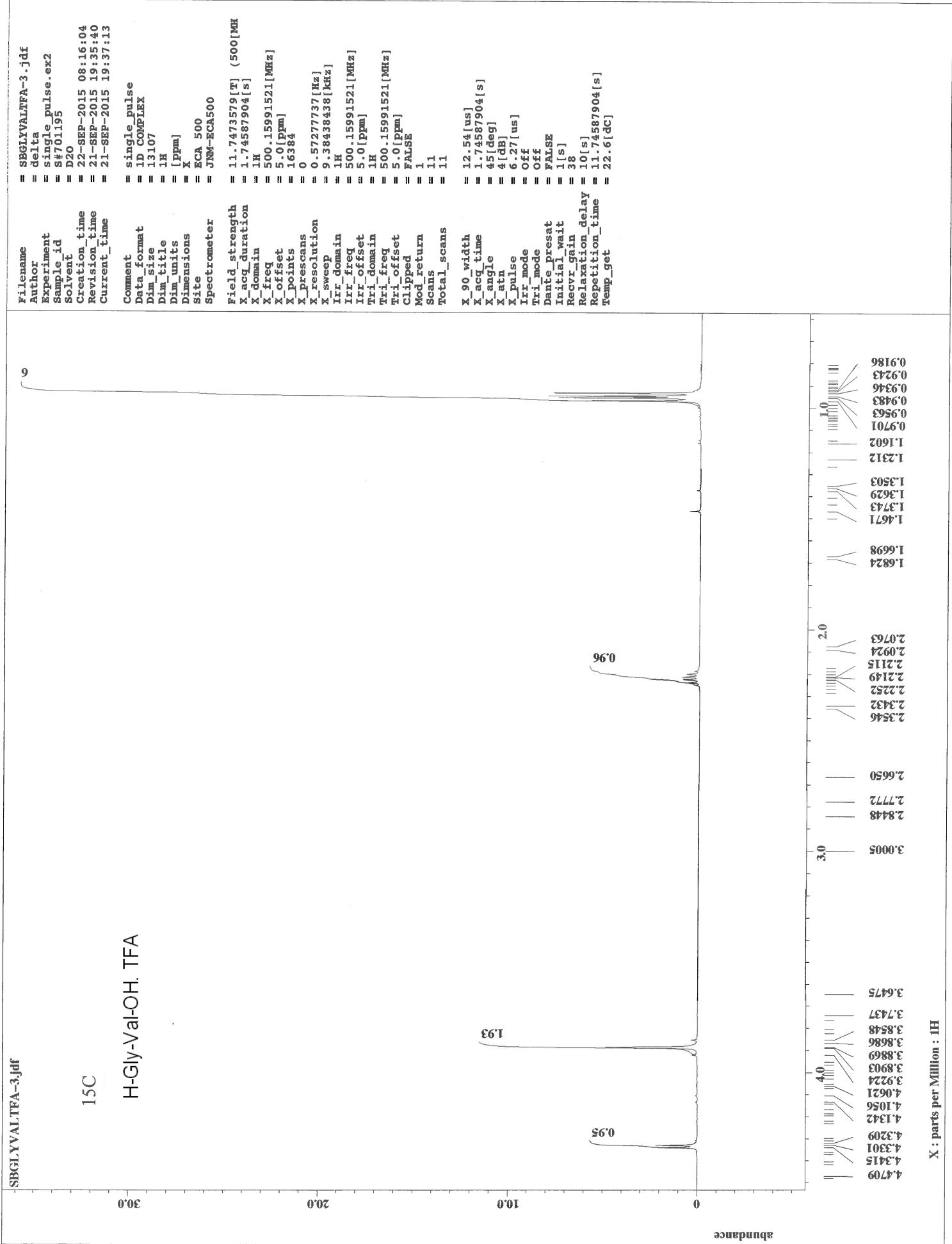
```











```

Filename = SBGLYVALTFAc-3.jdf
Author = delta
Experiment = single_pulse_decouple
Sample_id = S#103778
Solvent = D2O
Creation_time = 22-SEP-2015 08:27:39
Revision_time = 21-SEP-2015 19:43:48
Current_time = 21-SEP-2015 19:44:09

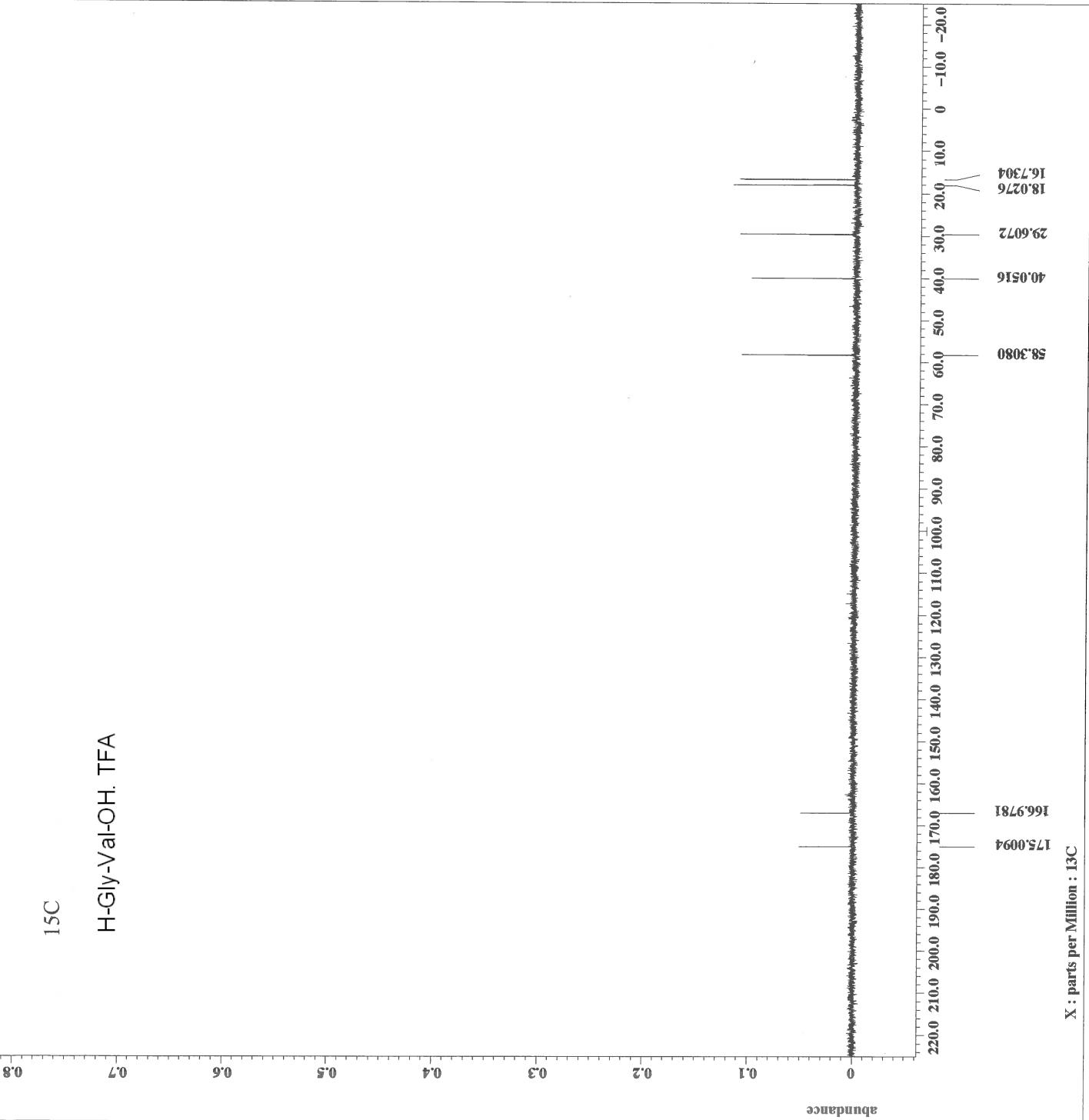
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 262,4
Dim_title = 13C
Dim_units = [PPM]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

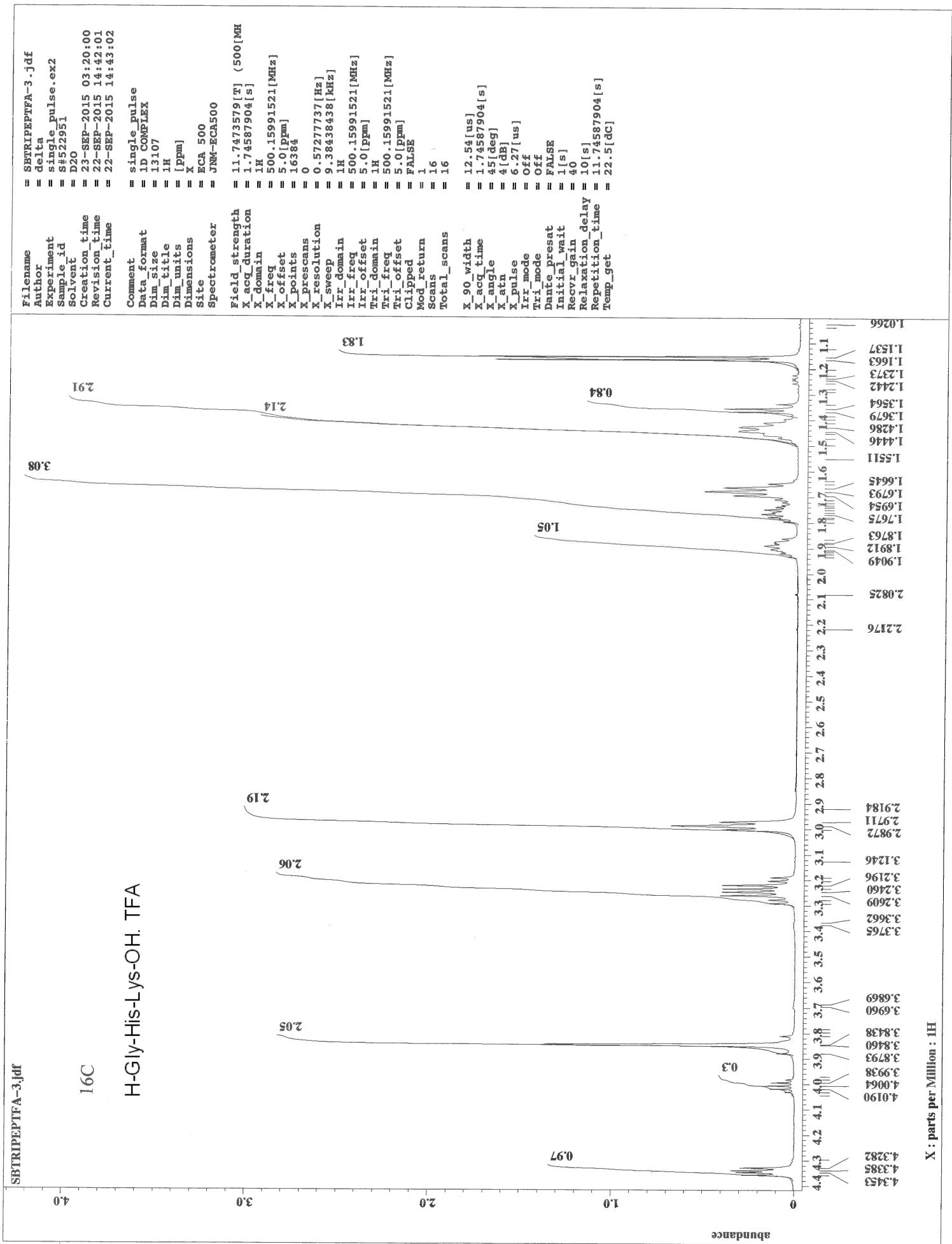
Field_strength = 11.7473579 [T] (500 [MHz])
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 125.76529768 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_Prescans = 4
X_resolution = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 10
Scans = 580
Total_scans = 580

X_90_width = 10.73 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.576666667 [us]
Irr_atn_dec = 20 [dB]
Irr_atn_noe = 20 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 0.2 [s]
Recvr_gain = 50
Relaxation_delay = 0.2 [s]
Repetition_time = 1.03361792 [s]
Temp_get = 23 [dC]

```

H-Gly-Val-OH. TFA





```

Filename = SBTRIPEPTFAC-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = #526053
Solvent = D2O
Creation_time = 23-SEP-2015 03:39:32
Revision_time = 22-SEP-2015 14:55:42
Current_time = 22-SEP-2015 14:56:50

Comment = single_pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MHz])
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 125.76529768 [MHz]
X_offset = 100.0 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 10
Scans = 1070
Total_scans = 1070

X_90_width = 10.73 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.57666667 [us]
Irr_atn_dec = 20 [dB]
Irr_atn_noe = 20 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 0.2 [s]
Recvr_gain = 50
Relaxation_delay = 0.2 [s]
Repetition_time = 1.03361792 [s]
Temp_Set = 22.9 [ac]

```

