

Novel Piperazine-1,2,3-Triazole Leads for the Potential Treatment of Pancreatic Cancer

Jufeng Sun,^[a,b] Jennifer R. Baker,^[a] Cecilia C Russell,^[a] Hong N. T. Pham,^[c] Chloe D. Goldsmith,^[c] Peter J. Cossar,^[a] Jennette A. Sakoff ^{*[c]} Christopher J. Scarlett,^[d] and Adam McCluskey ^{*[a]}

^a Chemistry, School of Environmental & Life Sciences, The University of Newcastle, University Drive, Callaghan, NSW 2308, Australia. Email: Adam.McCluskey@newcastle.edu.au

^b Medicinal Chemistry, School of Pharmacy, Binzhou Medical University, Yantai, 264003, China.

^c Experimental Therapeutics Group, Department of Medical Oncology, Calvary Mater Newcastle Hospital, Edith Street, Waratah, NSW 2298, Australia

^d School of Environmental & Life Sciences, The University of Newcastle, Ourimbah, NSW 2258, Australia.

Supporting Information

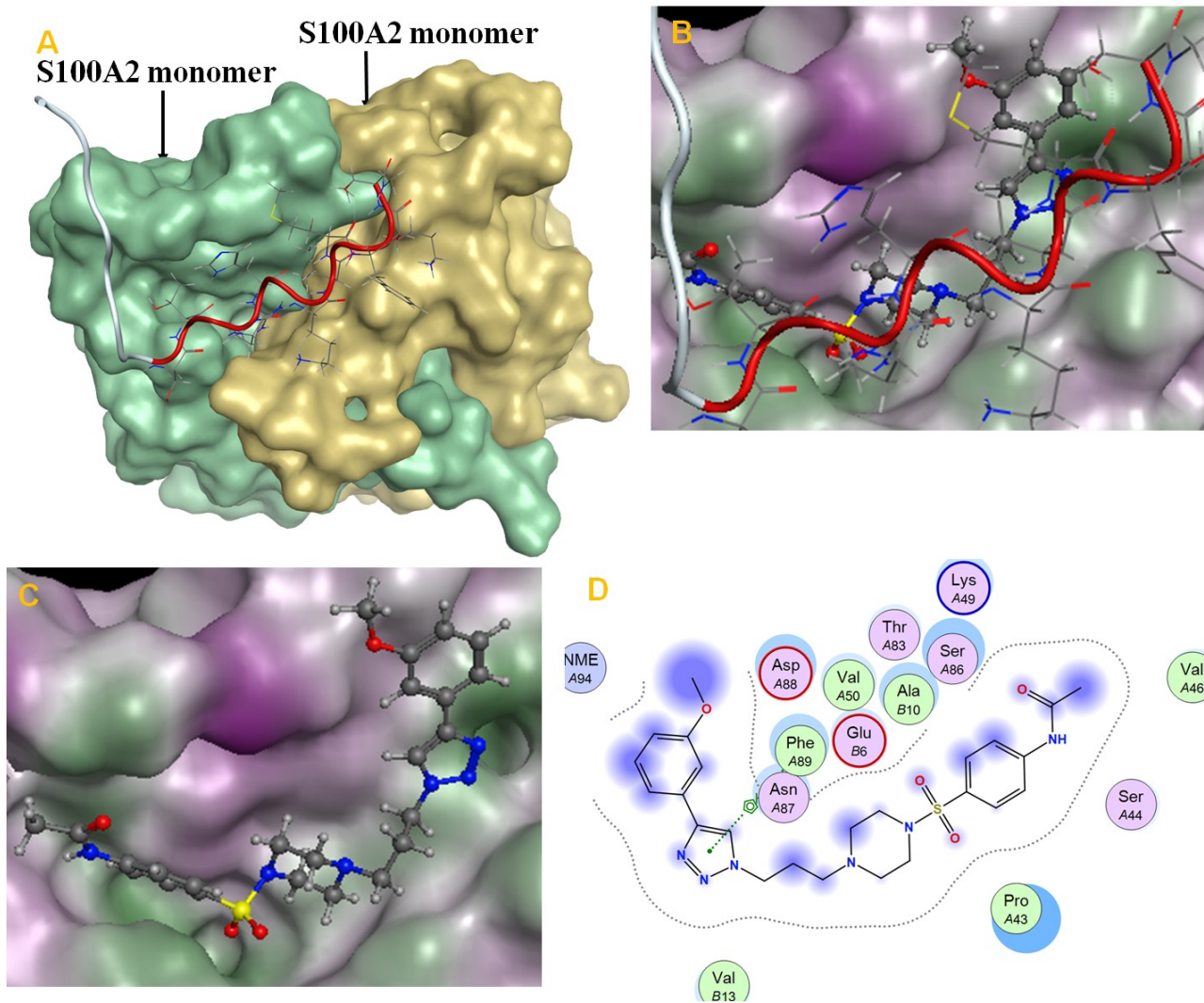
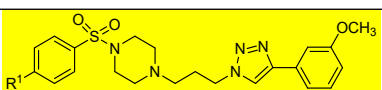


Figure 1. A. Top docking pose of S100A2 homodimer in complex with p53 peptide in binding pocket (in orange oval) similar dimensions to a small molecule; B. Overlay of lead 1 with p53 peptide (in red) in S100A2 binding pocket predicted by MOE and its structure (purple: hydrophilic area; green: hydrophobic area). C. Lead 1 docked in the S100A2 binding pocket (purple: hydrophilic area; green: hydrophobic area); D. Lead 1 Interaction plot of the MOE-dock. Lead 1 engages with S100A2 via arene-H interaction between triazole and PheA89 (A and B in codes of amino acids: sequence of S100A2 protein).

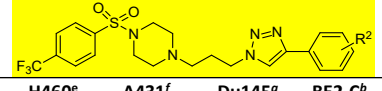
Table S1. Percentage growth inhibition evaluation (% at 25 μ M, MTT assay, n = 3) of *Library 1* analogues **2**, **14-24** in a panel of cancer cell lines and MCF10A cells. Higher values indicate higher compound potency.



| Comp. (R ¹) | HT29 ^a | U87 ^b | MCF-7 ^c | A2780 ^d | H460 ^e | A431 ^f | Du145 ^g | BE2-C ^b | SJ-G2 ^h | MiaPaCa-2 ⁱ | MCF10A ⁱ |
|--|-------------------|------------------|--------------------|--------------------|-------------------|-------------------|--------------------|--------------------|--------------------|------------------------|---------------------|
| 2 CH ₃ CONH | 25 ± 3 | 12 ± 3 | 21 ± 1 | 24 ± 2 | 14 ± 5 | 24 ± 10 | 12 ± 16 | 25 ± 8 | 11 ± 2 | 17 ± 4 | 29 ± 9 |
| 14 H | 43 ± 3 | <10 | 35 ± 7 | 28 ± 2 | 11 ± 3 | <10 | 14 ± 4 | 21 ± 3 | 20 ± 3 | <10 | <10 |
| 15 CH ₃ | 54 ± 2 | <10 | 38 ± 4 | 46 ± 2 | 27 ± 4 | 11 ± 7 | 10 ± 12 | 13 ± 8 | 34 ± 6 | <10 | 15 ± 20 |
| 16 (CH ₃) ₂ CH | ND | ND | ND | ND | ND | ND | ND | ND | ND | ND | ND |
| 17 (CH ₃) ₃ C | 48 ± 2 | <10 | 39 ± 3 | 51 ± 4 | 38 ± 9 | <10 | <10 | 40 ± 7 | 8 ± 6 | 29 ± 1 | 33 ± 5 |
| 18 OCH ₃ | 40 ± 1 | <10 | 33 ± 2 | 47 ± 2 | 10 ± 2 | 12 ± 2 | <10 | 5 ± 3 | 38 ± 3 | <10 | <10 |
| 19 F | 64 ± 1 | 12 ± 1 | 30 ± 3 | 32 ± 4 | 15 ± 9 | 11 ± 8 | <10 | 33 ± 8 | 10 ± 3 | 25 ± 6 | 21 ± 7 |
| 20 Cl | 72 ± 1 | <10 | 41 ± 7 | 45 ± 3 | 23 ± 5 | 10 ± 6 | <10 | 48 ± 4 | 15 ± 7 | 31 ± 6 | 31 ± 12 |
| 21 Br | 60 ± 3 | 10 ± 3 | 69 ± 4 | 56 ± 3 | 40 ± 3 | 35 ± 7 | 49 ± 2 | 56 ± 2 | 52 ± 3 | 26 ± 4 | 42 ± 7 |
| 22 CF ₃ | 55 ± 4 | 12 ± 3 | 46 ± 6 | 55 ± 4 | 25 ± 3 | <10 | 25 ± 7 | 23 ± 8 | 30 ± 4 | <10 | 27 ± 7 |
| 23 NO ₂ | 39 ± 2 | <10 | 28 ± 4 | 47 ± 1 | 14 ± 3 | 10 ± 1 | <10 | 12 ± 4 | 28 ± 4 | <10 | 13 ± 7 |
| 24 CH ₃ CO | 40 ± 2 | 14 ± 1 | 27 ± 2 | 30 ± 1 | 19 ± 7 | 18 ± 6 | 10 ± 16 | 41 ± 5 | 13 ± 2 | 27 ± 2 | 29 ± 11 |

^a colon; ^b glioblastoma; ^c breast; ^d ovarian; ^e lung; ^f skin; ^g prostate; ^h neuroblastoma; ⁱ pancreas; ^j normal breast. ND = Not determined due to insolubility in test vehicle.

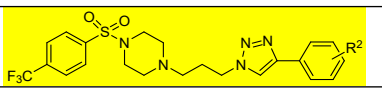
Table S2. Percentage growth inhibition evaluation (% at 25 μ M, MTT assay, n = 3) of *Library 3* analogues **33-42** in a panel of cancer cell lines and MCF10A cells. Higher values indicate higher compound potency.



| Comp. (R ²) | HT29 ^a | U87 ^b | MCF-7 ^c | A2780 ^d | H460 ^e | A431 ^f | Du145 ^g | BE2-C ^b | SJ-G2 ^h | MiaPaCa-2 ⁱ | MCF10A ⁱ |
|--|-------------------|------------------|--------------------|--------------------|-------------------|-------------------|--------------------|--------------------|--------------------|------------------------|---------------------|
| 33 H | 44±1 | 23±1 | 45±2 | 40±3 | 42±3 | 32±8 | <10 | 40±3 | 27±1 | 48±3 | 50±2 |
| 34 4-CH ₃ | 91±2 | 57±5 | 96±1 | 78±2 | 78±4 | 85±3 | 74±8 | 78±2 | 83±5 | 76±3 | 85±5 |
| 35 4-CH ₂ CH ₃ | 84±2 | 45±8 | 99±3 | 73±2 | 76±2 | 73±4 | 68±5 | 71±1 | 76±4 | 77±1 | 83±3 |
| 36 4-C(CH ₃) ₃ | 79±4 | 39±5 | 75±5 | 75±3 | 69±3 | 72±1 | 73±7 | 70±3 | 67±8 | 64±3 | 83±3 |
| 37 4-F | 59±6 | 30±2 | 69±9 | 55±9 | 57±8 | 49±15 | 49±12 | 54 ± 9 | 57±9 | 52±6 | 61±1 |
| 38 4-Br | 84±6 | 67±5 | 98±2 | 84±3 | 90±4 | 89±5 | 78±9 | 87±4 | 92±5 | 83±2 | 92±4 |
| 39 3-Cl | 71±2 | 29±4 | 75±0 | 57±5 | 56±0 | 51±6 | 41±5 | 61±1 | 58±1 | 62±1 | 67±3 |
| 40 4-CF ₃ | 73±5 | 74±5 | 90±5 | 78±5 | 90±5 | 83±7 | 91±8 | 82±6 | 88±2 | 72±7 | 87±3 |
| 41 4-NO ₂ | 41±0 | 13±5 | 84±4 | 43±6 | 47±2 | 27±1 | 34±2 | 48±8 | 30±2 | 58±5 | 52±17 |
| 42 4-N(CH ₃) ₂ | 52±3 | 14±0 | 60±4 | 53±1 | 58±0 | 47±12 | 50±2 | 48±1 | 70±30 | 42±1 | 61±3 |

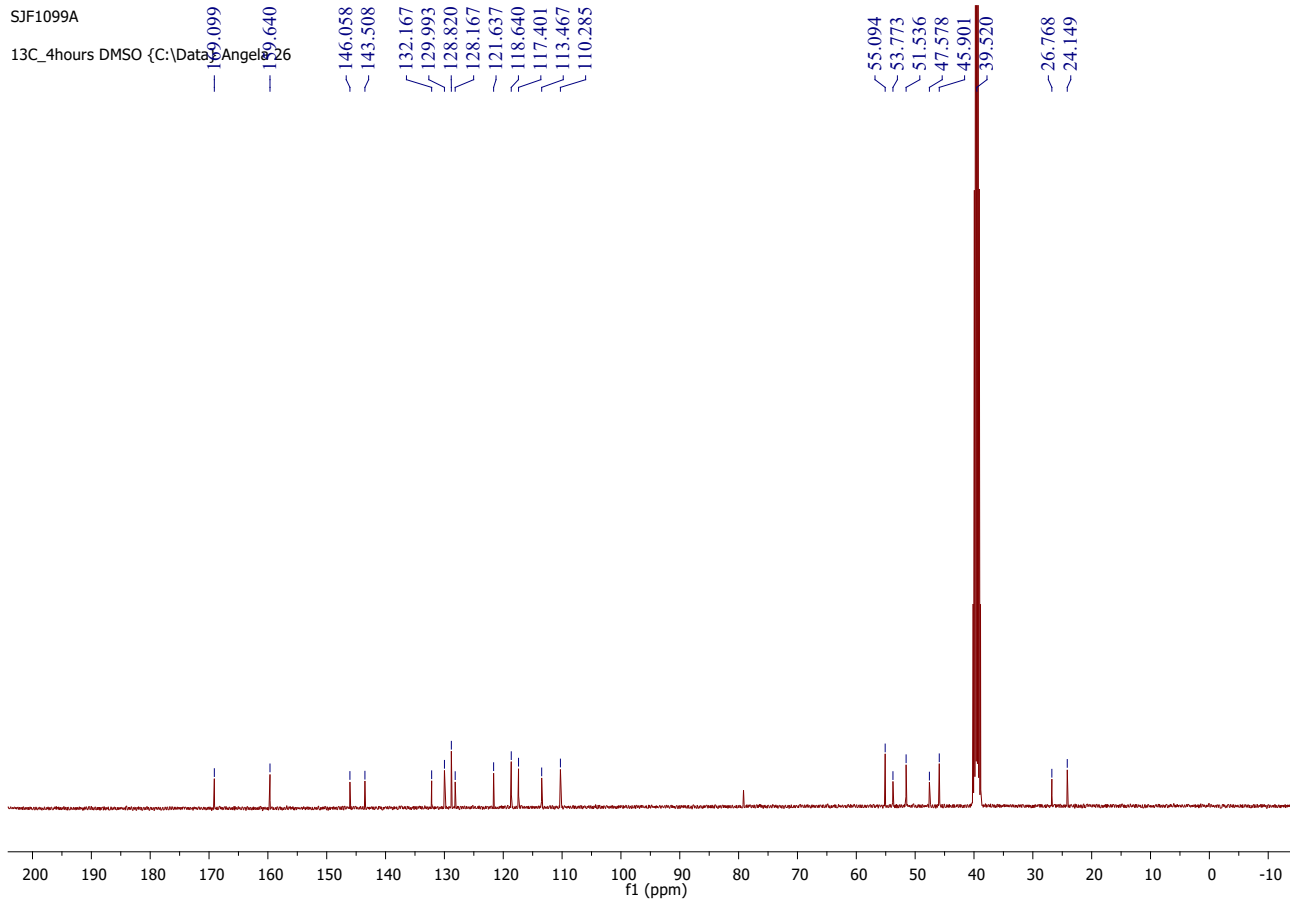
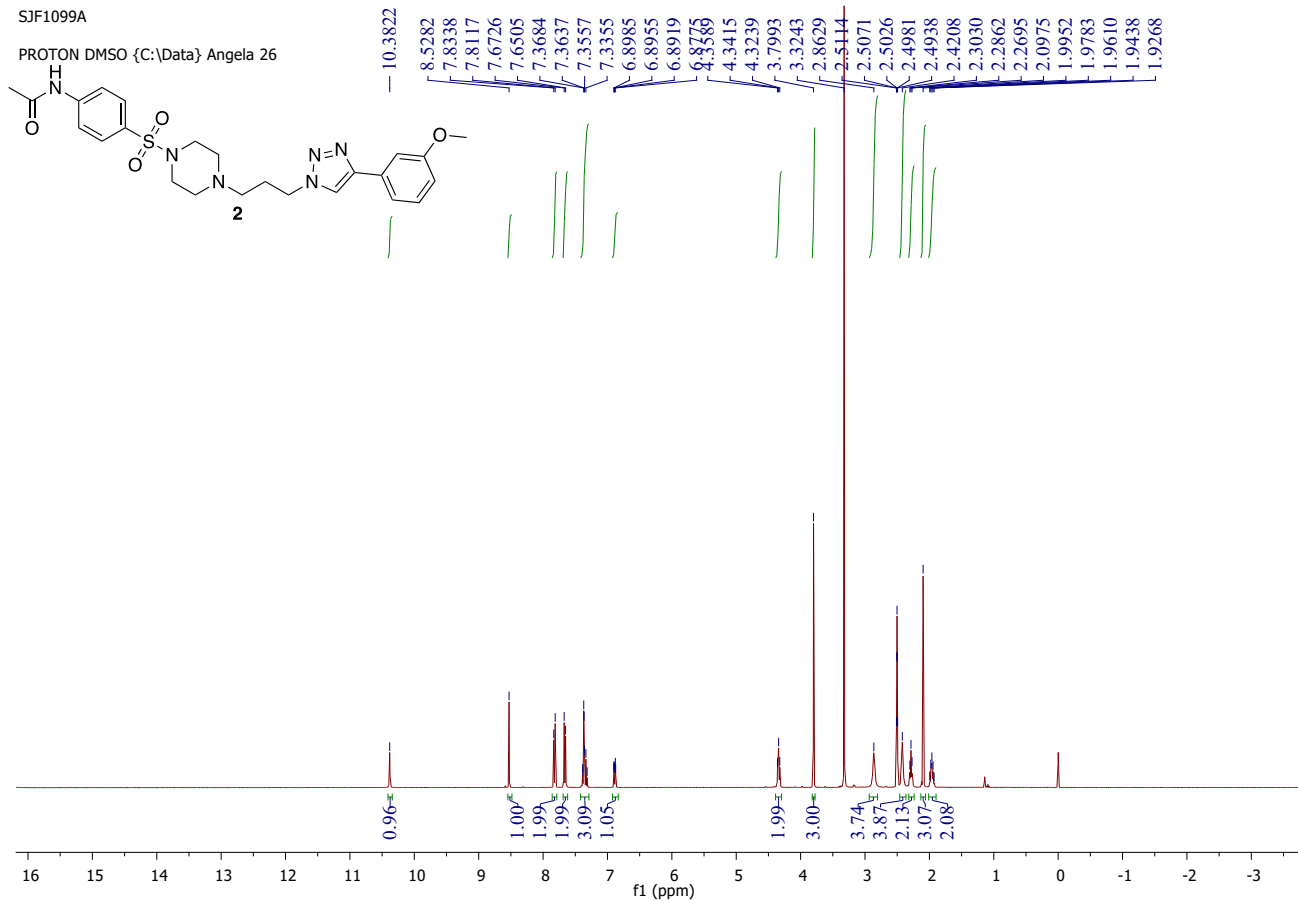
^a colon; ^b glioblastoma; ^c breast; ^d ovarian; ^e lung; ^f skin; ^g prostate; ^h neuroblastoma; ⁱ pancreas; ^j normal breast

Table S3. Percentage growth inhibition evaluation (% at 25 μ M, MTT assay, n = 3) of *Library 3* analogues **33-36** and **38-41** in an expanded Pancreatic Cancer cell line panel. Higher values indicate higher compound potency.



| Comp. (R ²) | BxPC-3 | AsPC-1 | Capan-2 | HPAC | PANC-1 |
|--|---------|--------|---------|--------|--------|
| 33 H | 34 ± 1 | 37 ± 1 | 23 ± 22 | 4 ± 11 | 50 ± 2 |
| 34 4-CH ₃ | 96 ± 1 | 77 ± 1 | 91 ± 4 | 93 ± 4 | 70 ± 1 |
| 35 4-CH ₂ CH ₃ | 48 ± 3 | 12 ± 4 | 18 ± 9 | 15 ± 6 | <0 |
| 36 4-C(CH ₃) ₃ | 95 ± 3 | 74 ± 1 | 83 ± 4 | 81 ± 2 | 63 ± 2 |
| 38 3-Cl | 19 ± 20 | 42 ± 6 | 32 ± 11 | 20 ± 9 | 49 ± 6 |
| 39 4-Br | 97 ± 1 | 79 ± 7 | 94 ± 15 | 92 ± 5 | 83 ± 7 |
| 40 4-CF ₃ | 78 ± 6 | 60 ± 2 | 76 ± 11 | 89 ± 5 | 66 ± 6 |
| 41 4-NO ₂ | 37 ± 0 | 22 ± 4 | 28 ± 19 | <0 | 34 ± 0 |

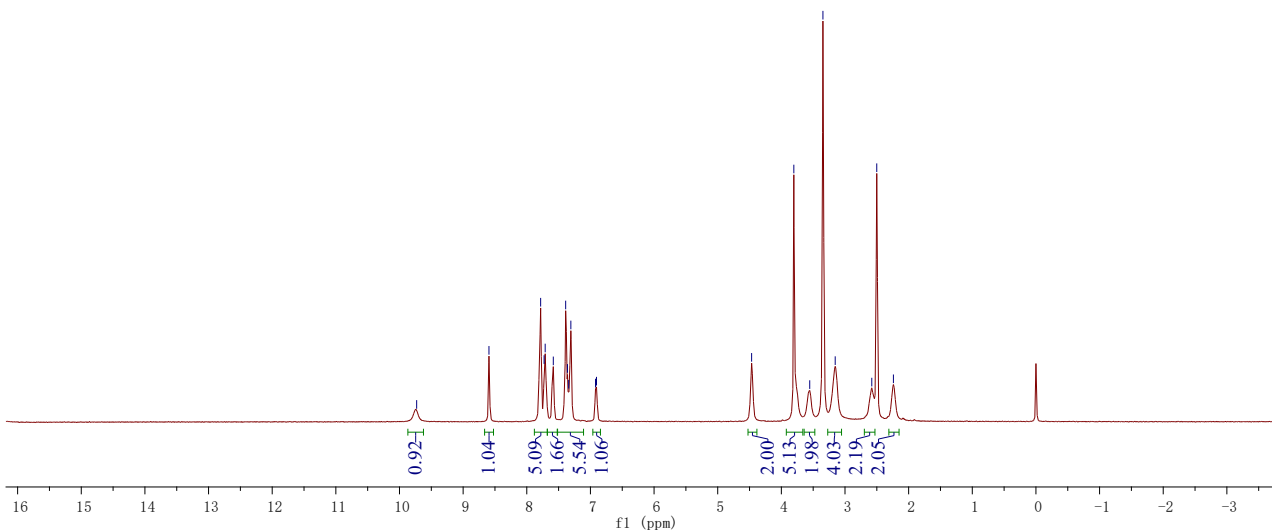
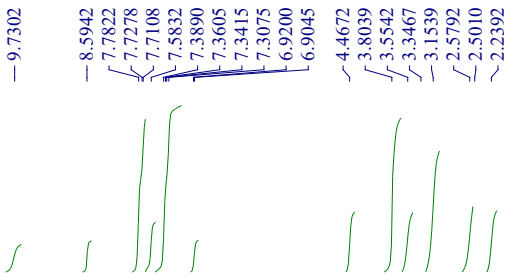
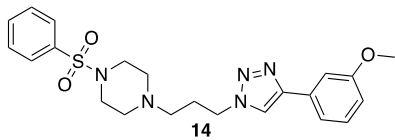
N-(4-((4-(3-(4-(3-Methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)propyl)piperazin-1-yl)-sulfonyl)phenyl)acetamide (**2**)



1-(3-(4-(3-Methoxyphenyl)-1H-1,2,3-triazol-1-yl)propyl)-4-(phenylsulfonyl)-piperazine benzene sulfonate (**14**)

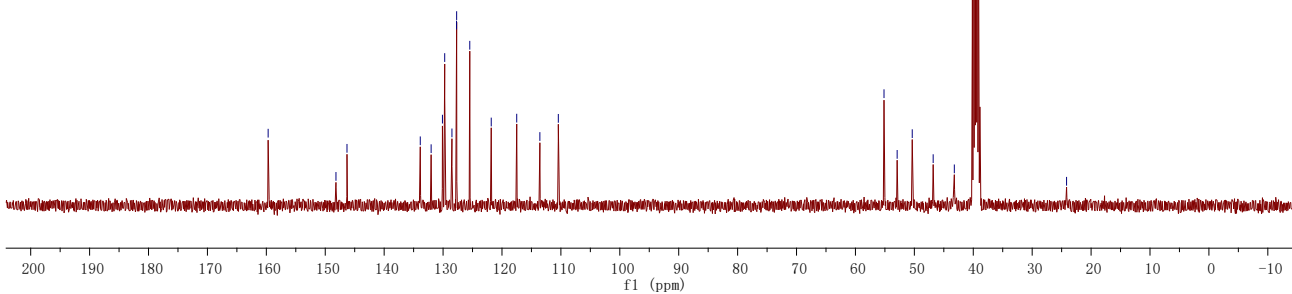
SJF1079A

PROTON HDMSO {C:\Data} Angela 36



SJF1079

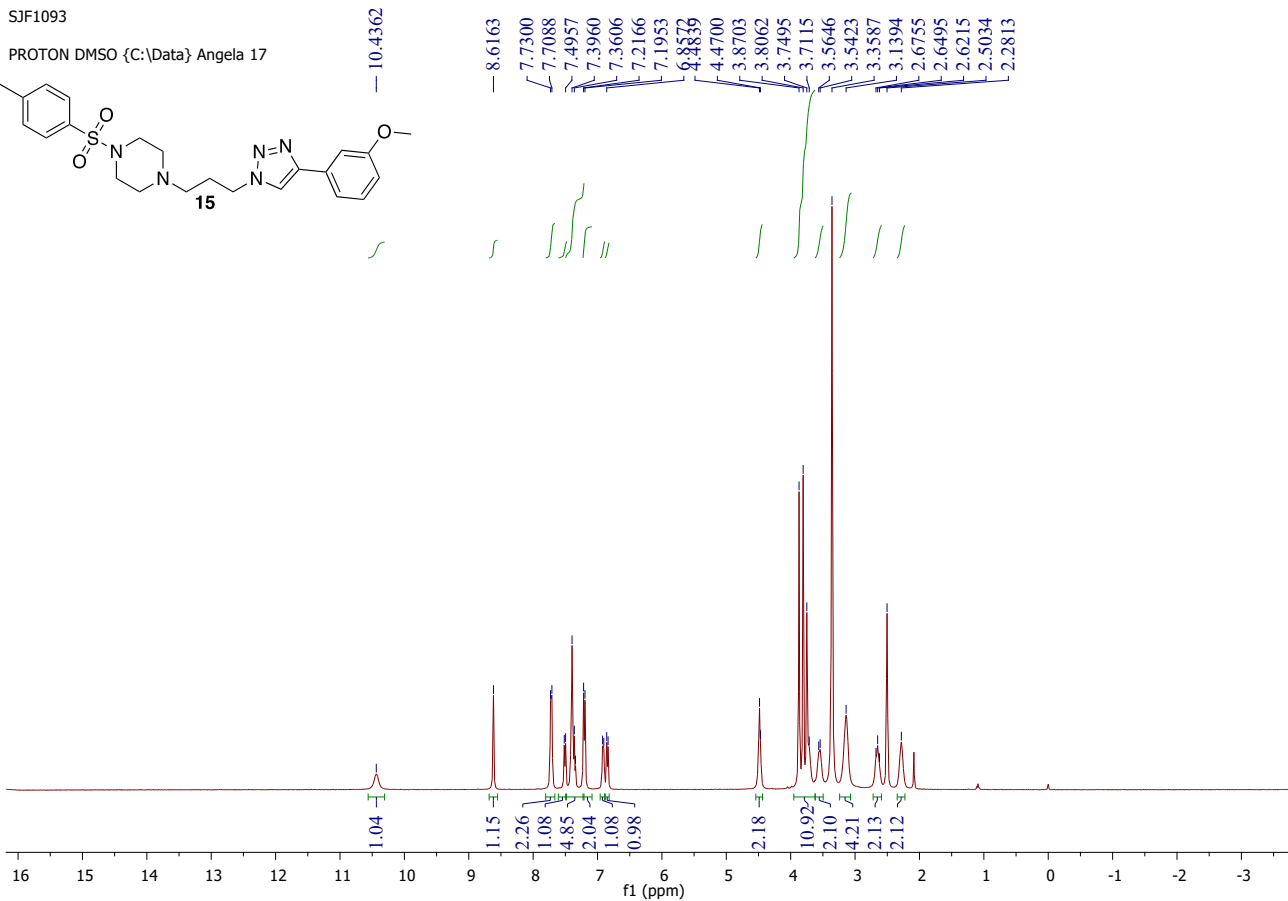
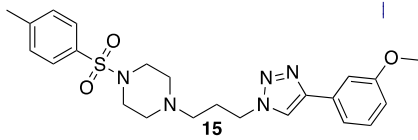
13C_30min DMSO {C:\Data} Angela 36



1-(3-(4-(3-Methoxyphenyl)-1H-1,2,3-triazol-1-yl)propyl)-4-tosylpiperazine (15)

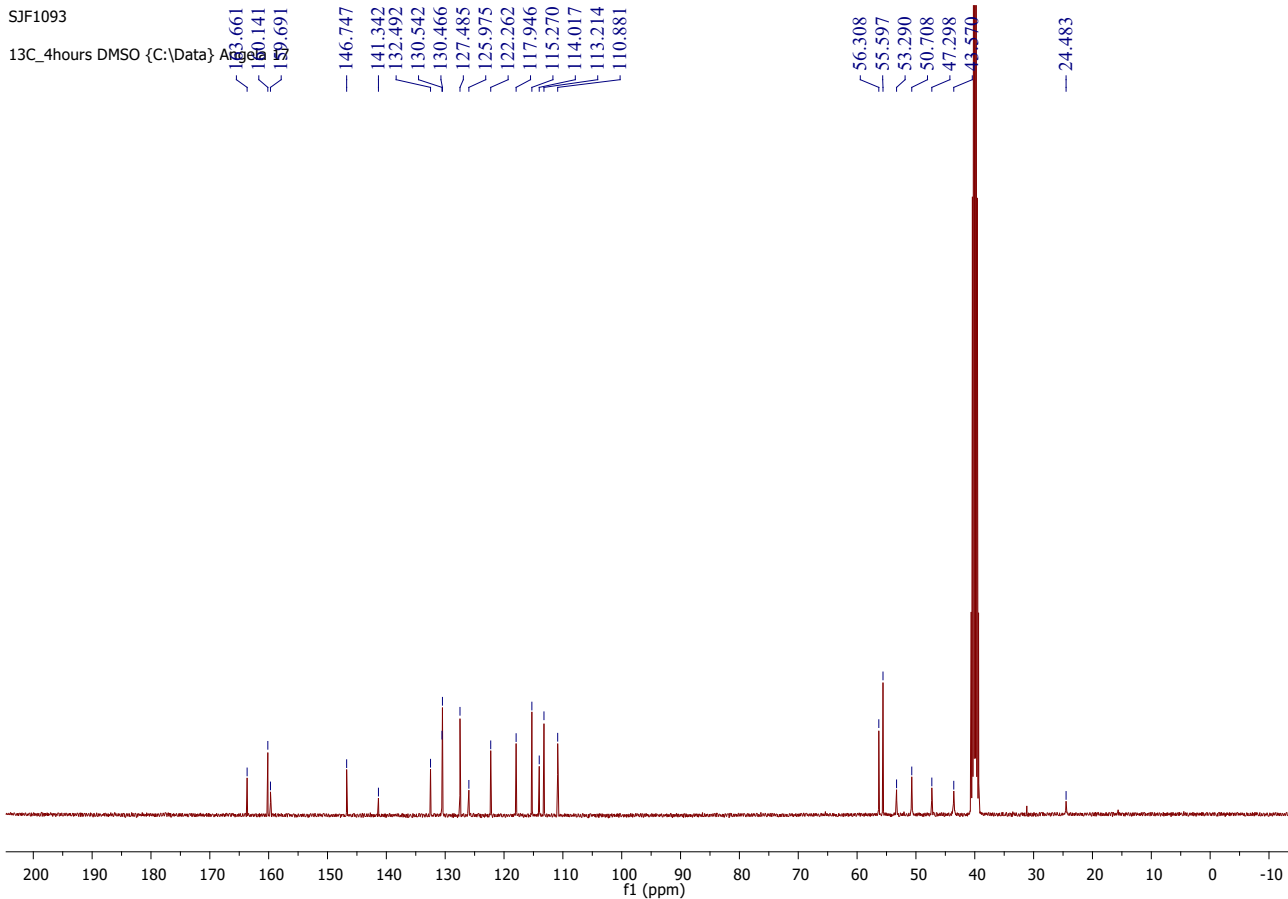
SJF1093

PROTON DMSO {C:\Data} Angela 17

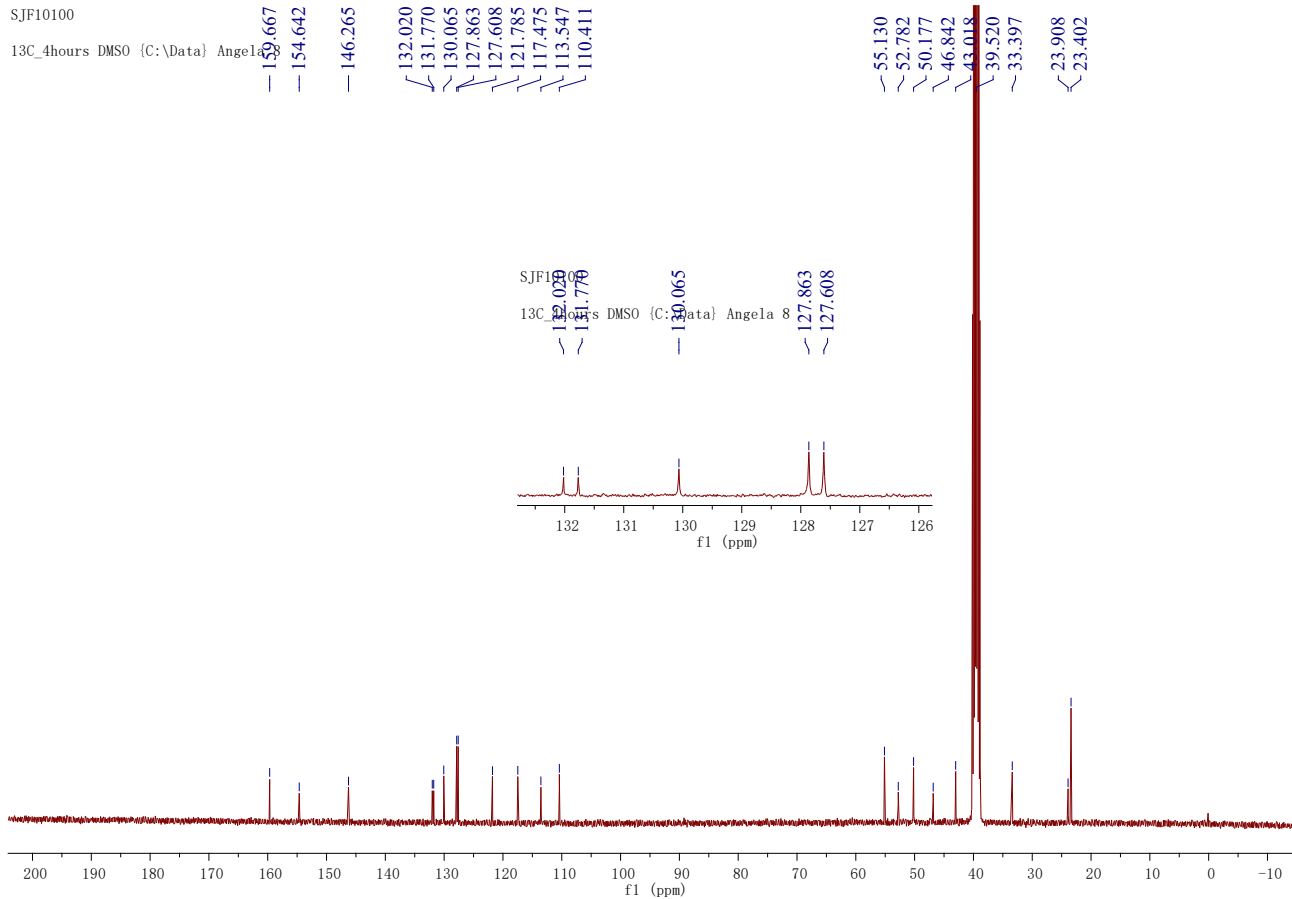
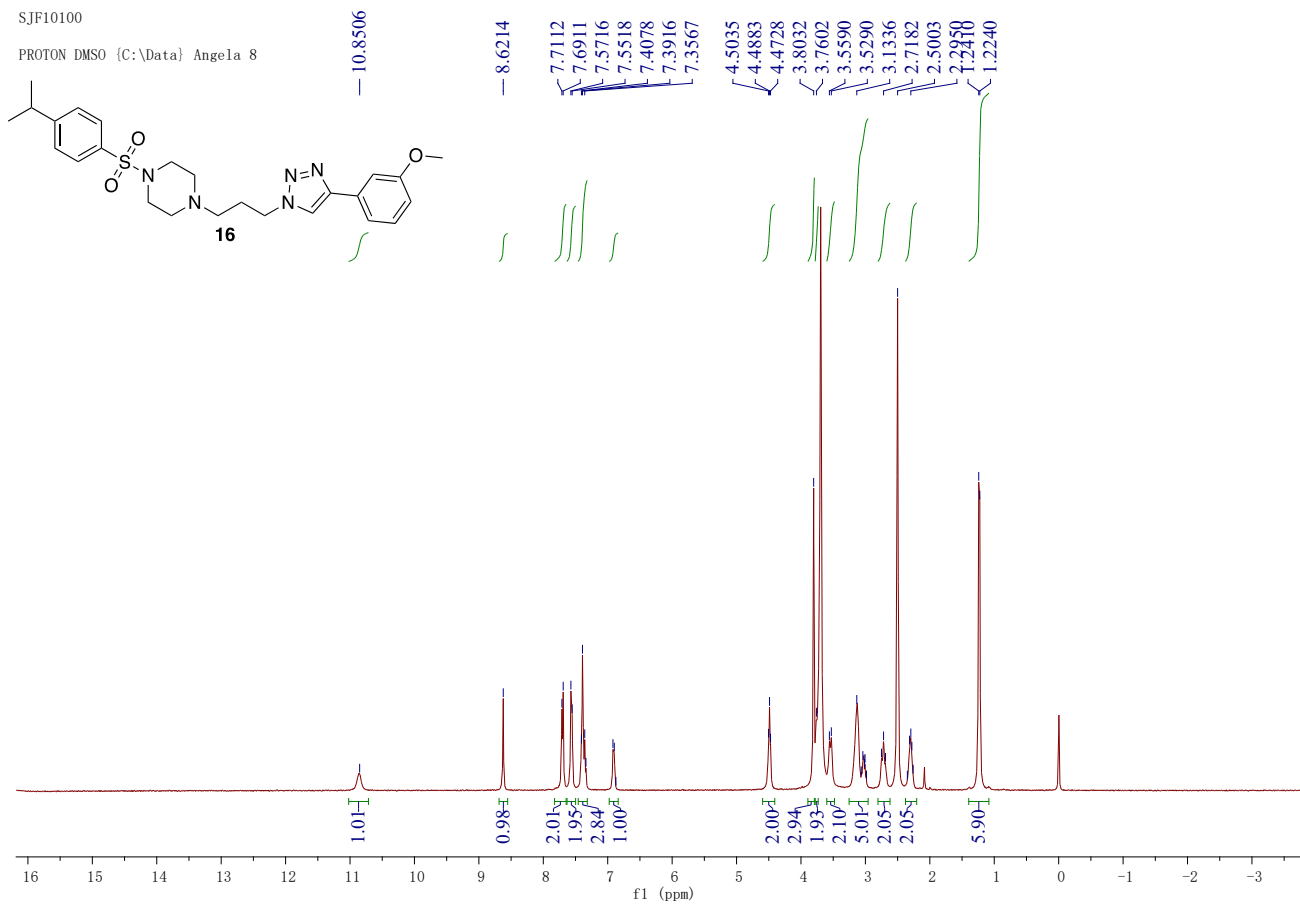


SJF1093

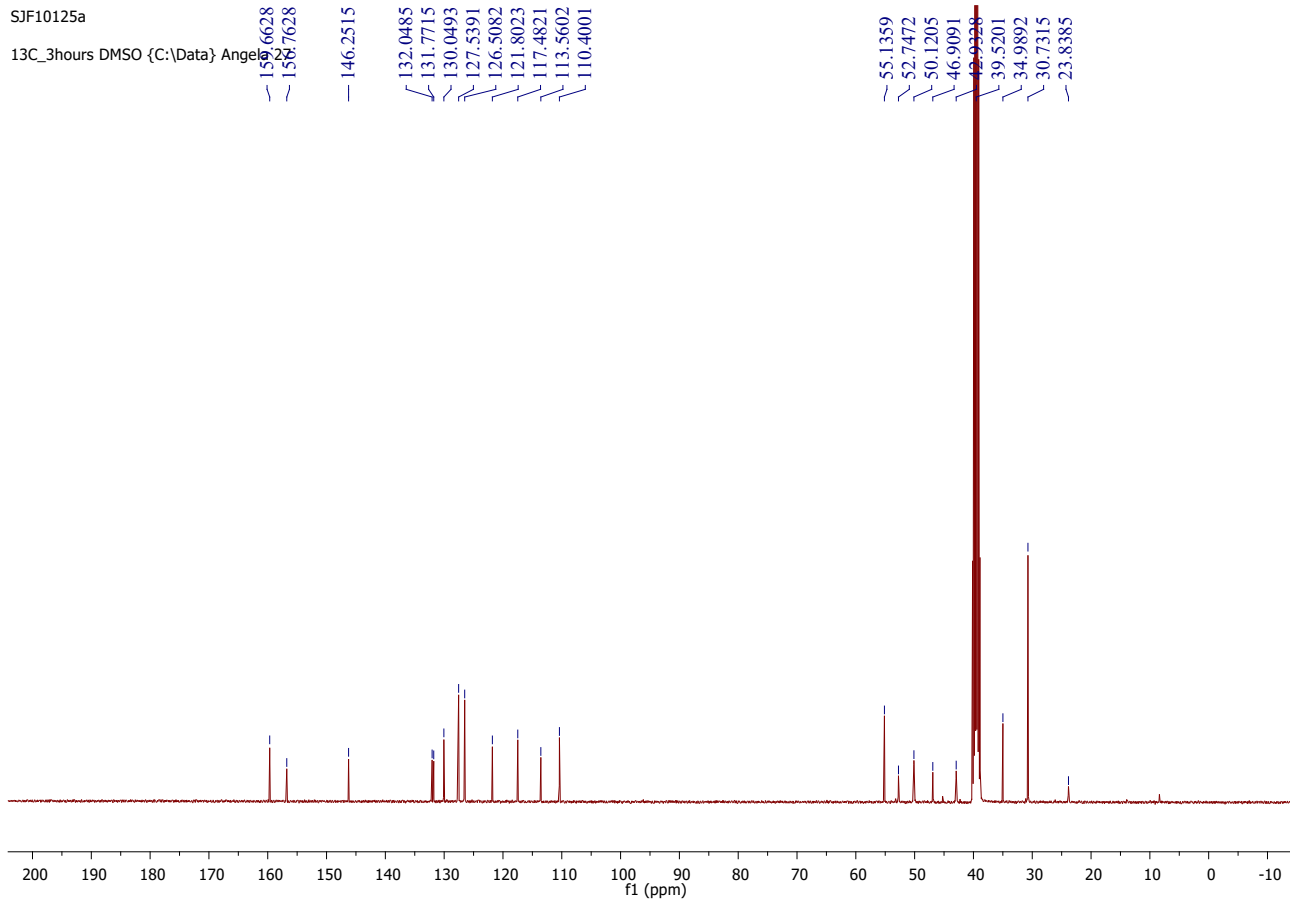
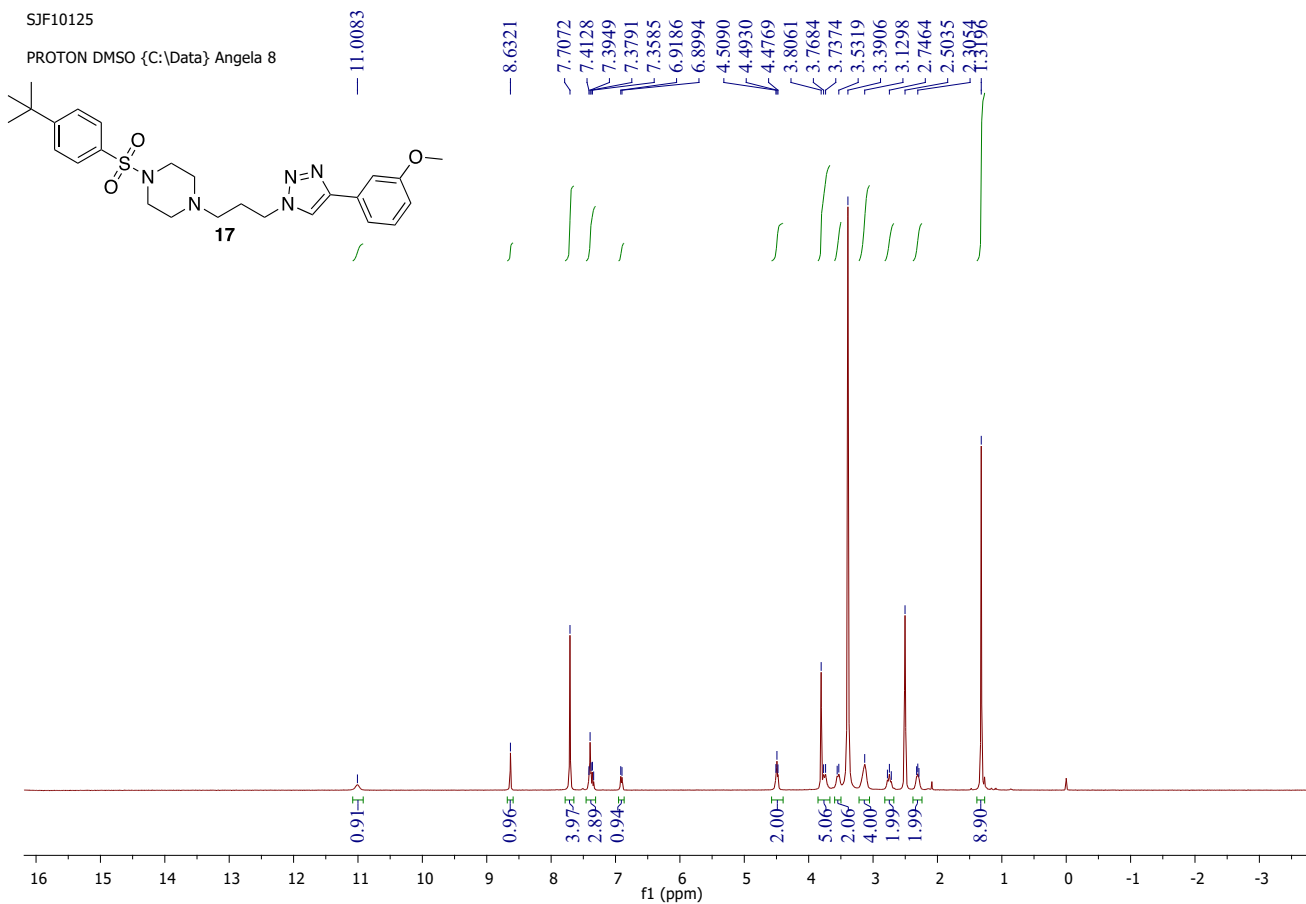
13C_4hours DMSO {C:\Data} Angela 17



1-(4-Isopropylphenylsulfonyl)-4-(3-(4-(3-methoxyphenyl)-1H-1,2,3-triazol-1-yl)-propyl) piperazine hydrochloride (**16**)



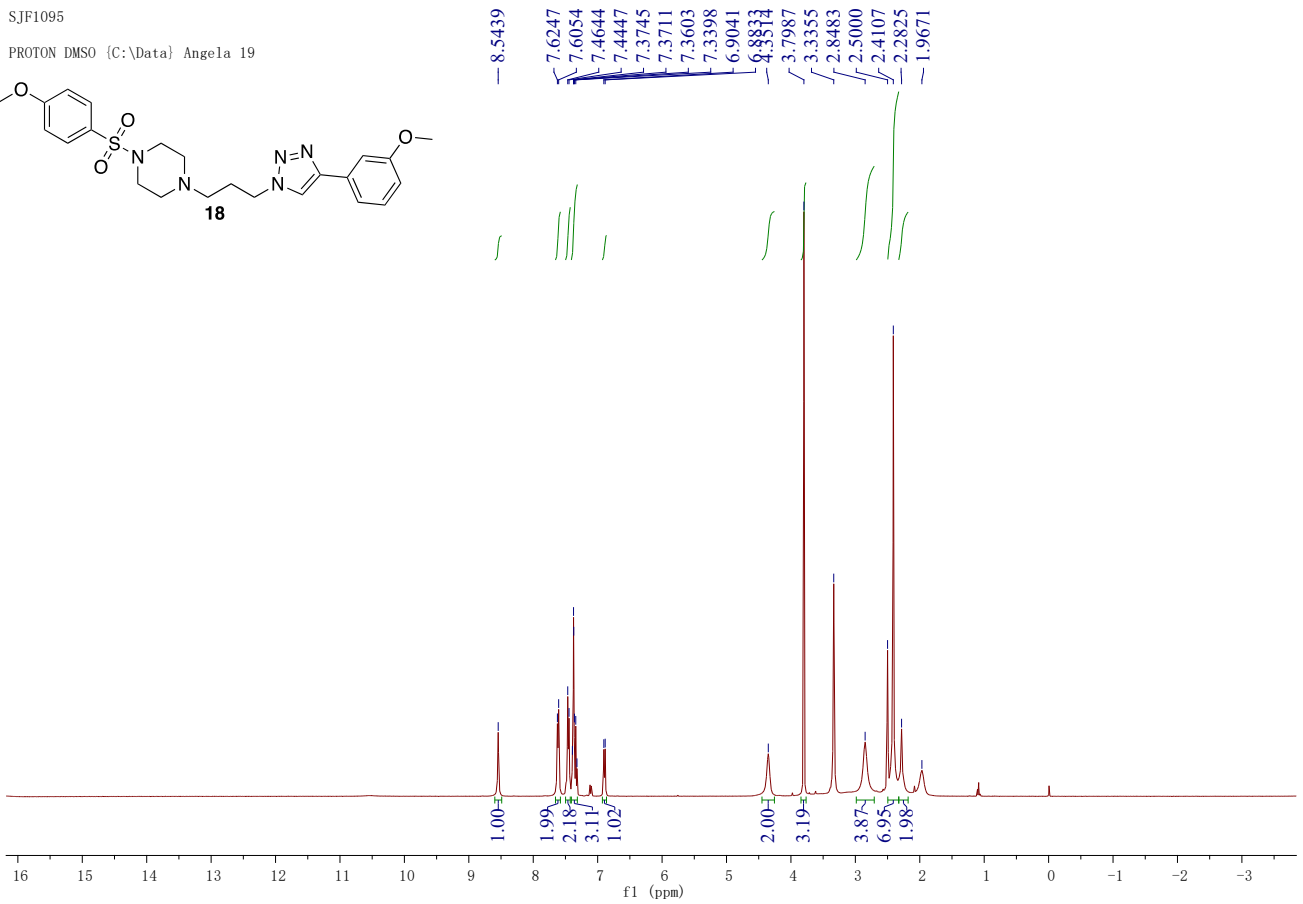
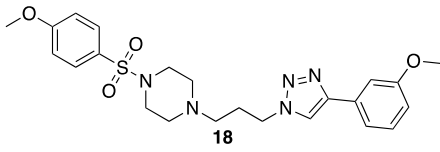
1-((4-(tert-Butyl)phenyl)sulfonyl)-4-(3-(4-(3-methoxyphenyl)-1H-1,2,3-triazol-1-yl)propyl)piperazine hydrochloride (**17**)



1-(3-(4-(3-Methoxyphenyl)-1H-1,2,3-triazol-1-yl)propyl)-4-((4-methoxyphenyl)-sulfonyl)piperazine 4-methoxy benzenesulfonate (**18**)

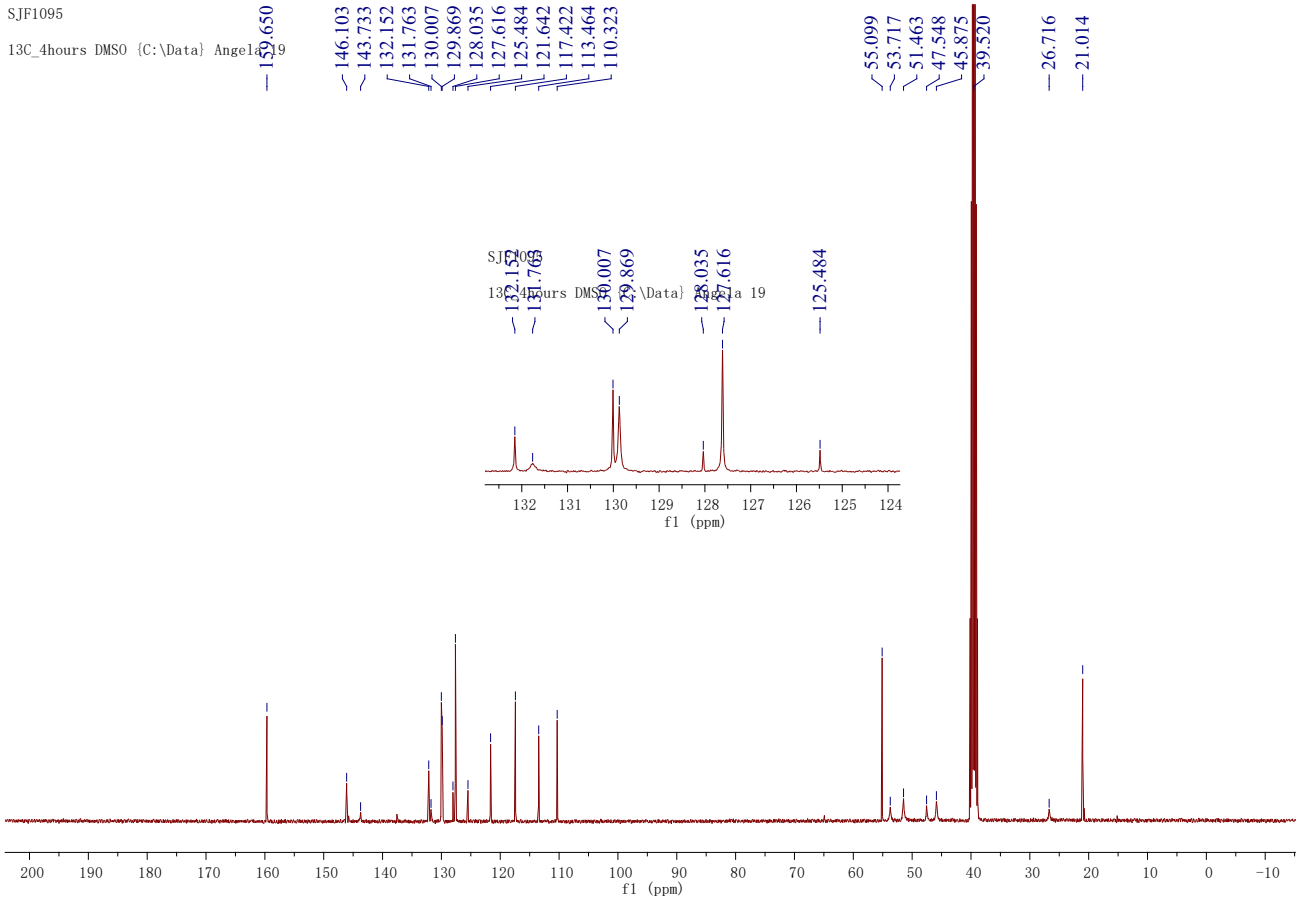
SJF1095

PROTON DMSO (C:\Data) Angela 19

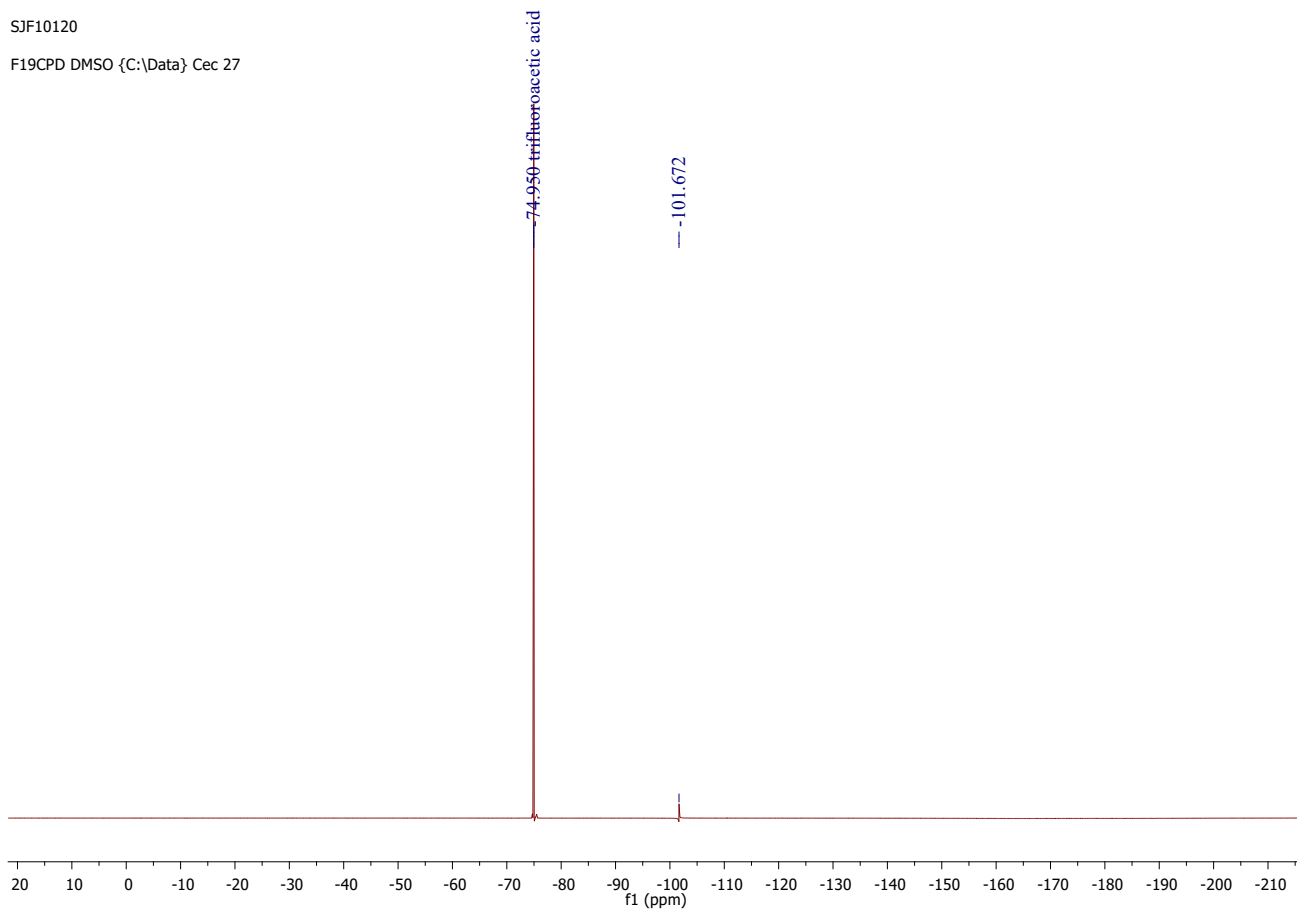
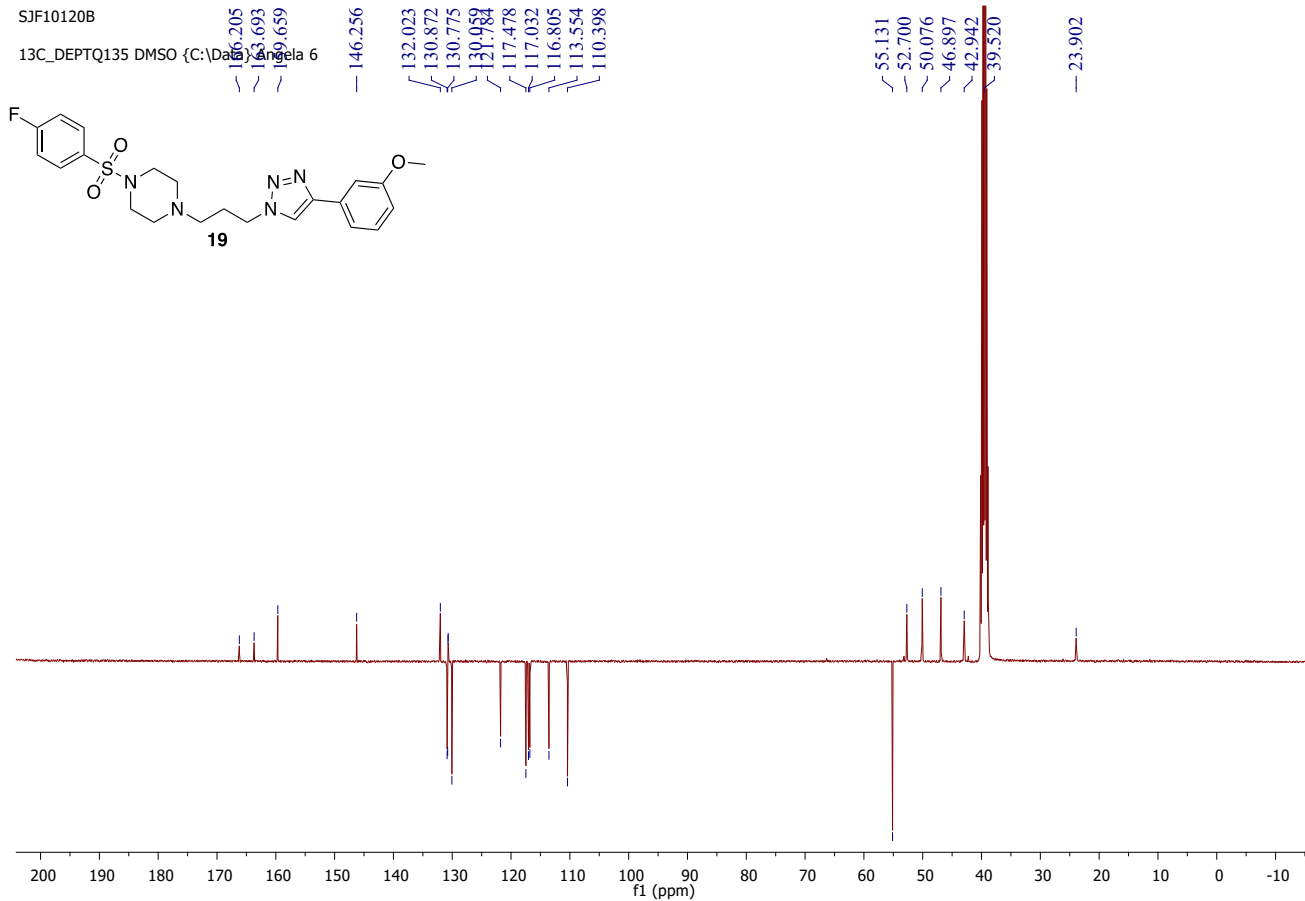


SJF1095

13C_4hours DMSO (C:\Data) Angel



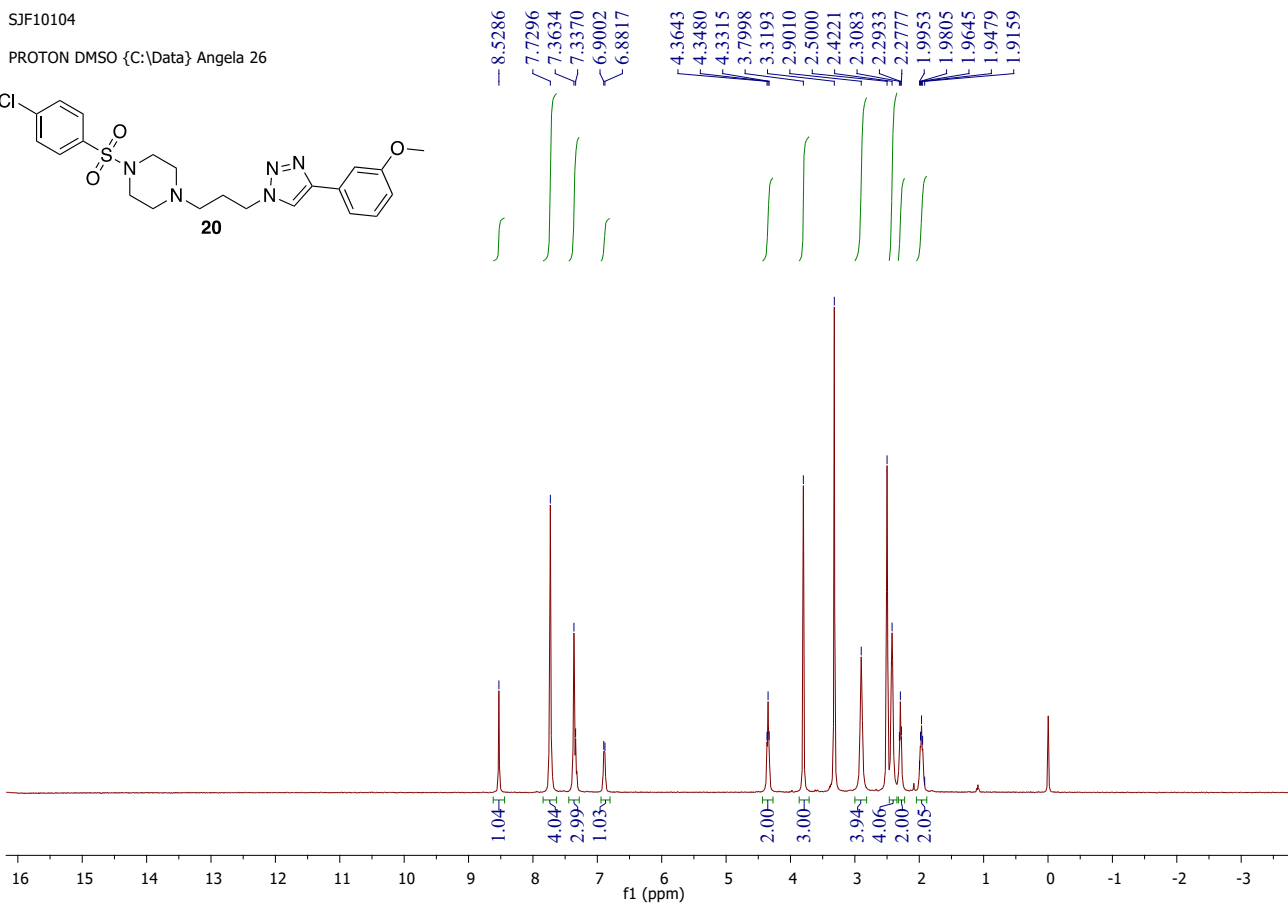
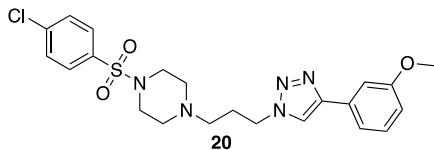
1-((4-Fluorophenyl)sulfonyl)-4-(3-(4-(3-methoxyphenyl)-1H-1,2,3-triazol-1-yl)-propyl)piperazine hydrochloride (19)



1-((4-Chlorophenyl)sulfonyl)-4-(3-(4-(3-methoxyphenyl)-1H-1,2,3-triazol-1-yl)-propyl)piperazine (20)

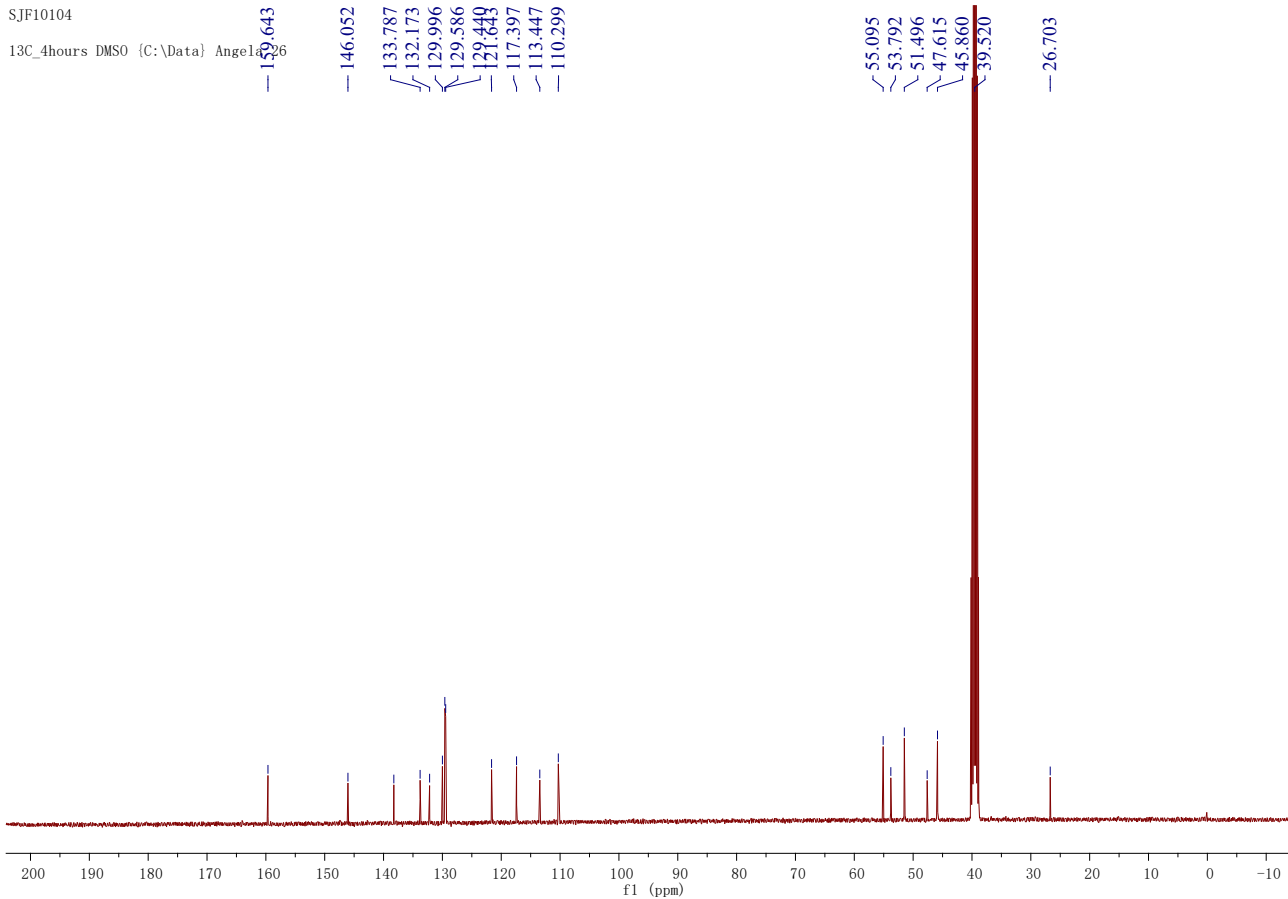
SJF10104

PROTON DMSO {C:\Data} Angela 26



SJF10104

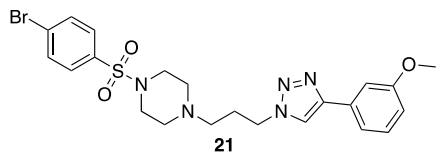
13C_4hours DMSO {C:\Data} Angela 26



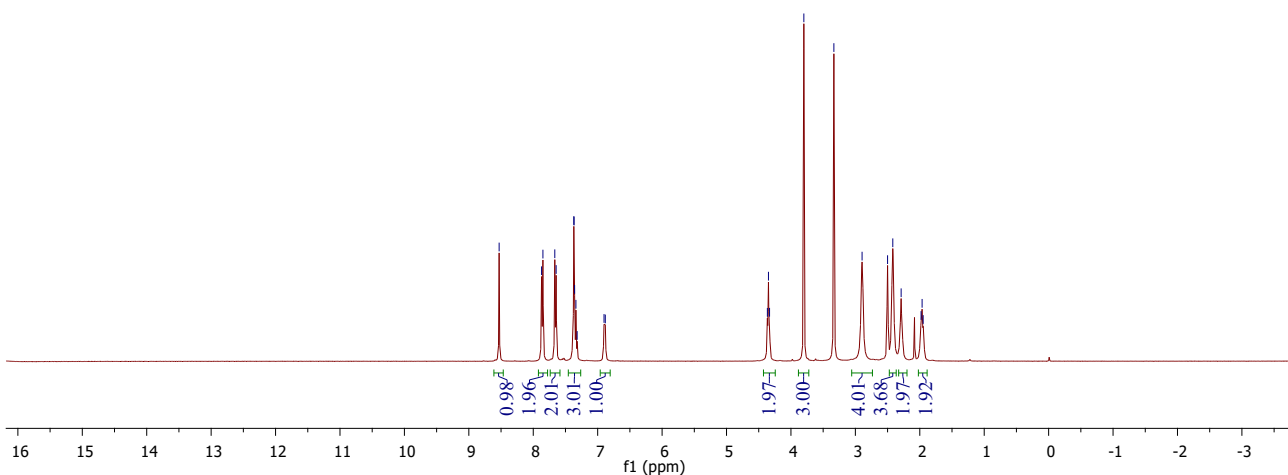
1-((4-Bromophenyl)sulfonyl)-4-(3-(4-(3-methoxyphenyl)-1H-1,2,3-triazol-1-yl) propyl)piperazine (21)

SJF1094

PROTON DMSO {C:\Data} Angela 18



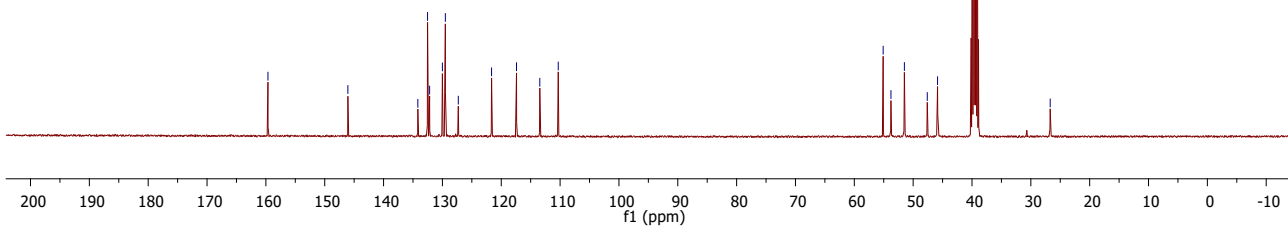
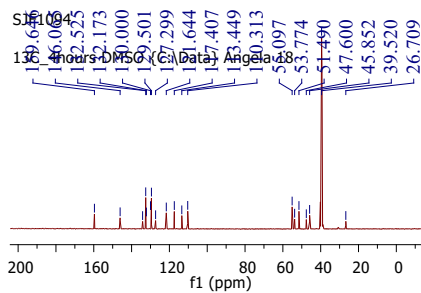
8.5296
7.8709
7.8499
7.6657
7.6447
7.3699
7.3669
7.3582
7.3377
7.3186
6.9015
6.8816
4.3659
4.3490
4.3321
3.7997
3.3336
2.8959
2.5001
2.4191
2.2895
1.9801
1.9641
1.9478



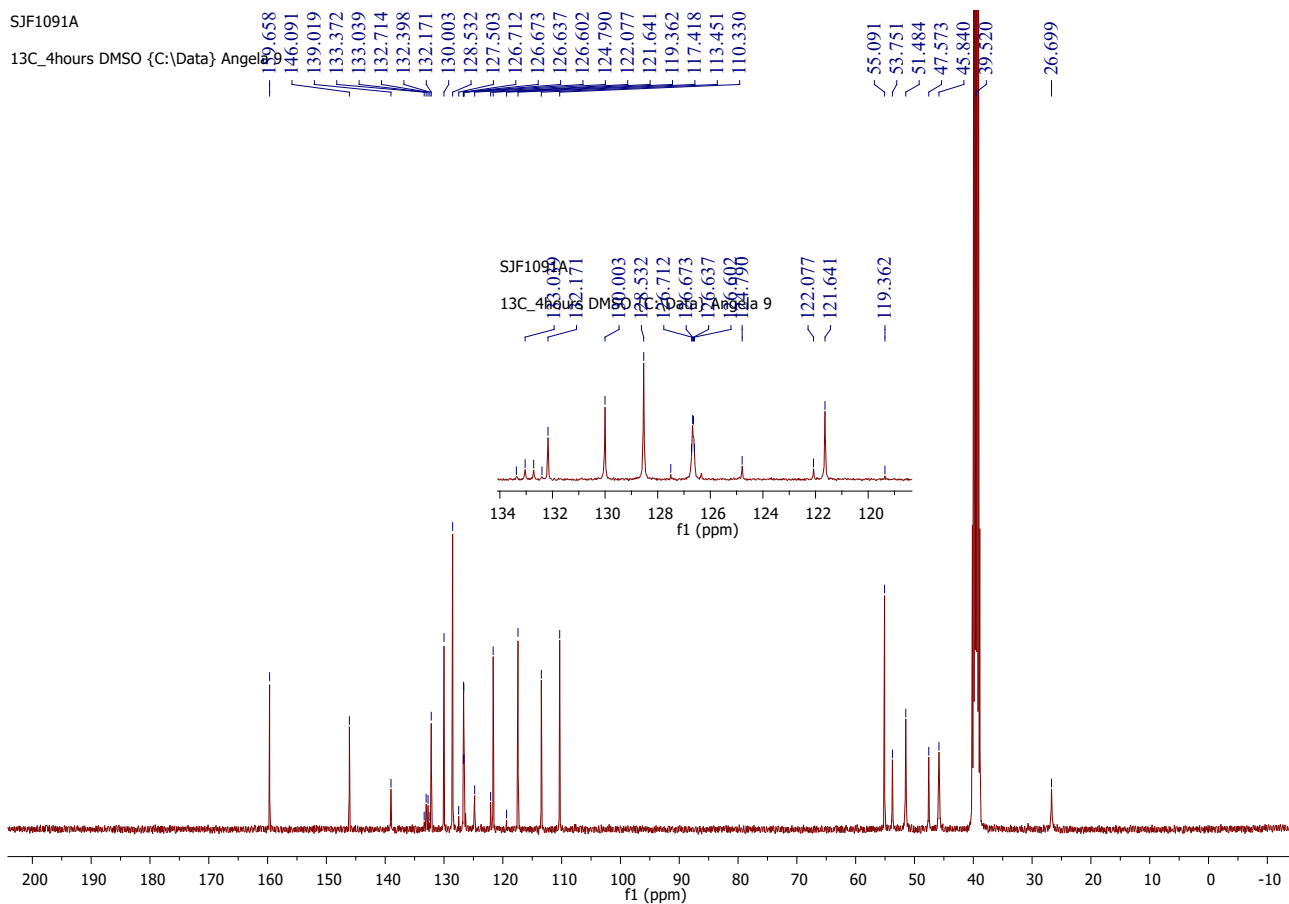
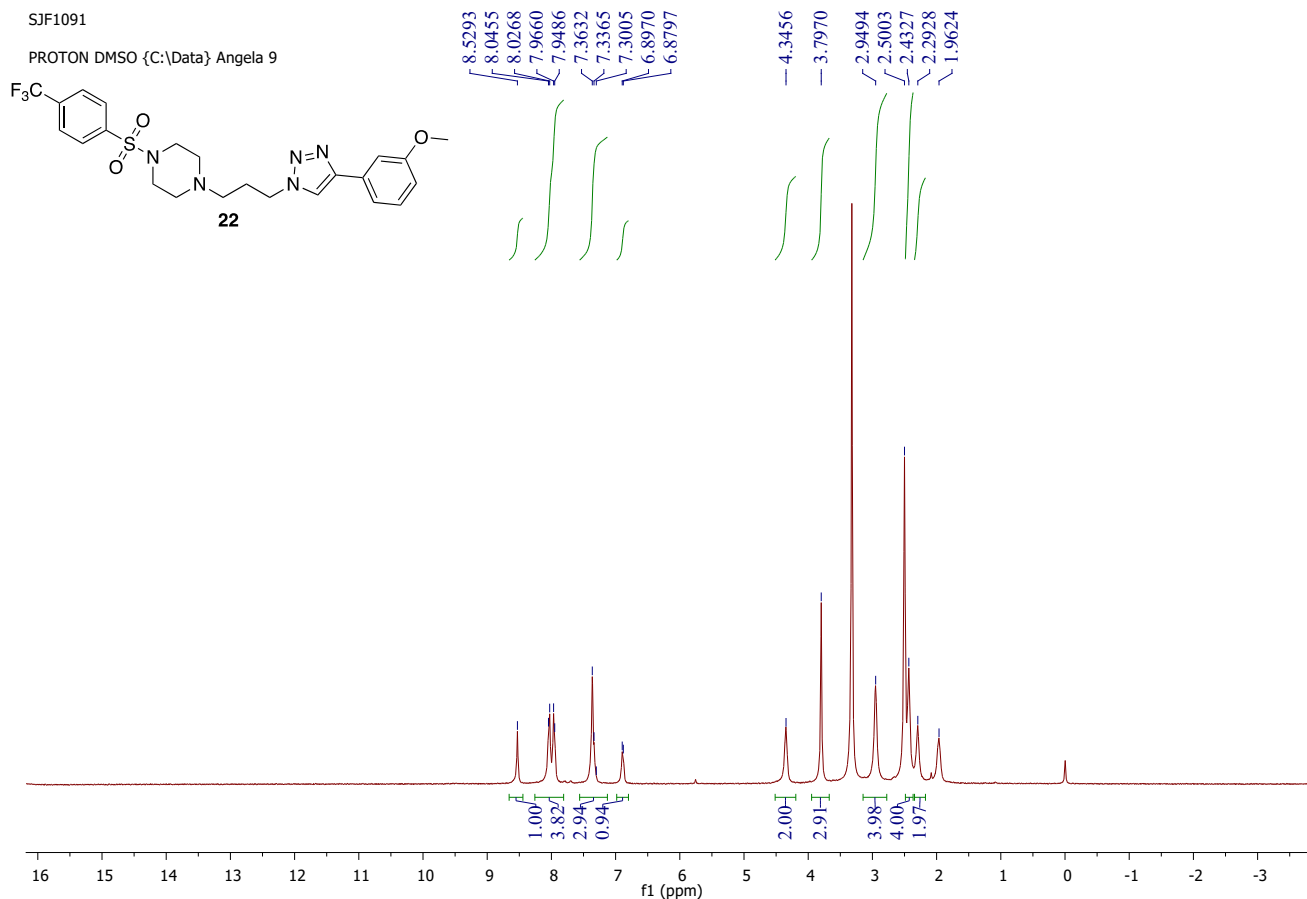
SJF1094

13C_4hours DMSO {C:\Data} Angela 18

129.646
146.065
134.174
132.525
132.173
130.000
129.501
127.299
121.644
117.407
113.449
110.313
55.097
53.774
51.490
47.600
45.852
39.520
26.709

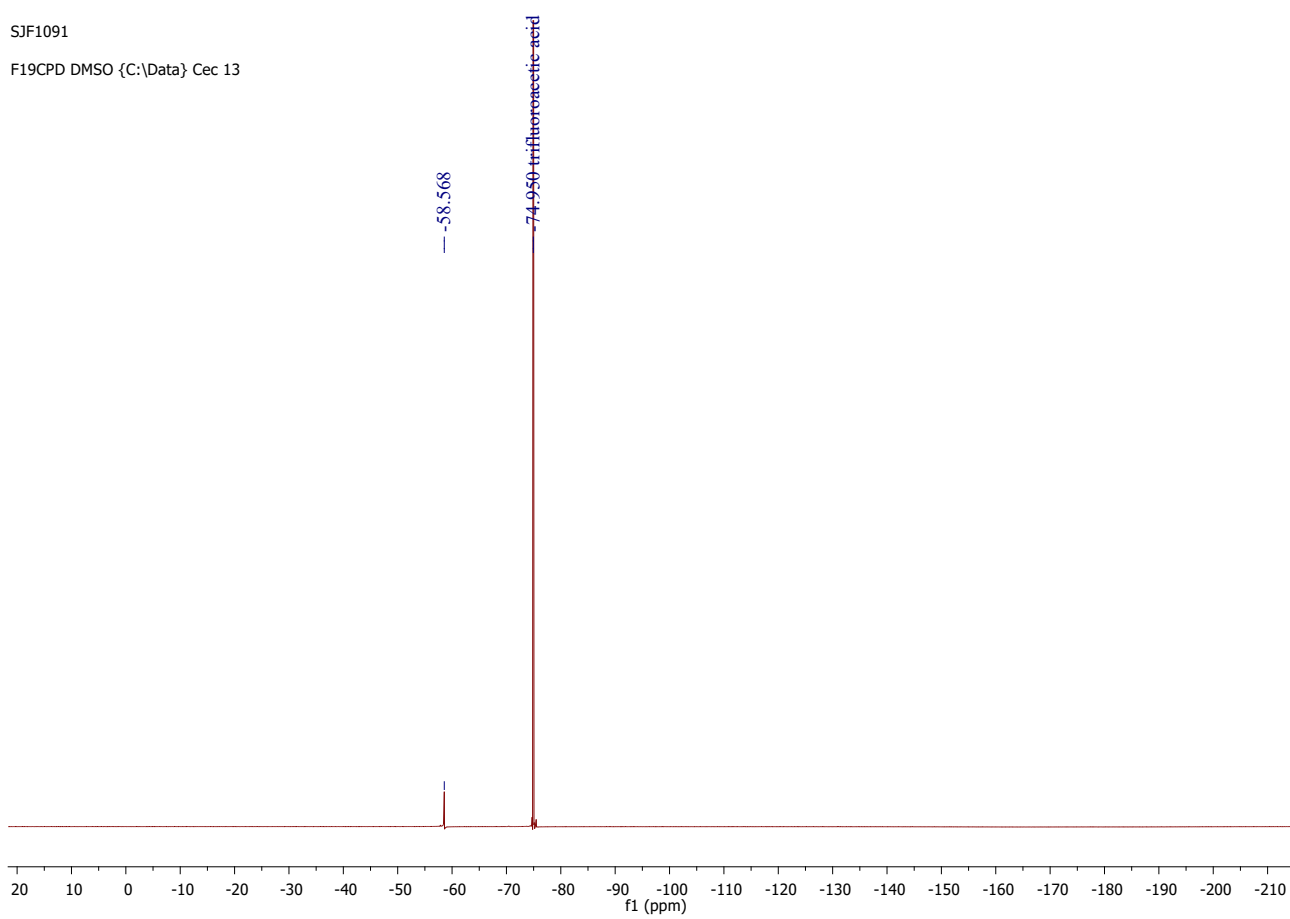


1-(3-(4-(3-Methoxyphenyl)-1H-1,2,3-triazol-1-yl)propyl)-4-((4-(trifluoromethyl)phenyl)sulfonyl) piperazine (**22**)

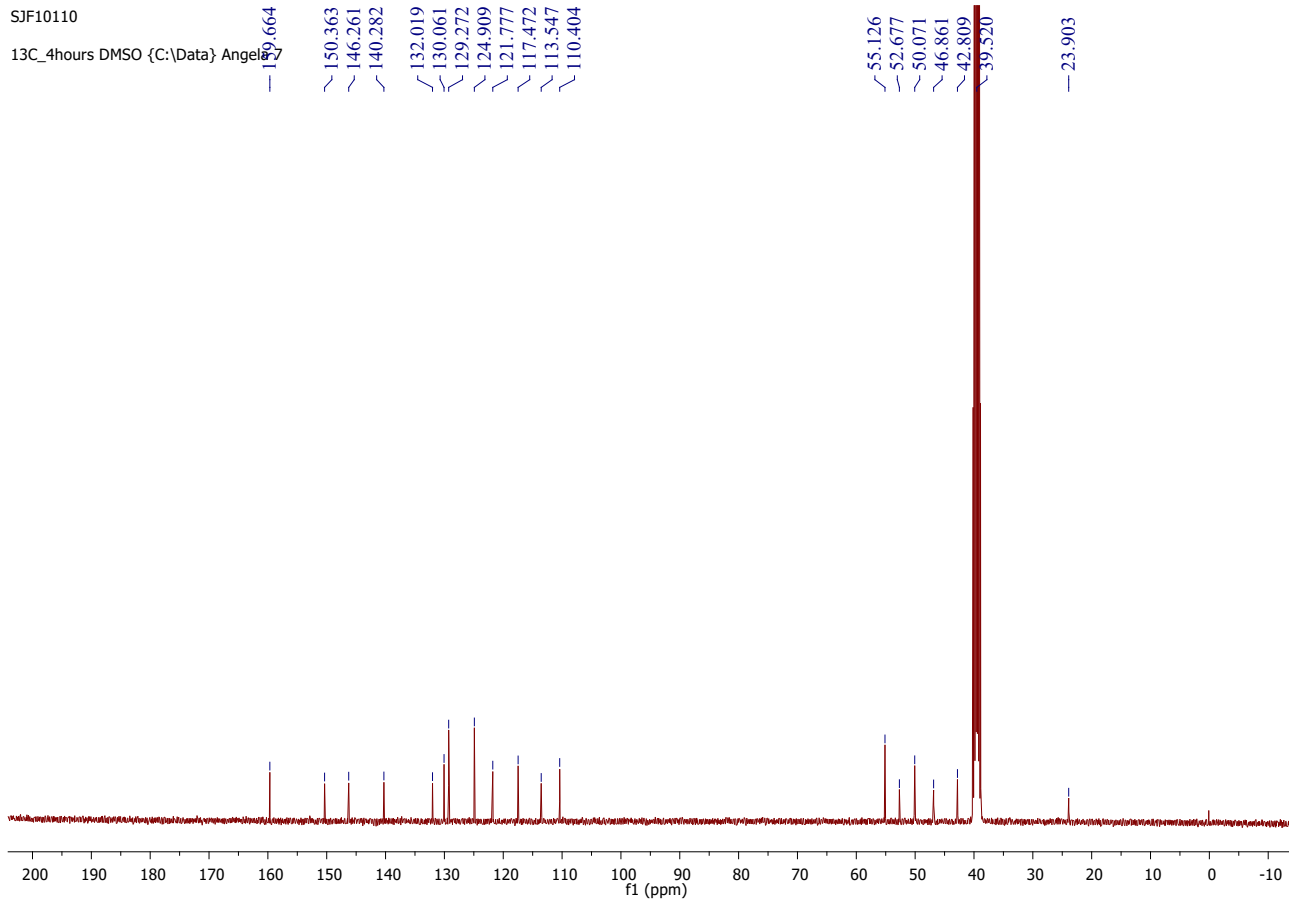
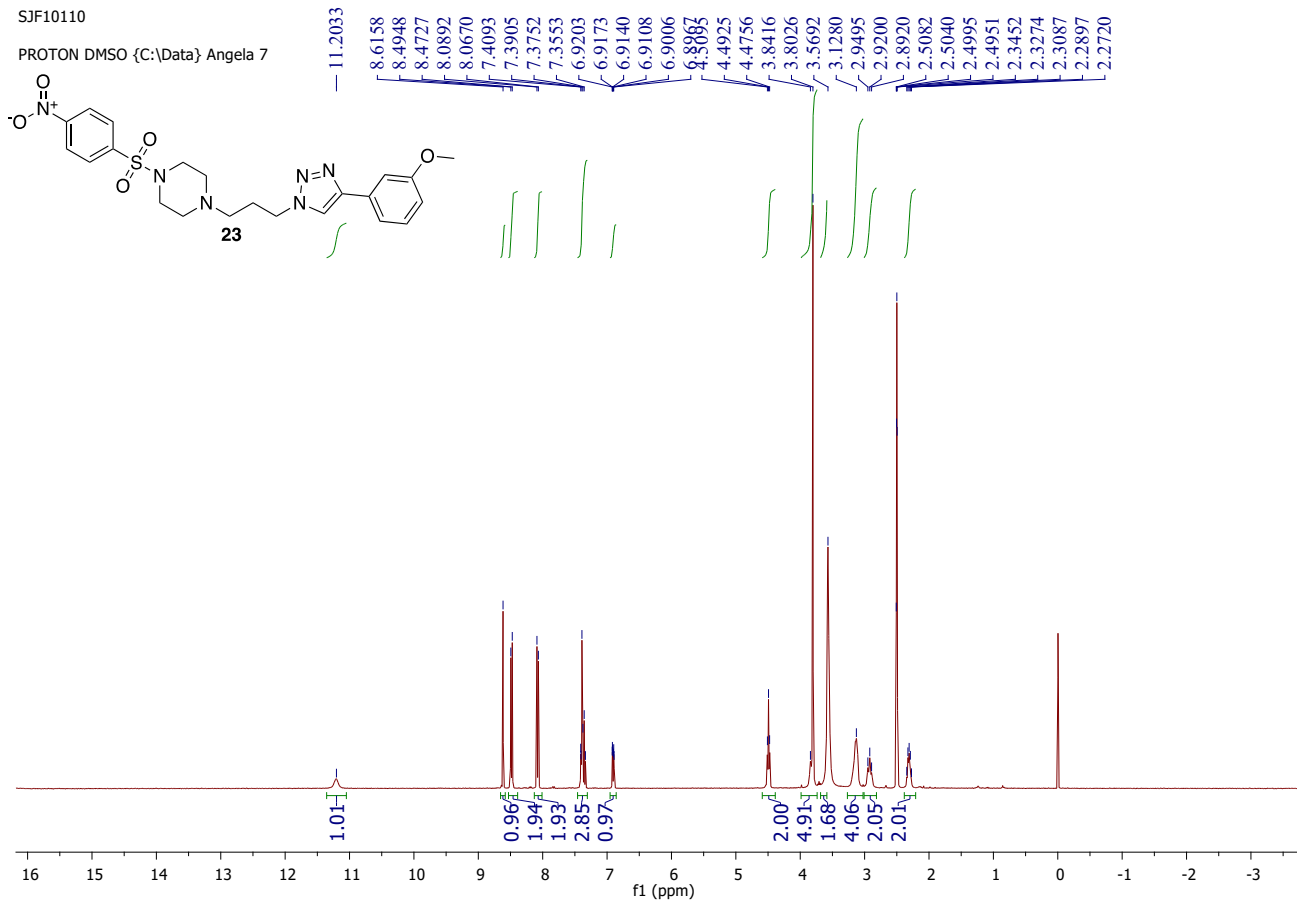


SJF1091

F19CPD DMSO {C:\Data} Cec 13



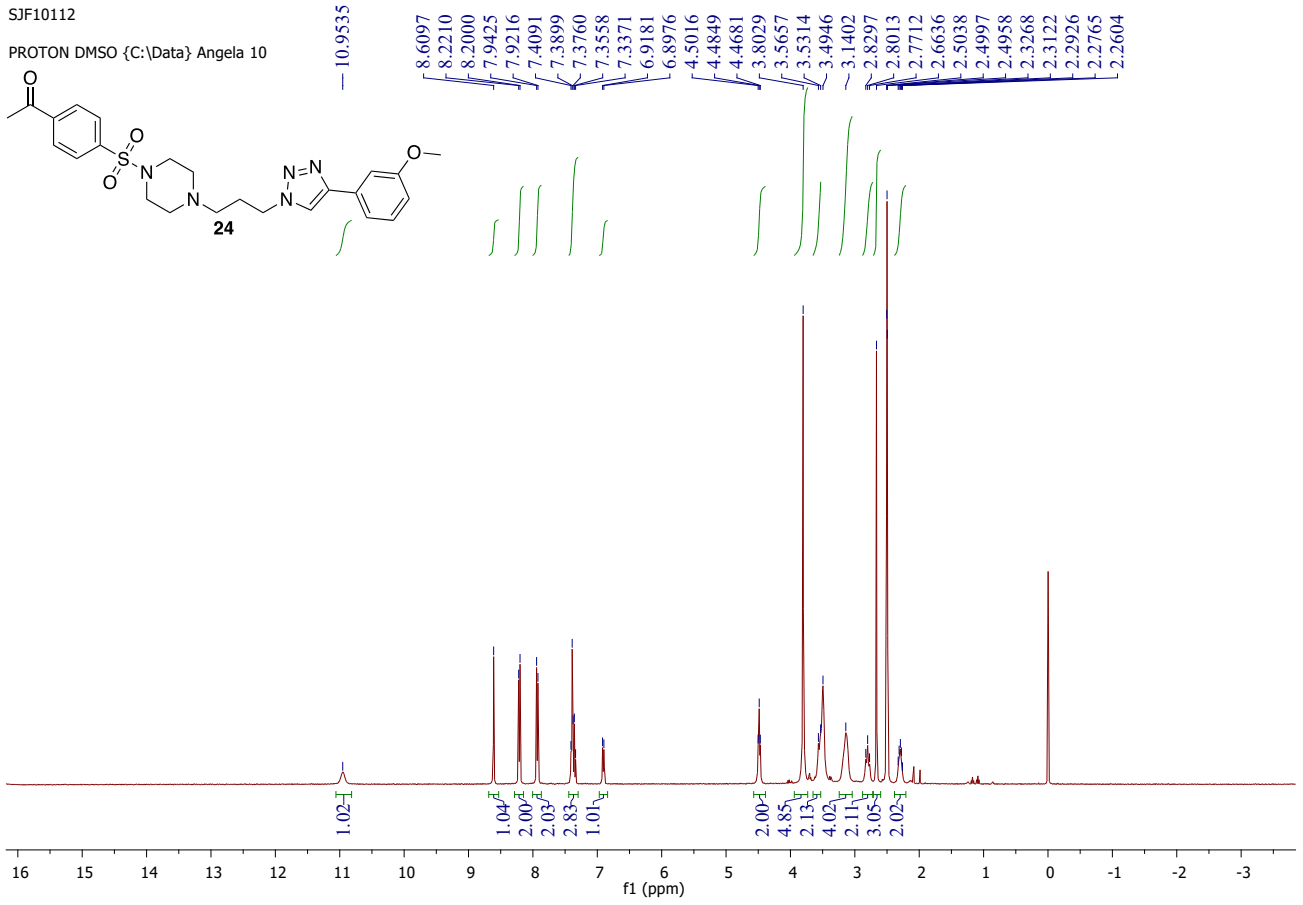
1-(3-(4-(3-Methoxyphenyl)-1H-1,2,3-triazol-1-yl)propyl)-4-((4-nitrophenyl)-sulfonyl)piperazine hydrochloride (**23**)



1-(4-((4-(3-(4-(3-Methoxyphenyl)-1H-1,2,3-triazol-1-yl)propyl)piperazin-1-yl)-sulfonyl)phenyl)ethanone hydrochloride
(24)

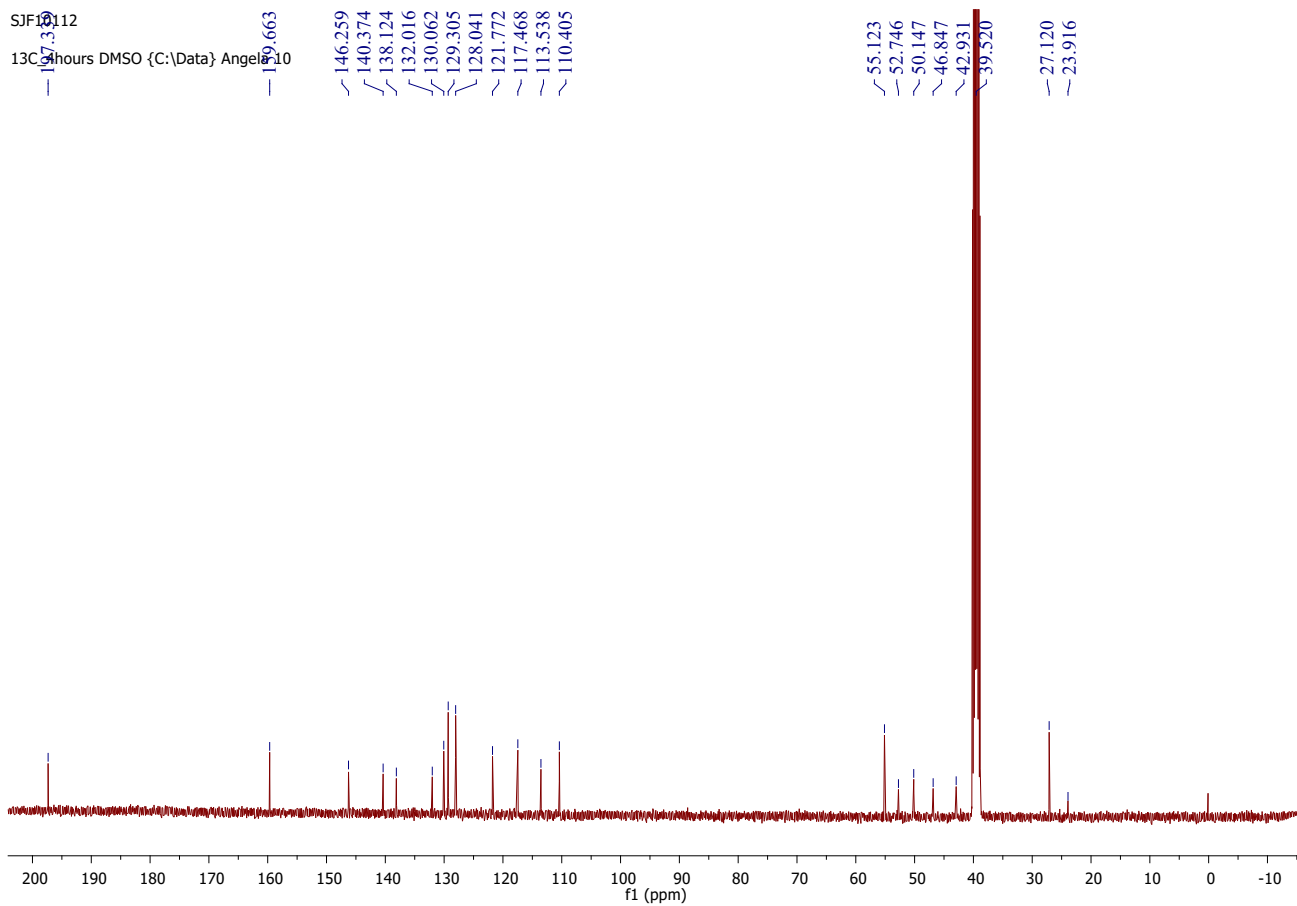
SJF10112

PROTON DMSO {C:\Data} Angela 10

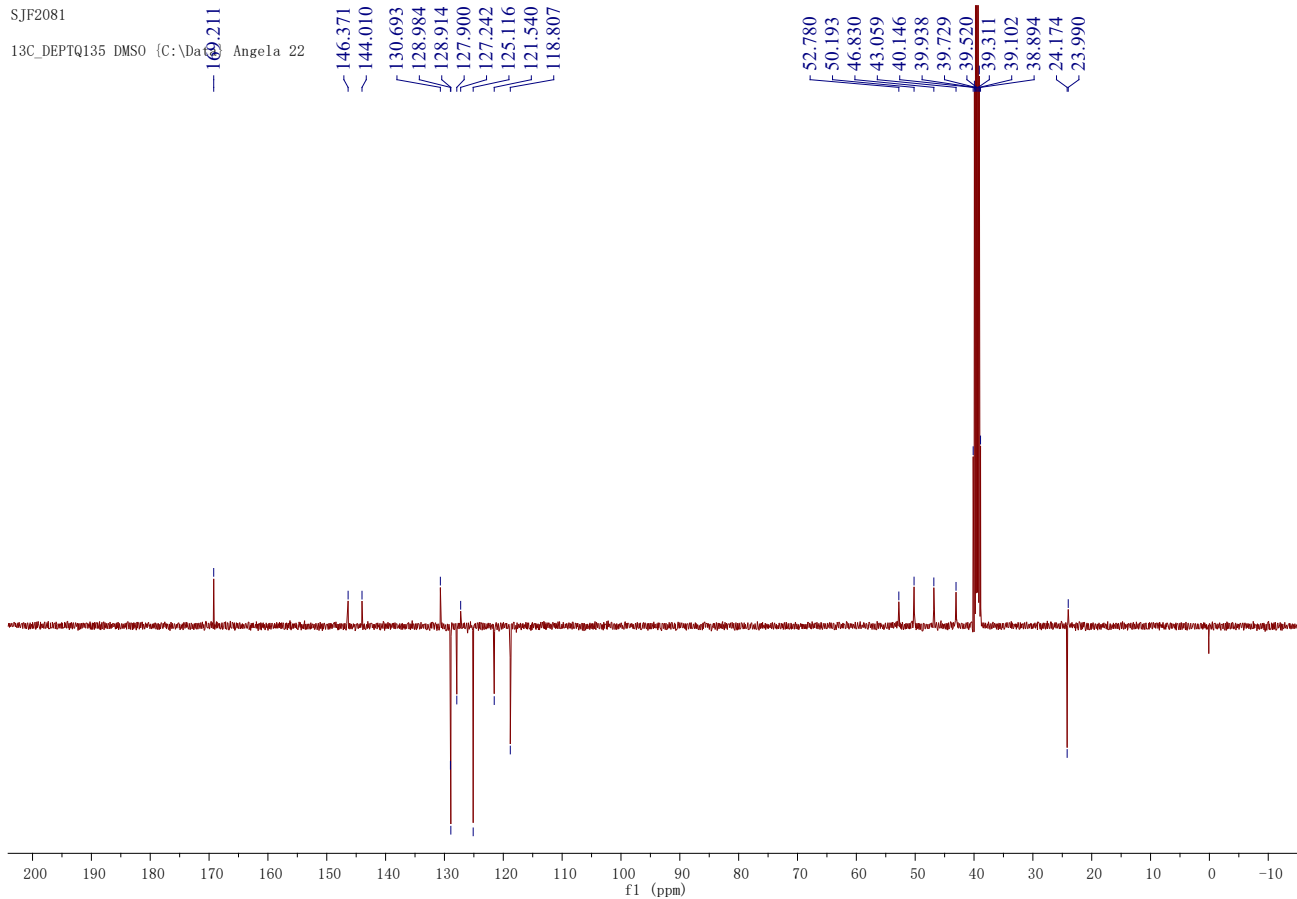
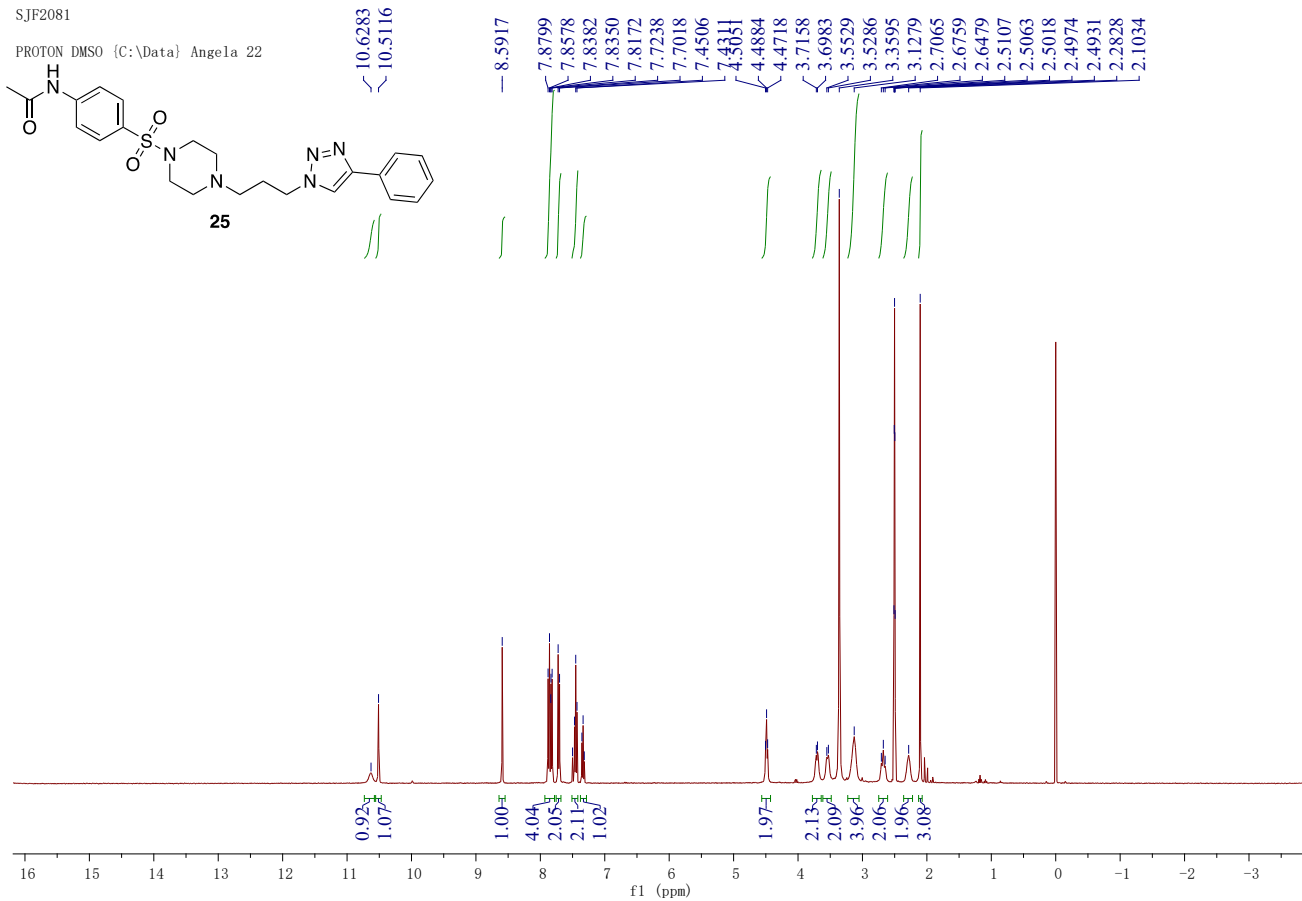


SJF10112

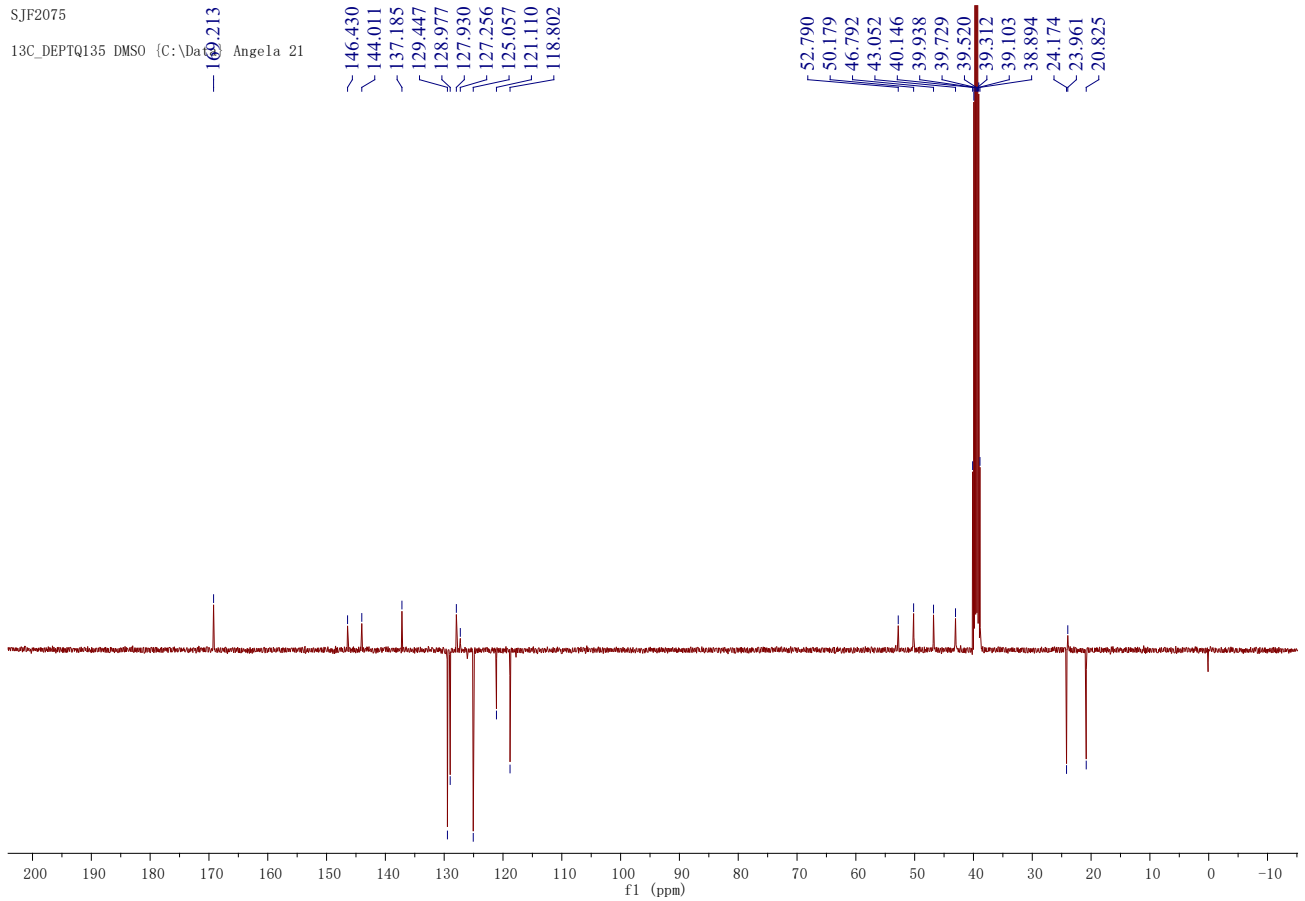
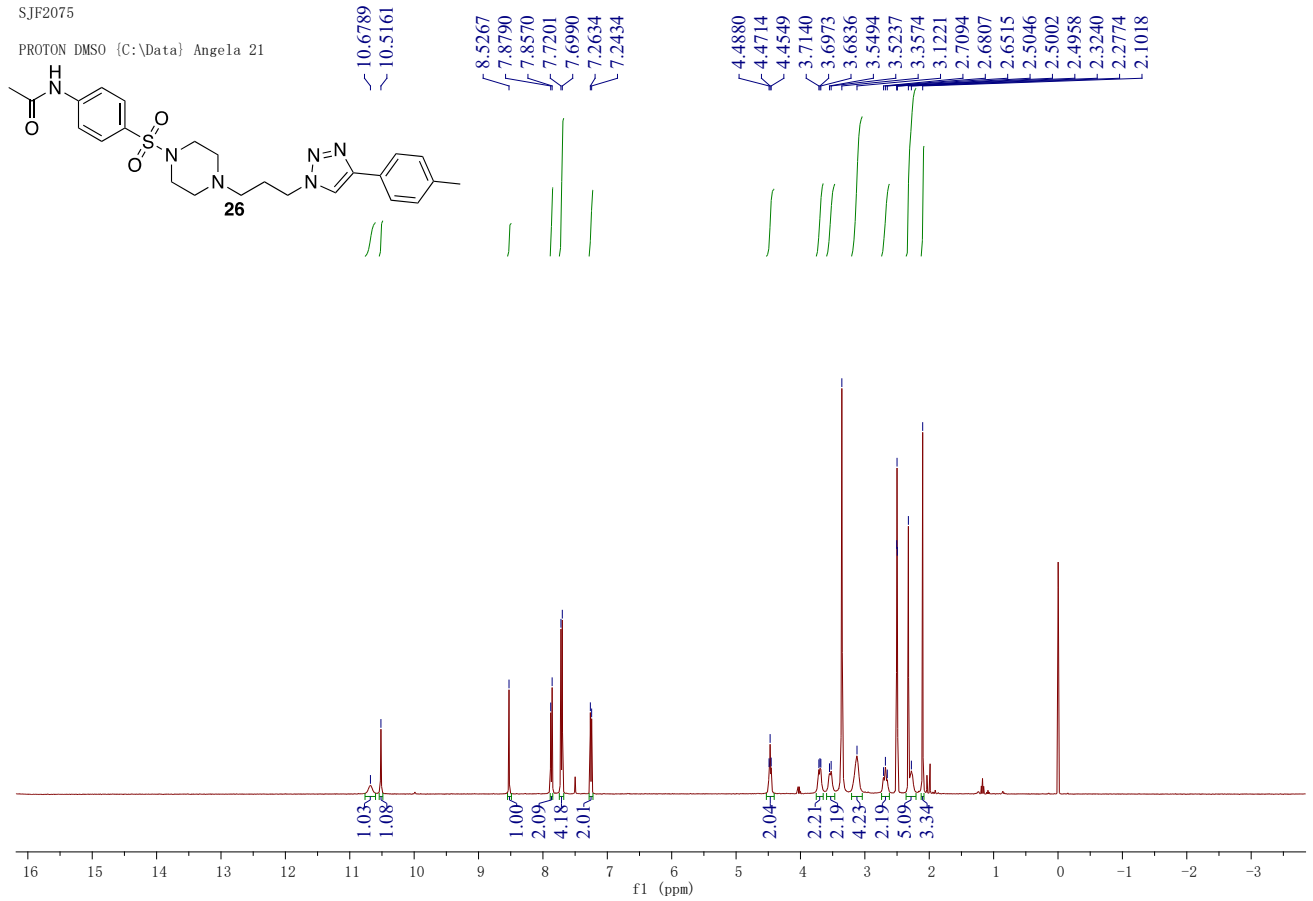
13C hours DMSO (C:\Data) Angel



N-(4-{4-[3-(4-Phenyl-[1,2,3]triazol-1-yl)-propyl]-piperazine-1-sulfonyl}-phenyl)-acetamide hydrochloride (**25**)



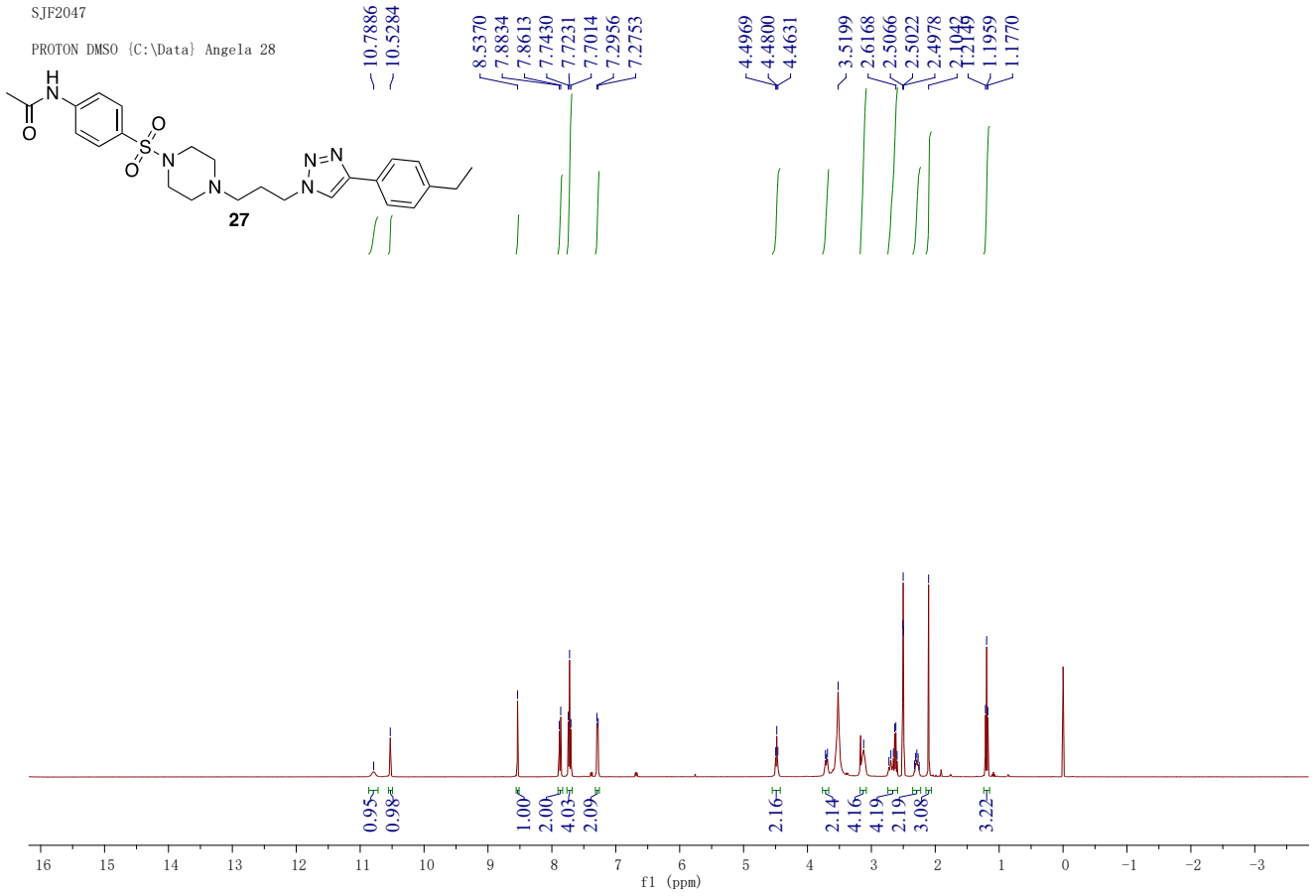
***N*-(4-{4-[3-(4-*p*-Tolyl-[1,2,3]triazol-1-yl)-propyl]-piperazine-1-sulfonyl}-phenyl)-acetamide hydrochloride (26)**



N-[4-(4-{3-[4-(4-Ethylphenyl)-[1,2,3]triazol-1-yl]-propyl}-piperazine-1-sulfonyl)-phenyl]-acetamide hydrochloride (**27**)

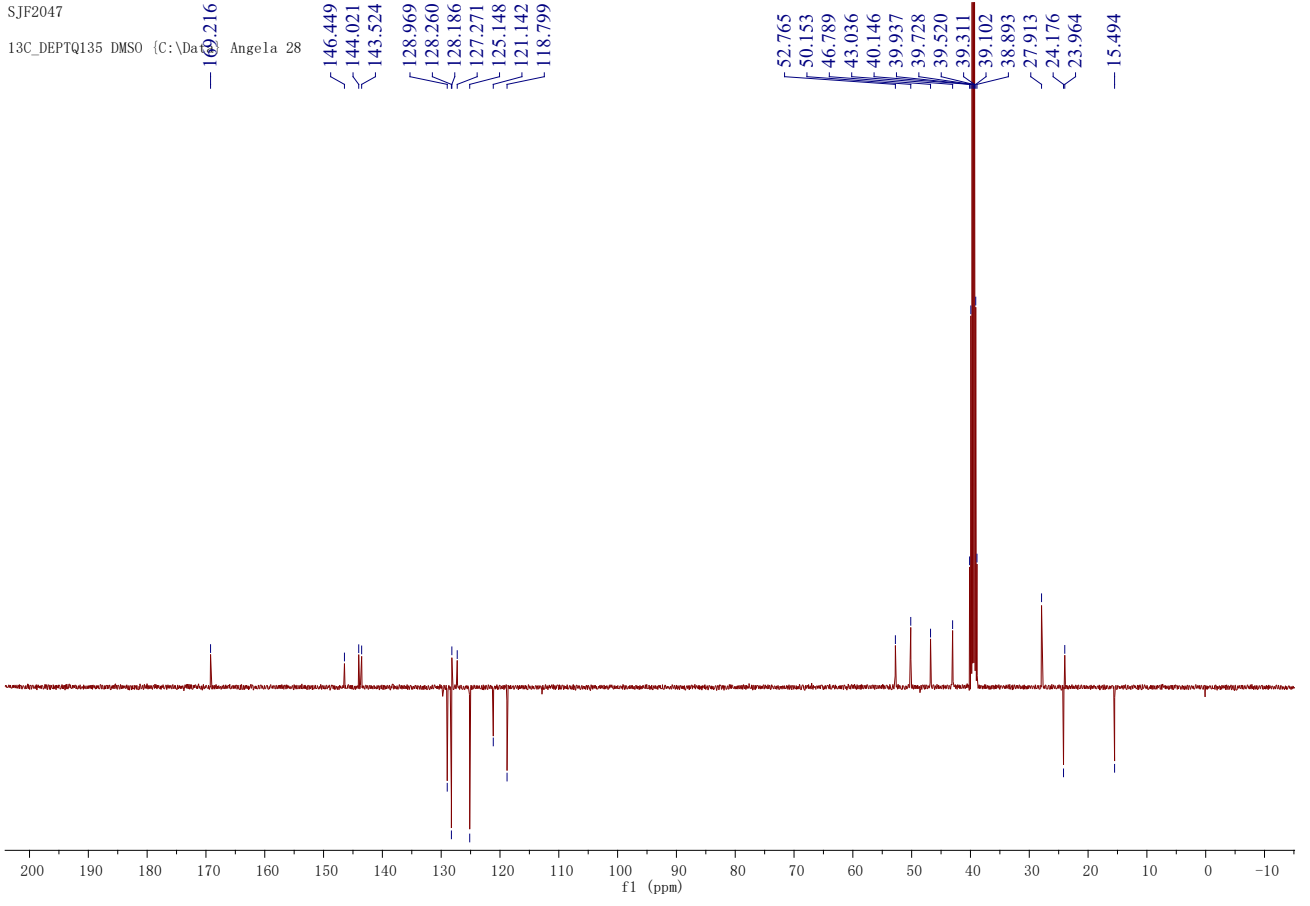
SJF2047

PROTON DMSO (C:\Data) Angela 28

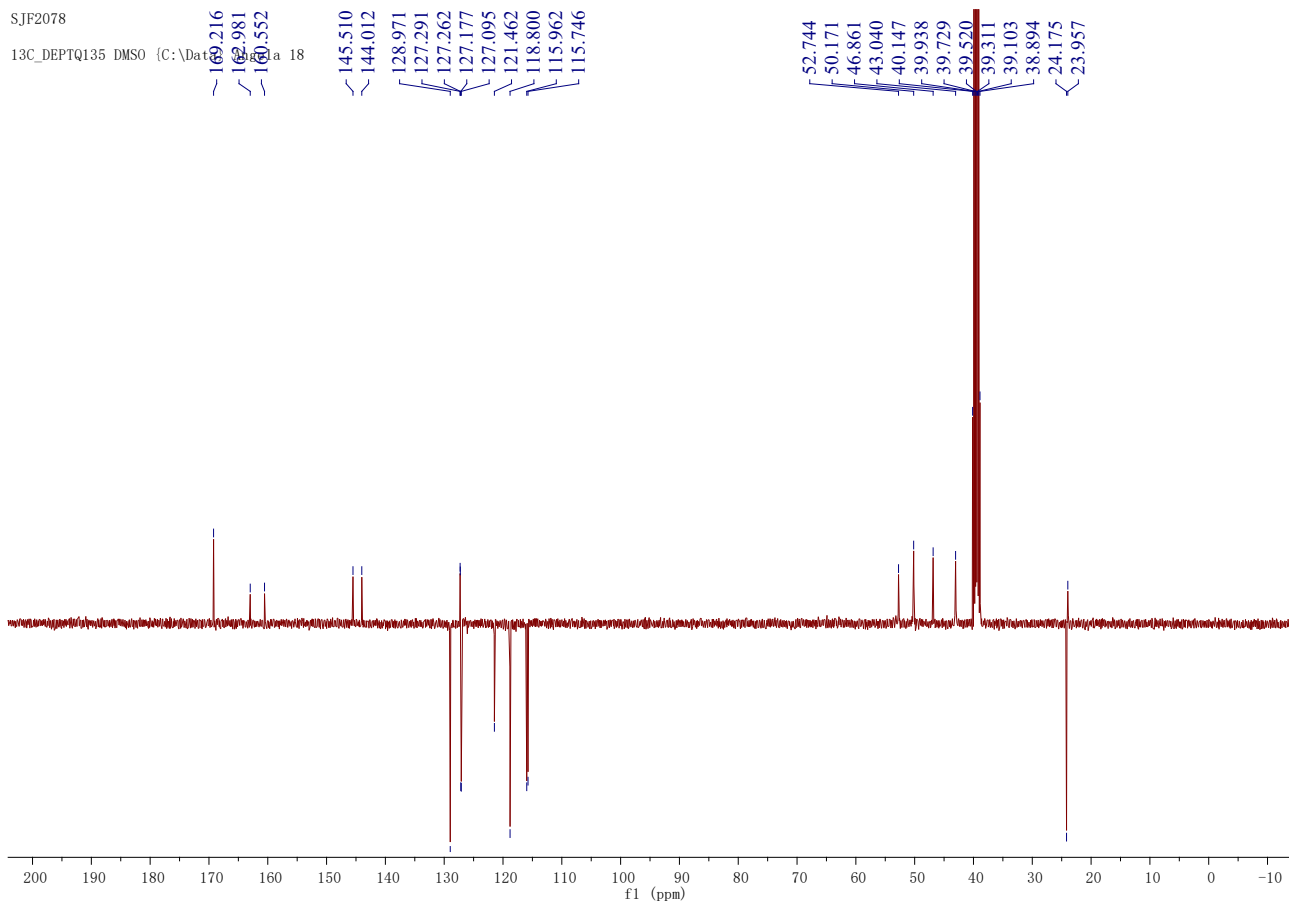
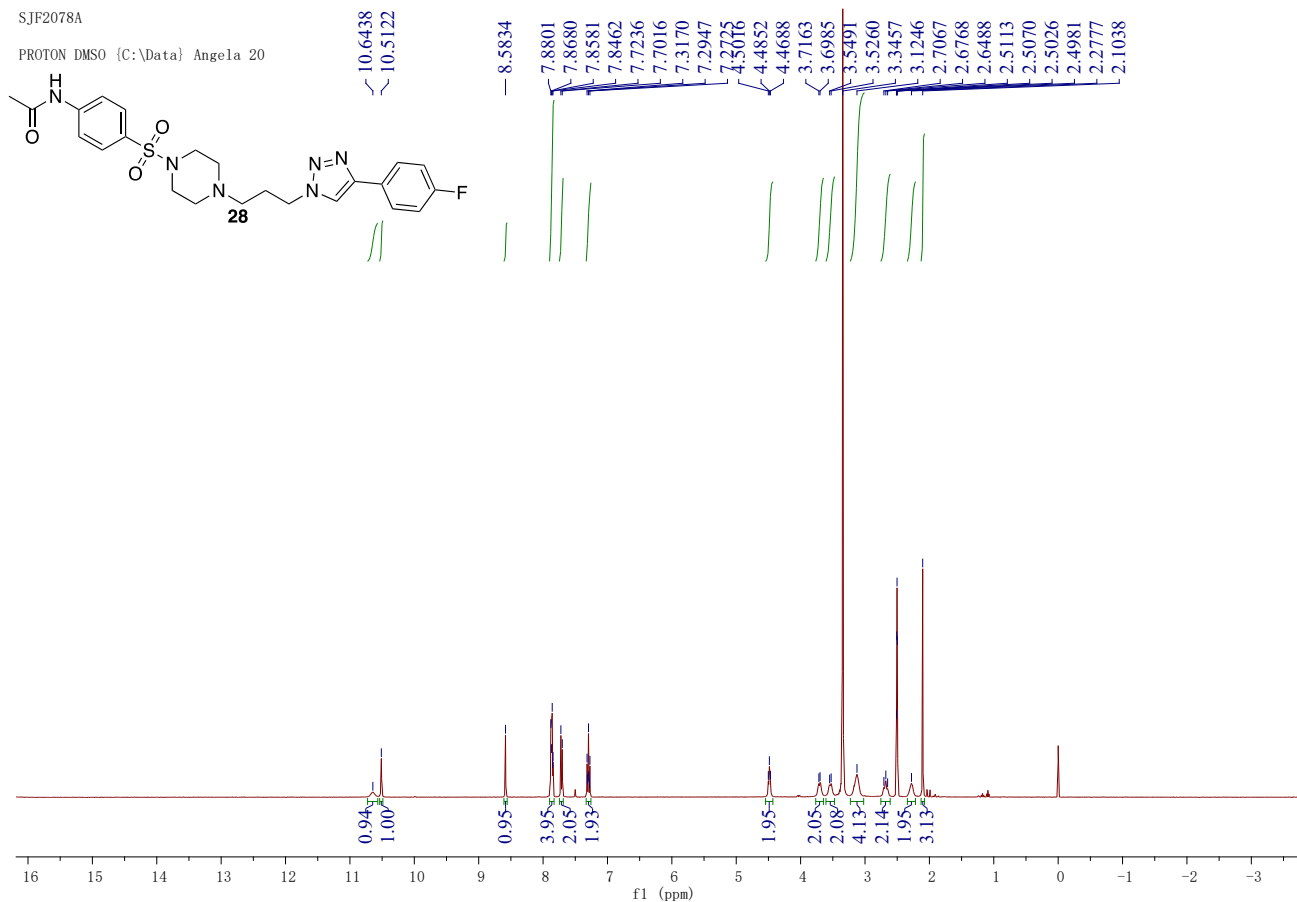


SJF2047

13C_DEPTQ135 DMSO {C:\Da Angela 28

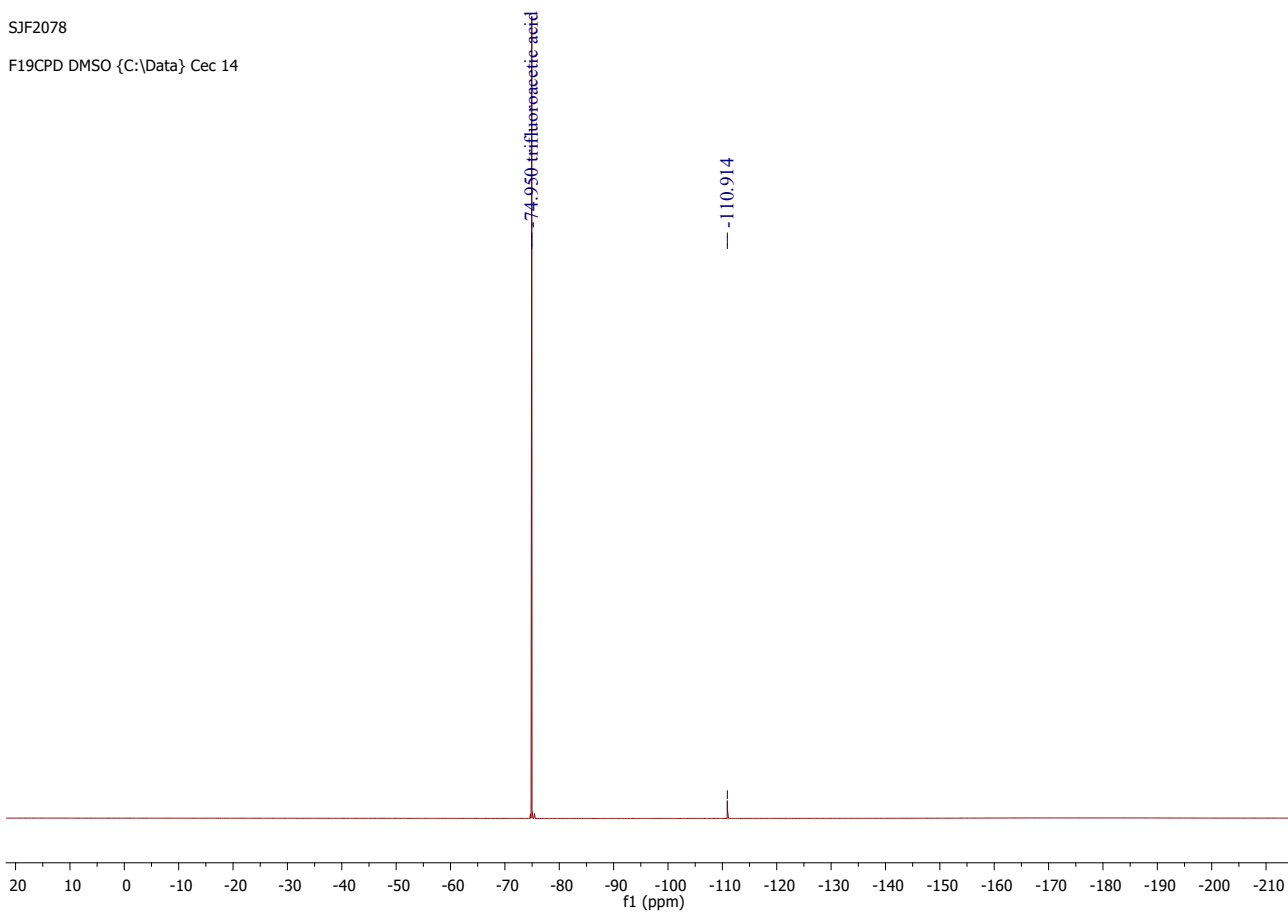


***N*-[4-(4-{3-[4-(4-Fluorophenyl)-[1,2,3]triazol-1-yl]-propyl}-piperazine-1-sulfonyl)-phenyl]-acetamide hydrochloride (28)**

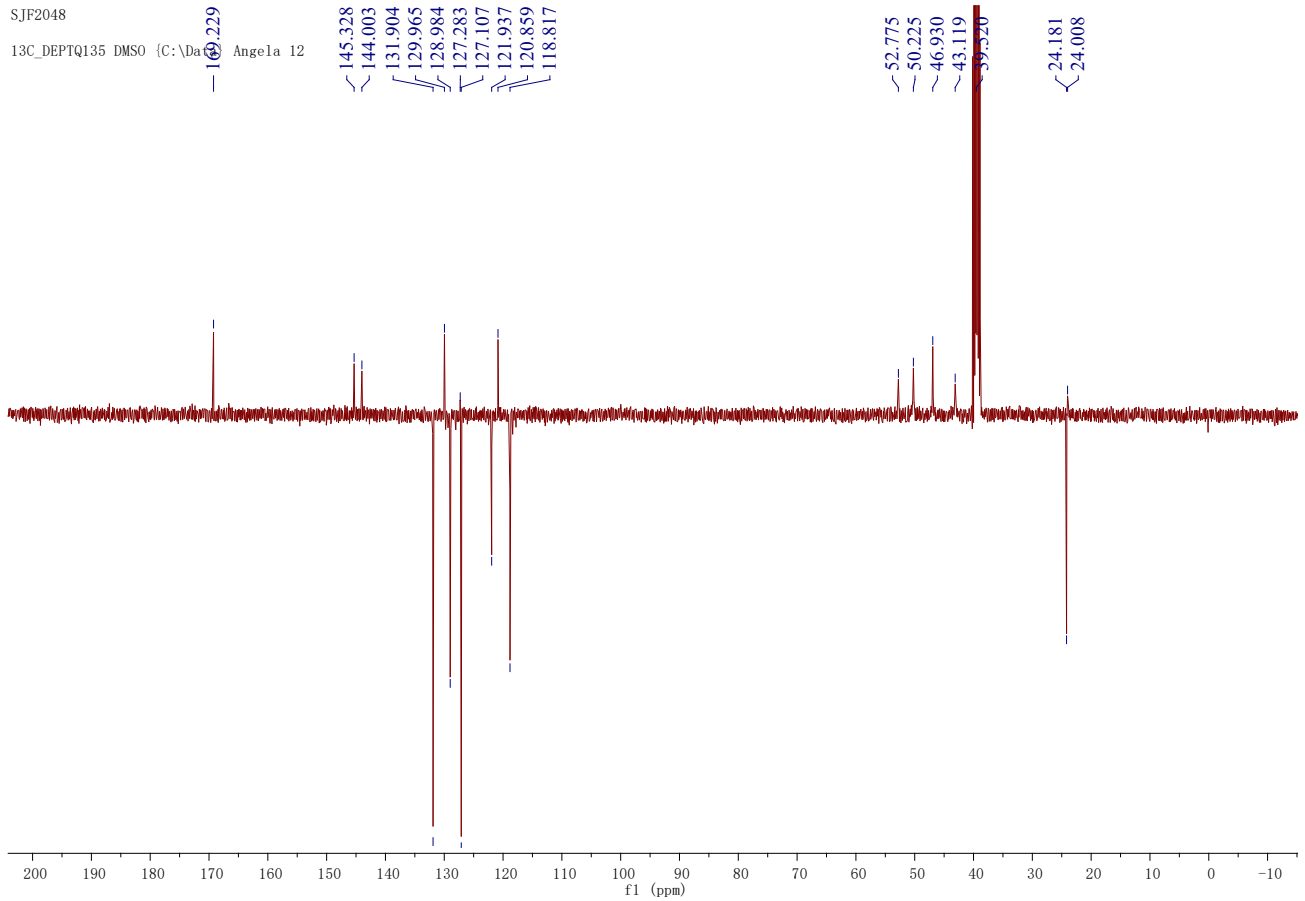
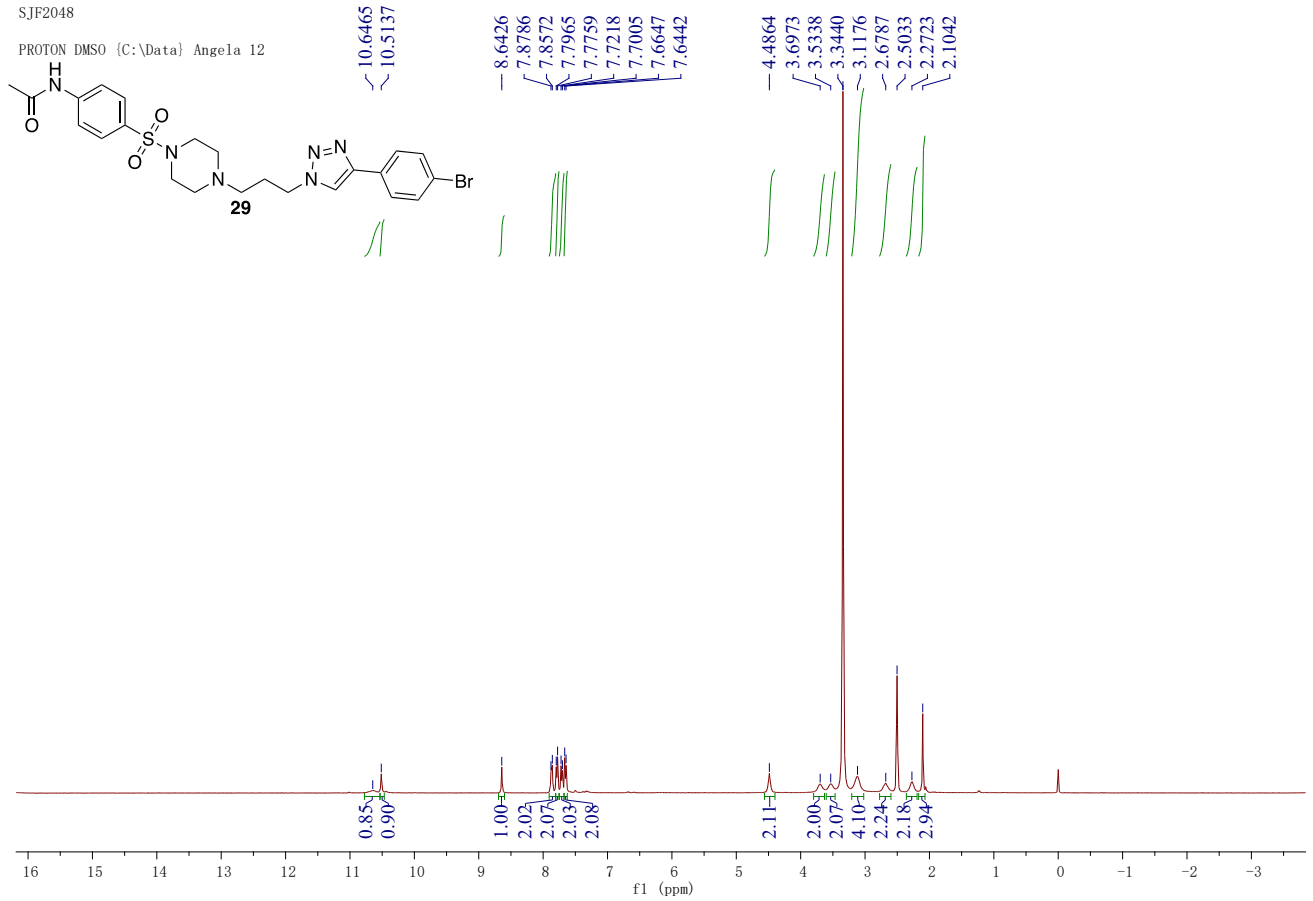


SJF2078

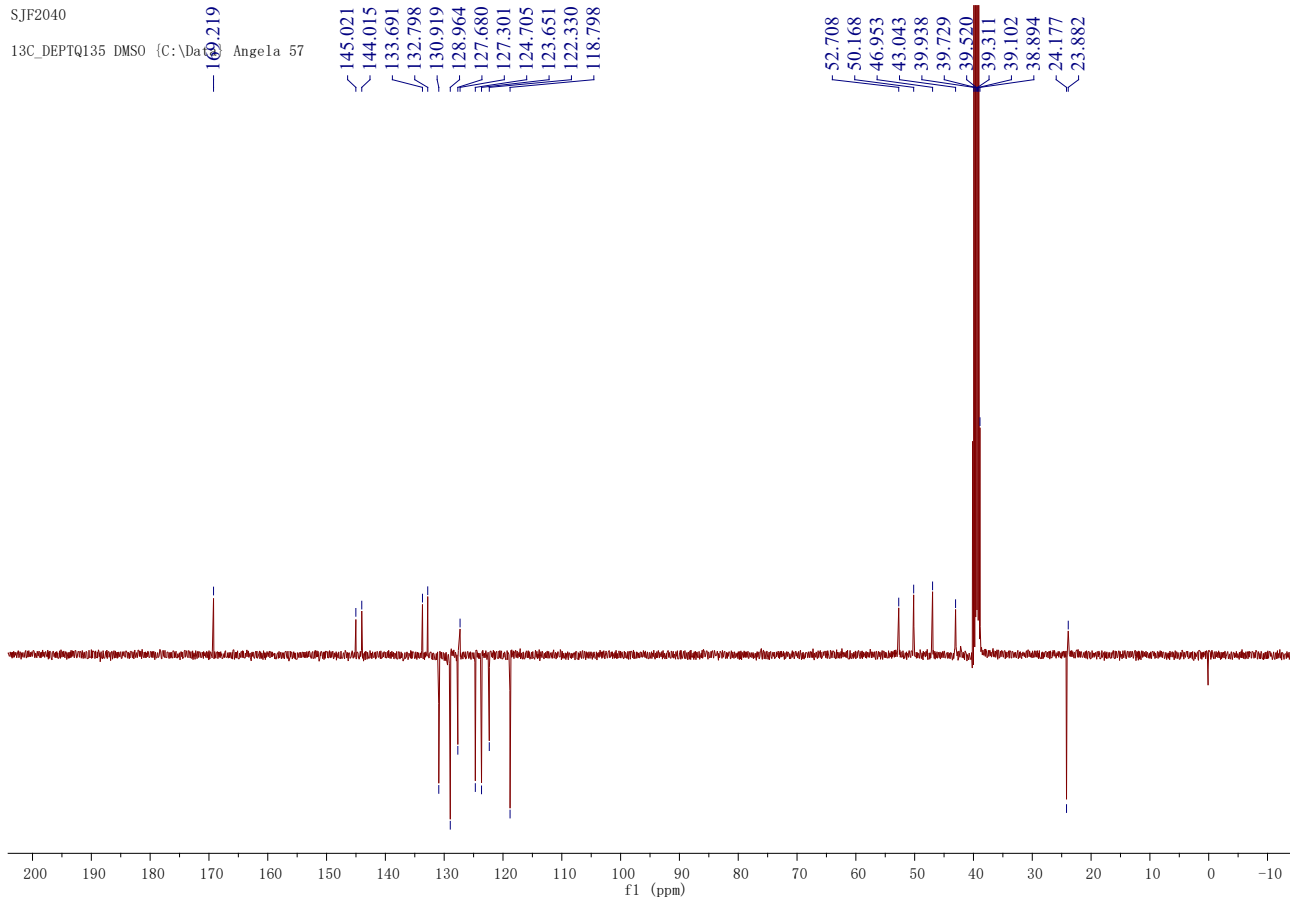
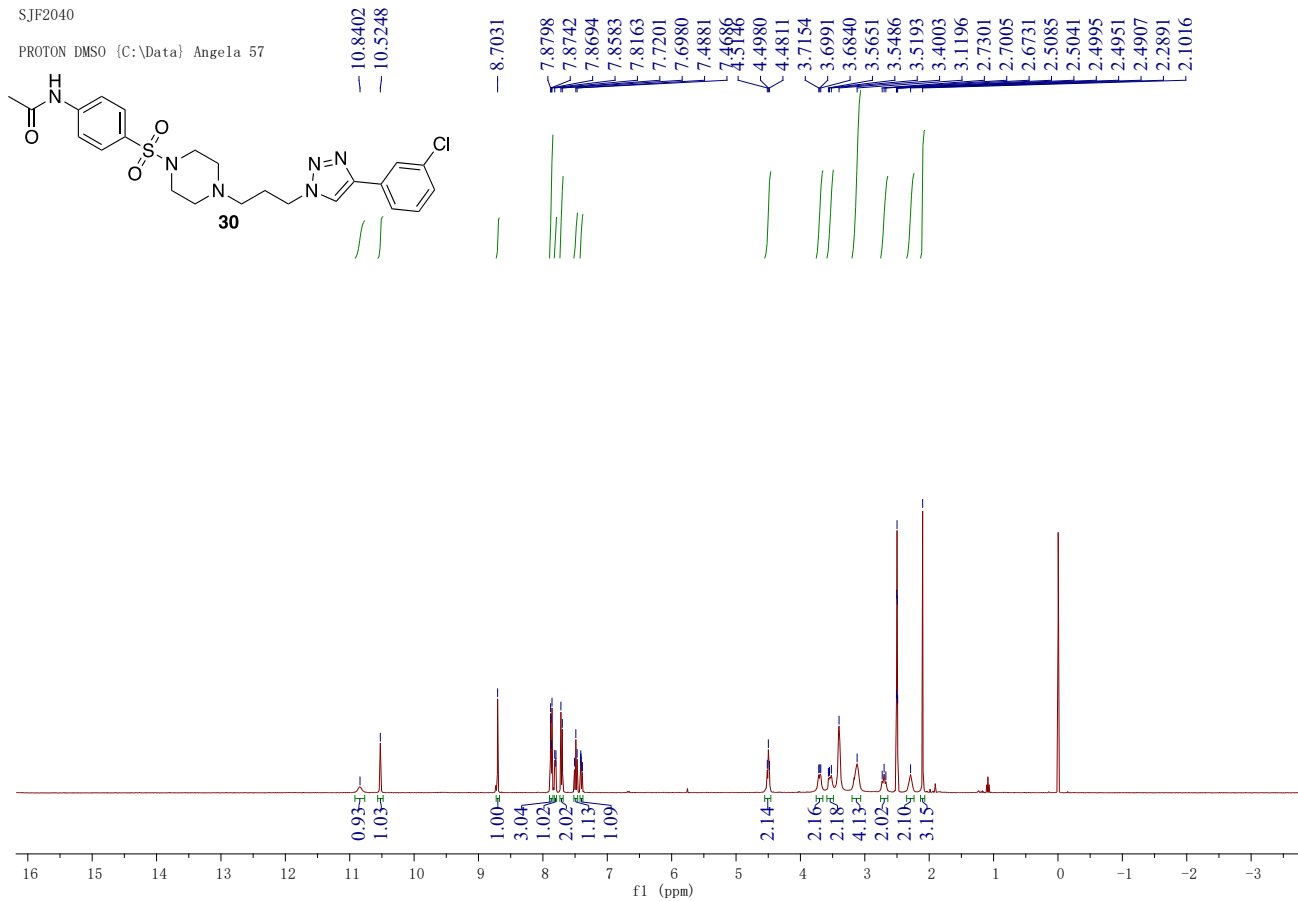
F19CPD DMSO {C:\Data} Cec 14



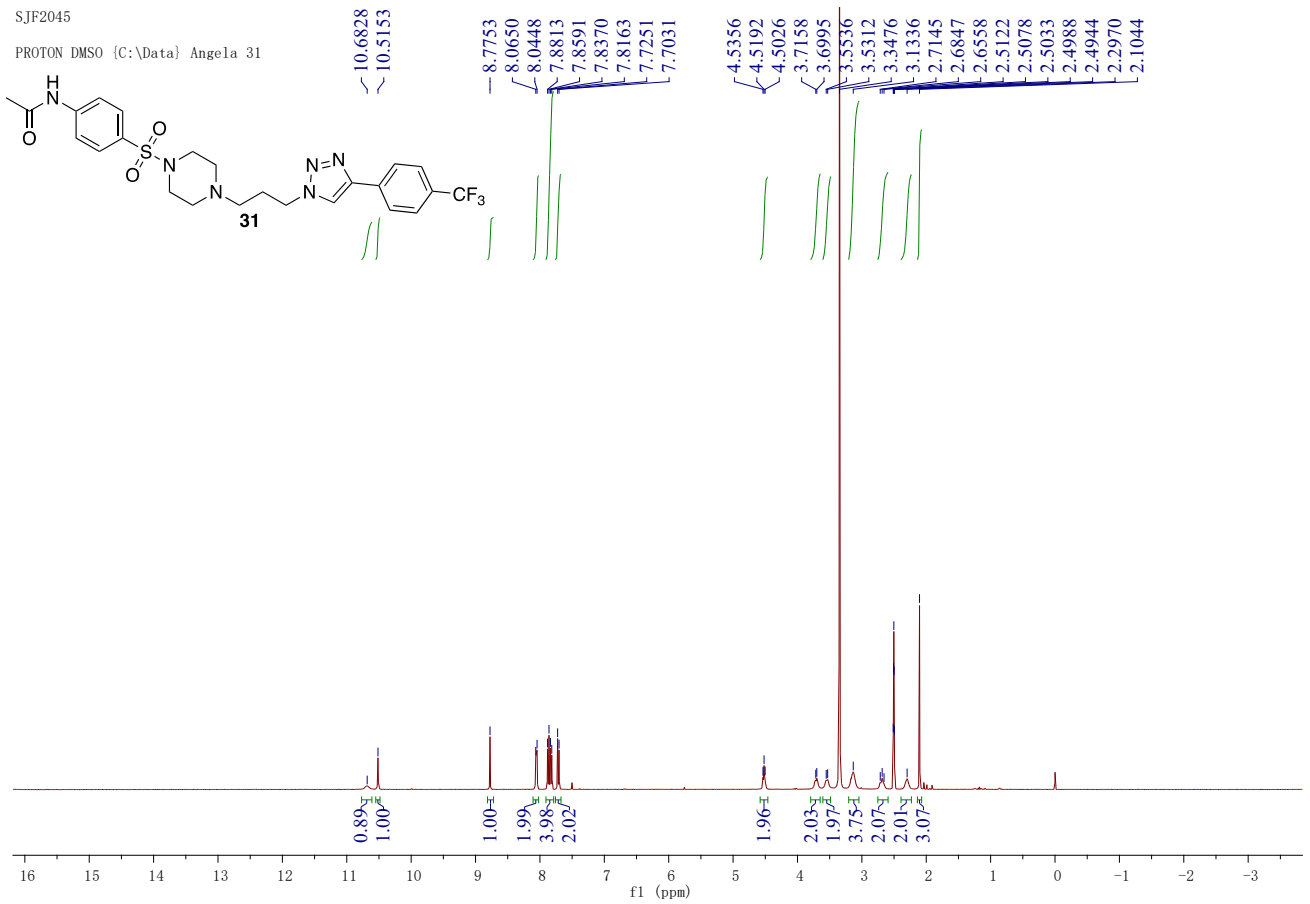
N-[4-(4-{3-[4-(4-Bromophenyl)-[1,2,3]triazol-1-yl]-propyl}-piperazine-1-sulfonyl)-phenyl]-acetamide hydrochloride (**29**)



N-[4-(4-{3-[4-(3-Chloro-phenyl)-[1,2,3]triazol-1-yl]-propyl}-piperazine-1-sulfonyl)-phenyl]-acetamide hydrochloride (30)

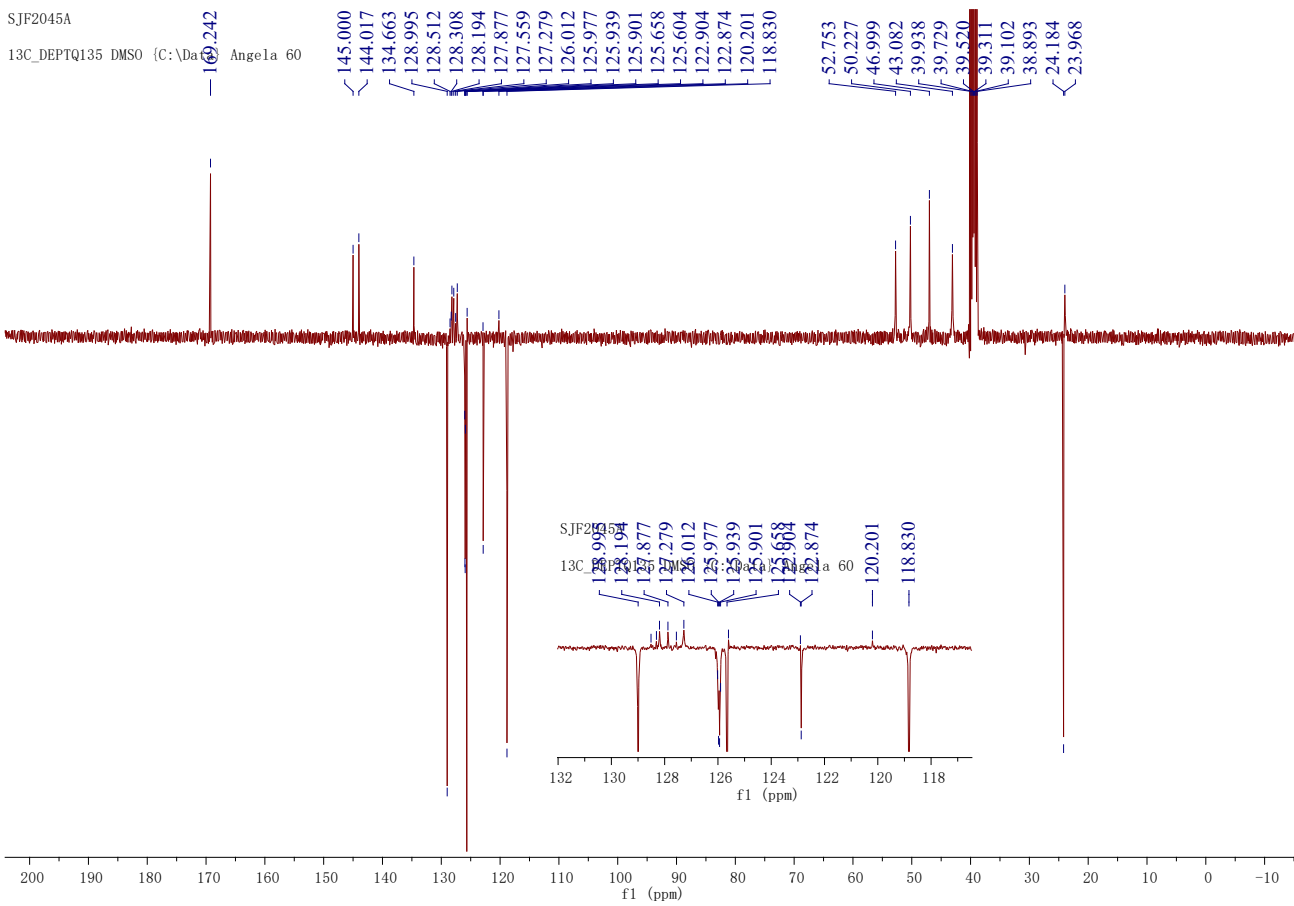


***N*-[4-(4-{3-[4-(4-Trifluoromethylphenyl)-[1,2,3]triazol-1-yl]-propyl}-piperazine-1-sulfonyl)-phenyl]-acetamide hydrochloride (**31**)**



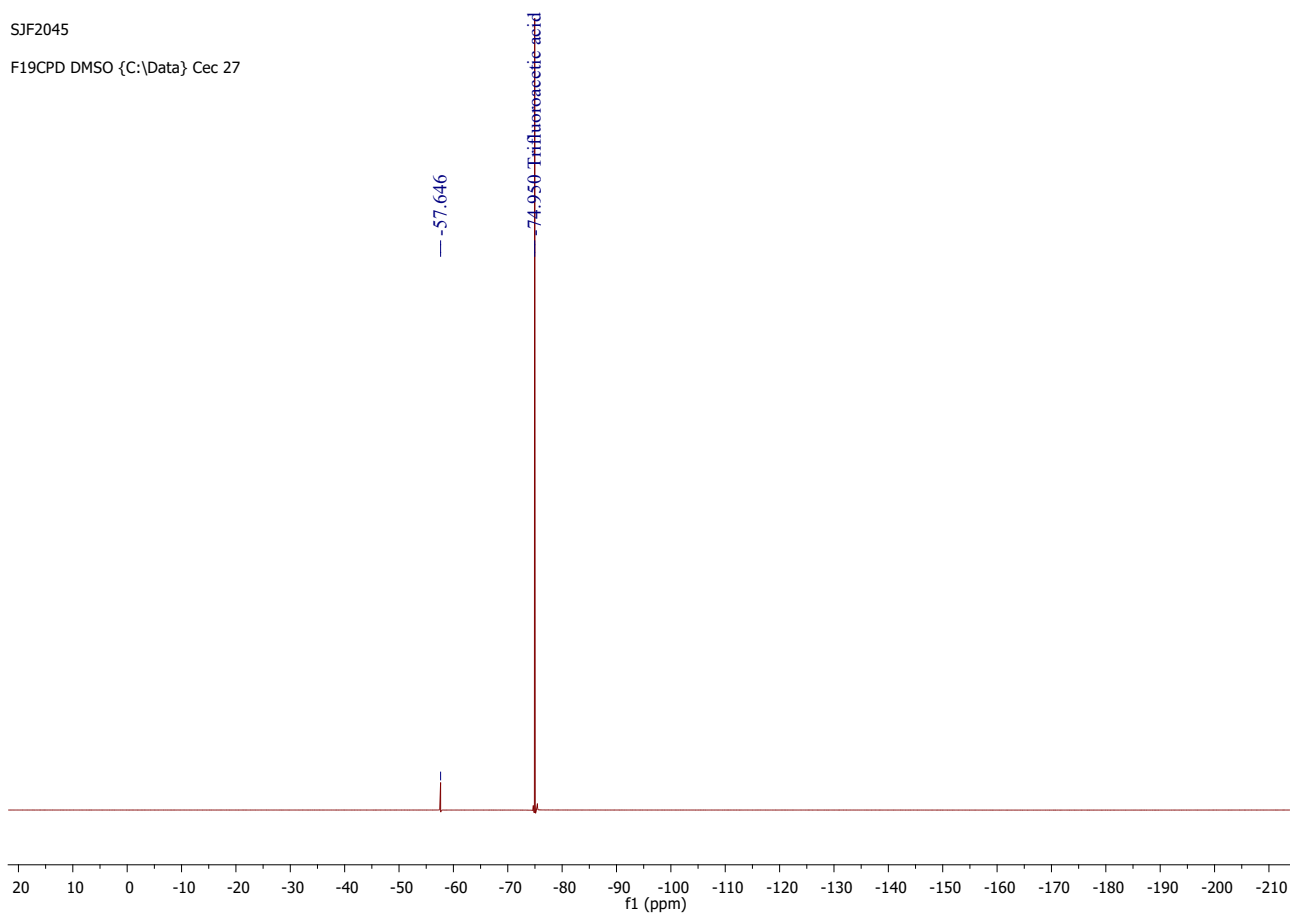
SJF2045A

13C_DEPTQ135 DMSO {C:\Da Angela 60

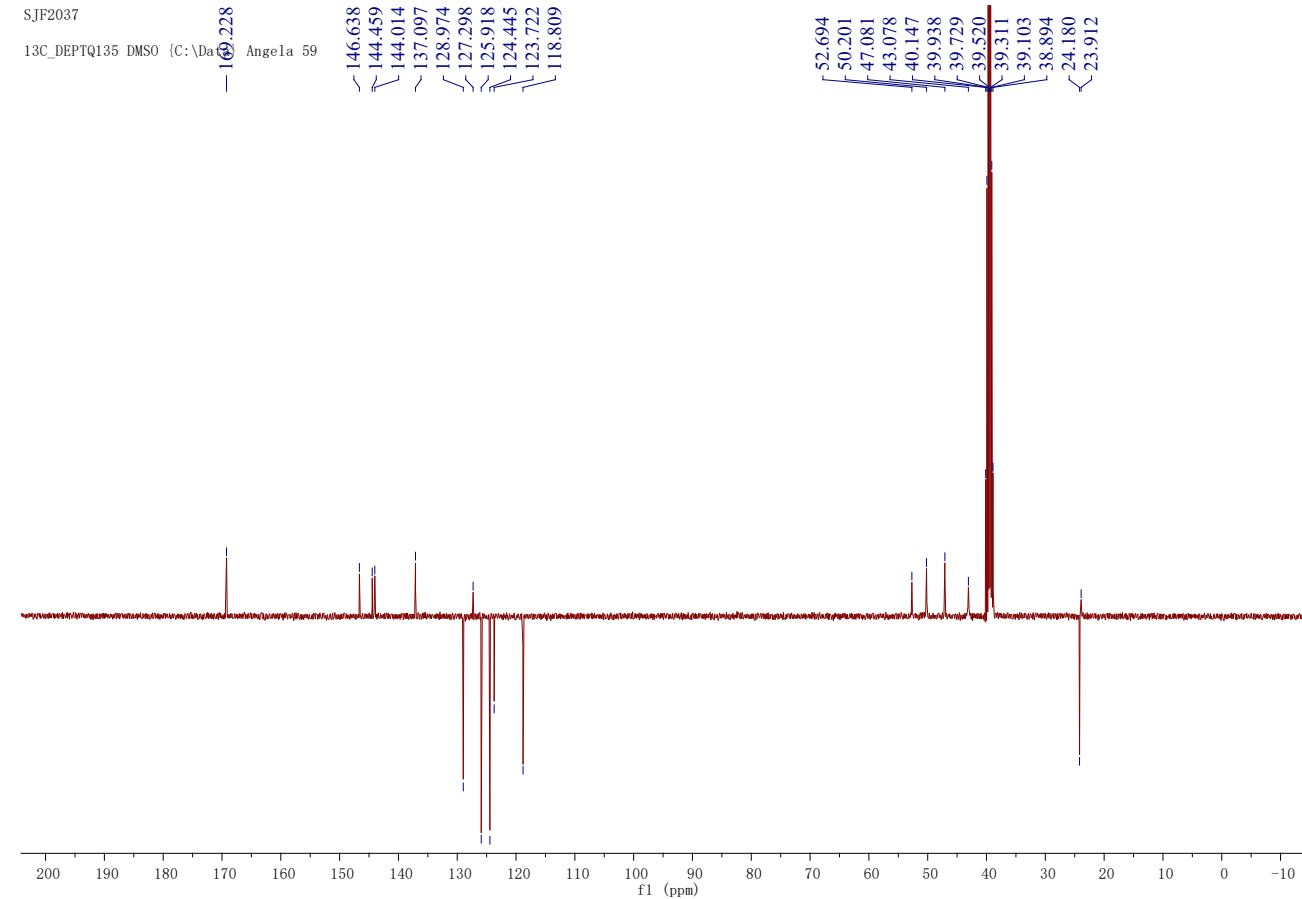
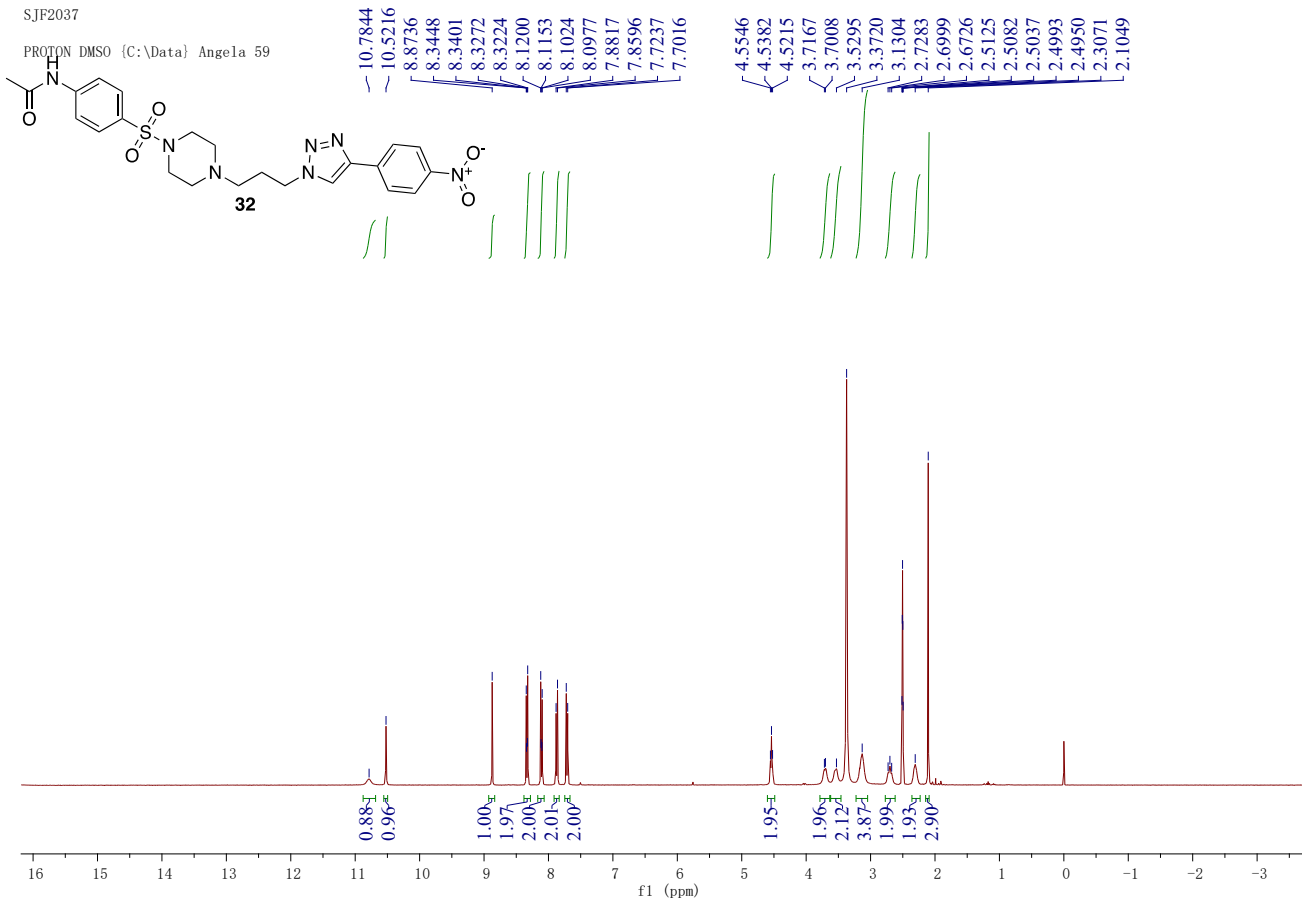


SJF2045

F19CPD DMSO {C:\Data} Cec 27



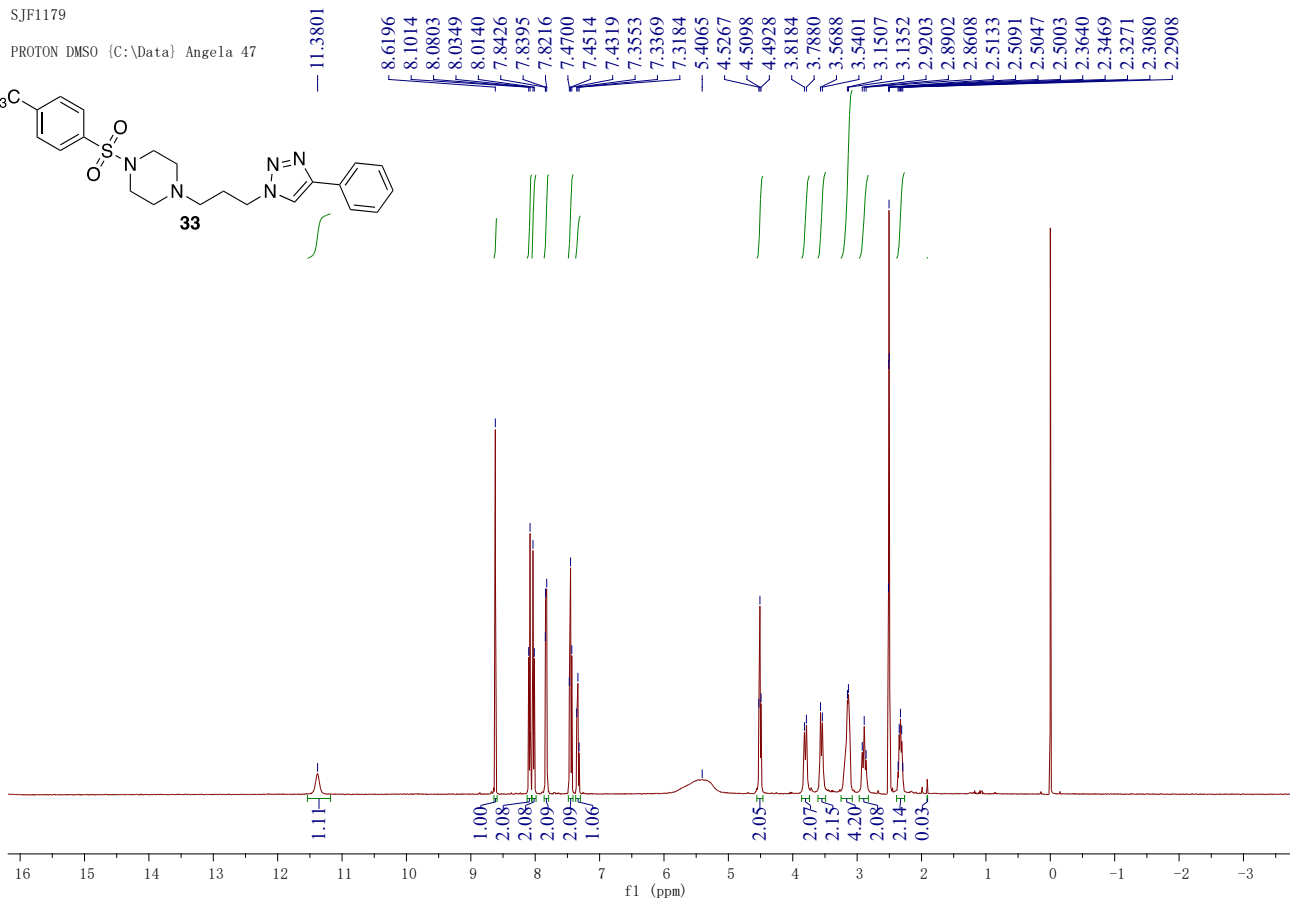
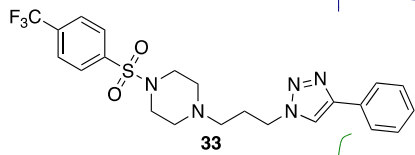
N-[4-(4-{3-[4-(4-Nitrophenyl)-[1,2,3]triazol-1-yl]-propyl]-piperazine-1-sulfonyl)-phenyl]-acetamide hydrochloride (32)



1-(3-(4-Phenyl-1H-1,2,3-triazol-1-yl)propyl)-4-((4-(trifluoromethyl)phenyl)-sulfonyl)piperazine hydrochloride (33)

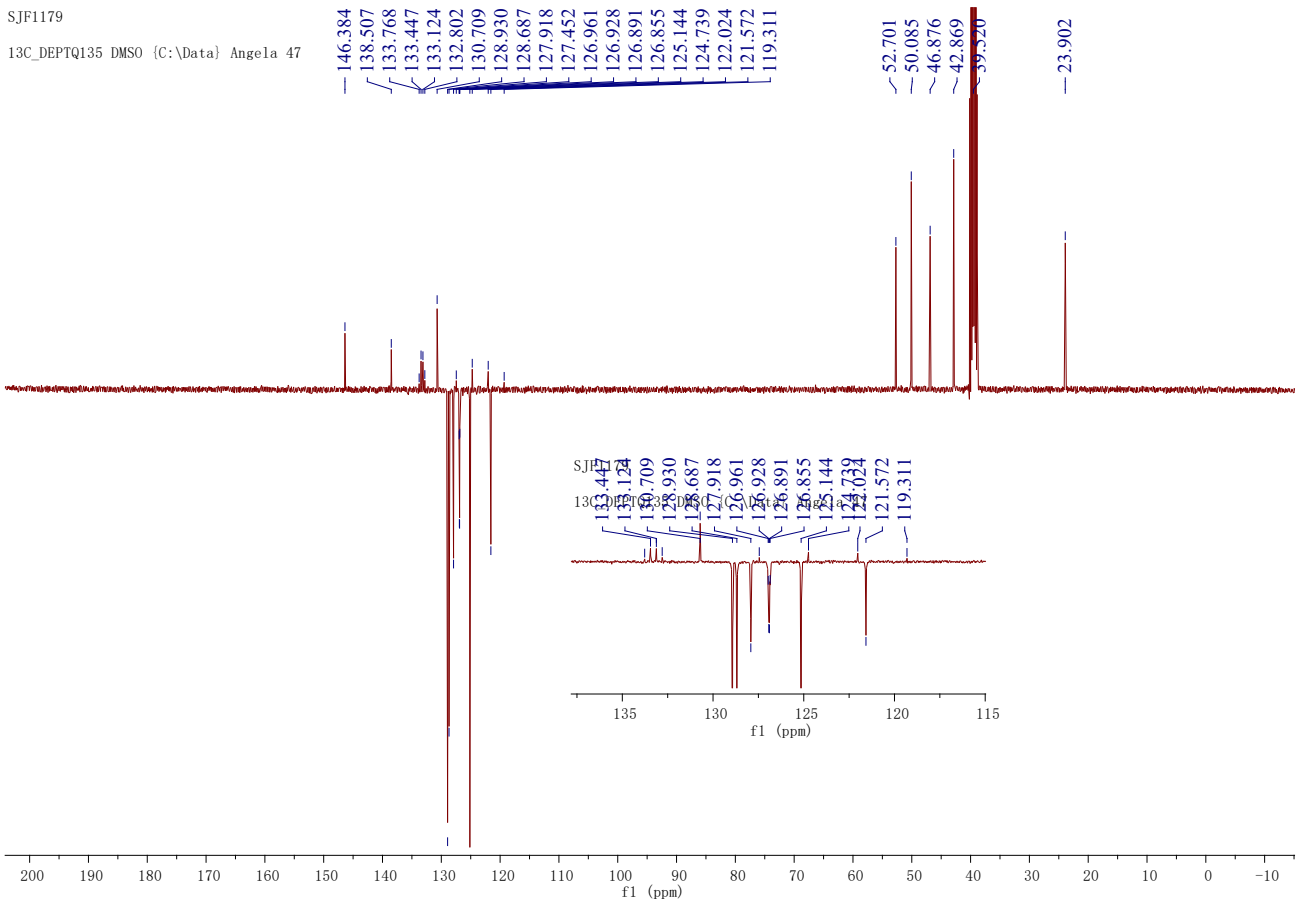
SJF1179

PROTON DMSO (C:\Data) Angela 47



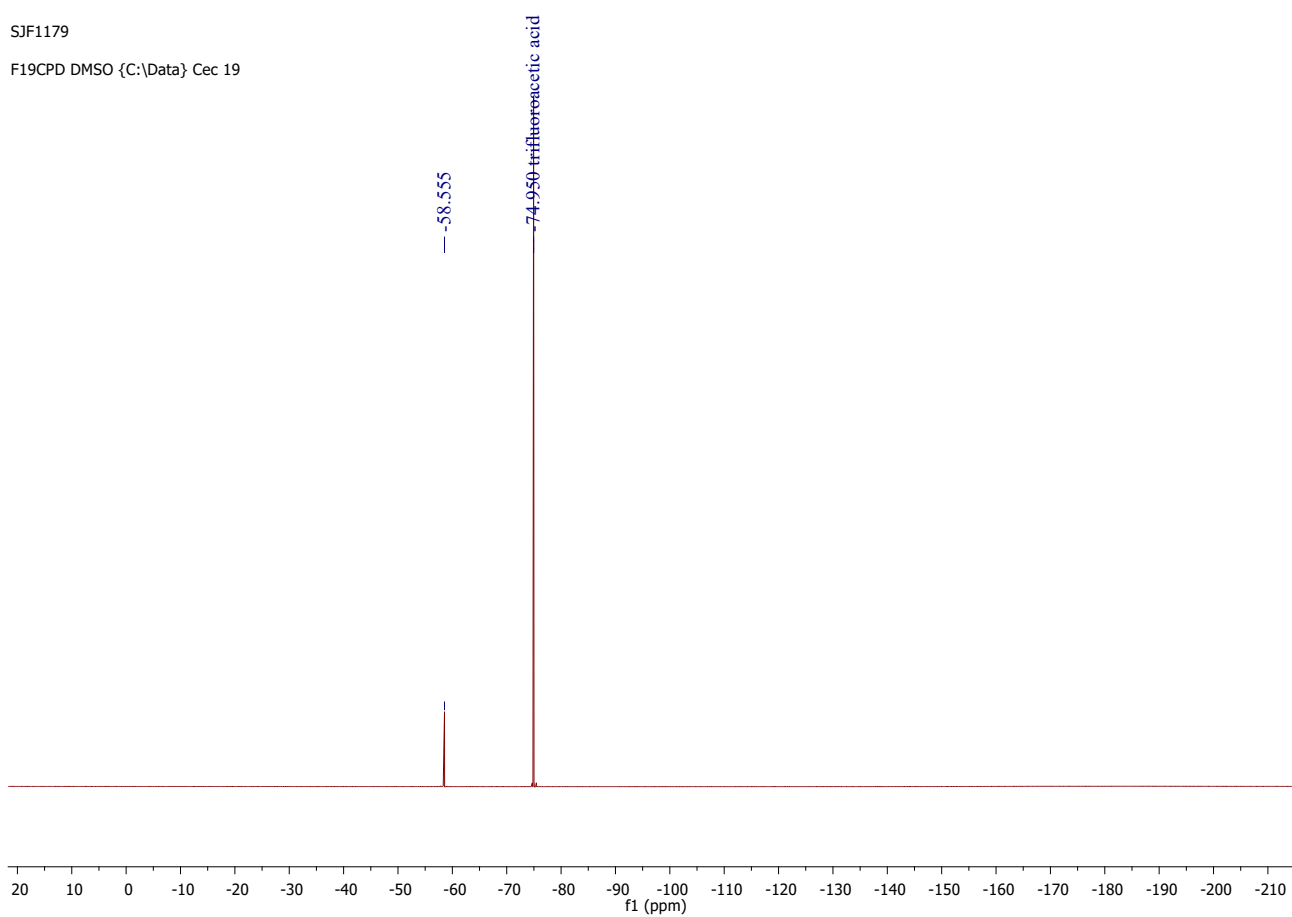
SJF1179

13C_DEPTQ135 DMSO {C:\Data} Angela 47

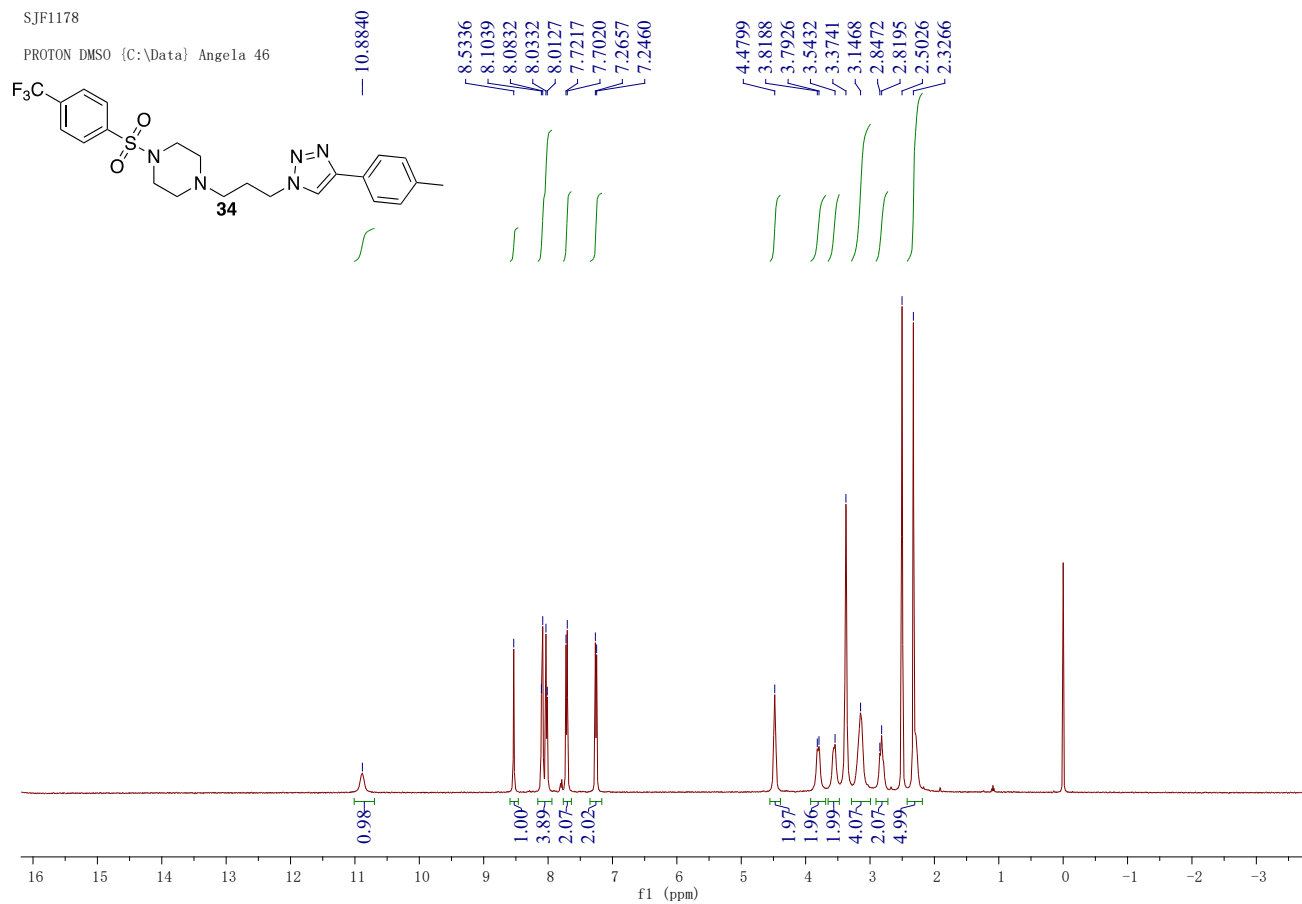


SJF1179

F19CPD DMSO {C:\Data} Cec 19

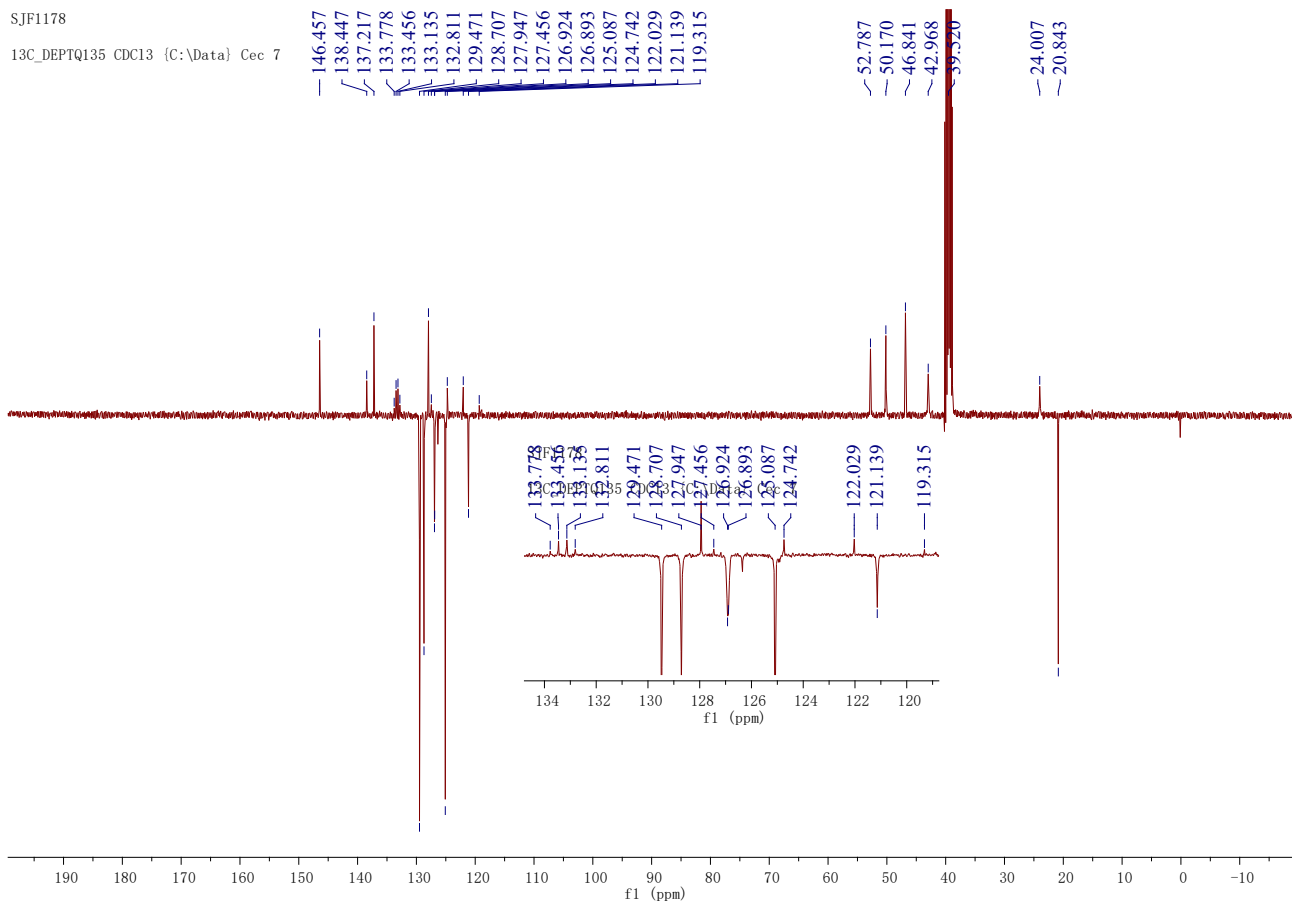


1-(3-(4-(p-Tolyl)-1H-1,2,3-triazol-1-yl)propyl)-4-((4-(trifluoromethyl)phenyl)sulfonyl)piperazine hydrochloride (34)



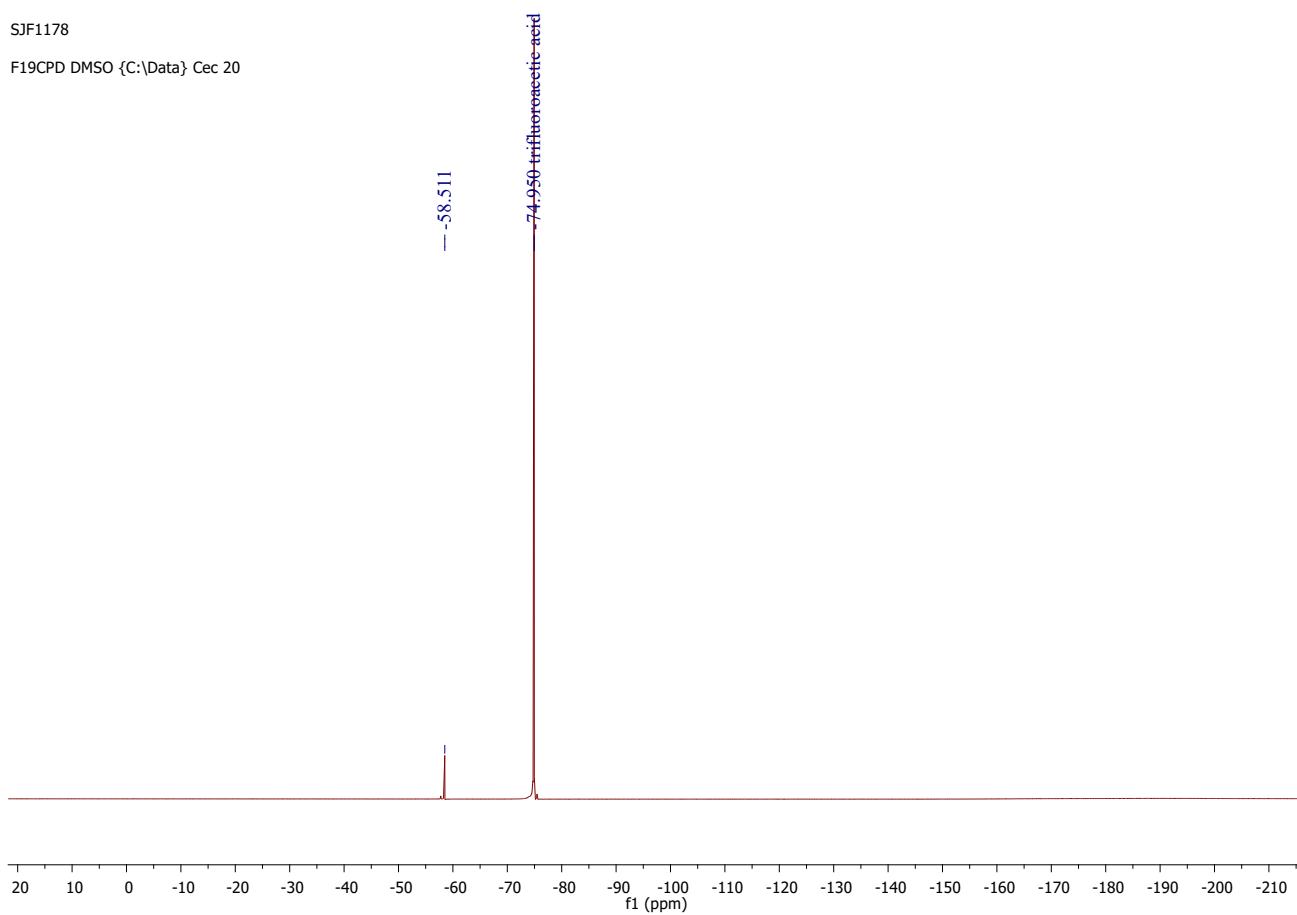
SJF1178

13C_DEPTQ135 CDC13 (C:\Data) Cec 7



SJF1178

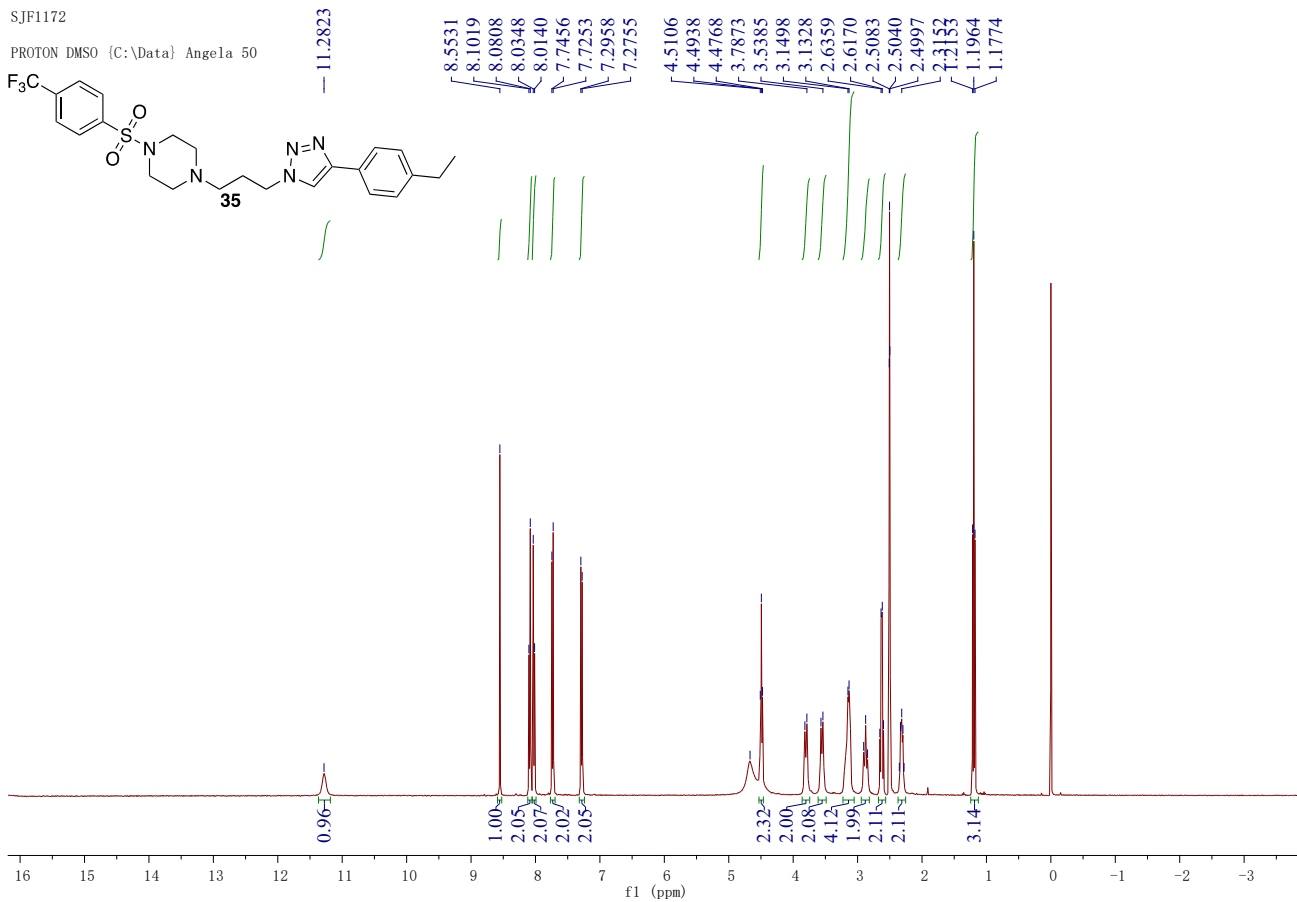
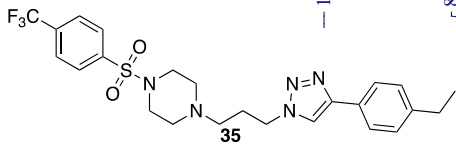
F19CPD DMSO {C:\Data} Cec 20



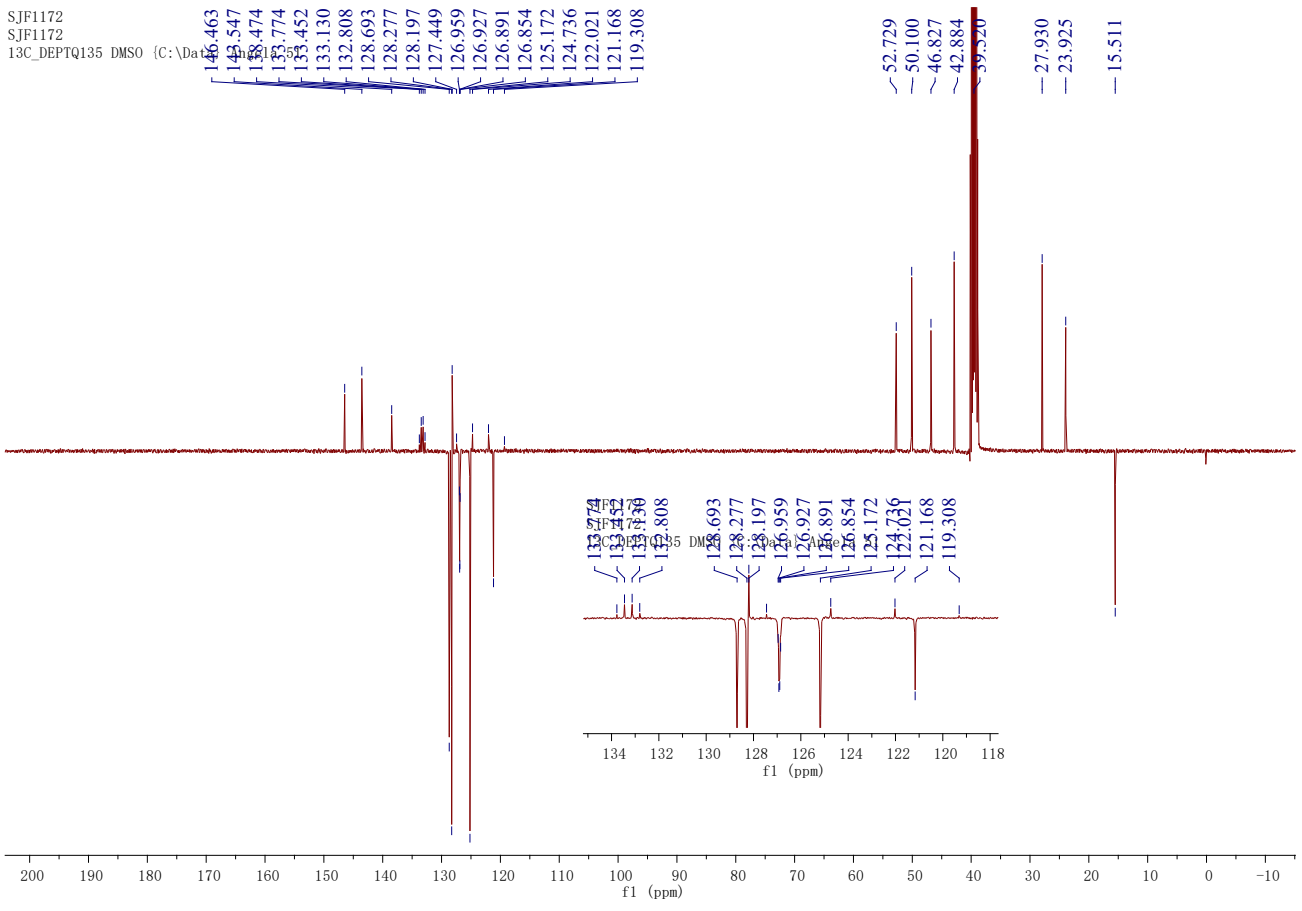
1-(3-(4-(4-Ethylphenyl)-1H-1,2,3-triazol-1-yl)propyl)-4-(4-(trifluoromethyl)phenyl)-sulfonylpiperazine hydrochloride
(35)

SJF1172

PROTON DMSO (C:\Data) Angela 50

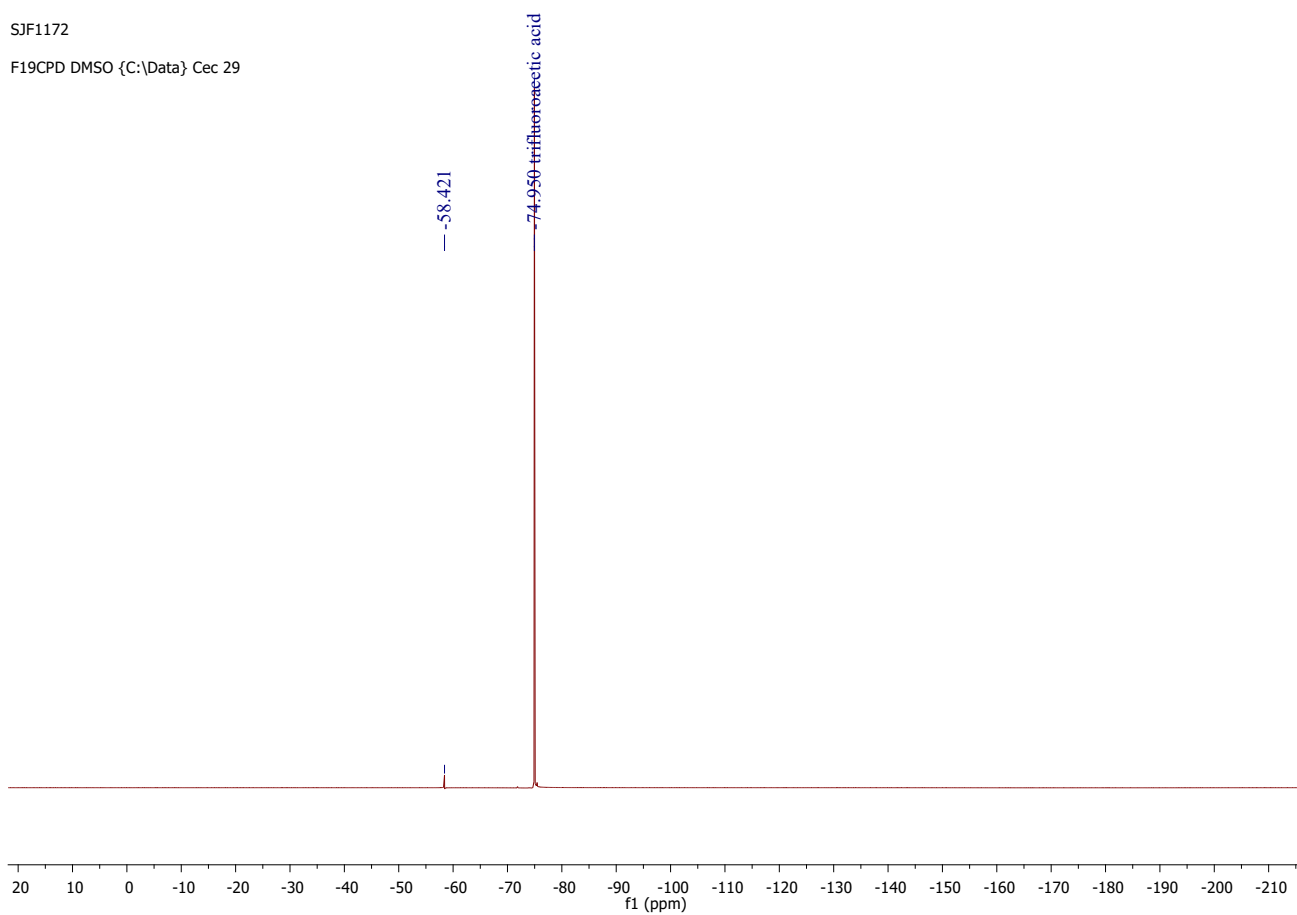


SJF1172
SJF1172
13C_DEPTQ135 DMSO {C:\Dat

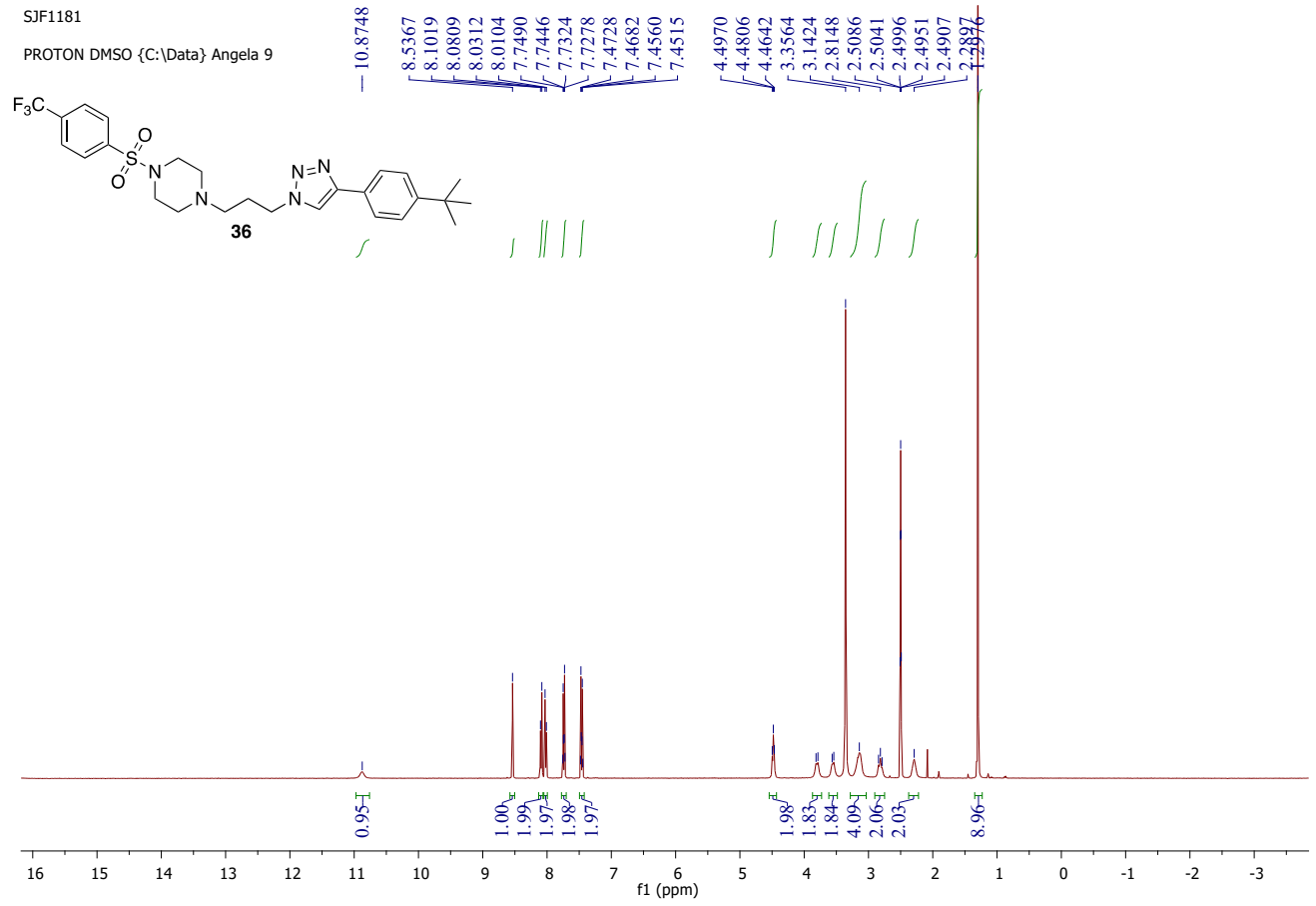


SJF1172

F19CPD DMSO {C:\Data} Cec 29

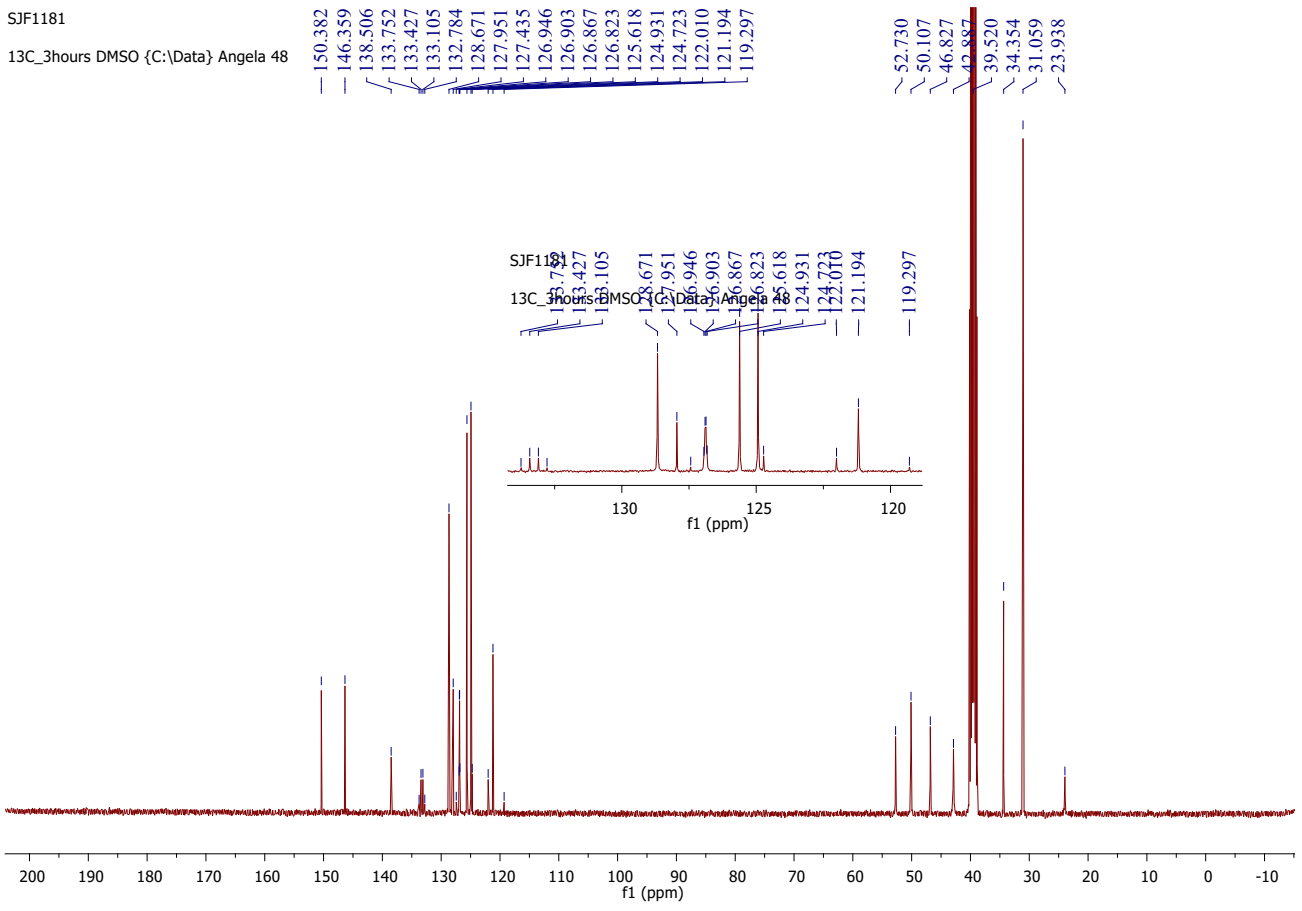


1-(3-(4-(4-(Tert-butyl)phenyl)-1H-1,2,3-triazol-1-yl)propyl)-4-((4-(trifluoromethyl)phenyl)sulfonyl) piperazine hydrochloride (36)



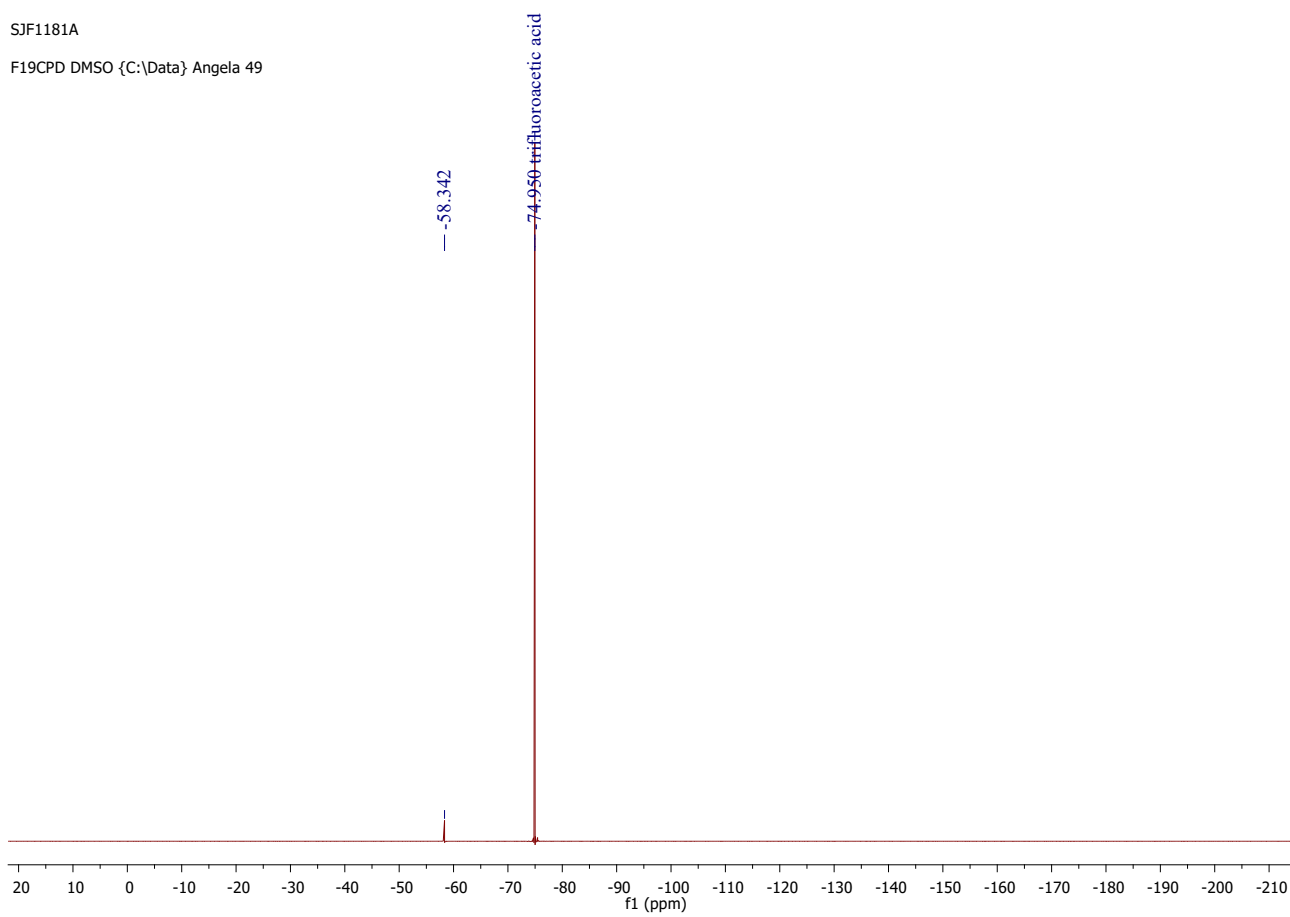
SJF1181

13C_3hours DMSO (C:\Data) Angela 48

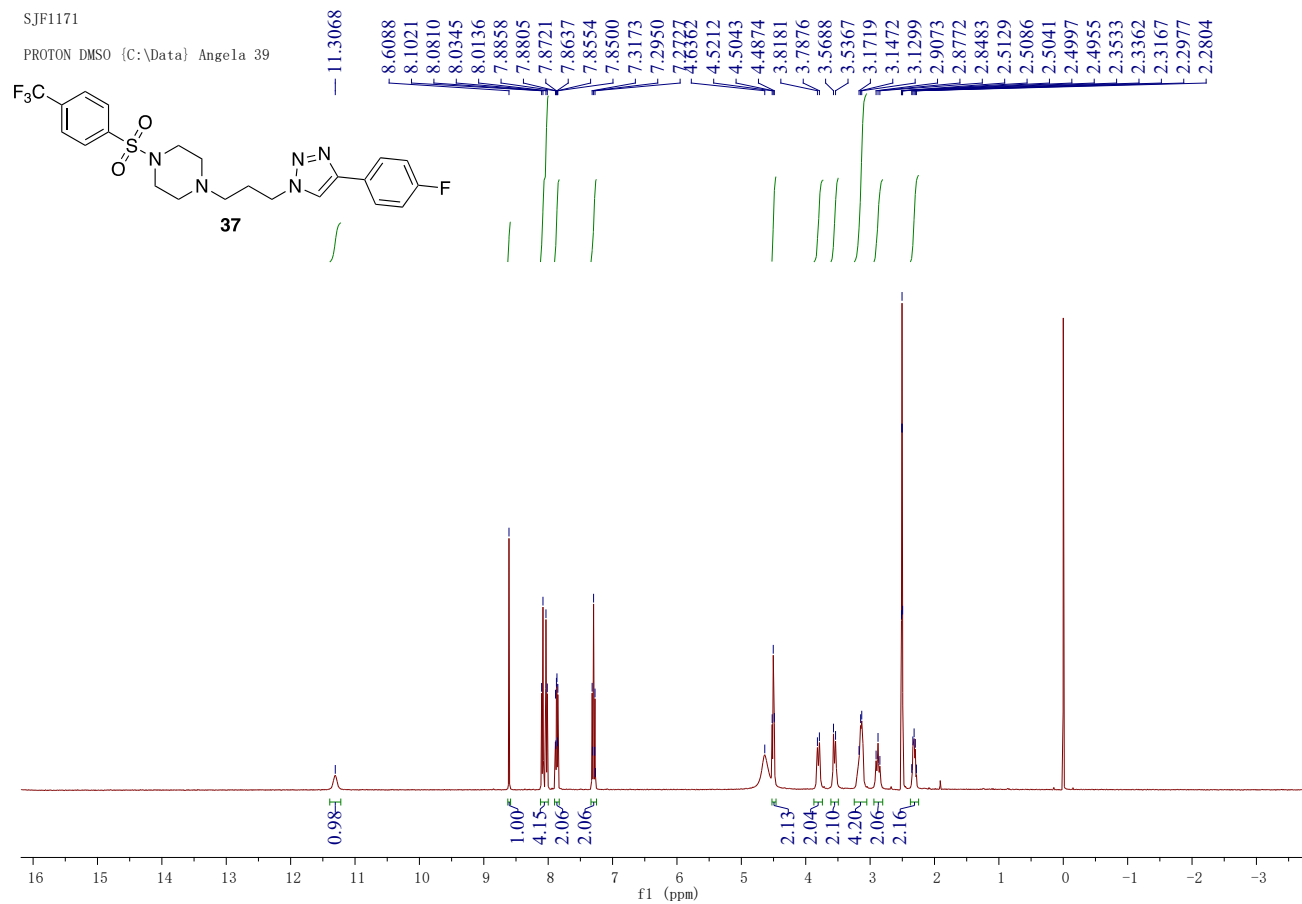


SJF1181A

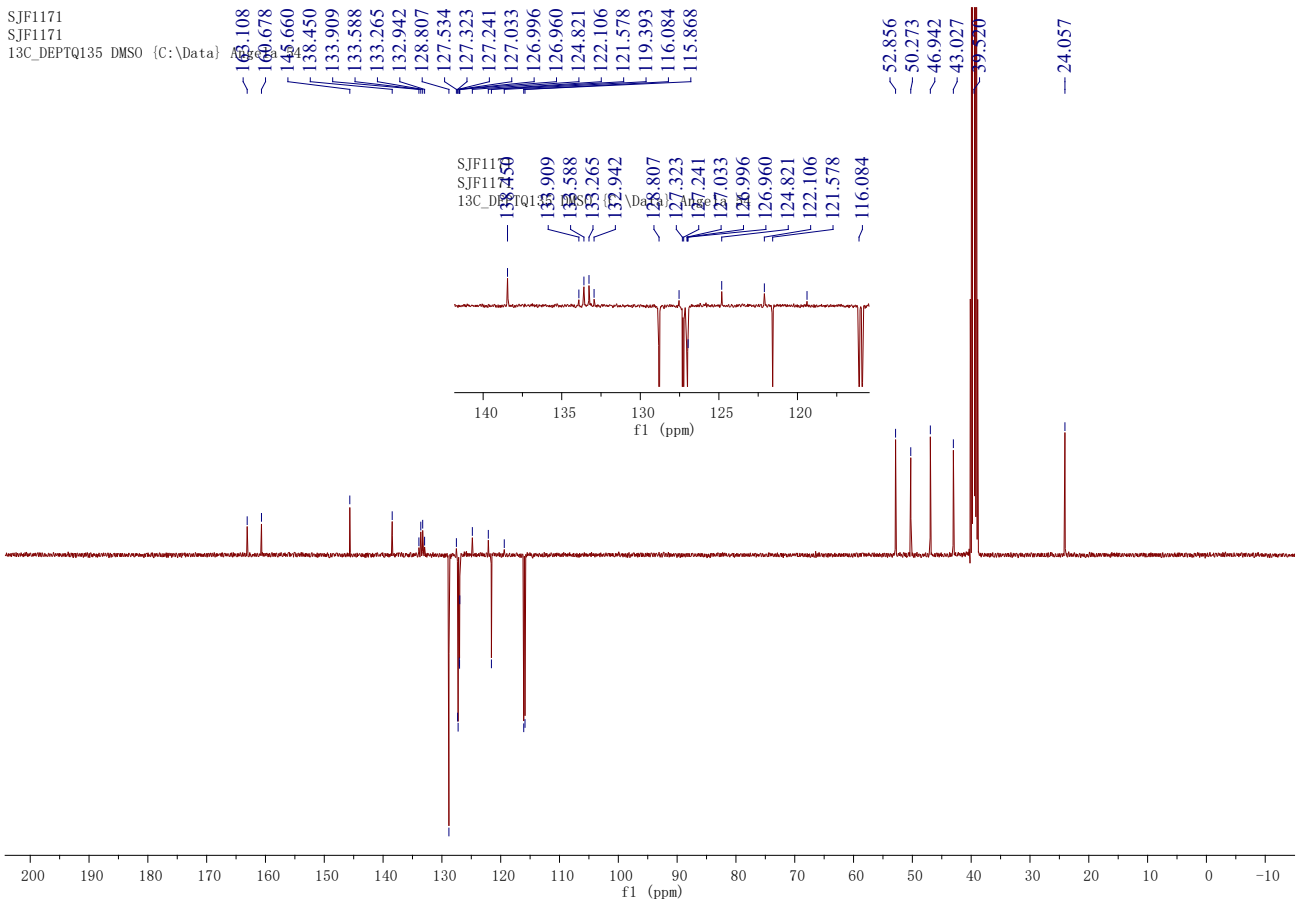
F19CPD DMSO {C:\Data} Angela 49



1-(3-(4-(4-Fluorophenyl)-1H-1,2,3-triazol-1-yl)propyl)-4-((4-(trifluoromethyl)-phenyl)sulfonyl)piperazine hydrochloride
(37)

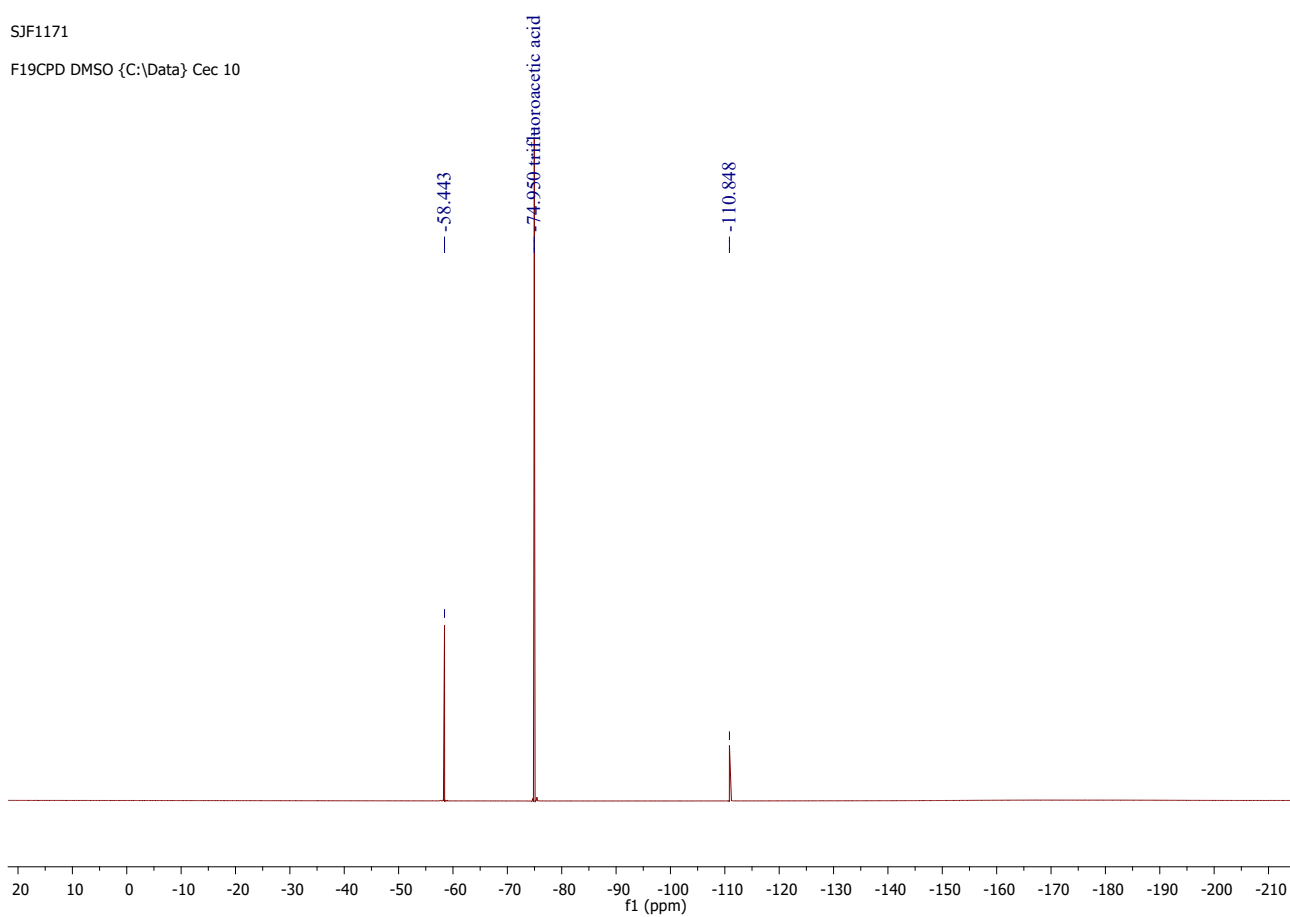


SJF1171
13C_DEPTQ135 DMSO {C:\Data}



SJF1171

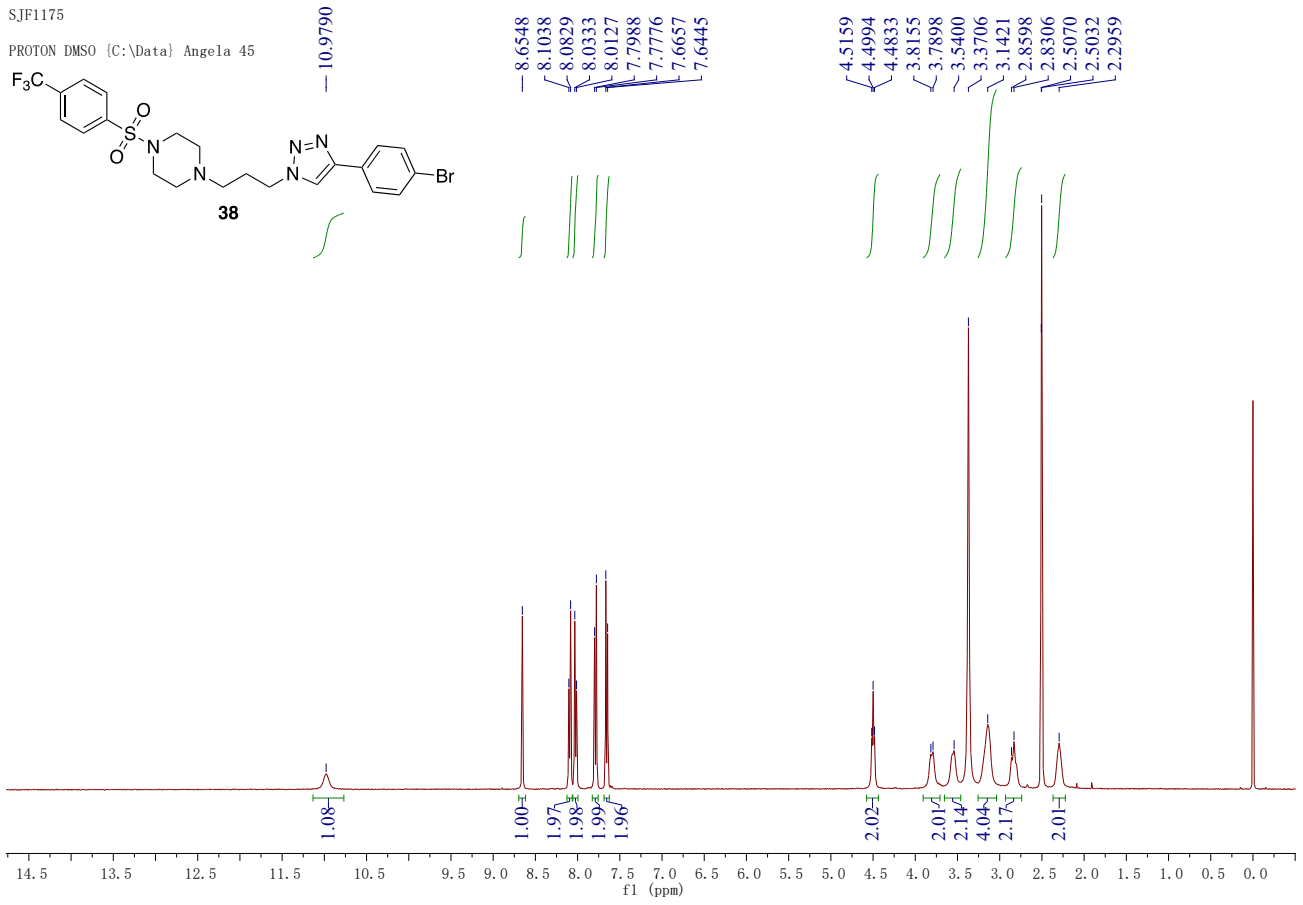
F19CPD DMSO {C:\Data} Ccc 10



1-(3-(4-(4-Bromophenyl)-1H-1,2,3-triazol-1-yl)propyl)-4-((4-(trifluoromethyl)phenyl)sulfonyl)piperazine hydrochloride
(38)

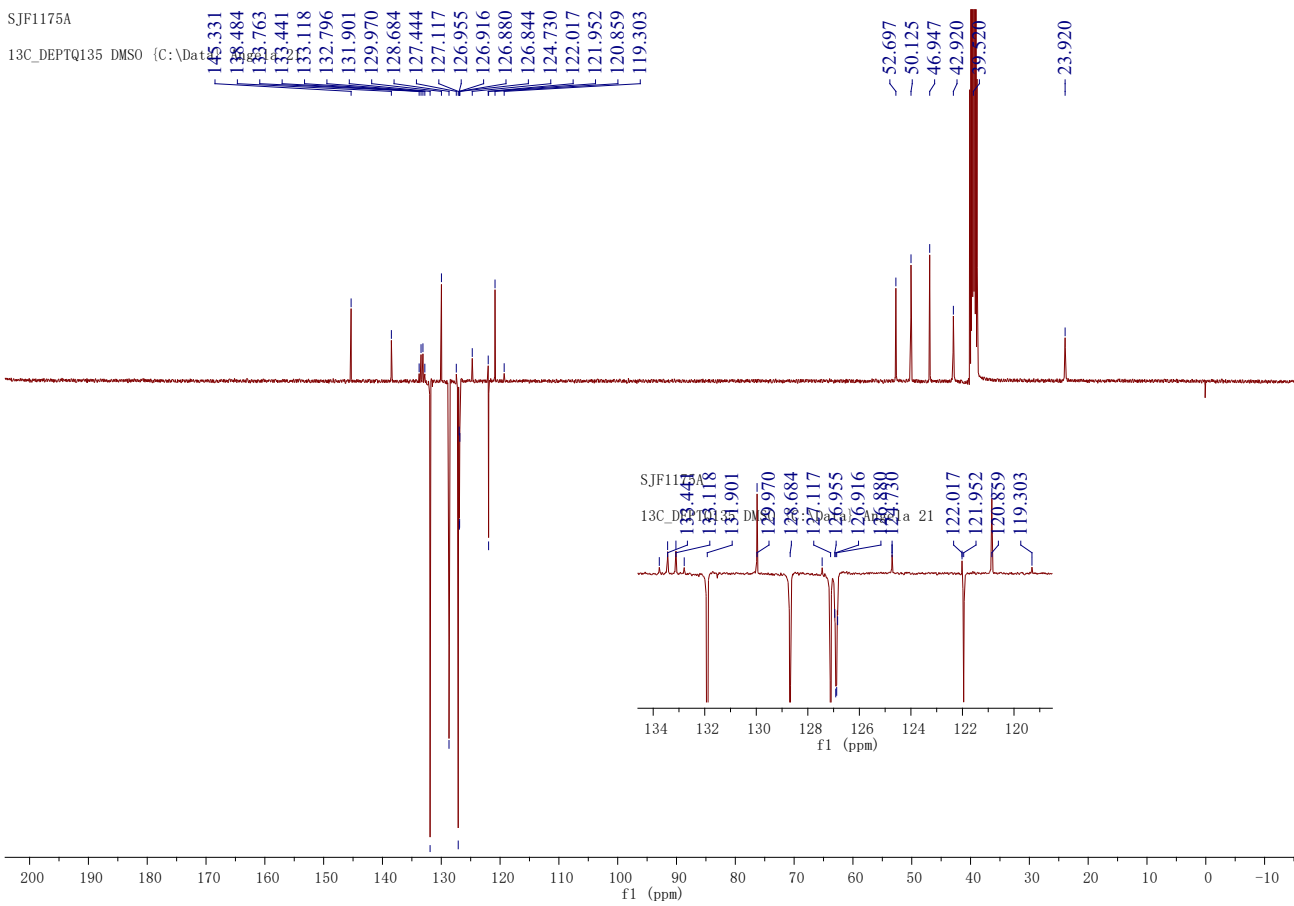
SJF1175

PROTON DMSO (C:\Data) Angela 45



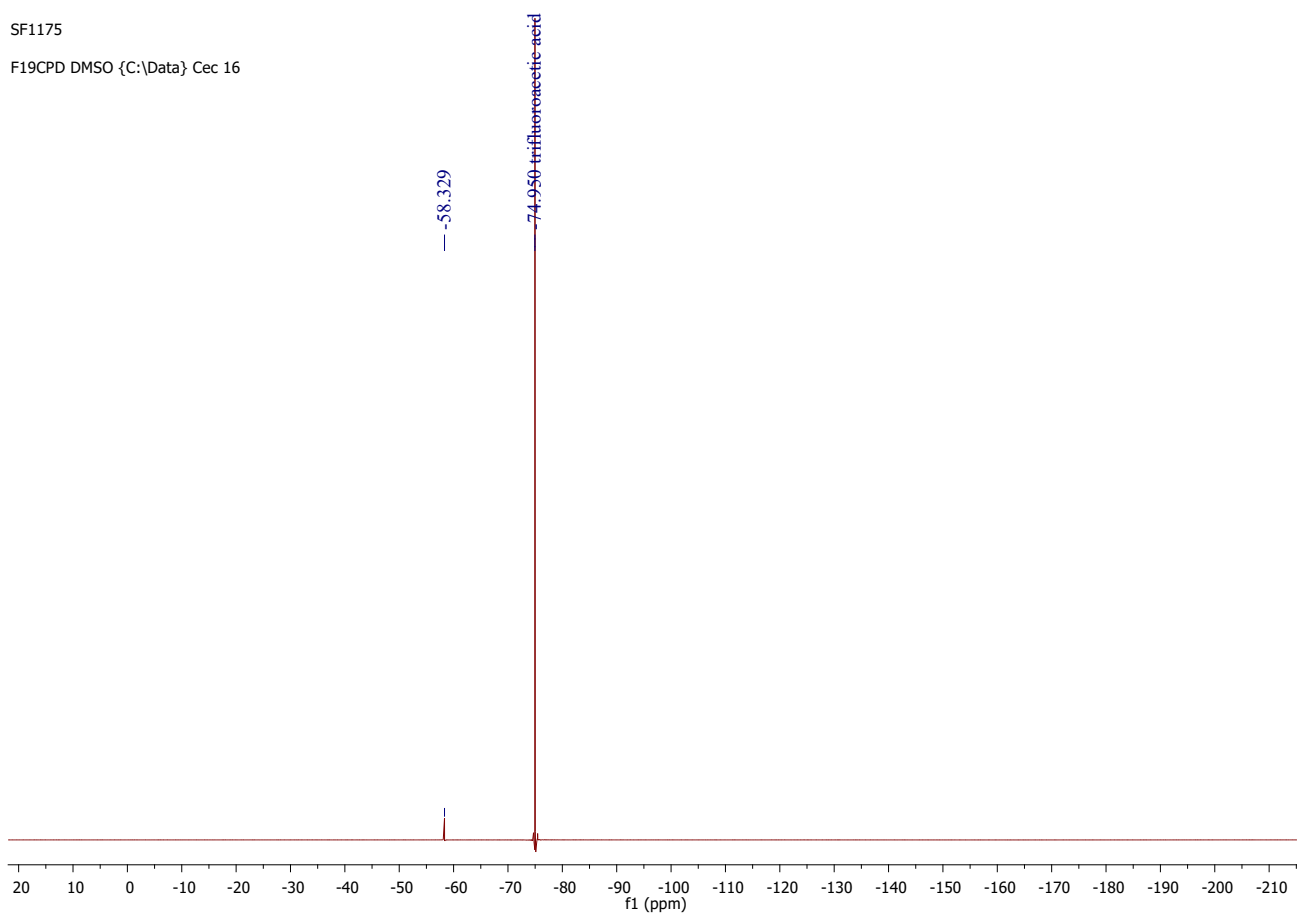
SJF1175A

13C_DEPTQ135 DMSO {C:\Dat

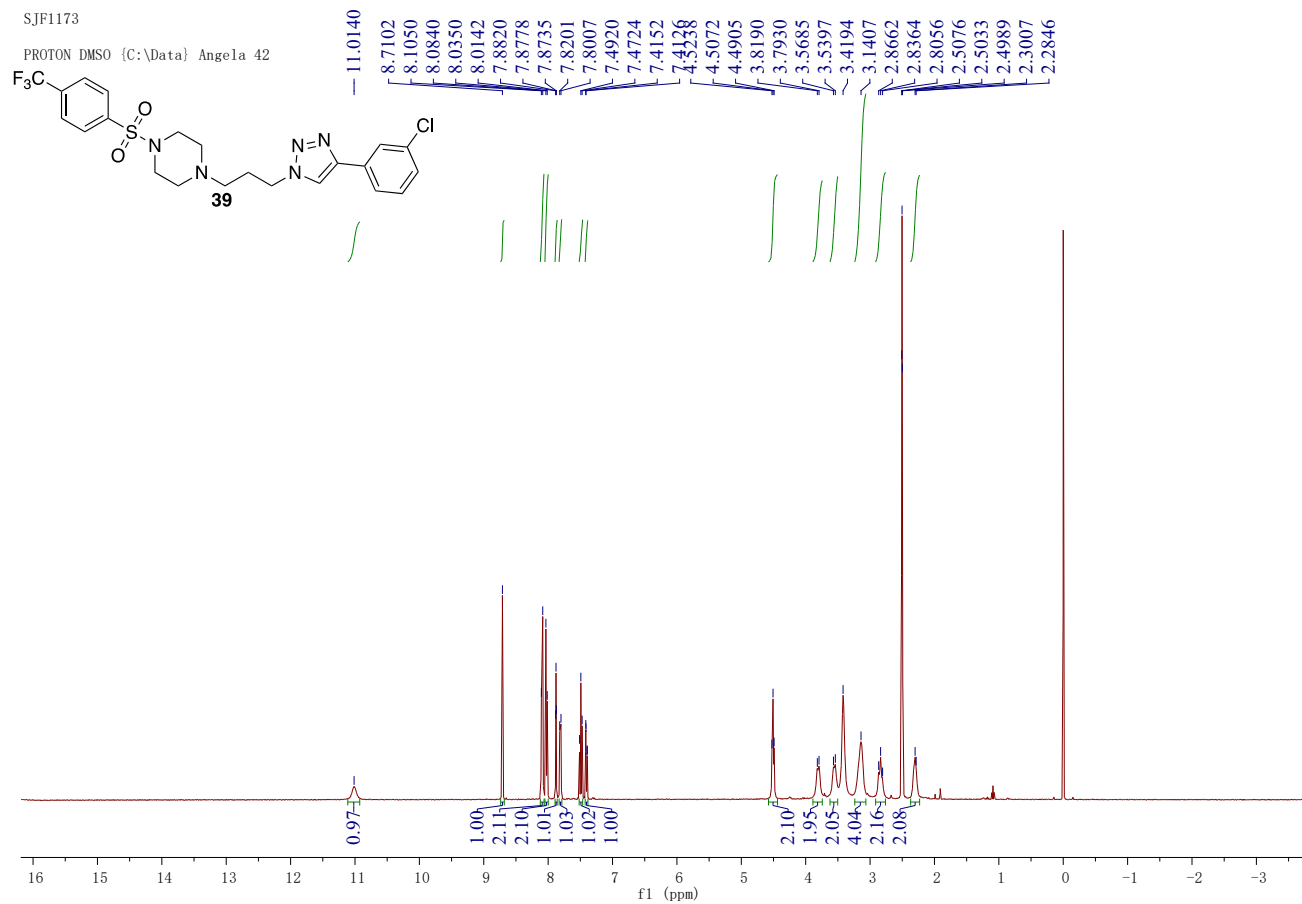


SF1175

F19CPD DMSO {C:\Data} Cec 16

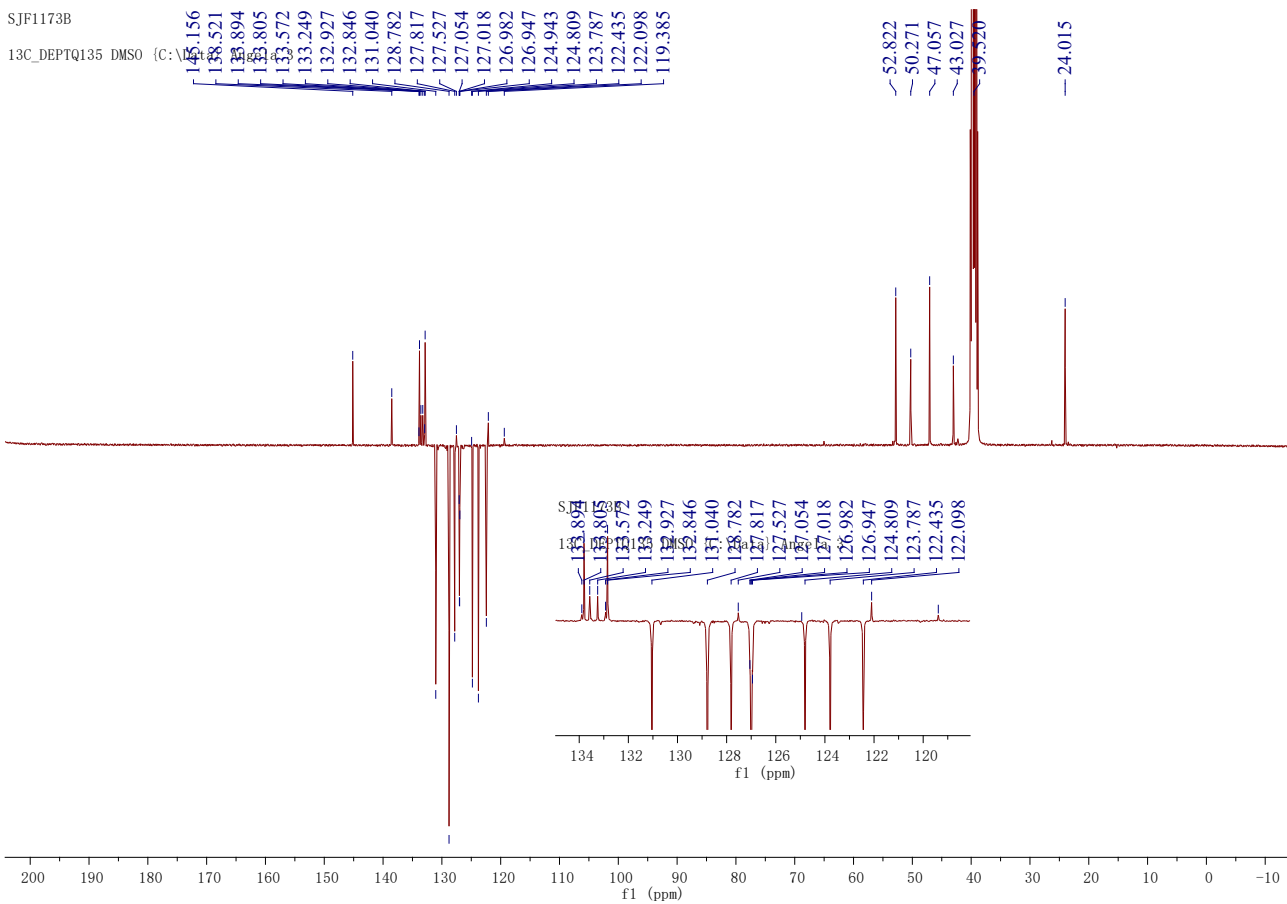


1-(3-(4-(3-Chlorophenyl)-1H-1,2,3-triazol-1-yl)propyl)-4-((4-(trifluoromethyl)-phenyl)sulfonyl)piperazine hydrochloride
(39)



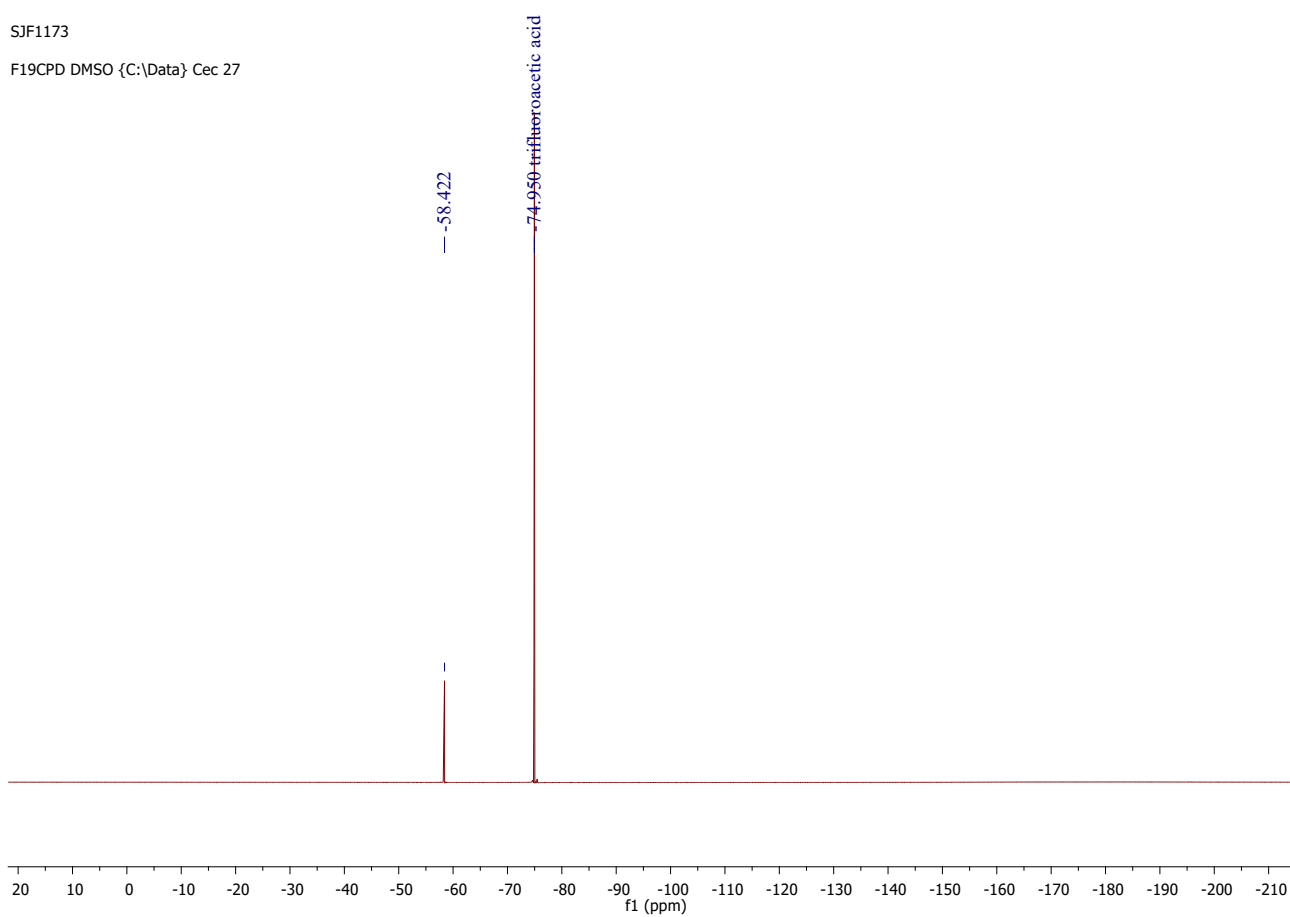
SJF1173B

13C_DEPTQ135 DMSO (C:



SJF1173

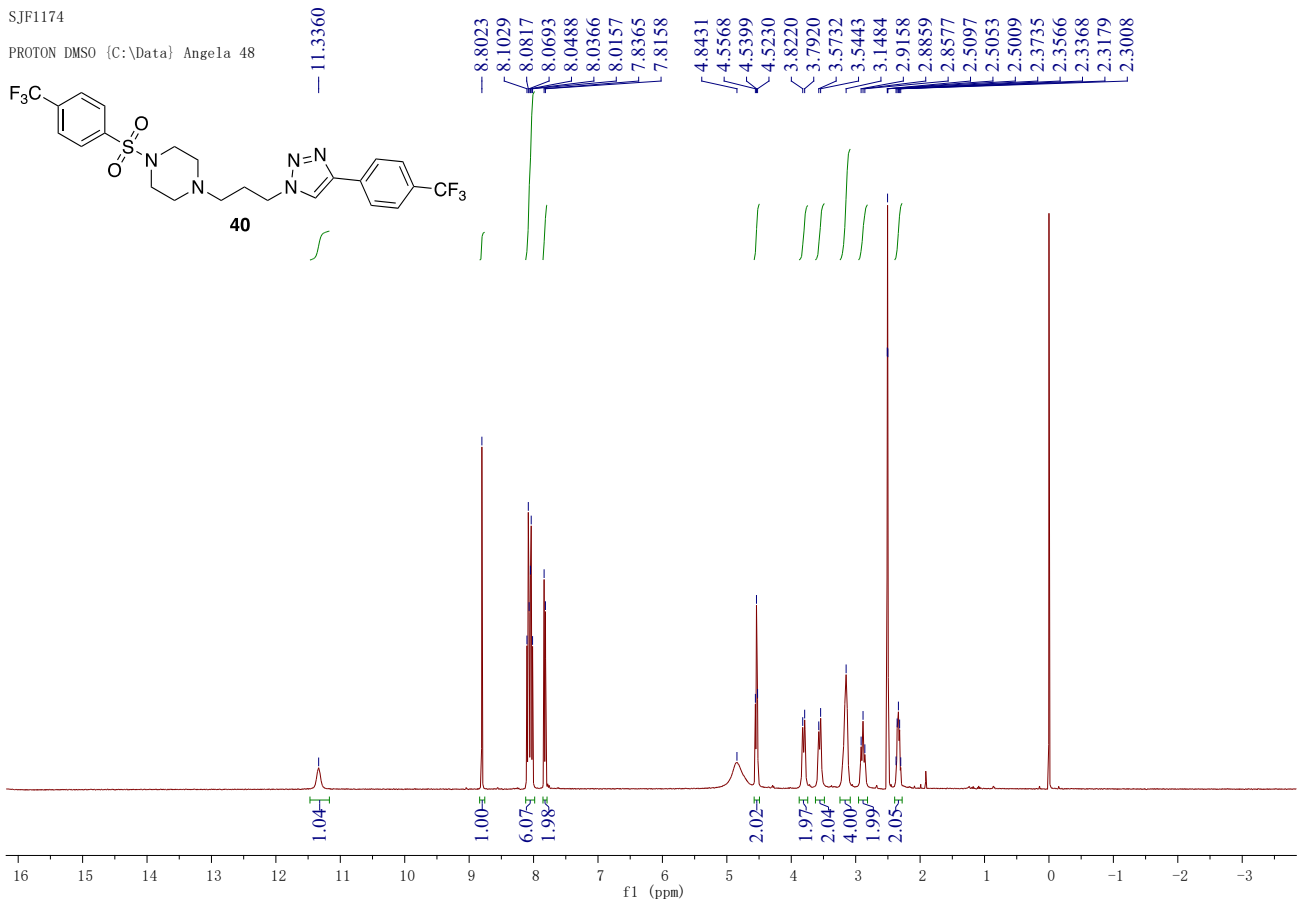
F19CPD DMSO {C:\Data} Cec 27



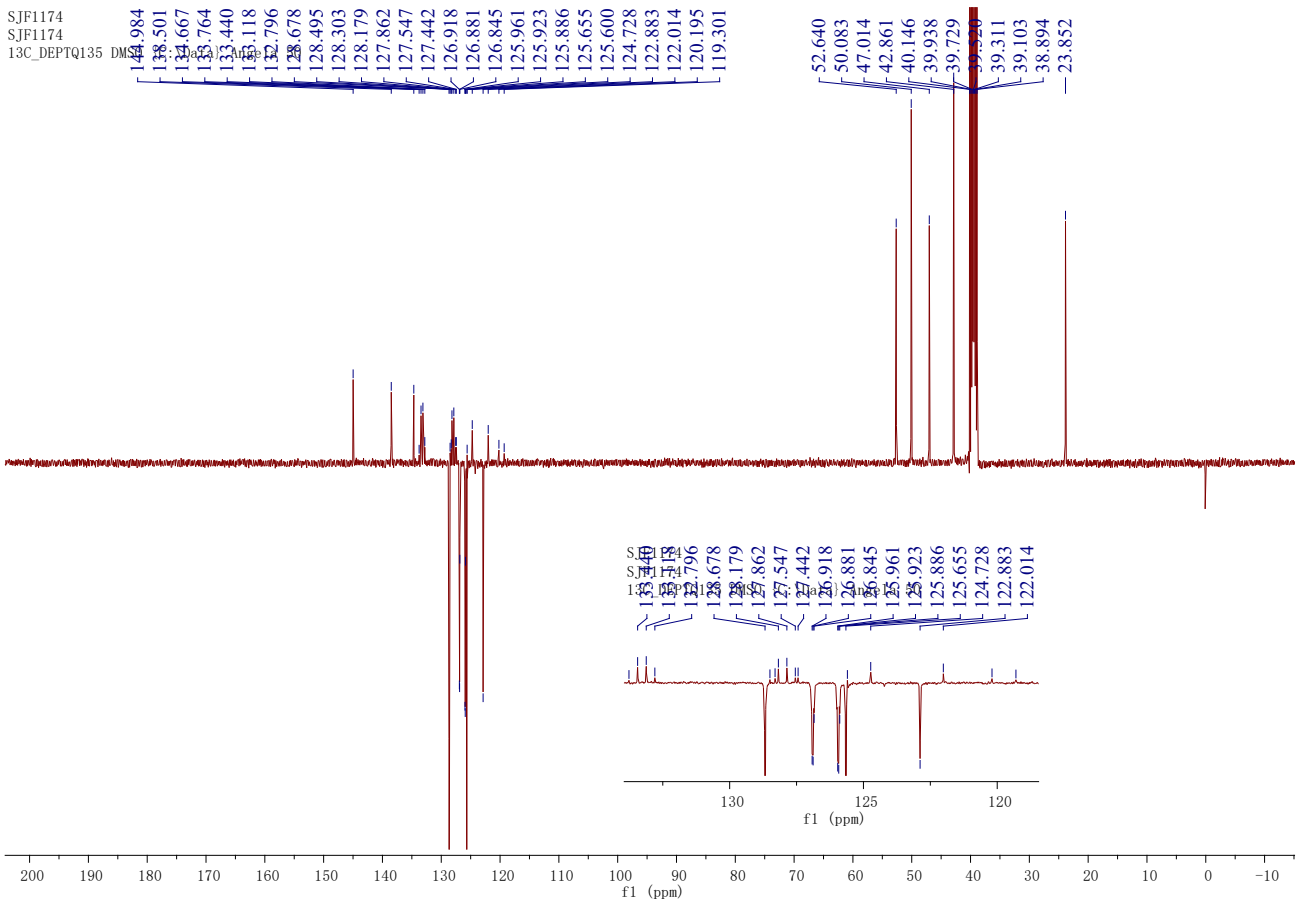
1-(4-Trifluoromethylbenzenesulfonyl)-4-{3-[4-(4-trifluoromethylphenyl)-[1,2,3]-triazol-1-yl]-propyl}-piperazine hydrochloride (**40**)

SJF1174

PROTON DMSO (C:\Data) Angela 48

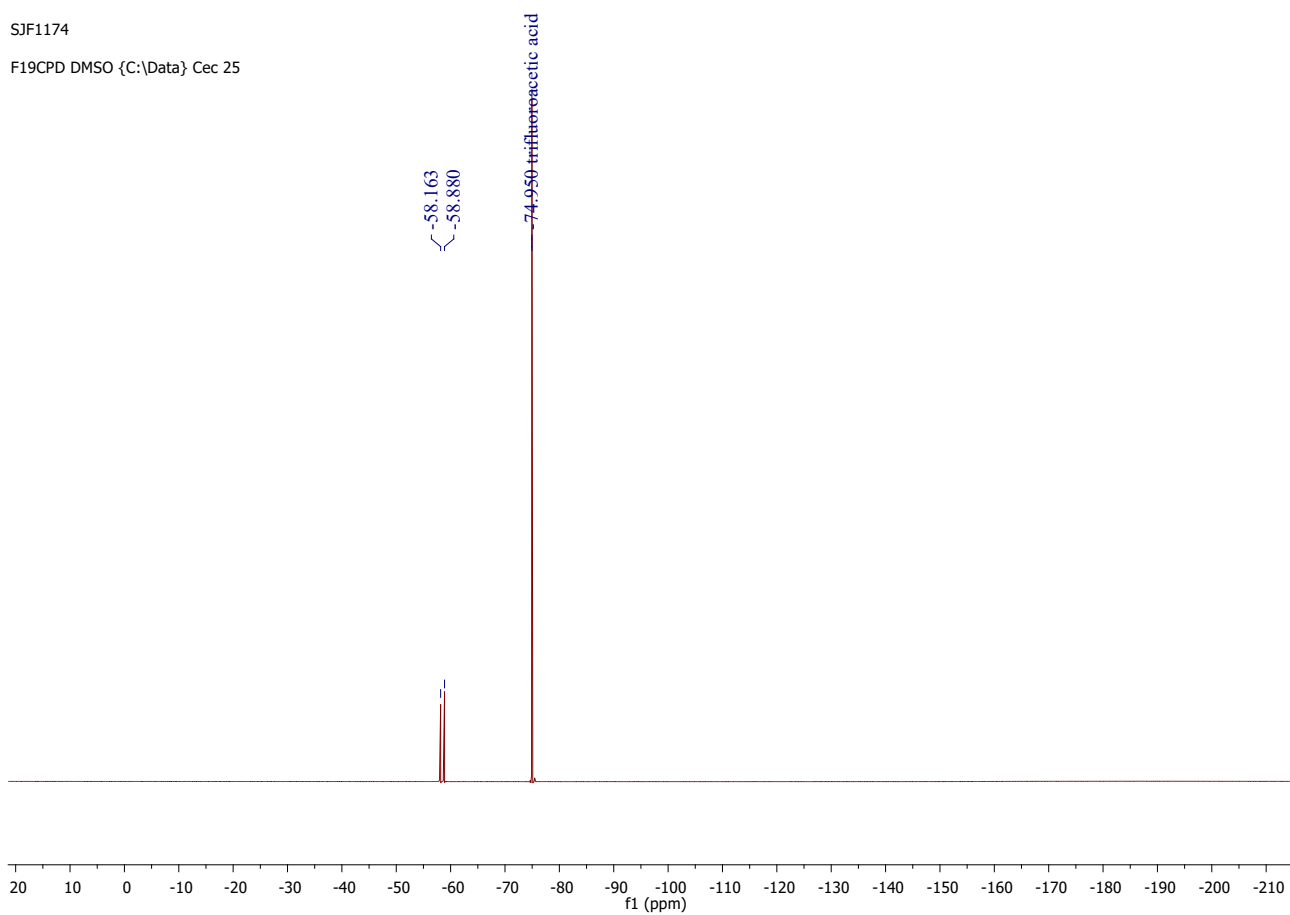


SJF1174
SJF1174
13C_DEPTQ135 DM

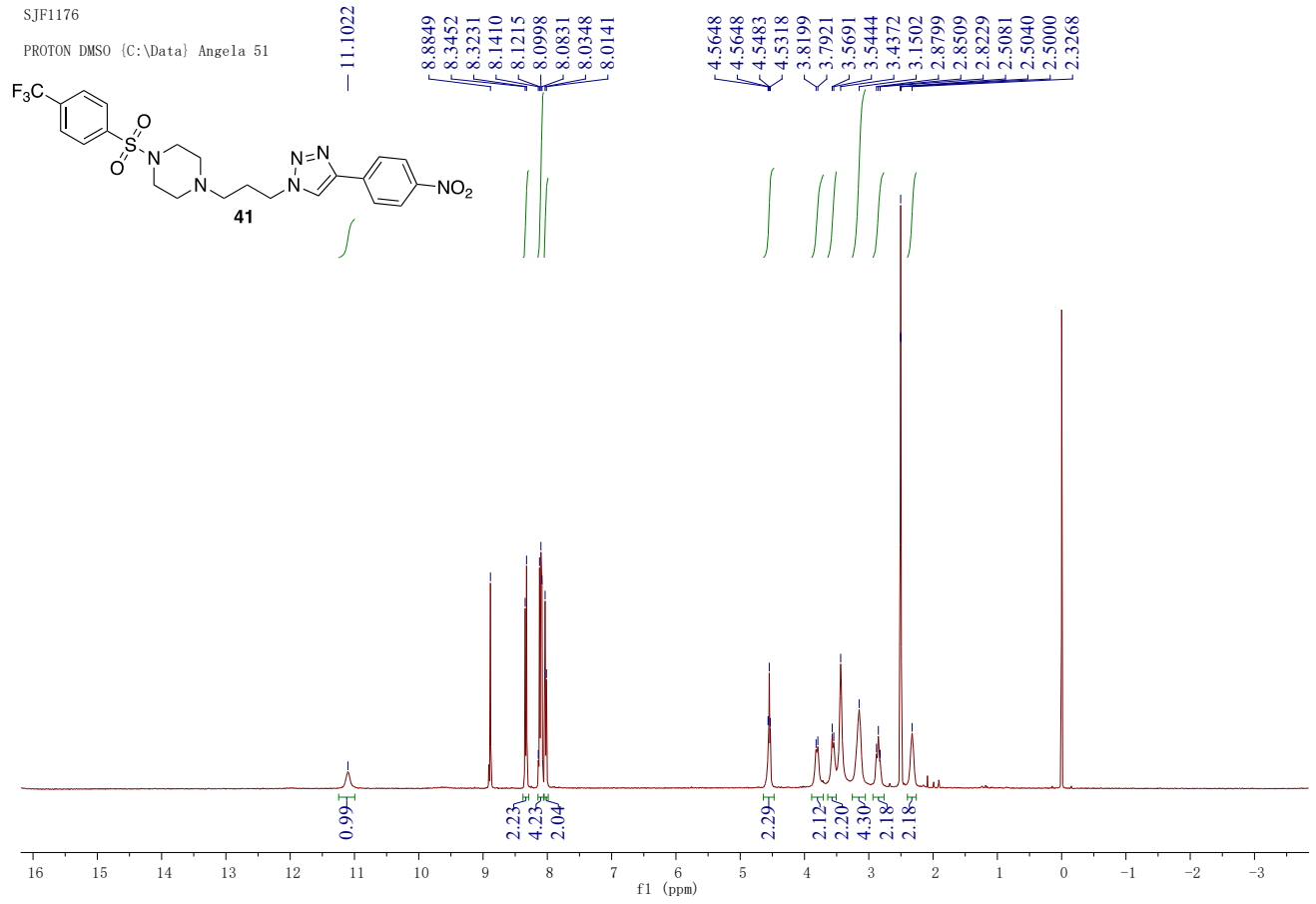


SJF1174

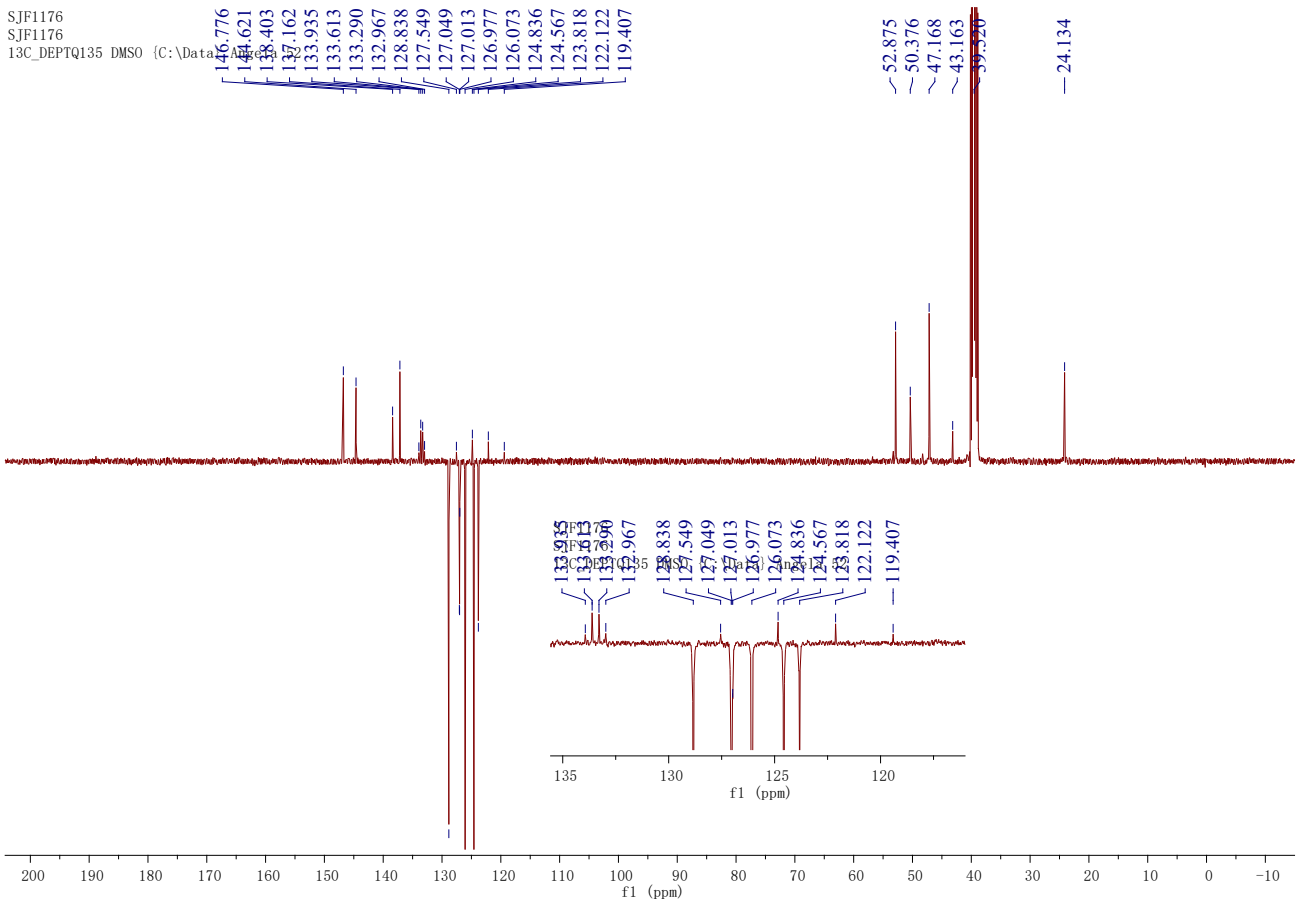
F19CPD DMSO {C:\Data} Cec 25



1-(3-(4-(4-Nitrophenyl)-1H-1,2,3-triazol-1-yl)propyl)-4-((4-(trifluoromethyl)-phenyl)sulfonyl)piperazine hydrochloride
(41)

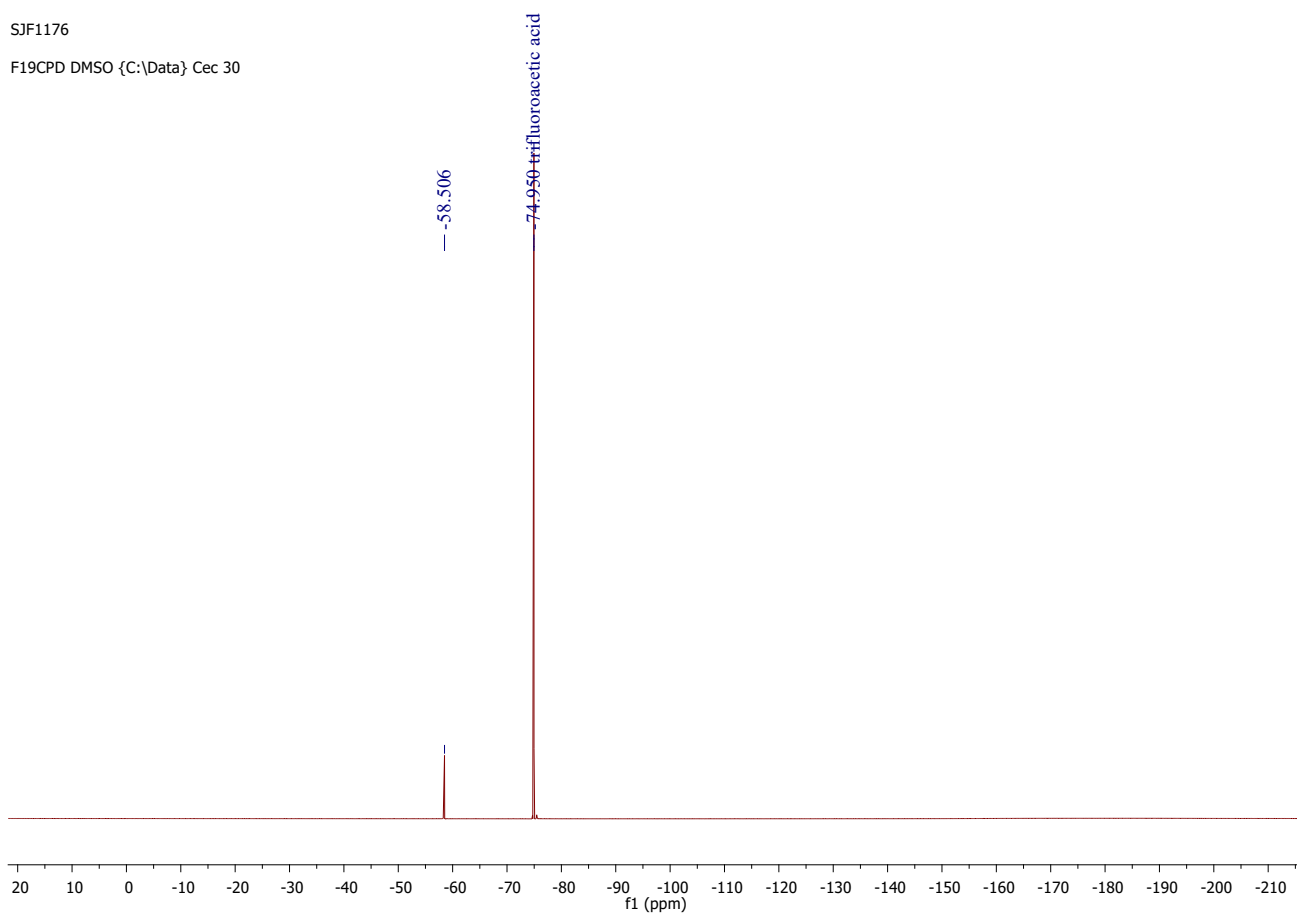


SJF1176
SJF1176
13C_DEPTQ135 DMSO {C:\Data

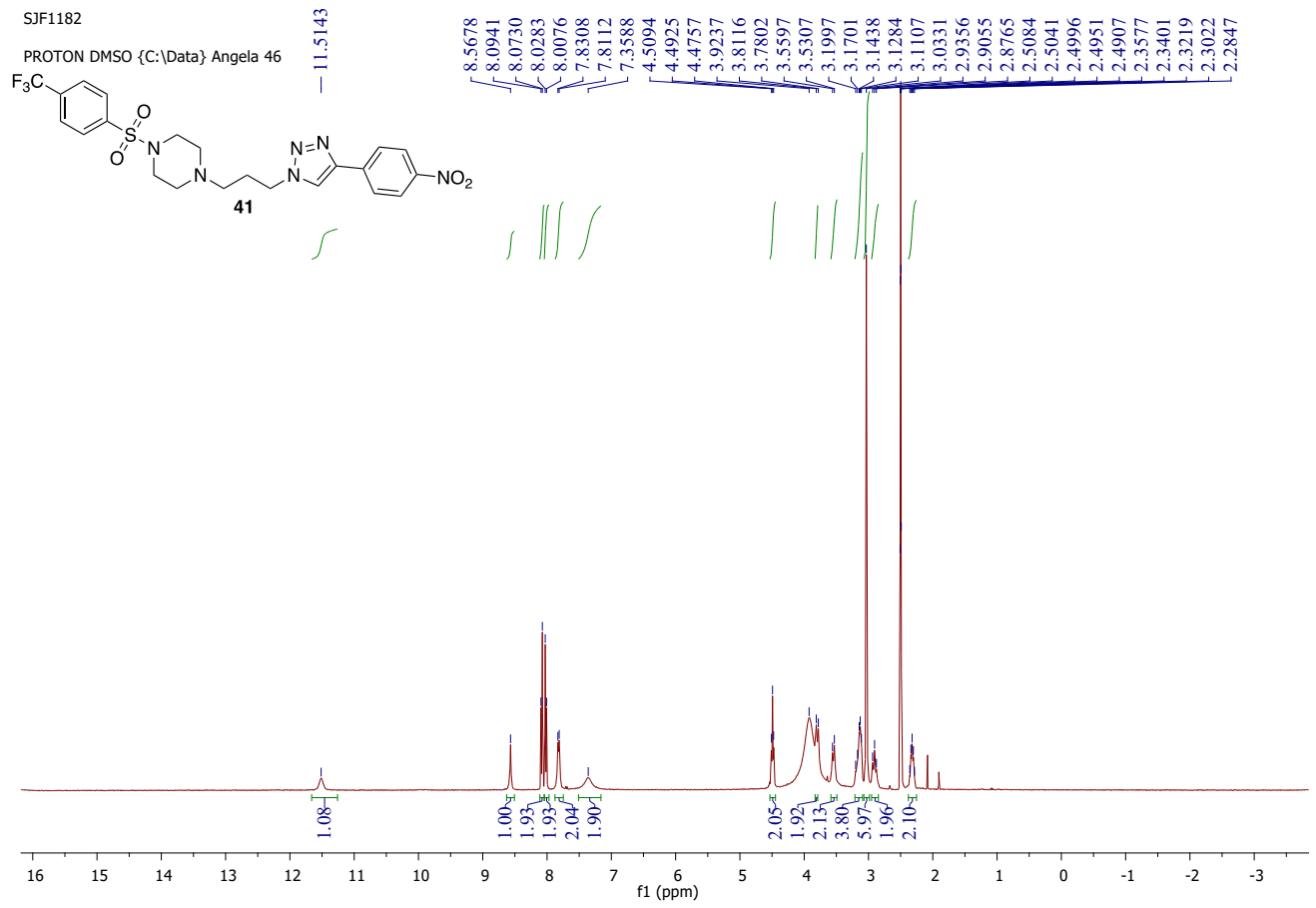


SJF1176

F19CPD DMSO {C:\Data} Ccc 30

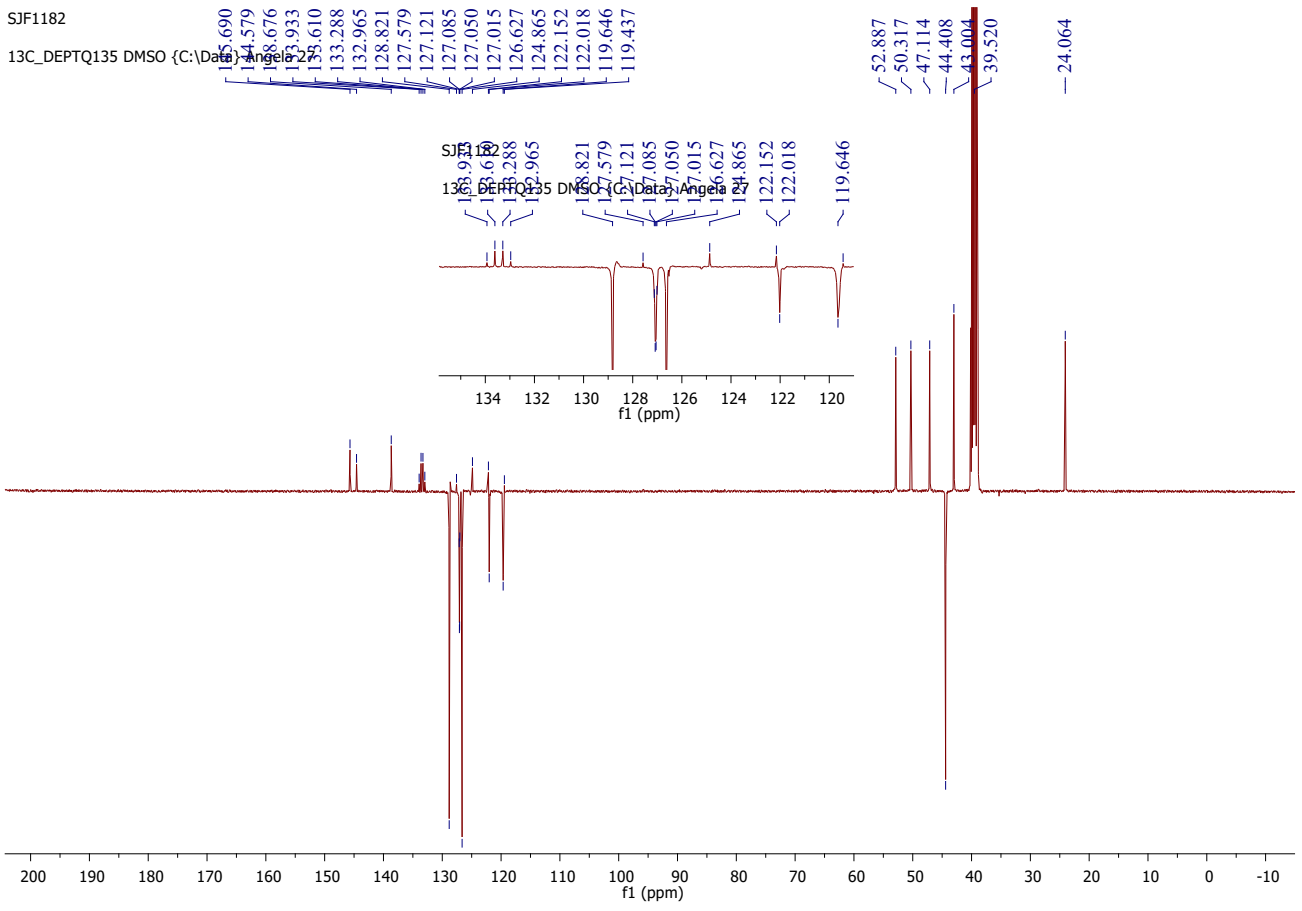


***N,N*-Dimethyl-4-(1-(3-(4-((4-(trifluoromethyl)phenyl)sulfonyl)piperazin-1-yl)-propyl)-1H-1,2,3-triazol-4-yl)aniline hydrochloride (42)**



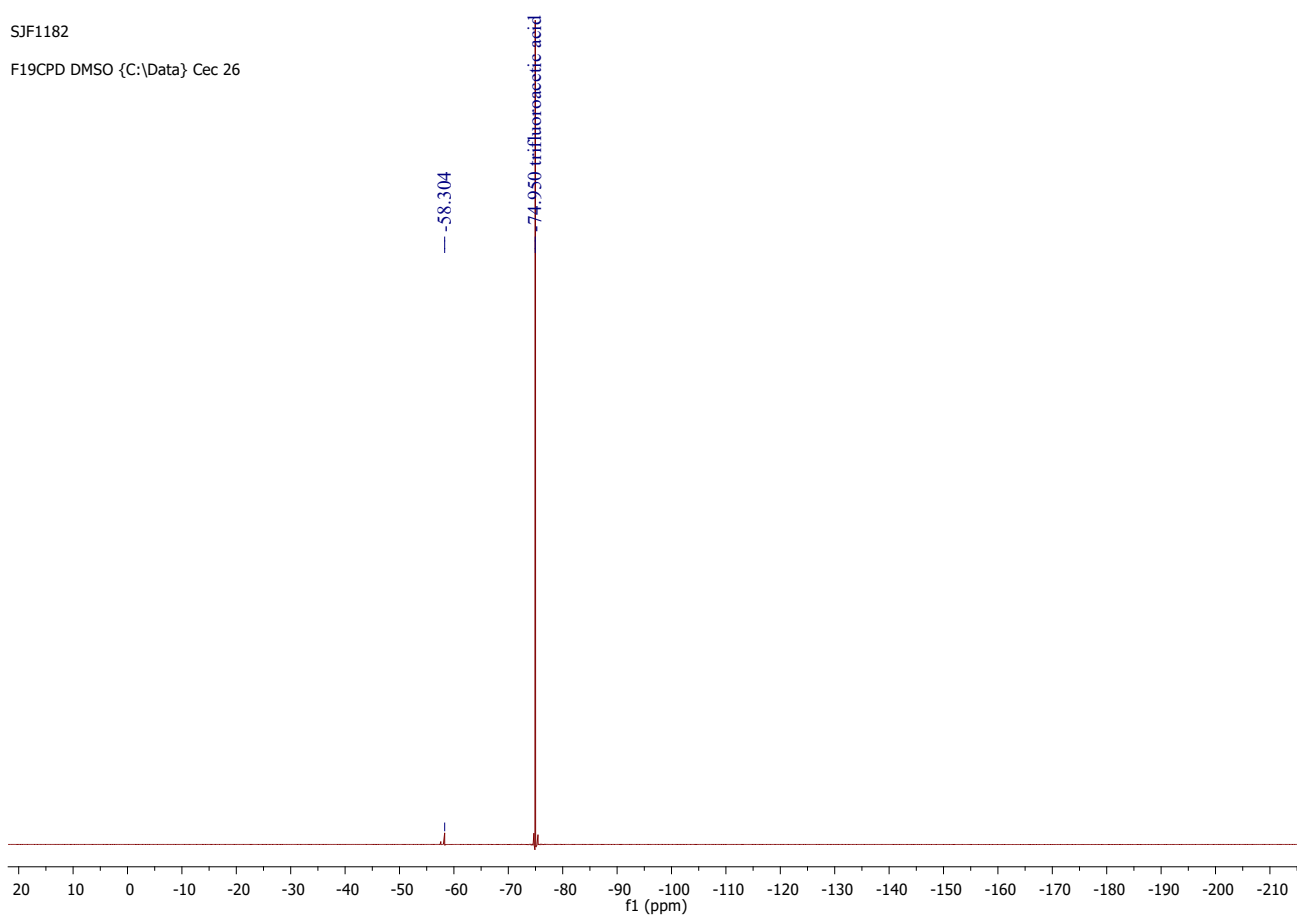
SJF1182

13C_DEPTQ135 DMSO (C:\Data\Angel

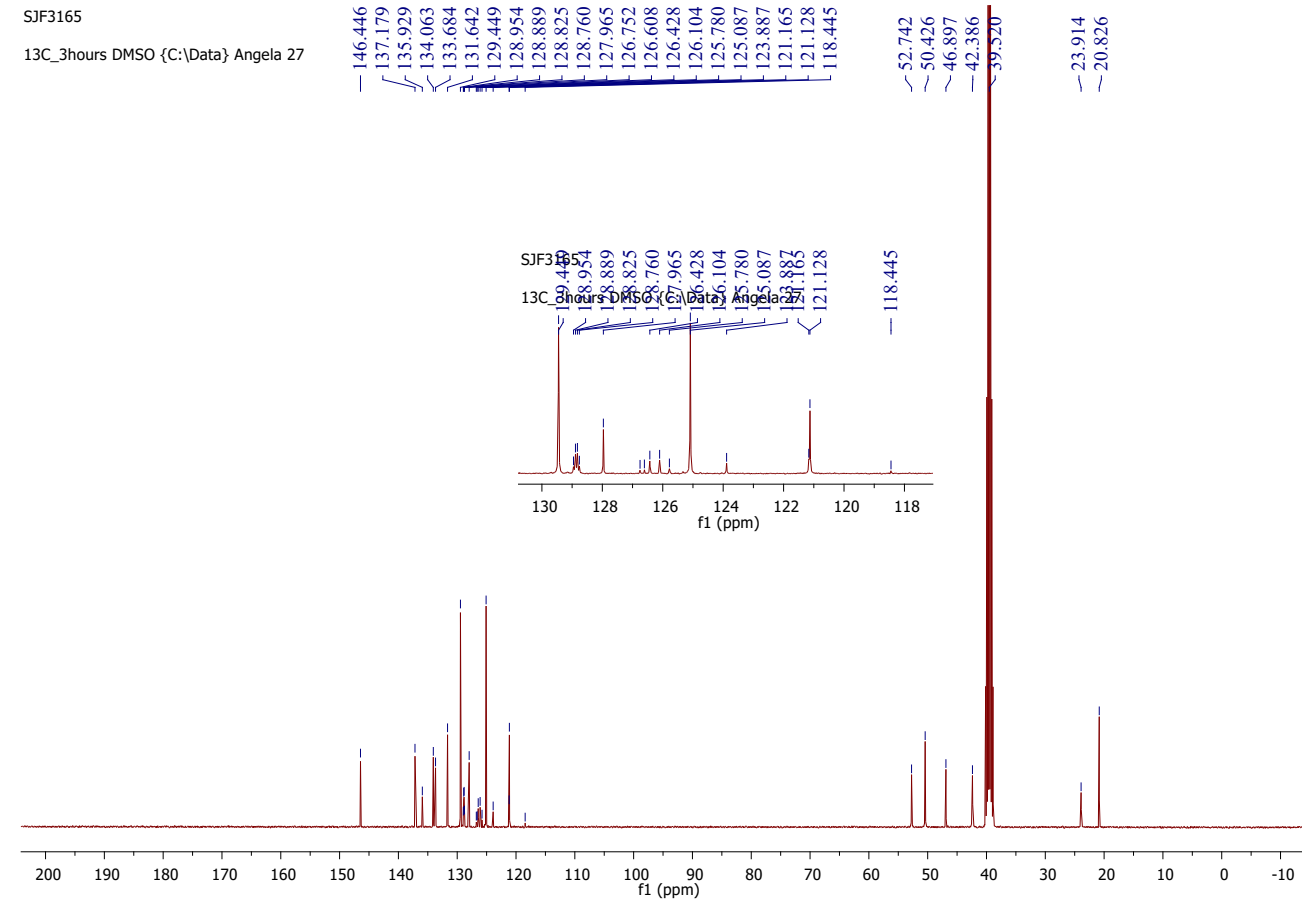
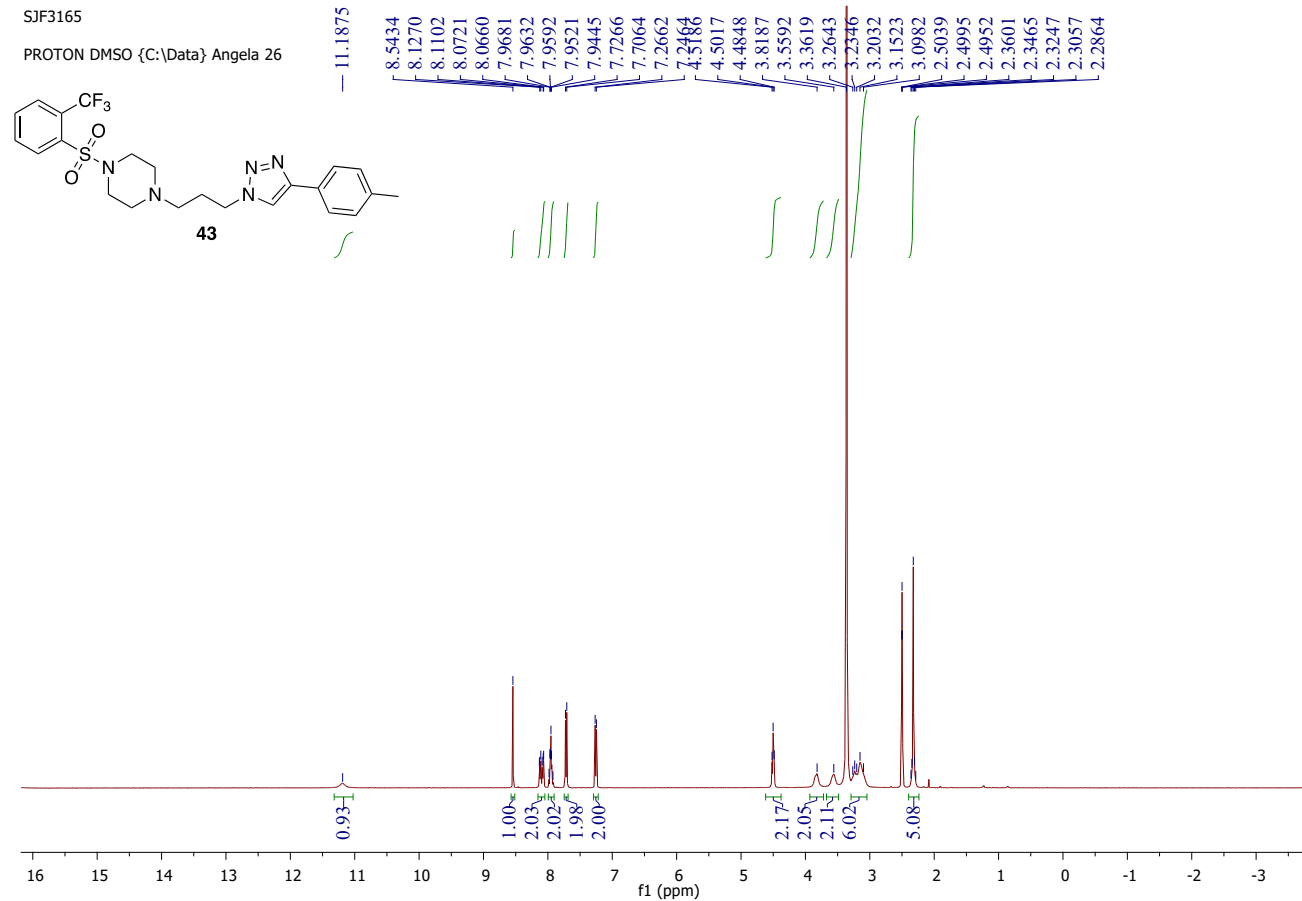


SJF1182

F19CPD DMSO {C:\Data} Cec 26

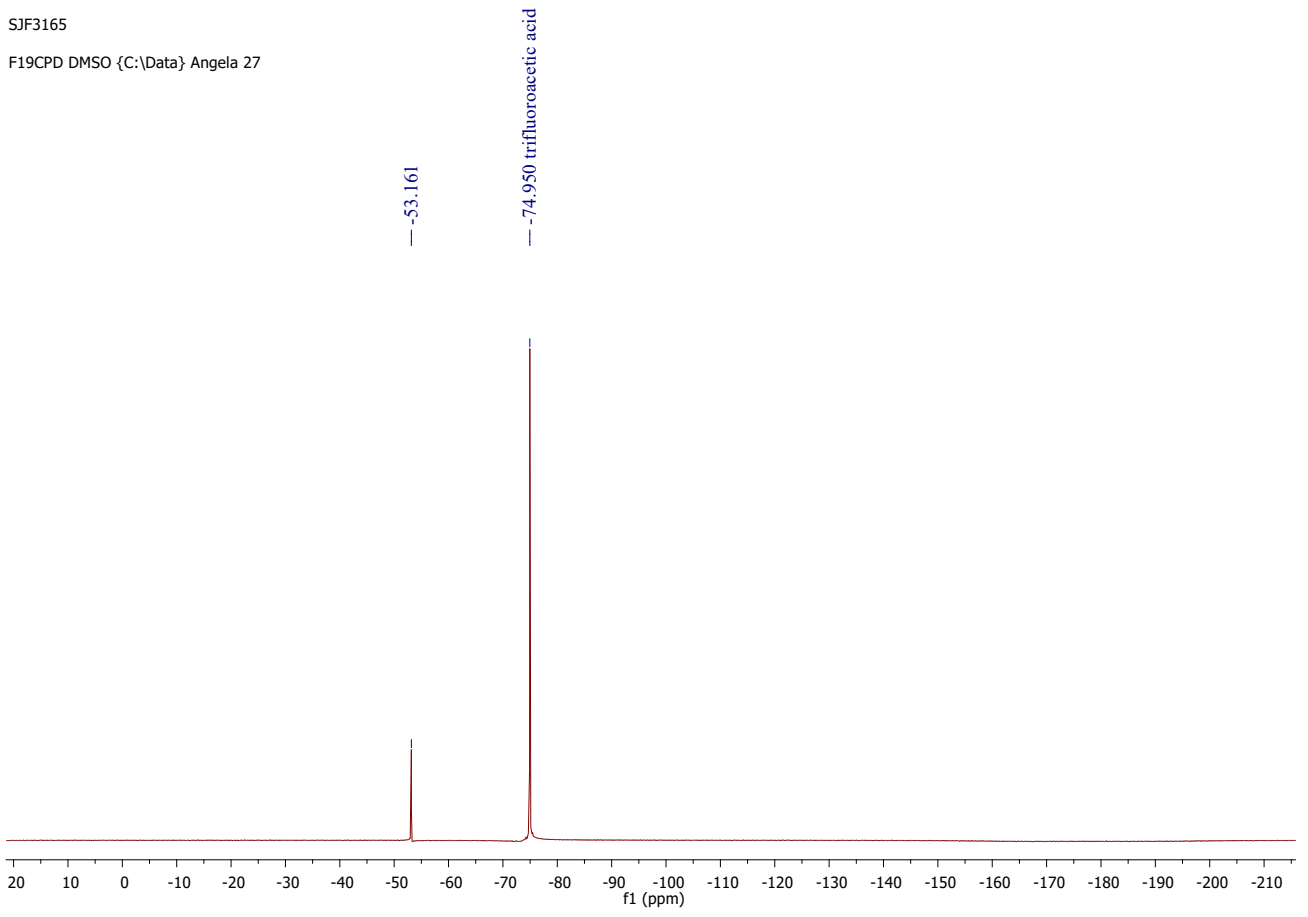


1-[3-(4-p-Tolyl-[1,2,3]triazol-1-yl)-propyl]-4-(2-trifluoromethylbenzenesulfonyl)-piperazine hydrochloride (43)

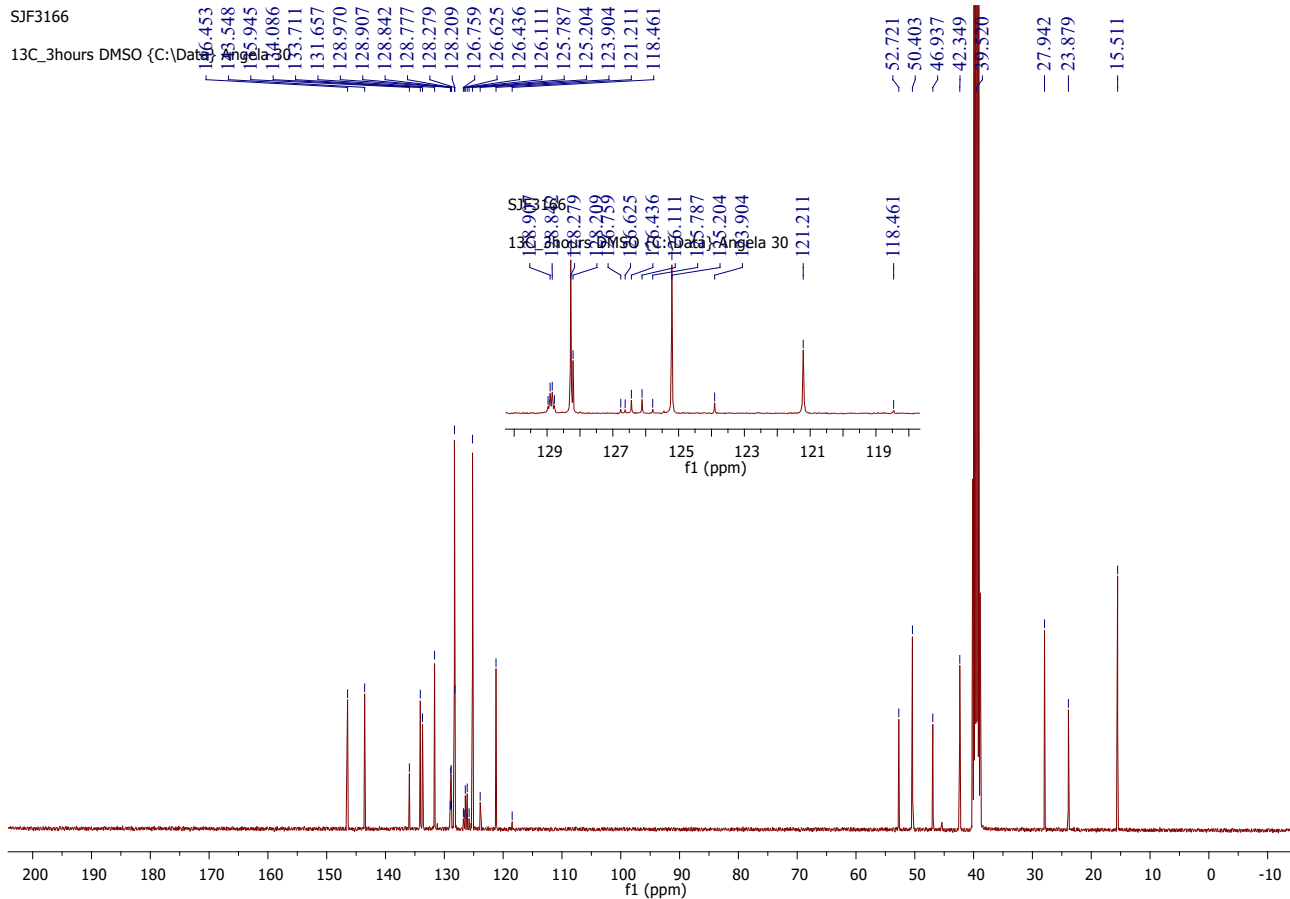
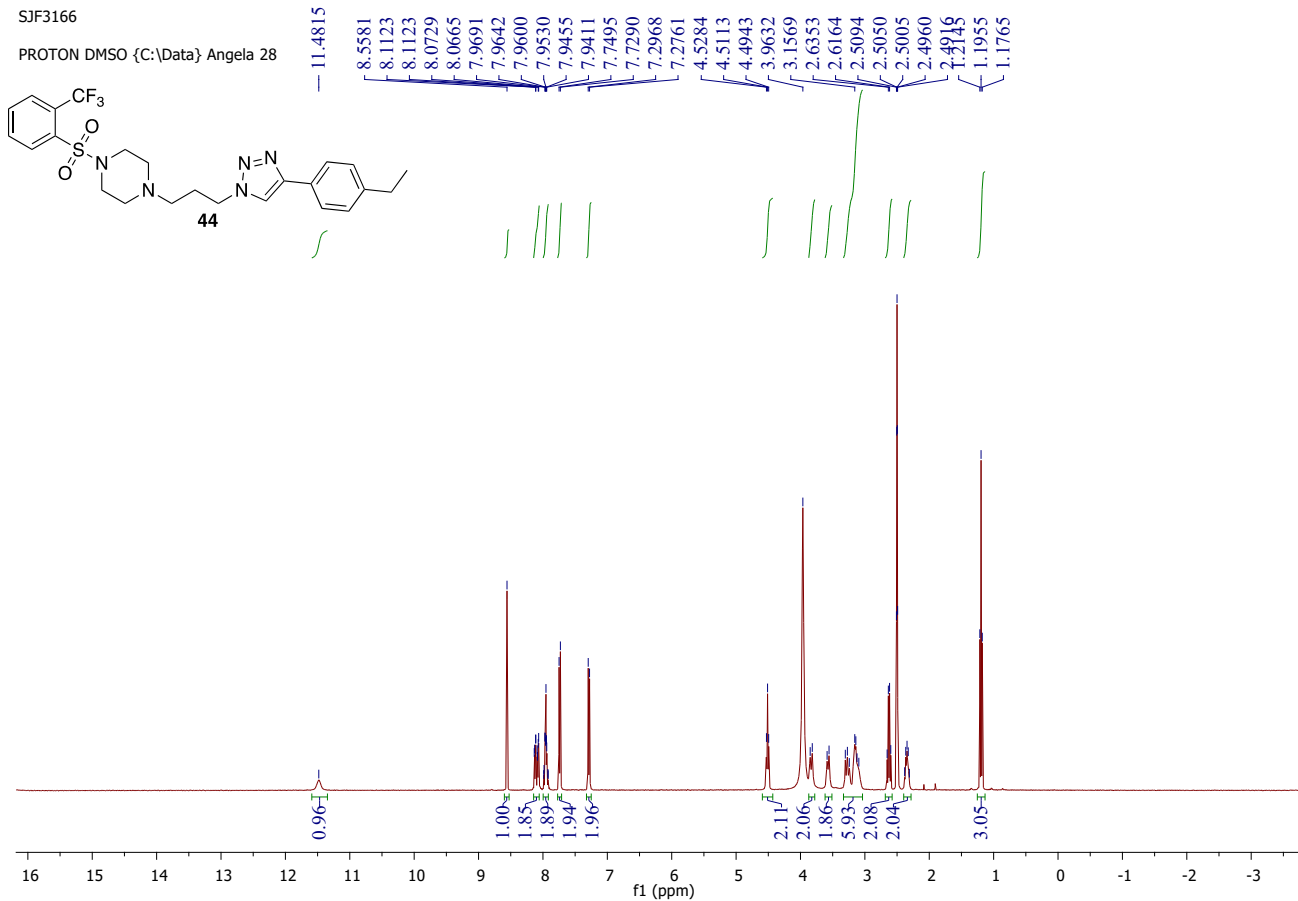


SJF3165

F19CPD DMSO {C:\Data} Angela 27

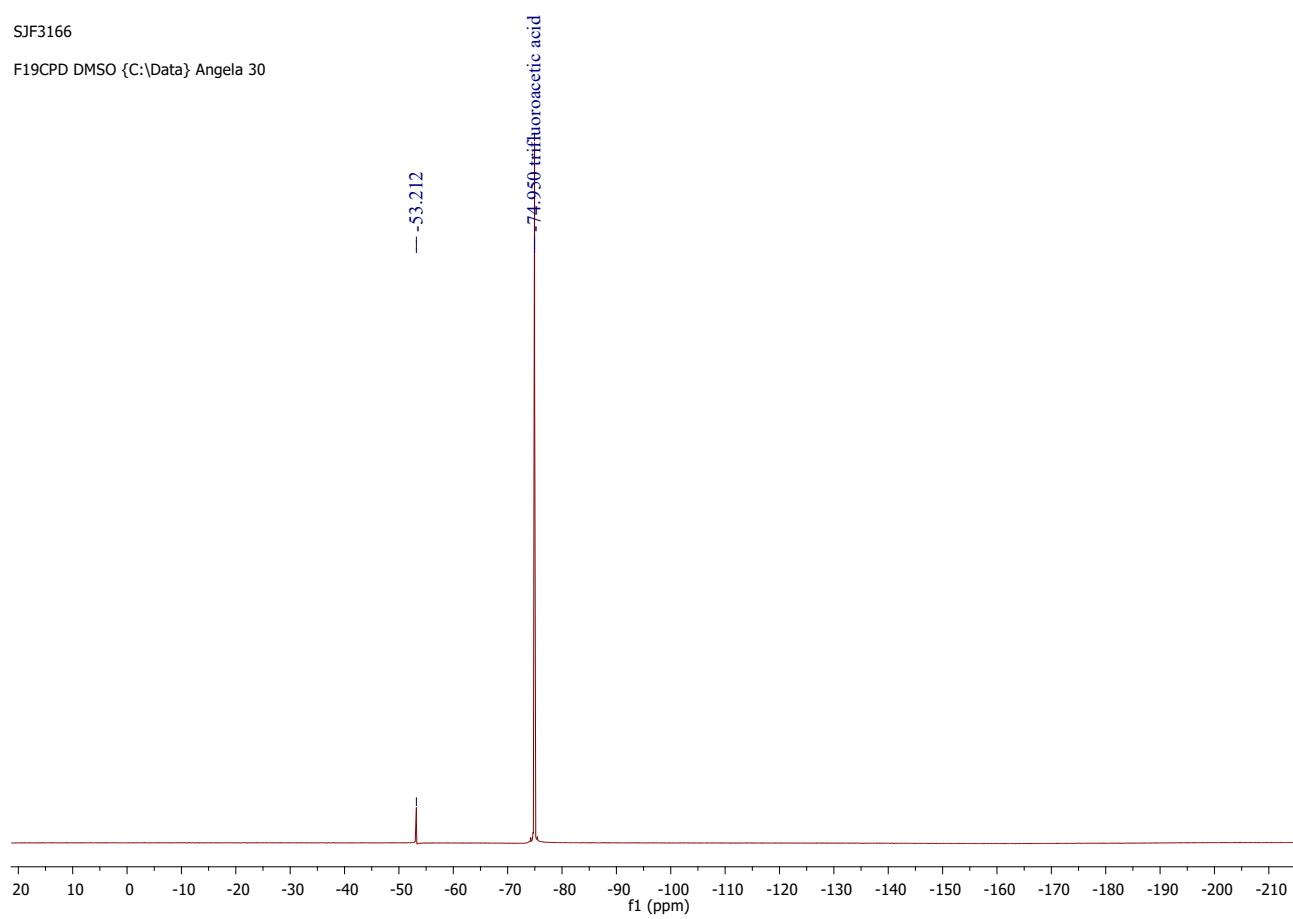


1-[3-[4-(4-Ethylphenyl)-[1,2,3]triazol-1-yl]-propyl]-4-(2-trifluoromethylbenzenesulfonyl)-piperazine hydrochloride (**44**)



SJF3166

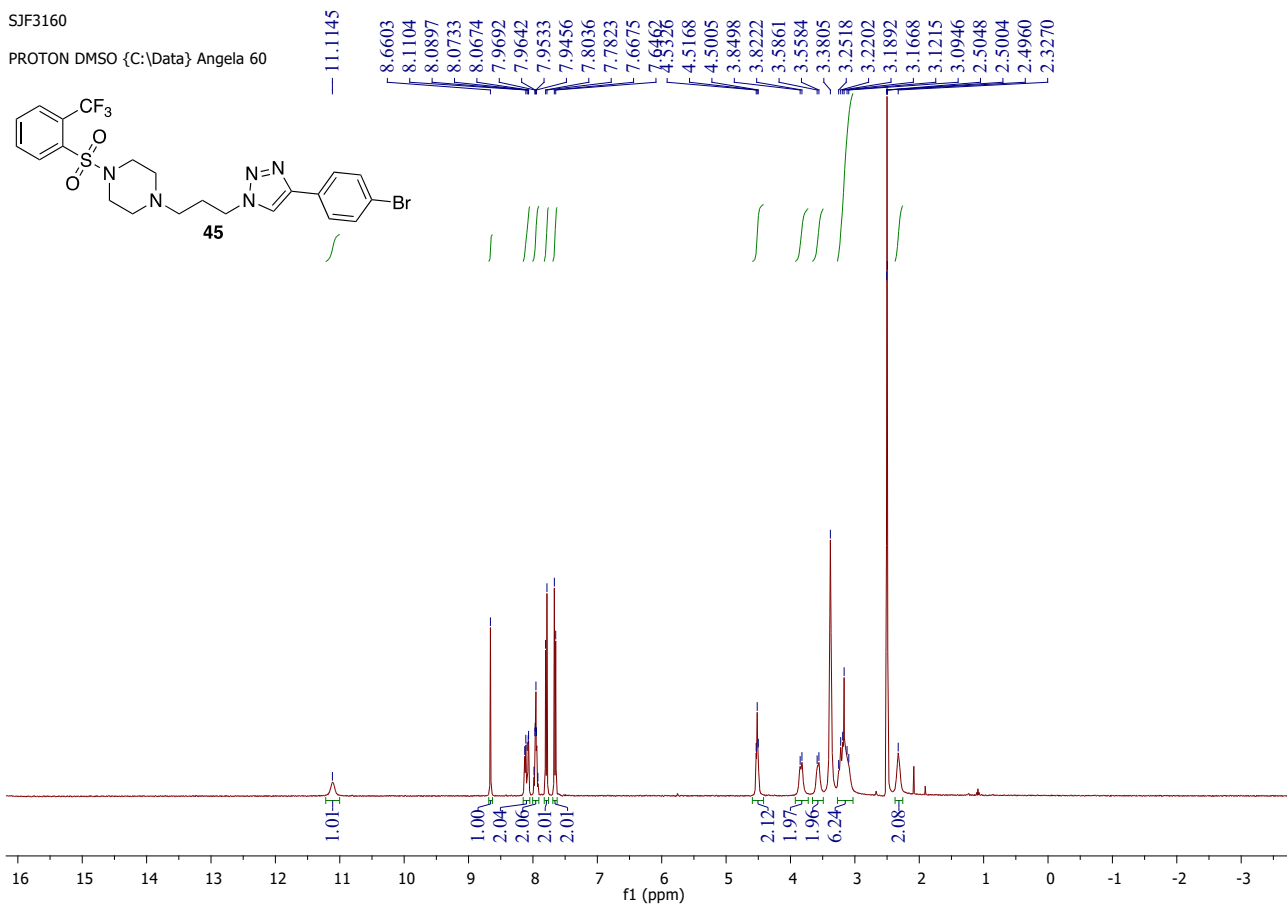
F19CPD DMSO {C:\Data} Angela 30



1-{3-[4-(4-Bromophenyl)-[1,2,3]triazol-1-yl]-propyl}-4-(2-trifluoromethylbenzene sulfonyl)-piperazine hydrochloride
(45)

SJF3160

PROTON DMSO {C:\Data} Angela 60



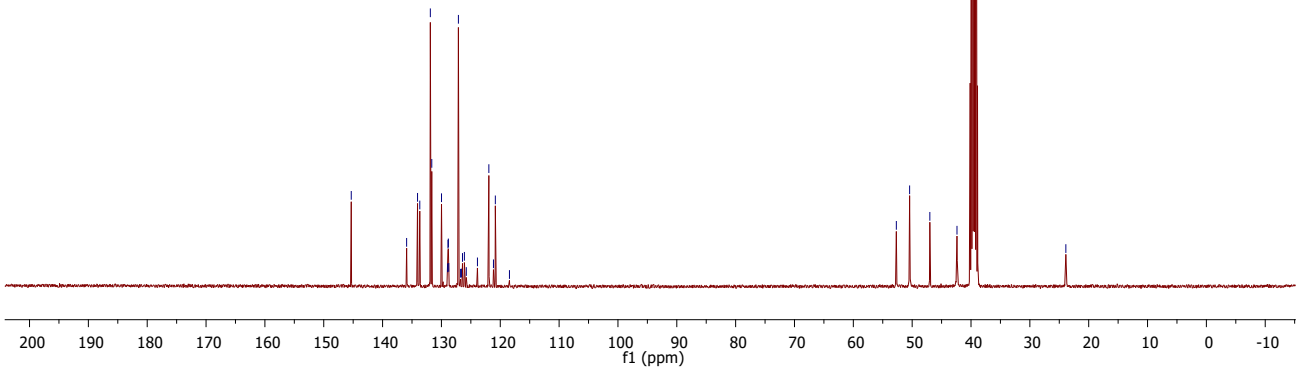
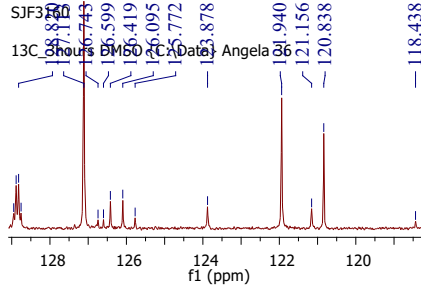
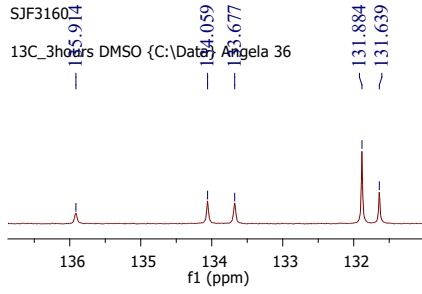
SJF3160

13C_3hours DMSO (C:\Data) Angela 36



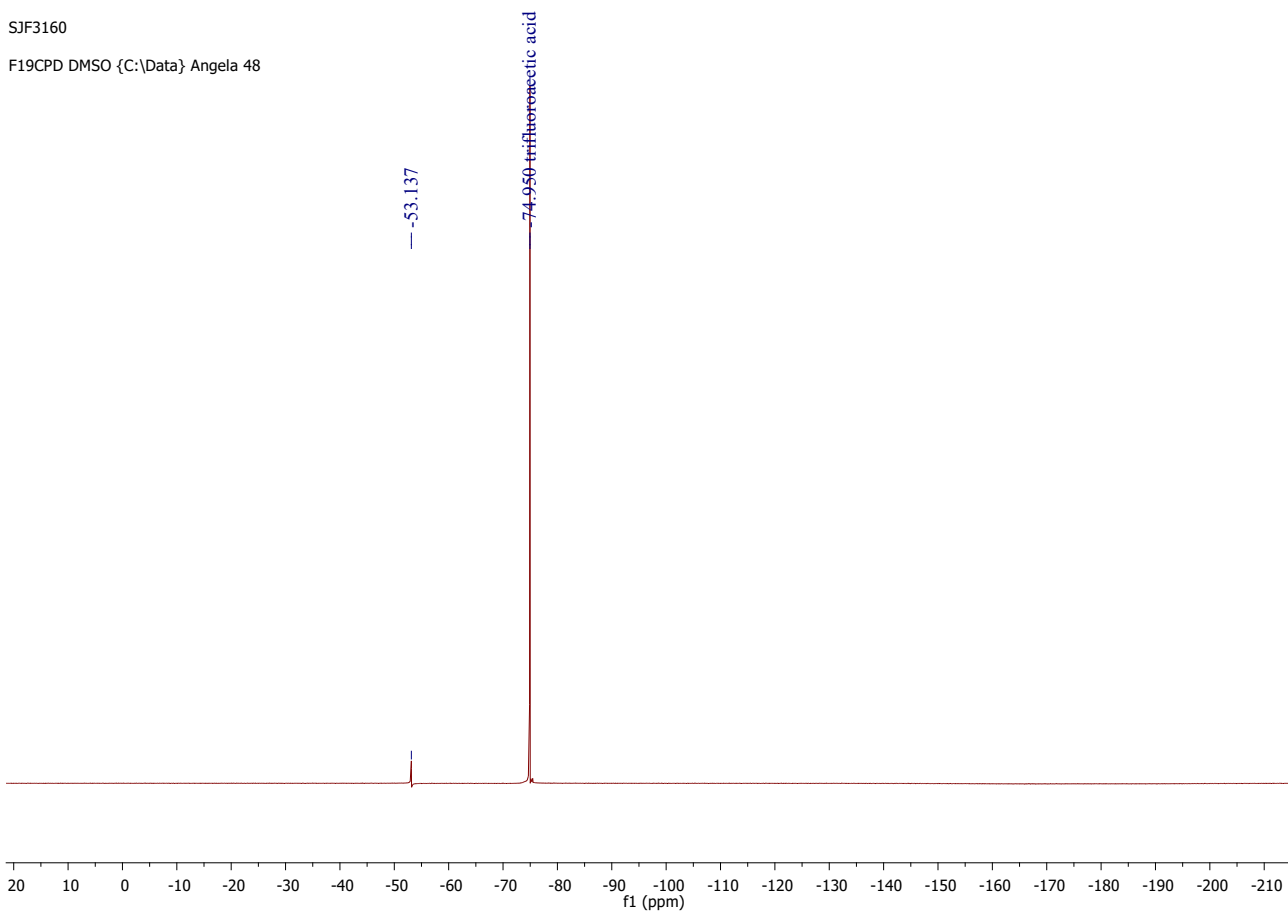
SJF3160

13C_3hours DMSO (C:\Data) Angela 36



SJF3160

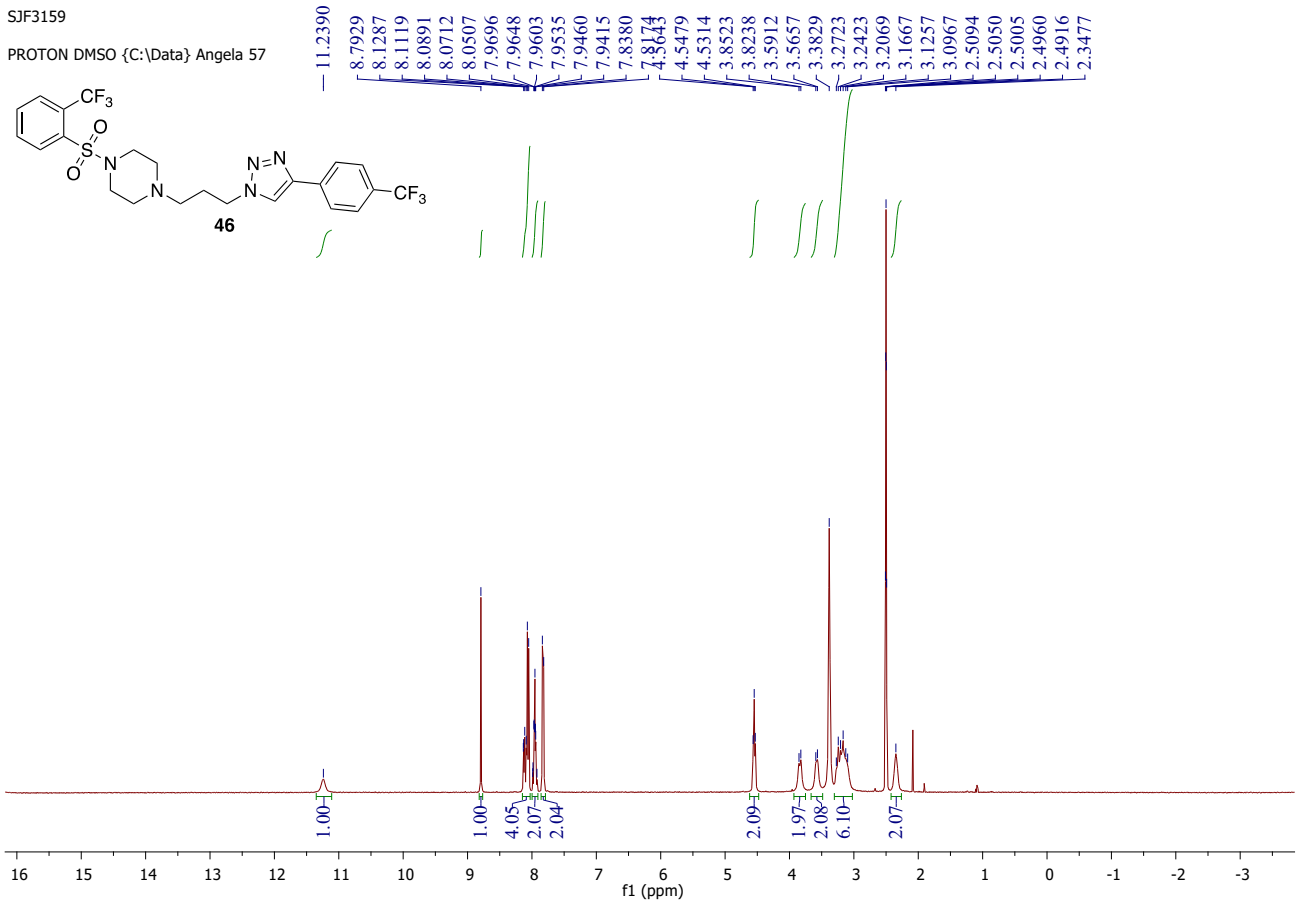
F19CPD DMSO {C:\Data} Angela 48



1-(2-Trifluoromethylbenzenesulfonyl)-4-{3-[4-(4-trifluoromethylphenyl)-[1,2,3]-triazol-1-yl]-propyl}-piperazine hydrochloride (**46**)

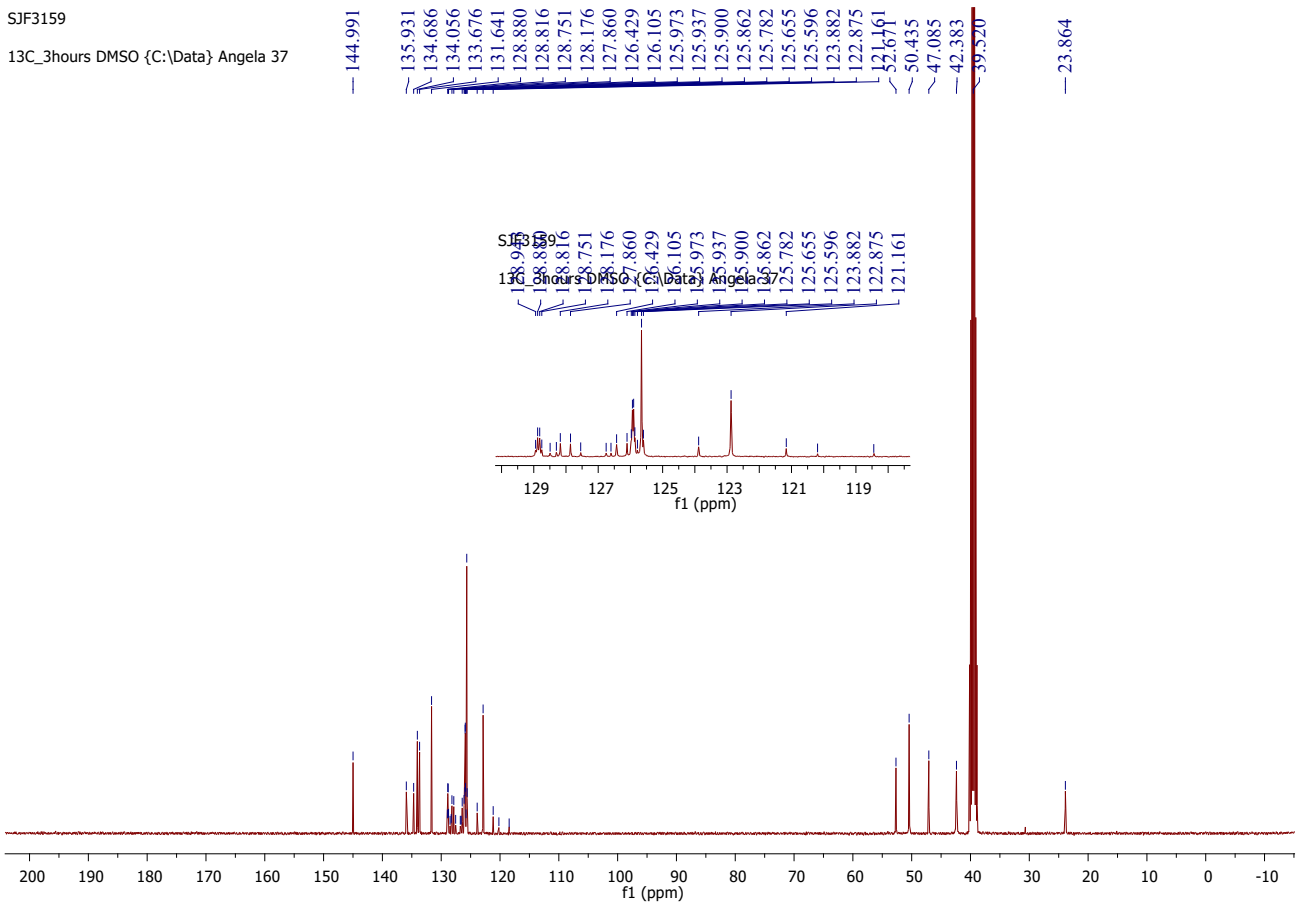
SJF3159

PROTON DMSO {C:\Data} Angela 57



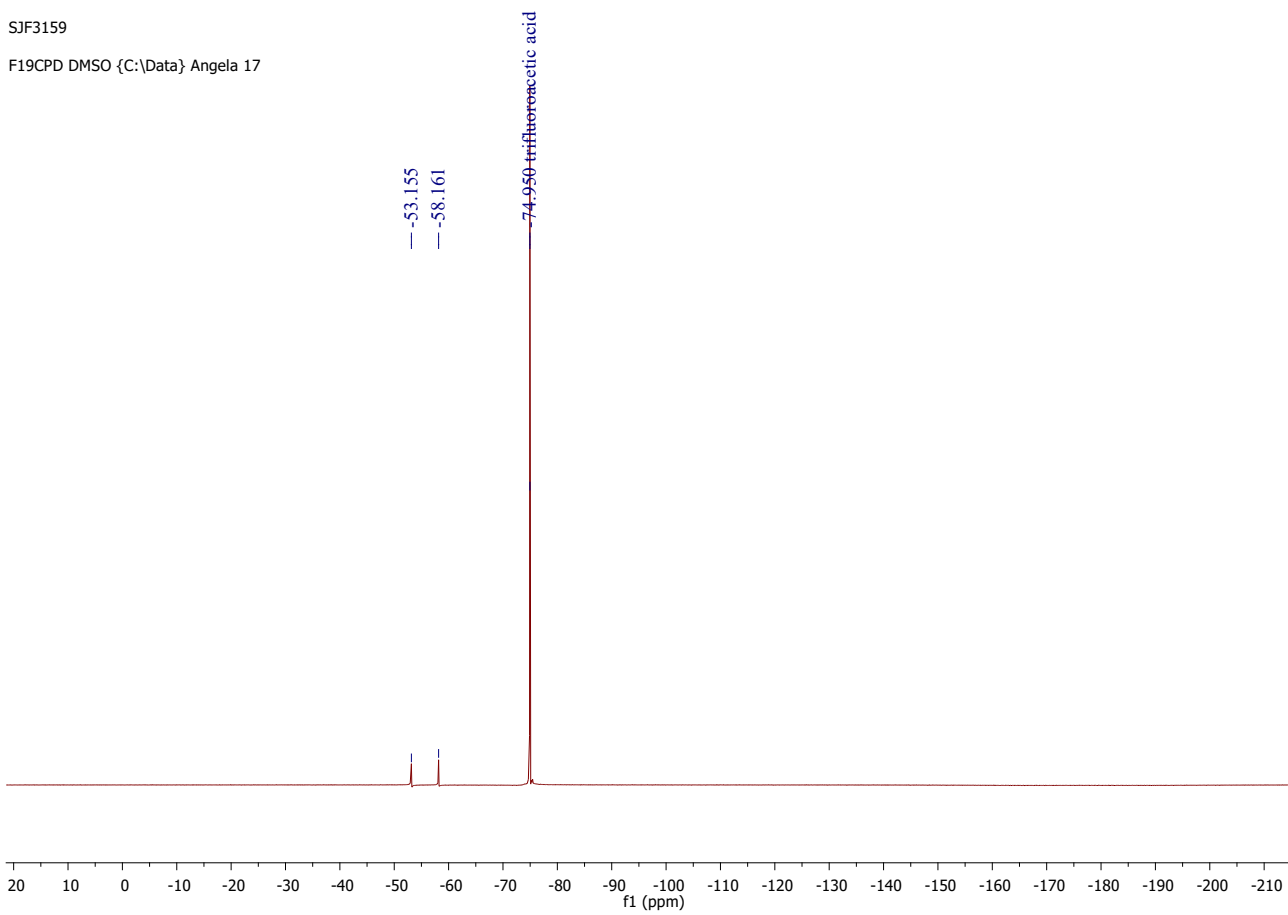
SJF3159

13C_3hours DMSO (C:\Data) Angela 37



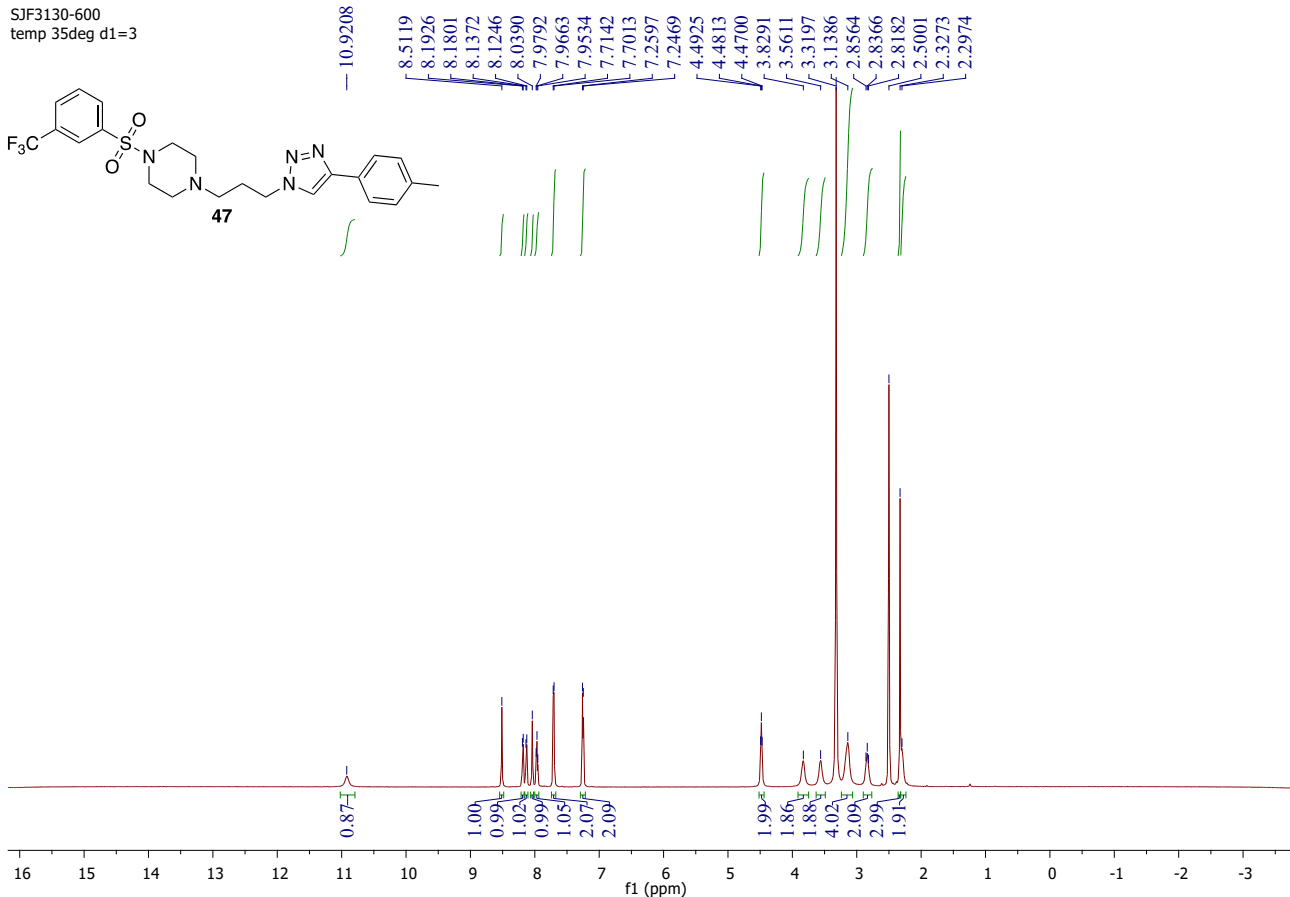
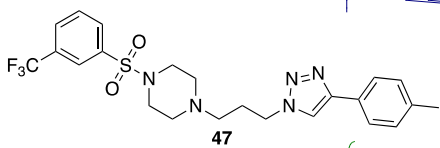
SJF3159

F19CPD DMSO {C:\Data} Angela 17



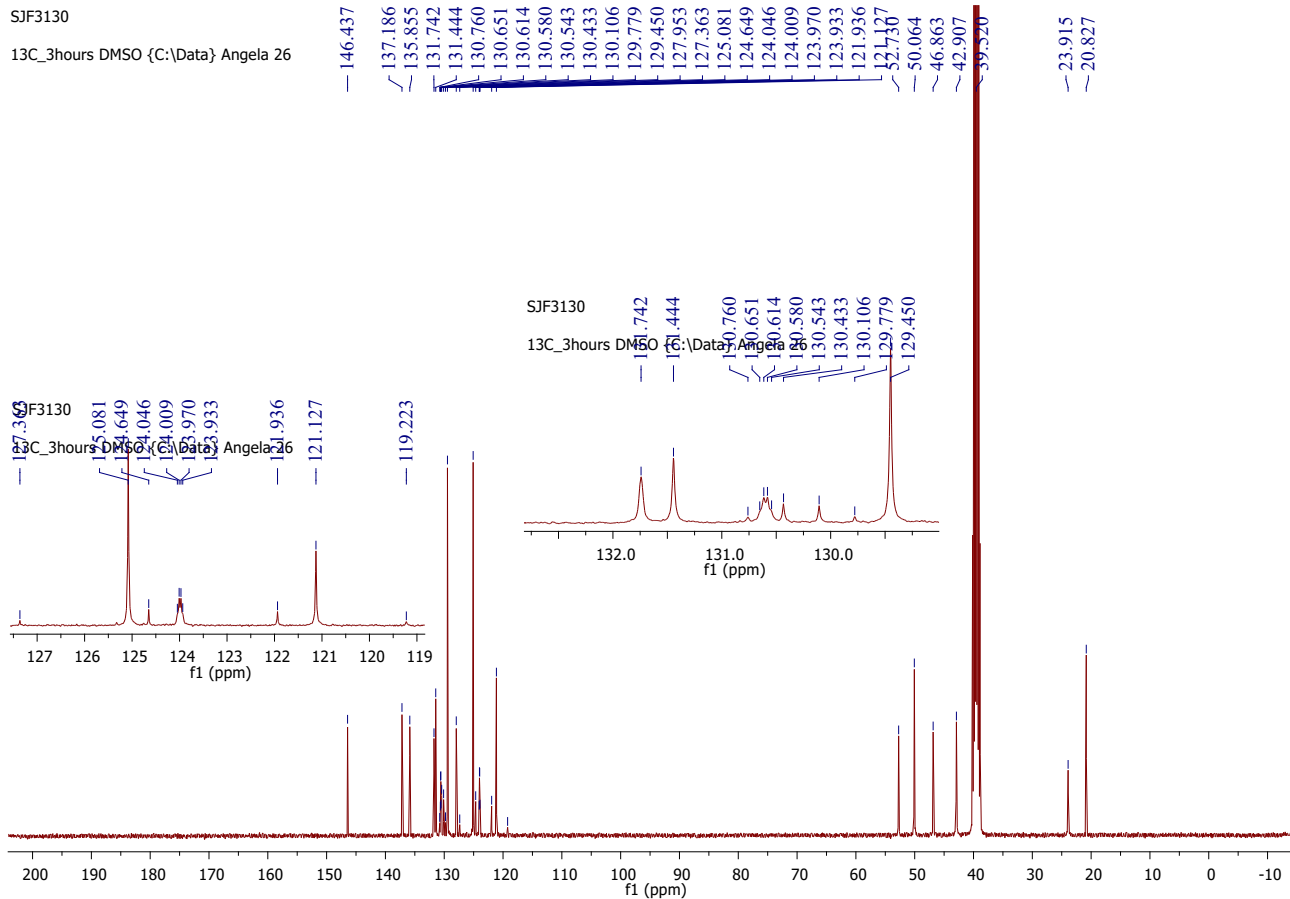
1-[3-(4-p-Tolyl-[1,2,3]triazol-1-yl)-propyl]-4-(3-trifluoromethylbenzenesulfonyl)-piperazine hydrochloride (47)

SJF3130-600
temp 35deg d1=3



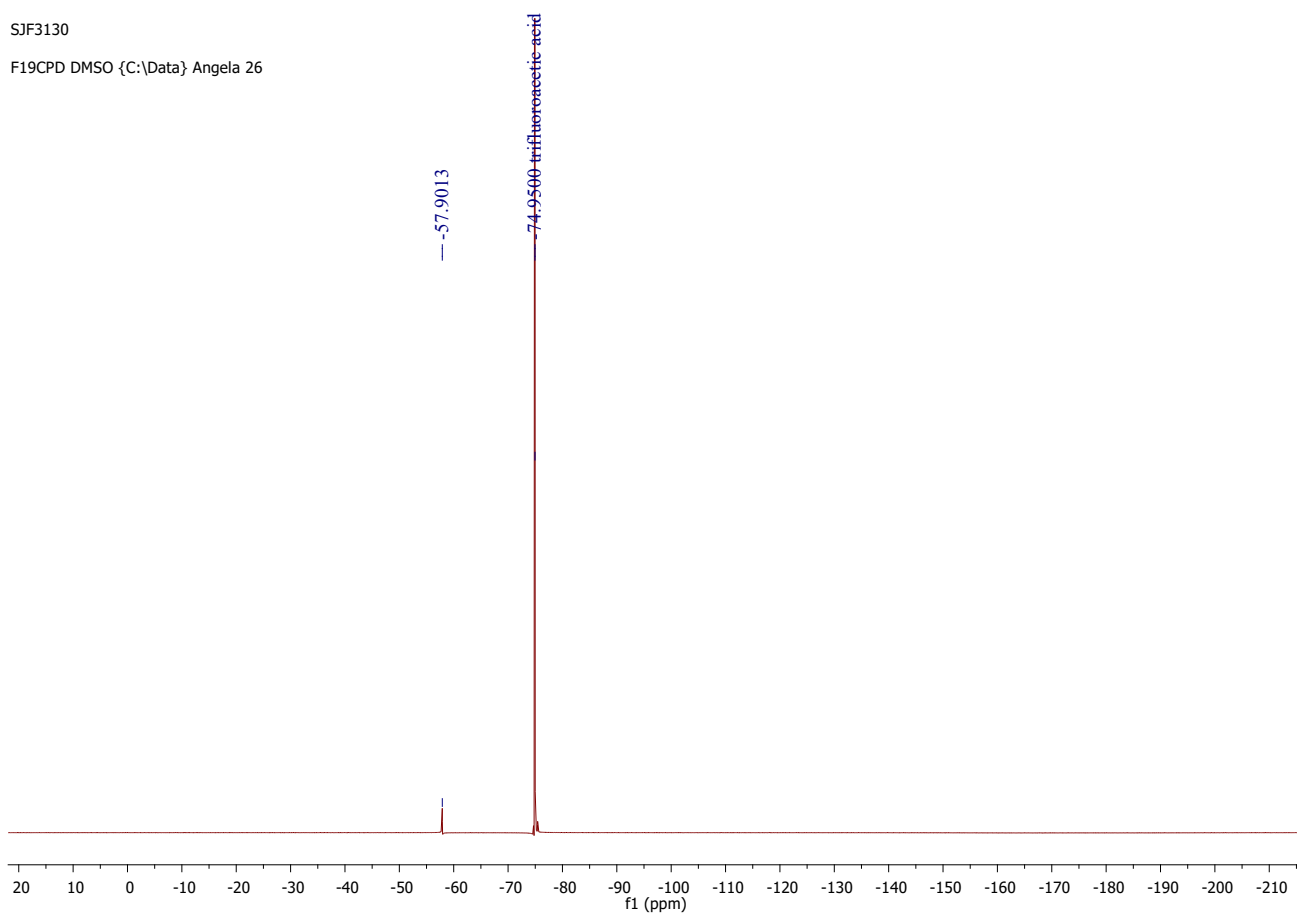
SJF3130

13C_3hours DMSO (C:\Data) Angela 26

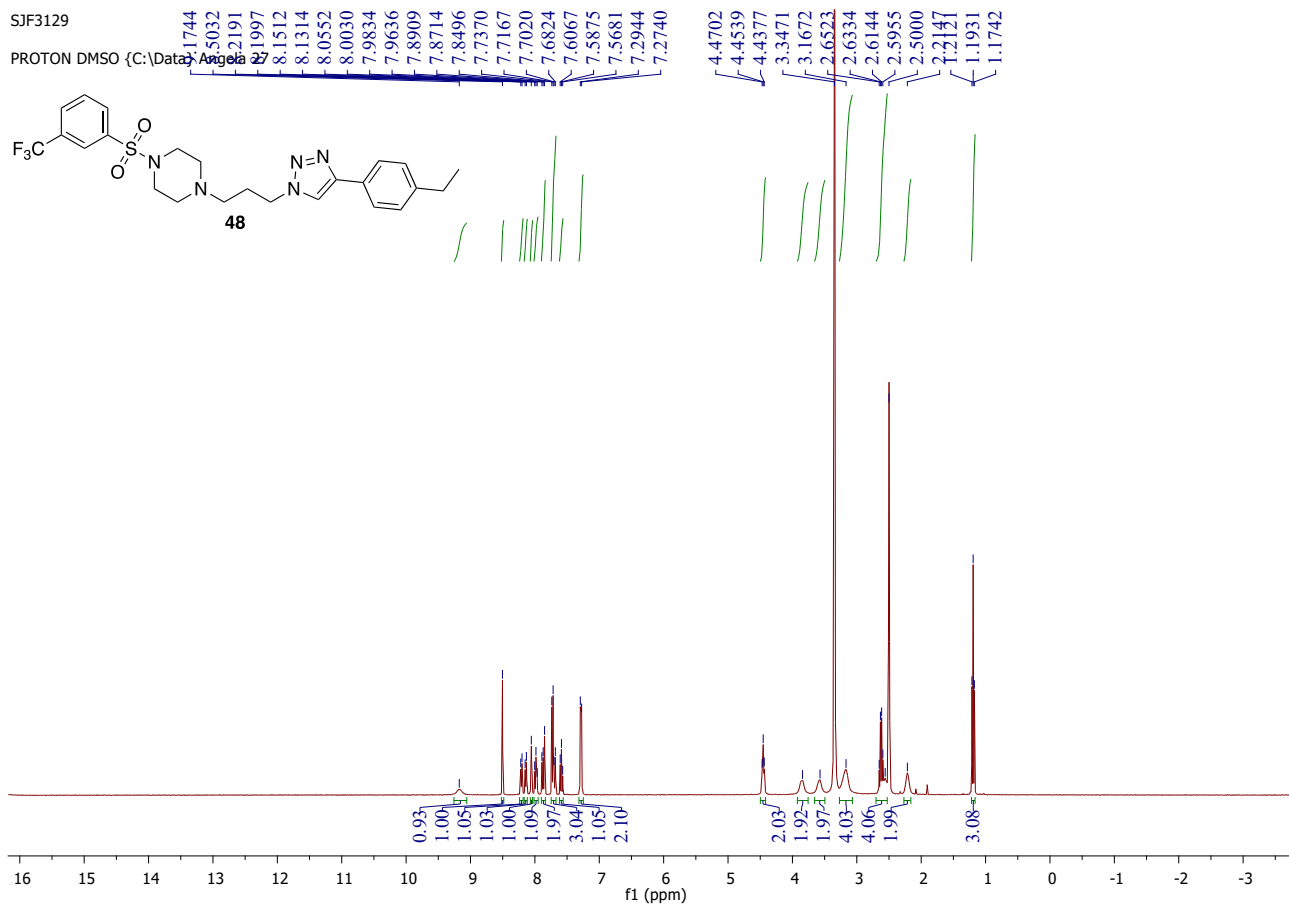


SJF3130

F19CPD DMSO {C:\Data} Angela 26

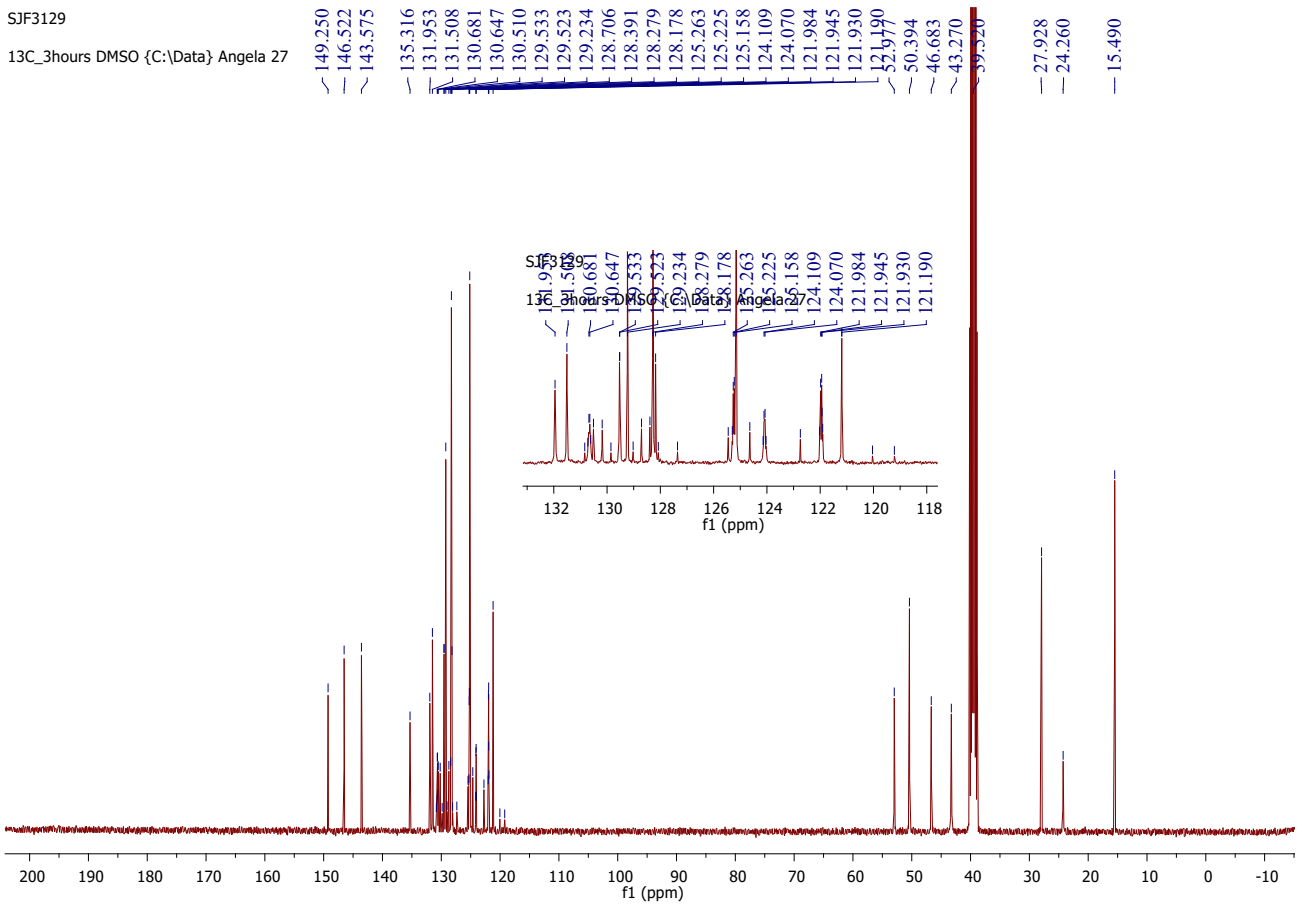


1-[3-[4-(4-Ethyl-phenyl)-[1,2,3]triazol-1-yl]-propyl]-4-(3-trifluoromethylbenzenesulfonyl)-piperazine 3-trifluoromethylbenzenesulfonate (48)



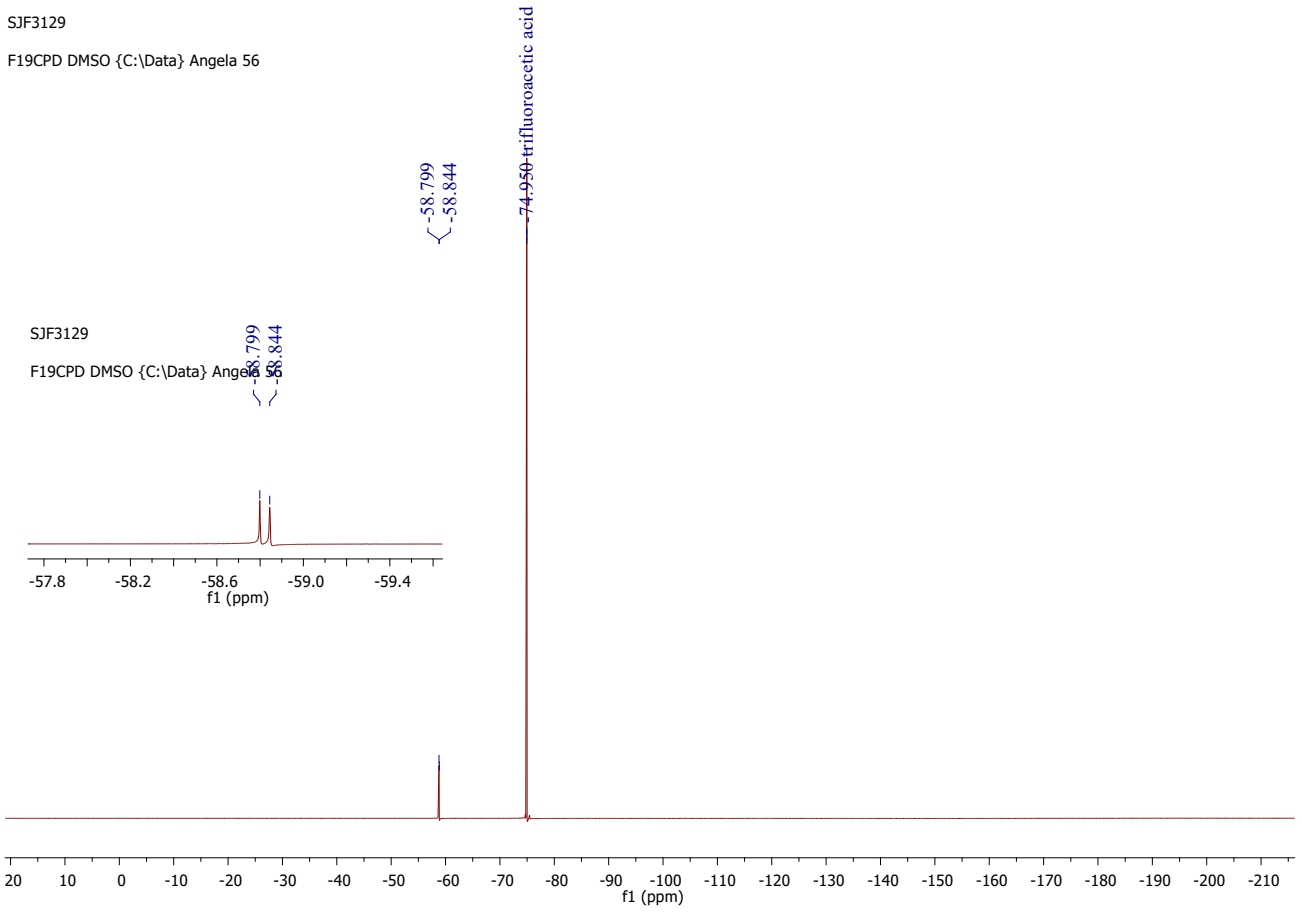
SJF3129

13C_3hours DMSO {C:\Data} Angela 27



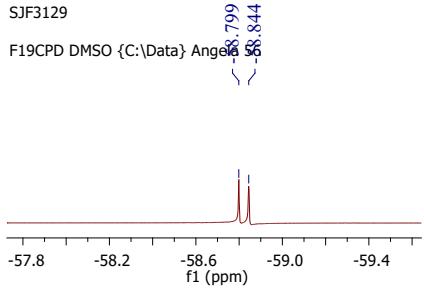
SJF3129

F19CPD DMSO {C:\Data} Angela 56



SJF3129

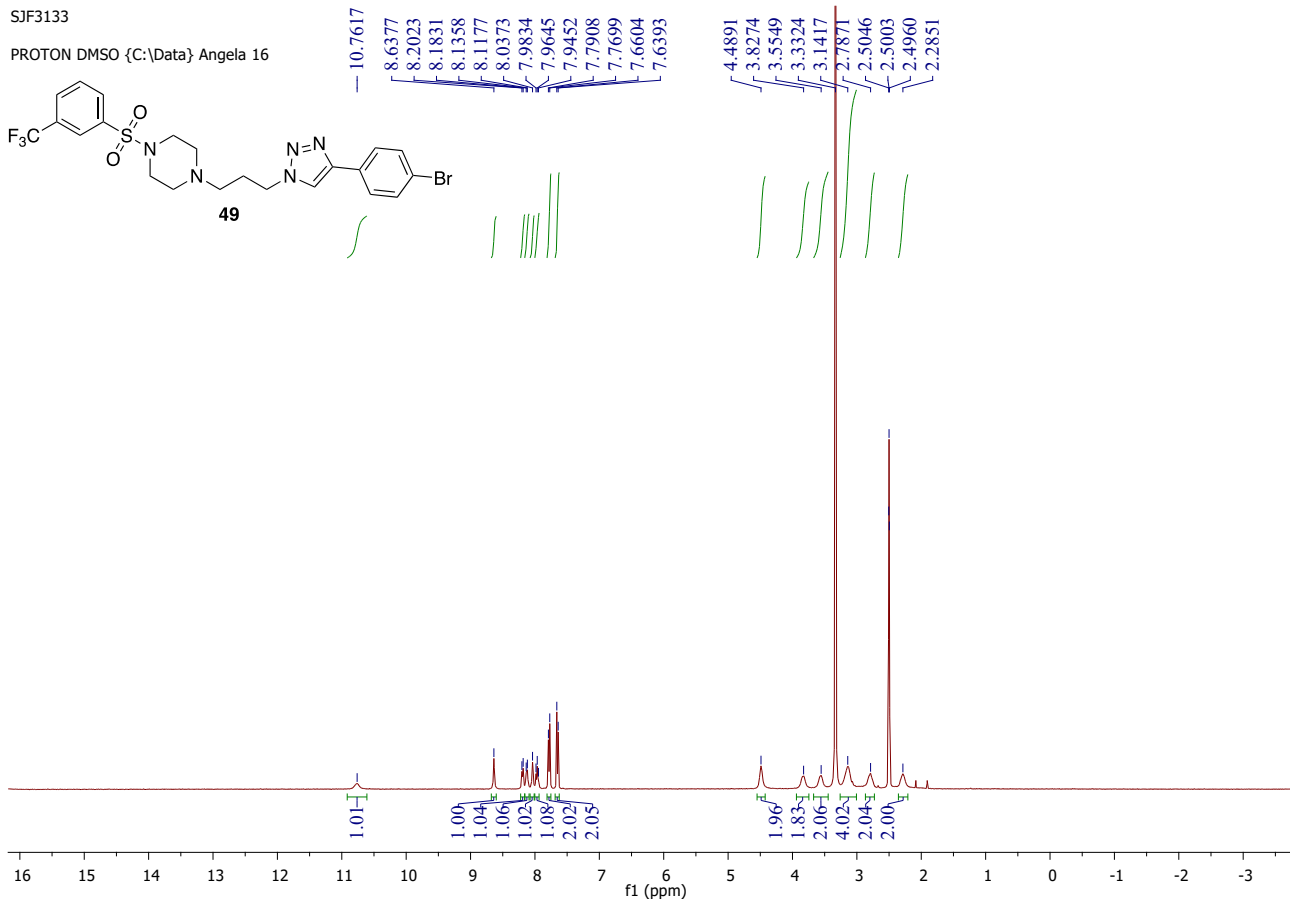
F19CPD DMSO {C:\Data} Angela 56



1-[3-[4-(4-Bromophenyl)-[1,2,3]triazol-1-yl]-propyl]-4-(3-trifluoromethylbenzenesulfonyl)-piperazine hydrochloride (49)

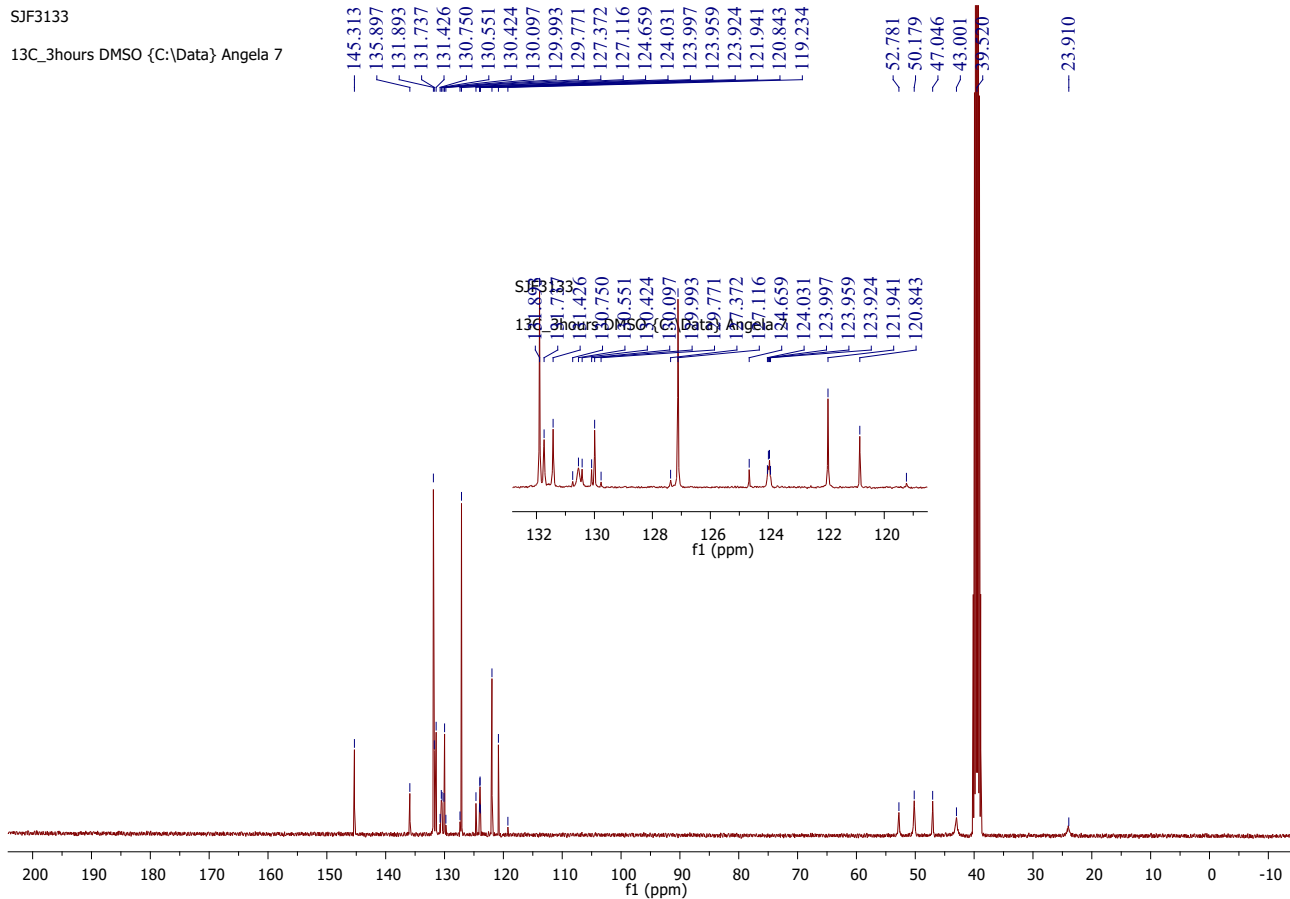
SJF3133

PROTON DMSO {C:\Data} Angela 16



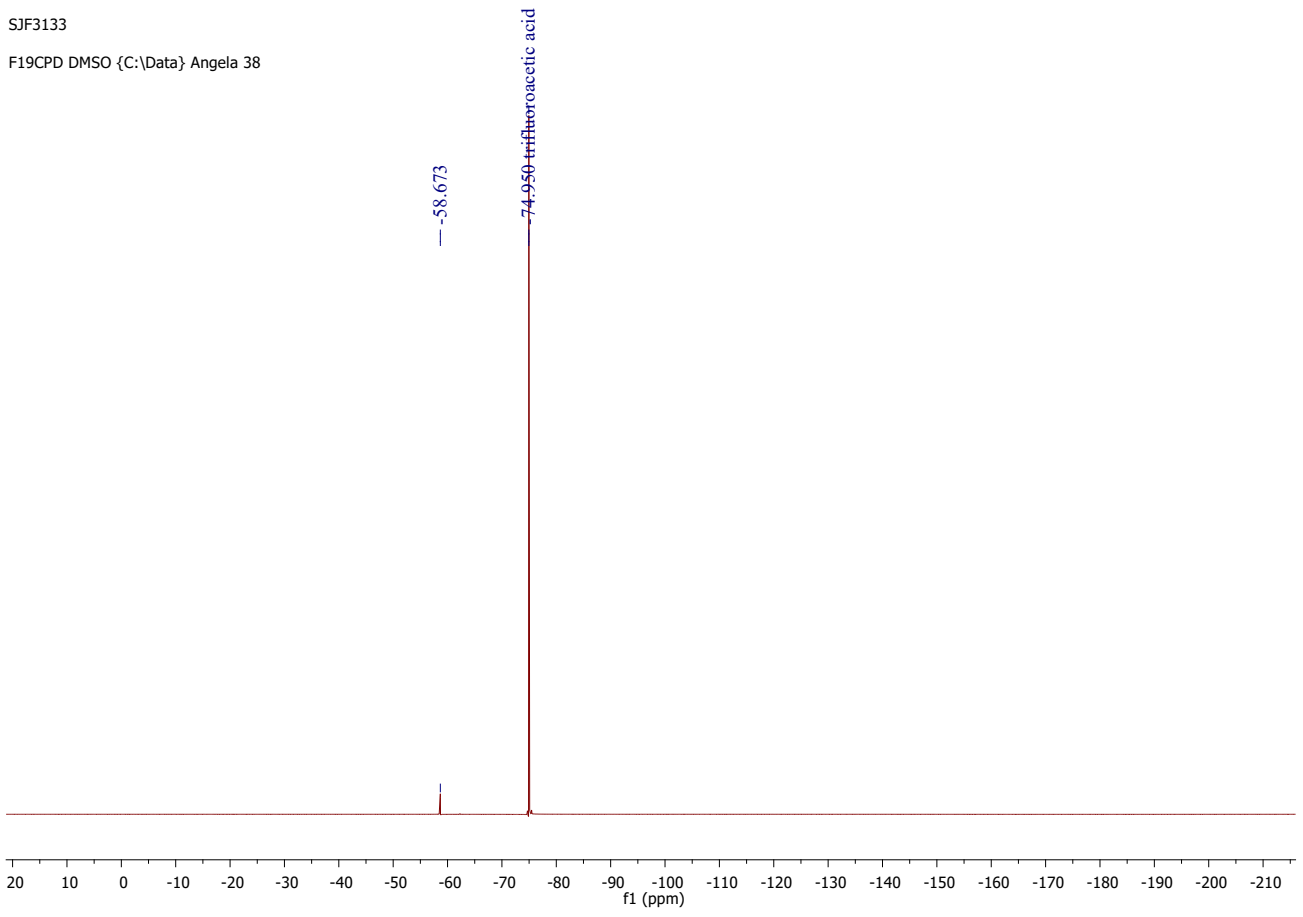
SJF3133

13C_3hours DMSO {C:\Data} Angela 7



SJF3133

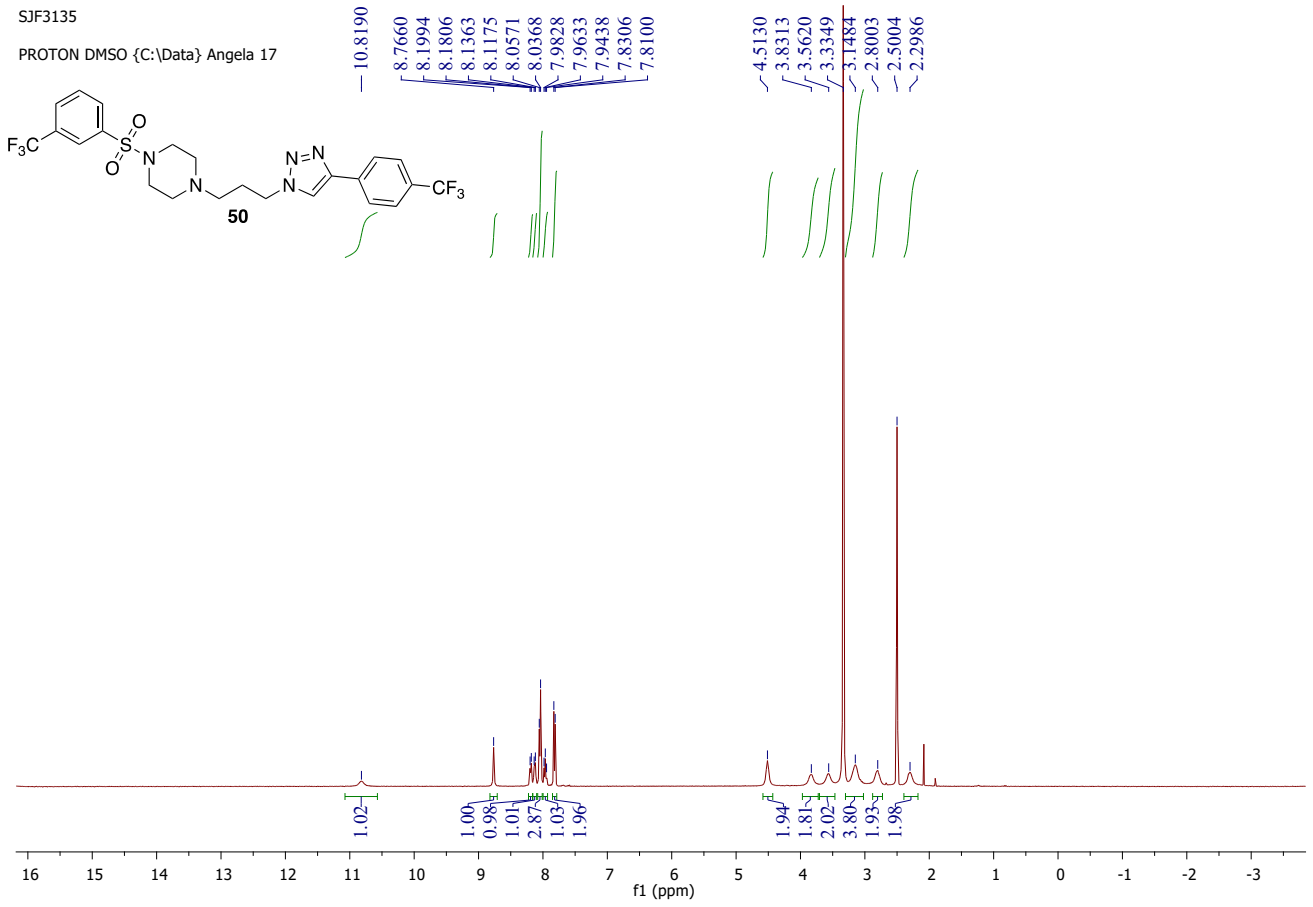
F19CPD DMSO {C:\Data} Angela 38



1-(3-Trifluoromethylbenzenesulfonyl)-4-{3-[4-(4-trifluoromethyl-phenyl)-[1,2,3]-triazol-1-yl]-propyl}-piperazine hydrochloride (50)

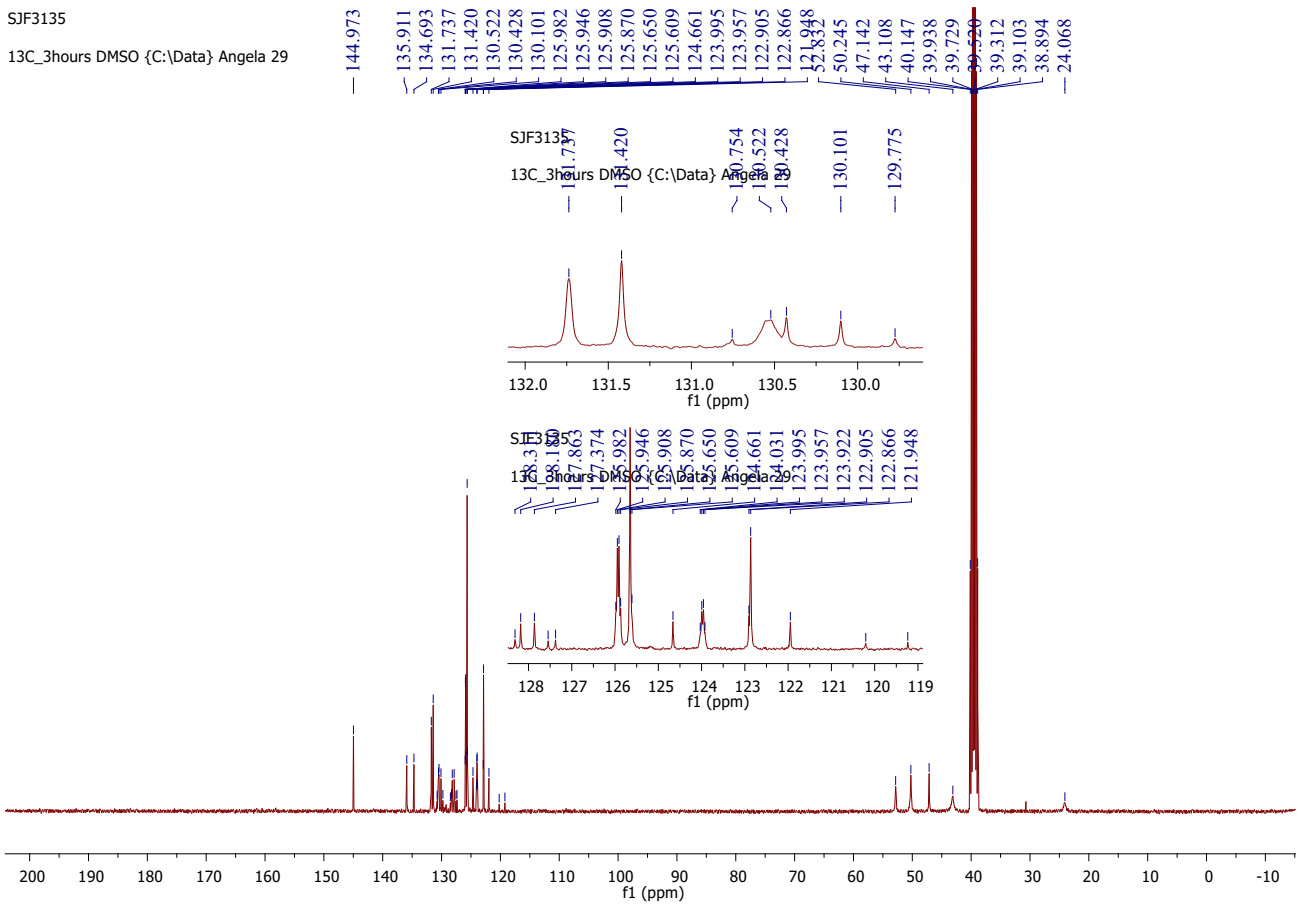
SJF3135

PROTON DMSO {C:\Data} Angela 17



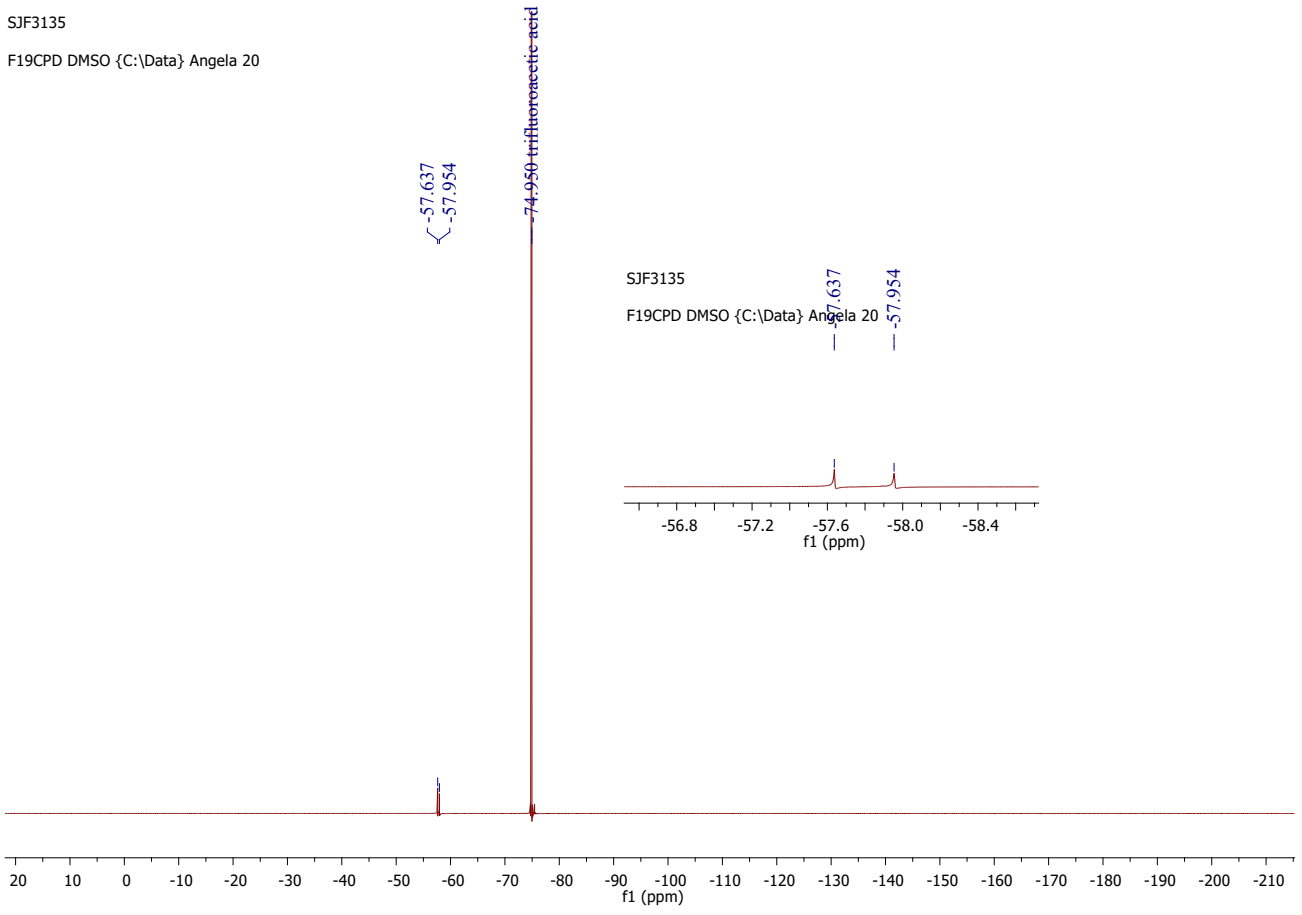
SJF3135

13C_3hours DMSO (C:\Data) Angela 29



SJF3135

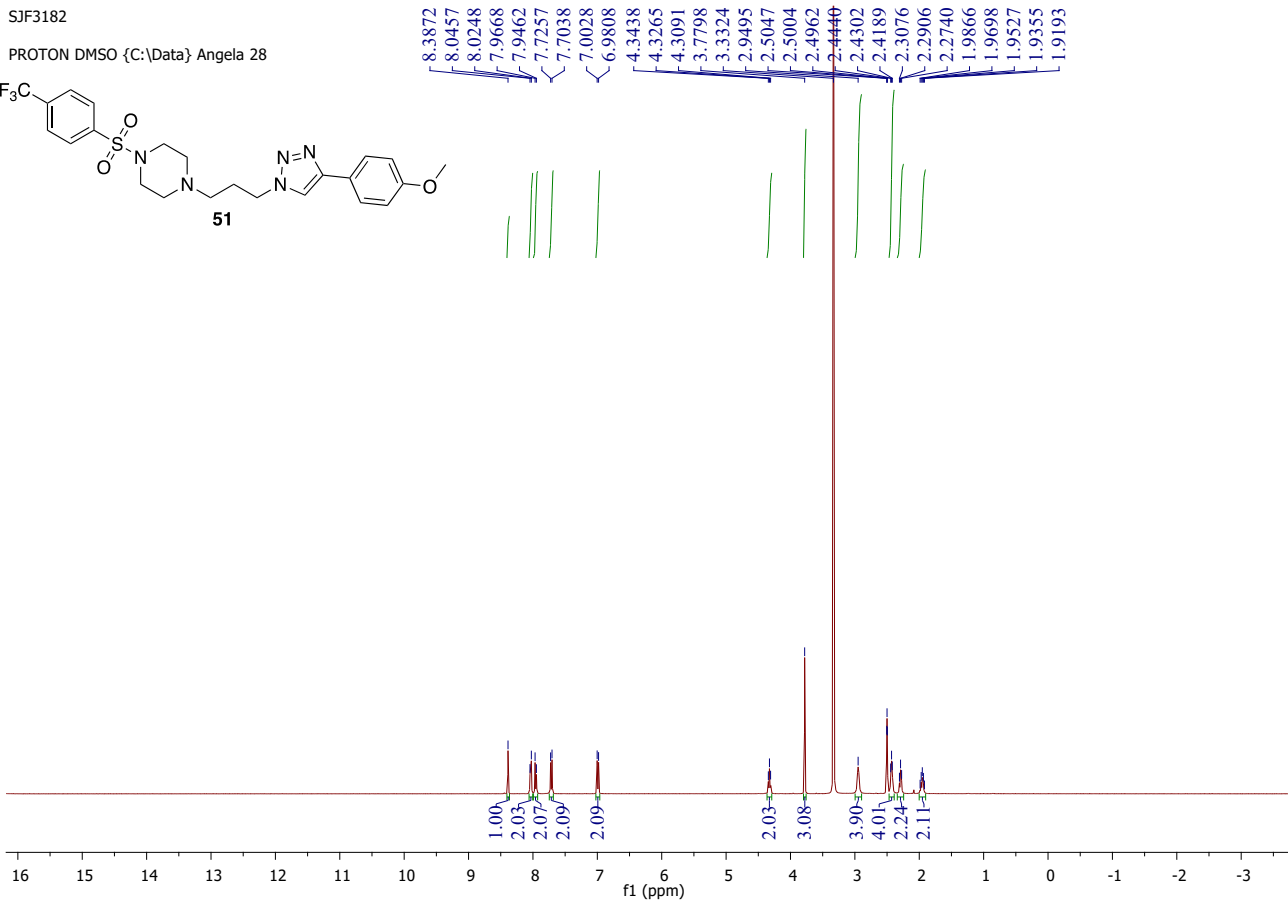
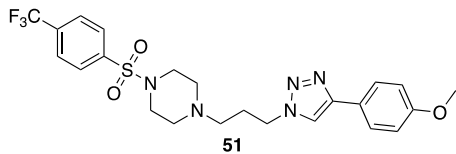
F19CPD DMSO {C:\Data} Angela 20



1-{3-[4-(4-Methoxyphenyl)-[1,2,3]triazol-1-yl]-propyl}-4-(4-trifluoromethylbenzenesulfonyl)-piperazine (51)

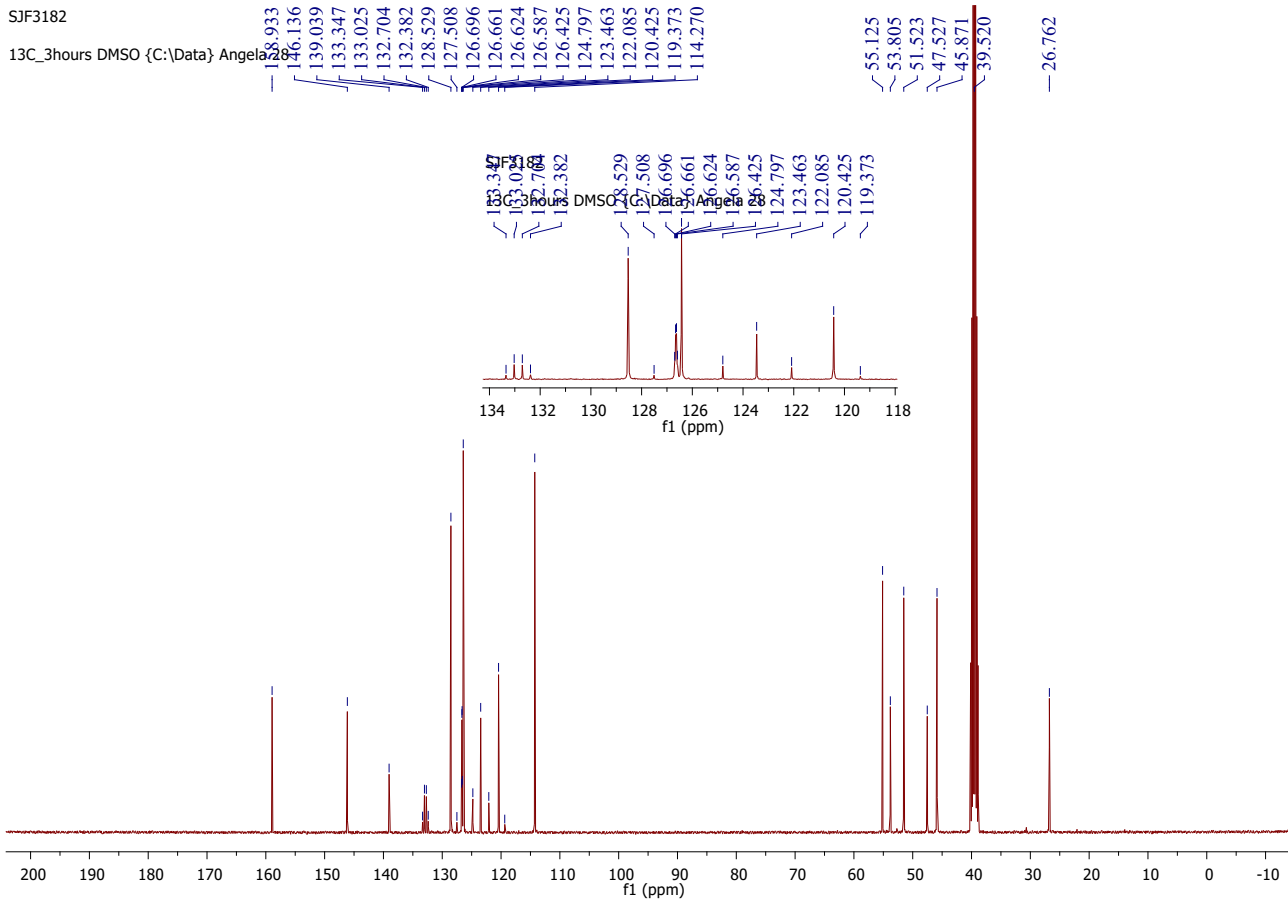
SJF3182

PROTON DMSO {C:\Data} Angela 28



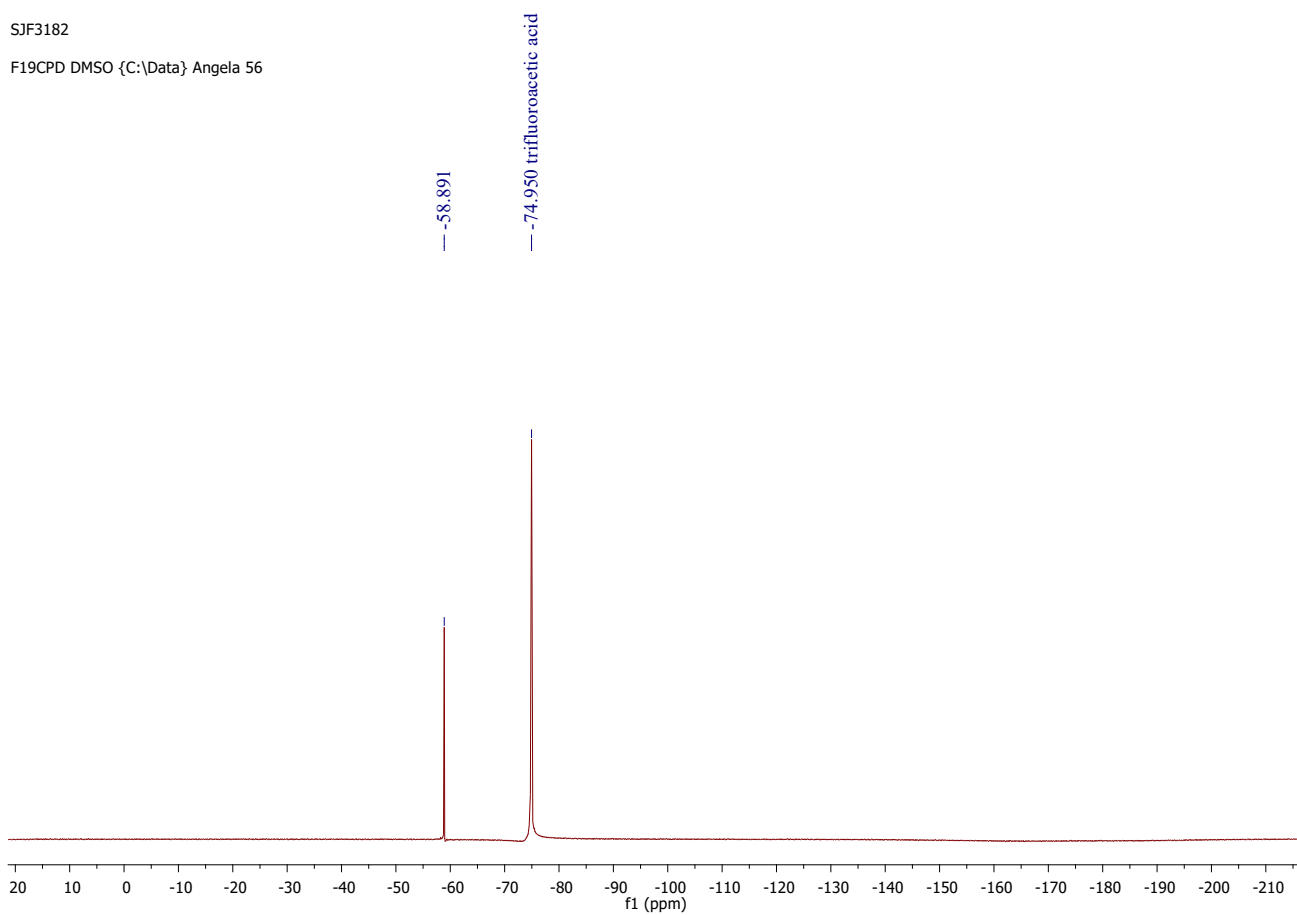
SJF3182

13C_3hours DMSO {C:\Data} Angela 28

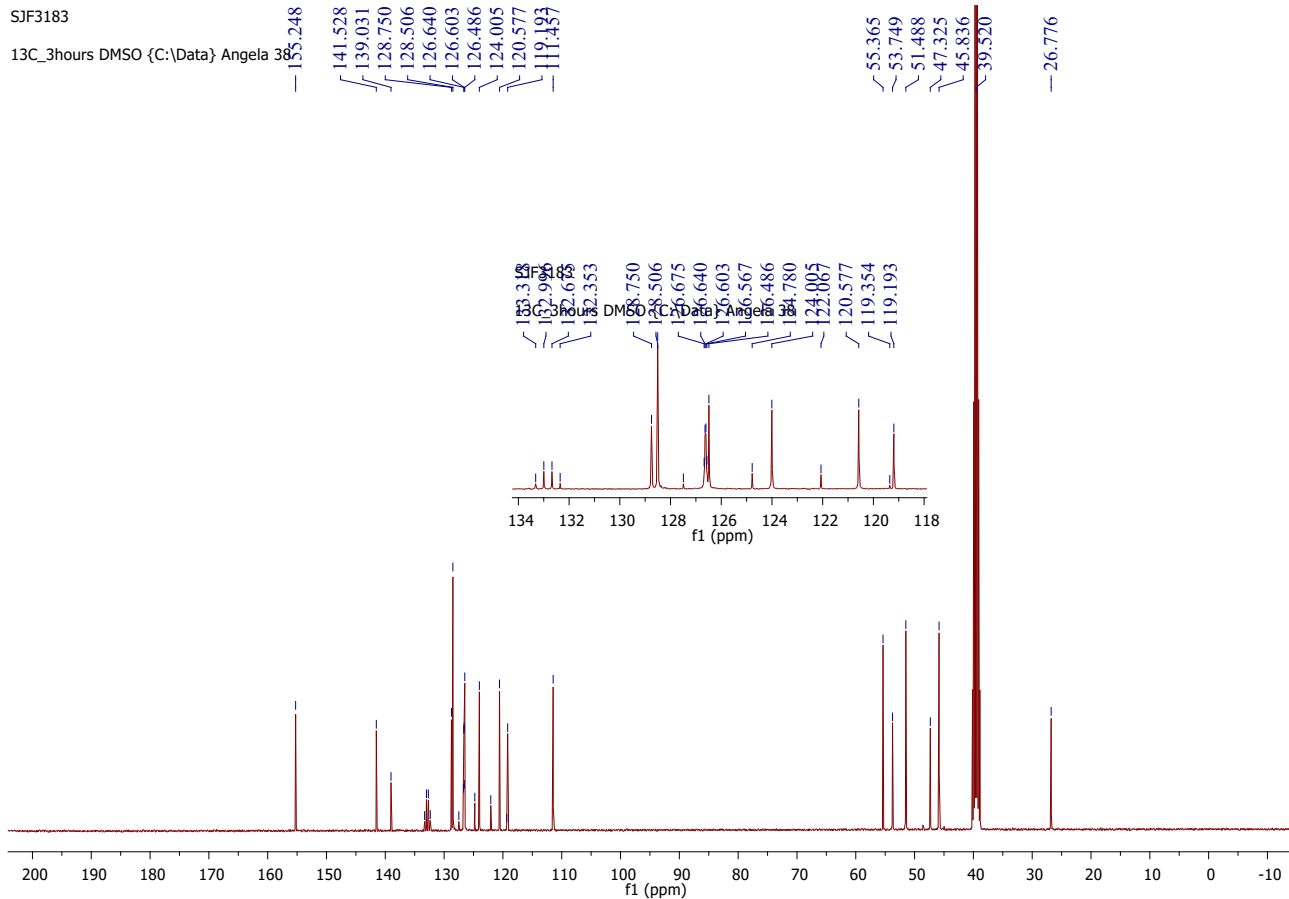
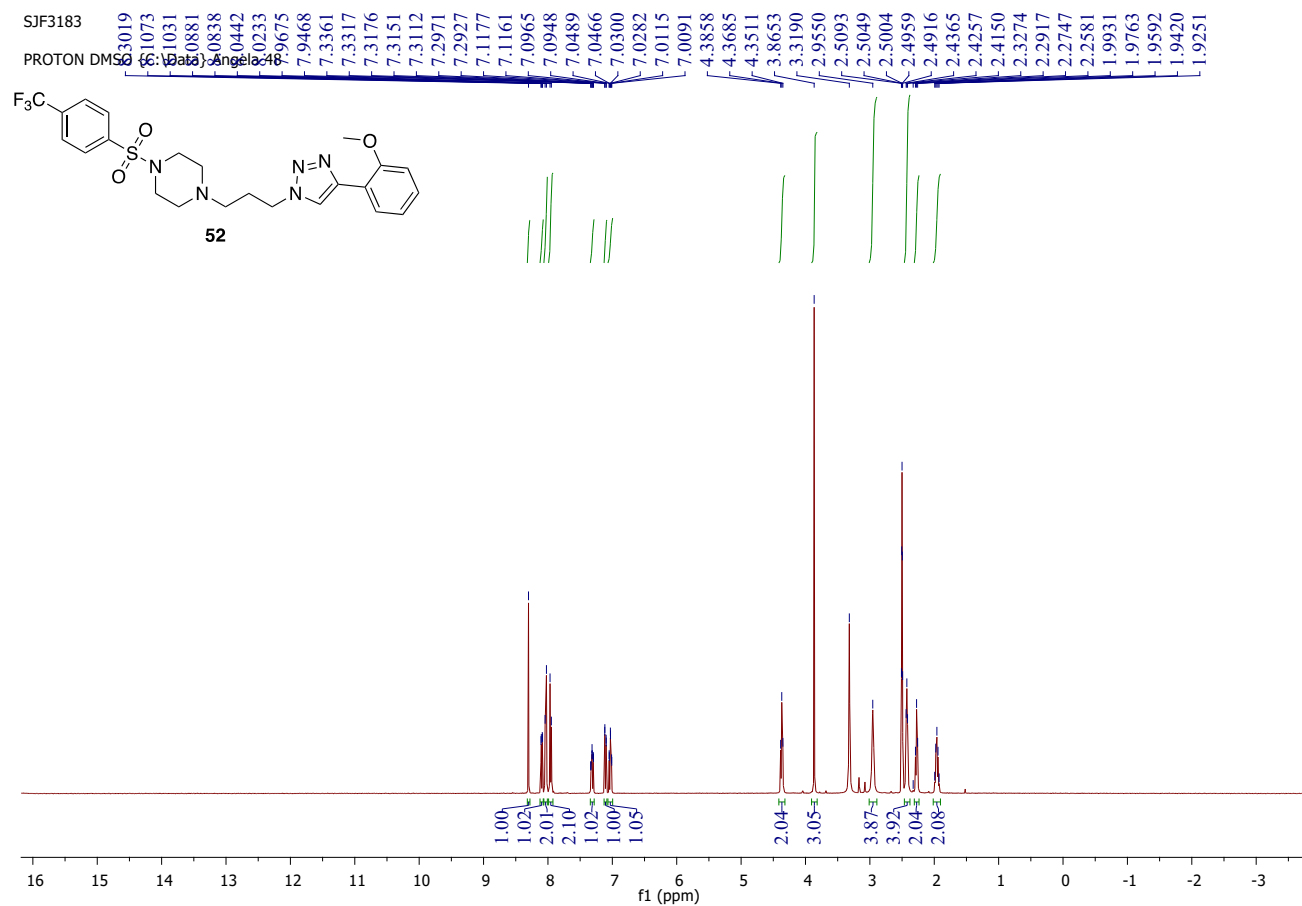


SJF3182

F19CPD DMSO {C:\Data} Angela 56



1-{3-[4-(2-Methoxyphenyl)-[1,2,3]triazol-1-yl]-propyl}-4-(4-trifluoromethylbenzenesulfonyl)-piperazine (52)



SJF3183

F19CPD DMSO {C:\Data} Angela 38

