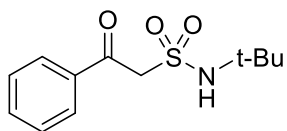
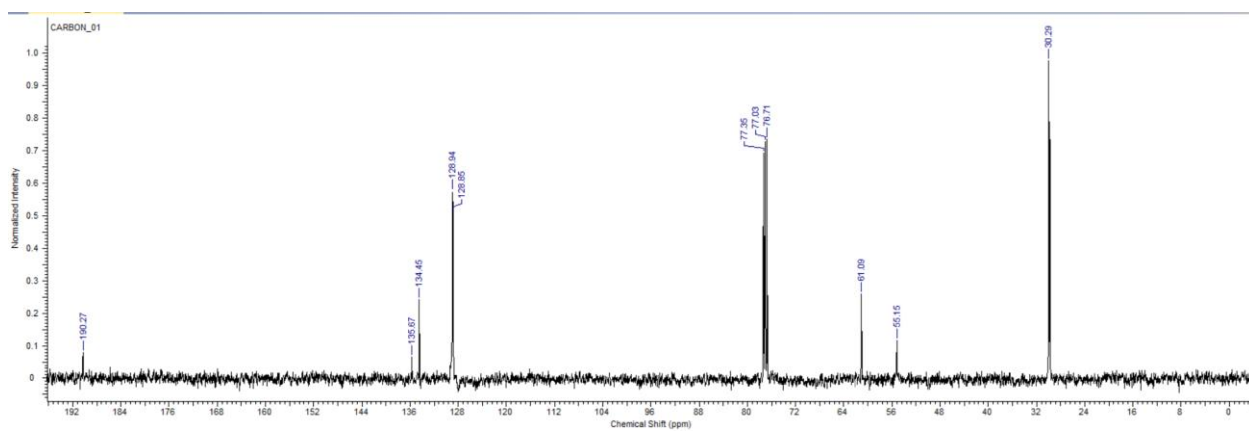
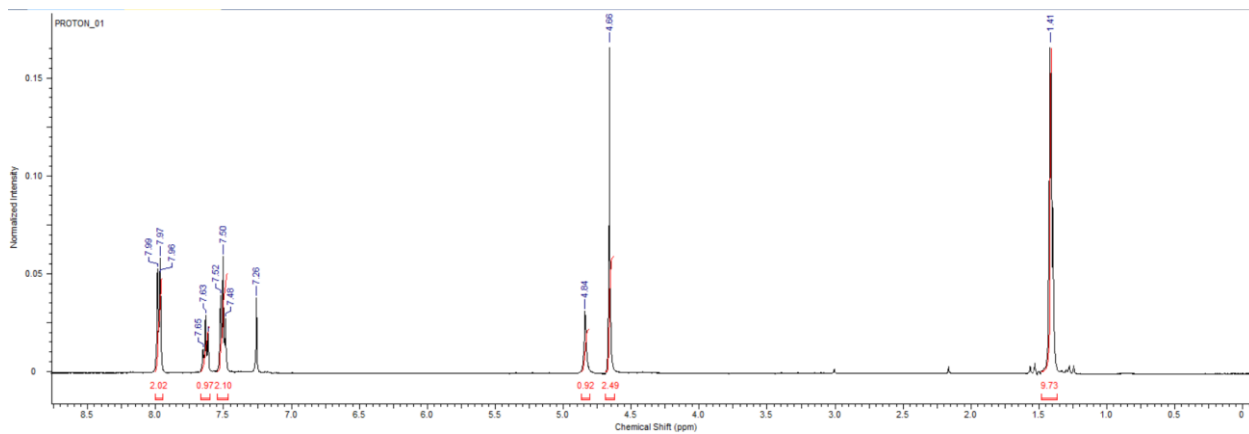


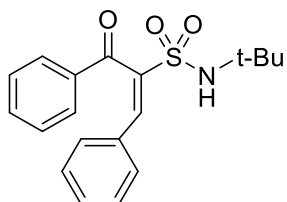
Supplementary material for the article

Synthesis and Biological Evaluation of Chalconesulfonamides: En Route to Proapoptotic
Agents with Antiestrogenic Potency

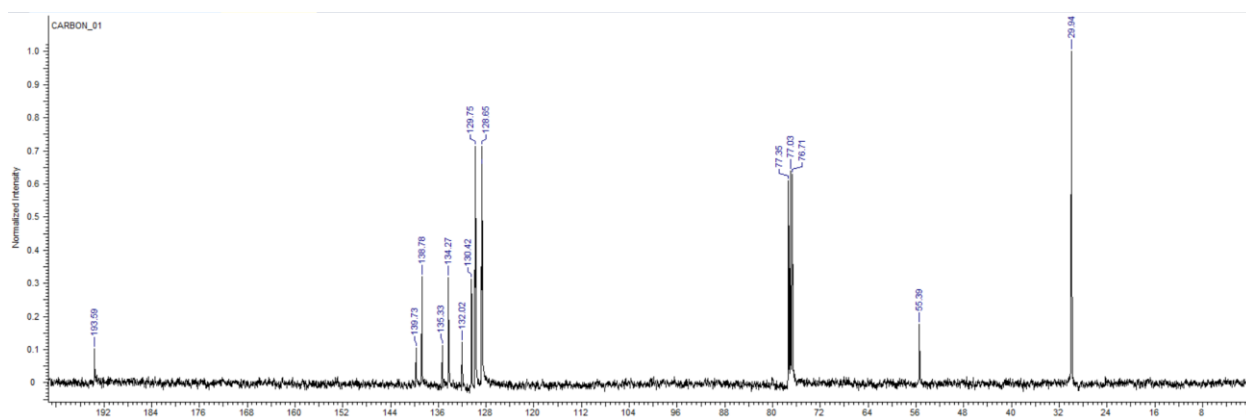
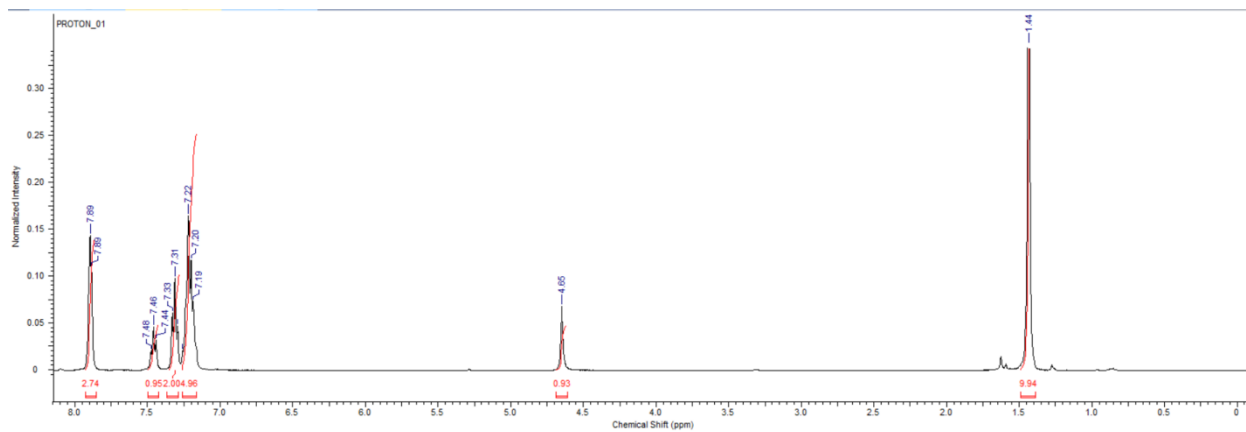


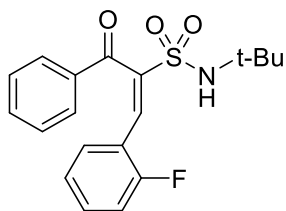
N-(*tert*-butyl)-2-oxo-2-phenylethane-1-sulfonamide (6)



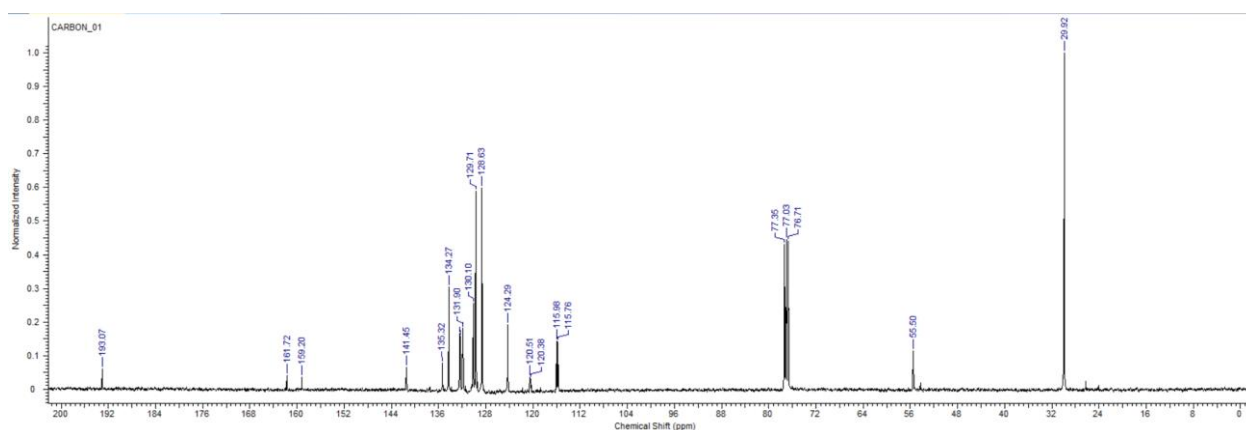
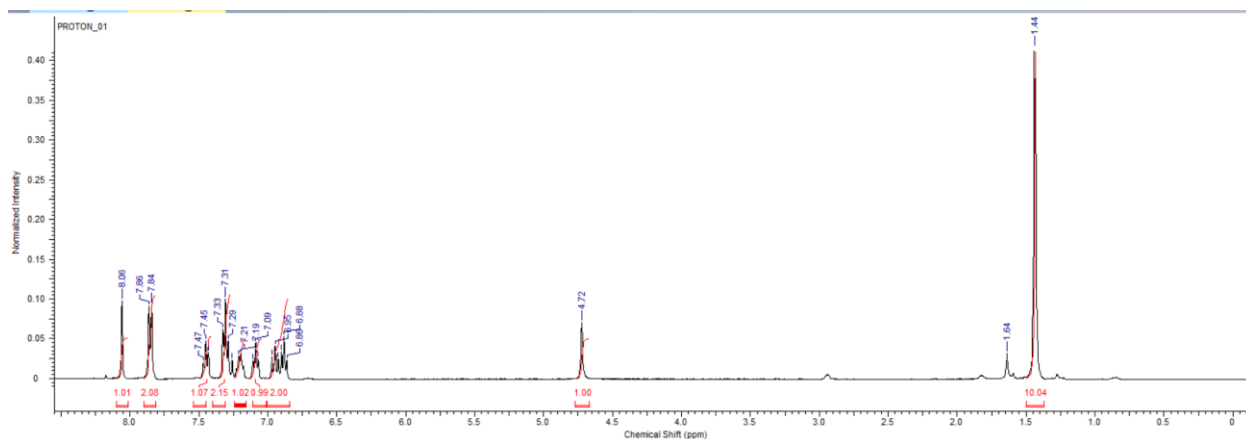


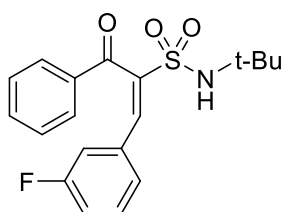
(*E*)-*N*-(*tert*-butyl)-3-oxo-1,3-diphenylprop-1-ene-2-sulfonamide (**10a**)



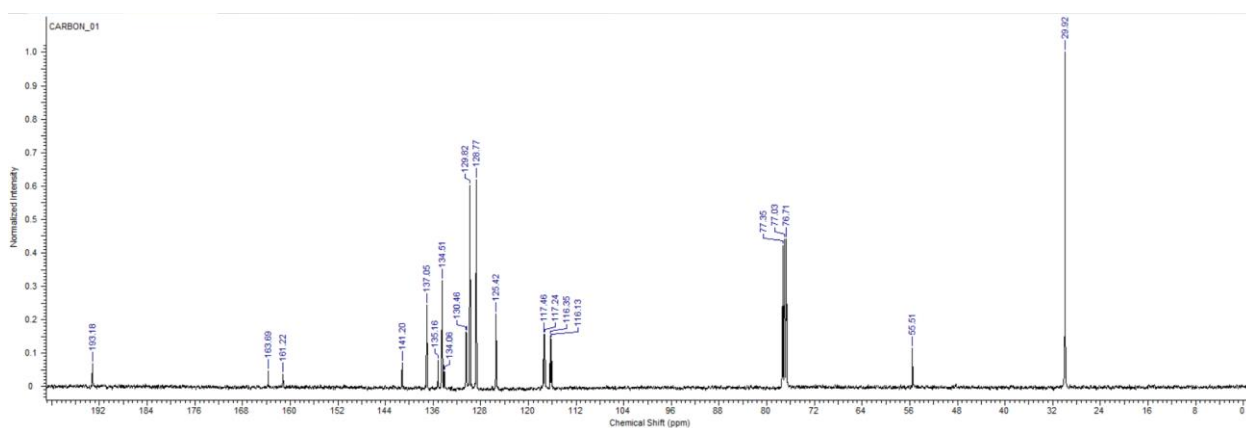
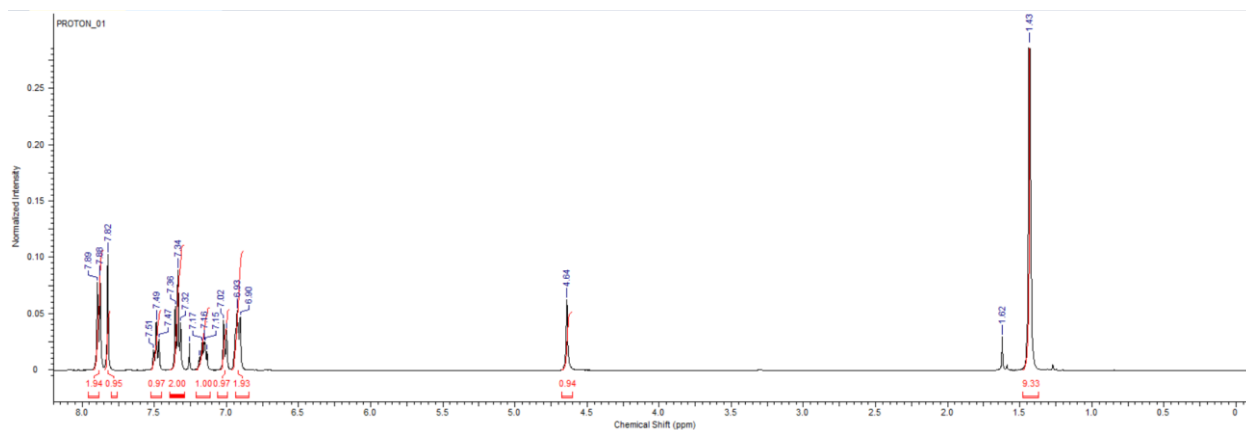


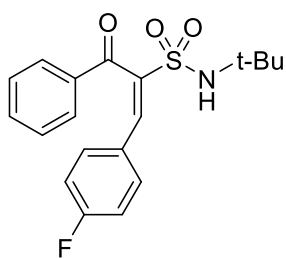
(*E*)-*N*-(*tert*-butyl)-1-(2-fluorophenyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**10b**)



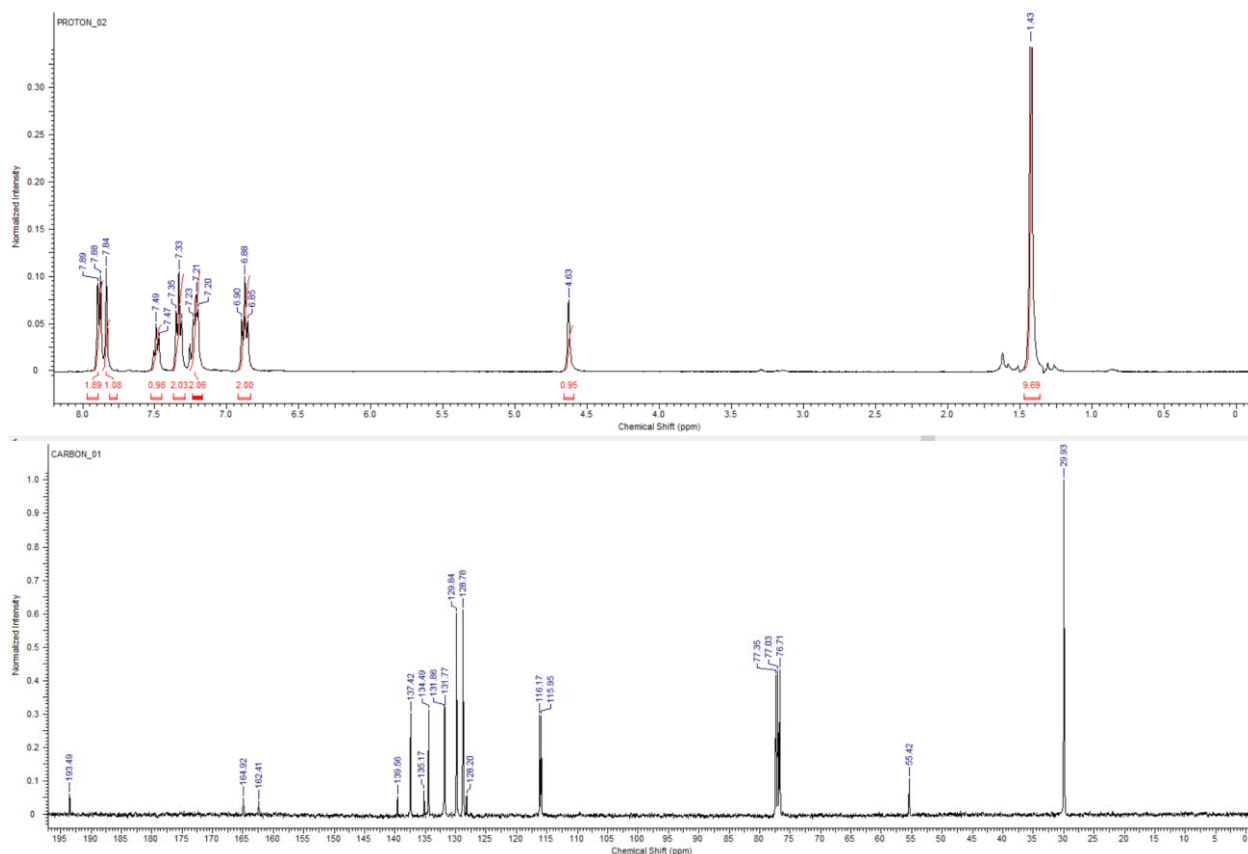


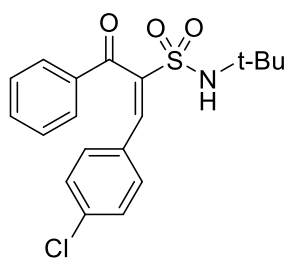
(*E*)-*N*-(*tert*-butyl)-1-(3-fluorophenyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**10c**)



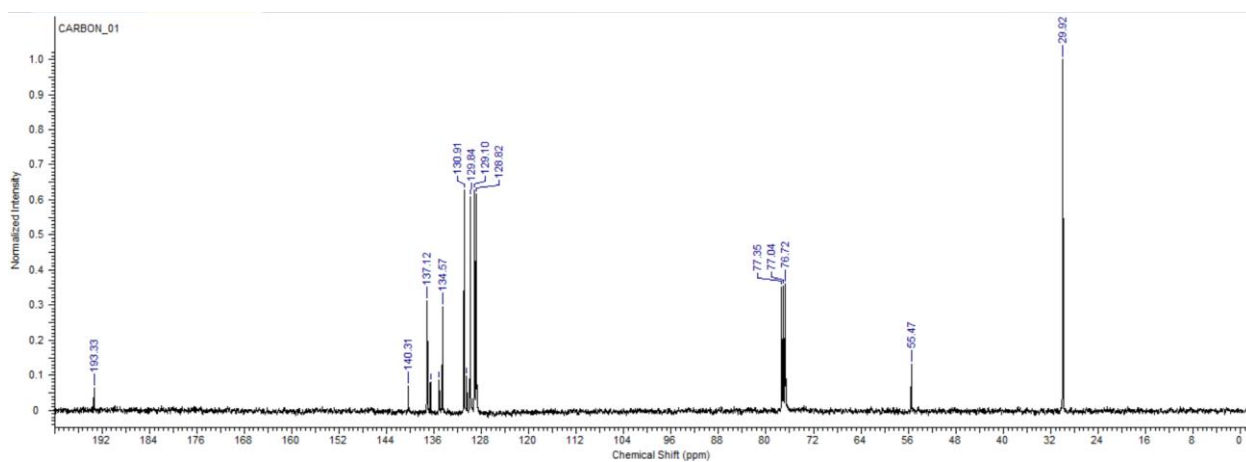
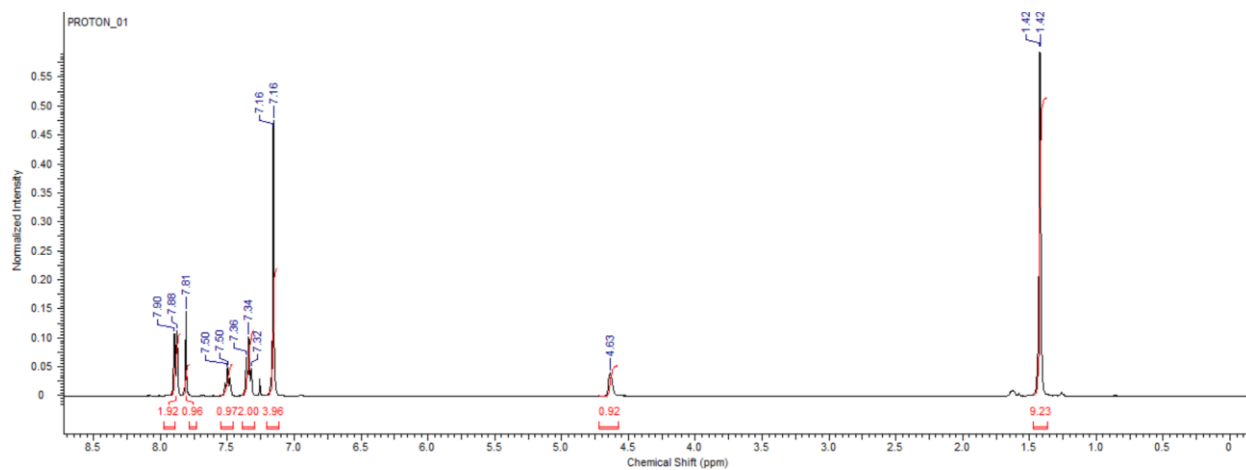


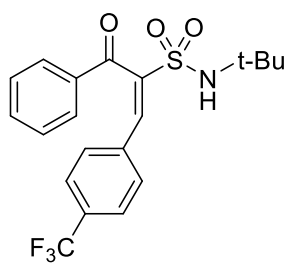
(*E*)-*N*-(*tert*-butyl)-1-(4-fluorophenyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**10d**)



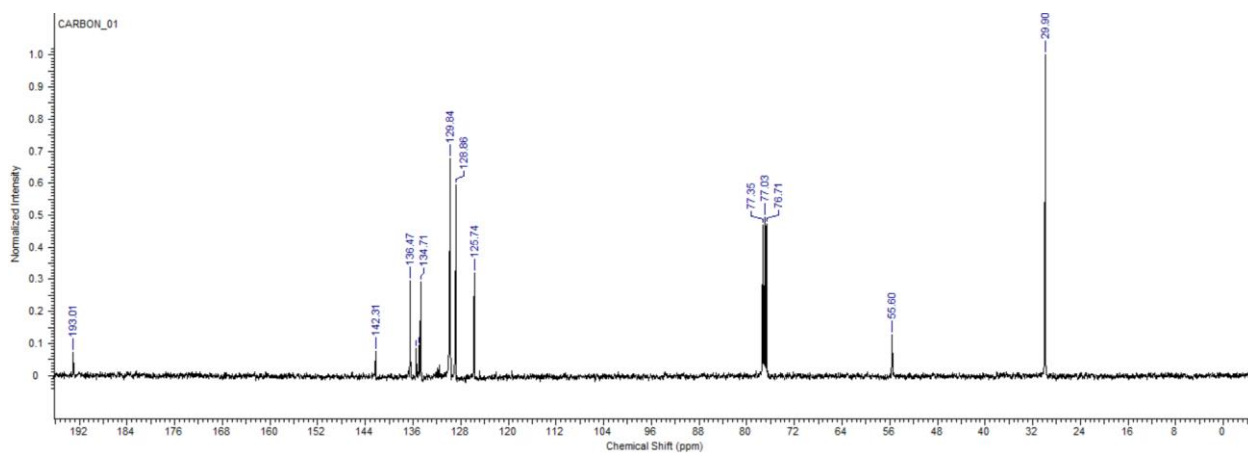
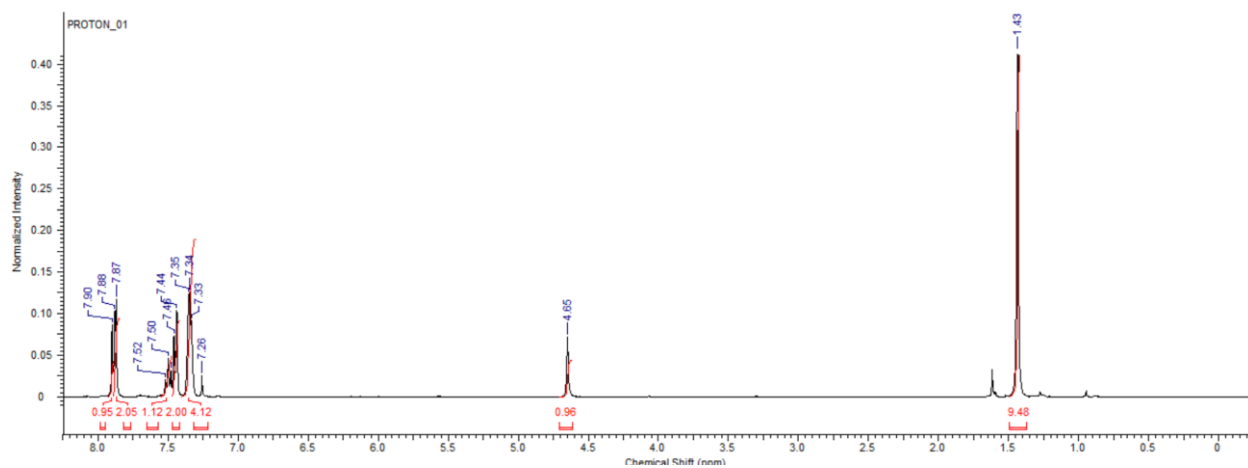


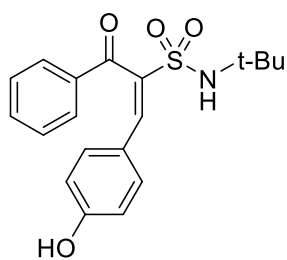
(*E*)-*N*-(*tert*-butyl)-1-(4-chlorophenyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**10e**)



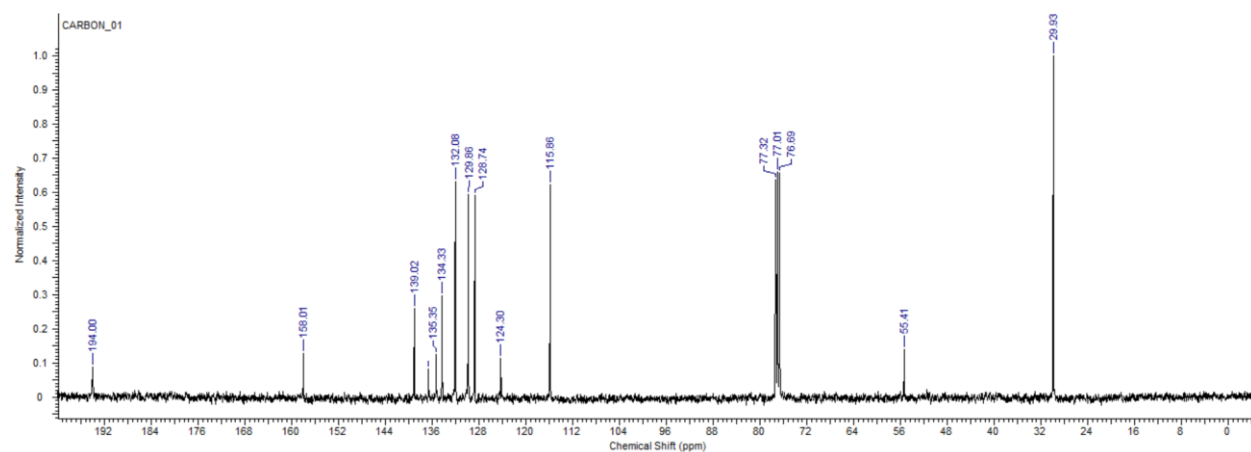
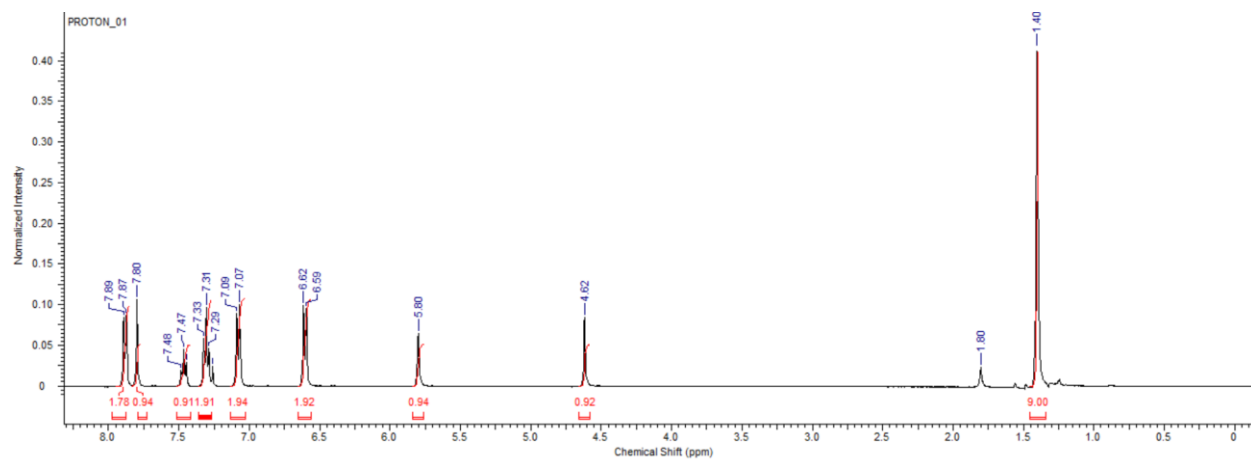


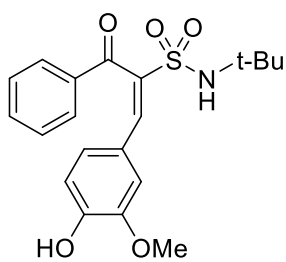
(*E*)-*N*-(*tert*-butyl)-3-oxo-3-phenyl-1-(4-(trifluoromethyl)phenyl)prop-1-ene-2-sulfonamide (**10f**)



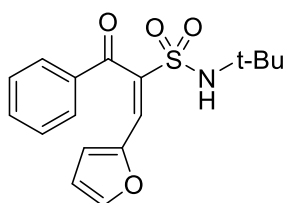
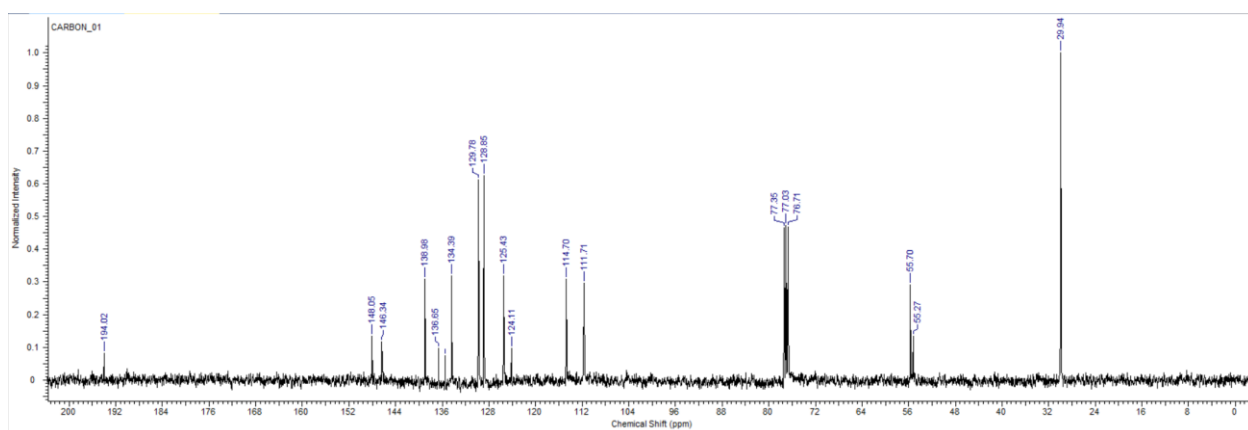
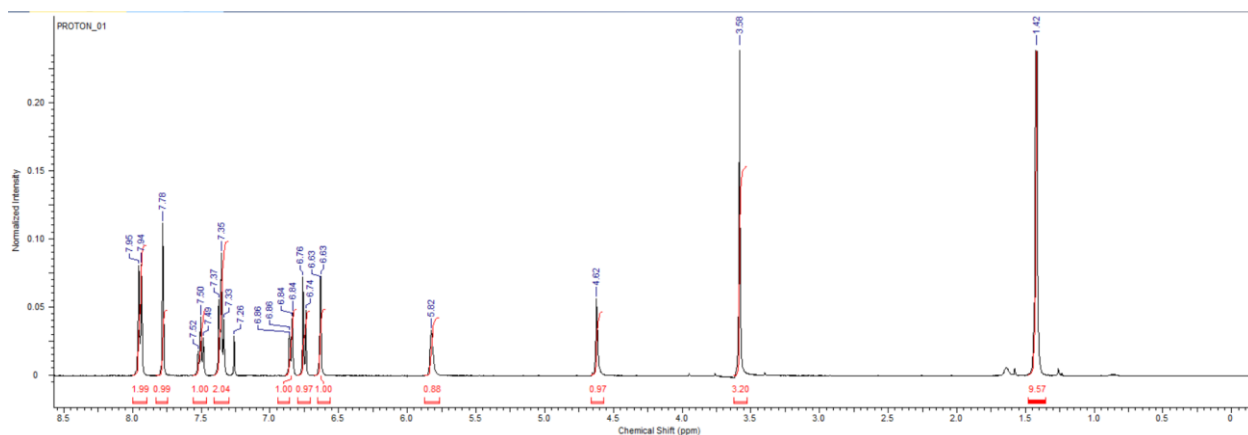


(*E*)-*N*-(*tert*-butyl)-1-(4-hydroxyphenyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**10g**)

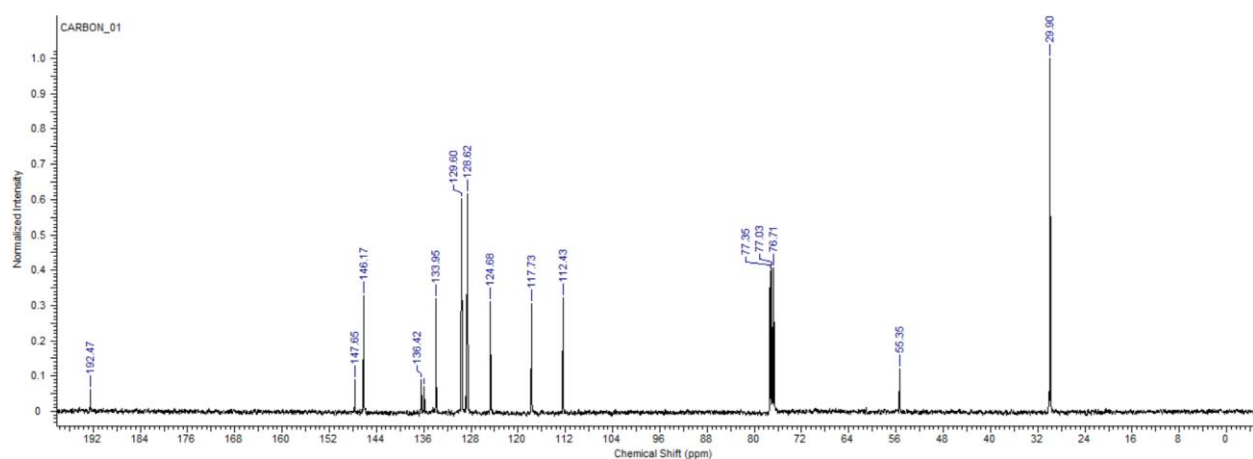
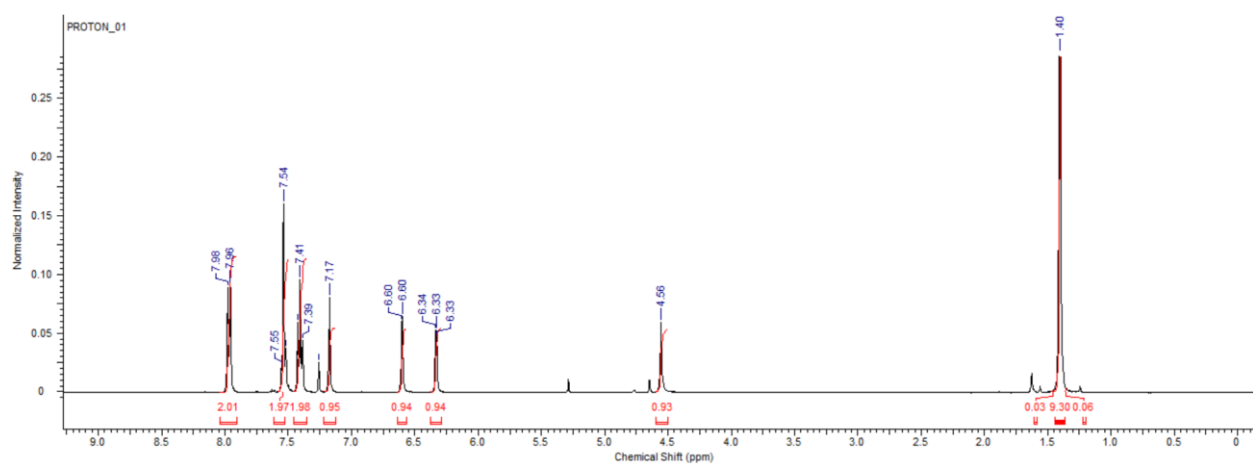


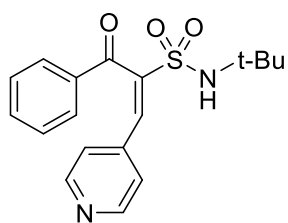


(*E*)-*N*-(*tert*-butyl)-1-(4-hydroxy-3-methoxyphenyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**10h**)

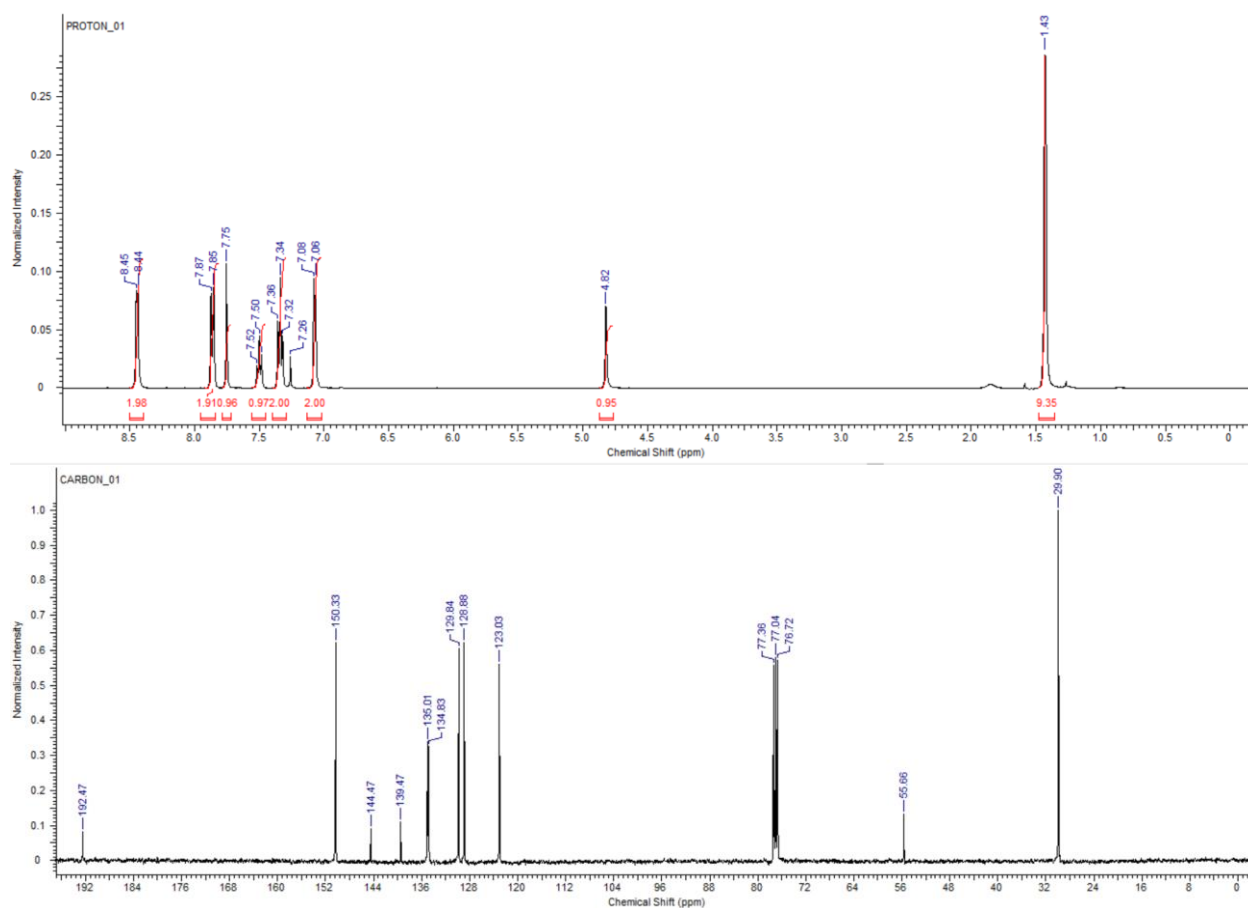


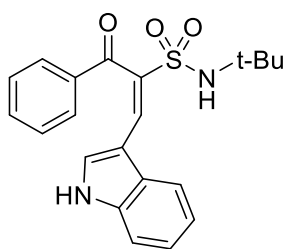
(*E*)-*N*-(*tert*-butyl)-1-(furan-2-yl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**10i**)



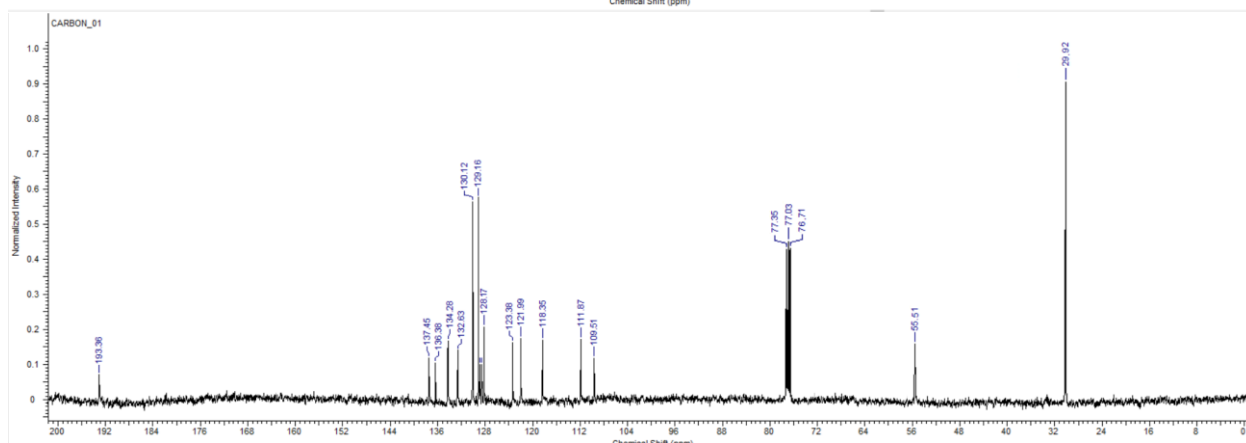
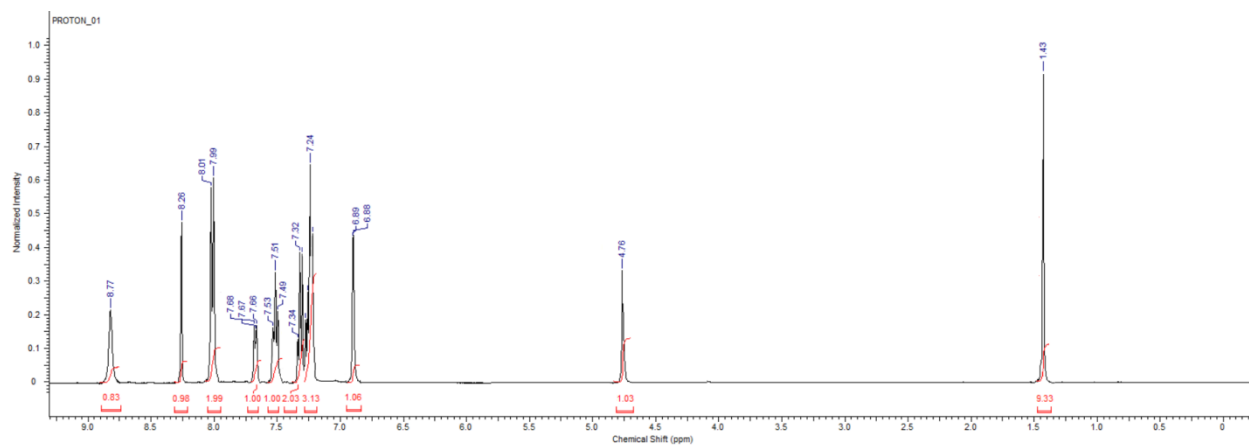


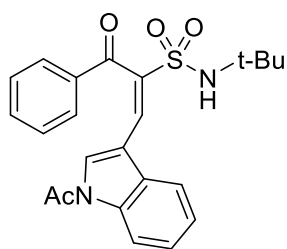
(E)-N-(*tert*-butyl)-3-oxo-3-phenyl-1-(pyridin-4-yl)prop-1-ene-2-sulfonamide (**10j**)



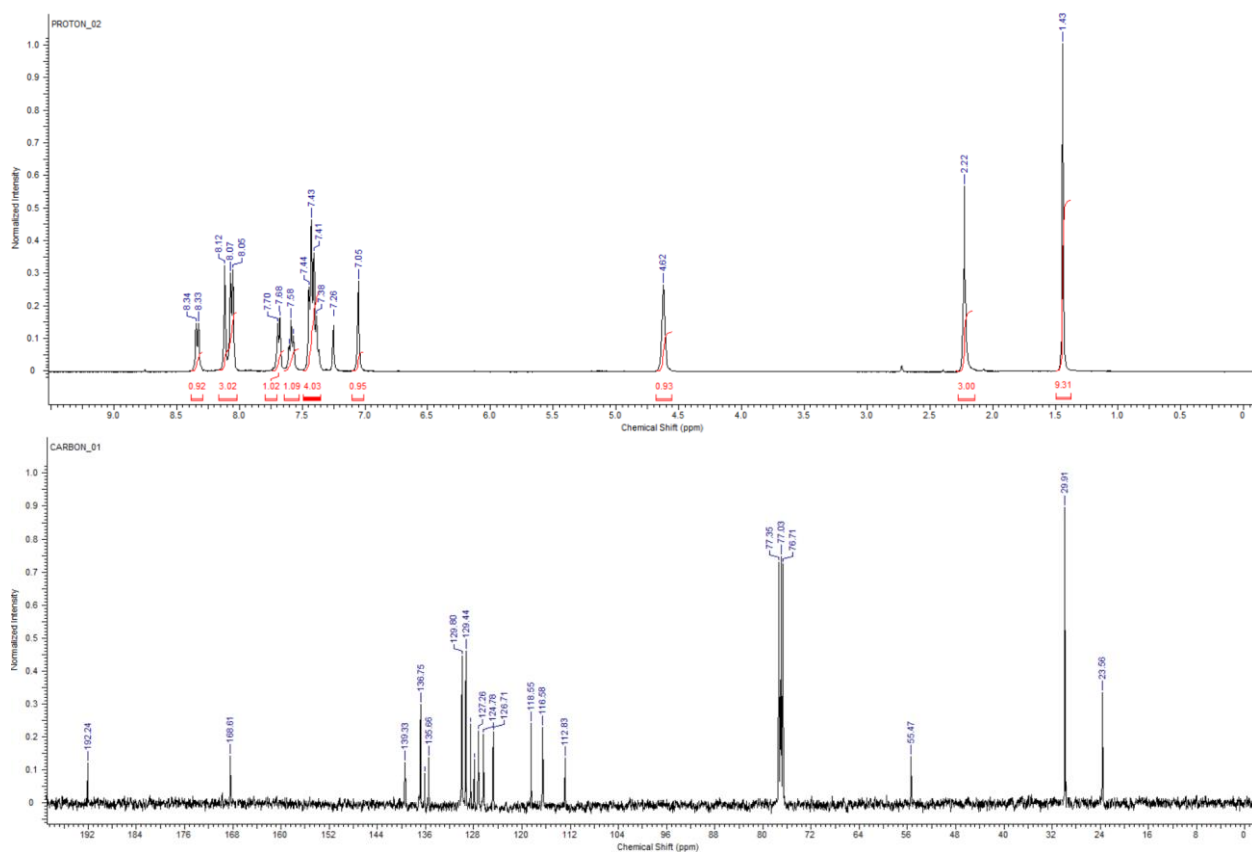


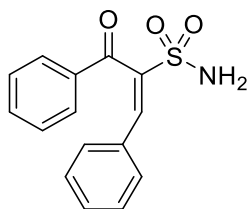
(*E*)-1-(1*H*-Indol-3-yl)- *N*-(*tert*-butyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**10k**).



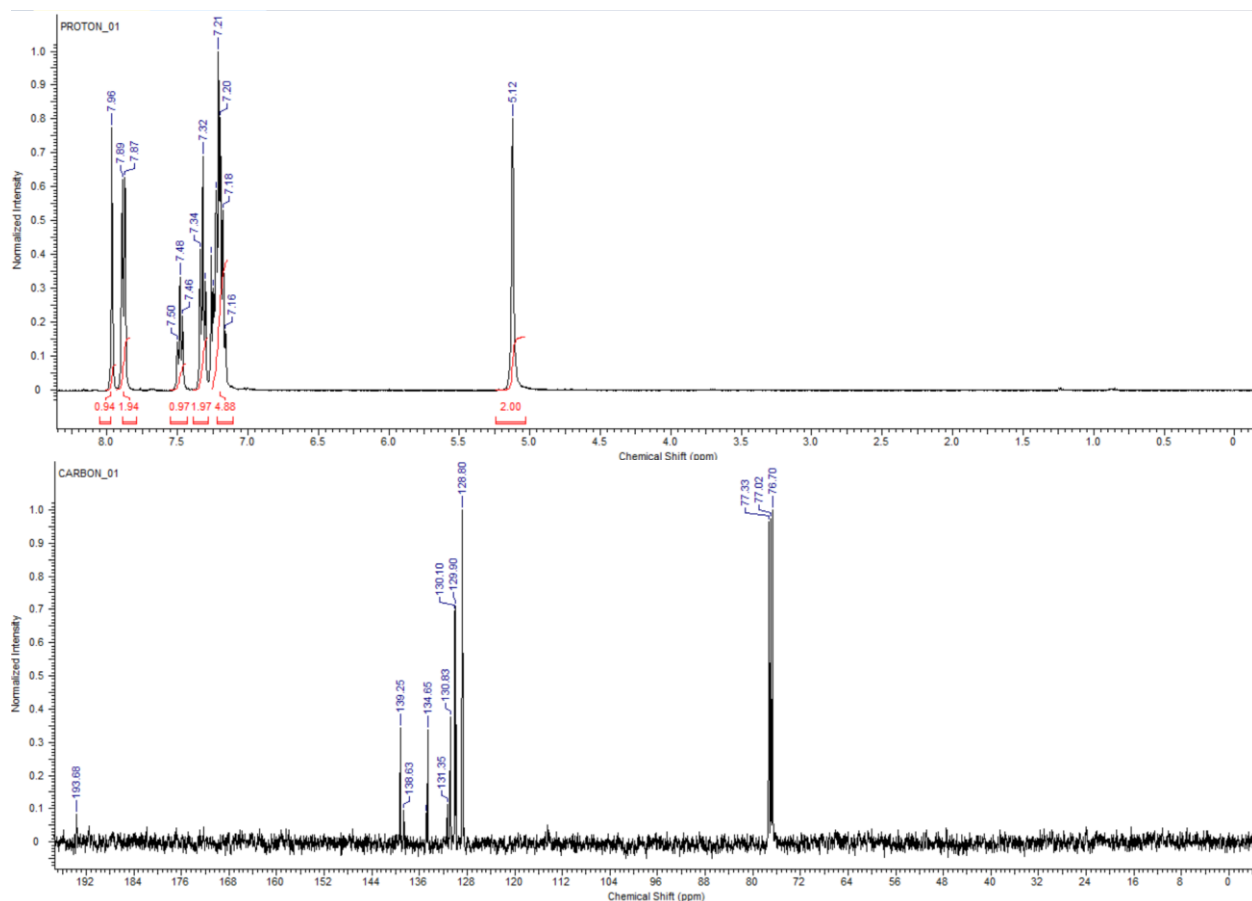


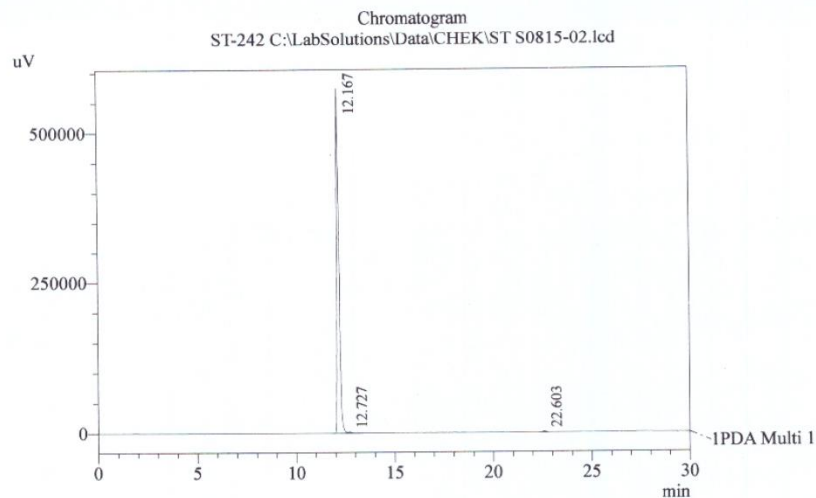
(E)-1-(1-Acetyl-1H-indol-3-yl)-N-(*tert*-butyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide
(101)





(E)-3-oxo-1,3-diphenylprop-1-ene-2-sulfonamide (7a)





1 PDA Multi 1 / 260nm 4nm

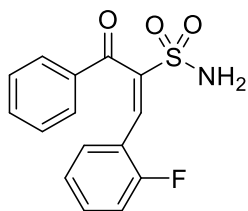
PDA Ch1 260nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	12.167	4937769	572939	99.332
2	12.727	21106	1981	0.425
3	22.603	12086	1517	0.243
Total		4970960	576437	100.000

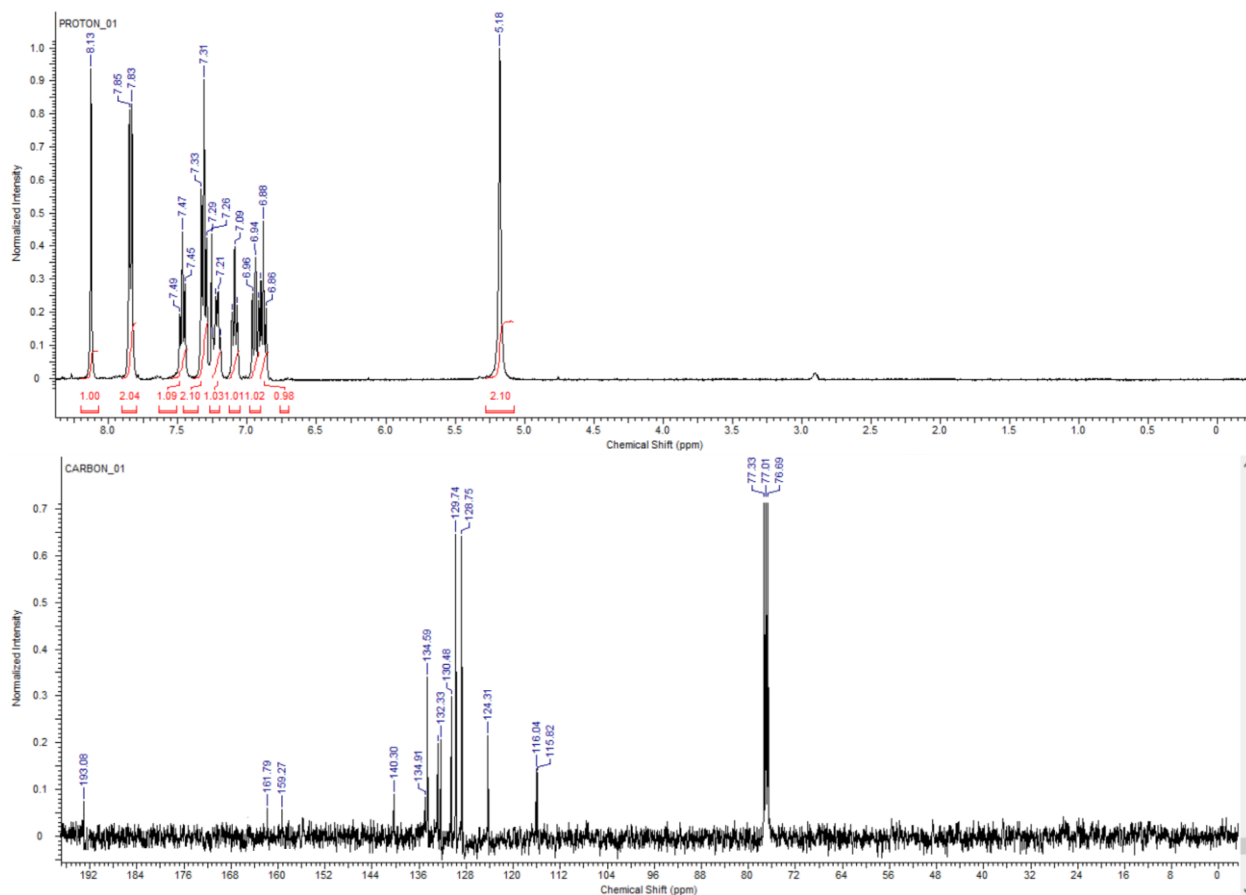
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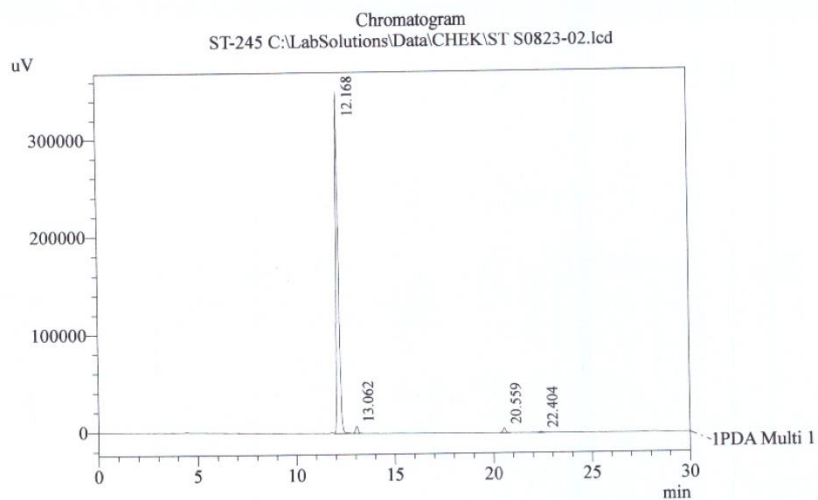
Time	Unit	Command	Value
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	90
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mk. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl



(*E*)-1-(2-fluorophenyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**7b**)





1 PDA Multi 1 / 260nm 4nm

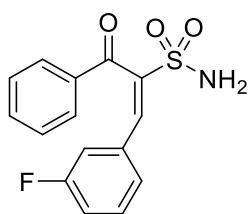
PDA Ch1 260nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	12.168	3230131	351062	96.099
2	13.062	68951	7340	2.051
3	20.559	51609	5055	1.535
4	22.404	10563	946	0.314
Total		3361254	364403	100.000

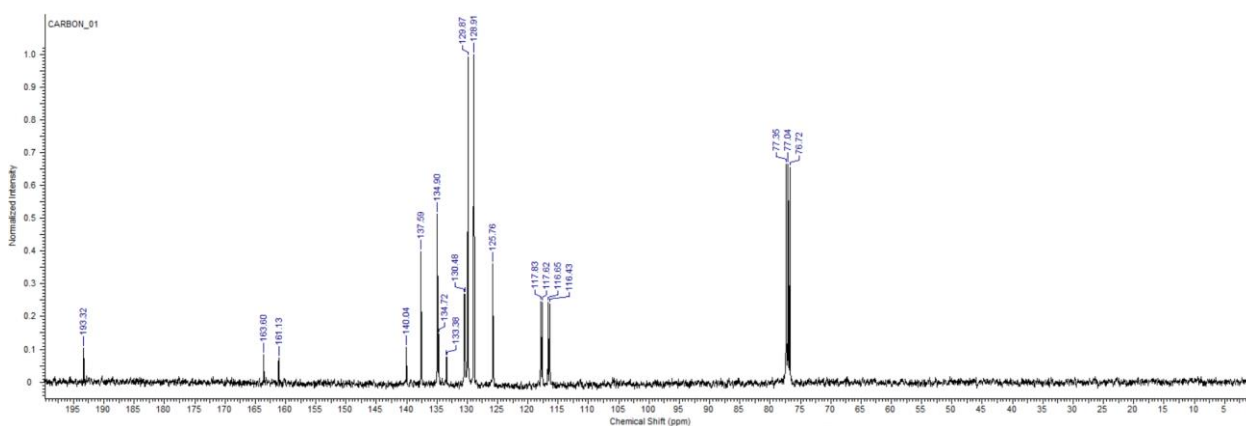
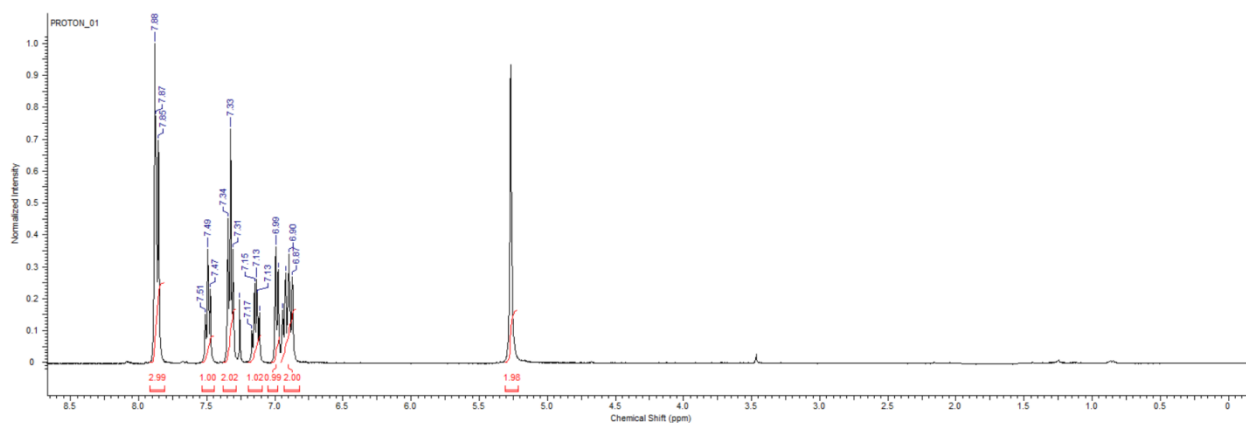
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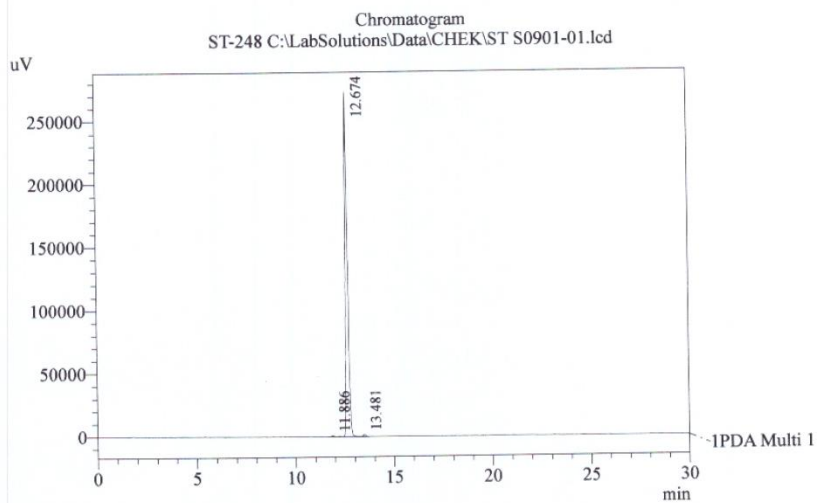
Time	Unit	Command	Value
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	90
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl



(*E*)-1-(3-fluorophenyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**7c**)





1 PDA Multi 1 / 260nm 4nm

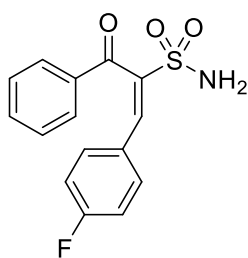
PDA Ch1 260nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	11.886	10774	877	0.441
2	12.674	2415255	273682	98.970
3	13.481	14374	1610	0.589
Total		2440404	276169	100.000

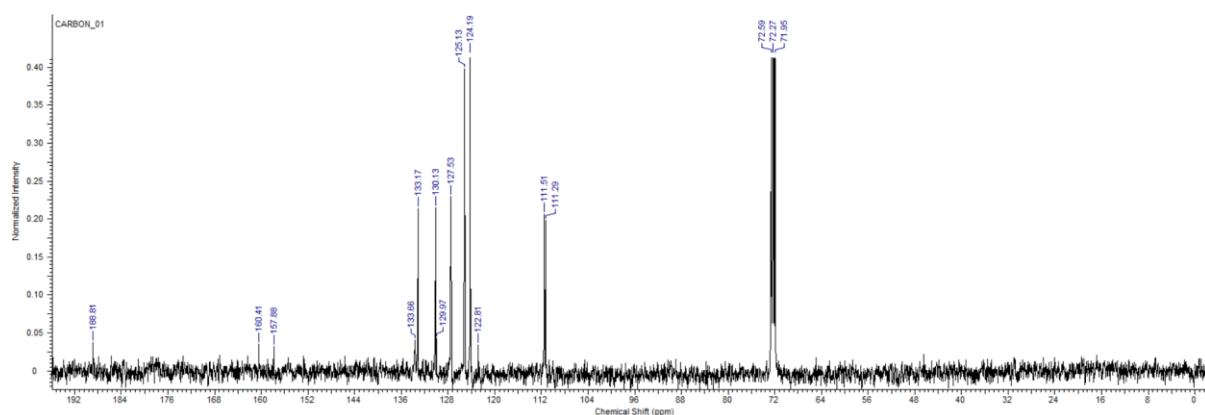
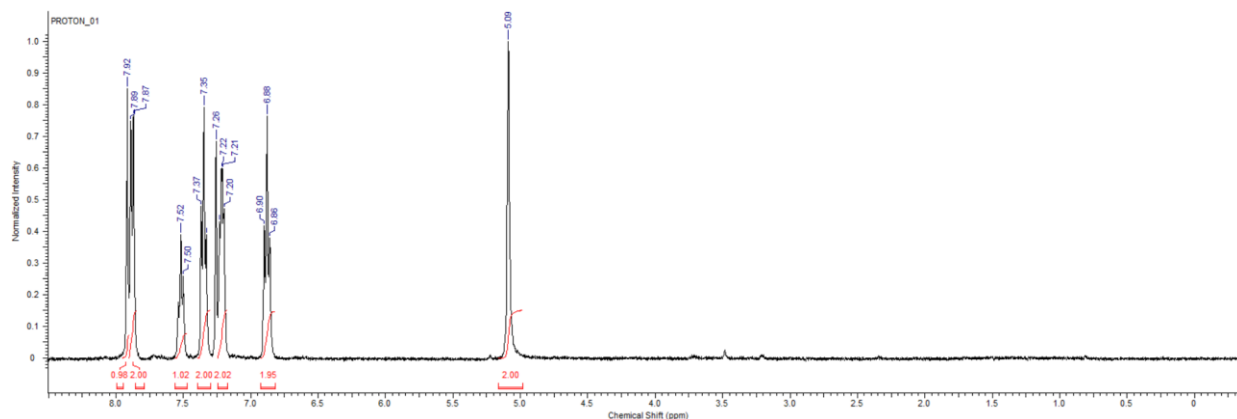
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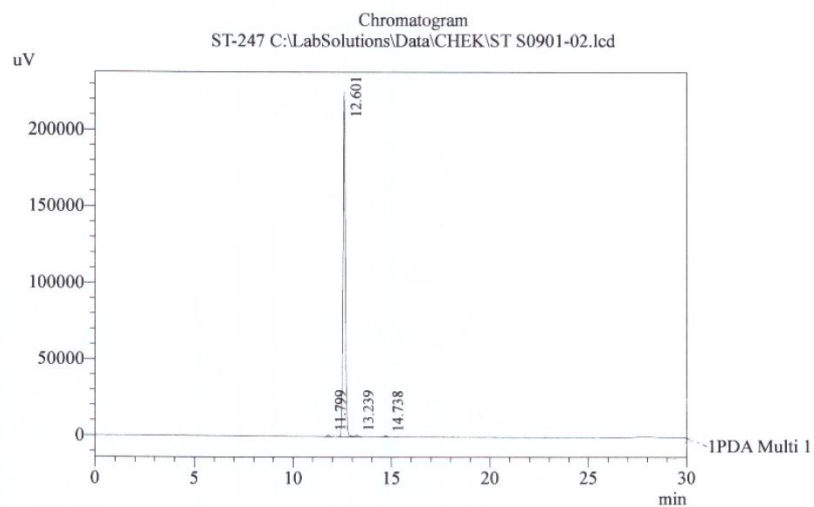
Time	Unit	Command	Valu
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	90
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl



(*E*)-1-(4-fluorophenyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**7d**)





1 PDA Multi 1 / 260nm 4nm

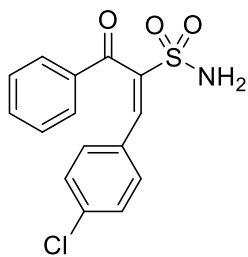
PDA Ch1 260nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	11.799	11438	1248	0.570
2	12.601	1975737	225727	98.414
3	13.239	13287	1223	0.662
4	14.738	7108	707	0.354
Total		2007569	228905	100.000

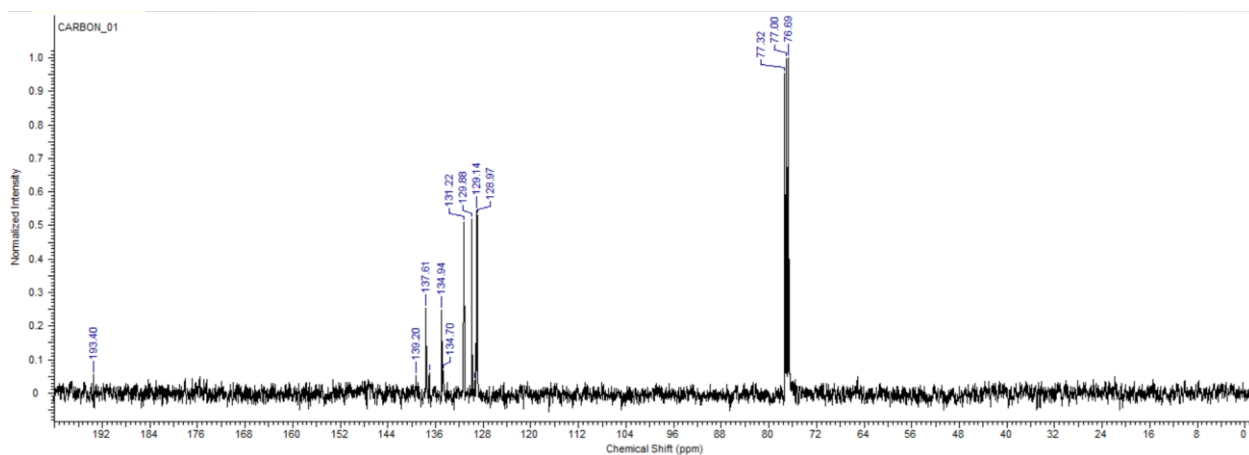
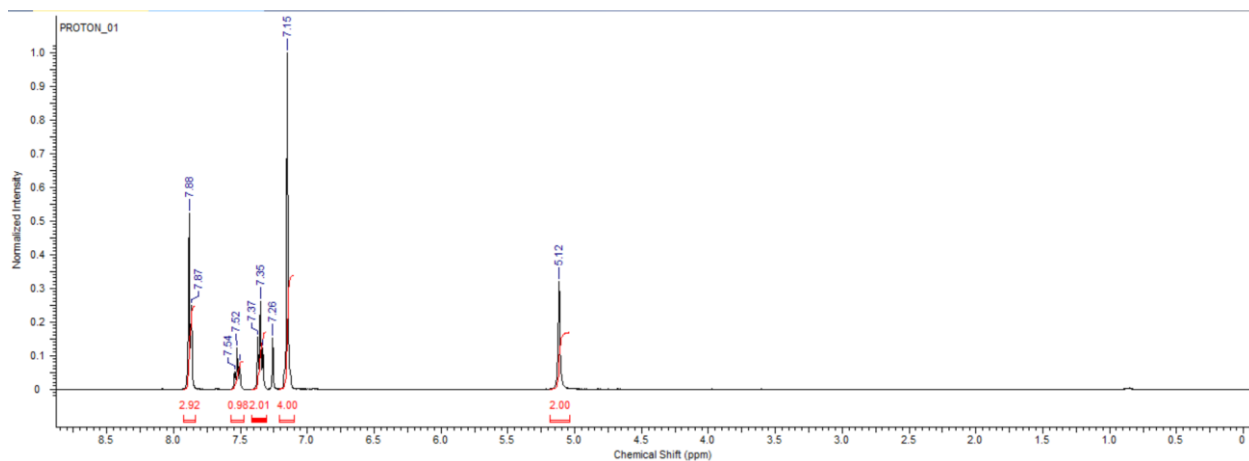
Method Filename : FOS B.lcm 01.09.2022 14:18:22

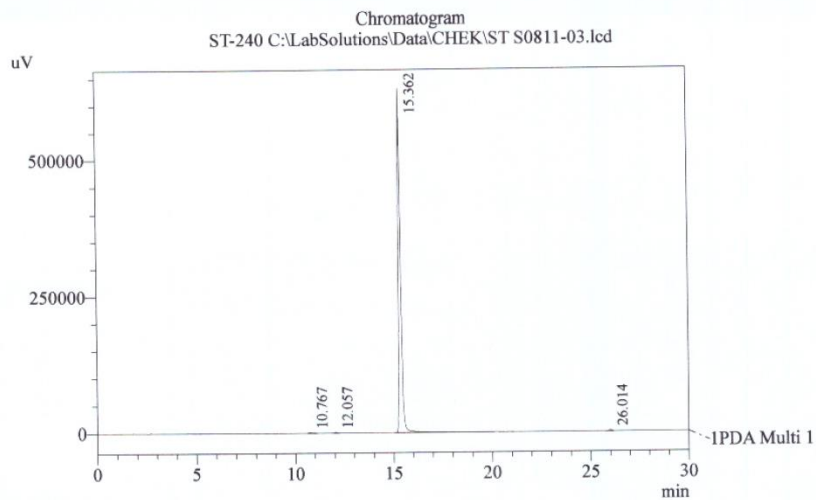
Time	Unit	Command	Valu
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	90
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl



(*E*)-1-(4-chlorophenyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**7e**)





1 PDA Multi 1 / 260nm 4nm

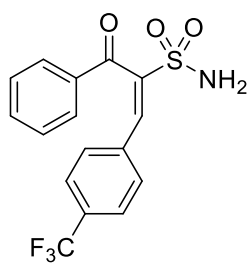
PDA Ch1 260nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	10.767	12669	1248	0.219
2	12.057	11371	1547	0.196
3	15.362	5745646	630596	99.268
4	26.014	18320	2184	0.317
Total		5788005	635575	100.000

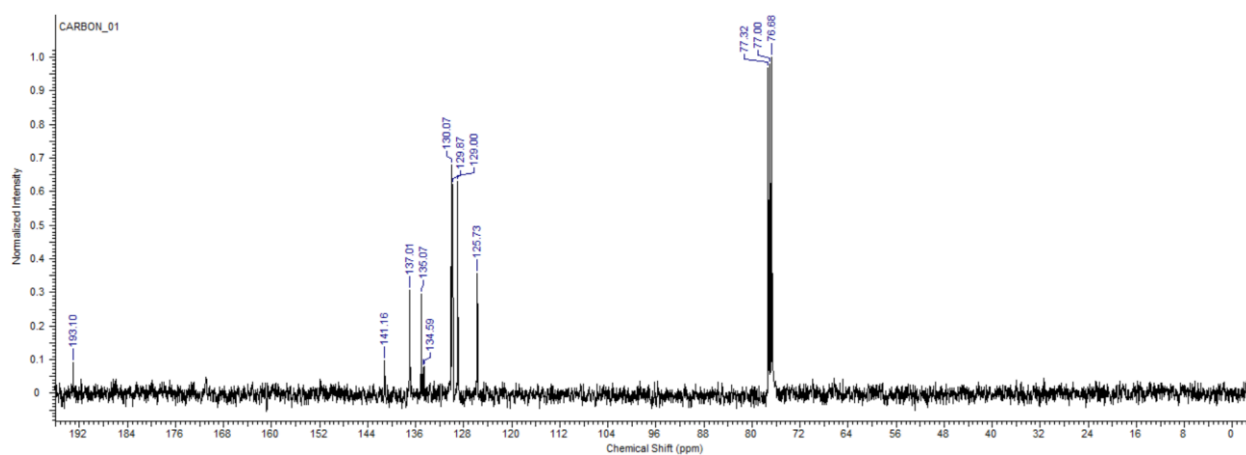
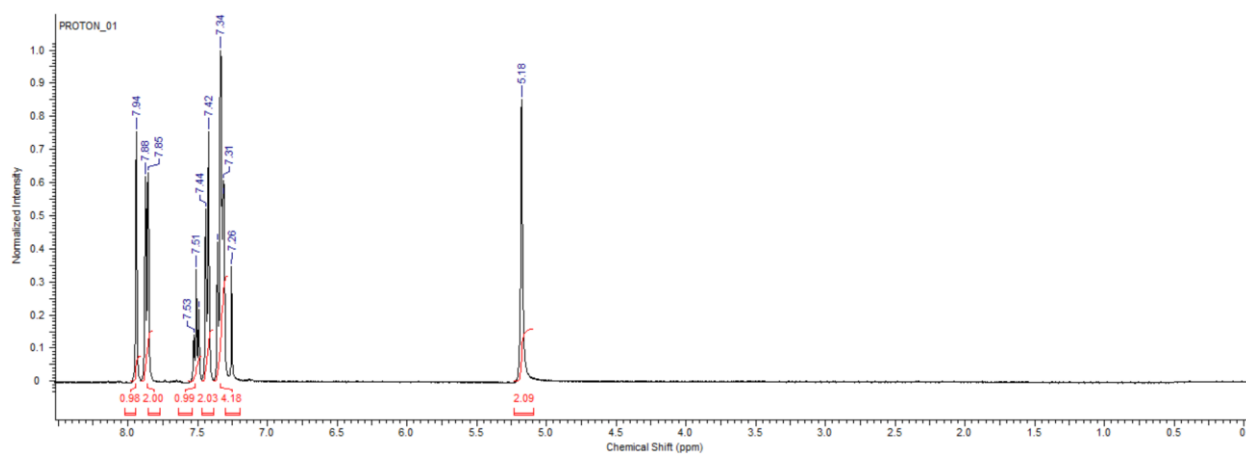
Method Filename : FOS B.lcm 11.08.2022 13:17:22

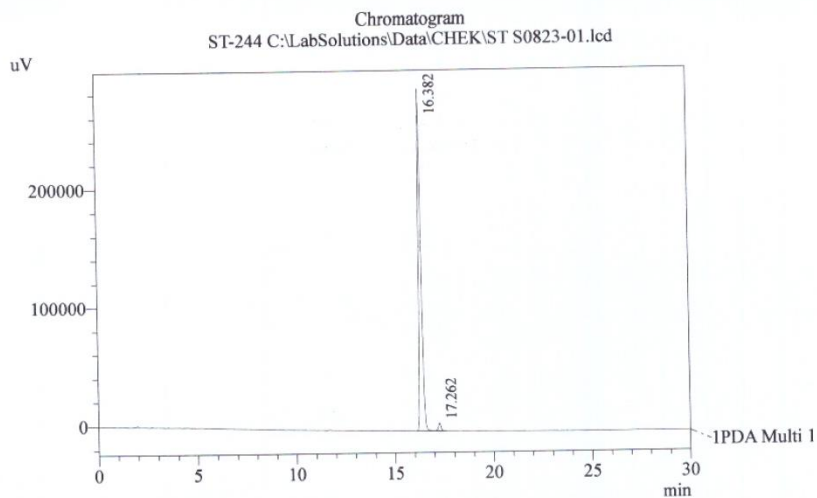
Time	Unit	Command	Valu
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	90
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl



(*E*)-3-oxo-3-phenyl-1-(4-(trifluoromethyl)phenyl)prop-1-ene-2-sulfonamide (**7f**)





1 PDA Multi 1 / 260nm 4nm

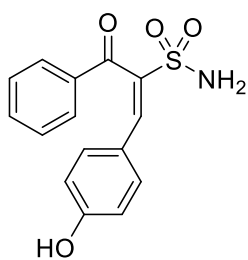
PDA Ch1 260nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	16.382	2750488	288752	97.867
2	17.262	59948	6427	2.133
Total		2810436	295179	100.000

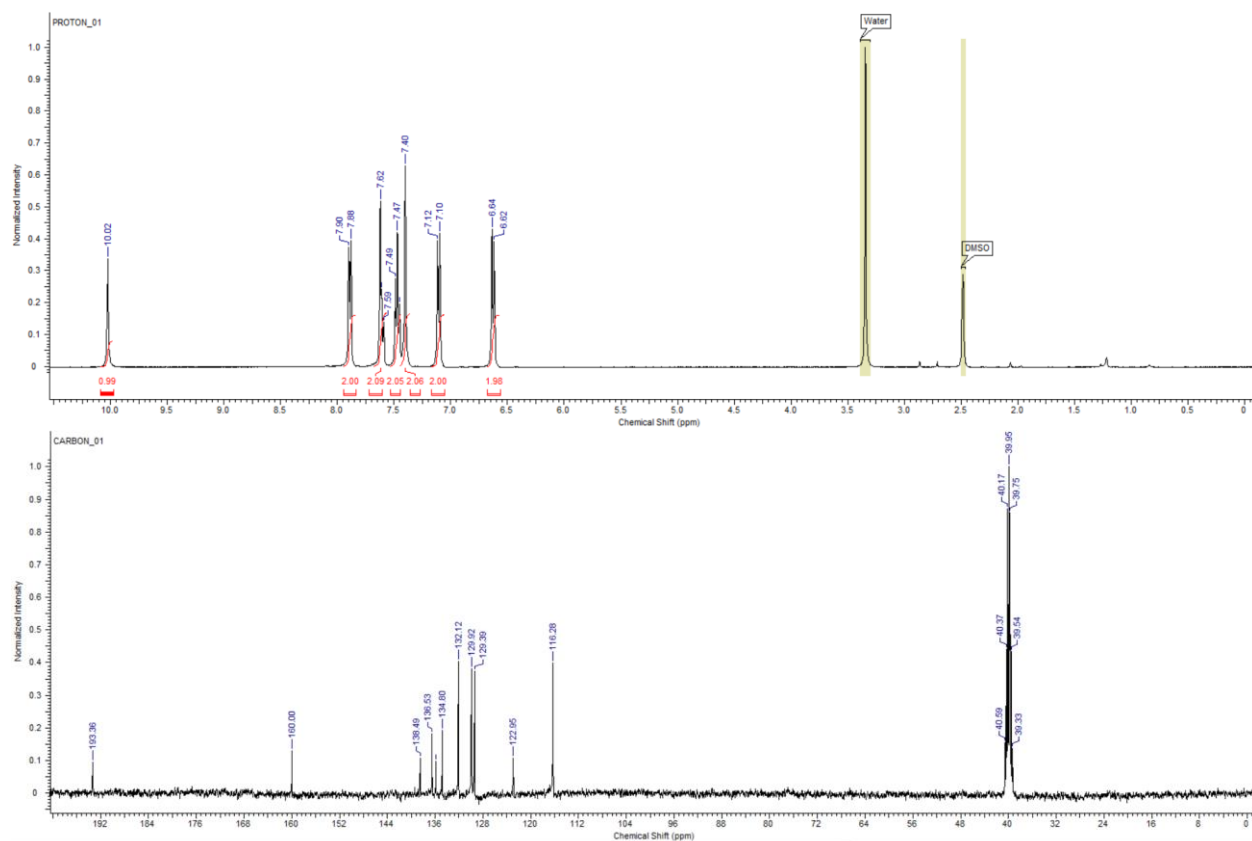
Method Filename : FOS B.lcm 23.08.2022 10:33:27

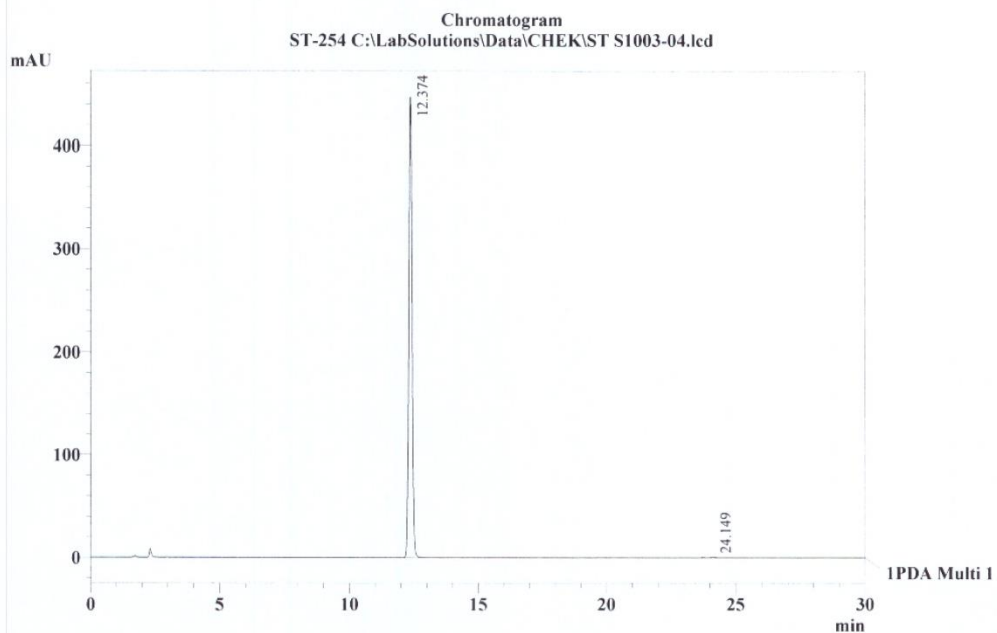
Time	Unit	Command	Valu
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	90
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl



(*E*)-1-(4-hydroxyphenyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**7g**)





1 PDA Multi 1 / 254nm 4nm

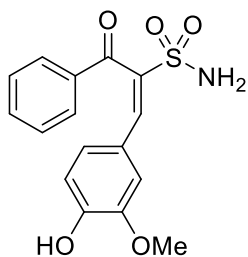
PeakTable

Peak#	Ret. Time	Area	Height	Area %
1	12.374	3953006	447406	99.714
2	24.149	11328	779	0.286
Total		3964334	448185	100.000

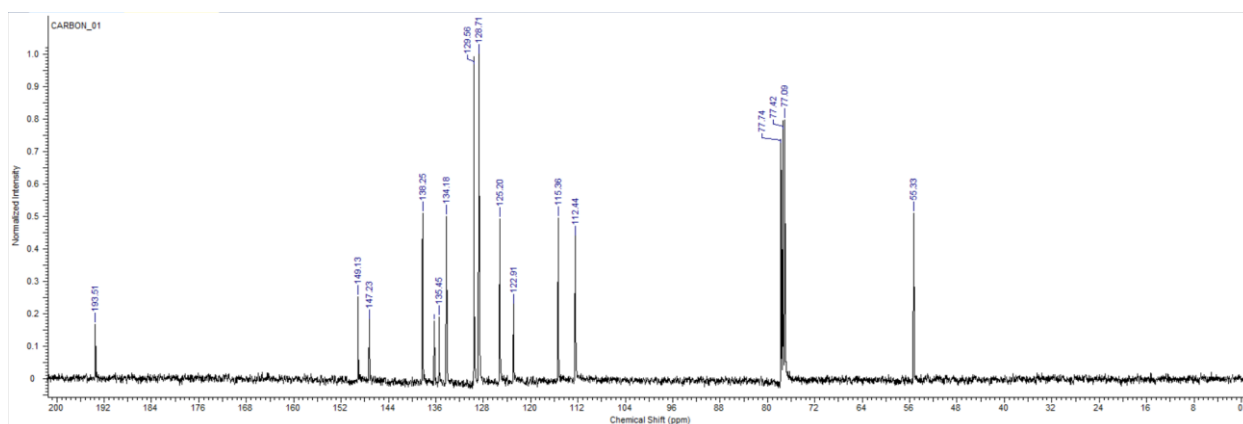
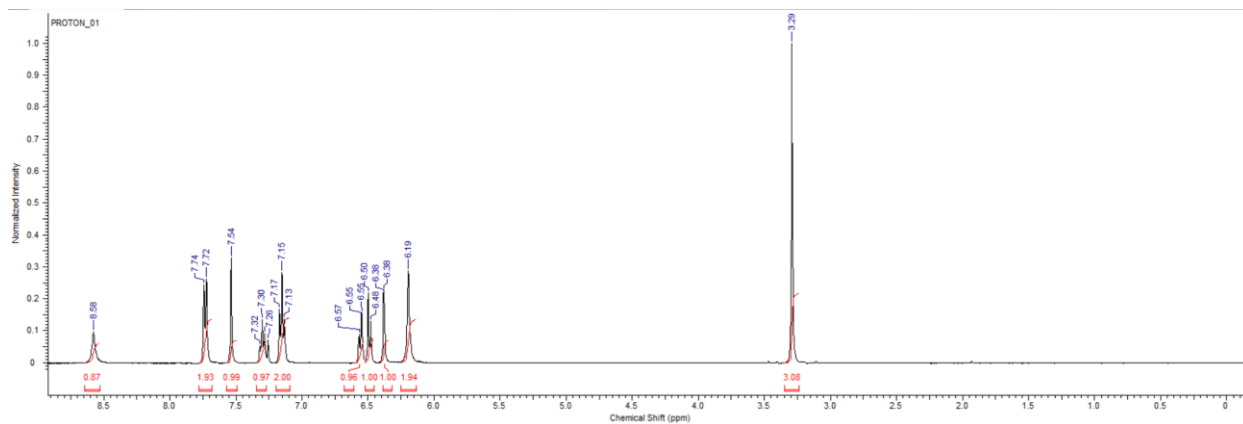
<<LC Program>>		Method		
Time	Unit	Command	Value	
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30.00	Pumps	B.Conc	70	
33.00	Pumps	B.Conc	30	
45.00	Controller	Stop		

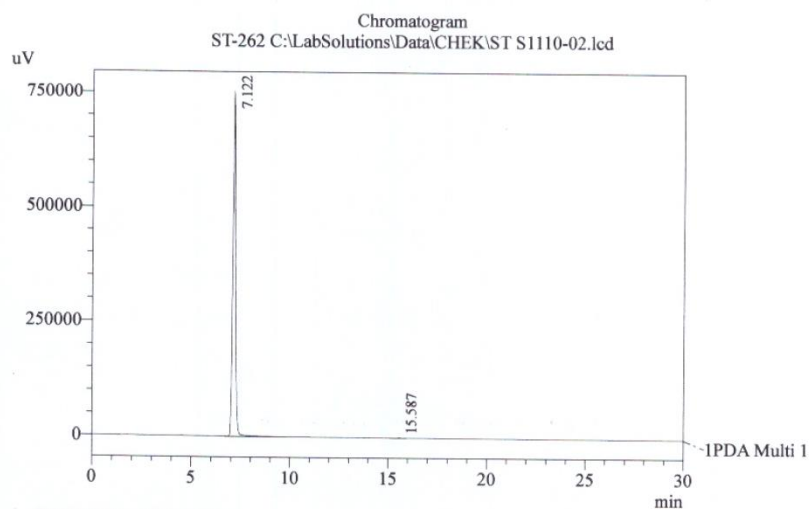
Method Filename : FOS Cv.lcm

Shimadzu LC-20AD; 2-System FOS, Colon Kromasil 100-C18, size 5µm, 4,6*250mm, N 86912
Elution: A - H₃PO₄ 0.01M pH 2.6; B - MeCN, fl. 1,0 ml/min, loop 20µl.



(*E*)-1-(4-hydroxy-3-methoxyphenyl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**7h**)





1 PDA Multi 1 / 260nm 4nm

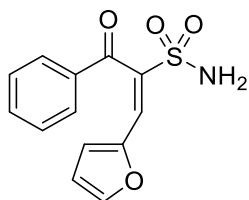
PDA Ch1 260nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	7.122	7702425	754910	99.891
2	15.587	8436	562	0.109
Total		7710860	755473	100.000

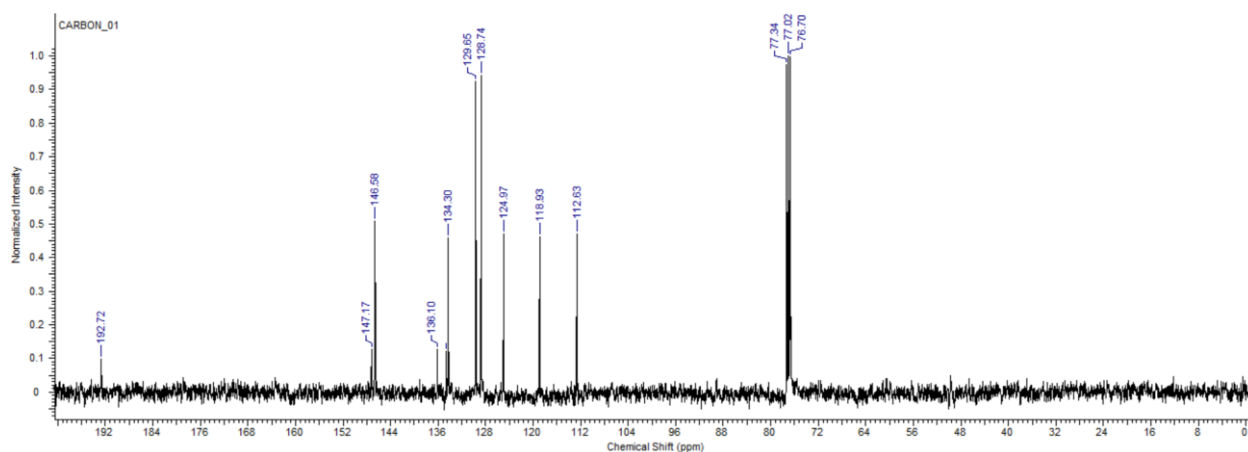
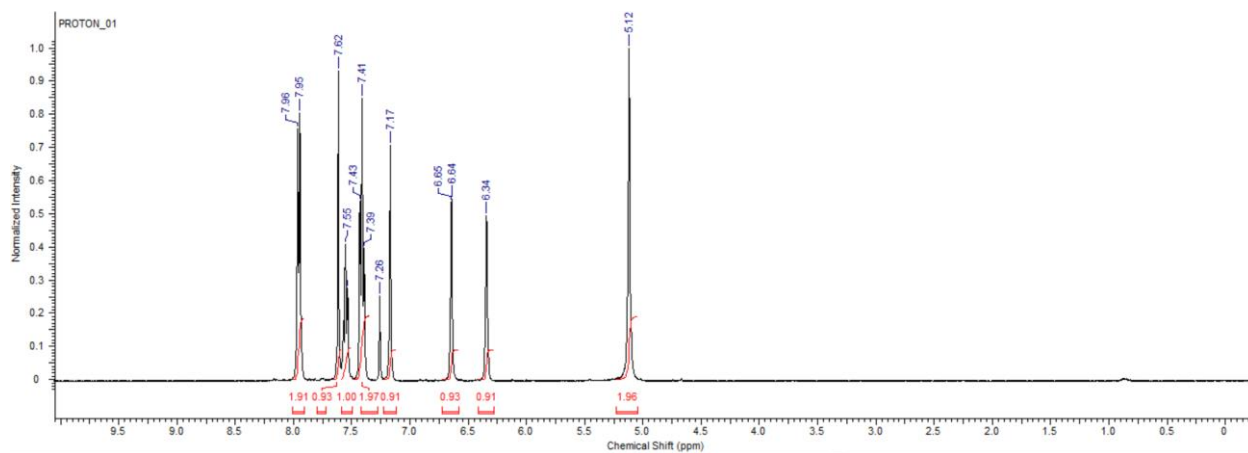
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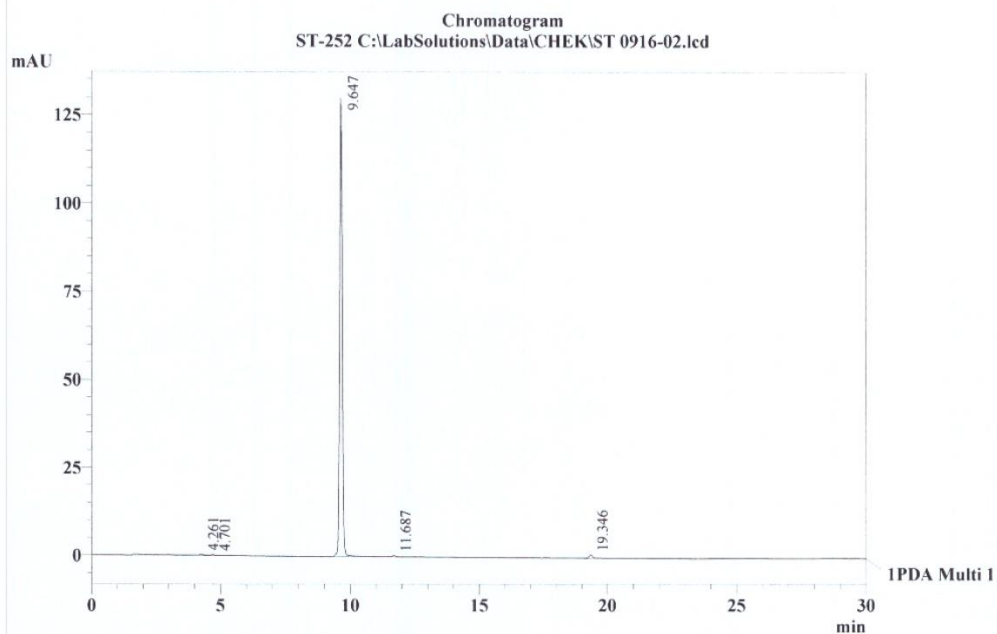
Time	Unit	Command	Valu
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	90
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mk. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl



(*E*)-1-(furan-2-yl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**7i**)





1 PDA Multi 1 / 260nm 4nm

PeakTable

PDA Ch1 260nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	4.261	2580	333	0.278
2	4.701	1013	175	0.109
3	9.647	915660	130177	98.490
4	11.687	2475	358	0.266
5	19.346	7969	989	0.857
Total		929697	132032	100.000

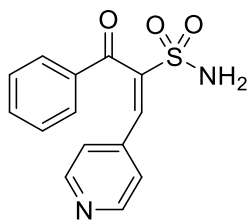
Method

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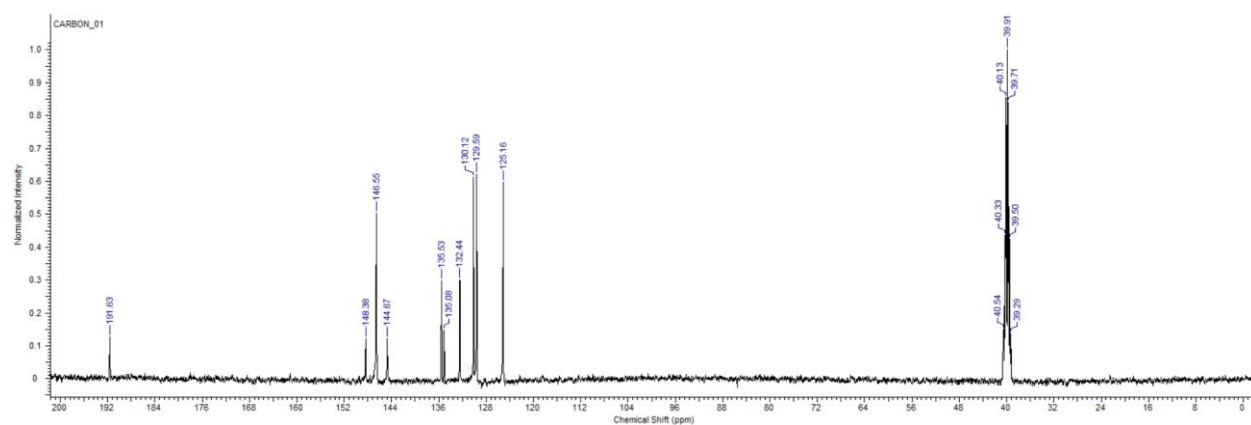
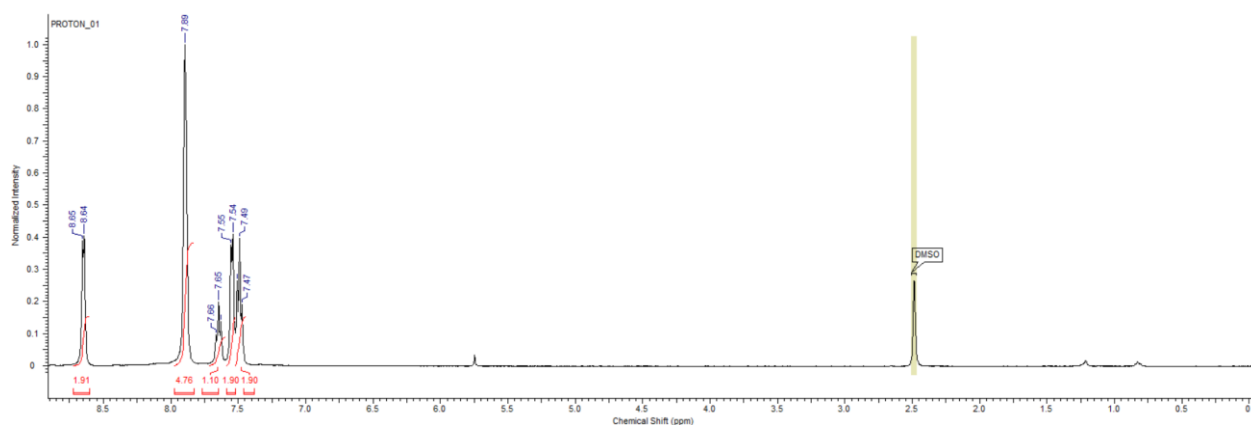
Time	Unit	Command	Value
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30.00	Pumps	B.Conc	90
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

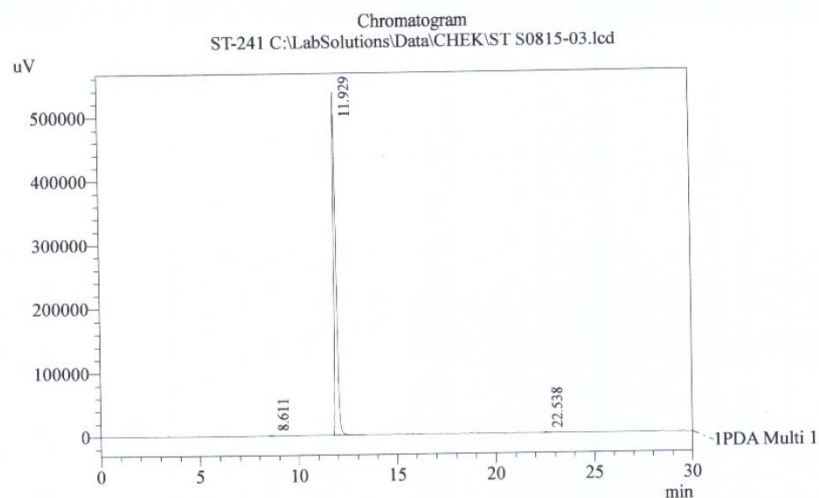
Method Filename : FOS C.lcm

Shimadzu LC-20AD; 2-System FOS, Colon Kromasil 100-C18, size 5µm, 4,6*250mm, N 86912
Elution: A - H3PO4 0.01M pH 2.6; B - MeCN, fl. 1,0 ml/min, loop 20µkl.



(*E*)-3-oxo-3-phenyl-1-(pyridin-4-yl)prop-1-ene-2-sulfonamide (**7j**)





1 PDA Multi 1 / 260nm 4nm

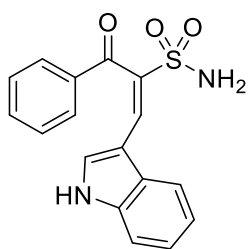
PDA Ch1 260nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	8.611	13630	1318	0.288
2	11.929	4705042	535625	99.465
3	22.538	11680	1272	0.247
Total		4730353	538214	100.000

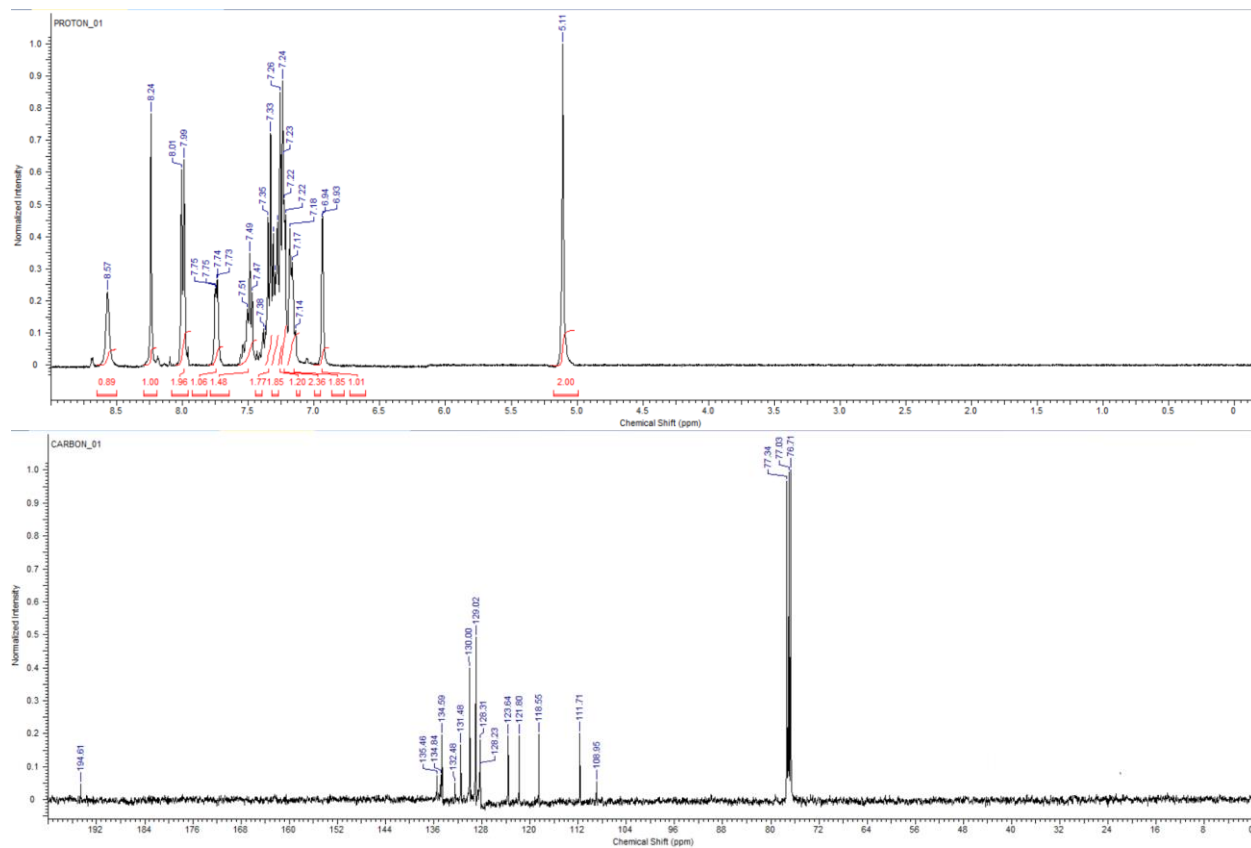
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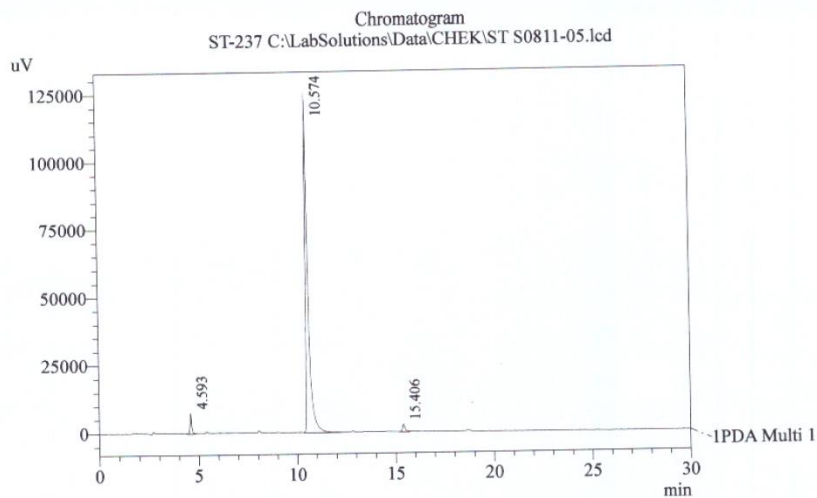
Time	Unit	Command	Valu
0.01	Pumps	B.Conc	10
30.00	Pumps	B.Conc	60
33.00	Pumps	B.Conc	10
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5nm. C-18, 4.6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl



(*E*)-1-(1*H*-indol-3-yl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**7k**)





1 PDA Multi 1 / 260nm 4nm

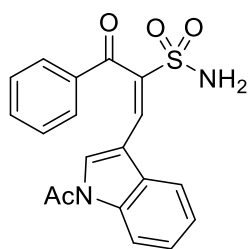
PDA Ch1 260nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	4.593	48833	7620	3.488
2	10.574	1265539	125908	94.566
3	15.406	27238	2757	1.945
Total		1400115	140131	100.000

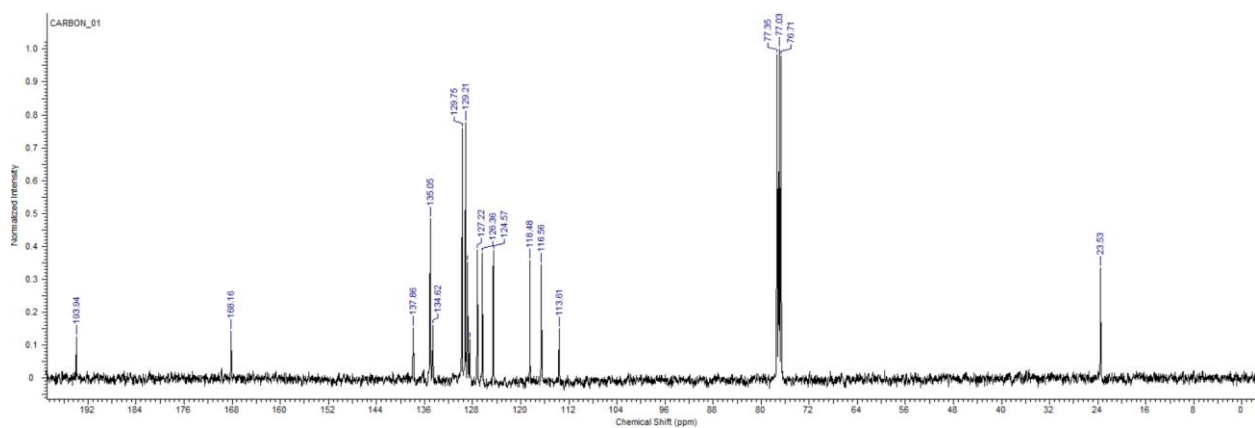
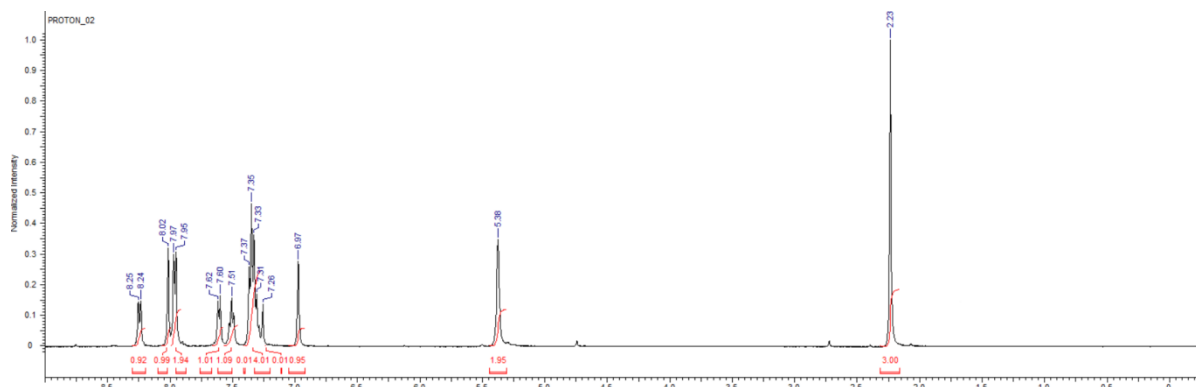
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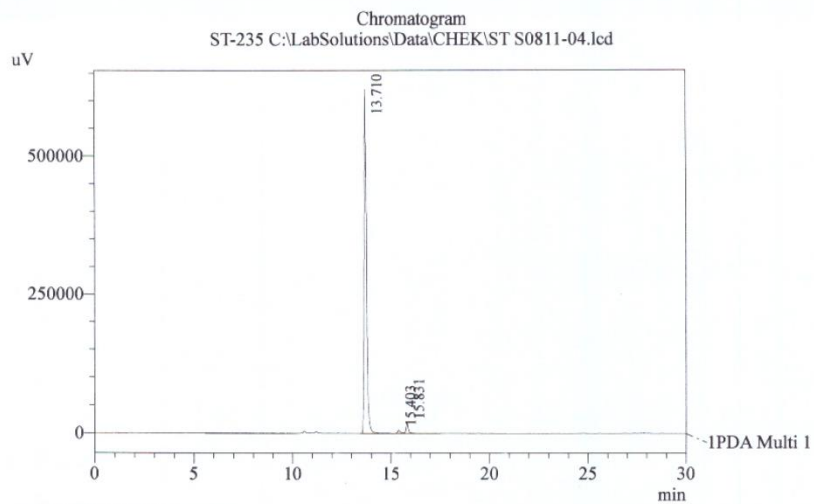
Time	Unit	Command	Valu
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	90
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Color- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl



(F)-1-(1-acetyl-1H-indol-3-yl)-3-oxo-3-phenylprop-1-ene-2-sulfonamide (**71**)





1 PDA Multi 1 / 254nm 4nm

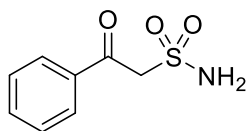
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	13.710	5650631	620863	96.285
2	15.403	61564	5805	1.049
3	15.831	156434	18107	2.666
Total		5868629	656912	100.000

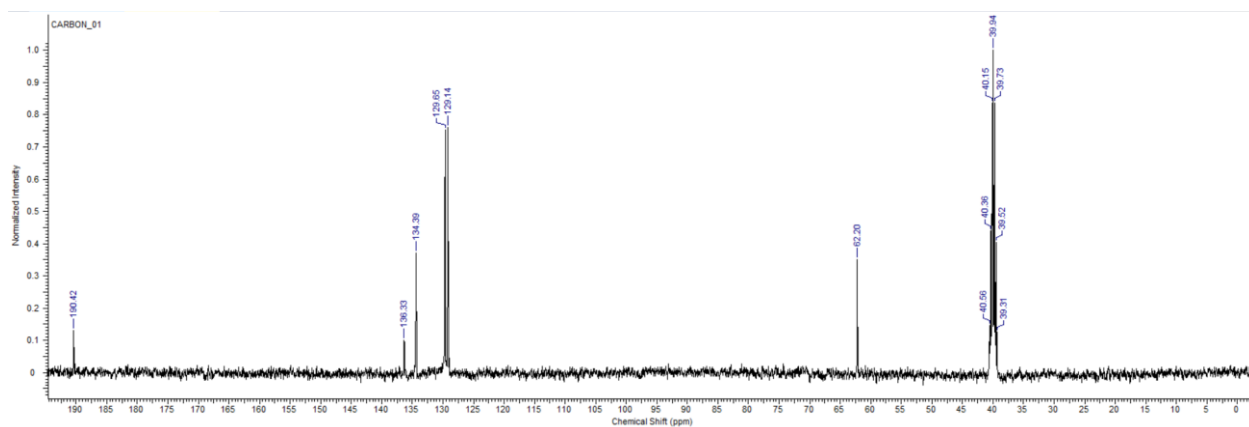
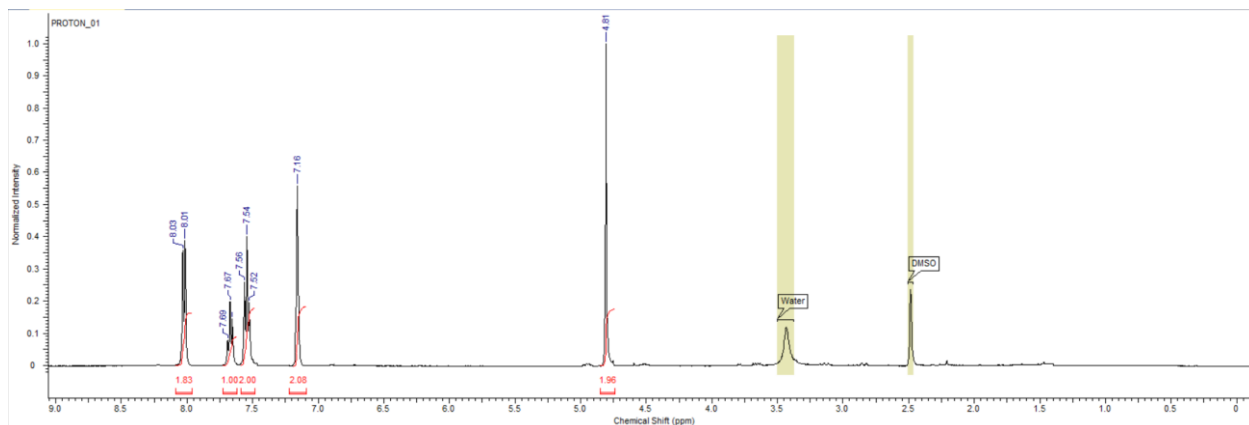
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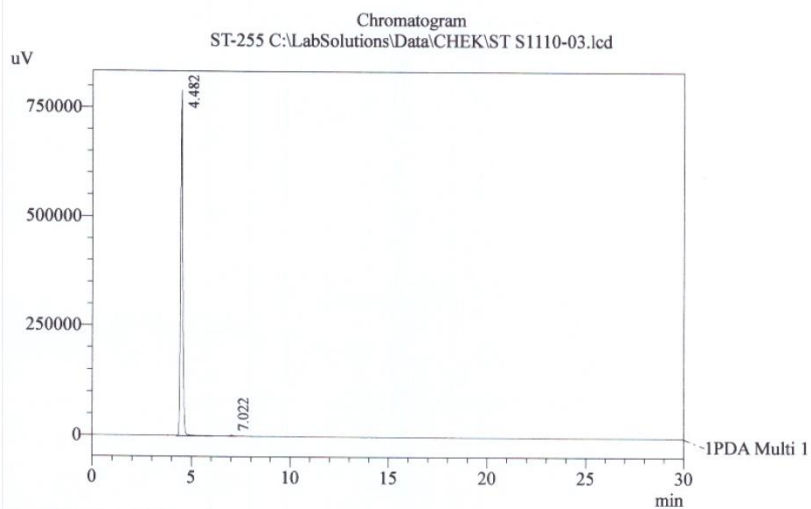
Time	Unit	Command	Value
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	90
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mk. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl



2-oxo-2-phenylethane-1-sulfonamide (11)





1 PDA Multi 1 / 254nm 4nm

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	4.482	6468293	790739	99.604
2	7.022	25725	2679	0.396
Total		6494018	793417	100.000

Method Filename : FOS B.lcm 10.11.2022 12:59:59

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	90
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl

Table S1. Crystallographic data for **7a**

Formula moiety	C ₁₅ H ₁₃ NO ₃ S
Brutto formula	C ₁₅ H ₁₃ NO ₃ S
Formula weight	287.32
Diffractometer	Bruker QUEST
Scan mode	ω and ϕ scans
Anode [Wavelength, Å]	MoK α [0.71073] microfocus sealed X-ray tube
Crystal Dimensions, mm	0.07 \times 0.31 \times 0.31
Crystal color	colourless
Crystal system	monoclinic
a, Å	10.3899(3)
b, Å	33.2046(9)
c, Å	16.2988(4)
α , °	90
β , °	102.374(2)
γ , °	90
Volume, Å ³	5492.3(3)
Density, gcm ⁻³	1.390
Temperature, K	100
T _{min} /T _{max}	0.4273/0.4998
μ , mm ⁻¹	0.242
Space group	Cc
Z	16
F(000)	2400

Reflections collected	39106
Independent reflections	14133
Reflections ($I > 2\sigma(I)$)	12646
Parameters	729
R_{int}	0.0419
$2\theta_{\text{min}} - 2\theta_{\text{max}}, ^\circ$	4.196 - 61.016
wR_2 (all reflections)	0.1181
$R_1(I > \sigma(I))$	0.0485
GOF	1.060
$Q_{\text{min}}/Q_{\text{max}}, \text{e}\text{\AA}^{-3}$	-0.404/0.948
Restraints	2

Hydrogen bonding in 7a

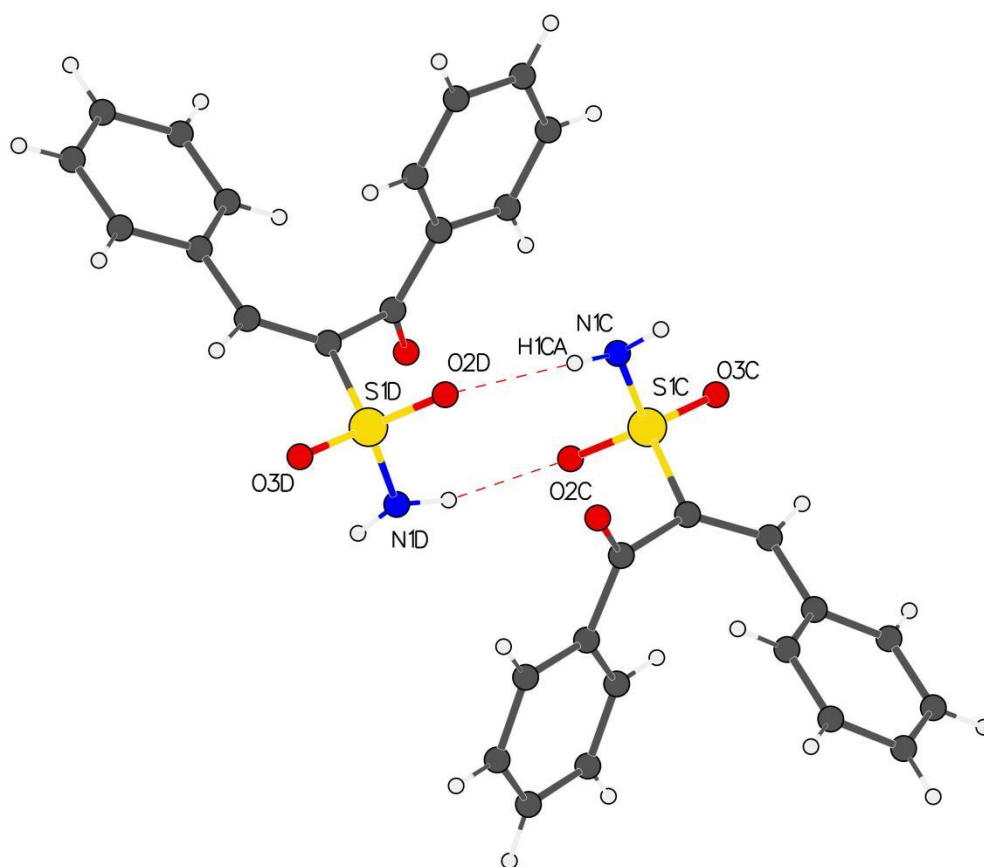


Figure S1. Centrosymmetric dimer in crystal structure of **7a** formed by hydrogen bonds between sulfonamide groups.

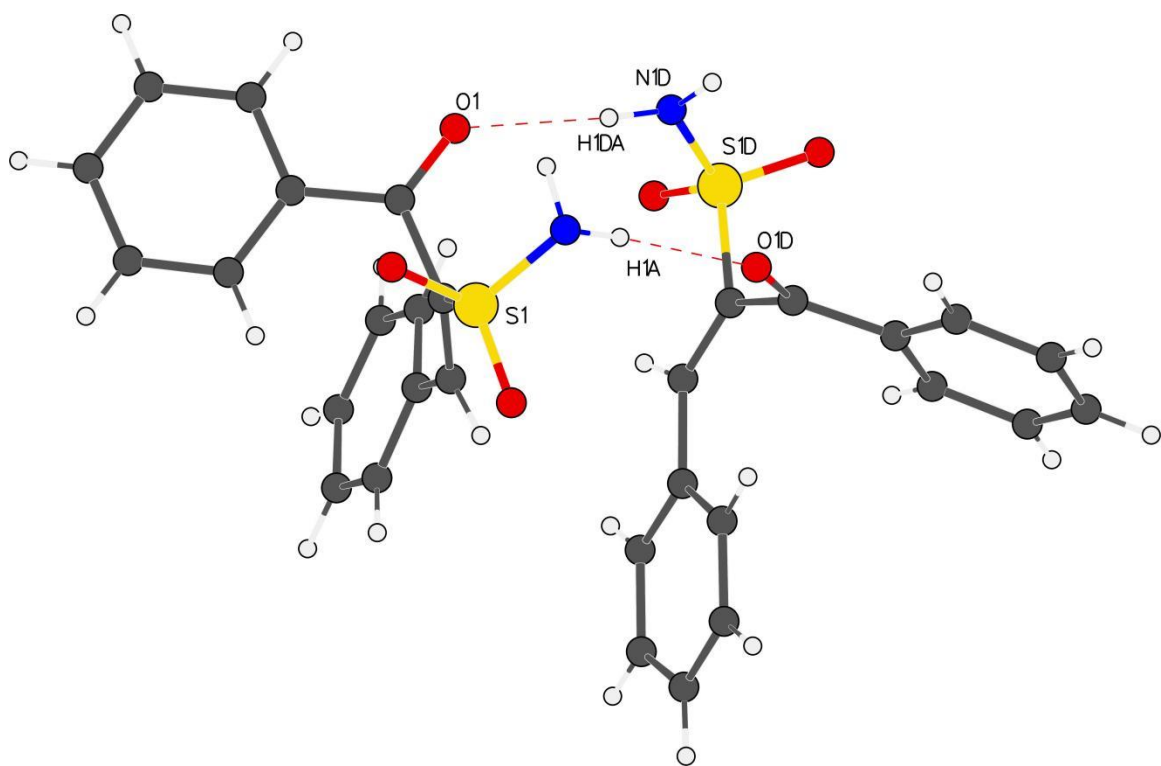


Figure S2. Centrosymmetric dimer in crystal structure of **7a** formed by hydrogen bonds between sulfonamide and carbonyl groups.

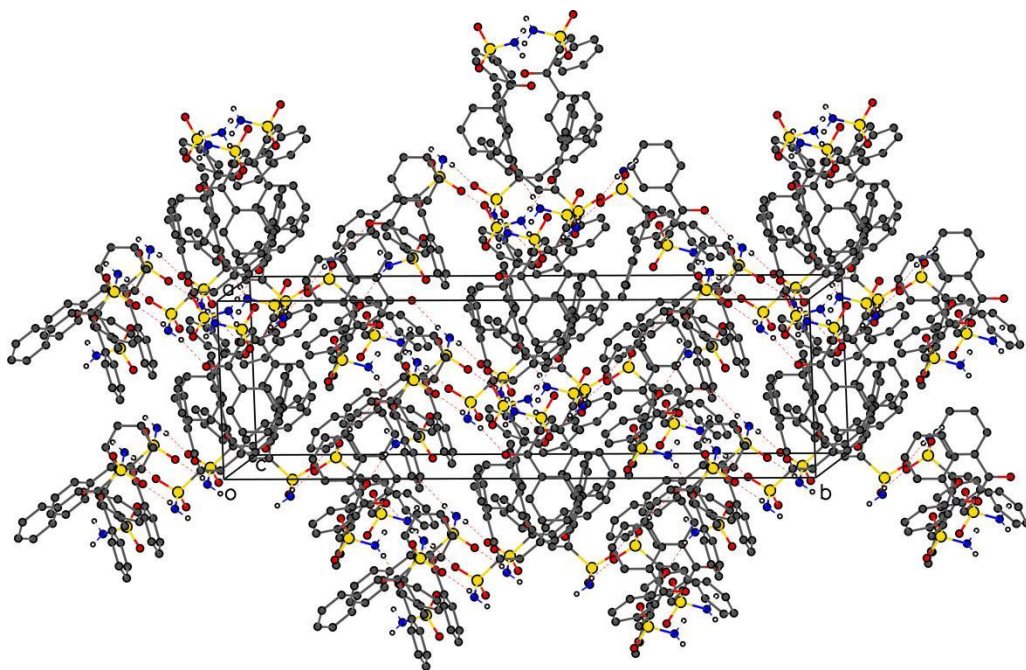


Figure S3. Crystal packing of **7a**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N1	H1A	O1D ¹	0.90	1.99	2.864(4)	163.4
N1A	H1AA	O1C ²	0.90	2.06	2.941(4)	166.6
N1C	H1CA	O2D	0.90	2.10	2.905(4)	147.5
N1C	H1CB	O1A ³	0.90	2.06	2.942(4)	167.6
N1D	H1DA	O1 ⁴	0.90	2.12	3.013(4)	170.6
N1D	H1DB	O2C	0.90	2.10	2.971(4)	164.0

Table S2. Hydrogen Bonds for **7a**

¹-1/2+X,-1/2+Y,+Z; ²1+X,+Y,+Z; ³-1+X,+Y,+Z; ⁴1/2+X,1/2+Y,+Z