Synthesis, In silico Pharmacokinetic Analysis and Anticancer Activity Evaluation of Benzothiazole-Triazole Hybrids

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Table of Contents	**Page No**
S1. Anticancer activity i.e. one-dose data for Benzothiazole-triazole hybrids retrieved from NCI database	2-4
S2: Lipinski's 'ruleof 5'parametersfor Benzothiazole-triazole hybrids	5
S3: ADME predictions for Benzothiazole-triazole hybrids	6
S4: Spectras ^{1}Hand ^{13}C:	7-32

Table S1. Anticancer activity i.e. one-dose data for Benzothiazole-triazole hybrids retrieved from NCI database

Cell Line	Mean Growth percent									
	(4a)	(5a)	(5b)	(4b)	(4c)	(4d)	(5c)	(5d)	(5e)	(5f)
Leukemia										
CCRF-CEM	97.53	103.39	97.10	99.95					100.65	99.73
HL-60(TB)	99.41	97.05	97.67	99.01	98.78	99.76	97.39	98.11	100.28	97.57
K-562	100.10	94.76	96.78	98.85	102.94	103.40	100.23	90.24	97.30	99.57
MOLT	100.90	104.00	99.08	100.72	105.60	101.11	100.97	102.35	109.76	109.86
RPMI-8226	94.32	107.09	95.72	104.78	95.34	98.00	98.74	100.33	106.11	114.31
SR	96.21	100.05	91.37	95.19	109.51	105.34	104.25	99.06	99.57	106.74
Non-Small Cell Lung Cancer										
A549/ATCC	106.31	97.15	103.71	98.98	105.08	100.06	100.85	104.02	102.80	99.86
EKVX	94.06	94.13	91.48	104.19	94.86	98.74	102.71	92.51	94.85	101.96
HOP-62	100.98	100.51	101.77	101.37	100.99	100.29	103.65	102.29	113.39	106.66
HOP-92	102.44	105.96	106.90	113.47	107.42	105.93	103.60	101.85	114.81	113.12
NCI-H226	102.77	103.21	103.98	105.19	98.93	102.16	101.68	100.92	101.64	104.48
NCI-H23	96.65	101.29	97.03	100.52	99.88	96.52	101.16	100.12	102.91	108.79
NCI-H460	104.23	106.33	104.28	104.38	101.22	101.67	103.48	102.81	107.71	109.28
NCI-H522	97.92	93.74	92.52	89.39	97.81	90.05	95.33	94.50	96.78	92.19
Colon Cancer										
COLO 205	111.39	111.48	109.30	108.02	110.76	105.84	109.41	107.57	112.53	109.56
HCC-2998	108.72	109.28	102.79	108.56	105.00	115.24	104.66	109.53	106.50	109.79
HCT-116	107.09	97.21	101.04	100.38	96.09	95.89	98.03	96.49	105.67	103.33
HCT-15	102.74	105.01	104.66	105.66	107.13	104.31	105.42	102.21	109.68	108.98
HT29	117.78	99.48	106.33	106.51	103.46	96.05	106.18	106.32	106.76	105.35
KM12	105.95	107.16	107.67	101.87	103.17	104.94	102.68	103.16	111.54	108.08
SW-620	100.31	106.40	98.53	102.55	95.84	95.96	95.20	101.12	107.64	112.89
CNS Cancer										
SF-268	95.83	99.00	98.36	97.94	96.37	96.44	97.04	94.95	101.03	103.18
SF-295	107.57	105.54	103.20	106.30	100.96	104.72	101.50	102.15	105.34	98.93
SF-539	101.91	95.02	95.33	94.83	95.18	92.49	95.59	90.09	99.94	100.28
SNB-19	101.93	96.85	98.84	99.91	100.32	98.00	100.88	96.23	102.55	100.74
SNB-75	85.59	92.38	90.69	95.29	95.26	84.42	83.70	86.06	92.65	98.92
U251	107.42	102.29	101.54	99.56	103.60	97.08	102.75	100.16	105.51	100.73
Melanoma										
LOX IMVI	90.45	95.08	91.49	94.19	93.50	99.99	92.33	93.59	95.86	98.74
MALME-3M	96.29	93.84	89.95	106.80	102.26	101.01	95.16	97.75	104.21	99.13
M14	98.84	94.70	95.59	100.63	95.98	97.53	97.51	93.53	99.62	100.38
MDA-MB-435	103.83	99.70	104.25	103.46	101.01	98.74	98.97	101.01	103.21	104.23
SK-MEL-2	108.33	106.56	101.37	104.40	104.67	106.38	103.82	107.11	105.55	110.57
SK-MEL-28	103.73	106.24	99.94	103.49	101.78	101.52	99.22	97.50	109.71	108.49
SK-MEL-5	99.53	102.47	100.10	102.72	98.47	99.83	99.26	100.11	99.12	102.74
UACC-257	105.90	103.90	108.36	99.26	104.79	102.16	97.53	104.60	110.64	106.40
UACC-62	97.45	97.03	95.98	94.64	96.56	91.66	92.05	95.66	103.16	99.80
Ovarian Cancer										
IGROV1	97.87	97.83	92.80	98.69	98.16	96.46	96.39	99.77	102.43	102.84
OVCAR-3	106.25	100.96	102.85	106.62	105.95	102.98	101.46	106.39	107.34	103.94
OVCAR-4	115.78	107.60	113.41	109.59	107.80	101.51	104.32	110.06	119.05	111.40
OVCAR-5	96.32	100.71	100.30	100.63	97.59	92.94	94.71	94.98	103.00	102.53
OVCAR-8	102.82	99.35	103.93	101.50	100.81	99.00	101.20	99.92	103.34	100.68
NCI/ADR-RES	97.51	99.35	101.07	98.86	102.58	102.72	101.82	102.76	110.88	113.07
SK-OV-3	104.58	104.43	96.62	104.08	102.49	94.52	105.26	104.42	111.76	116.42
Renal Cancer										
786-0	106.47	103.33	102.09	102.05	100.61	103.81	100.98	102.57	105.53	106.21
A498	121.94	118.17	121.98	123.86	113.91	110.84	113.12	110.32	133.78	120.25
ACHN	101.88	104.48	101.69	104.48	103.60	104.51	98.83	98.25	102.54	107.16
CAKI-1	84.79	88.92	86.14	91.11	89.17	86.56	91.02	80.65	90.12	93.18
RXF 393	108.56	112.49	106.62	115.48	114.05	112.92	111.86	111.48	116.86	120.13
SN12C	98.92	96.52	99.43	101.48	95.93	98.28	95.53	96.24	98.60	100.68
TK-10	113.31	105.99	113.01	101.86	110.00	104.12	103.09	105.01	110.63	109.47
UO-31	67.66	72.64	63.90	72.11	70.56	65.42	76.52	60.63	71.10	78.40
Prostate Cancer										
PC-3	93.13	96.33	96.06	95.35	92.90	93.64	92.34	91.54	100.23	99.89
DU-145	111.47	113.10	115.55	109.63	113.64	112.22	113.02	113.34	113.59	115.54
Breast Cancer										
MCF7	96.27	97.85	96.02	97.69	95.19	96.70	96.21	93.41	100.10	99.86
MDA-MB-231/ATCC	98.76	100.32	96.41	103.00	102.57	99.41	102.07	99.48	101.03	105.54
HS 578T	108.55	108.86	104.42	106.06	102.15	100.28	101.96	95.63	114.64	115.46
BT-549	102.49	105.74	104.06	103.83	101.49	95.56	100.00	97.41	106.65	108.30
T-47D	113.29	110.14	104.84	92.51	107.08	102.66	109.76	104.88	112.33	106.17
MDA-MB-468	103.40	101.24	104.47	105.06	103.59	106.14	105.47	105.62	108.10	108.88

Cell Line	Mean Growth percent (5g)	(5h)	(5i)	(5j)	(5k)	(5l)	(5m)	(4e)	(4f)	(4g)
Leukemia										
CCRF-CEM	94.31	103.21					97.51	98.23	103.27	101.75
HL-60(TB)	99.11	99.74	98.47`	100.66	98.02	101.23	99.70	98.34	98.93	99.51
K-562	104.12	103.93	104.99	105.78	105.56	95.85	96.82	96.48	95.29	98.85
MOLT-4	108.34	111.87	106.25	110.47	105.91	104.09	103.80	100.95	99.68	98.54
RPMI-8226	104.54	106.26	100.16	112.34	104.63	96.62	102.50	99.53	93.11	97.25
SR	101.36	99.99	120.31	109.76	104.29	105.22	103.17	94.89	104.41	111.04
Non-Small Cell Lung Cancer										
A549/ATCC	105.93	103.95	108.71	98.41	106.72	102.46	102.18	97.48	103.88	101.17
EKVX	104.27	103.35	102.71	100.77	112.00	91.74	88.53	91.54	95.17	98.33
HOP-62	105.54	101.43	97.82	102.20	102.03	102.60	101.57	100.96	101.54	98.30
HOP-92	105.06	118.78	116.47	108.77	114.16	104.21	95.43	105.77	97.29	107.01
NCI-H226	104.34	105.35	101.81	105.86	109.40	96.98	95.26	100.31	101.15	103.12
NCI-H23	105.52	105.48	99.85	109.59	105.16	105.61	102.10	99.90	102.60	106.38
NCI-H460	107.25	105.63	103.16	103.18	104.11	104.74	105.75	107.45	105.82	105.78
NCI-H522	93.26	89.66	102.21	93.85	94.89	96.39	92.78	96.03	89.87	88.08
Colon Cancer										
COLO 205	110.95	111.65	108.56	108.64	110.11	109.39	109.65	111.96	110.29	108.49
HCC-2998	106.55	113.26	107.61	115.63	106.47	107.29	105.71	103.44	102.96	102.81
HCT-116	104.50	102.54	101.10	100.71	99.84	104.34	98.94	99.37	98.58	105.59
HCT-15	106.72	104.12	107.45	107.89	108.52	104.12	105.45	106.83	105.48	111.03
HT29	101.30	103.38	101.18	103.69	107.27	105.56	104.05	103.33	97.46	101.87
KM12	106.26	103.28	104.51	108.56	106.14	101.87	104.75	104.02	106.66	102.60
SW-620	104.82	104.87	96.41	99.91	98.28	96.43	102.44	113.32	103.63	107.05
CNS Cancer										
SF-268	103.31	101.62	101.71	98.82	99.59	101.14	95.71	97.76	99.26	101.76
SF-295	100.76	104.77	103.94	103.66	102.68	101.40	102.38	103.21	99.72	102.98
SF-539	104.69	99.44	99.68	99.54	93.86	95.02	95.24	96.16	99.04	91.11
SNB-19	97.68	101.99	99.23	102.36	100.52	99.31	96.42	97.94	96.77	100.85
SNB-75	103.14`	93.60	103.43	100.70	97.45	94.47	76.55	78.19	99.84	91.98
U251	100.53	102.07	103.67	97.83	103.10	97.24	107.80	98.86	99.01	98.25
Melanoma										
LOX IMVI	97.94	93.71	95.65	96.57	96.23	95.99	90.93	96.03	92.68	94.20
MALME-3M	99.85	101.71	114.08	101.03	93.12	97.63	95.06	88.20	92.67	103.64
M14	100.73	103.47	99.89	102.00	100.69	98.08	97.11	98.20	98.86	105.43
MDA-MB-435	108.58	110.06	105.18	105.12	105.95	104.77	101.67	100.23	107.46	106.13
SK-MEL-2	104.43	102.08	105.35	105.29	107.25	108.78	103.27	107.61	100.06	103.68
SK-MEL-28	104.05	108.09	101.02	102.99	104.67	103.65	103.85	101.86	98.83	102.58
SK-MEL-5	101.24	104.06	97.36	99.49	99.06	100.48	96.50	101.60	99.58	101.33
UACC-257	110.78	106.18	110.09	106.03	106.22	105.05	103.68	100.44	107.95	96.51
UACC-62	100.27	99.47	100.10	98.08	99.38	99.59	96.85	97.75	96.60	93.07
Ovarian Cancer										
IGROV1	101.04	96.59	96.77	97.28	96.33	100.17	94.30	98.11	96.16	99.00
OVCAR-3	110.30	111.48	107.45	107.12	105.20	104.18	104.79	101.09	104.66	106.17
OVCAR-4	120.33	115.56	113.29	109.05	112.32	113.16	111.58	101.15	116.91	108.48
OVCAR-5	99.68	103.56	99.69	98.61	101.07	99.88	100.54	102.81	99.71	105.65
OVCAR-8	103.60	101.27	100.37	100.31	101.49	100.26	103.81	95.96	100.60	96.69
NCI/ADR-RES	112.36	109.24	107.51	106.55	110.90	105.22	103.52	99.85	102.68	104.22
SK-OV-3	110.66	101.62	101.87	109.71	111.09	107.57	101.35	88.01	100.29	95.44
Renal Cancer										
786-0	105.42	102.39	106.44	108.46	104.35	103.82	103.41	101.15	101.28	102.43
A498	110.32	133.83	112.31	129.30	120.57	125.04	133.11	116.28	116.05	108.64
ACHN	109.34	102.97	101.68	101.32	101.52	102.80	95.84	100.69	104.62	97.92
CAKI-1	97.87	89.94	87.41	87.57	87.49	86.79	82.89	91.50	91.13	90.25
RXF 393	120.16	120.33	116.15	113.61	116.09	118.26	111.59	121.19	110.15	114.54
SN12C	105.48	101.85	98.28	98.53	100.47	100.05	94.62	97.59	102.37	99.36
TK-10	109.50	107.37	113.43	102.57	106.34	107.85	112.36	104.28	104.84	97.87
UO-31	76.30	66.75	67.01	65.95	67.06	70.22	62.14	73.14	70.06	74.23
Prostate Cancer										
PC-3	98.03	95.55	97.94	96.31	96.70	93.25	93.11	97.59	95.10	97.74
DU-145	118.63	112.98	118.79	117.27	118.08	115.86	112.86	111.69	113.78	113.66
Breast Cancer										
MCF7	98.72	101.01	98.13	99.97	100.68	95.53	91.70	91.72	92.68	98.41
MDA-MB-231/ATCC	102.30	101.55	105.44	98.88	104.61	102.09	94.79	101.18	92.55	97.17
HS 578T	111.44	104.36	103.38	100.61	104.56	100.71	107.86	112.66	101.90	108.83
BT-549	104.80	112.45	113.43	103.05	107.26	102.12	102.55	102.40	101.56	103.02
T-47D	109.58	102.93	102.06	102.41	110.99	101.72	108.12	96.21	101.04	95.84
MDA-MB-468	105.42	112.96	113.60	109.92	116.25	111.95	102.51	105.42	105.17	105.50

Cell Line	Mean Growth percent				
	(4h)	(4i)	(4j)	(5n)	
Leukemia					
HL-60(TB)	97.87	99.08	97.93	97.71	
K-562	102.10	99.53	98.53	90.47	
MOLT-4	102.16	105.42	97.99	103.66	
RPMI-8226	95.18	91.94	93.08	85.17	
SR	114.45	108.71	110.71	95.98	
Non-Small Cell Lung Cancer					
A549/ATCC	104.79	98.45	104.05	101.19	
EKVX	101.87	84.66	111.43	86.44	
HOP-62	95.20	99.37	100.98	95.69	
HOP-92	107.23	99.12	102.94	93.26	
NCI-H226	97.30	101.06	102.80	102.58	
NCI-H23	95.32	101.68	103.71	101.15	
NCI-H460	100.80	102.45	102.23	102.78	
NCI-H522	97.44	91.71	95.93	94.81	
Colon Cancer					
COLO 205	113.25	109.71	111.72	103.98	
HCC-2998	101.16	107.87	101.80	105.81	
HCT-116	99.51	100.07	103.91	98.23	
HCT-15	103.83	109.02	110.83	102.67	
HT29	97.04	102.57	110.63	100.18	
KM12	105.31	107.15	103.27	100.12	
SW-620	95.36	97.67	99.37	98.97	
CNS Cancer					
SF-268	97.21	97.14	99.39	97.07	
SF-295	99.16	101.19	100.49	99.54	
SF-539	95.44	94.01	91.00	85.36	
SNB-19	95.37	97.51	95.88	95.16	
SNB-75	92.61	88.11	85.40	77.68	
U251	102.90	99.05	100.85	95.23	
Melanoma					
LOX IMVI	90.63	99.50	94.59	92.63	
MALME-3M	99.97	91.50	96.67	88.76	
M14	99.63	98.73	100.38	94.48	
MDA-MB-435	108.39	102.08	98.33	101.03	
SK-MEL-2	104.13	101.40	104.92	105.07	
SK-MEL-28	101.16	97.28	100.67	96.25	
SK-MEL-5	96.23	98.46	98.03	98.87	
UACC-257	103.57	97.50	100.77	102.65	
UACC-62	97.89	96.36	97.39	94.90	
Ovarian Cancer					
IGROV1	98.35	93.96	92.19	93.89	
OVCAR-3	103.29	103.28	101.00	100.93	
OVCAR-4	105.43	104.30	102.65	106.84	
OVCAR-5	98.74	97.12	97.91	95.07	
OVCAR-8	96.69	99.73	102.07	97.78	
NCI/ADR-RES	100.25	105.76	105.79	102.59	
SK-OV-3	98.41	99.72	99.74	97.89	
Renal Cancer					
786-0	104.23	106.42	104.17	100.57	
A498	108.24	108.28	112.09	120.55	
ACHN	99.70	99.30	97.58	95.73	
CAKI-1	88.09	93.08	86.72	77.29	
RXF 393	113.63	115.73	115.61	120.59	
SN12C	96.38	97.67	98.28	96.31	
TK-10	103.94	97.23	104.52	107.55	
UO-31	69.14	73.35	67.09	62.89	
Prostate Cancer					
PC-3	96.47	98.27	94.20	86.82	
DU-145	117.52	109.39	113.51	110.12	
Breast Cancer					
MCF7	92.22	94.50	95.18	90.31	
MDA-MB-231/ATCC	100.23	100.00	95.29	91.76	
HS 578T	98.60	99.89	95.72	97.09	
BT-549	103.74	97.64	101.87	97.06	
T-47D	103.07	96.21	103.96	94.81	
MDA-MB-468	105.42	106.29	109.08	106.26	

In silico ADME prediction

The pharmacokinetics of the compounds under study, ADME predictions were done for the compounds using Qikprop v3.5 (Schrödinger, Inc., New York, NY, 2012).[5] All the compounds prepared by LigPrep were used for the calculation of pharmacokinetic properties by QikProp. The program QikProp, utilizes the method of Jorgensen to compute pharmacokinetic properties and descriptors such as octanol/water partitioning coefficient, aqueous solubility, brain/blood partition coefficient, intestinal wall permeability, plasma protein binding and others.

TableS2.Calculation of Lipinski's 'ruleof 5'parametersfor Benzothiazole-triazole hybrids

S.No (Molecule)	Mol wt	donor HB(<5)	Accpt HB (<10)	QP logPo/w (<5)	Rule of five (<4)
(4a)	393.419	0	7.25	2.819	0
(4b)	365.409	1	7.25	3.118	0
(4c)	379.436	1	7.25	3.534	0
(4d)	393.462	1	7.25	3.898	0
(4e)	393.419	0	7.25	2.738	0
(4f)	407.446	0	7.25	3.104	0
(4g)	410.406	0	6.25	3.088	0
(4h)	444.305	1	7.25	3.681	0
(4i)	390.419	0	6.75	2.995	0
(4j)	393.419	0	7.25	2.379	0
(5a)	289.311	1	6.2	1.348	0
(5b)	335.383	1	6.5	2.976	0
(5c)	357.429	2	7.25	2.579	0
(5d)	353.373	1	6.5	3.208	0
(5e)	365.409	1	7.25	3.067	0
(5f)	299.35	1	6.5	2.275	0
(5g)	341.43	1	6.5	3.155	0
(5h)	360.392	0	6	2.576	0
(5i)	349.409	1	6.5	3.279	0
(5j)	301.365	1	6.5	2.421	0
(5k)	315.392	1	6.5	2.76	0
(5l)	329.419	1	6.5	3.094	0
(5m)	343.446	1	6.5	3.022	0
(5n)	377.463	1	6.5	4.0090	0

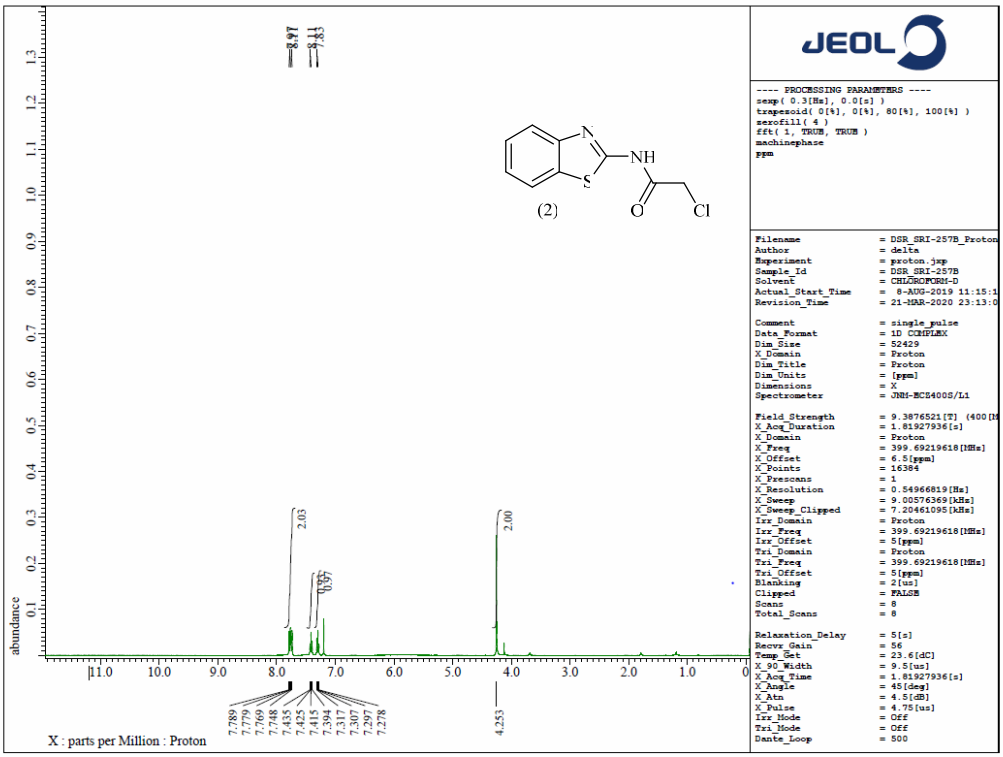
[a] Calculated using Qikprop v3.5.

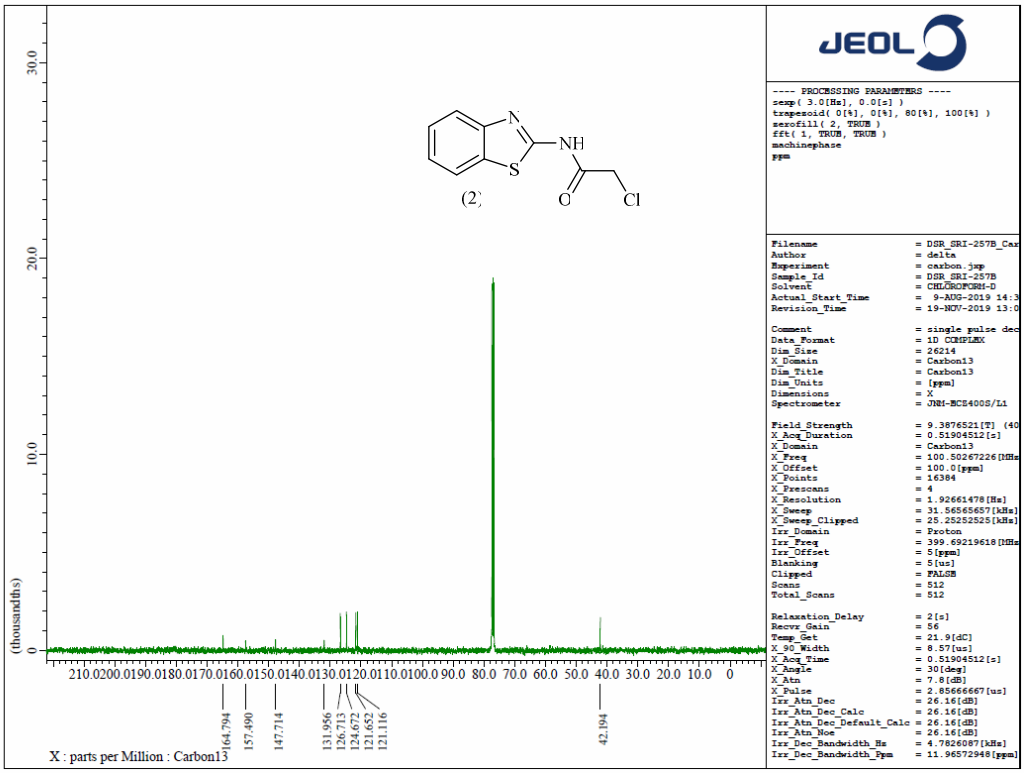
Table S3.ADME predictions for Benzothiazole-triazole hybrids

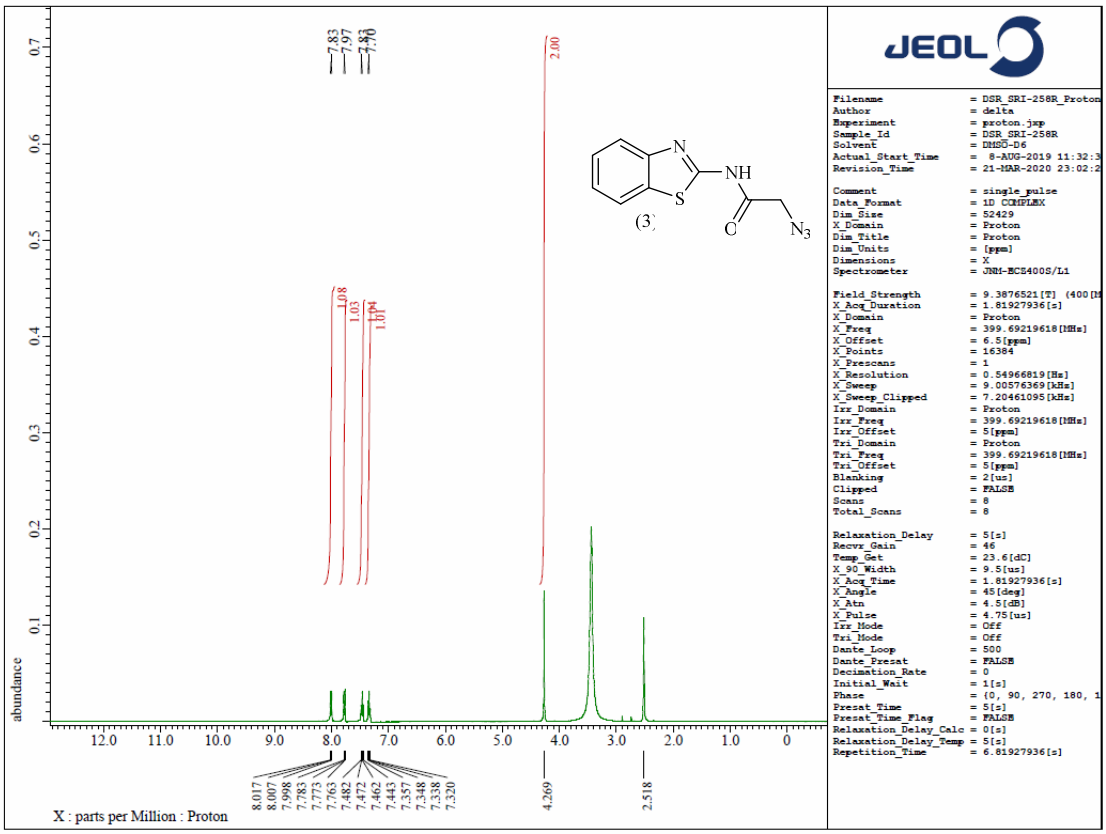
S.No (Molecule)	PercentHumanOralAbsorption(>80%-high,<25% poor)[a]	QPPCaco nms^{-1} (<25 poor,>500 great) [a]	QPlogBB (-3.0-1.2) [a]	QPPMDCK (<25 poor >500 great) [a]	QPlogKhsa (-1.5to1.5) [a]	QPlogHERG (<-5 causes concern) [a]	#rotor (0-15) [a]
(4a)	80.36	115.33	-2.03	83.90	-0.156	-6.754	8
(4b)	93.48	498.26	-1.17	396.68	0.023	-7.066	6
(4c)	100.00	628.38	-1.09	553.86	0.178	-7.03	6
(4d)	100.00	644.312	-1.166	568.357	0.29	-7.118	7
(4e)	82.395	159.323	-1.694	123.119	-0.236	-6.152	8
(4f)	85.26	174.83	-1.85	98.14	-0.043	-6.604	8
(4g)	80.00	89.92	-2.02	66.43	0.052	-6.341	8
(4h)	96.78	498.11	-1.02	1050.36	0.157	-6.986	6
(4i)	83.77	156.63	-1.77	120.95	-0.106	-6.5	8
(4j)	79.702	147.672	-1.56	111.635	-0.349	-5.206	8
(5a)	75.22	180.27	-1.47	100.38	-0.399	-5.143	6
(5b)	95.50	719.50	-0.73	640.72	0.062	-6.672	3
(5c)	88.43	390.52	-1.08	330.57	0.073	-5.723	4
(5d)	96.85	718.39	-0.62	1154.75	0.102	-6.547	3
(5e)	96.08	723.20	-0.82	644.07	0.063	-6.573	4
(5f)	92.43	821.13	-0.63	738.68	-0.15	-5.572	3
(5g)	100.00	807.14	-0.69	724.64	0.219	-5.814	3
(5h)	81.84	167.72	-1.32	130.28	-0.106	-5.344	5
(5i)	100.00	717.60	-0.76	638.91	0.214	-6.584	3
(5j)	92.27	721.27	-0.84	642.11	-0.159	-5.707	5
(5k)	94.29	724.28	-0.93	644.64	-0.06	-5.862	6
(5l)	95.08	622.87	-1.10	547.97	0.055	-6.02	7
(5m)	94.52	612.34	-1.04	440.99	0.052	-4.929	8
(5n)	100.00	734.11	-0.94	654.31	0.436	-6.845	5

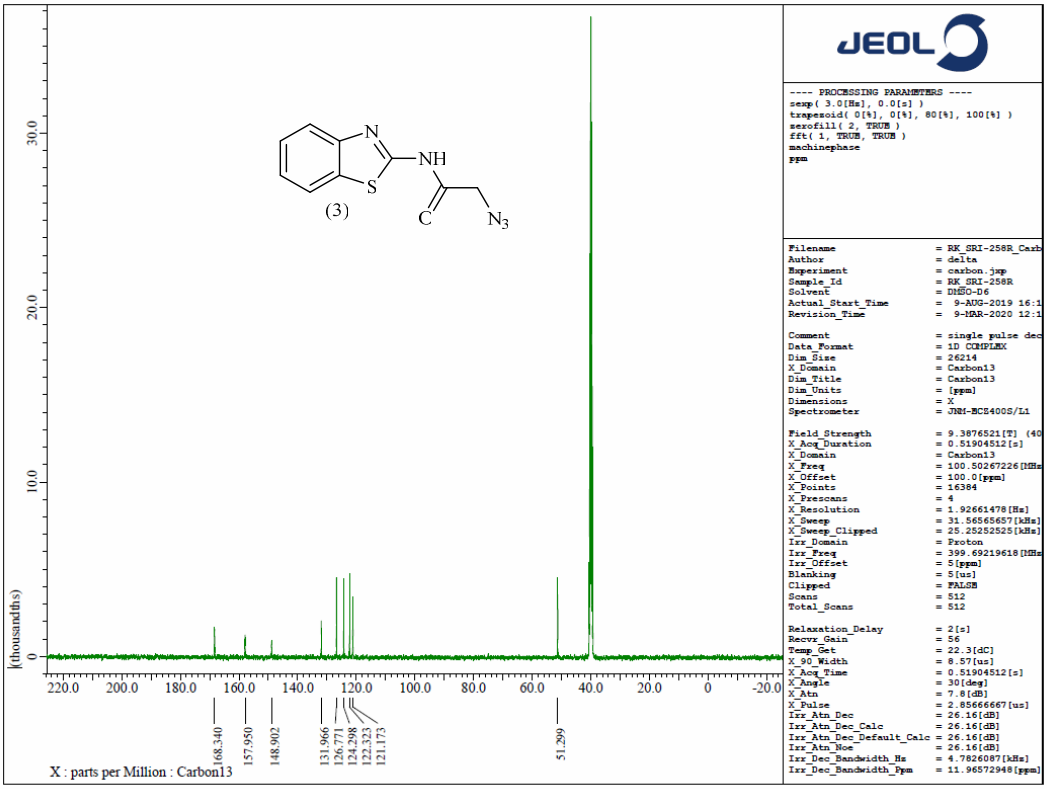
[a] Calculated using Qikprop v3.5. The ranges/recommended values, shown in parenthesis, were calculated from 95% of known drugs

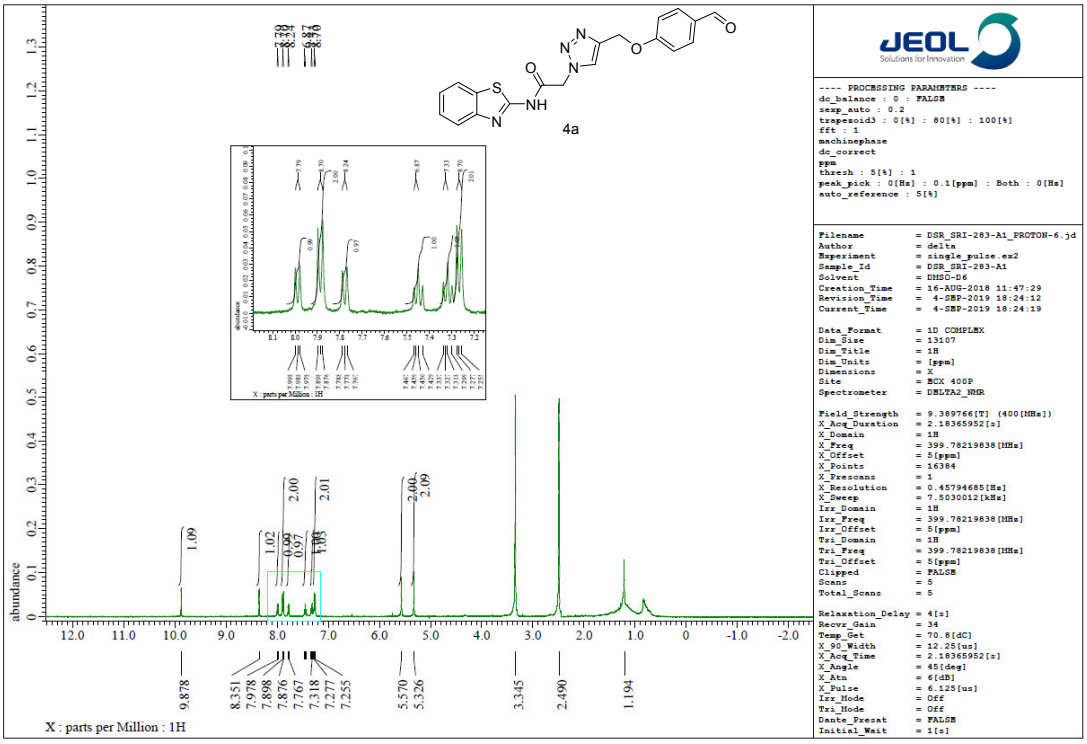
S4. Spectras ^{1}Hand ^{13}C:

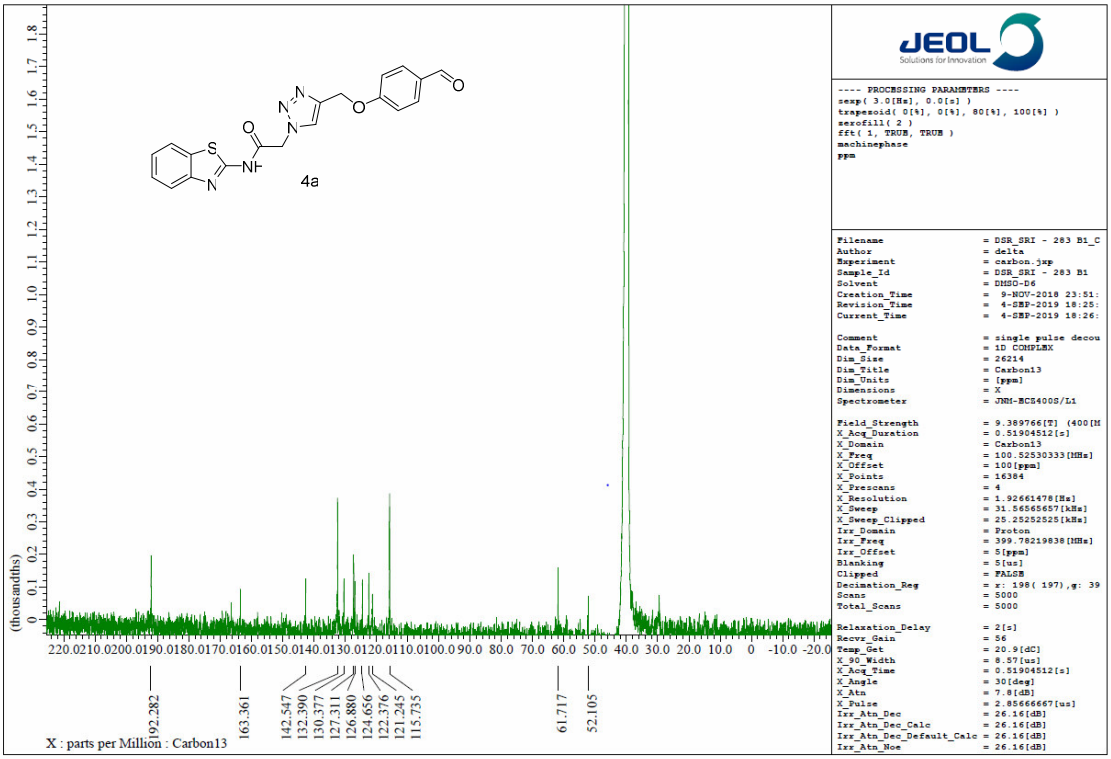


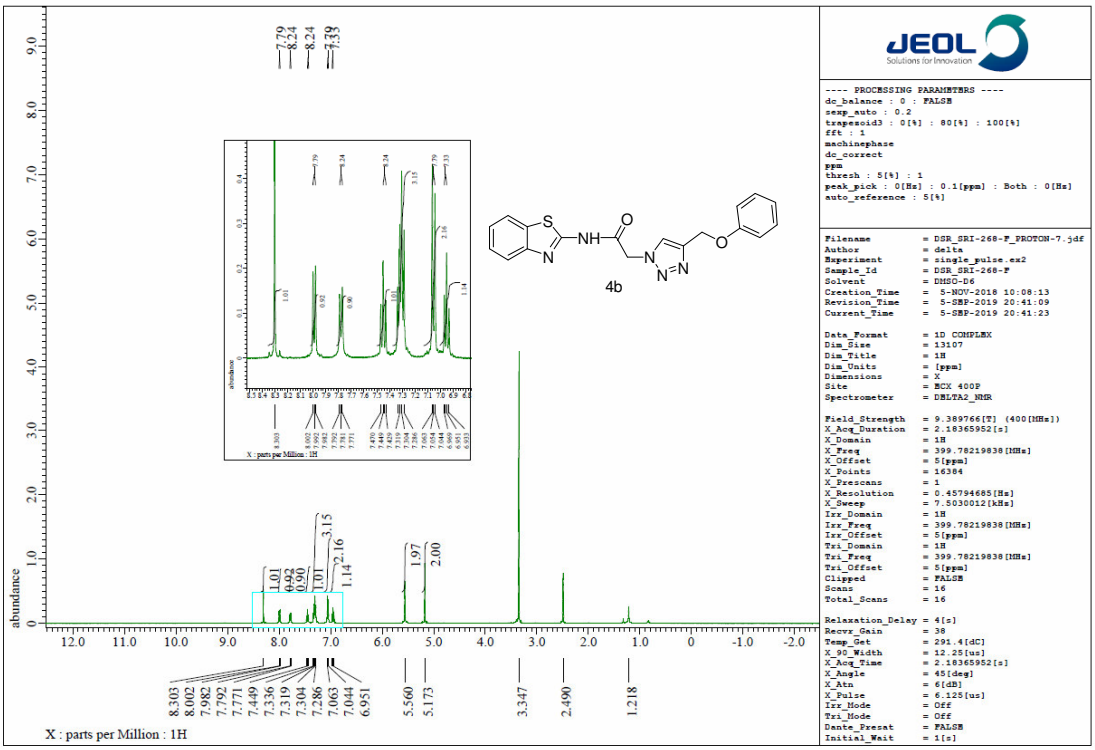


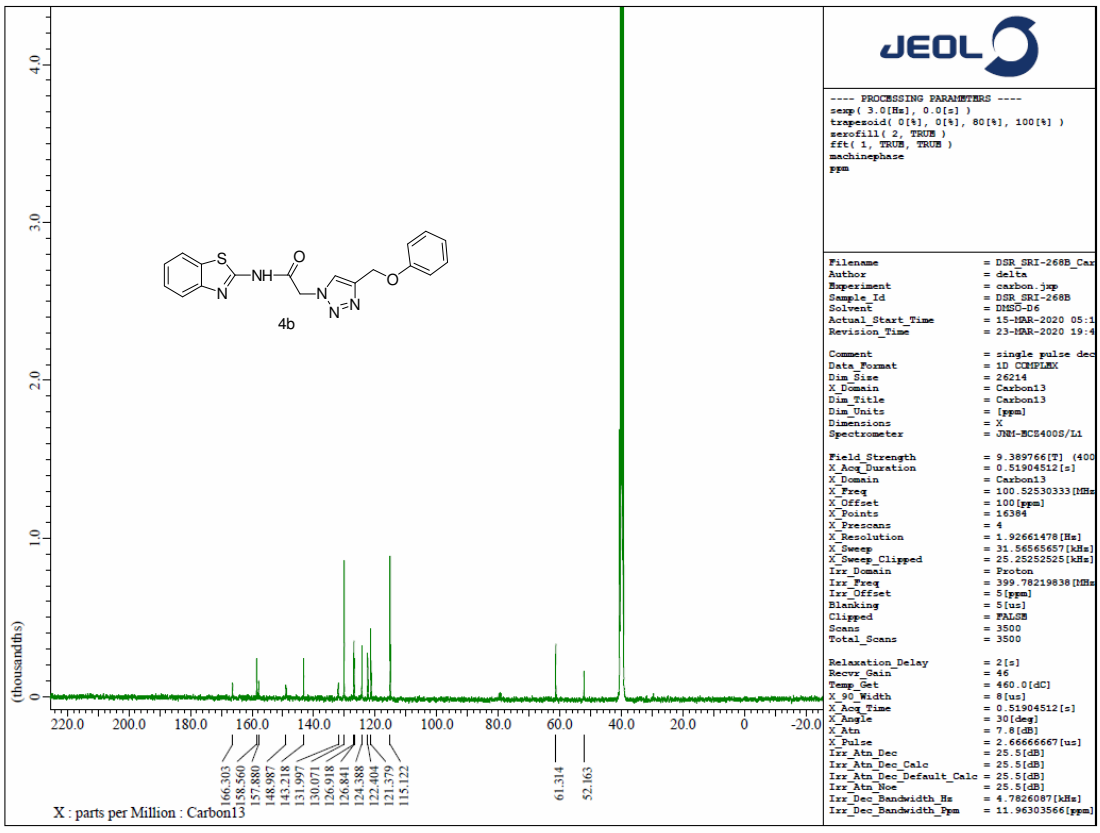

7.83
7.97
7.98
7.70
2.00
1.08
1.03
1.04
1.00
(3)
abundance
X : parts per Million : Proton
8.017
8.007
7.998
7.783
7.773
7.763
7.482
7.472
7.462
7.443
7.357
7.348
7.338
7.320
4.269
2.518
Filename = DSR_SRI-258R_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = DSR_SRI-258R
Solvent = DMSO-D6
Actual_Start_Time = 8-AUG-2019 11:32:3
Revision_Time = 21-MAR-2020 23:02:2
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.3876521[T] (400[M
X_Acq_Duration = 1.81927936[s]
X_Domain = Proton
X_Freq = 399.69219618[MHz]
X_Offset = 6.5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.54966819[Hz]
X_Sweep = 9.00576369[kHz]
X_Sweep_Clipped = 7.20461095[kHz]
Irr_Domain = Proton
Irr_Freq = 399.69219618[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.69219618[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 23.6[dC]
X_90_Width = 9.5[us]
X_Acq_Time = 1.81927936[s]
X_Angle = 45[deg]
X_Atn = 4.5[dB]
X_Pulse = 4.75[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 1
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.81927936[s]

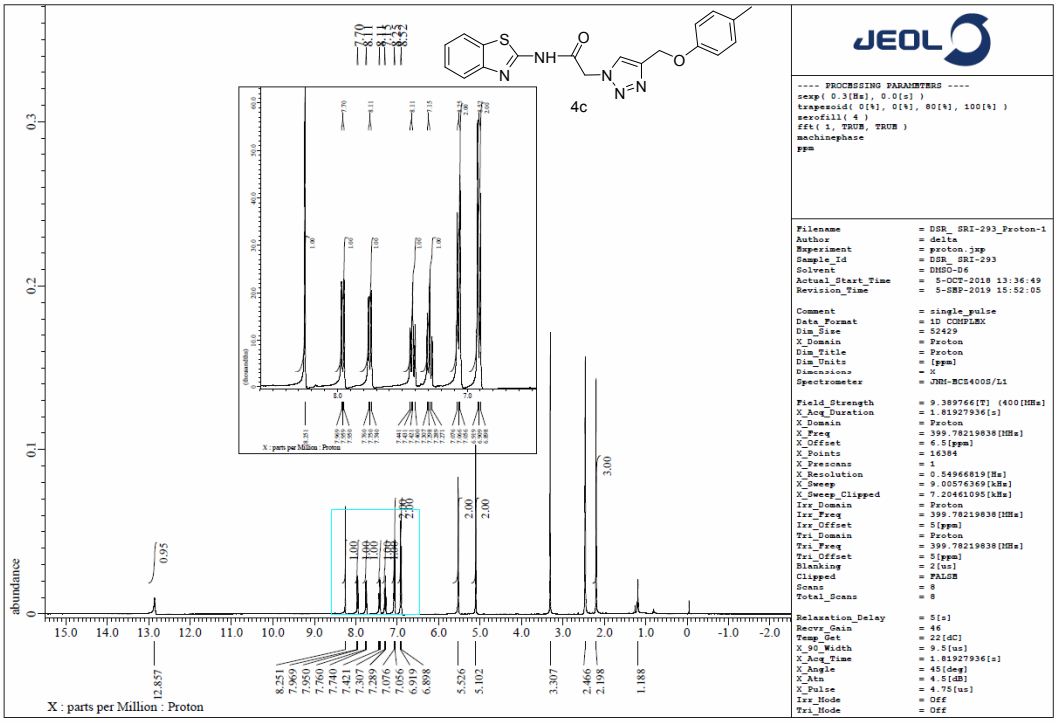

(3)
(thousandths)
X : parts per Million : Carbon13
168.340
157.950
148.902
131.966
126.771
124.298
122.323
121.173
51.299
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = RK_SRI-258R_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = RK_SRI-258R
Solvent = DMSO-D6
Actual_Start_Time = 9-AUG-2019 16:1
Revision_Time = 9-MAR-2020 12:1
Comment = single pulse dec
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.3876521[T] (40
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.50267226[MHz
X_Offset = 100.0[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.69219618[MHz
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.3[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96572948[ppm]

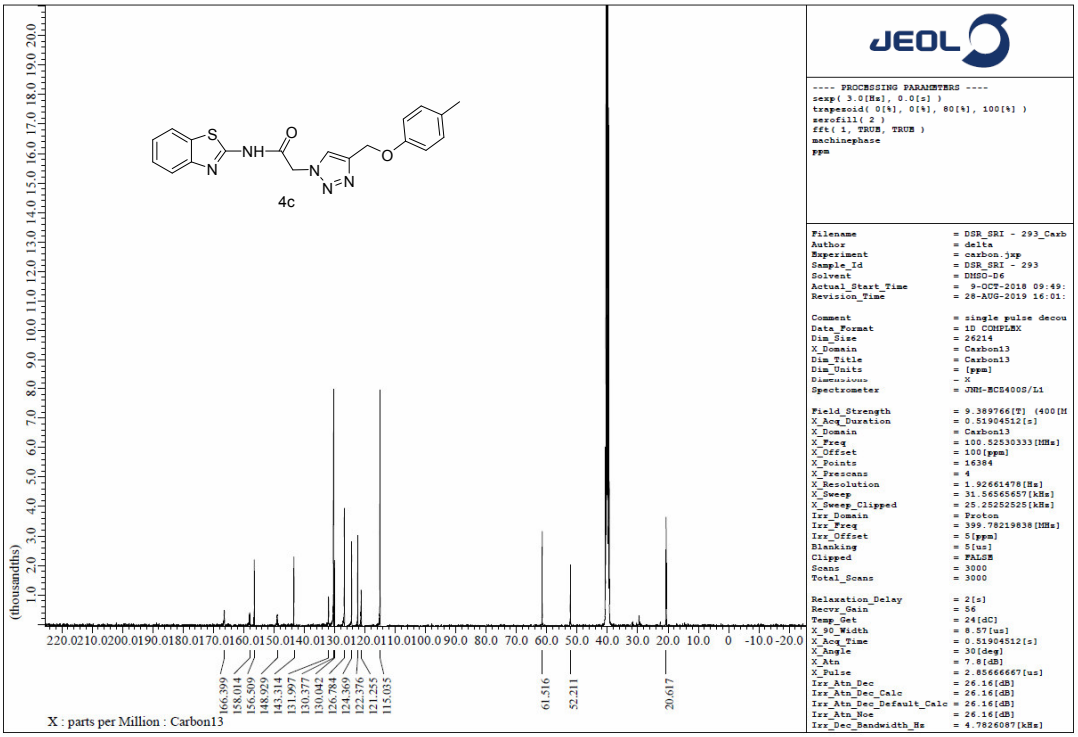

4a
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-283-A1_PROTON-6.jd
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-283-A1
Solvent = DMSO-D6
Creation_Time = 16-AUG-2018 11:47:29
Revision_Time = 4-SEP-2019 18:24:12
Current_Time = 4-SEP-2019 18:24:19
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = RCX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 5
Total_Scans = 5
Relaxation_Delay = 4[s]
Recvr_Gain = 34
Temp_Get = 70.8[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

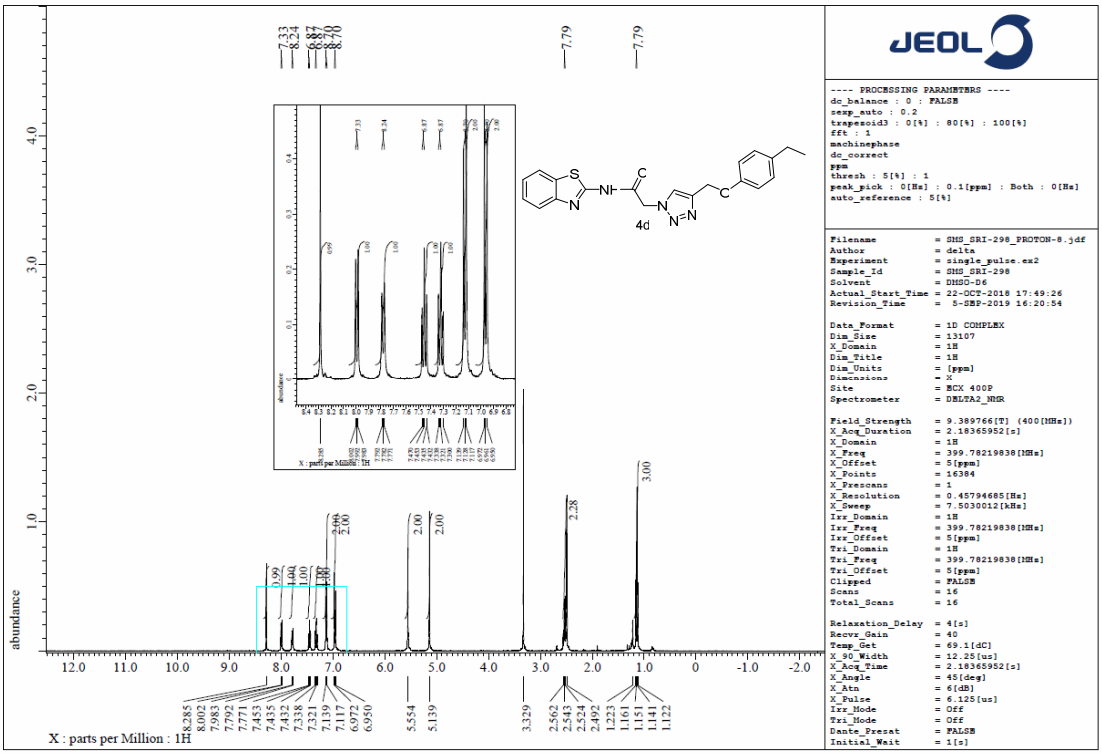

4a
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(5[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI - 283 B1_C
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_SRI - 283 B1
Solvent = DMSO-D6
Creation_Time = 9-NOV-2018 23:51:
Revision_Time = 4-SEP-2019 18:25:
Current_Time = 4-SEP-2019 18:26:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = r: 198(197),q: 39
Scans = 5000
Total_Scans = 5000
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 20.9[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.0[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

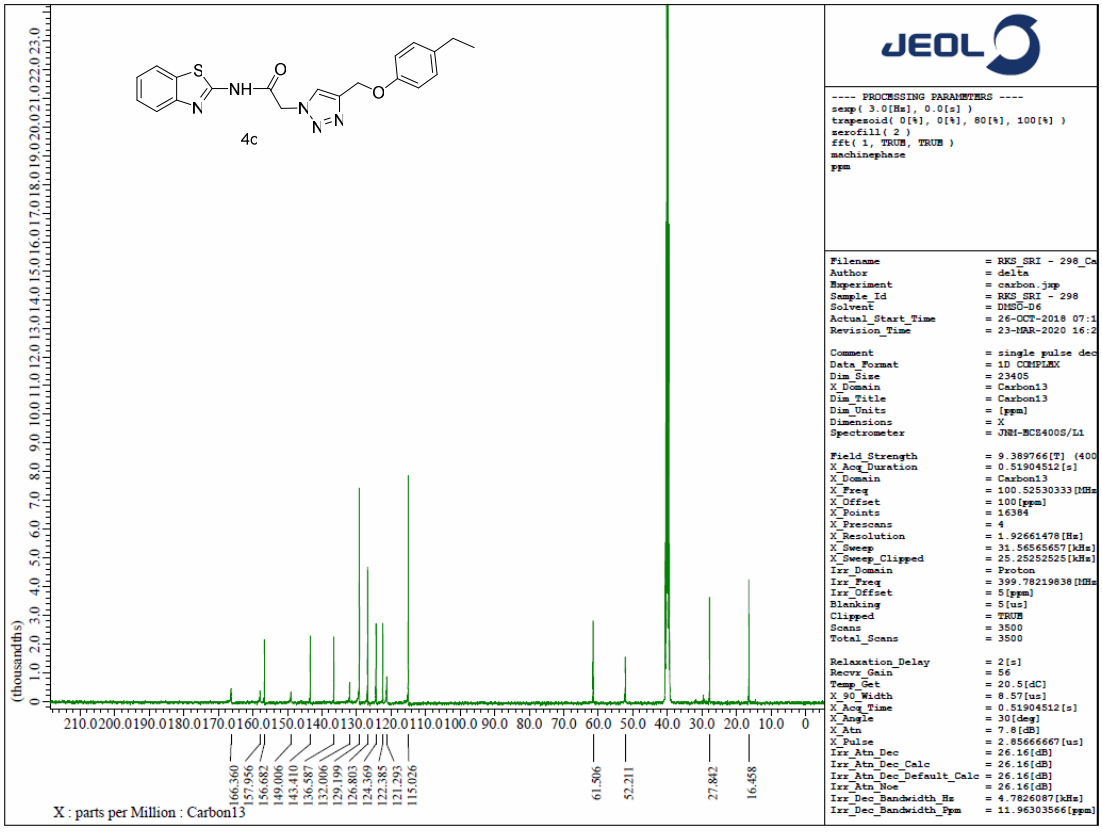

4b
X : parts per Million : 1H
abundance
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-268-F_PROTON-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-268-F
Solvent = DMSO-D6
Creation_Time = 5-NOV-2018 10:08:13
Revision_Time = 5-SEP-2019 20:41:09
Current_Time = 5-SEP-2019 20:41:23
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = BCX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 38
Temp_Get = 291.4[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

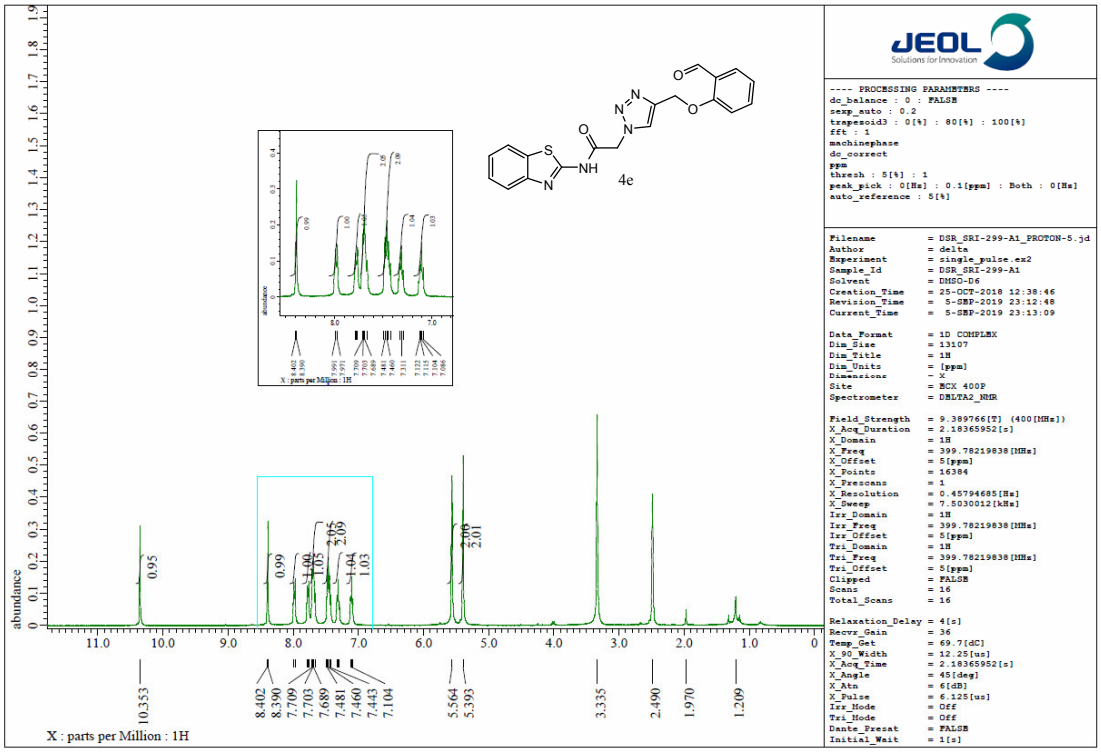

4b
X : parts per Million : Carbon13
(thousandths)
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI-268B_Car
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_SRI-268B
Solvent = DMSO-D6
Actual_Start_Time = 15-MAR-2020 05:1
Revision_Time = 23-MAR-2020 19:4
Comment = single pulse dec
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.389766[T] (400
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 3500
Total_Scans = 3500
Relaxation_Delay = 2[s]
Recvr_Gain = 46
Temp_Get = 460.0[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.66666667[us]
Irr_Atn_Dec = 25.5[dB]
Irr_Atn_Dec_Calc = 25.5[dB]
Irr_Atn_Dec_Default_Calc = 25.5[dB]
Irr_Atn_Noe = 25.5[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]

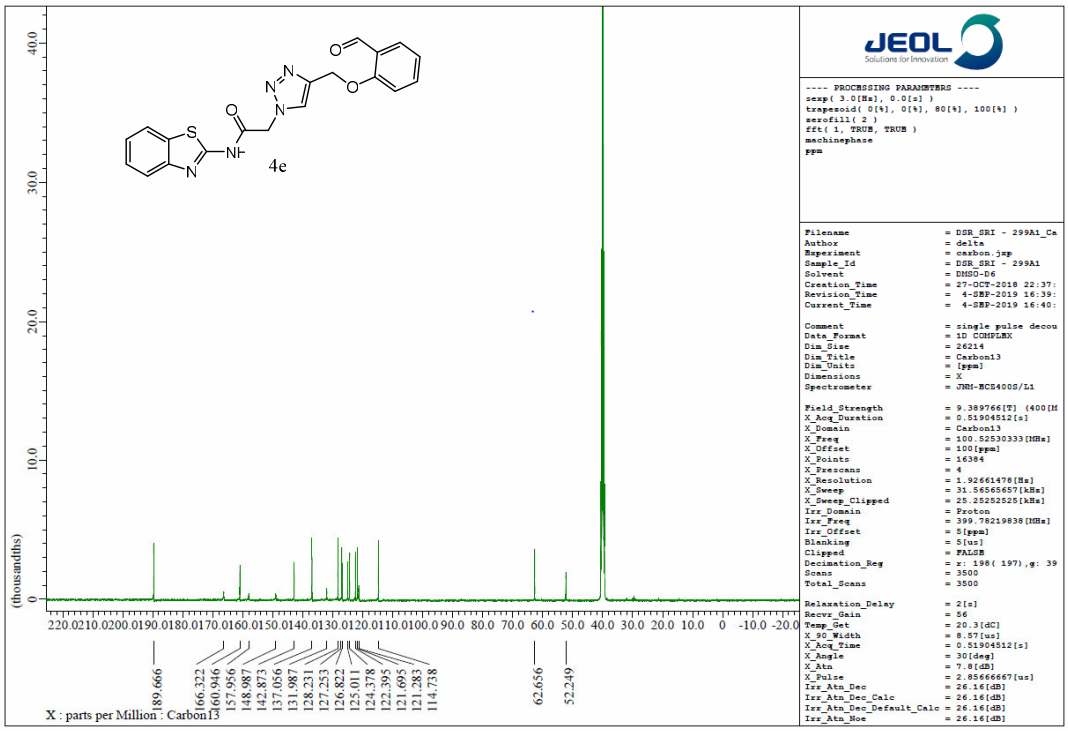

4c
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.3[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(4)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_ SRI-293_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = DSR_ SRI-293
Solvent = DMSO-D6
Actual_Start_Time = 5-OCT-2018 13:36:49
Revision_Time = 5-SEP-2019 15:52:05
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimension = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.389766[T] (400[MHz]
X_Acq_Duration = 1.81927936[s]
X_Domain = Proton
X_Freq = 399.78219838[MHz]
X_Offset = 6.5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.54966819[Hz]
X_Sweep = 9.00576369[kHz]
X_Sweep_Clipped = 7.20461095[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22[dC]
X_90_Width = 9.5[us]
X_Acq_Time = 1.81927936[s]
X_Angle = 45[deg]
X_Atn = 4.5[dB]
X_Pulse = 4.75[us]
Irr_Mode = Off
Tri_Mode = Off

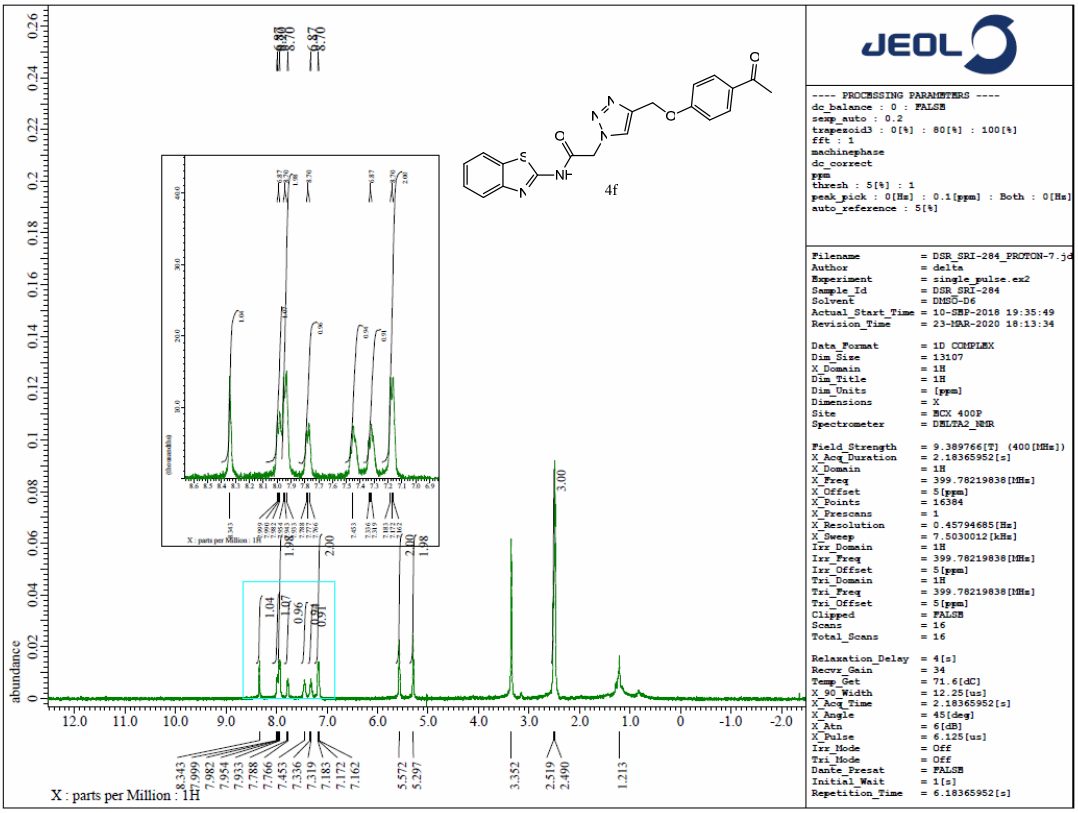

4c
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI - 293_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_SRI - 293
Solvent = DMSO-D6
Actual_Start_Time = 9-OCT-2018 09:49:
Revision_Time = 28-AUG-2019 16:01:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimension = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 3000
Total_Scans = 3000
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 24[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]

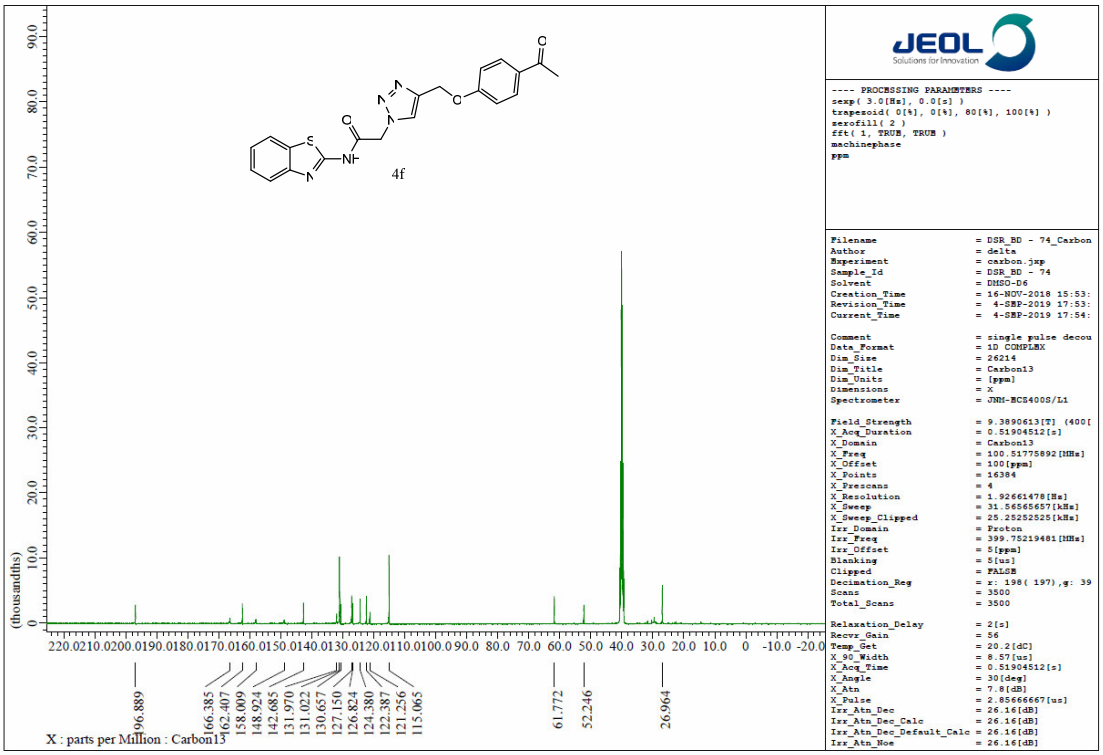

4d
abundance
X : parts per Million : 1H

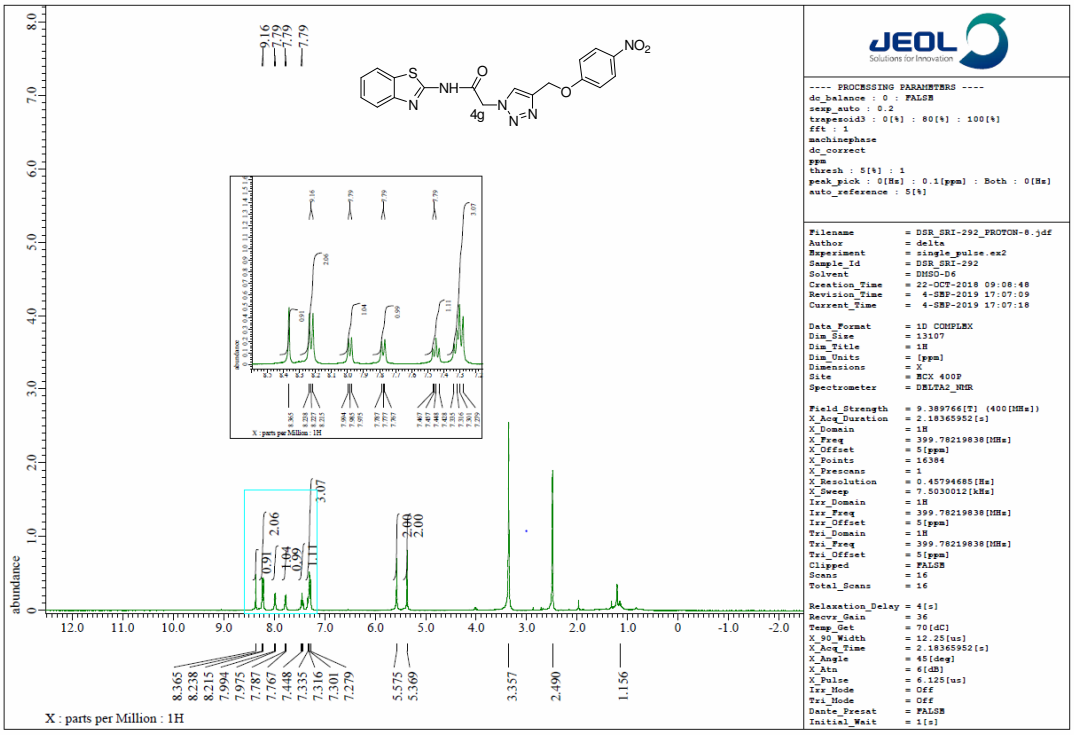

4c
(thousandths)
X : parts per Million : Carbon13

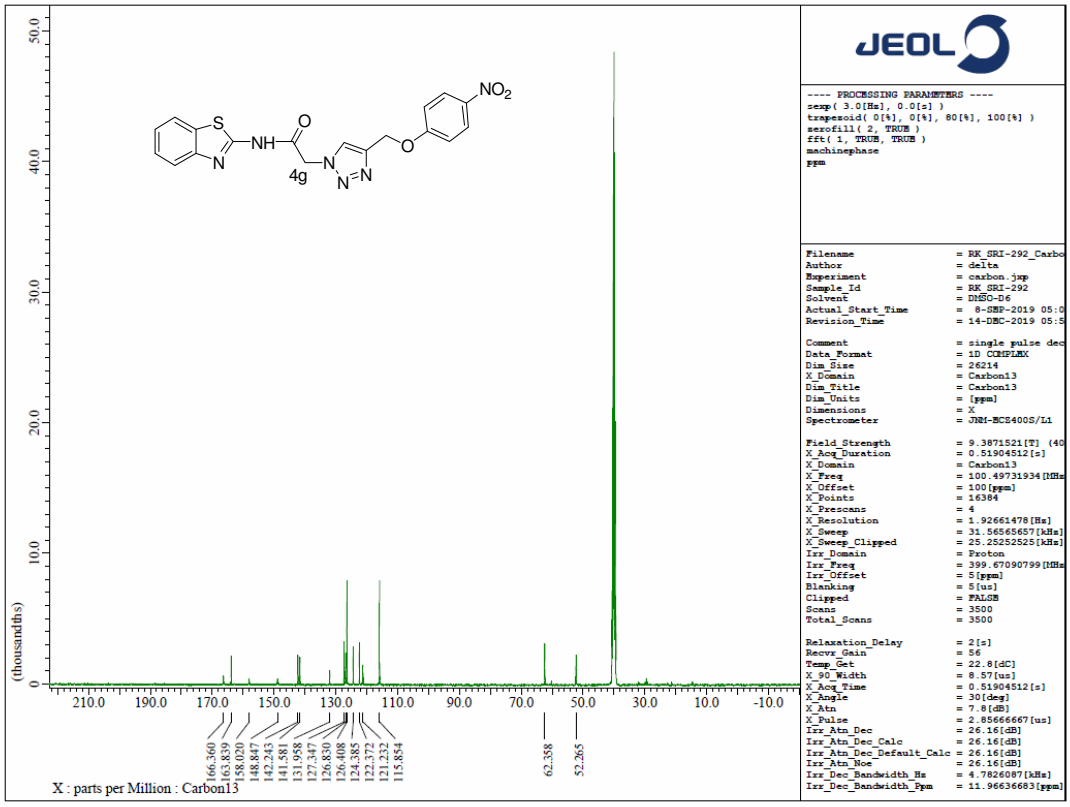

4e
abundance
X : parts per Million : 1H
10.353
8.402
8.390
7.709
7.703
7.689
7.481
7.460
7.443
7.104
5.564
5.393
3.335
2.490
1.970
1.209
0.95
0.99
1.00
1.05
2.05
2.09
1.04
1.03
2.00
2.01
JEOL
Solutions for Innovation
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-299-A1_PROTON-5.jd
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-299-A1
Solvent = DMSO-D6
Creation_Time = 25-OCT-2018 12:38:46
Revision_Time = 5-SEP-2019 23:12:48
Current_Time = 5-SEP-2019 23:13:09
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = BCX 400P
Spectrometer = DBL/TA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 69.7[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

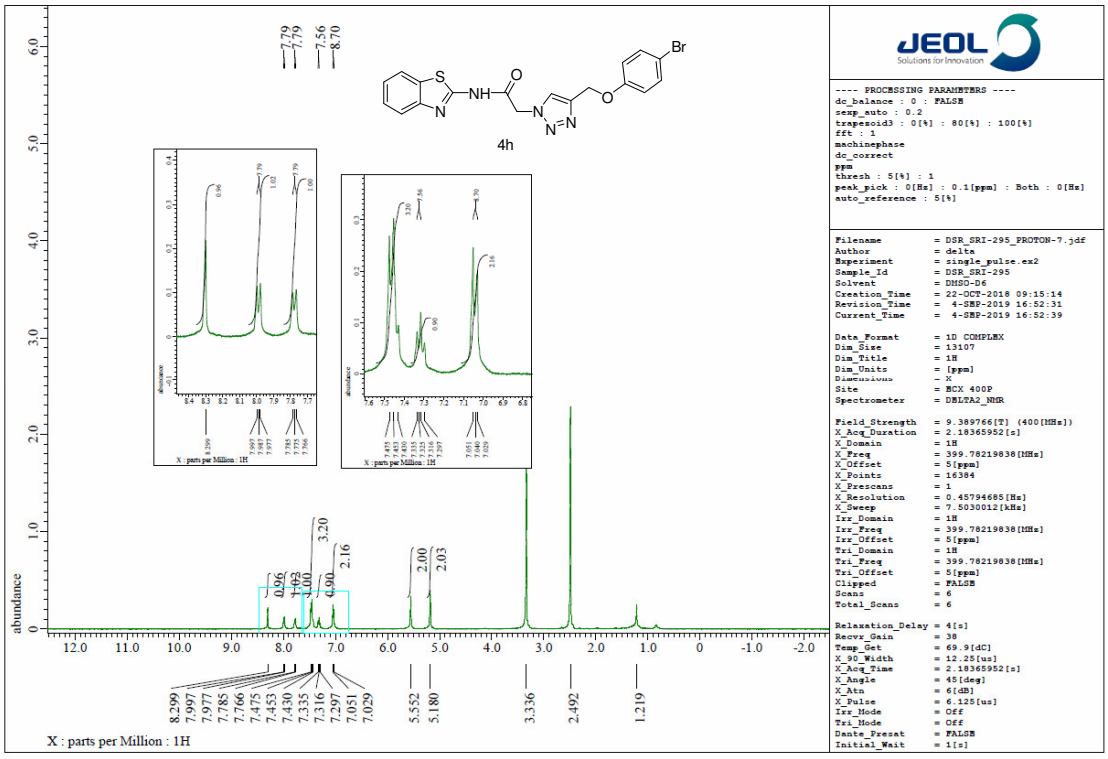

4e
(thousandths)
X : parts per Million : Carbon13
189.666
166.322
160.946
157.956
148.987
142.873
137.056
131.987
128.231
127.253
126.822
125.011
124.378
122.395
121.695
121.283
114.738
62.656
52.249
JEOL
Solutions for Innovation
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI - 299A1_Ca
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_SRI - 299A1
Solvent = DMSO-D6
Creation_Time = 27-OCT-2018 22:37:
Revision_Time = 4-SEP-2019 16:39:
Current_Time = 4-SEP-2019 16:40:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = x: 198(197),y: 39
Scans = 3500
Total_Scans = 3500
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 20.3[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

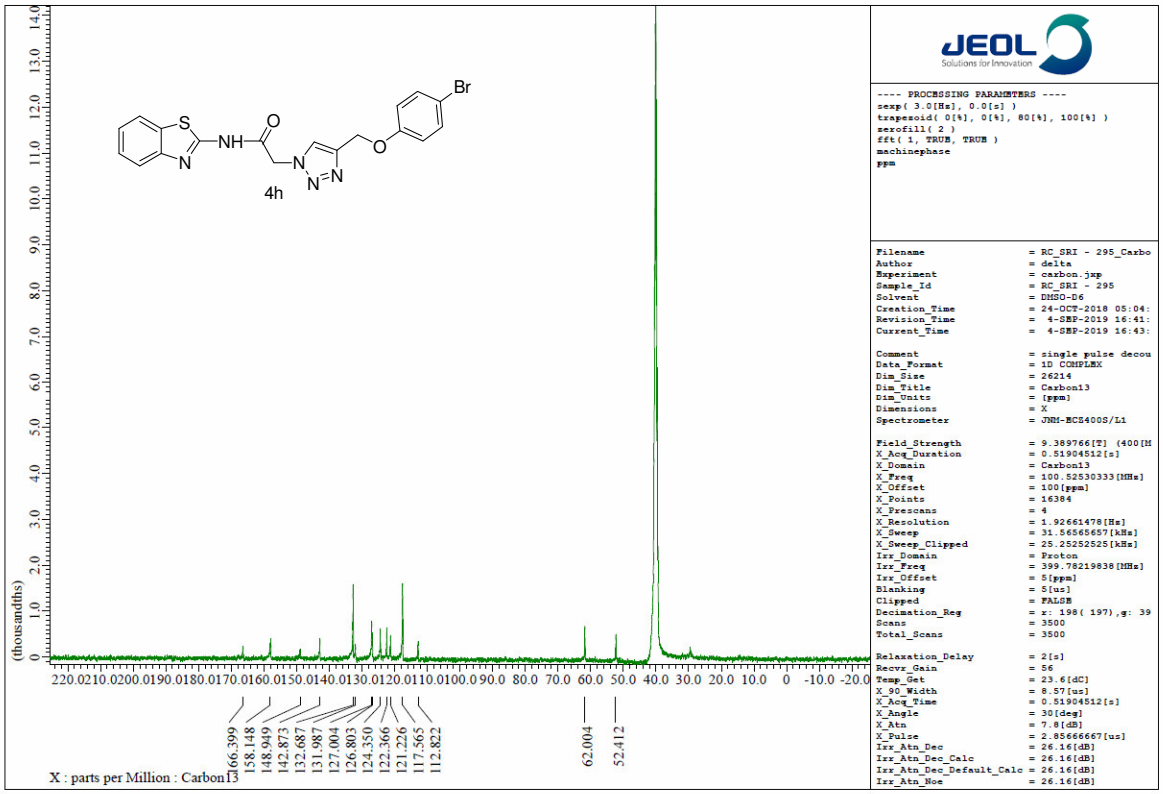

4f
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-284_PROTON-7.jd
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-284
Solvent = DMSO-D6
Actual_Start_Time = 10-SEP-2018 19:35:49
Revision_Time = 23-MAR-2020 18:13:34
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = NCX 400P
Spectrometer = DEL/TA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 34
Temp_Get = 71.6[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.18365952[s]

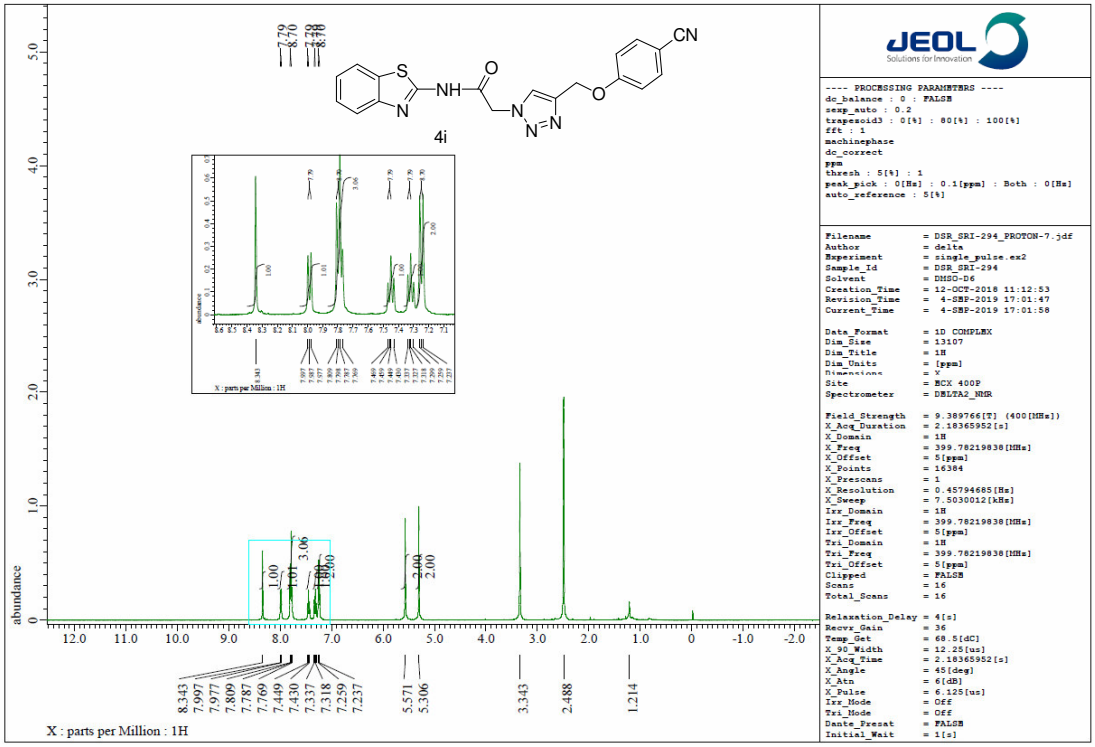

4f
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_BD - 74_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_BD - 74
Solvent = DMSO-D6
Creation_Time = 16-NOV-2018 15:53:
Revision_Time = 4-SEP-2019 17:53:
Current_Time = 4-SEP-2019 17:54:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.3890613[T] (400[
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.51775892[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.75219481[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = x: 198(197),y: 39
Scans = 3500
Total_Scans = 3500
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 20.2[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

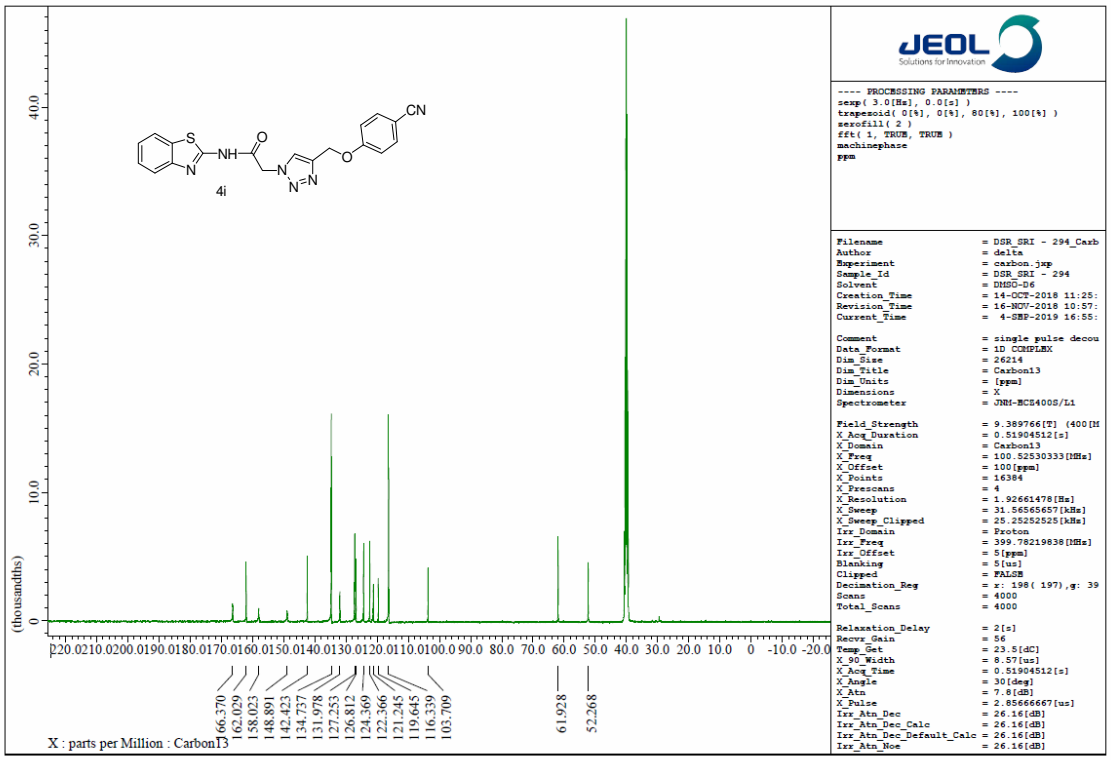

4g
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapesoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-292_PROTON-8.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-292
Solvent = DMSO-D6
Creation_Time = 22-OCT-2018 09:08:48
Revision_Time = 4-SEP-2019 17:07:09
Current_Time = 4-SEP-2019 17:07:18
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = BCX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 6[s]
Recvr_Gain = 36
Temp_Get = 70[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

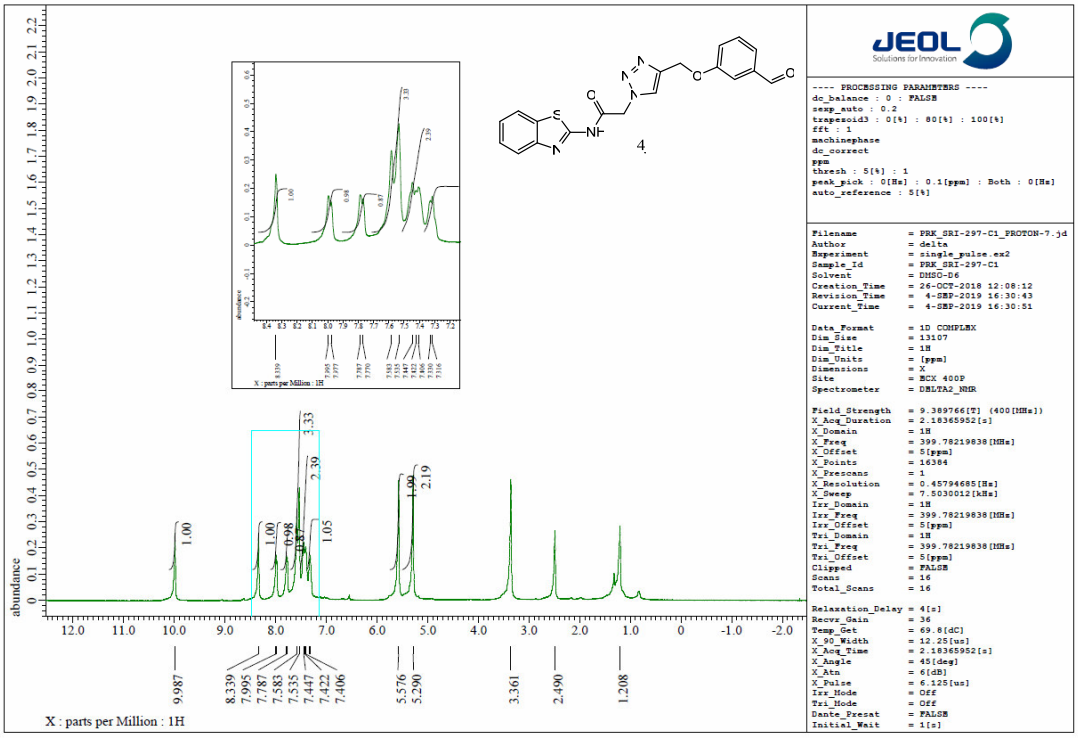

4g
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapesoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = RK_SRI-292_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = RK_SRI-292
Solvent = DMSO-D6
Actual_Start_Time = 8-SEP-2019 05:0
Revision_Time = 14-DEC-2019 05:5
Comment = single pulse dec
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.3871521[T] (40
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.49731934[MHz
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.67090799[MHz
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 3500
Total_Scans = 3500
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.8[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96636683[ppm]

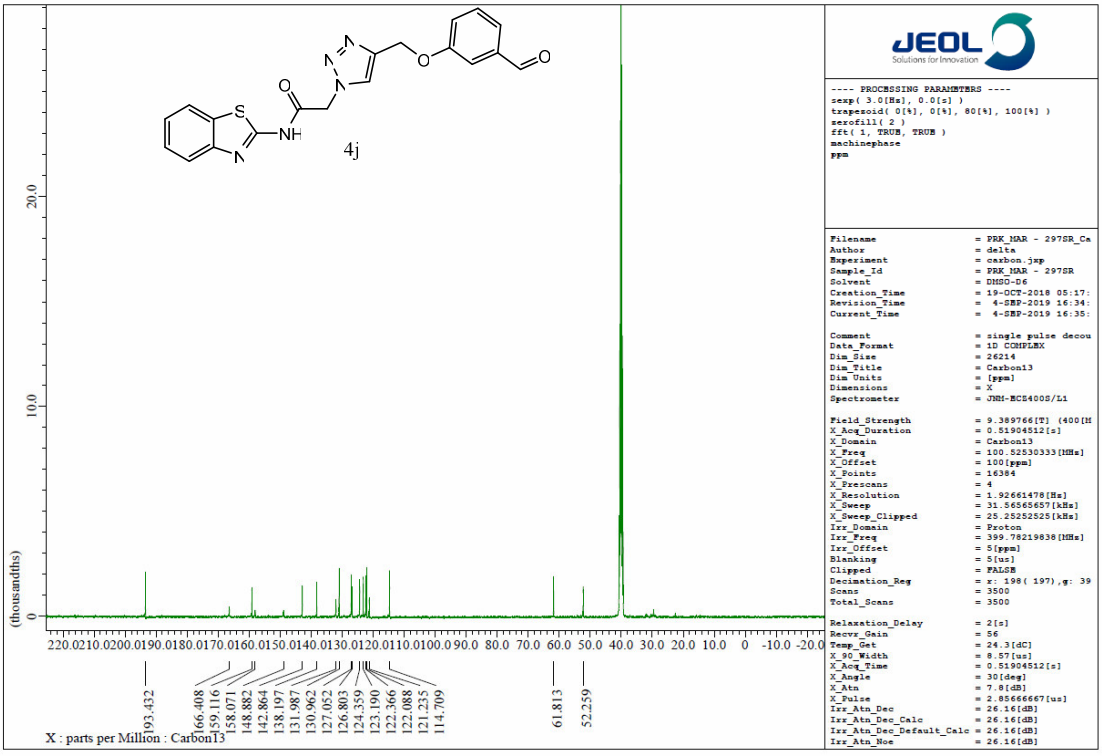

4h
X : parts per Million : 1H
abundance
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-295_PROTON-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-295
Solvent = DMSO-D6
Creation_Time = 22-OCT-2018 09:15:14
Revision_Time = 4-SEP-2019 16:52:31
Current_Time = 4-SEP-2019 16:52:39
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Site = RCX 400P
Spectrometer = DBL7A2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 6
Total_Scans = 6
Relaxation_Delay = 4[s]
Recvr_Gain = 38
Temp_Get = 69.9[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

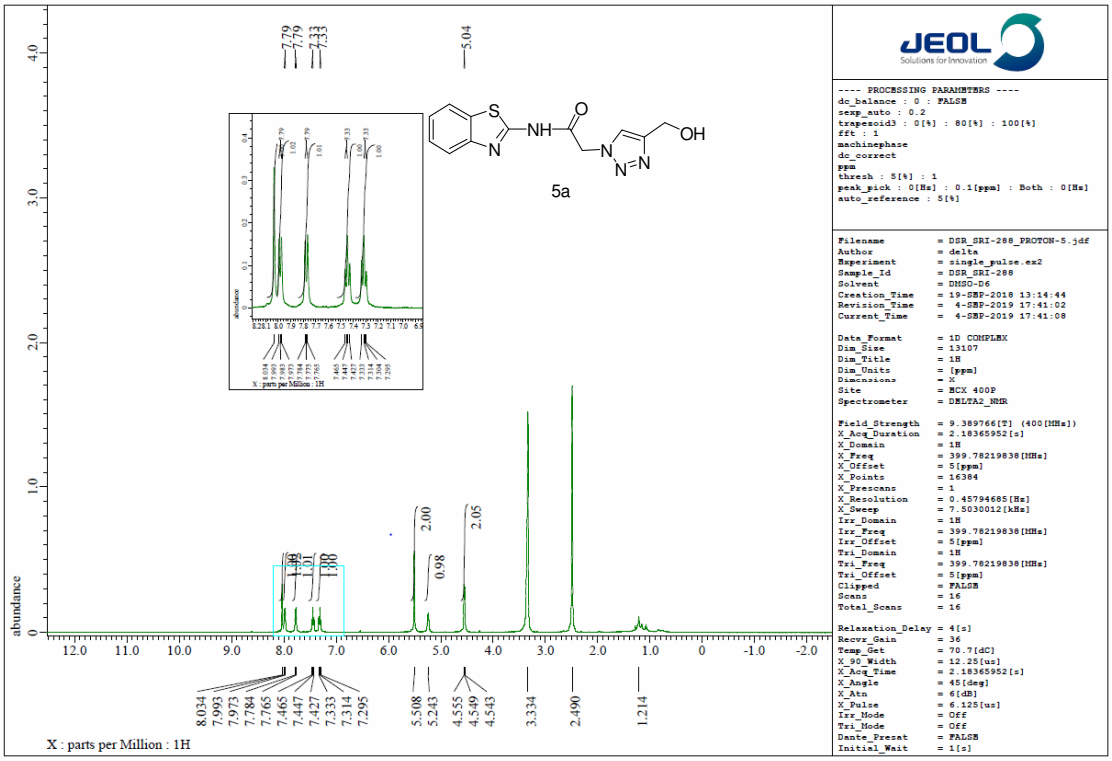

4h
X : parts per Million : Carbon13
(thousandths)
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = RC_SRI - 295_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = RC_SRI - 295
Solvent = DMSO-D6
Creation_Time = 24-OCT-2018 05:04:
Revision_Time = 4-SEP-2019 16:41:
Current_Time = 4-SEP-2019 16:43:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = x: 198(197),y: 39
Scans = 3500
Total_Scans = 3500
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 23.6[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

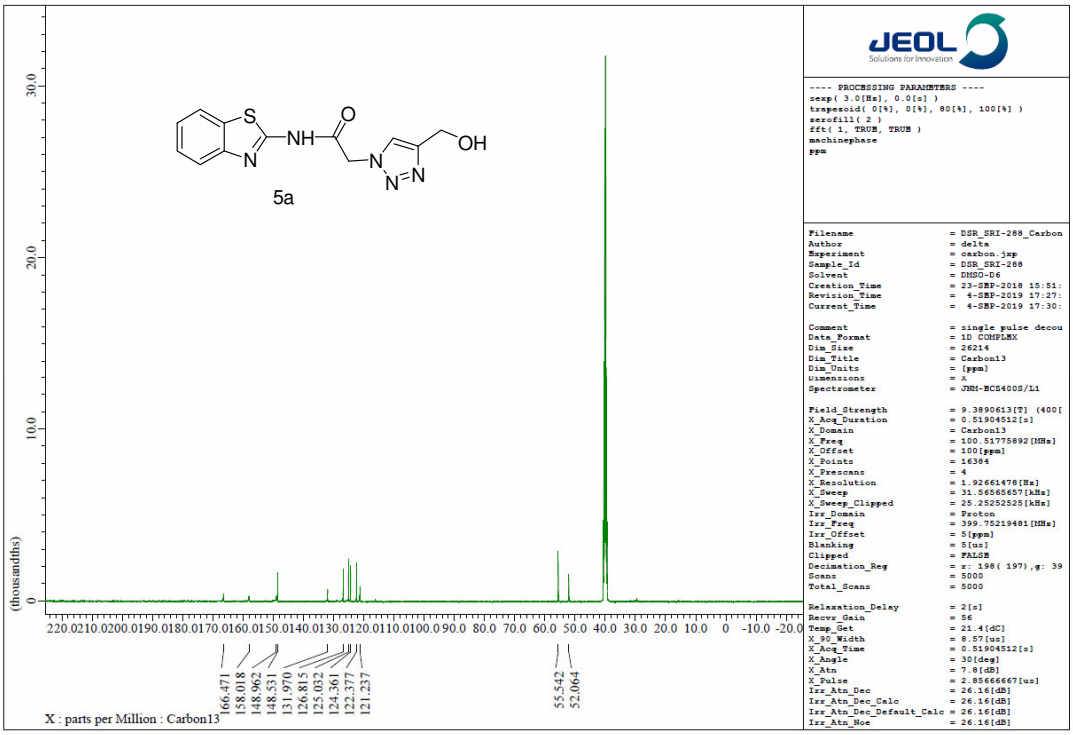

4i
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-294_PROTON-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-294
Solvent = DMSO-D6
Creation_Time = 12-OCT-2018 11:12:53
Revision_Time = 4-SEP-2019 17:01:47
Current_Time = 4-SEP-2019 17:01:58
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Site = BCX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 68.5[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

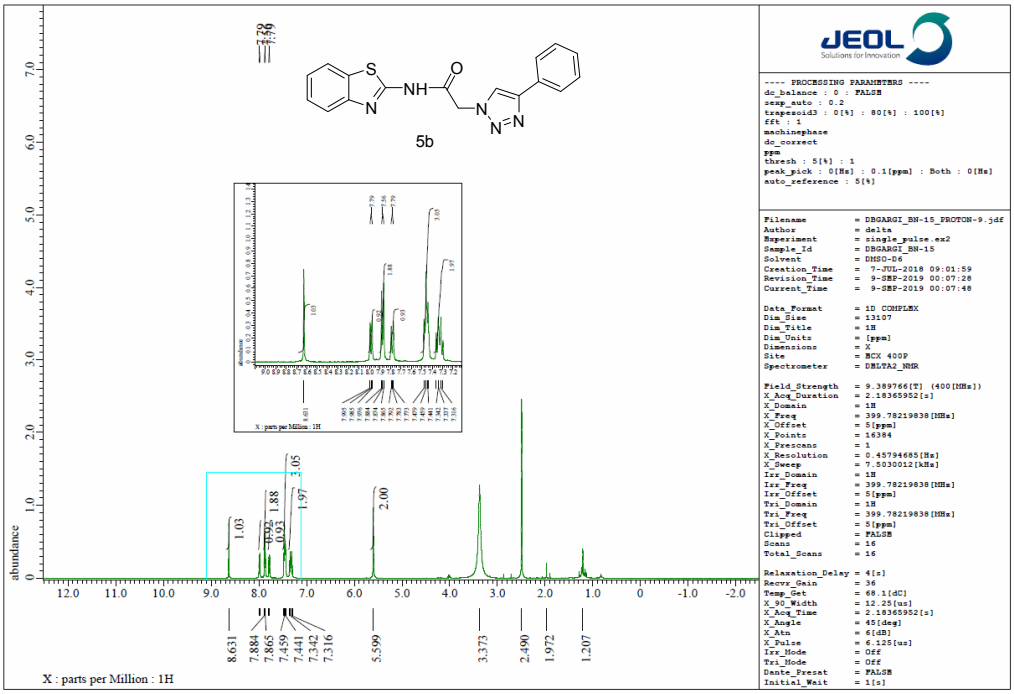

4i
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI - 294_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_SRI - 294
Solvent = DMSO-D6
Creation_Time = 14-OCT-2018 11:25:
Revision_Time = 16-NOV-2018 10:57:
Current_Time = 4-SEP-2019 16:55:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = x: 198(197),y: 39
Scans = 4000
Total_Scans = 4000
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 23.5[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

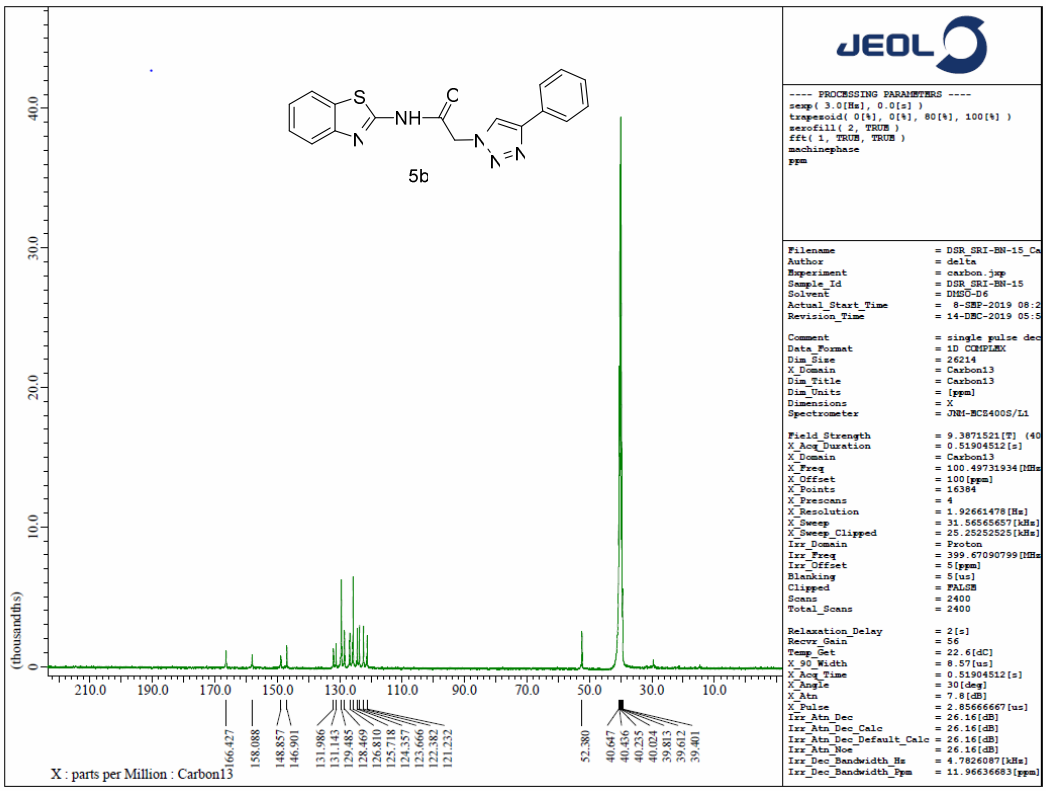

4
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = PRK_SRI-297-C1_PROTON-7.jd
Author = delta
Experiment = single_pulse.ex2
Sample_Id = PRK_SRI-297-C1
Solvent = DMSO-D6
Creation_Time = 26-OCT-2018 12:08:12
Revision_Time = 4-SEP-2019 16:30:43
Current_Time = 4-SEP-2019 16:30:51
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = NCX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 69.8[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

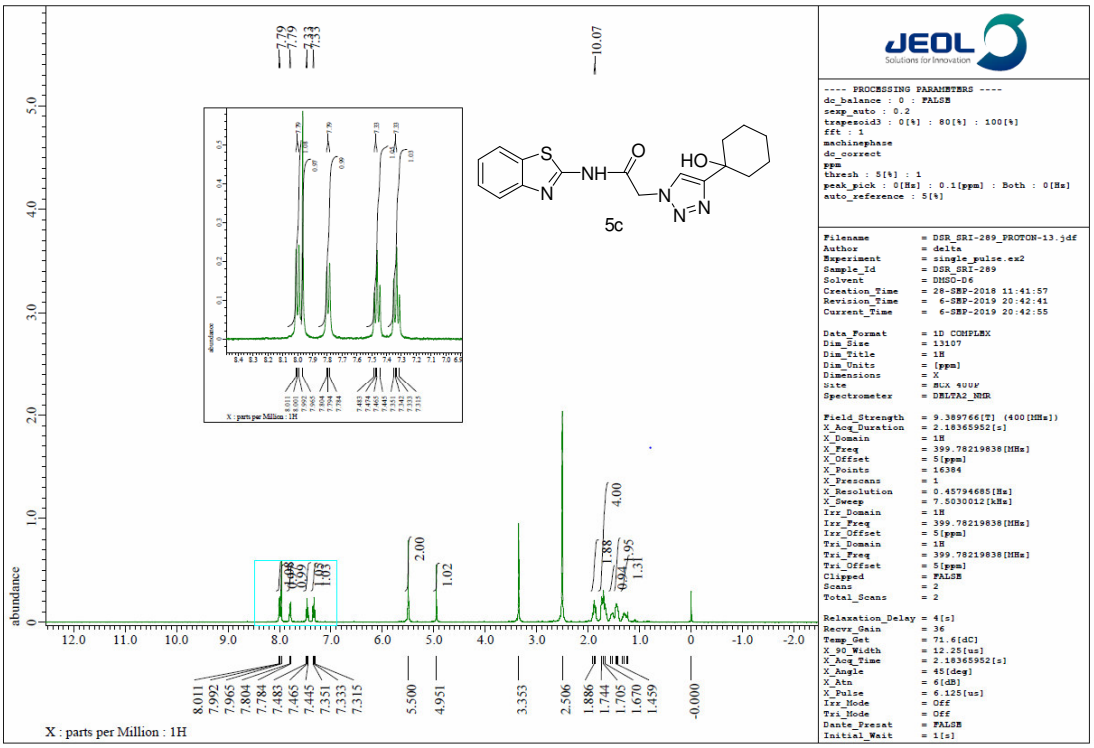

4j
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = PRK_MAR - 297SR_Ca
Author = delta
Experiment = carbon.jxp
Sample_Id = PRK_MAR - 297SR
Solvent = DMSO-D6
Creation_Time = 19-OCT-2018 05:17:
Revision_Time = 4-SEP-2019 16:34:
Current_Time = 4-SEP-2019 16:35:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = x: 198(197),y: 39
Scans = 3500
Total_Scans = 3500
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 24.3[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

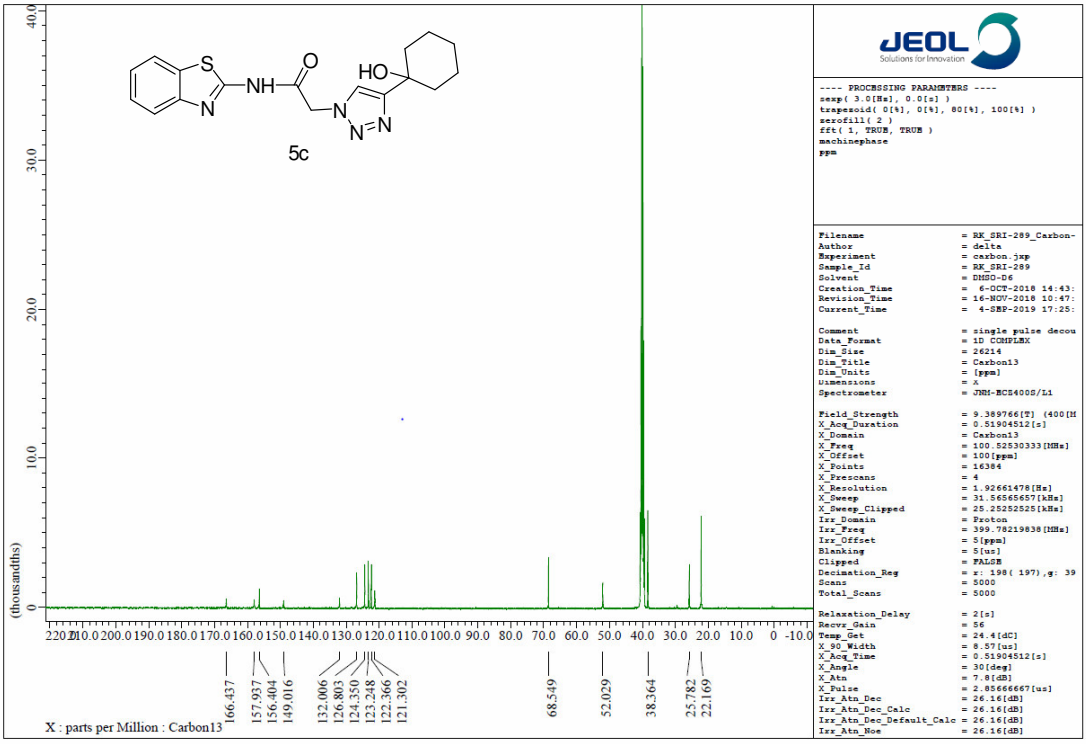

7.79
7.79
7.33
7.33
5.04
S
NH
O
N
N
N
OH
5a
2.00
2.05
0.98
1.03
1.01
1.00
abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
8.034
7.993
7.973
7.784
7.765
7.465
7.447
7.427
7.333
7.314
7.295
5.508
5.243
4.555
4.549
4.543
3.334
2.490
1.214
X : parts per Million : 1H
JEOL
Solutions for Innovation
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-288_PROTON-5.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-288
Solvent = DMSO-D6
Creation_Time = 19-SEP-2018 13:14:44
Revision_Time = 4-SEP-2019 17:41:02
Current_Time = 4-SEP-2019 17:41:08
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = RCX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 70.7[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

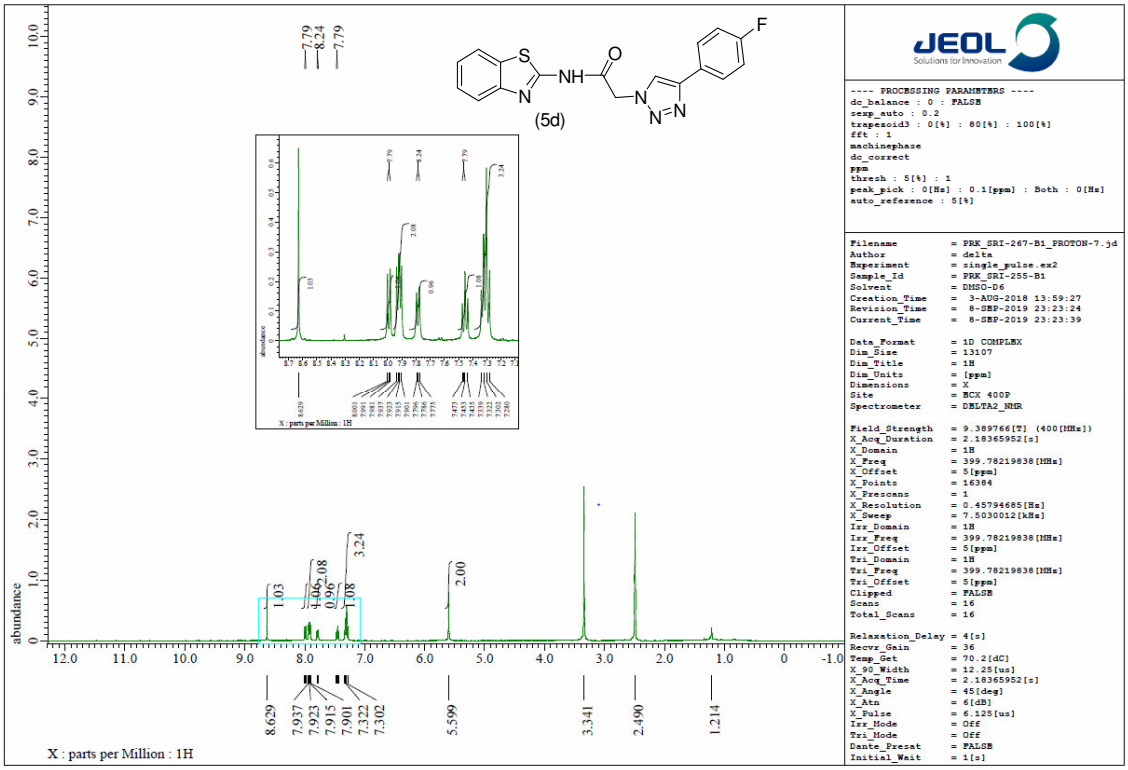

S
NH
O
N
N
N
OH
5a
(thousandths)
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
166.471
158.018
148.962
148.531
131.970
126.815
125.032
124.361
122.377
121.237
55.542
52.064
X : parts per Million : Carbon13
JEOL
Solutions for Innovation
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI-288_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_SRI-288
Solvent = DMSO-D6
Creation_Time = 23-SEP-2018 15:51:
Revision_Time = 4-SEP-2019 17:27:
Current_Time = 4-SEP-2019 17:30:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.3890613[T] (400[
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.51775892[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.75219481[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = x: 198(197),y: 39
Scans = 5000
Total_Scans = 5000
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 21.4[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

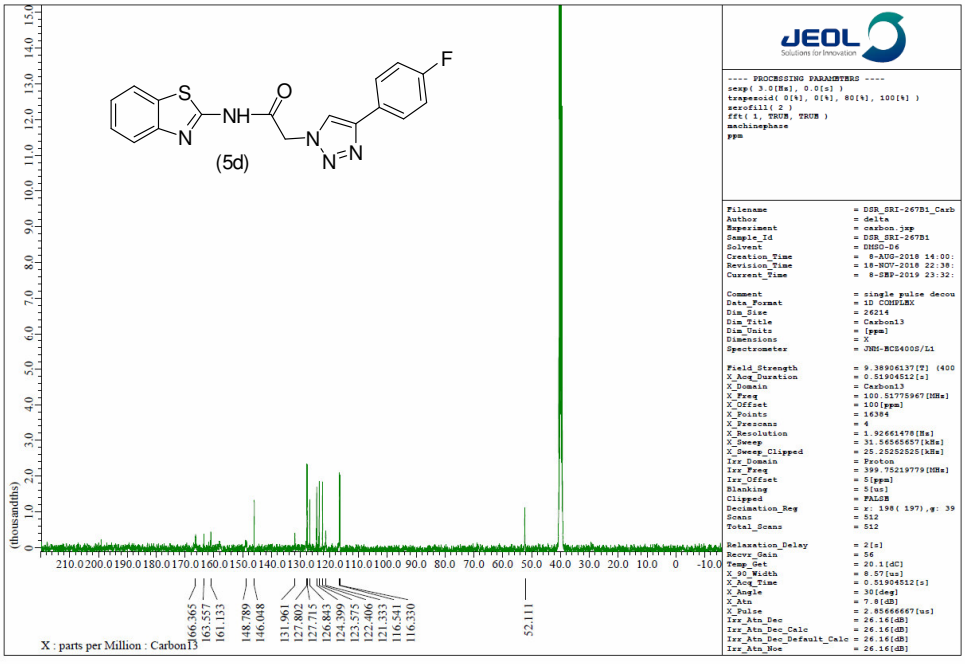

5b
abundance
X : parts per Million : 1H
8.631
7.884
7.865
7.459
7.441
7.342
7.316
5.599
3.373
2.490
1.972
1.207
1.03
1.88
3.05
1.97
2.00
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DBGARGI_BN-15_PROTON-9.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DBGARGI_BN-15
Solvent = DMSO-D6
Creation_Time = 7-JUL-2018 09:01:59
Revision_Time = 9-SEP-2019 00:07:28
Current_Time = 9-SEP-2019 00:07:48
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = NCX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Trz_Domain = 1H
Trz_Freq = 399.78219838[MHz]
Trz_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 68.1[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Trz_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

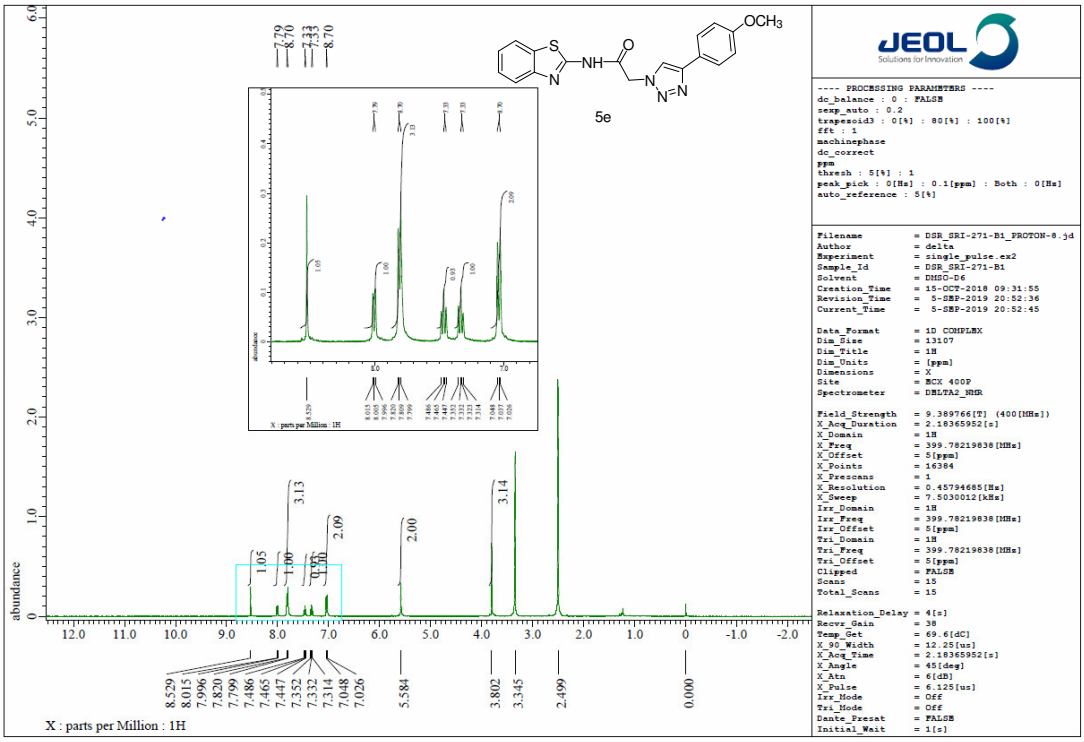

5b
(thousandths)
X : parts per Million : Carbon13
166.427
158.088
148.857
146.901
131.986
131.143
129.485
128.469
126.810
125.718
124.357
123.666
122.382
121.232
52.380
40.647
40.456
40.235
40.024
39.813
39.612
39.401
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI-BN-15_Ca
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_SRI-BN-15
Solvent = DMSO-D6
Actual_Start_Time = 8-SEP-2019 08:2
Revision_Time = 14-DEC-2019 05:5
Comment = single pulse dec
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.3871521[T] (40
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.49731934[MHz
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.67090799[MHz
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 2400
Total_Scans = 2400
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.6[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96636683[ppm]

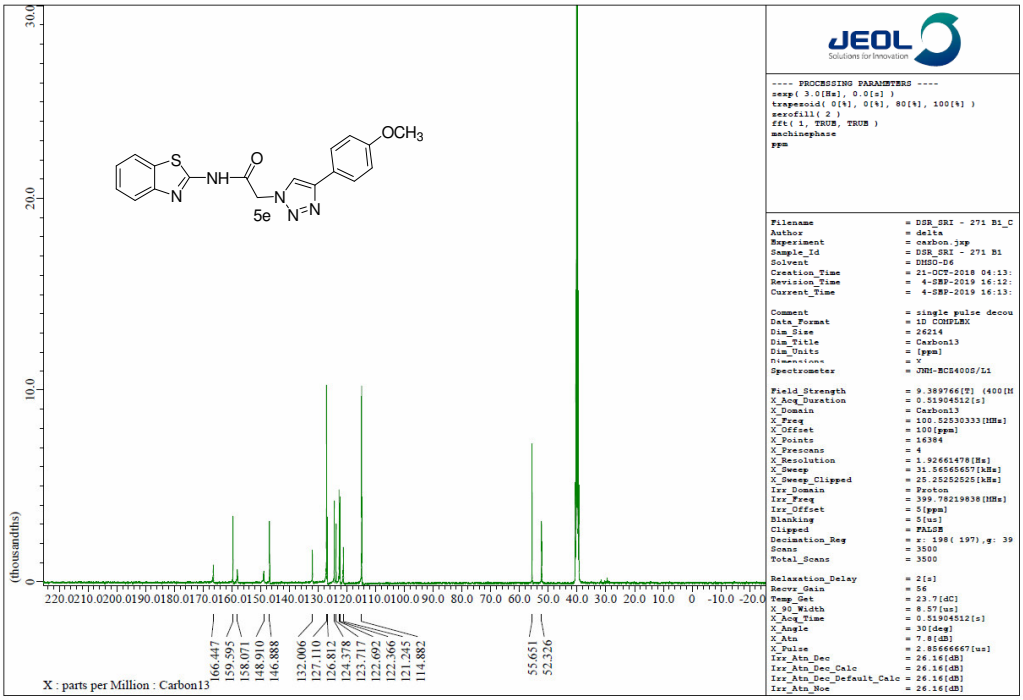

5c
X : parts per Million : 1H
abundance
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-289_PROTON-13.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-289
Solvent = DMSO-D6
Creation_Time = 28-SEP-2018 11:41:57
Revision_Time = 6-SEP-2019 20:42:41
Current_Time = 6-SEP-2019 20:42:55
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = MLX 400W
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 2
Total_Scans = 2
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 71.6[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

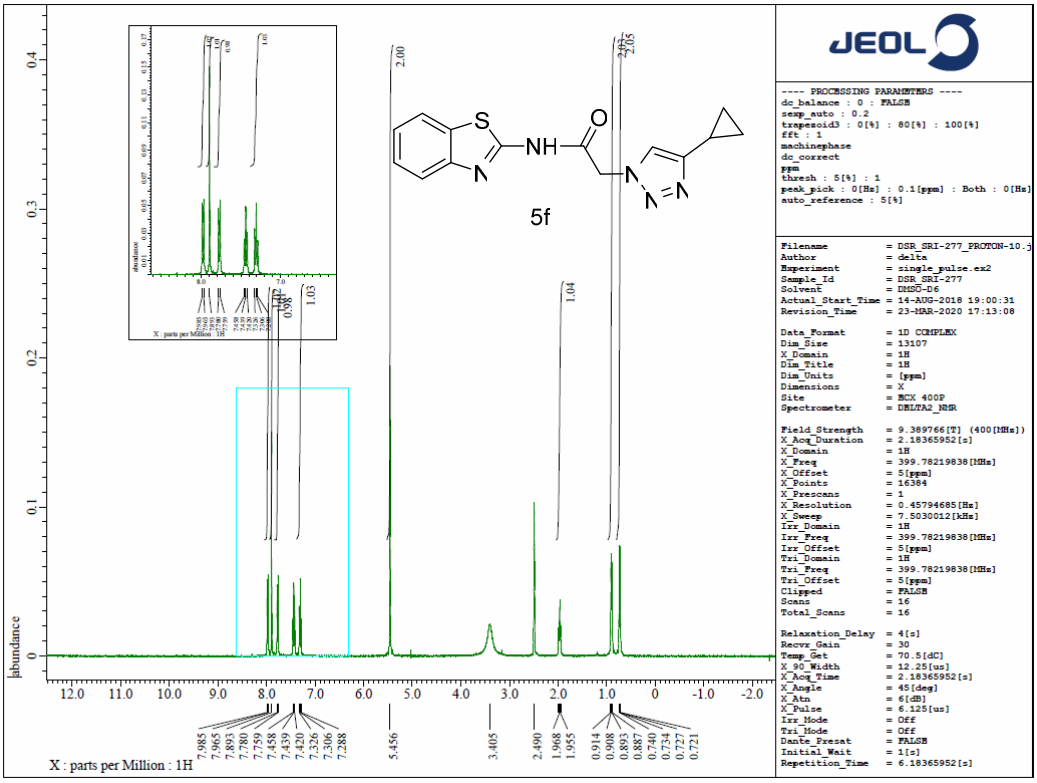

5c
X : parts per Million : Carbon13
(thousandths)
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = RK_SRI-289_Carbon-
Author = delta
Experiment = carbon.jxp
Sample_Id = RK_SRI-289
Solvent = DMSO-D6
Creation_Time = 6-OCT-2018 14:43:
Revision_Time = 16-NOV-2018 10:47:
Current_Time = 4-SEP-2019 17:25:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = r: 198(197),g: 39
Scans = 5000
Total_Scans = 5000
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 24.4[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

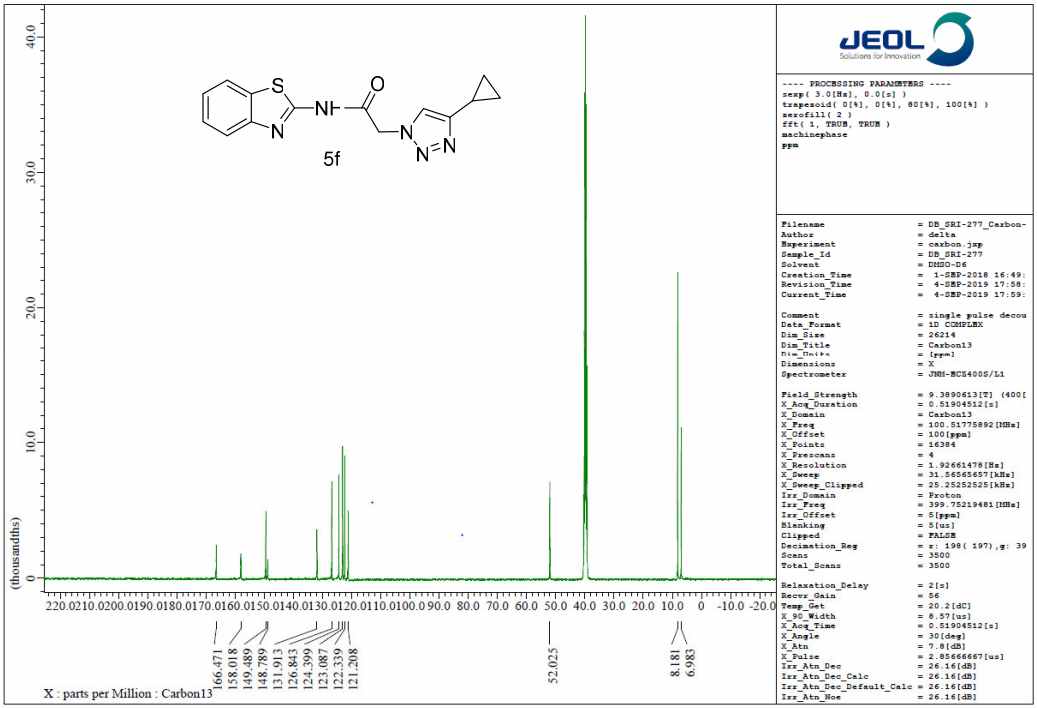

(5d)
X : parts per Million : 1H
abundance
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = PRK_SRI-267-B1_PROTON-7.jd
Author = delta
Experiment = single_pulse.ex2
Sample_Id = PRK_SRI-255-B1
Solvent = DMSO-D6
Creation_Time = 3-AUG-2018 13:59:27
Revision_Time = 8-SEP-2019 23:23:24
Current_Time = 8-SEP-2019 23:23:39
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = NCX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 70.2[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

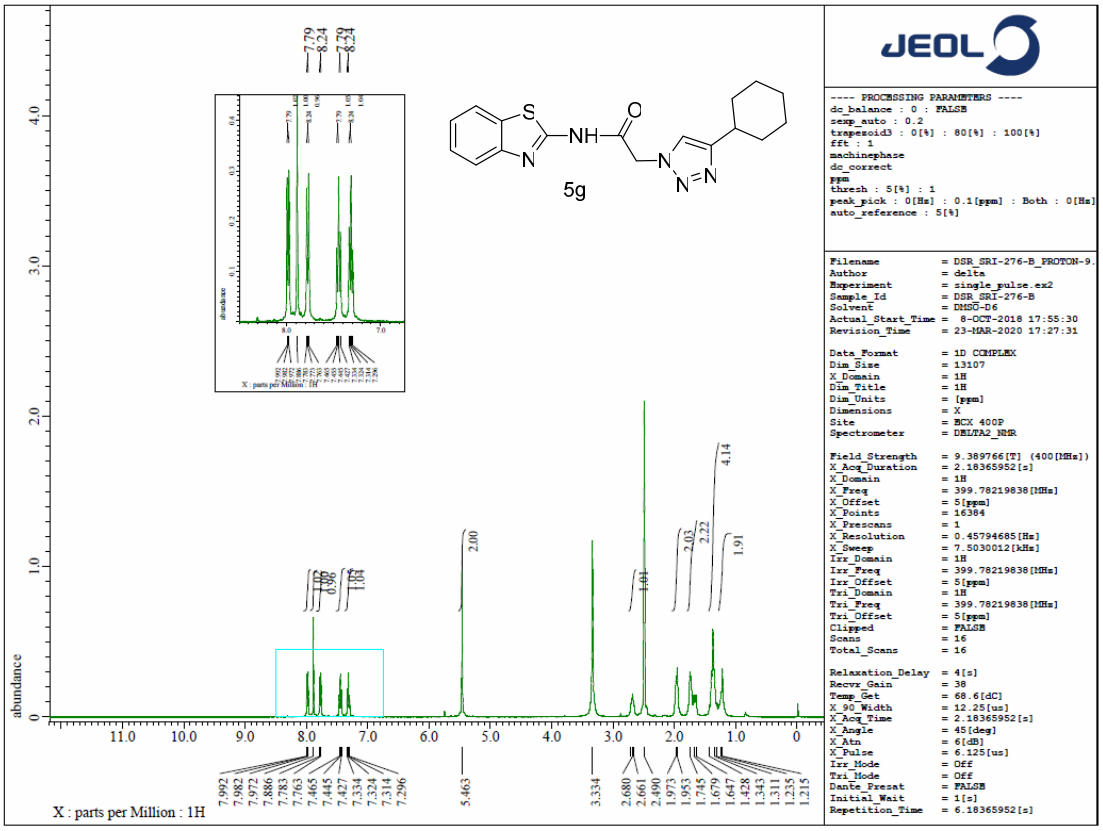

(5d)
X : parts per Million : Carbon13
(thousandths)
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI-267B1_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_SRI-267B1
Solvent = DMSO-D6
Creation_Time = 8-AUG-2018 14:00:
Revision_Time = 18-NOV-2018 22:38:
Current_Time = 8-SEP-2019 23:32:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.38906137[T] (400
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.51775967[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.75219779[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = x: 198(197),y: 39
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 20.1[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

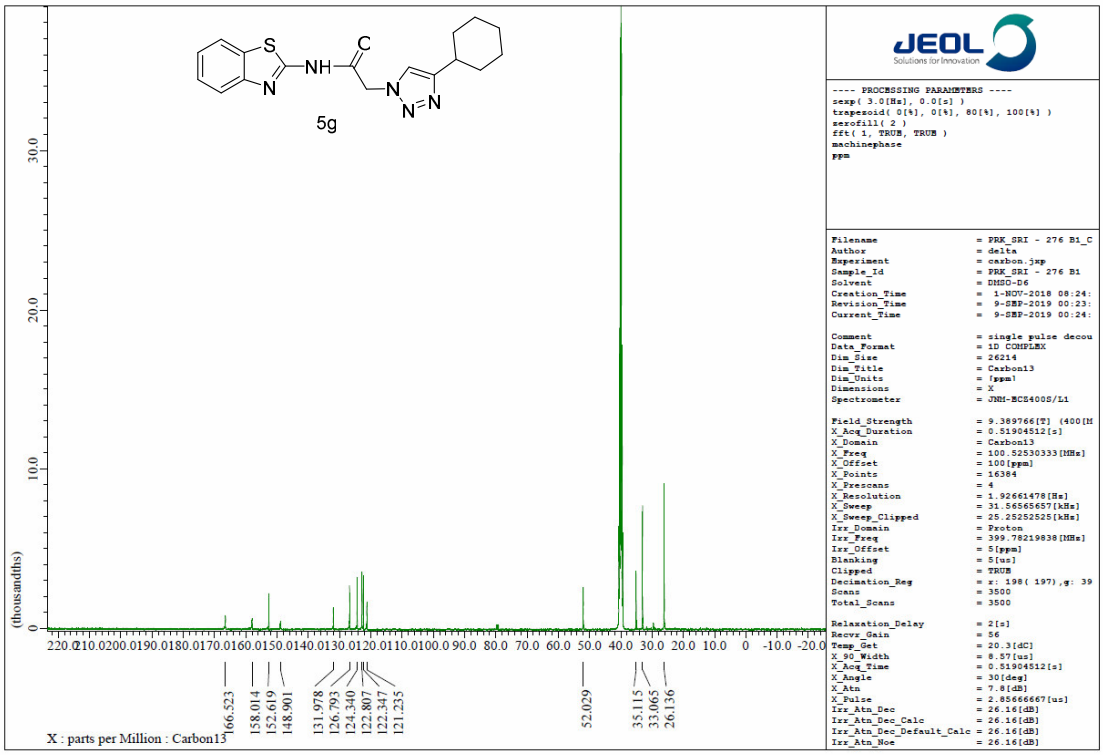

5e
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapesoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-271-B1_PROTON-8.jd
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-271-B1
Solvent = DMSO-D6
Creation_Time = 15-OCT-2018 09:31:55
Revision_Time = 5-SEP-2019 20:52:36
Current_Time = 5-SEP-2019 20:52:45
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = BCX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 15
Total_Scans = 15
Relaxation_Delay = 4[s]
Recvr_Gain = 38
Temp_Get = 69.6[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

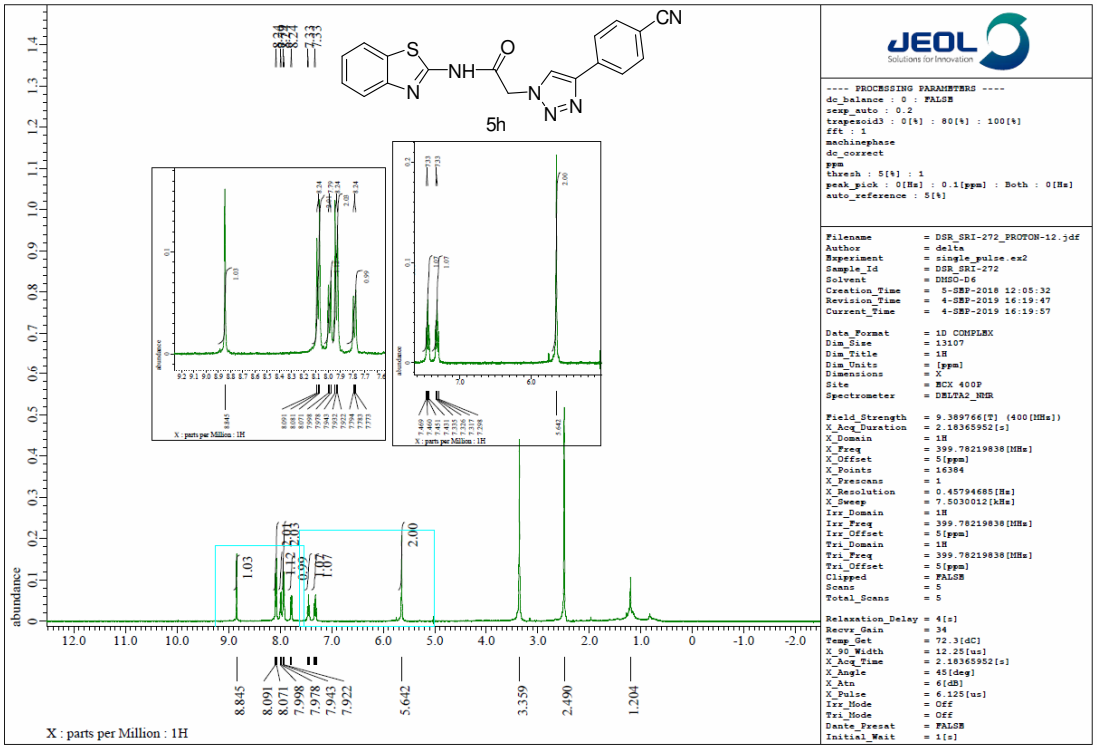

5e
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapesoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI - 271 B1_C
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_SRI - 271 B1
Solvent = DMSO-D6
Creation_Time = 21-OCT-2018 04:13:
Revision_Time = 4-SEP-2019 16:12:
Current_Time = 4-SEP-2019 16:13:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = x: 198(197),y: 39
Scans = 3500
Total_Scans = 3500
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 23.7[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

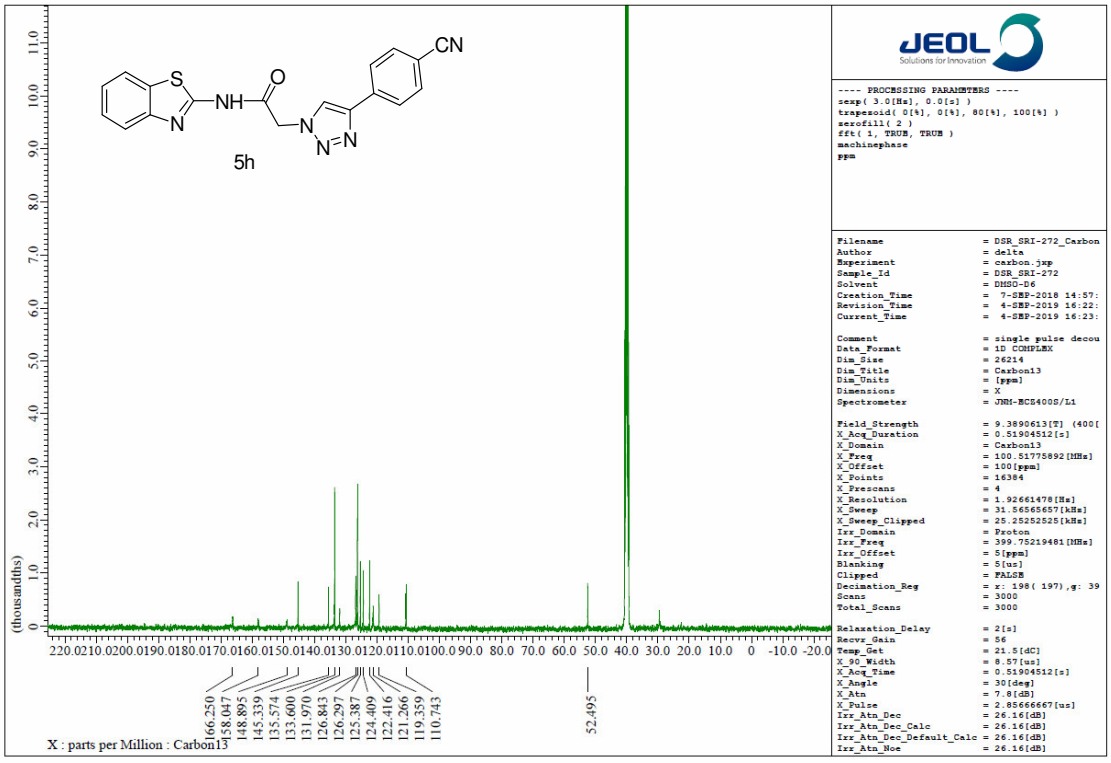

5f
X : parts per Million : 1H
abundance

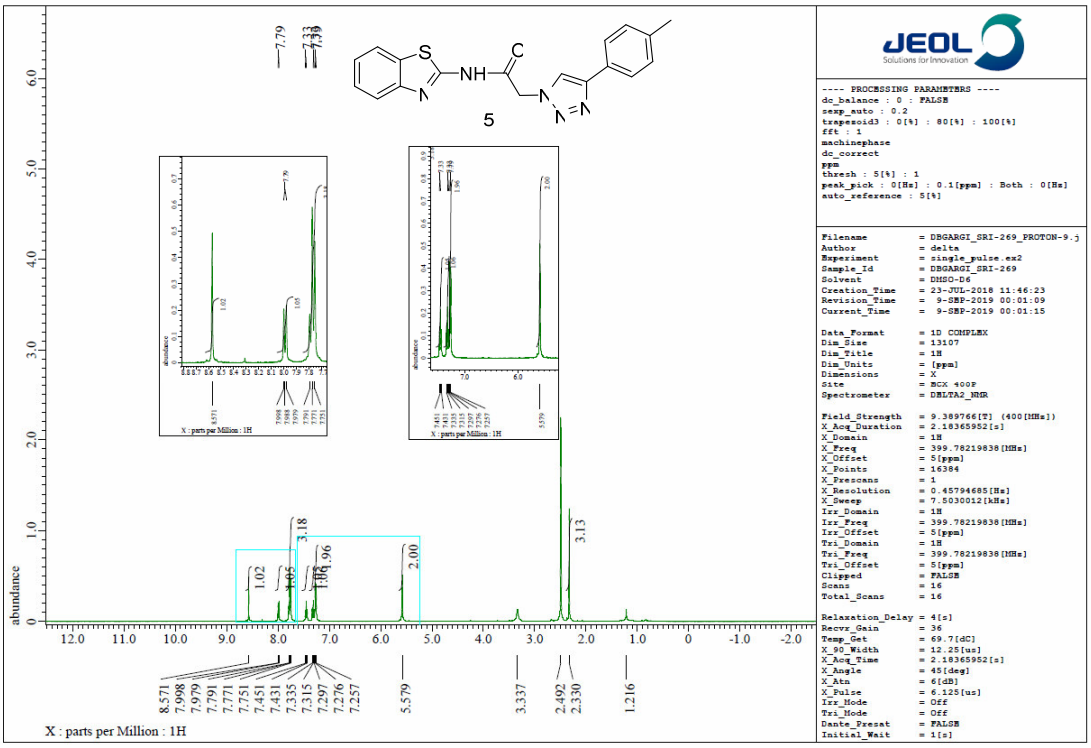

5f
X : parts per Million : Carbon13
(thousandths)

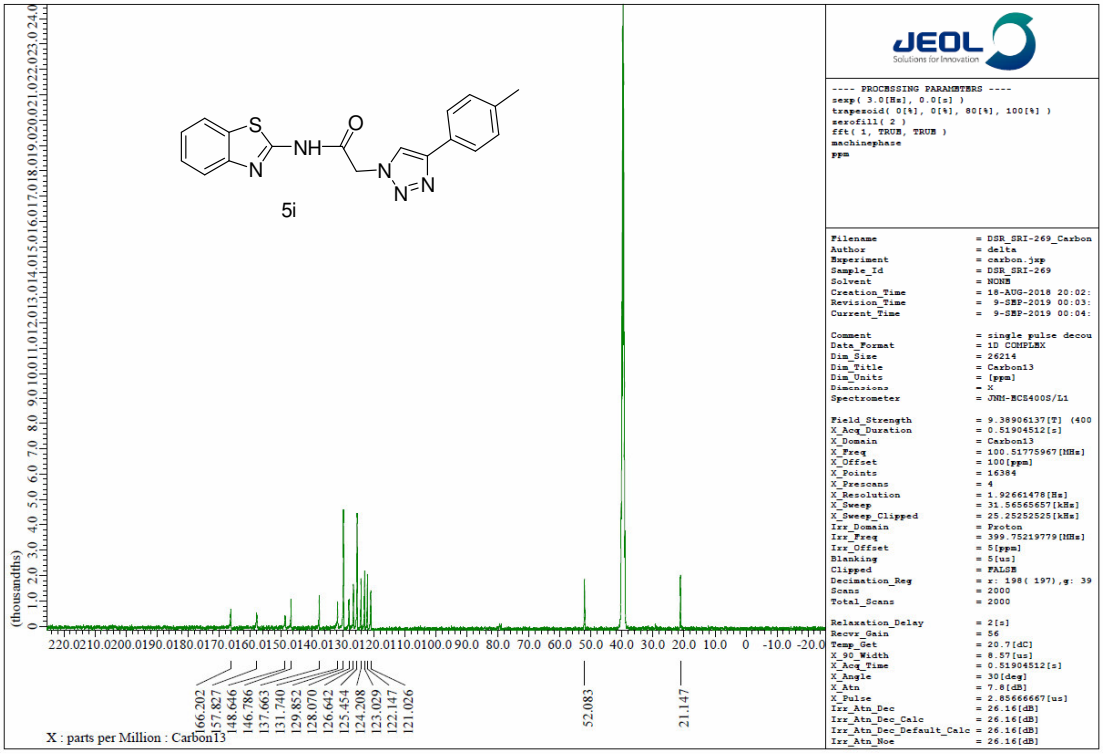

7.79
8.24
7.79
8.24
5g
4.14
2.00
2.03
2.22
1.91
1.01
0.98
1.03
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-276-B_PROTON-9.
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-276-B
Solvent = DMSO-D6
Actual_Start_Time = 8-OCT-2018 17:55:30
Revision_Time = 23-MAR-2020 17:27:31
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = RCX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 38
Temp_Get = 68.6[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.18365952[s]

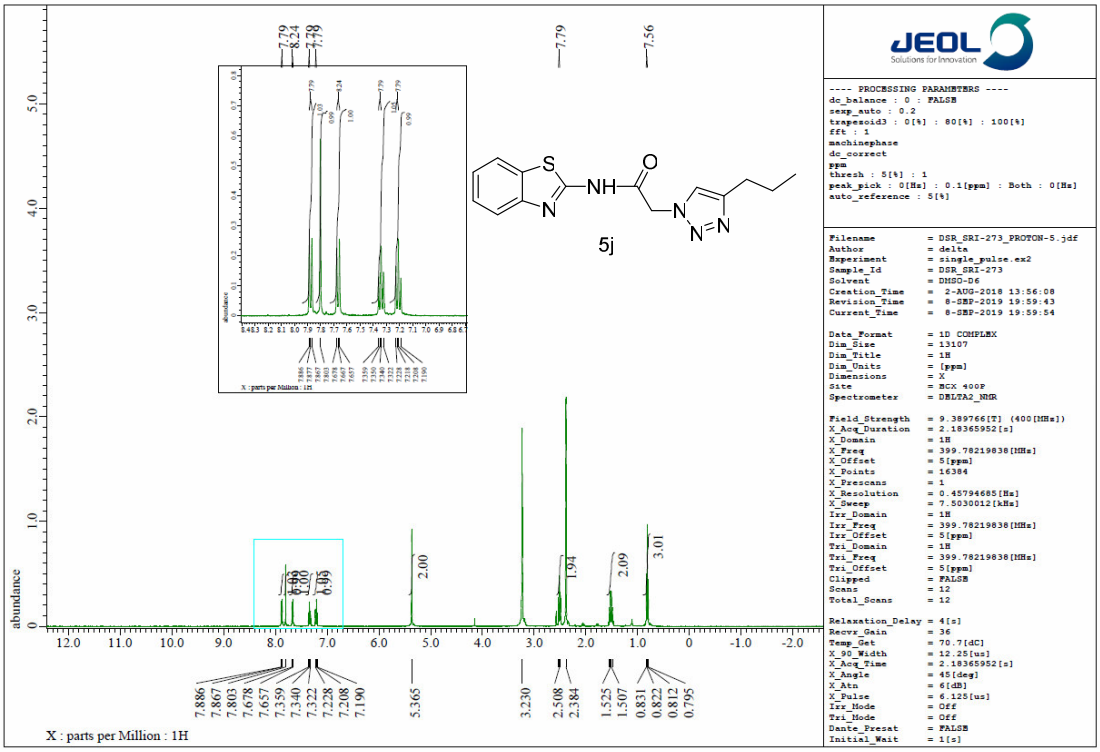

5g
(thousandths)
166.523
158.014
152.619
148.901
131.978
126.793
124.340
122.807
122.347
121.235
52.029
35.115
33.065
26.136
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = PRK_SRI - 276 B1_C
Author = delta
Experiment = carbon.jxp
Sample_Id = PRK_SRI - 276 B1
Solvent = DMSO-D6
Creation_Time = 1-NOV-2018 08:24:
Revision_Time = 9-SEP-2019 00:23:
Current_Time = 9-SEP-2019 00:24:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Decimation_Reg = x: 198(197),y: 39
Scans = 3500
Total_Scans = 3500
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 20.3[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

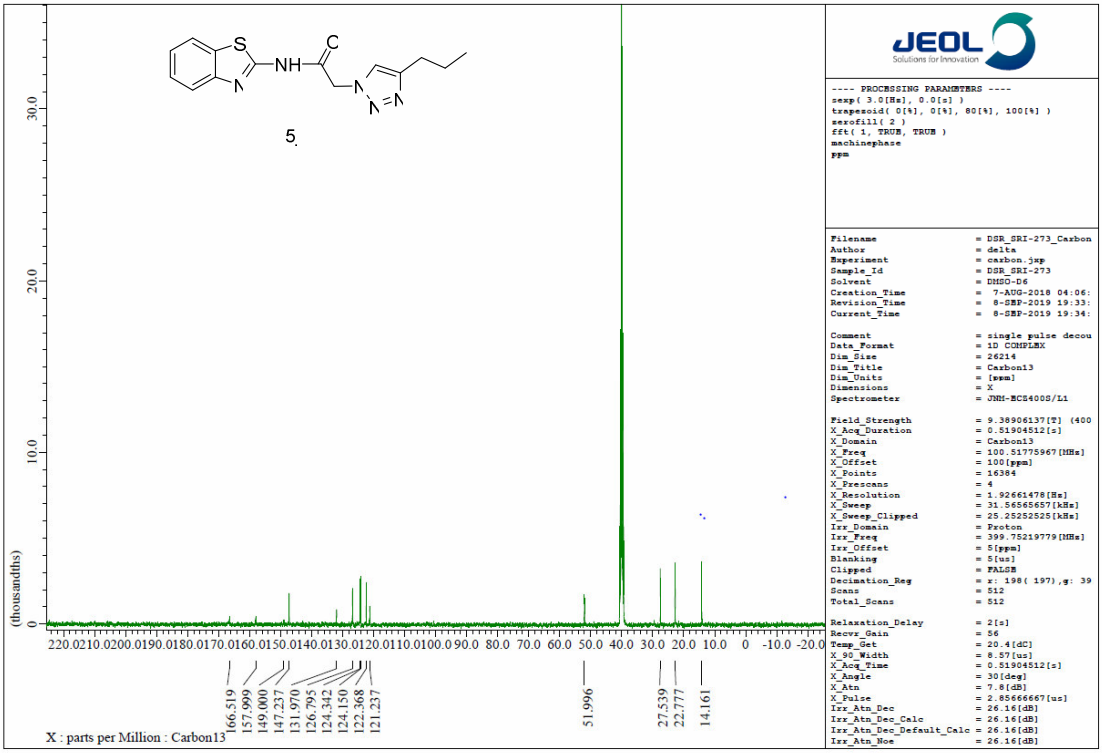

5h
X : parts per Million : 1H
abundance
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-272_PROTON-12.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-272
Solvent = DMSO-D6
Creation_Time = 5-SEP-2018 12:05:32
Revision_Time = 4-SEP-2019 16:19:47
Current_Time = 4-SEP-2019 16:19:57
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = NCX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 5
Total_Scans = 5
Relaxation_Delay = 4[s]
Recvr_Gain = 34
Temp_Get = 72.3[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

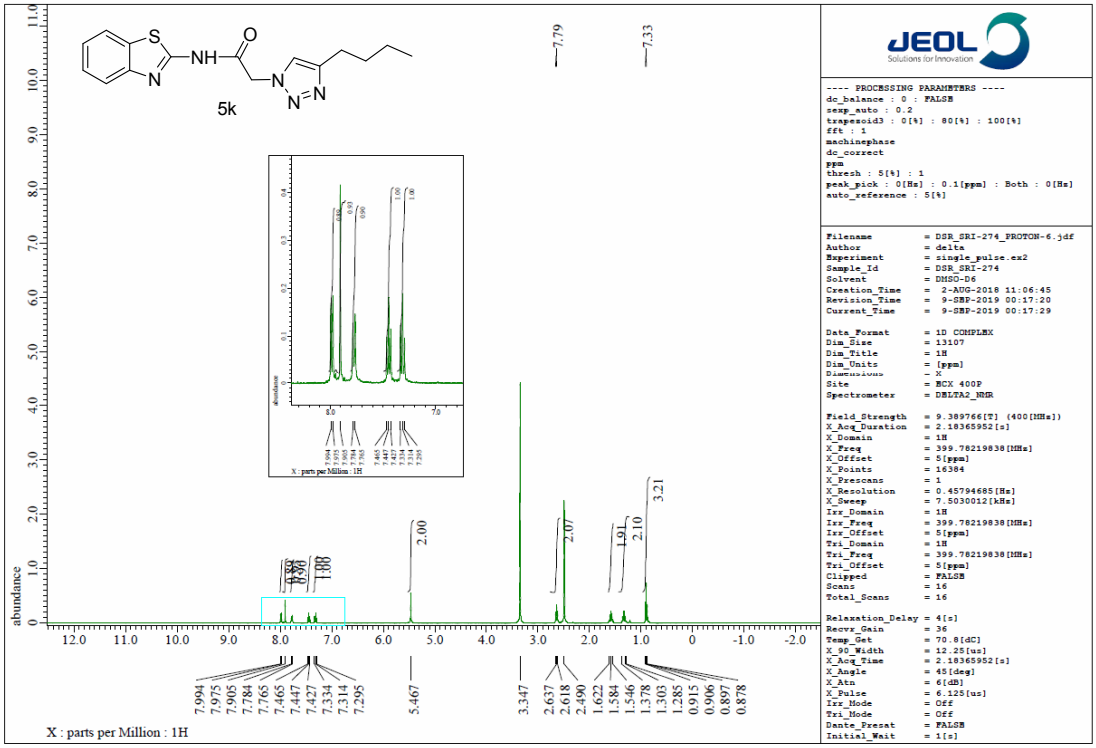

5h
X : parts per Million : Carbon13
(thousandths)
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI-272_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_SRI-272
Solvent = DMSO-D6
Creation_Time = 7-SEP-2018 14:57:
Revision_Time = 4-SEP-2019 16:22:
Current_Time = 4-SEP-2019 16:23:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.3890613[T] (400[
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.51775892[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.75219481[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = x: 198(197),y: 39
Scans = 3000
Total_Scans = 3000
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 21.5[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

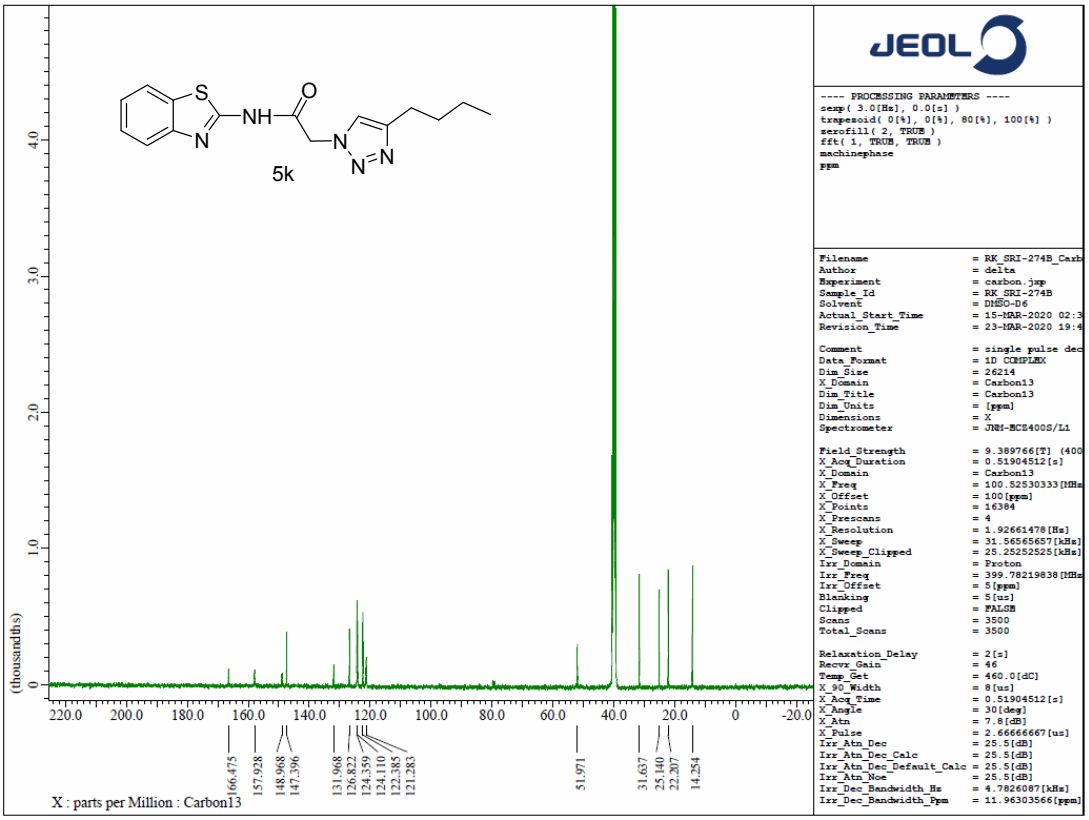

5
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DBGARGI_SRI-269_PROTON-9.j
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DBGARGI_SRI-269
Solvent = DMSO-D6
Creation_Time = 23-JUL-2018 11:46:23
Revision_Time = 9-SEP-2019 00:01:09
Current_Time = 9-SEP-2019 00:01:15
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = BCX 400P
Spectrometer = DBLTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 69.7[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

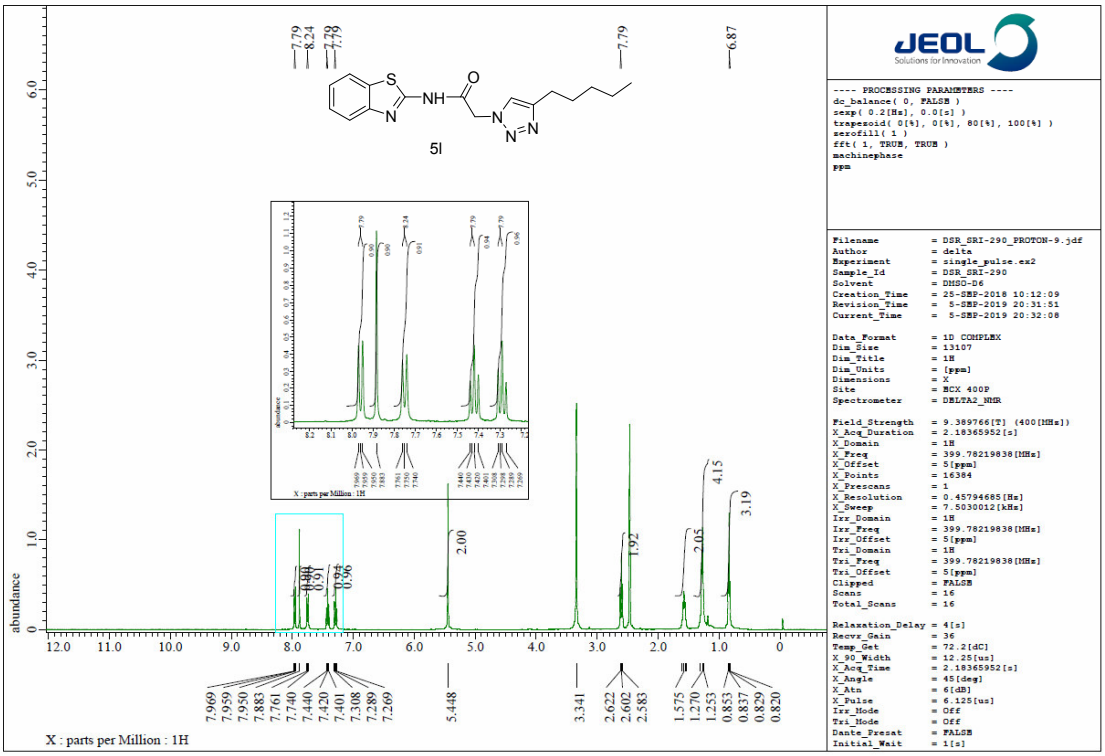

5i
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI-269_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_SRI-269
Solvent = NONE
Creation_Time = 18-AUG-2018 20:02:
Revision_Time = 9-SEP-2019 00:03:
Current_Time = 9-SEP-2019 00:04:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.38906137[T] (400
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.51775967[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.75219779[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = x: 198(197),y: 39
Scans = 2000
Total_Scans = 2000
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 20.7[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

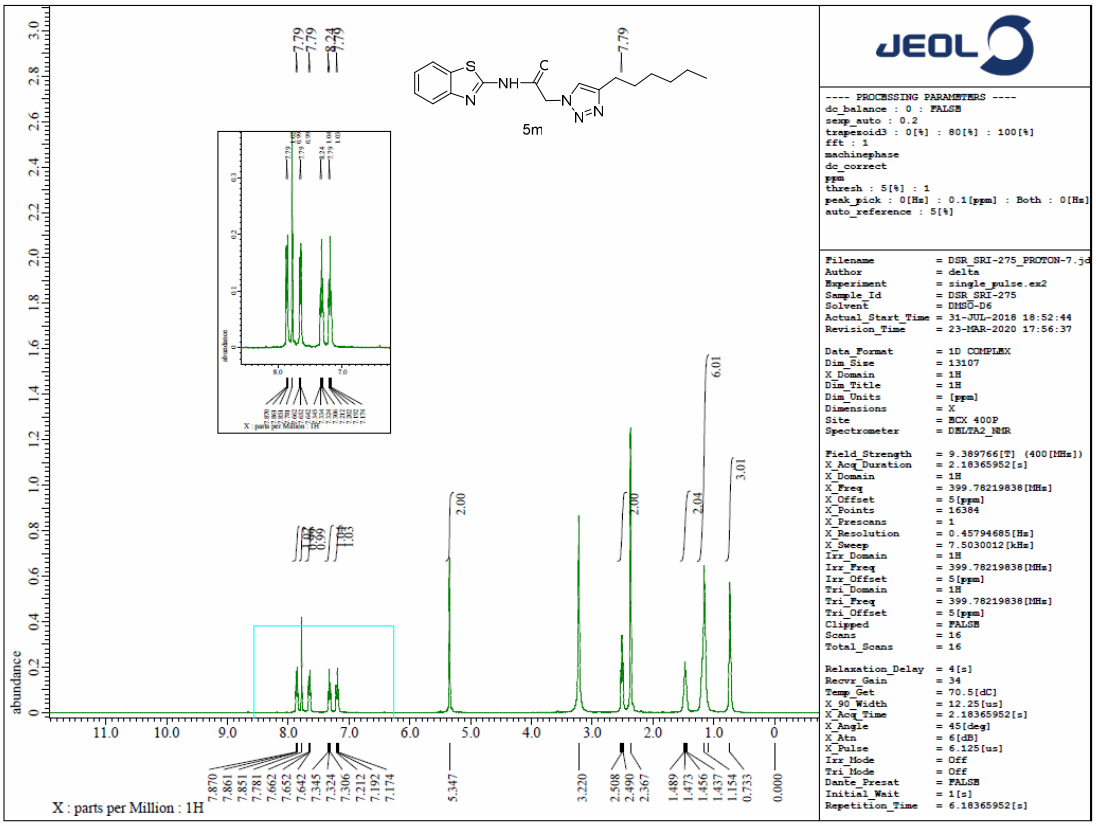

5j
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-273_PROTON-5.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-273
Solvent = DMSO-D6
Creation_Time = 2-AUG-2018 13:56:08
Revision_Time = 8-SEP-2019 19:59:43
Current_Time = 8-SEP-2019 19:59:54
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = BCX 400P
Spectrometer = DBLTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 12
Total_Scans = 12
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 70.7[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

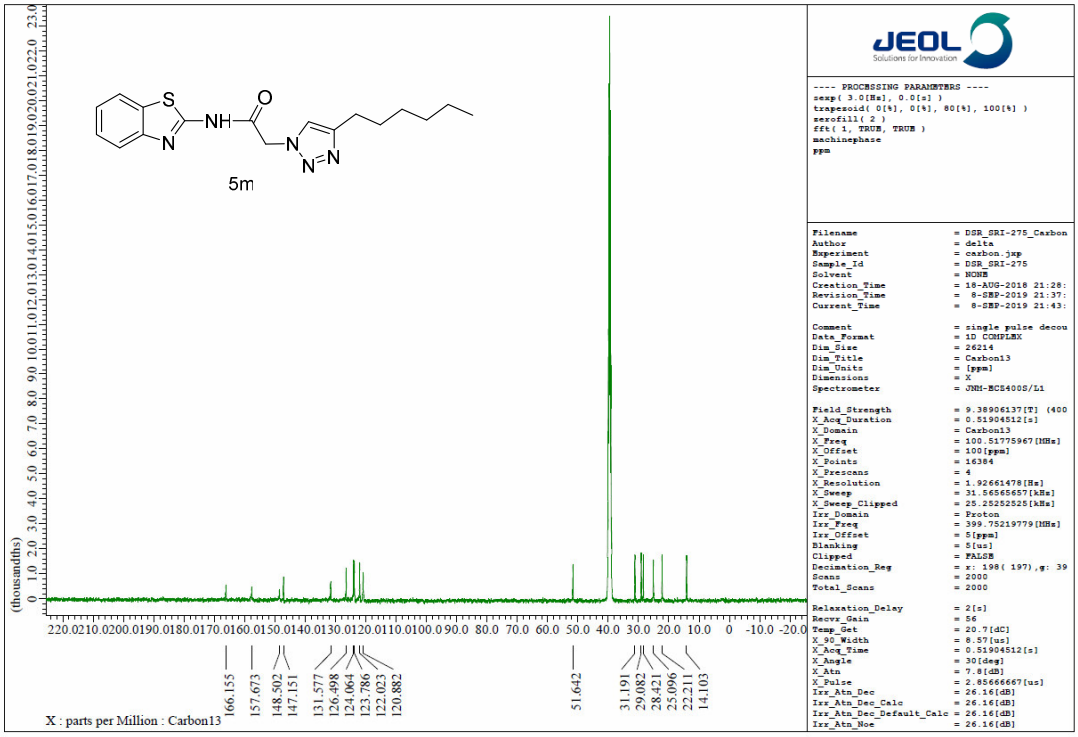

5
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI-273_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_SRI-273
Solvent = DMSO-D6
Creation_Time = 7-AUG-2018 04:06:
Revision_Time = 8-SEP-2019 19:33:
Current_Time = 8-SEP-2019 19:34:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.38906137[T] (400
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.51775967[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.75219779[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = x: 198(197),y: 39
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 20.4[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]

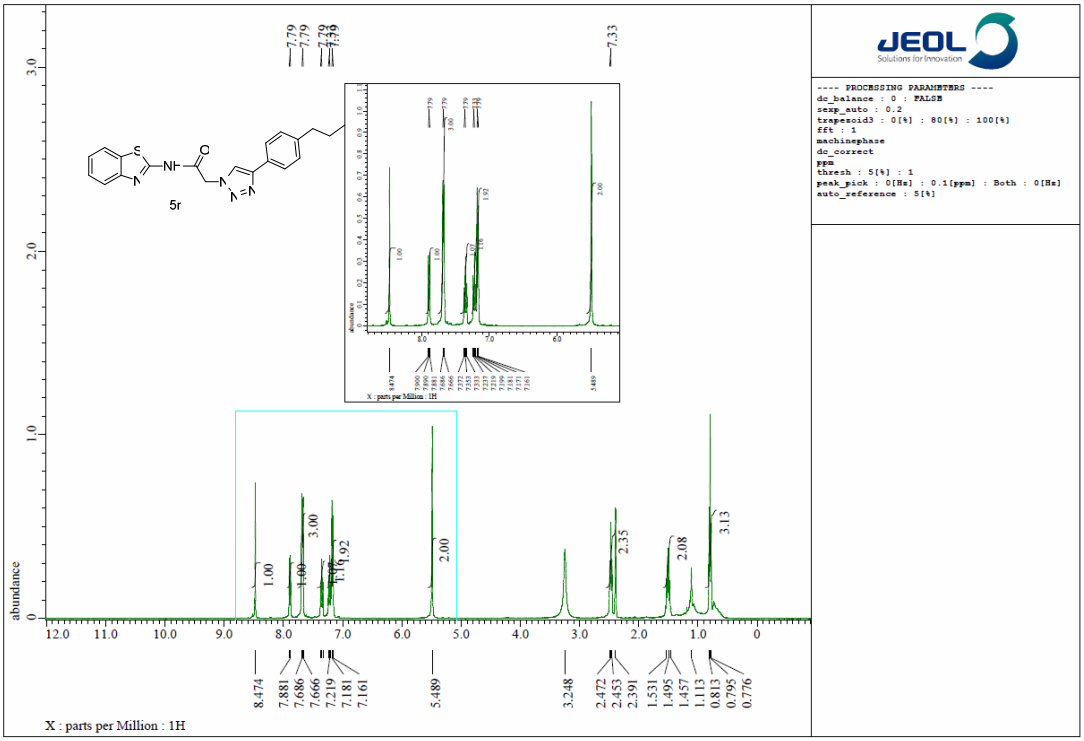

5k
X : parts per Million : 1H
abundance

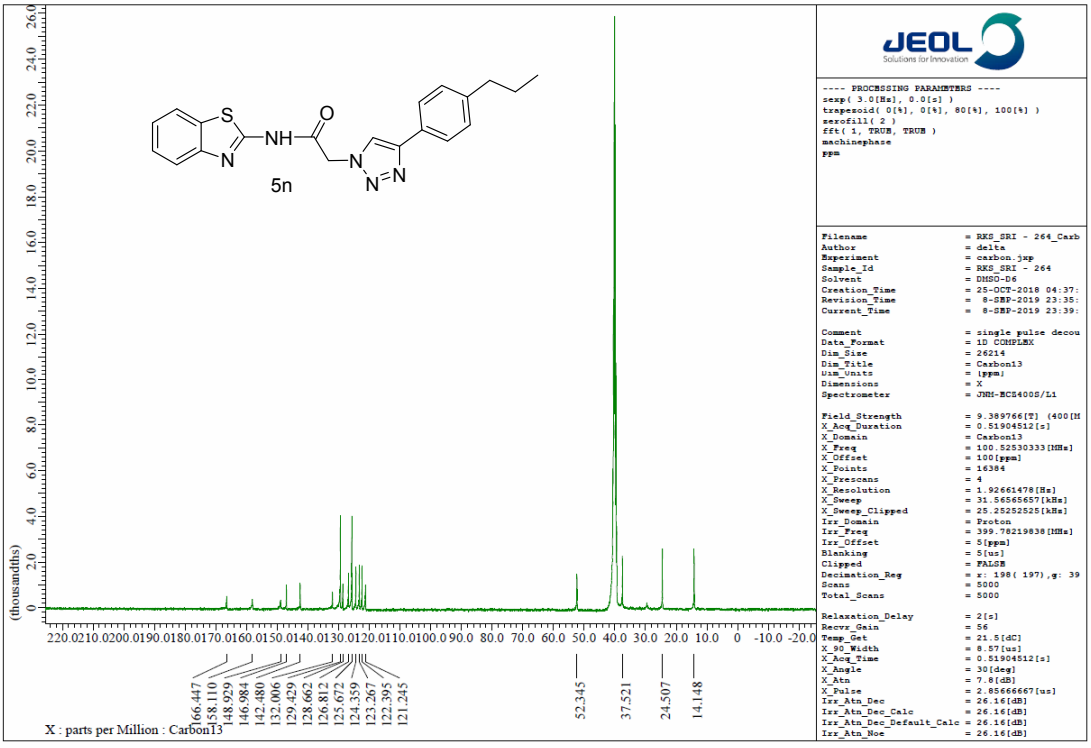

5k
X : parts per Million : Carbon13
(thousandths)


5l
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI-290_PROTON-9.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-290
Solvent = DMSO-D6
Creation_Time = 25-SEP-2018 10:12:09
Revision_Time = 5-SEP-2019 20:31:51
Current_Time = 5-SEP-2019 20:32:08
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = NCX 400P
Spectrometer = DNLTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 72.2[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]


5m
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = DSR_SRI-275_PROTON-7.jd
Author = delta
Experiment = single_pulse.ex2
Sample_Id = DSR_SRI-275
Solvent = DMSO-D6
Actual_Start_Time = 31-JUL-2018 18:52:44
Revision_Time = 23-MAR-2020 17:56:37
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = NCX 400P
Spectrometer = DNLTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 34
Temp_Get = 70.5[dC]
X_90_Width = 12.25[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 6.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.18365952[s]


5m
(thousandths)
X : parts per Million : Carbon13
166.155
157.673
148.502
147.151
131.577
126.498
124.064
123.786
122.023
120.882
51.642
31.191
29.082
28.421
25.096
22.211
14.103
---- PROCESSING PARAMETERS ----
exp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSR_SRI-275_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = DSR_SRI-275
Solvent = NONE
Creation_Time = 18-AUG-2018 21:28:
Revision_Time = 8-SEP-2019 21:37:
Current_Time = 8-SEP-2019 21:43:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.38906137[T] (400
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.51775967[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.75219779[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = x: 198(197),y: 39
Scans = 2000
Total_Scans = 2000
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 20.7[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]


5r
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]


5n
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = RKS_SRI - 264_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = RKS_SRI - 264
Solvent = DMSO-D6
Creation_Time = 25-OCT-2018 04:37:
Revision_Time = 8-SEP-2019 23:35:
Current_Time = 8-SEP-2019 23:39:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = (ppm)
Dimensions = X
Spectrometer = JNM-ECS400S/L1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0.51904512[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 16384
X_Prescans = 4
X_Resolution = 1.92661478[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Decimation_Reg = x: 198(197),y: 39
Scans = 5000
Total_Scans = 5000
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 21.5[dC]
X_90_Width = 8.57[us]
X_Acq_Time = 0.51904512[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 2.85666667[us]
Irr_Atn_Dec = 26.16[dB]
Irr_Atn_Dec_Calc = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe = 26.16[dB]