Supporting Information

Identification of Biologically Active Pyrimido[5,4-*b*]indoles that Prolong NF-κB Activation Without Intrinsic Activity

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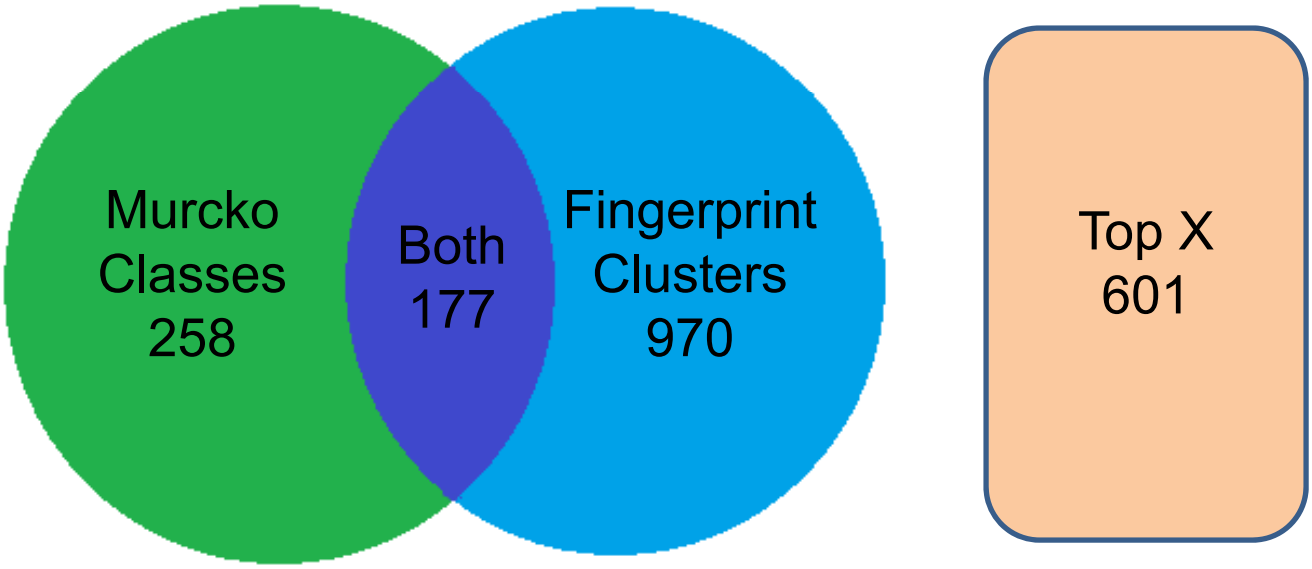
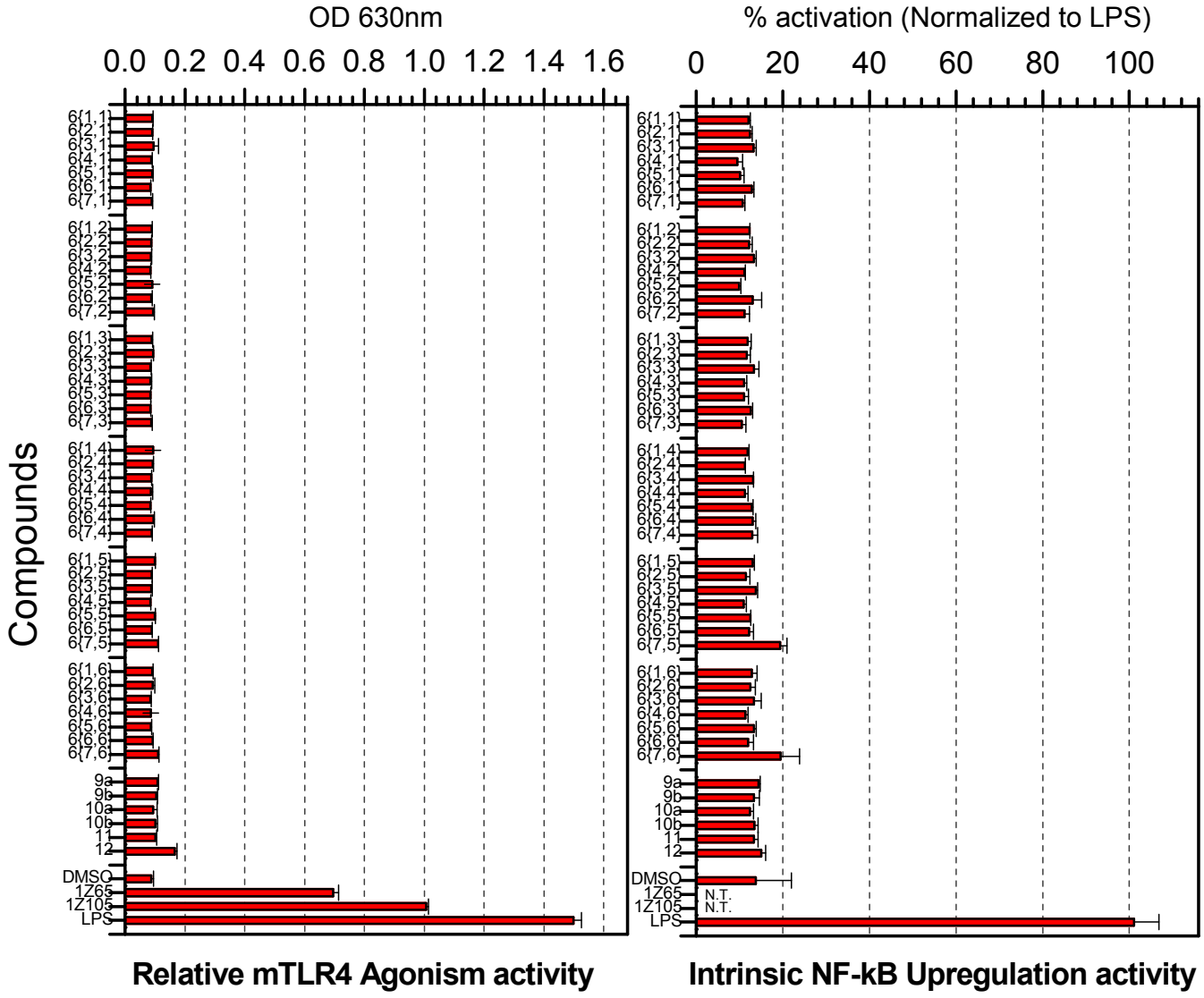
Supporting Information Figure S1
Hit confirmation rates using different approaches of hit selection [a]



Confirmation rates by different approaches for hit selection			
Approach methods	# hits in primary screen	# confirmed hits	Confirmation rates (%)
Structural approach	**1405**	**295**	**21**
a. Murcko	435	134	30.80
b. Daylight	1147	232	20.2
c. Murcko+Daylight	177	71	40.1
TopX	**601**	**112**	**18.6**

[a] Confirmation rates by different approaches used for hits selection shows that structural clustering approach improves confirmation rates.

Supporting Information Figure S2
(Left) mTLR4 agonistic activities and (Right) Intrinsic NF-κB inducing activities of synthesized compounds [a]



[a] Left: Relative murine TLR4 agonistic activity of compounds at 5 μM were determined using HEK-TLR4 based SEAP assay. 1Z65 and 1Z105 (compounds **1** and **42**, respectively; reference 1) are pyrimidoindole class of TLR4 agonists.[1] Right: Intrinsic NF-κB inducing activity of compound alone at 5h in NF-κB FRET cells as percent activation normalized to LPS (10ng/mL) as 100%. The response ratio for LPS was 8.61 ± 1.7. N.T. is not tested.

Supporting Information Figure S3
Compound collection library used for HTS [a]

	Vendor	#384 plate	# compounds
Diversity Collection	ChemBridge	74	23,370
	ChemDiv	157	49,997
	SPECS	95	30,106
	ChemBridge Premium	95	29,998
	Celera_ChemRx	9	2,767
	Subtotal		***136,238***
Kinase Targeted Collection	ChemDiv	32	9,993
	I.F. Labs	40	12,696
	Celera_ARS	4	1,236
	Celera_Asinex	2	369
	Subtotal		***24,294***
Known Bioactive Collection	Microsource	6	1,898
	Iconix	1	200
	Subtotal		***2,098***
Drug	FDA Supplemental Purchase	1	270
	Pharmakon	5	1,591
	Subtotal		***1,861***
Protease library (Cysteine protease, Deubiquitinase, MMP)	Celera	6	1,813
	Subtotal		***1,813***
Total		**527**	**166,304**

[a] Collection of compounds used for HTS were obtained from a variety of libraries including diversity collection and kinase as well as protease libraries.

Supporting Information Table S1
Data from 5h and 12h NF-κB FRET assay and THP-1 MTT Assay [a]

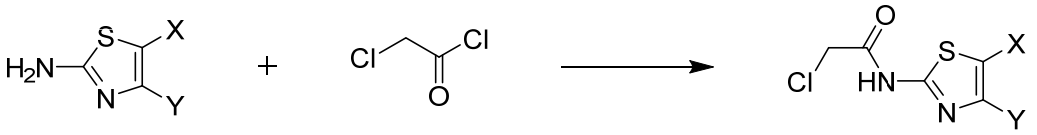
	5h NF-κB Induction with LPS		20h NF-κB Induction with LPS		THP-1 MTT Relative Viability	
Compound #	**Mean (% act)**	**SD**	**Mean(% act)**	**SD**	**Mean (% viability)**	**SD**
LPS (10ng/mL)	100.0	6.0	100.0	8.1	97.8	7.0
DMSO (0.5%)	13.2	2.1	39.8	7.8	100.0	5.9
6{1,1}	103.3	4.9	110.6	13.2	96.6	5.5
6{2,1}	98.4	4.2	122.2	8.8	95.3	4.5
6{3,1}	101.3	6.3	102.0	7.9	95.8	8.9
6{4,1}	104.8	4.8	114.8	10.0	105.9	5.3
6{5,1}	97.3	3.5	94.8	9.6	98.7	5.7
6{6,1}	93.8	4.8	103.3	7.1	96.4	4.8
6{7,1}	97.9	1.9	121.4	14.5	103.6	3.7
6{1,2}	104.0	7.1	116.7	8.4	95.2	5.9
6{2,2}	102.6	3.1	117.7	7.6	96.3	4.0
6{3,2}	104.3	3.2	103.1	7.7	97.7	5.2
6{4,2}	102.7	4.4	97.0	9.3	99.4	3.8
6{5,2}	102.3	3.5	114.4	12.2	98.0	6.3
6{6,2}	94.5	5.8	110.3	13.1	95.8	6.1
6{7,2}	92.7	4.4	107.7	6.3	100.5	5.6
6{1,3}	104.9	5.4	112.4	3.1	101.2	7.2
6{2,3}	104.8	3.2	110.0	10.9	105.2	4.8
6{3,3}	111.6	12.3	101.5	10.7	97.0	3.7
6{4,3}	100.6	5.6	98.5	11.8	89.0	13.7
6{5,3}	105.6	5.8	101.9	10.2	102.4	6.1
6{6,3}	96.7	3.9	107.9	5.7	98.2	7.1
6{7,3}	100.9	2.3	111.0	12.8	94.9	5.4
6{1,4}	100.4	6.7	108.0	12.9	73.8	4.7
6{2,4}	109.2	15.2	137.1	8.2	79.2	5.3
6{3,4}	102.7	4.5	112.7	10.9	69.4	4.6
6{4,4}	98.6	2.9	107.3	10.6	77.4	3.7
6{5,4}	100.5	3.6	114.0	7.2	73.8	2.6
6{6,4}	95.0	8.5	121.2	7.9	78.2	4.8
6{7,4}	100.0	5.7	120.5	8.9	75.1	5.2
6{1,5}	94.2	6.8	130.7	15.5	99.8	1.5
6{2,5}	98.6	5.9	107.1	9.5	103.0	4.7
6{3,5}	89.2	4.0	73.5	6.4	101.6	3.6
6{4,5}	97.1	9.1	97.5	11.7	74.3	4.7
6{5,5}	97.4	7.2	117.4	9.4	79.4	4.6
6{6,5}	98.0	11.3	115.0	11.8	97.8	3.3
6{7,5}	102.3	6.0	176.0	19.1	88.1	6.5
6{1,6}	91.9	6.9	152.0	14.7	84.5	2.4
6{2,6}	98.0	5.9	138.0	14.9	97.7	6.7
6{3,6}	87.5	7.1	83.1	8.0	103.2	3.8
6{4,6}	90.5	3.5	115.2	1.3	70.7	2.4
6{5,6}	93.4	5.3	171.1	9.7	76.6	4.1
6{6,6}	106.2	9.6	190.0	4.9	97.6	5.6
6{7,6}	109.4	10.3	190.8	17.3	79.9	5.3
9a	102.6	6.8	153.7	17.4	87.2	5.1
9b	99.9	3.7	143.3	13.3	85.4	4.4
10a	96.3	6.2	138.6	6.9	87.4	3.7
10b	91.0	2.4	142.0	11.0	76.4	3.3
11	98.9	8.6	94.0	8.7	63.8	2.4
12	96.7	6.4	91.4	11.6	61.5	2.4

[a] The %act values in NF-κB induction assay was normalized to LPS (10ng/mL) as 100%. The mean response ratio for LPS was 8.00±1.2 and 2.57±0.5 at 5h and 20h respectively. The %viability values in MTT assay was normalized to DMSO as 100%. The mean OD value for DMSO was 0.92±0.1. All raw values used for normalization are represented as mean±SD.

References

1. Chan, M.; Hayashi, T.; Mathewson, R. D.; Nour, A.; Hayashi, Y.; Yao, S.; Tawatao, R. I.; Crain, B.; Tsigelny, I. F.; Kouznetsova, V. L.; Messer, K.; Pu, M.; Corr, M.; Carson, D. A.; Cottam, H. B., Identification of Substituted Pyrimido[5,4-*b*]indoles as Selective Toll-Like Receptor 4 Ligands. *J. Med. Chem.* **2013,** *56* (11), 4206-4223.

Syntheses of Compounds **5**{4-6}



2-aminothiazole,
X, Y = H
2-aminobenzothiazole,
X-Y = -CH=CH-CH=CH-
2-amino-6-methylbenzothiazole,
X-Y = -CH=C(CH3)-CH=CH-

5{4}, X, Y = H
5{5}, X-Y = -CH=CH-CH=CH-
5{6}, X-Y = -CH=C(CH3)-CH=CH-

General procedure for the synthesis of Compound 5{4-6}. To a solution of 2-aminothiazole (for compound **5**{4}) or 2-aminobenzothiazole (for compound **5**{5}) or 2-amino-6-methylbenzothiazole (for compound **5**{6}) (1 eq.) in toluene was added chloroacetyl chloride (1.5 eq.). The reaction mixture was heated at 70 ^{o}C for 9h and the precipitated were filtered and washed with excess toluene to obtain compound **5**{4-6}.
5{4}; 2-chloro-N-(thiazol-2-yl)acetamide (yield = 74%): MS (ESI-TOF) for $C_5H_5ClN_2OS[M + H]^+$ calculated 177.0, found 176.9.
5{5}; N-(benzo[d]thiazol-2-yl)-2-chloroacetamide (yield = 80%): MS (ESI-TOF) for $C_9H_7ClN_2OS[M + H]^+$ calculated 227.0, found 226.9.
5{6}; 2-chloro-N-(6-methylbenzo[d]thiazol-2-yl)acetamide (yield = 88%): MS (ESI-TOF) for $C_{10}H_9ClN_2OS[M + H]^+$ calculated 241.0, found 240.9.

Experimental Section: Compound names, reaction yields, ^{1}H NMR and MS characterization data for all the final compounds, ^{13}C NMR and HRMS characterization data for key compounds.

6{1,1}; **methyl 2-((3-(4-fluorophenyl)-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 68%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.15 (s, 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.56 (d, *J* = 4.88 Hz, 1H), 7.59 (d, *J* = 4.88 Hz, 1H), 7.42 - 7.55 (m, 4H), 7.26 (t, *J* = 7.32 Hz, 1H), 4.04 (s, 2H), 3.71 (s, 3H). MS (ESI-TOF) for $C_{19}H_{14}FN_3O_3S[M + H]^+$ calculated 384.1, found 384.0.

6{2,1}; **methyl 2-((3-(4-methoxyphenyl)-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 58%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.11 (s, 1H), 7.90 (d, *J* = 7.81 Hz, 1H), 7.46 (d, *J* = 8.29 Hz, 1H), 7.51 (t, *J* = 8.30 Hz, 1H), 7.38 (d, *J* = 8.78 Hz, 2H), 7.25 (t, *J* = 7.32 Hz, 1H), 7.14 (d, *J* = 8.78 Hz, 2H), 4.01 (s, 2H), 3.86 (s, 3H), 3.71 (s, 3H). MS (ESI-TOF) for $C_{20}H_{17}N_3O_4S[M - H]^-$ calculated 394.1, found 393.9.

6{3,1}; **methyl 2-((3-isopropyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 18%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.91 (s, 1H), 7.83 (d, *J* = 7.81 Hz, 1H), 7.49 (d, *J* = 8.29 Hz, 1H), 7.44 (t, *J* = 7.32 Hz, 1H), 7.22 (t, *J* = 7.32 Hz, 1H), 4.51 - 4.79 (m, 1H), 4.14 (s, 2H), 3.72 (s, 3H), 1.65 (d, *J* = 6.34 Hz, 6H). MS (ESI-TOF) for $C_{16}H_{17}N_3O_3S[M - H]^-$ calculated 330.1, found 330.0.

6{4,1}; **methyl 2-((3-methyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 64%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.01 (s, 1H), 7.86 (d, *J* = 7.81 Hz, 1H), 7.45 (t, *J* = 7.30 Hz, 1H), 7.50 (d, *J* = 8.29 Hz, 1H), 7.22 (t, *J* = 7.32 Hz, 1H), 4.19 (s, 2H), 3.71 (s, 3H), 3.62 (s, 3H). MS (ESI-TOF) for $C_{14}H_{13}N_3O_3S[M + H]^+$ calculated 304.1, found 304.0.

6{5,1}; **methyl 2-((3-ethyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 41%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.01 (s, 1H), 7.85 (d, *J* = 7.81 Hz, 1H), 7.44 (d, *J* = 7.80 Hz, 1H), 7.49 (t, *J* = 8.30 Hz, 2H), 7.23 (t, *J* = 7.32 Hz, 1H), 4.08 - 4.28 (m, 2H), 4.20 (q, *J* = 6.80 Hz, 1H), 3.72 (s, 3H), 1.33 (t, *J* = 7.07 Hz, 3H). MS (ESI-TOF) for $C_{15}H_{15}N_3O_3S[M + H]^+$ calculated 318.1, found 318.0.

6{6,1}; **methyl 2-((4-oxo-3-propyl-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 39%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.84 (d, *J* = 7.81 Hz, 1H), 7.48 (t, *J* = 8.30 Hz, 1H), 7.43 (d, *J* = 7.81 Hz, 1H), 7.22 (t, *J* = 7.56 Hz, 1H), 4.18 (s, 2H), 4.04 - 4.14 (m, 2H), 3.70 (s, 3H), 1.76 (sxt, *J* = 7.80 Hz, 2H), 0.97 (t, *J* = 7.32 Hz, 3H). MS (ESI-TOF) for $C_{16}H_{17}N_3O_3S[M + H]^+$ calculated 332.1, found 332.0.

6{7,1}; **methyl 2-((3-butyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 82%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.85 (d, *J* = 7.81 Hz, 1H), 7.49 (t, *J* = 8.30 Hz, 1H), 7.44 (d, *J* = 8.29 Hz, 1H), 7.23 (t, *J* = 7.30 Hz, 1H), 4.19 (s, 2H), 4.14 (t, *J* = 7.80 Hz, 2H), 3.72 (s, 3H), 1.73 (quin, *J* = 7.30 Hz, 2H), 1.42 (sxt, *J* = 7.80 Hz, 2H), 0.96 (t, *J* = 7.32 Hz, 3H). MS (ESI-TOF) for $C_{17}H_{19}N_3O_3S[M - H]^-$ calculated 344.1, found 344.0

6{1,2}; **ethyl 2-((3-(4-fluorophenyl)-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 66%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.15 (s, 1H), 7.91 (d, *J* = 8.29 Hz, 1H), 7.42 - 7.61 (m, 6H), 7.25 (t, *J* = 7.56 Hz, 1H), 4.15 (q, *J* = 6.83 Hz, 2H), 4.03 (s, 2H), 1.23 (t, *J* = 7.07 Hz, 3H). MS (ESI-TOF) for $C_{20}H_{16}FN_3O_3S[M - H]^-$ calculated 396.1, found 395.8.

6{2,2}; **ethyl 2-((3-(4-methoxyphenyl)-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 51%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.12 (s, 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.47 (t, *J* = 7.60 Hz, 1H), 7.52 (d, *J* = 8.30 Hz, 1H), 7.38 (d, *J* = 7.81 Hz, 2H), 7.25

(t, *J* = 6.80 Hz, 1H), 7.14 (d, *J* = 8.29 Hz, 2H), 4.15 (q, *J* = 6.83 Hz, 2H), 4.00 (s, 2H), 3.87 (s, 3H), 1.22 (t, *J* = 6.83 Hz, 3H). MS (ESI-TOF) for $C_{21}H_{19}N_3O_4S[M - H]^-$ calculated 408.1, found 408.0.

6{3,2}; **ethyl 2-((3-isopropyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 41%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.91 (s, 1H), 7.83 (d, *J* = 7.80 Hz, 1H), 7.43 (t, *J* = 7.60 Hz, 1H), 7.49 (d, *J* = 8.30 Hz, 1H), 7.21 (t, *J* = 7.56 Hz, 1H), 4.52 - 4.78 (m, 1H), 4.13 (s, 2H), 4.14 (q, *J* = 7.30 Hz, 2H), 1.65 (d, *J* = 6.83 Hz, 6H), 1.21 (t, *J* = 7.07 Hz, 3H). MS (ESI-TOF) for $C_{17}H_{19}N_3O_3S[M + H]^+$ calculated 346.1, found 346.0.

6{4,2}; **ethyl 2-((3-methyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 54%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.84 (d, *J* = 7.81 Hz, 1H), 7.46 (t, *J* = 8.30 Hz, 1H), 7.42 (d, *J* = 8.30 Hz, 1H), 7.20 (t, *J* = 7.60 Hz, 1H), 4.15 (s, 2H), 4.14 (q, *J* = 7.10 Hz, 2H), 3.59 (s, 3H), 1.20 (t, *J* = 7.07 Hz, 3H). MS (ESI-TOF) for $C_{15}H_{15}N_3O_3S[M + H]^+$ calculated 318.1, found 318.0.

6{5,2}; **ethyl 2-((3-ethyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 42%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.99 (br. s., 1H), 7.84 (d, *J* = 7.32 Hz, 1H), 7.43 (t, *J* = 7.30 Hz, 1H), 7.48 (d, *J* = 8.29 Hz, 1H), 7.20 (t, *J* = 6.80 Hz, 1H), 4.00 - 4.22 (m, 6H), 1.31 (t, *J* = 7.30 Hz, 3H), 1.18 (t, *J* = 6.80 Hz, 3H). MS (ESI-TOF) for $C_{16}H_{17}N_3O_3S[M + H]^+$ calculated 332.1, found 332.0.

6{6,2}; **ethyl 2-((4-oxo-3-propyl-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 48%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.01 (br. s., 1H), 7.85 (d, *J* = 8.29 Hz, 1H), 7.50 (d, *J* = 8.30 Hz, 1H), 7.44 (t, *J* = 7.80 Hz, 1H), 7.22 (t, *J* = 7.07 Hz, 1H), 4.03 - 4.21 (m, 6H), 1.76 (q, *J* = 7.30 Hz, 2H), 1.19 (t, *J* = 7.07 Hz, 3H), 0.97 (t, *J* = 7.56 Hz, 3H). MS (ESI-TOF) for $C_{17}H_{19}N_3O_3S[M + H]^+$ calculated 346.1, found 346.0.

6{7,2}; **ethyl 2-((3-butyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 49%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.85 (d, *J* = 8.29 Hz, 1H), 7.49 (d, *J* = 8.30 Hz, 1H), 7.44 (t, *J* = 8.30 Hz, 1H), 7.22 (t, *J* = 7.56 Hz, 1H), 4.06 - 4.23 (m, 6H), 1.72 (quin, *J* = 7.56 Hz, 2H), 1.41 (sxt, *J* = 7.41 Hz, 2H), 1.20 (t, *J* = 7.07 Hz, 3H), 0.96 (t, *J* = 7.31 Hz, 3H). MS (ESI-TOF) for $C_{16}H_{21}N_3O_3S[M + H]^+$ calculated 360.1, found 360.1.

6{1,3}; ***tert*-butyl 2-((3-(4-** ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.15 (s, 1H), 7.95 (d, *J* = 8.29 Hz, 1H), 7.41 - 7.60 (m, 6H), 7.26 (t, *J* = 7.32 Hz, 1H), 3.92 (s, 2H), 1.40 (s, 9H). MS (ESI-TOF) for $C_{22}H_{20}FN_3O_3S[M + H]^+$ calculated 426.1, found 426.0.

6{2,3}; ***tert*-butyl 2-((3-(4-methoxyphenyl)-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 34%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.11 (s, 1H), 7.95 (d, *J* = 7.81 Hz, 1H), 7.51 (d, *J* = 8.29 Hz, 1H), 7.46 (t, *J* = 7.30 Hz, 1H), 7.37 (d, *J* = 8.29 Hz, 2H), 7.25 (t, *J* = 7.07 Hz, 1H), 7.14 (d, *J* = 8.78 Hz, 2H), 3.90 (s, 2H), 3.86 (s, 3H), 1.40 (s, 9H) . MS (ESI-TOF) for $C_{23}H_{23}N_3O_4S[M - H]^-$ calculated 436.1, found 436.0.

6{3,3}; ***tert*-butyl 2-((3-isopropyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 33%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.90 (br. s., 1H), 7.89 (d, *J* = 7.81 Hz, 1H), 7.49 (d, *J* = 8.29 Hz, 1H), 7.43 (t, *J* = 7.80 Hz, 1H), 7.22 (t, *J* = 7.32 Hz, 1H), 4.57 - 4.75 (m, 1H), 4.04 (s, 2H), 1.65 (d, *J* = 6.34 Hz, 6H), 1.37 (s, 9H). MS (ESI-TOF) for $C_{19}H_{23}N_3O_3S[M - H]^-$ calculated 372.1, found 372.1.

6{4,3}; ***tert*-butyl 2-((3-methyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 52%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.01 (br. s., 1H), 7.92 (d, *J* = 7.81 Hz, 1H), 7.49 (d, *J* = 8.30 Hz, 1H), 7.44 (t, *J* = 7.80 Hz, 1H), 7.22 (t, *J* = 7.32 Hz, 1H), 4.08 (s, 2H), 3.61 (s, 3H), 1.41 (s, 9H). MS (ESI-TOF) for $C_{17}H_{19}N_3O_3S[M + H]^+$ calculated 346.1, found 346.0.

6{5,3}; ***tert*-butyl 2-((3-ethyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 70%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.01 (s, 1H), 7.91 (d, *J* = 8.05 Hz, 1H), 7.49 (d, *J* = 8.54 Hz, 1H), 7.44 (t, *J* = 7.80 Hz, 1H), 7.22 (t, *J* = 7.44 Hz, 1H), 4.20 (q, *J* = 6.83 Hz, 2H), 4.08 (s, 2H), 1.38 (s, 9H), 1.33 (t, *J* = 7.07 Hz, 3H). MS (ESI-TOF) for $C_{18}H_{21}N_3O_3S$[M - H]$^-$ calculated 358.1, found 358.1.

6{6,3}; ***tert*-butyl 2-((4-oxo-3-propyl-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 52%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.01 (s, 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.49 (d, *J* = 8.29 Hz, 1H), 7.44 (t, *J* = 7.80 Hz, 1H), 7.22 (t, *J* = 7.32 Hz, 1H), 4.07 (s, 2H), 4.10 (t, *J* = 7.80 Hz, 2H), 1.77 (sxt, *J* = 7.30 Hz, 2H), 1.37 (s, 9H), 0.97 (t, *J* = 7.32 Hz, 3H). MS (ESI-TOF) for $C_{19}H_{23}N_3O_3S$[M - H]$^-$ calculated 372.1, found 372.0.

6{7,3}; ***tert*-butyl 2-((3-butyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 70%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.90 (d, *J* = 8.29 Hz, 1H), 7.50 (d, *J* = 8.29 Hz, 1H), 7.44 (t, *J* = 7.80 Hz, 1H), 7.22 (t, *J* = 7.32 Hz, 1H), 4.14 (t, *J* = 7.80 Hz, 2H), 4.07 (s, 2H), 1.73 (quin, *J* = 7.70 Hz, 2H), 1.30 - 1.48 (m, 11H), 0.95 (t, *J* = 7.32 Hz, 3H). MS (ESI-TOF) for $C_{20}H_{25}N_3O_3S$[M - H]$^-$ calculated 386.2, found 386.1.

6{1,4}; **2-((3-(4-fluorophenyl)-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(thiazol-2-yl)-acetamide** (yield = 44%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.56 (s, 1H), 12.08 (s, 1H), 7.80 (d, *J* = 8.29 Hz, 1H), 7.54 - 7.63 (m, 2H), 7.51 (d, *J* = 3.42 Hz, 1H), 7.35 - 7.48 (m, 4H), 7.16 (d, *J* = 3.42 Hz, 1H), 7.08 (t, *J* = 7.56 Hz, 1H), 4.16 (s, 2H). MS (ESI-TOF) for $C_{21}H_{14}FN_5O_2S_2$ [M - H]$^-$ calculated 450.1, found 449.9.

6{2,4}; **2-((3-(4-methoxyphenyl)-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(thiazol-2-yl)-acetamide** (yield = 66%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.57 (s, 1H), 12.07 (s, 1H), 7.81 (d, *J* = 7.81 Hz, 1H), 7.50 - 7.56 (m, 1H), 7.47 (d, *J* = 8.29 Hz, 1H), 7.36 - 7.43 (m,

3H), 7.05 - 7.21 (m, 3H), 7.09 (t, *J* = 7.40 Hz, 1H), 4.15 (s, 2H), 3.87 (s, 3H). MS (ESI-TOF) for $C_{22}H_{17}N_3O_3S[M - H]^-$ calculated 462.1, found 462.0.

6{3,4}; **2-((3-isopropyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(thiazol-2-yl)-acetamide** (yield = 68%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.64 (br. s., 1H), 11.86 (br. s., 1H), 7.73 (d, *J* = 7.81 Hz, 1H), 7.53 (br. s., 1H), 7.43 (d, *J* = 7.81 Hz, 1H), 7.36 (t, *J* = 7.30 Hz, 1H), 7.17 (br. s., 1H), 7.02 (t, *J* = 7.32 Hz, 1H), 4.57 - 4.74 (m, 1H), 4.28 (s, 2H), 1.66 (d, *J* = 6.34 Hz, 6H). MS (ESI-TOF) for $C_{18}H_{17}N_5O_2S_2$ $[M + H]^+$ calculated 400.1, found 400.0.

6{4,4}; **2-((3-methyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(thiazol-2-yl)-acetamide** (yield = 64%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.62 (s, 1H), 11.97 (s, 1H), 7.77 (d, *J* = 7.81 Hz, 1H), 7.50 - 7.59 (m, 1H), 7.44 (d, *J* = 8.29 Hz, 1H), 7.38 (t, *J* = 7.30 Hz, 1H), 7.17 (d, *J* = 2.44 Hz, 1H), 7.06 (t, *J* = 7.30 Hz, 1H), 4.33 (s, 2H), 3.62 (s, 3H). MS (ESI-TOF) for $C_{16}H_{13}N_5O_2S_2$ $[M + H]^+$ calculated 372.1, found 371.9.

6{5,4}; **2-((3-ethyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(thiazol-2-yl)-acetamide** (yield = 81%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.63 (br. s., 1H), 11.97 (br. s., 1H), 7.75 (d, *J* = 8.29 Hz, 1H), 7.28 - 7.56 (m, 2H), 7.38 (t, *J* = 7.00 Hz, 1H), 7.17 (br. s., 1H), 7.05 (t, *J* = 7.30 Hz, 1H), 4.32 (s, 2H), 4.20 (q, *J* = 6.80 Hz, 2H), 1.34 (t, *J* = 6.80 Hz, 3H). MS (ESI-TOF) for $C_{17}H_{15}N_5O_2S_2$ $[M + H]^+$ calculated 386.1, found 385.9.

6{6,4}; **2-((4-oxo-3-propyl-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(thiazol-2-yl)-acetamide** (yield = 73%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.63 (s, 1H), 11.97 (s, 1H), 7.76 (d, *J* = 8.29 Hz, 1H), 7.53 (d, *J* = 3.90 Hz, 1H), 7.44 (d, *J* = 8.29 Hz, 1H), 7.38 (t, *J* = 7.60 Hz, 1H), 7.17 (d, *J* = 3.42 Hz, 1H), 7.05 (t, *J* = 7.80 Hz, 1H), 4.32 (s, 2H), 4.11 (t, *J* = 7.56 Hz, 2H), 1.78 (sxt, *J* = 7.30 Hz, 2H), 0.98 (t, *J* = 7.56 Hz, 3H). MS (ESI-TOF) for $C_{18}H_{17}N_5O_2S_2$ $[M - H]^-$ calculated 398.1, found 397.9.

6{7,4}; **2-((3-butyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(thiazol-2-yl)-acetamide** (yield = 92%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.61 (s, 1H), 11.94 (s, 1H), 7.73 (d, *J* = 7.81 Hz, 1H), 7.51 (d, *J* = 2.93 Hz, 1H), 7.42 (d, *J* = 7.81 Hz, 1H), 7.36 (t, *J* = 7.80 Hz, 1H), 7.15 (d, *J* = 2.93 Hz, 1H), 7.03 (t, *J* = 7.30 Hz, 1H), 4.30 (s, 2H), 4.13 (t, *J* = 7.32 Hz, 2H), 1.72 (quin, *J* = 7.30 Hz, 2H), 1.40 (sxt, *J* = 7.30 Hz, 2H), 0.95 (t, *J* = 7.32 Hz, 3H). MS (ESI-TOF) for $C_{19}H_{19}N_5O_2S_2$ [M - H]$^-$ calculated 412.1, found 411.9.

6{1,5}; ***N*-(benzo[*d*]thiazol-2-yl)-2-((3-(4-fluorophenyl)-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 67%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.86 (s, 1H), 12.10 (s, 1H), 7.92 (d, *J* = 7.81 Hz, 1H), 7.85 (t, *J* = 7.56 Hz, 2H), 7.58 - 7.66 (m, 2H), 7.40 - 7.53 (m, 4H), 7.35 (t, *J* = 7.30 Hz, 1H), 7.29 (t, *J* = 7.80 Hz, 1H), 6.97 (t, *J* = 7.56 Hz, 1H), 4.23 (s, 2H). MS (ESI-TOF) for $C_{25}H_{16}FN_5O_2S_2$ [M - H]$^-$ calculated 500.1, found 499.9.

6{2,5}; ***N*-(benzo[*d*]thiazol-2-yl)-2-((3-(4-methoxyphenyl)-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 64%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.85 (s, 1H), 12.07 (s, 1H), 7.92 (d, *J* = 7.81 Hz, 1H), 7.85 (t, *J* = 6.59 Hz, 2H), 7.39 - 7.52 (m, 4H), 7.34 (t, *J* = 7.30 Hz, 1H), 7.29 (t, *J* = 7.30 Hz, 1H), 7.15 (d, *J* = 8.78 Hz, 2H), 6.97 (t, *J* = 7.56 Hz, 1H), 4.21 (s, 2H), 3.87 (s, 3H). MS (ESI-TOF) for $C_{26}H_{19}N_5O_3S_2$ [M - H]$^-$ calculated 512.1, found 512.0.

6{3,5}; ***N*-(benzo[*d*]thiazol-2-yl)-2-((3-isopropyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 67%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.91 (s, 1H), 11.86 (br. s., 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.85 (d, *J* = 7.81 Hz, 1H), 7.79 (d, *J* = 7.81 Hz, 1H), 7.46 (t, *J* = 7.56 Hz, 1H), 7.40 (d, *J* = 8.29 Hz, 1H), 7.24 - 7.34 (m, *J* = 6.80 Hz, 2H), 6.89 (t, *J* = 7.56 Hz, 1H), 4.59 - 4.75 (m, 1H), 4.34 (s, 2H), 1.67 (d, *J* = 6.83 Hz, 6H). MS (ESI-TOF) for $C_{22}H_{19}N_5O_2S_2$ [M + Na^+] calculated 472.1, found 471.9.

6{4,5}; ***N*-(benzo[*d*]thiazol-2-yl)-2-((3-methyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 55%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.90 (s, 1H), 11.96 (s, 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.84 (d, *J* = 8.10 Hz, 1H), 7.81 (d, *J* = 8.10 Hz, 1H), 7.45 (t, *J* = 7.81 Hz, 1H), 7.41 (d, *J* = 8.78 Hz, 1H), 7.32 (t, *J* = 7.30 Hz, 1H), 7.28 (t, *J* = 7.30 Hz, 1H), 6.92 (t, *J* = 7.56 Hz, 1H), 4.39 (s, 2H), 3.63 (s, 3H). MS (ESI-TOF) for $C_{20}H_{15}N_5O_2S_2$ $[M + H]^+$ calculated 422.1, found 421.9.

6{5,5}; ***N*-(benzo[*d*]thiazol-2-yl)-2-((3-ethyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 83%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.91 (br. s., 1H), 11.96 (s, 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.82 (dd, *J* = 8.29, 16.59 Hz, 2H), 7.46 (t, *J* = 7.80 Hz, 1H), 7.41 (d, *J* = 8.29 Hz, 1H), 7.32 (t, *J* = 7.40 Hz, 1H), 7.28 (t, *J* = 7.50 Hz, 1H), 6.92 (t, *J* = 7.32 Hz, 1H), 4.38 (s, 2H), 4.21 (q, *J* = 7.30 Hz, 2H), 1.35 (t, *J* = 6.83 Hz, 3H). MS (ESI-TOF) for $C_{21}H_{17}N_5O_2S_2$ $[M - H]^-$ calculated 434.1, found 433.9.

6{6,5}; ***N*-(benzo[*d*]thiazol-2-yl)-2-((4-oxo-3-propyl-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 83%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.91 (s, 1H), 11.97 (s, 1H), 7.91 (d, *J* = 7.80 Hz, 1H), 7.82 (dd, *J* = 8.29, 14.63 Hz, 2H), 7.46 (t, *J* = 7.56 Hz, 1H), 7.41 (d, *J* = 8.29 Hz, 1H), 7.32 (t, *J* = 7.80 Hz, 1H), 7.28 (t, *J* = 7.80 Hz, 1H), 6.92 (t, *J* = 7.56 Hz, 1H), 4.38 (s, 2H), 4.12 (t, *J* = 7.80 Hz, 2H), 1.79 (sxt, *J* = 7.80 Hz, 2H), 0.99 (t, *J* = 7.31 Hz, 3H). MS (ESI-TOF) for $C_{22}H_{19}N_5O_2S_2$ $[M - H]^-$ calculated 448.1, found 448.0.

6{7,5}; ***N*-(benzo[*d*]thiazol-2-yl)-2-((3-butyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 74%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.91 (s, 1H), 11.96 (s, 1H), 7.91 (d, *J* = 7.80 Hz, 1H), 7.82 (dd, *J* = 8.04, 16.82 Hz, 2H), 7.46 (t, *J* = 7.30 Hz, 1H), 7.41 (d, *J* = 8.29 Hz, 1H), 7.30 (td, *J* = 7.31, 12.68 Hz, 2H), 6.92 (t, *J* = 7.31 Hz, 1H), 4.38 (s, 2H), 4.16 (t, *J* = 7.80 Hz, 2H), 1.75 (quin, *J* = 7.68 Hz, 2H), 1.43 (sxt, *J* = 7.41 Hz, 2H), 0.98 (t, *J* = 7.31 Hz,

3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 167.9, 158.1, 154.5, 150.9, 148.7, 138.8, 136.7, 131.4, 127.1, 126.1, 123.5, 121.7, 120.5, 120.1, 120.1, 119.7, 118.9, 112.6, 43.9, 35.9, 29.9, 19.6, 13.6. HRMS for $C_{23}H_{21}N_5O_2S_2$ [M + Na^+] calculated 486.1029, found 486.1028.

6{1,6}; **2-((3-(4-fluorophenyl)-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(6-methylbenzo[*d*]thiazol-2-yl)-acetamide** (yield = 62%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.77 (br. s., 1H), 12.10 (br. s., 1H), 7.86 (d, *J* = 8.29 Hz, 1H), 7.68 - 7.75 (m, 2H), 7.58 - 7.66 (m, *J* = 3.90 Hz, 2H), 7.41 - 7.52 (m, *J* = 8.30, 16.60 Hz, 3H), 7.35 (t, *J* = 6.80 Hz, 1H), 7.27 (d, *J* = 8.29 Hz, 1H), 6.98 (t, *J* = 7.30 Hz, 1H), 4.21 (s, 2H), 2.39 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 167.7, 163.6, 161.6, 157.2, 154.9, 152.1, 146.6, 138.8, 137.0, 132.9, 132.2, 132.0, 131.9, 131.5, 127.4, 127.2, 121.3, 120.2, 120.0, 119.1, 116.6, 116.5, 112.7, 104.5, 36.3, 20.9. HRMS for $C_{26}H_{18}FN_5O_2S_2$ [M + Na^+] calculated 538.0778, found 538.0781.

6{2,6}; **2-((3-(4-methoxyphenyl)-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(6-methylbenzo[*d*]thiazol-2-yl)-acetamide** (yield = 53%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.76 (s, 1H), 12.06 (s, 1H), 7.86 (d, *J* = 8.29 Hz, 1H), 7.68 - 7.76 (m, 2H), 7.39 - 7.48 (m, 3H), 7.31 - 7.38 (m, 1H), 7.27 (d, *J* = 8.29 Hz, 1H), 7.10 - 7.19 (m, 2H), 6.98 (t, *J* = 7.32 Hz, 1H), 4.19 (s, 2H), 3.87 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 167.8, 160.1, 157.2, 155.0, 152.8, 146.6, 138.8, 137.0, 132.9, 131.6, 130.7, 128.3, 127.4, 127.1, 121.3, 120.2, 120.2, 120.2, 119.9, 119.2, 114.7, 112.7, 55.5, 36.3, 20.9. HRMS for $C_{27}H_{21}N_5O_3S_2$ [M + Na^+] calculated 550.0978, found 550.0982.

6{3,6}; **2-((3-isopropyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(6-methylbenzo[*d*]thiazol-2-yl)-acetamide** (yield = 64%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.83 (s, 1H), 11.86 (s, 1H), 7.78 (d, *J* = 7.81 Hz, 1H), 7.67 - 7.76 (m, 2H), 7.40 (d, *J* = 7.81 Hz, 1H),

7.24 - 7.35 (m, 2H), 6.89 (t, *J* = 7.30 Hz, 1H), 4.57 - 4.74 (m, 1H), 4.32 (s, 2H), 2.38 (br. s., 3H), 1.66 (d, *J* = 6.34 Hz, 6H). MS (ESI-TOF) for $C_{23}H_{21}N_5O_2S_2$ [M + Na^+] calculated 486.1, found 486.0.

6{4,6}; **2-((3-methyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(6-methylbenzo[*d*]thiazol-2-yl)-acetamide** (yield = 64%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.81 (br. s., 1H), 11.96 (s, 1H), 7.81 (d, *J* = 8.29 Hz, 1H), 7.66 - 7.75 (m, 2H), 7.41 (d, *J* = 8.29 Hz, 1H), 7.32 (t, *J* = 7.80 Hz, 1H), 7.27 (d, *J* = 8.29 Hz, 1H), 6.93 (t, *J* = 7.32 Hz, 1H), 4.37 (s, 2H), 3.63 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 167.7, 157.2, 154.6, 151.6, 146.6, 138.7, 136.7, 132.9, 131.5, 127.4, 127.4, 127.1, 121.3, 120.2, 120.1, 119.7, 118.7, 112.6, 35.9, 30.0, 20.9. HRMS for $C_{21}H_{17}N_5O_2S_2$ [M + Na^+] calculated 458.0716, found 458.0720.

6{5,6}; **2-((3-ethyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(6-methylbenzo[*d*]thiazol-2-yl)-acetamide** (yield = 88%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.82 (s, 1H), 11.95 (s, 1H), 7.80 (d, *J* = 7.81 Hz, 1H), 7.69 (s, 1H), 7.72 (d, *J* = 8.29 Hz, 1H), 7.41 (d, *J* = 8.29 Hz, 1H), 7.26 (d, *J* = 8.29 Hz, 1H), 7.32 (t, *J* = 7.80 Hz, 1H), 6.93 (t, *J* = 7.56 Hz, 1H), 4.36 (s, 2H), 4.21 (q, *J* = 7.32 Hz, 2H), 2.38 (s, 3H), 1.35 (t, *J* = 7.07 Hz, 3H). ^{13}C NMR (126 MHz, TFA-d) δ 170.7, 155.9, 140.6, 140.1, 132.5, 131.8, 131.7, 126.0, 123.7, 121.9, 119.2, 118.6, 115.7, 114.9, 114.2, 113.5, 113.4, 112.6, 110.4, 44.6, 19.6, 11.5. HRMS for $C_{22}H_{19}N_5O_2S_2$ [M + Na^+] calculated 472.0872, found 472.0873.

6{6,6}; **2-((4-oxo-3-propyl-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(6-methylbenzo[*d*]thiazol-2-yl)-acetamide** (yield = 90%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.83 (s, 1H), 11.96 (s, 1H), 7.81 (d, *J* = 7.81 Hz, 1H), 7.59 - 7.74 (m, 2H), 7.37 - 7.47 (m, 1H), 7.32 (t, *J* = 7.80 Hz, 1H), 7.27 (d, *J* = 8.29 Hz, 1H), 6.93 (t, *J* = 7.56 Hz, 1H), 4.36 (br. s., 2H), 4.11 (t, *J* = 7.80 Hz, 2H), 2.38 (br. s., 3H), 1.79 (sxt, *J* = 7.30 Hz, 2H), 0.99 (t, *J* = 7.30 Hz, 3H). ^{13}C NMR

(126 MHz, DMSO-d_6) δ 167.8, 157.2, 154.5, 151.0, 146.6, 138.8, 136.7, 132.9, 131.5, 127.4, 127.2, 121.3, 120.2, 120.1, 119.8, 118.9, 112.6, 45.5, 35.9, 21.3, 21.0, 11.1. HRMS for $C_{23}H_{21}N_5O_2S_2$ [M + Na^+] calculated 486.1029, found 486.1029.

6{7,6}; **2-((3-butyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(6-methylbenzo[*d*]thiazol-2-yl)-acetamide** (yield = 67%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.82 (s, 1H), 11.95 (s, 1H), 7.80 (d, *J* = 7.81 Hz, 1H), 7.72 (d, *J* = 8.29 Hz, 1H), 7.70 (s, 1H), 7.41 (d, *J* = 7.81 Hz, 1H), 7.32 (t, *J* = 7.40 Hz, 1H), 7.26 (d, *J* = 8.29 Hz, 1H), 6.93 (t, *J* = 7.56 Hz, 1H), 4.36 (s, 2H), 4.15 (t, *J* = 7.56 Hz, 2H), 2.38 (s, 3H), 1.75 (quin, *J* = 7.30 Hz, 2H), 1.43 (sxt, *J* = 7.40 Hz, 2H), 0.98 (t, *J* = 7.32 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 167.8, 157.2, 154.5, 150.9, 146.6, 138.8, 136.7, 132.9, 131.5, 127.4, 127.2, 121.3, 120.2, 120.1, 119.8, 118.9, 112.6, 43.9, 35.9, 29.9, 20.9, 19.7, 13.6. HRMS for $C_{24}H_{23}N_5O_2S_2$ [M + Na^+] calculated 500.1185, found 500.1182.

9a; ***N*-(benzo[*d*]thiazol-2-yl)-2-((4-oxo-3-pentyl-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 82%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.90 (br. s., 1H), 11.94 (s, 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.84 (d, *J* = 7.80 Hz, 1H), 7.80 (d, *J* = 7.81 Hz, 1H), 7.45 (t, *J* = 7.81 Hz, 1H), 7.41 (d, *J* = 8.29 Hz, 1H), 7.32 (t, *J* = 7.30 Hz, 1H), 7.28 (t, *J* = 7.80 Hz, 1H), 6.92 (t, *J* = 7.07 Hz, 1H), 4.38 (s, 2H), 4.07 - 4.25 (m, 2H), 1.76 (quin, *J* = 7.30 Hz, 2H), 1.26 - 1.52 (m, 6H), 0.89 (t, *J* = 7.32 Hz, 3H). MS (ESI-TOF) for $C_{24}H_{23}N_5O_2S_2$ [M - H]$^-$ calculated 476.1, found 475.9.

9b; **2-((4-oxo-3-pentyl-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(6-methylbenzo[*d*]thiazol-2-yl)-acetamide** (yield = 87%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.81 (s, 1H), 11.95 (s, 1H), 7.80 (d, *J* = 7.81 Hz, 1H), 7.69 (s, 1H), 7.72 (d, *J* = 7.81 Hz, 1H), 7.39 - 7.45 (m, 1H), 7.29 - 7.35 (m, 1H), 7.26 (d, *J* = 8.29 Hz, 1H), 6.93 (t, *J* = 7.32 Hz, 1H), 4.36 (s,

2H), 4.09 - 4.19 (m, 2H), 2.38 (s, 3H), 1.76 (quin, *J* = 7.80 Hz, 2H), 1.23 - 1.50 (m, 6H), 0.89 (t, *J* = 6.83 Hz, 3H). MS (ESI-TOF) for $C_{25}H_{25}N_5O_2S_2$ $[M + H]^+$ calculated 490.1, found 491.9.

10a; ***N*-(benzo[*d*]thiazol-2-yl)-2-((3-hexyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 67%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.90 (s, 1H), 11.95 (s, 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.80 (d, *J* = 7.80 Hz, 1H), 7.84 (d, *J* = 7.80 Hz, 1H), 7.42 (d, *J* = 8.29 Hz, 1H), 7.46 (t, *J* = 7.32 Hz, 1H), 7.32 (t, *J* = 7.30 Hz, 1H), 7.29 (t, *J* = 7.80 Hz, 1H), 6.92 (t, *J* = 7.56 Hz, 1H), 4.38 (s, 2H), 4.08 - 4.25 (m, 2H), 1.77 (quin, *J* = 7.30 Hz, 2H), 1.29 - 1.50 (m, 4H), 0.92 (t, *J* = 7.30 Hz, 3H). MS (ESI-TOF) for $C_{25}H_{25}N_5O_2S_2$ $[M + Na^+]$ calculated 514.1, found 514.0.

10b; **2-((3-hexyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(6-methylbenzo[*d*]thiazol-2-yl)-acetamide** (yield = 73%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.82 (s, 1H), 11.95 (s, 1H), 7.81 (d, *J* = 7.81 Hz, 1H), 7.70 (s, 1H), 7.72 (d, *J* = 8.29 Hz, 1H), 7.42 (d, *J* = 8.29 Hz, 1H), 7.32 (t, *J* = 7.81 Hz, 1H), 7.27 (d, *J* = 8.29 Hz, 1H), 6.93 (t, *J* = 7.07 Hz, 1H), 4.37 (s, 2H), 4.07 - 4.21 (m, 2H), 2.39 (s, 3H), 1.77 (quin, *J* = 7.30 Hz, 2H), 1.31 - 1.47 (m, 4H), 0.92 (t, *J* = 6.83 Hz, 3H). MS (ESI-TOF) for $C_{26}H_{27}N_5O_2S_2$ $[M - H]^-$ calculated 504.2, found 504.0.

11; ***N*-(benzo[*d*]thiazol-2-yl)-2-((3-butyl-5-methyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)acetamide** (yield = 26%): ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.90 (s, 1H), 7.90 (d, *J* = 7.80 Hz, 1H), 7.84 (d, *J* = 7.80 Hz, 2H), 7.56 (d, *J* = 8.78 Hz, 1H), 7.45 (t, *J* = 7.80 Hz, 1H), 7.40 (t, *J* = 7.30 Hz, 1H), 7.28 (t, *J* = 7.56 Hz, 1H), 6.96 (t, *J* = 7.56 Hz, 1H), 4.38 (s, 2H), 4.10 - 4.16 (m, 2H), 4.08 (s, 3H), 1.74 (quin, *J* = 15.10 Hz, 2H), 1.44 (sxt, *J* = 7.31 Hz, 2H), 0.98 (t, *J* = 7.31 Hz, 3H). MS (ESI-TOF) for $C_{24}H_{23}N_5O_2S_2$ $[M + H]^+$ calculated 478.1, found 478.0.

12; **2-((3-butyl-5-methyl-4-oxo-4,5-dihydro-3*H*-pyrimido[5,4-*b*]indol-2-yl)thio)-*N*-(6-methylbenzo[*d*]thiazol-2-yl)acetamide** (yield = 33%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.82 (s, 1H), 7.84 (d, *J* = 7.81 Hz, 1H), 7.72 (d, *J* = 8.29 Hz, 1H), 7.67 - 7.74 (m, 1H), 7.57 (d, *J* = 8.29 Hz, 1H), 7.41 (t, *J* = 7.81 Hz, 1H), 7.26 (d, *J* = 8.29 Hz, 1H), 6.97 (t, *J* = 7.32 Hz, 1H), 4.36 (s, 2H), 4.09 (s, 3H), 4.13 (t, *J* = 7.80 Hz, 2H), 2.38 (s, 3H), 1.74 (quin, *J* = 7.81 Hz, 2H), 1.44 (sxt, *J* = 7.32 Hz, 2H), 0.98 (t, *J* = 7.32 Hz, 3H). MS (ESI-TOF) for $C_{25}H_{25}N_5O_2S_2$ $[M + H]^+$ calculated 492.2, found 492.0.

^{1}H NMR, LC-MS **6**{1,1}

4/21/2017 10:09:13 AM

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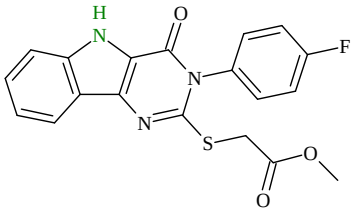
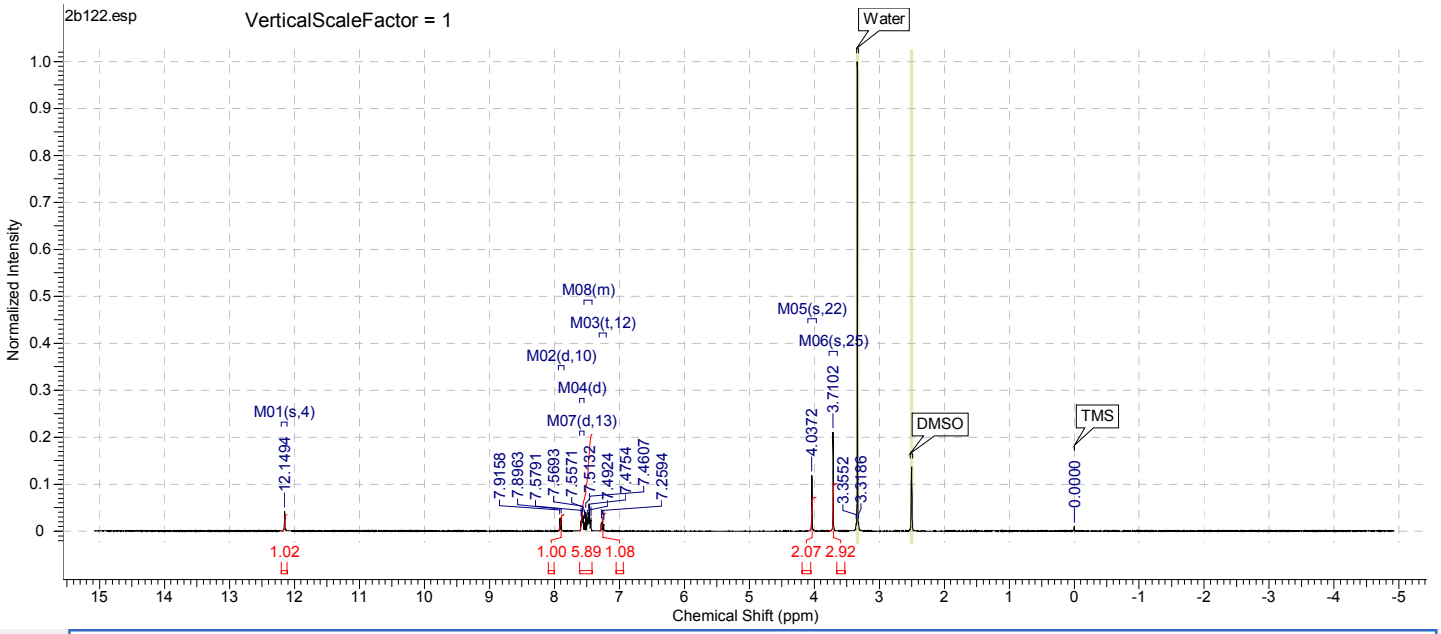
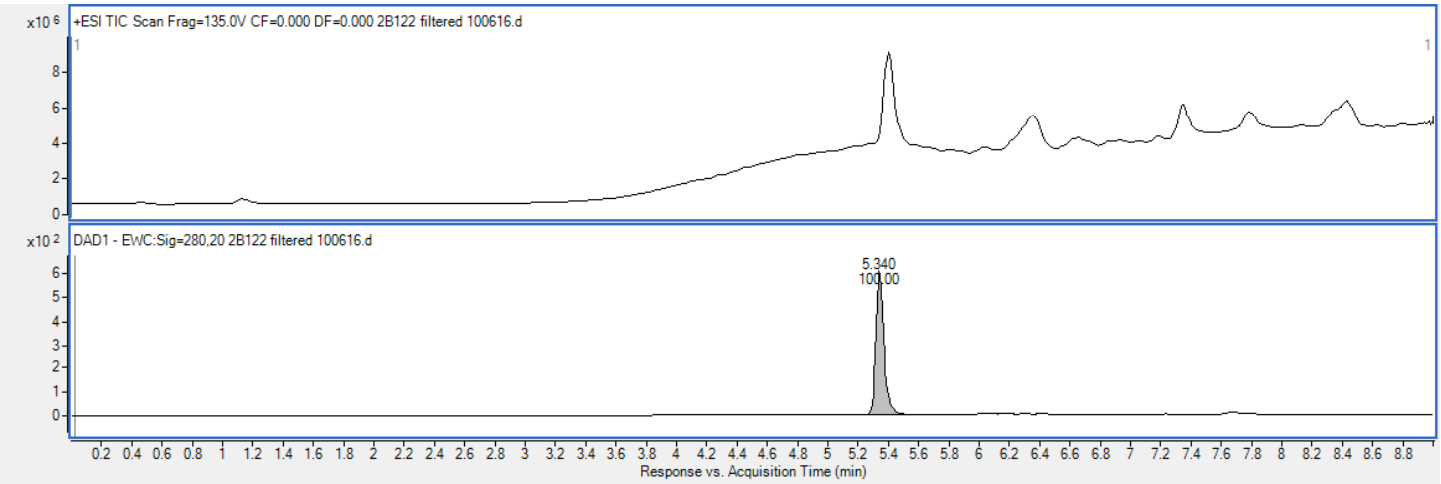
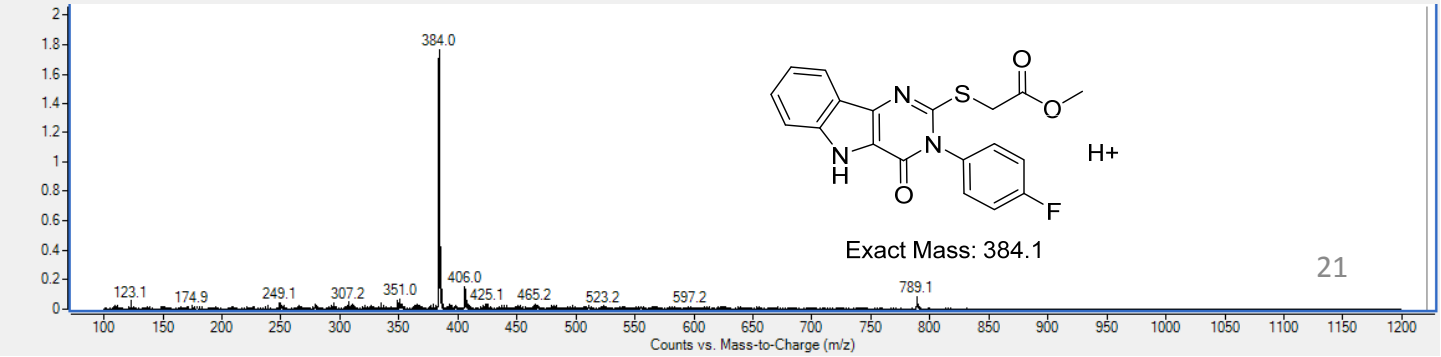
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2029.0183	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.15 (s, 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.56 (d, *J* = 4.88 Hz, 1H), 7.59 (d, *J* = 4.88 Hz, 1H), 7.42 - 7.55 (m, 4H), 7.26 (t, *J* = 7.32 Hz, 1H), 4.04 (s, 2H), 3.71 (s, 3H)









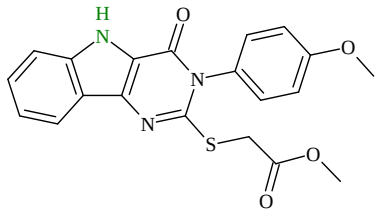
Exact Mass: 384.1

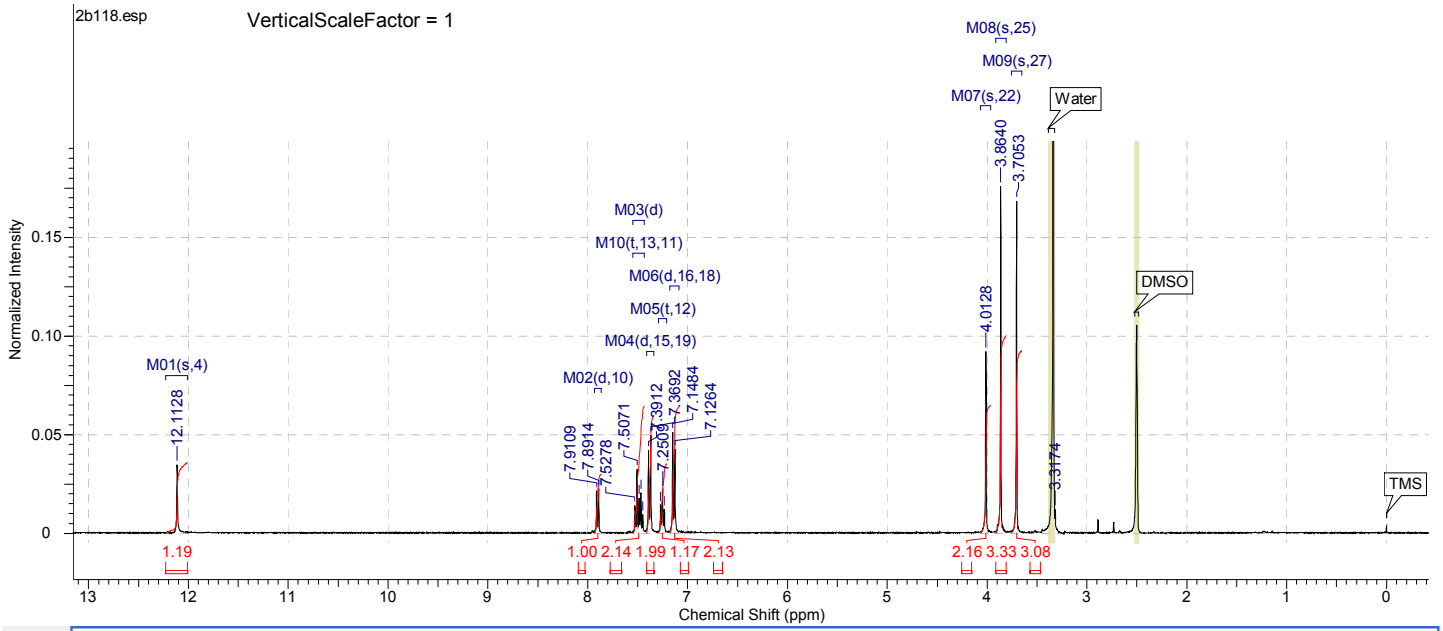
^{1}H NMR, LC-MS **6**{2,1}

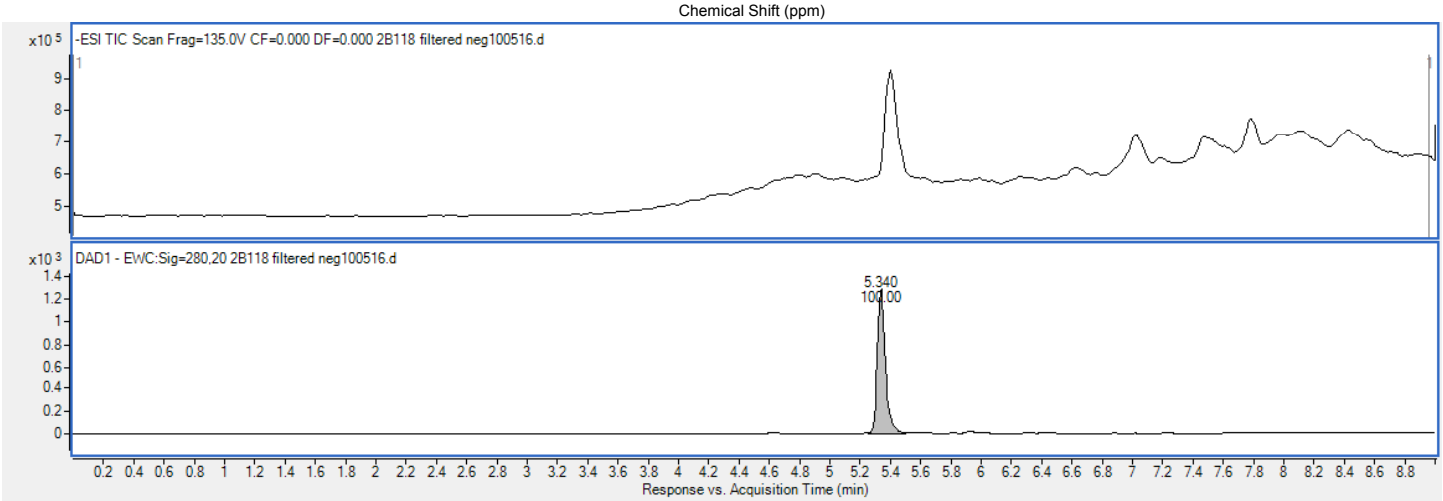
4/21/2017 10:10:53 AM

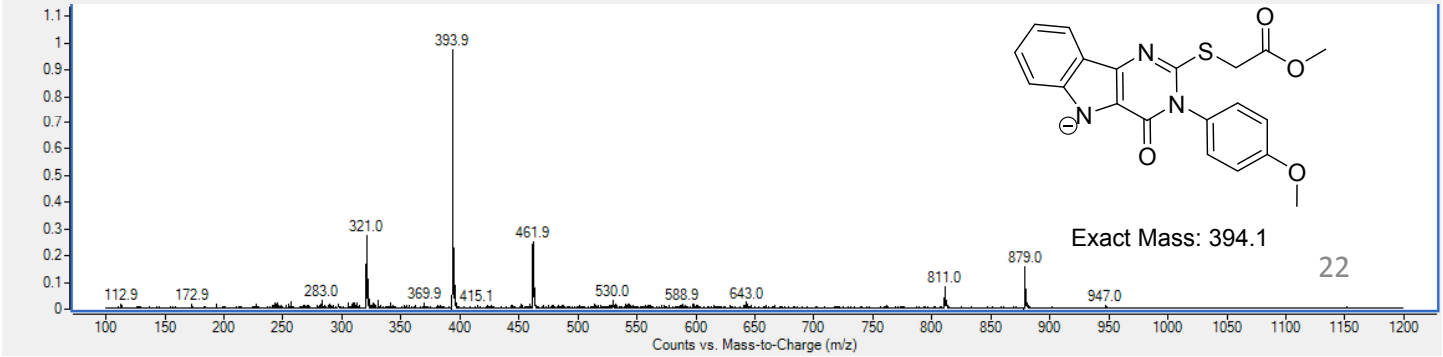
Acquisition Time (sec)	2.0097	***Comment***	STANDARD 1H OBSERVE			***Date***	Mar 24 2017
Date Stamp	Mar 24 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b118.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16065
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2029.5062	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.11 (s, 1H), 7.90 (d, *J* = 7.81 Hz, 1H), 7.46 (d, *J* = 8.29 Hz, 1H), 7.51 (t, *J* = 8.30 Hz, 1H), 7.38 (d, *J* = 8.78 Hz, 2H), 7.25 (t, *J* = 7.32 Hz, 1H), 7.14 (d, *J* = 8.78 Hz, 2H), 4.01 (s, 2H), 3.86 (s, 3H), 3.71 (s, 3H)









Exact Mass: 394.1

^{1}H NMR, LC-MS **6**{3,1}

4/21/2017 10:11:55 AM

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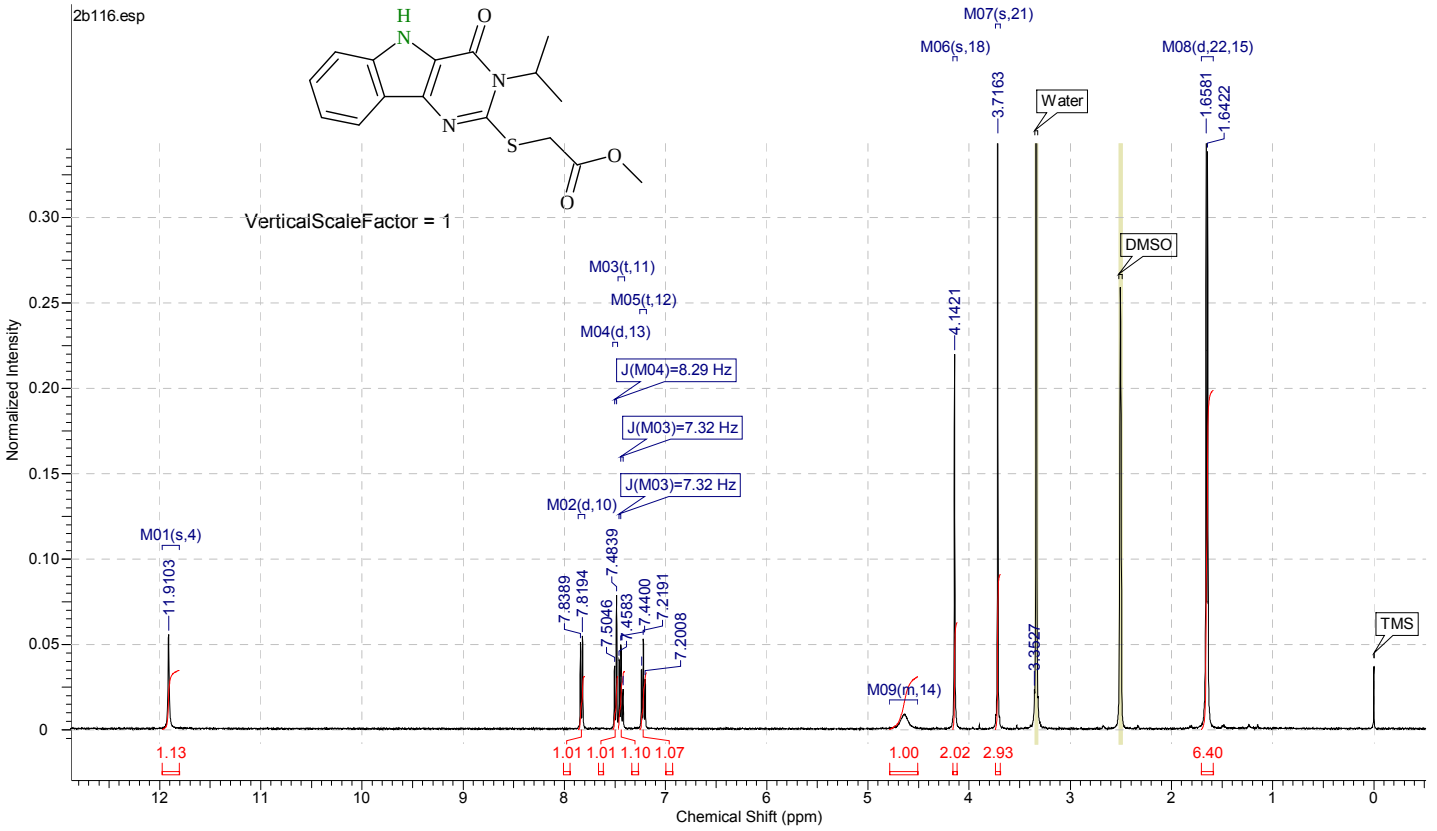
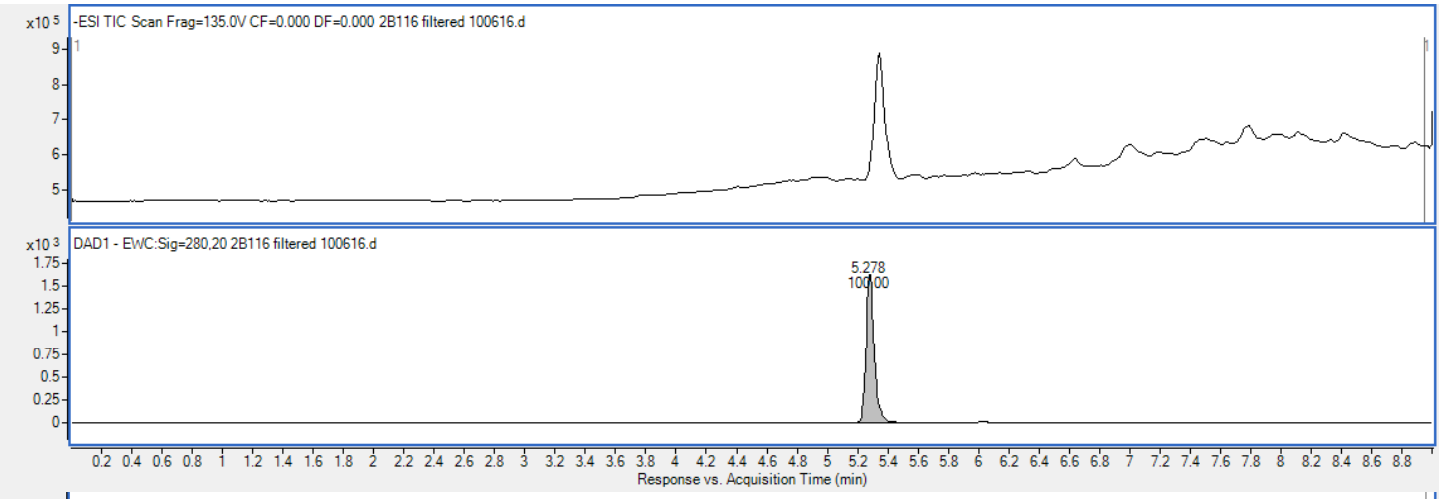
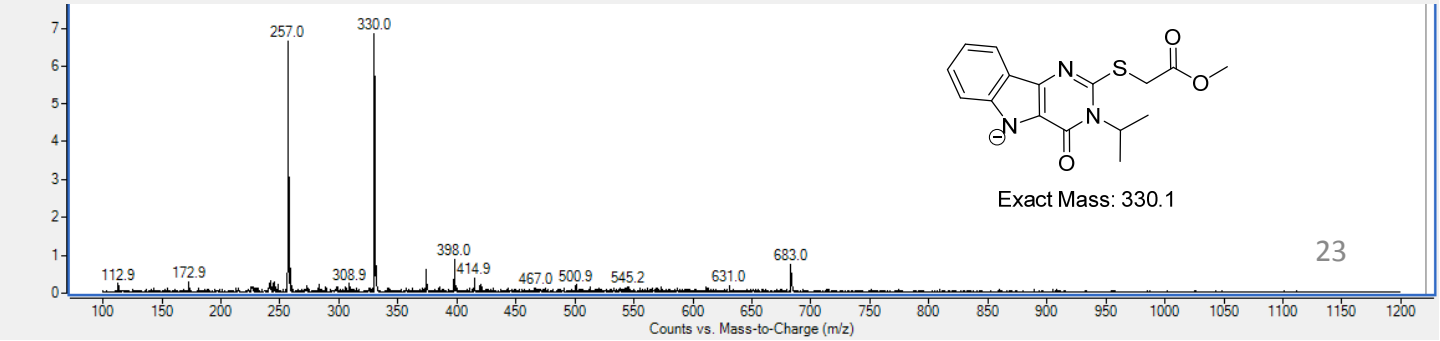
Date Stamp	Mar 24 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b116.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16156
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2029.9941	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.91 (s, 1H), 7.83 (d, *J* = 7.81 Hz, 1H), 7.49 (d, *J* = 8.29 Hz, 1H), 7.44 (t, *J* = 7.32 Hz, 1H), 7.22 (t, *J* = 7.32 Hz, 1H), 4.51 - 4.79 (m, 1H), 4.14 (s, 2H), 3.72 (s, 3H), 1.65 (d, *J* = 6.34 Hz, 6H)







Exact Mass: 330.1

^{1}H NMR, LC-MS **6**{4,1}

4/21/2017 10:14:03 AM

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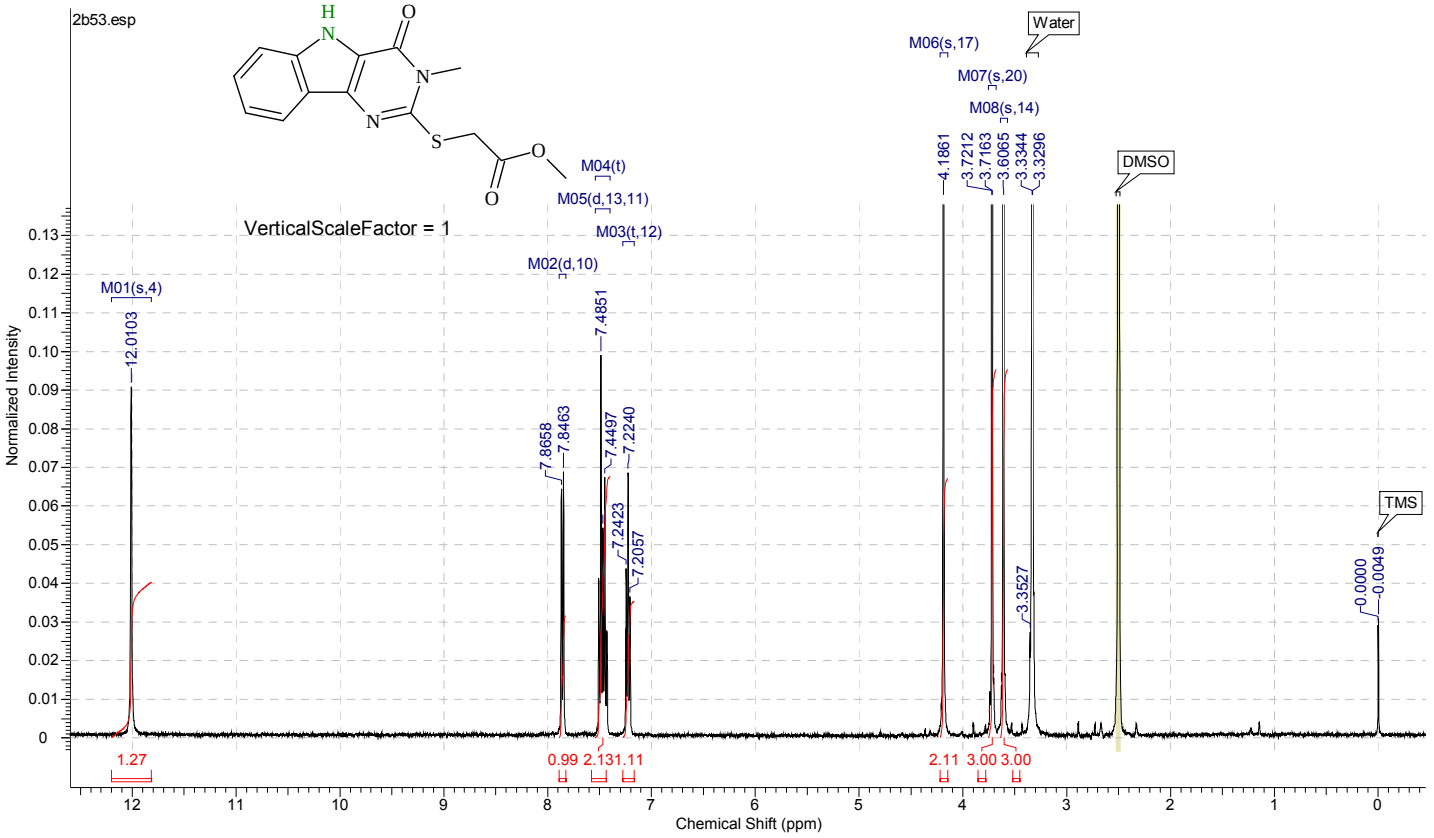
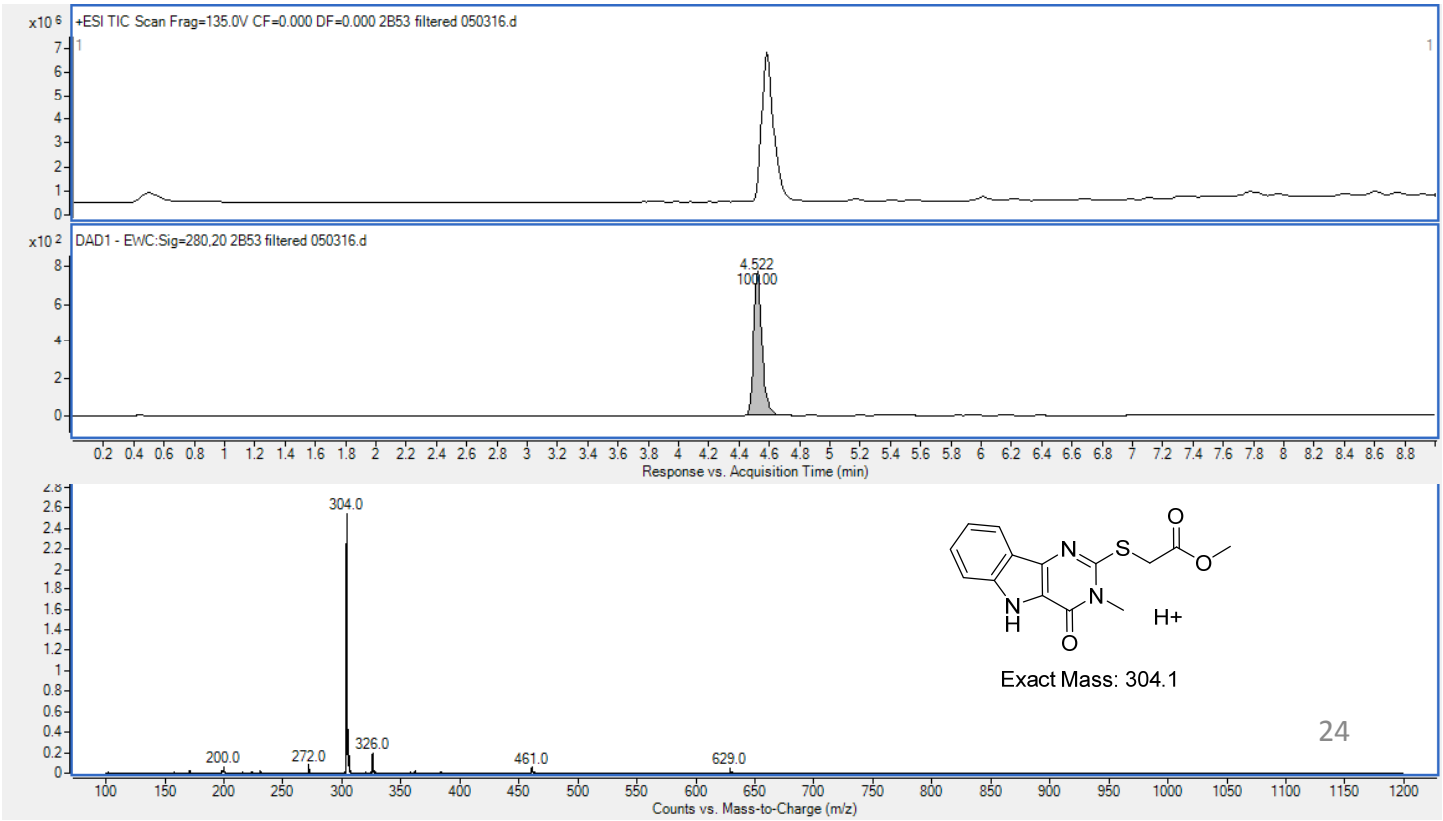
Date Stamp	Mar 24 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b53.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16130
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2028.5304	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.01 (s, 1H), 7.86 (d, *J* = 7.81 Hz, 1H), 7.45 (t, *J* = 7.30 Hz, 1H), 7.50 (d, *J* = 8.29 Hz, 1H), 7.22 (t, *J* = 7.32 Hz, 1H), 4.19 (s, 2H), 3.71 (s, 3H), 3.62 (s, 3H)



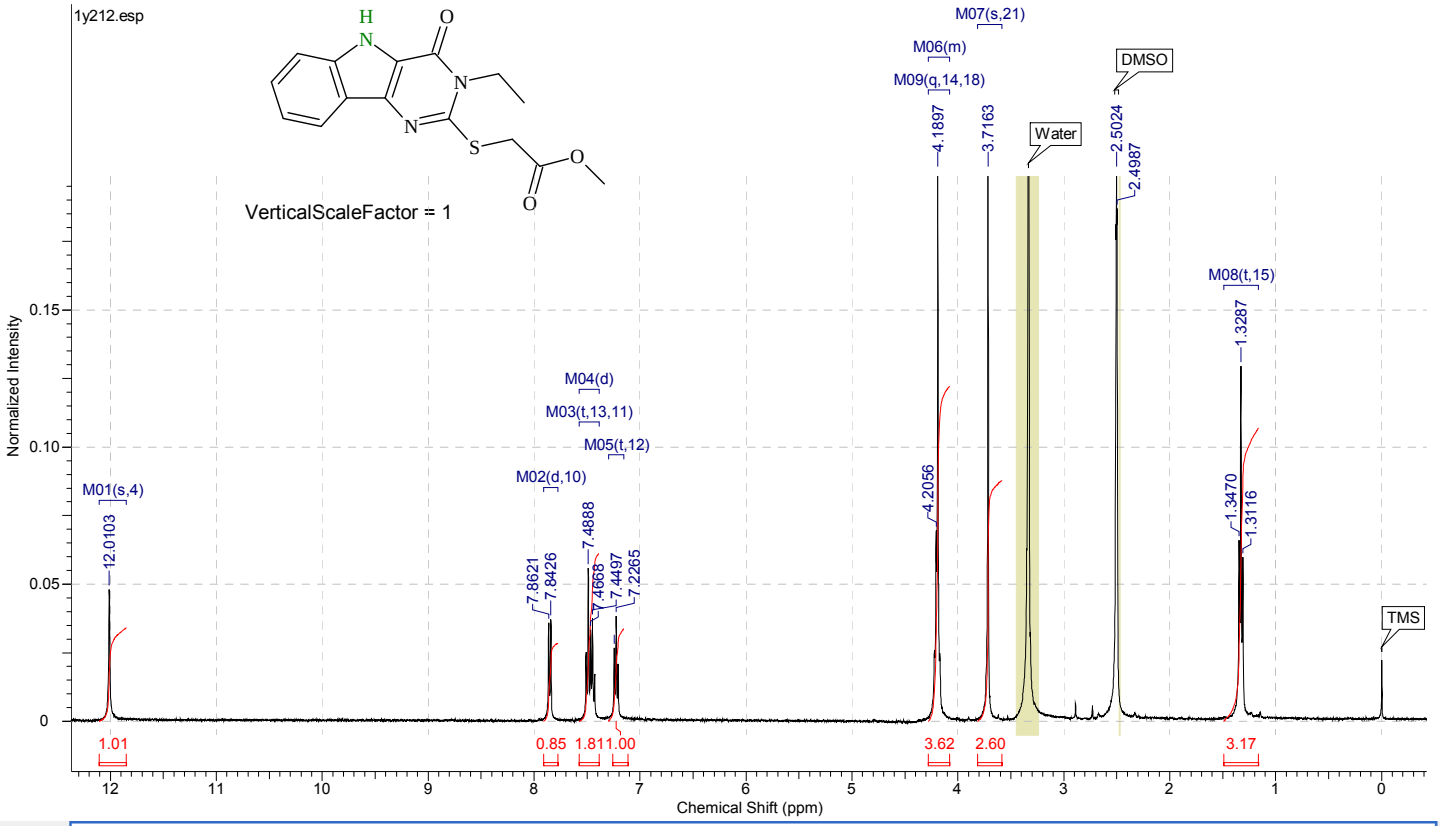


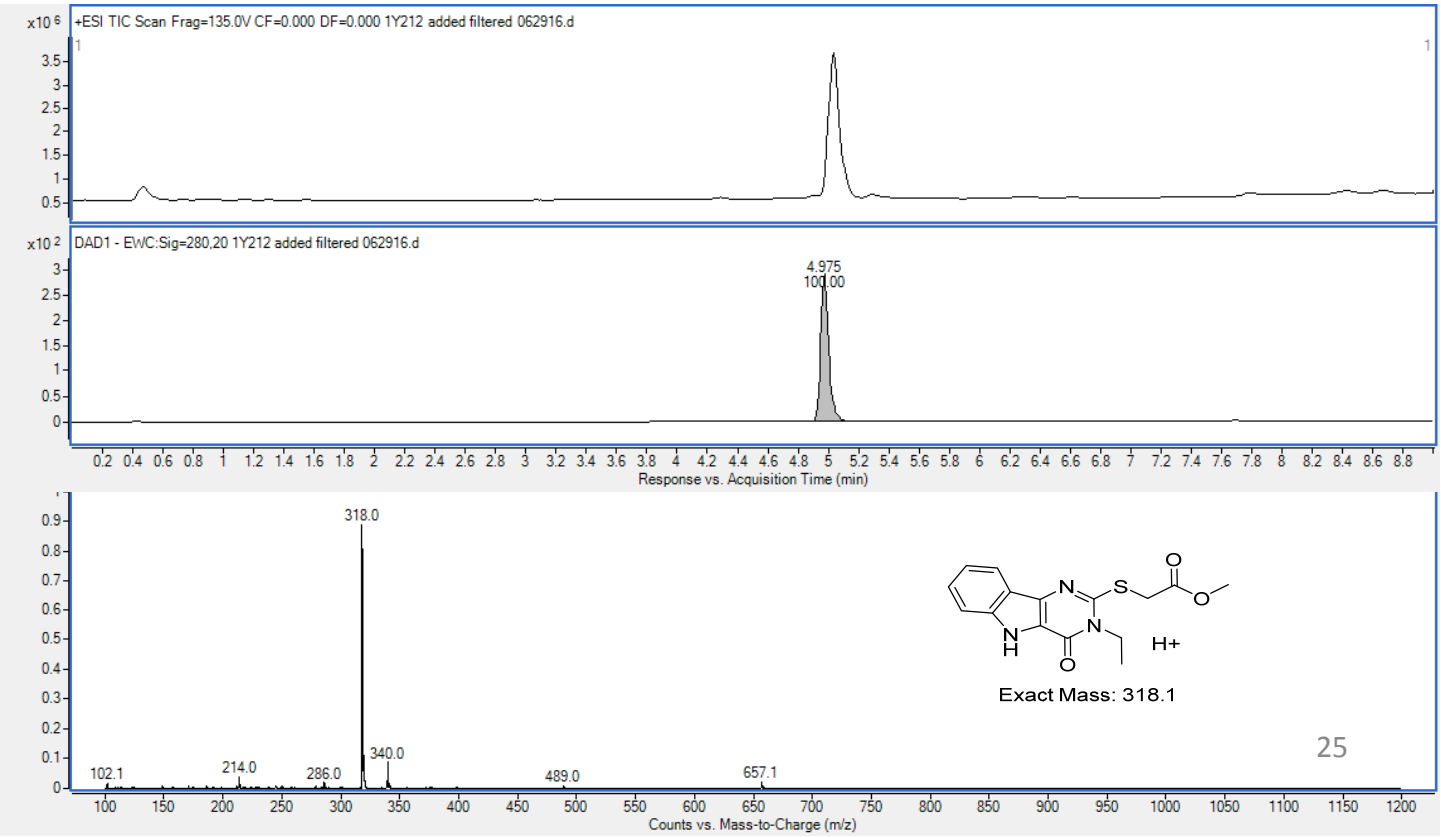
^{1}H NMR, LC-MS **6**{5,1}

4/21/2017 10:15:11 AM

Acquisition Time (sec)	2.0195	***Comment***	STANDARD 1H OBSERVE			***Date***	Mar 24 2017
Date Stamp	Mar 24 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\1y212.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16143
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2029.5062	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.01 (s, 1H), 7.85 (d, *J* = 7.81 Hz, 1H), 7.44 (d, *J* = 7.80 Hz, 1H), 7.49 (t, *J* = 8.30 Hz, 2H), 7.23 (t, *J* = 7.32 Hz, 1H), 4.08 - 4.28 (m, 2H), 4.20 (q, *J* = 6.80 Hz, 1H), 3.72 (s, 3H), 1.33 (t, *J* = 7.07 Hz, 3H)



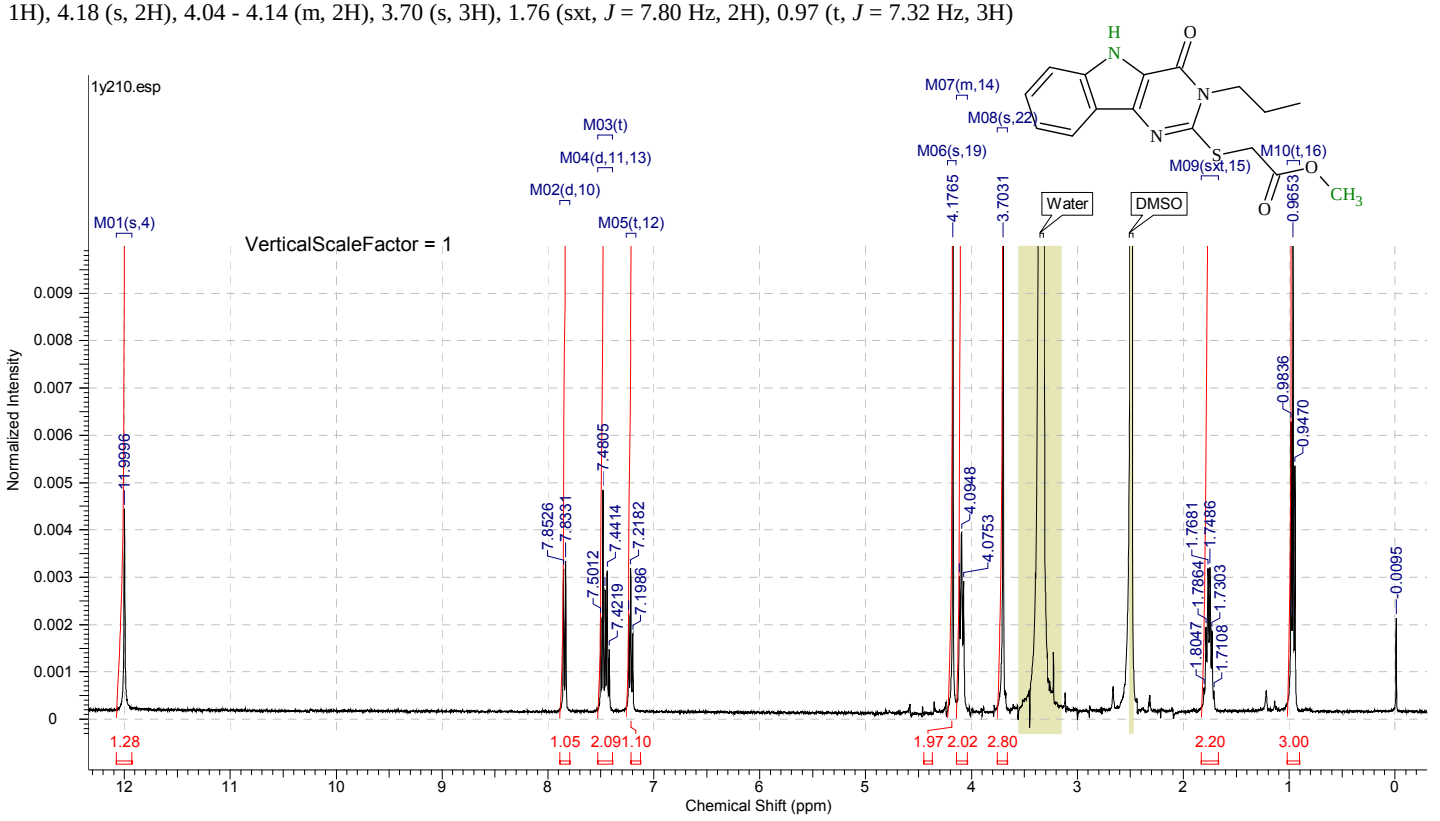


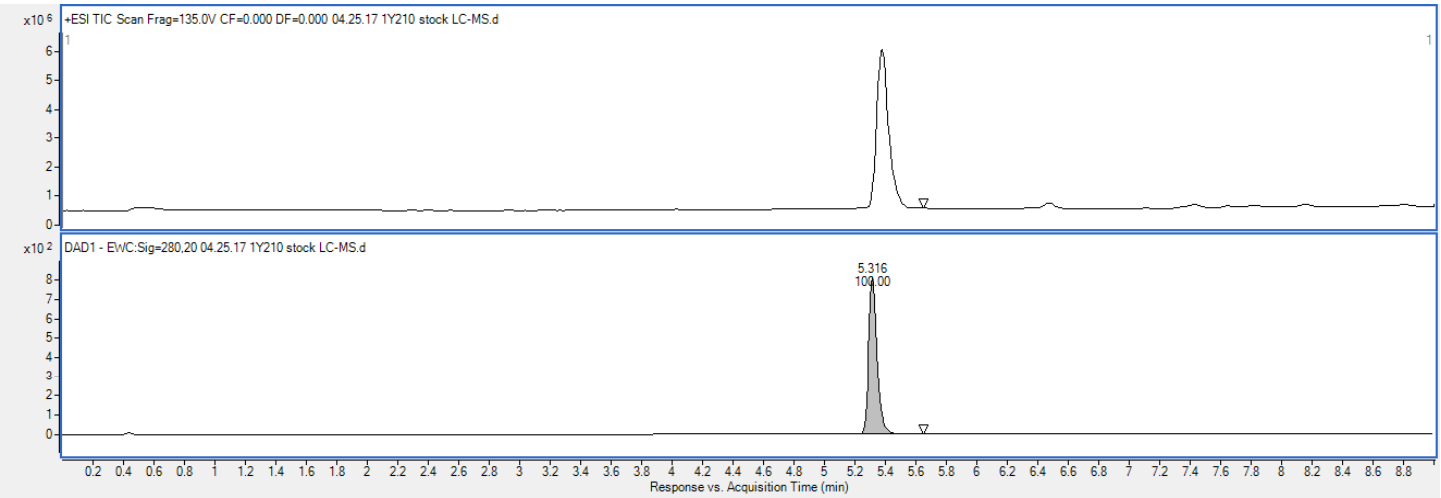
^{1}H NMR, LC-MS **6**{6,1}

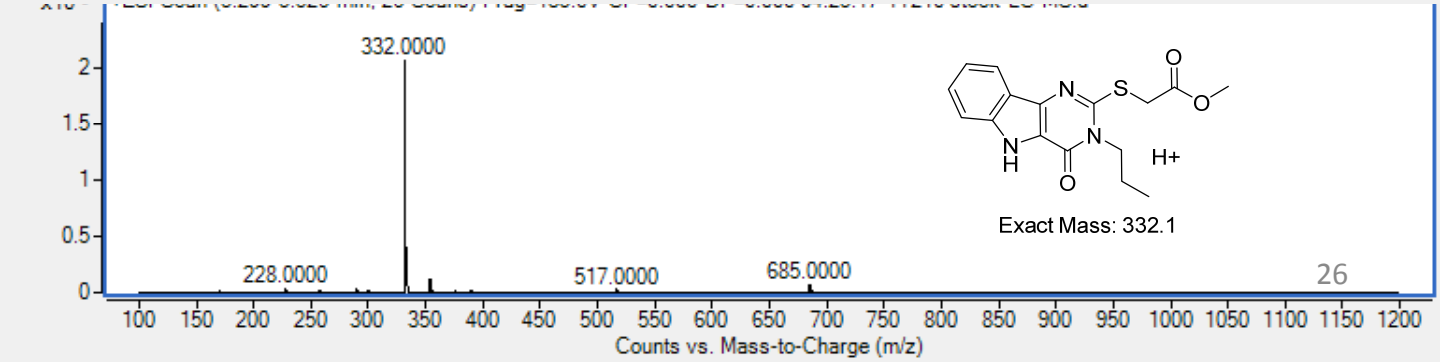
3/27/2017 10:57:42 AM

Acquisition Time (sec)	2.0227	***Comment***	STANDARD 1H OBSERVE			***Date***	Mar 24 2017
Date Stamp	Mar 24 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\1y210.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	64	***Original Points Count***	16169
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2025.6981	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.84 (d, *J* = 7.81 Hz, 1H), 7.48 (t, *J* = 8.30 Hz, 1H), 7.43 (d, *J* = 7.81 Hz, 1H), 7.22 (t, *J* = 7.56 Hz, 1H), 4.18 (s, 2H), 4.04 - 4.14 (m, 2H), 3.70 (s, 3H), 1.76 (sxt, *J* = 7.80 Hz, 2H), 0.97 (t, *J* = 7.32 Hz, 3H)





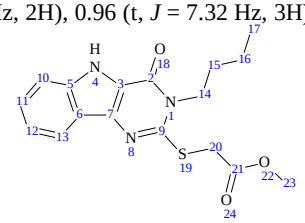


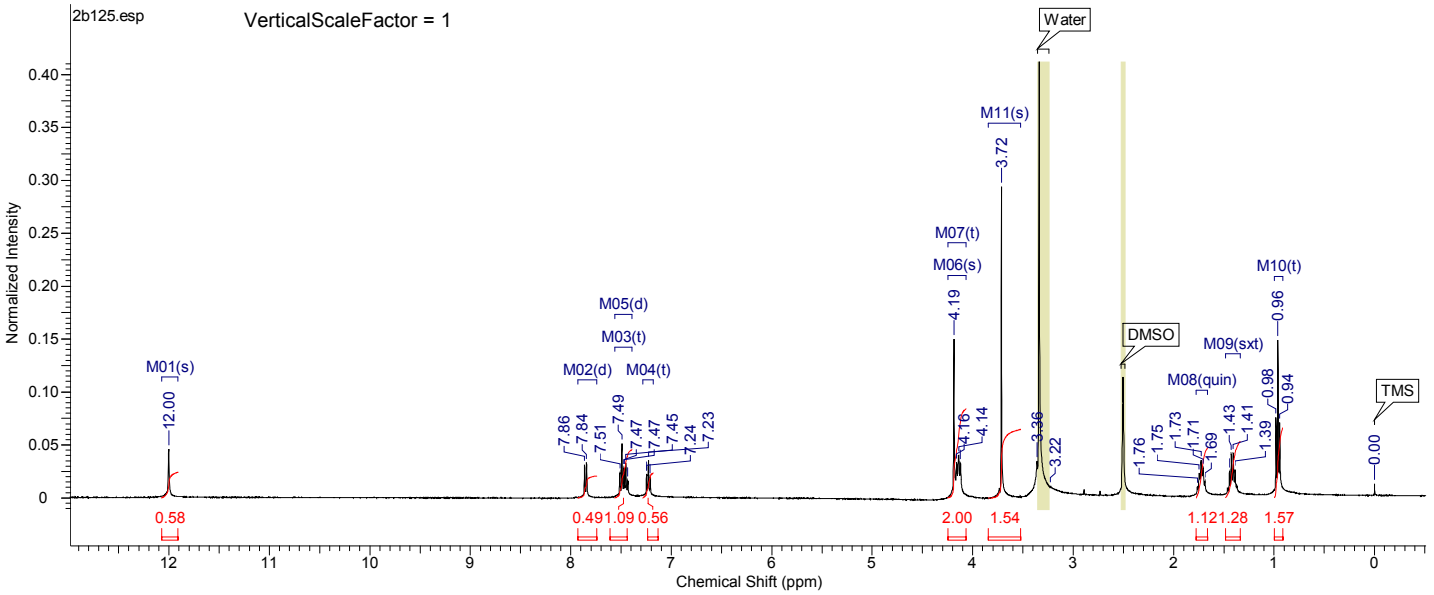
^{1}H NMR, LC-MS **6**{7,1}

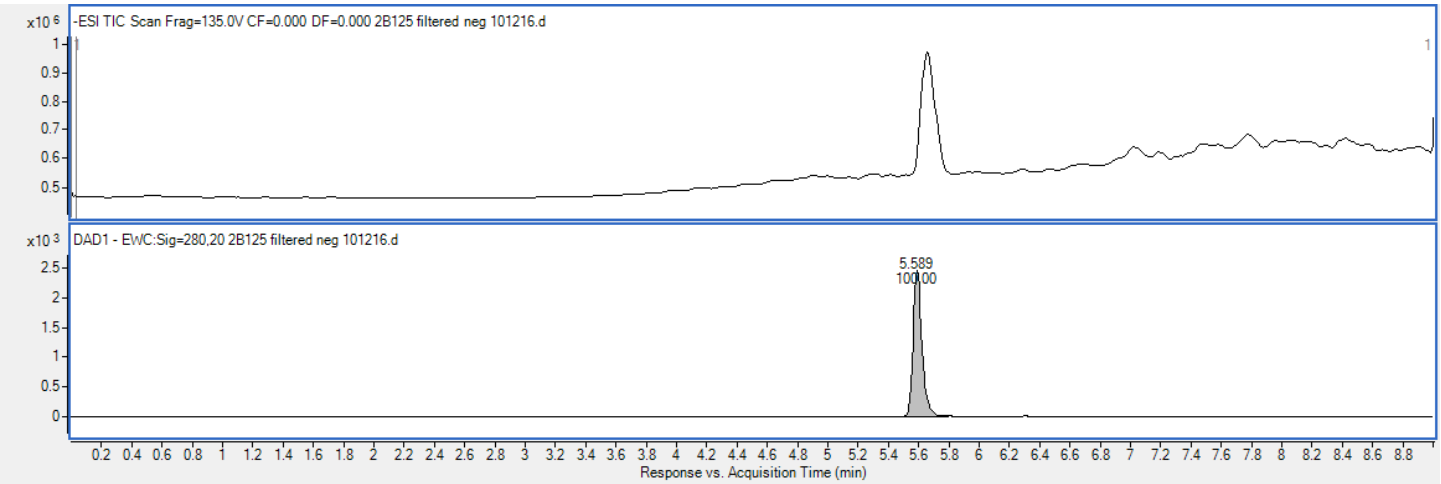
4/6/2017 4:50:00 PM

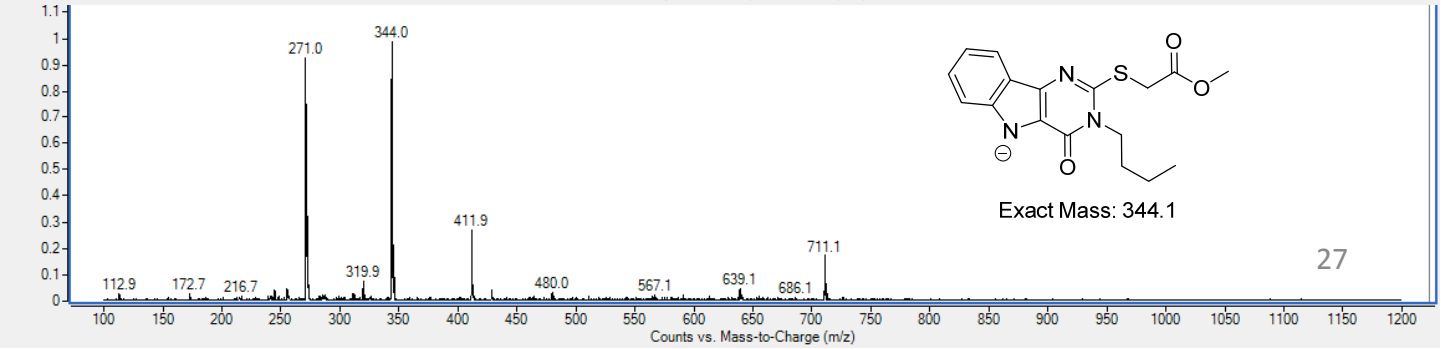
Acquisition Time (sec)	2.0081	***Comment***	STANDARD 1H OBSERVE			***Date***	Mar 24 2017
Date Stamp	Mar 24 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b125.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16052
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2030.9700	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.85 (d, *J* = 7.81 Hz, 1H), 7.49 (t, *J* = 8.30 Hz, 1H), 7.44 (d, *J* = 8.29 Hz, 1H), 7.23 (t, *J* = 7.30 Hz, 1H), 4.19 (s, 2H), 4.14 (t, *J* = 7.80 Hz, 2H), 3.72 (s, 3H), 1.73 (quin, *J* = 7.30 Hz, 2H), 1.42 (sxt, *J* = 7.80 Hz, 2H), 0.96 (t, *J* = 7.32 Hz, 3H)









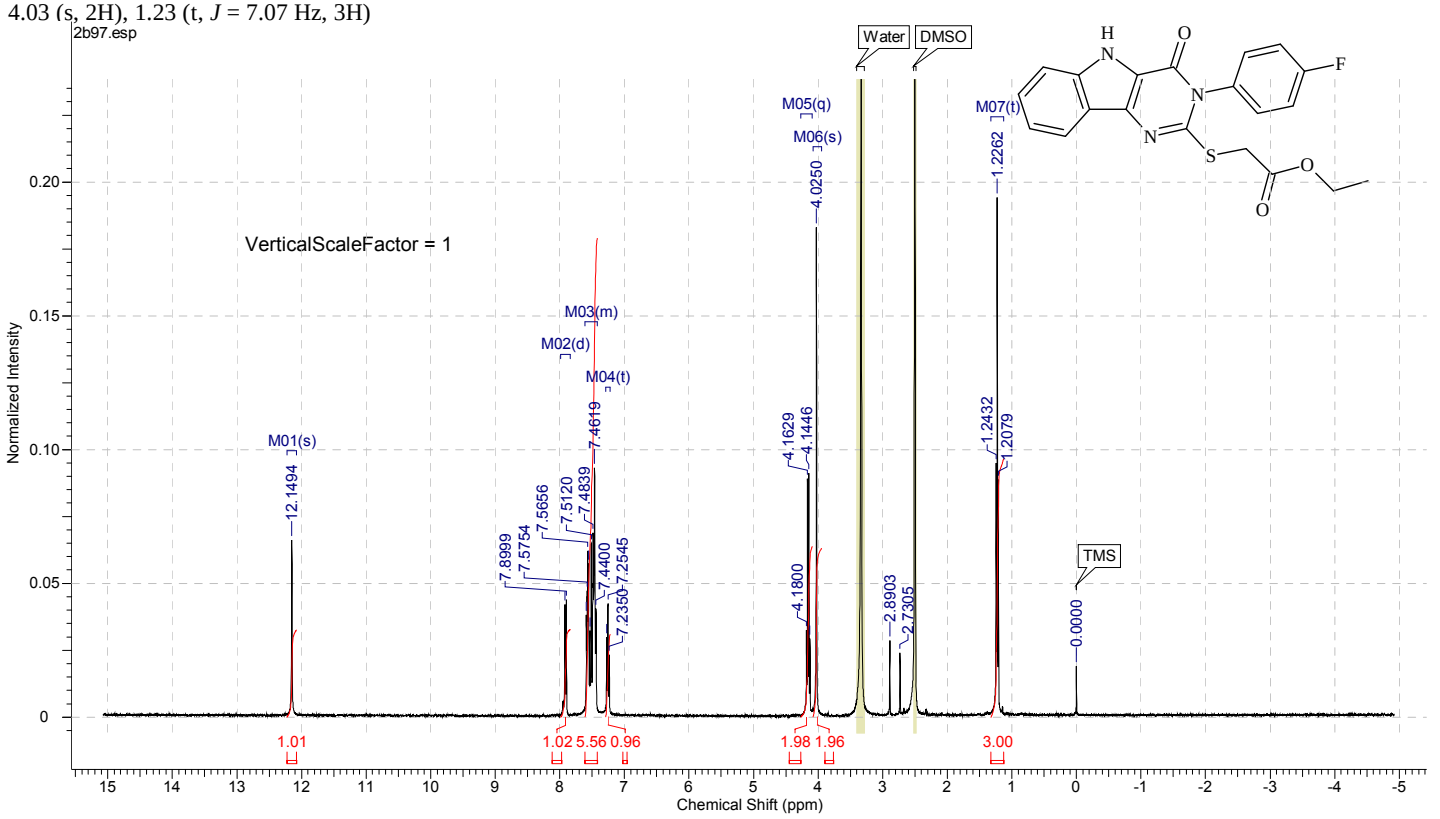
Exact Mass: 344.1

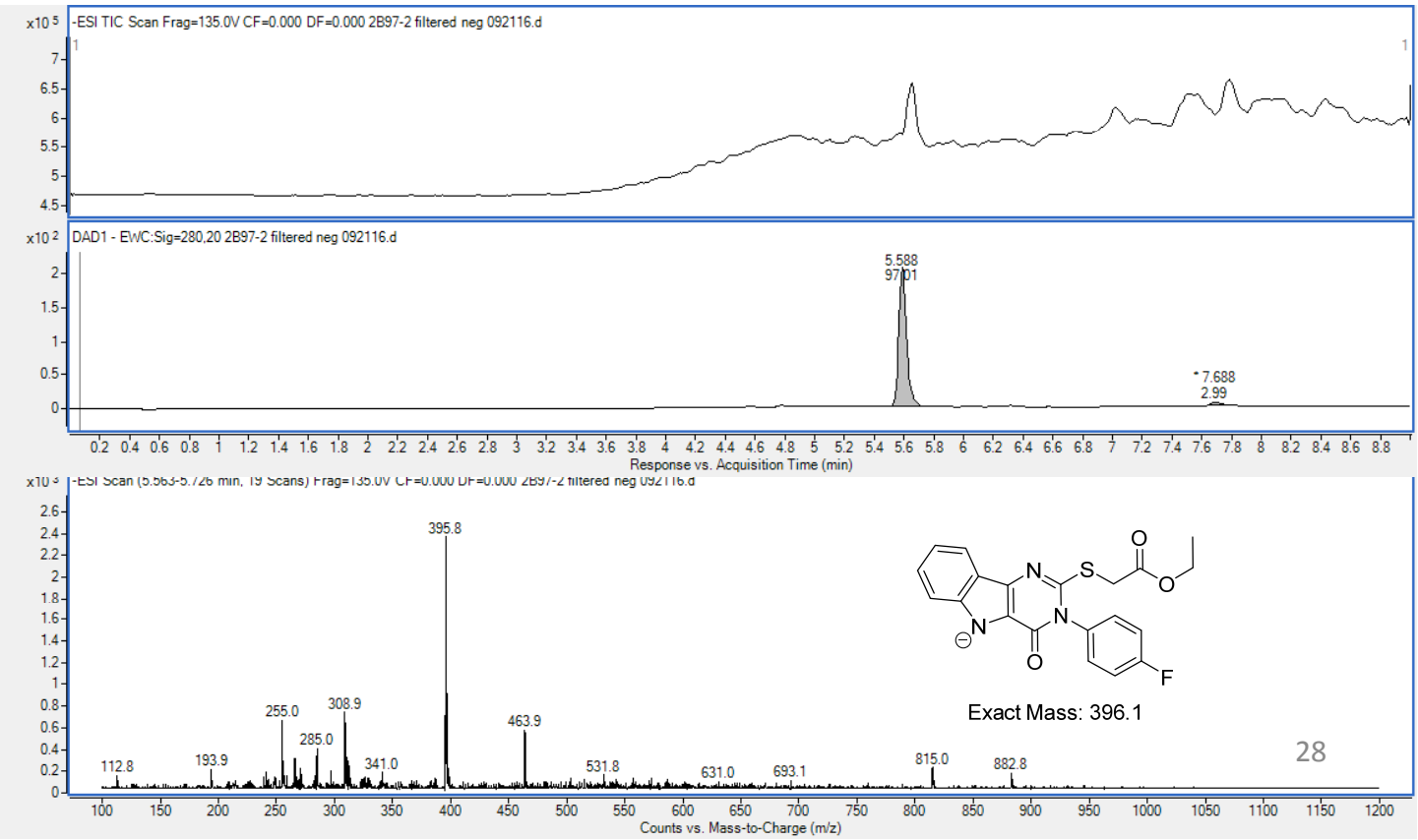
^{1}H NMR, LC-MS **6**{1,2}

4/25/2017 10:05:56 AM

Acquisition Time (sec)	2.0162	***Comment***	STANDARD 1H OBSERVE			***Date***	Mar 24 2017
Date Stamp	Mar 24 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b97.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16117
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2029.0183	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.15 (s, 1H), 7.91 (d, *J* = 8.29 Hz, 1H), 7.42 - 7.61 (m, 6H), 7.25 (t, *J* = 7.56 Hz, 1H), 4.15 (q, *J* = 6.83 Hz, 2H), 4.03 (s, 2H), 1.23 (t, *J* = 7.07 Hz, 3H)





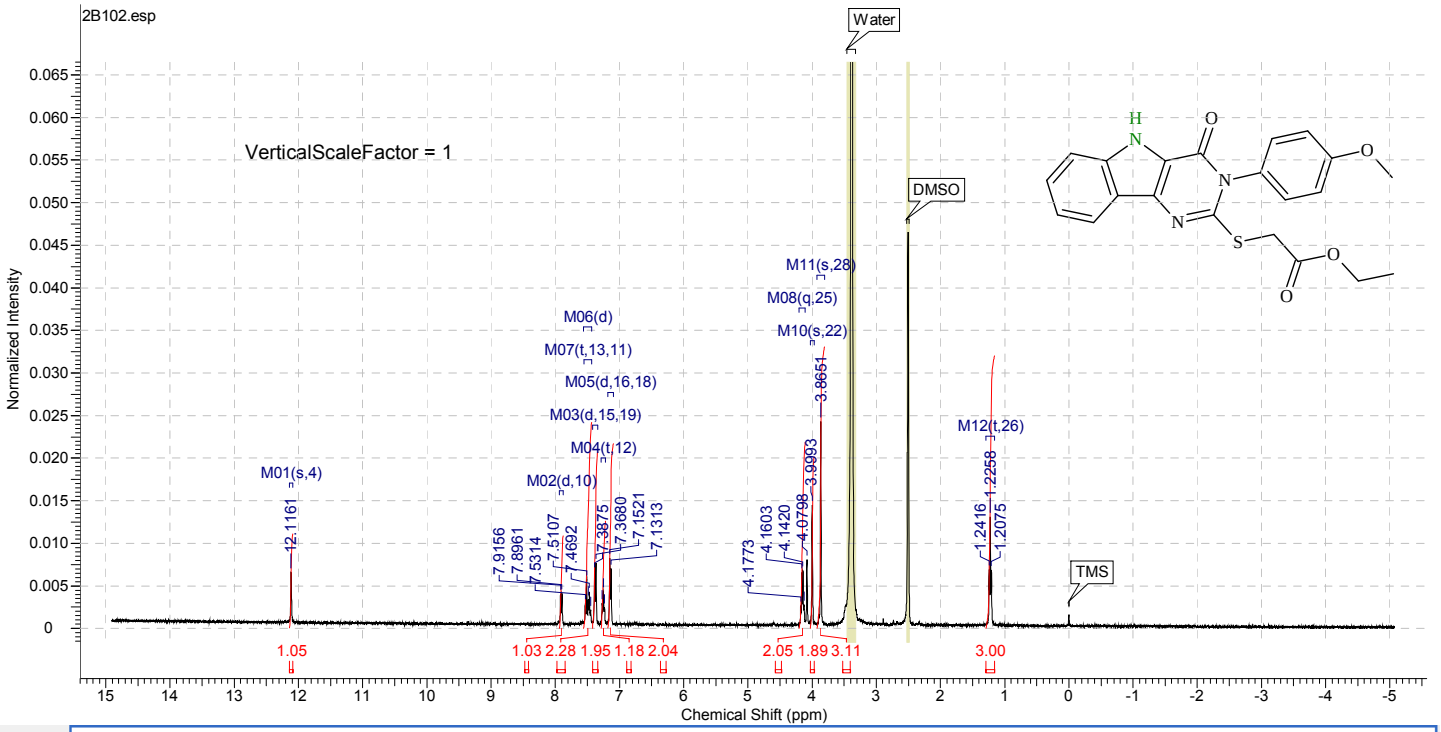
Exact Mass: 396.1

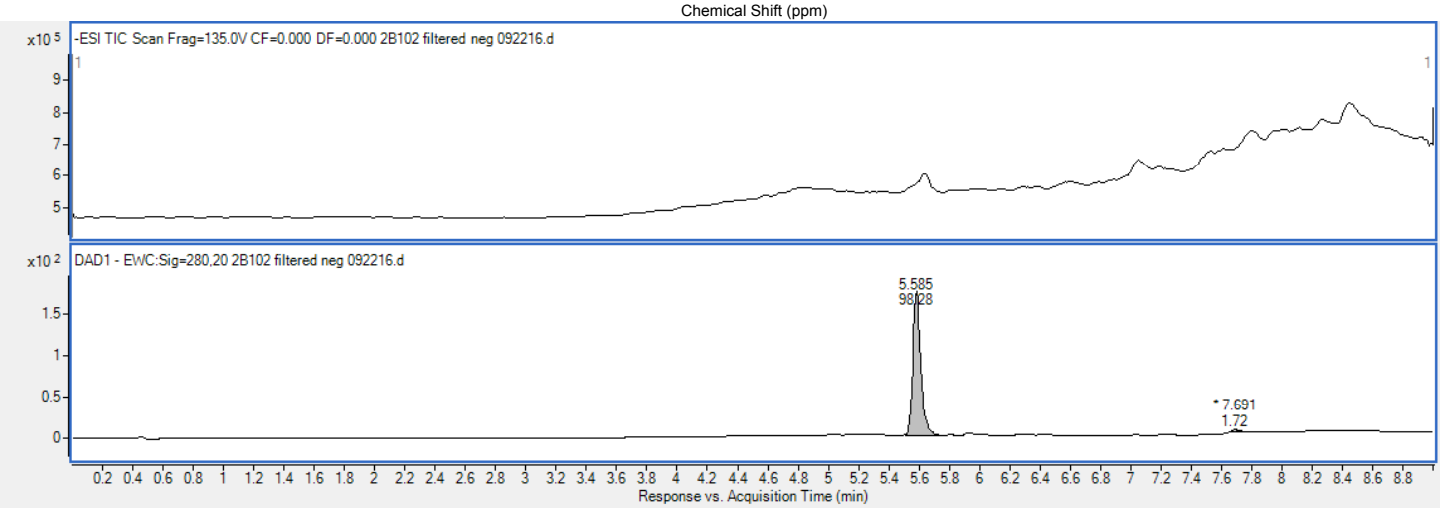
^{1}H NMR, LC-MS **6**{2,2}

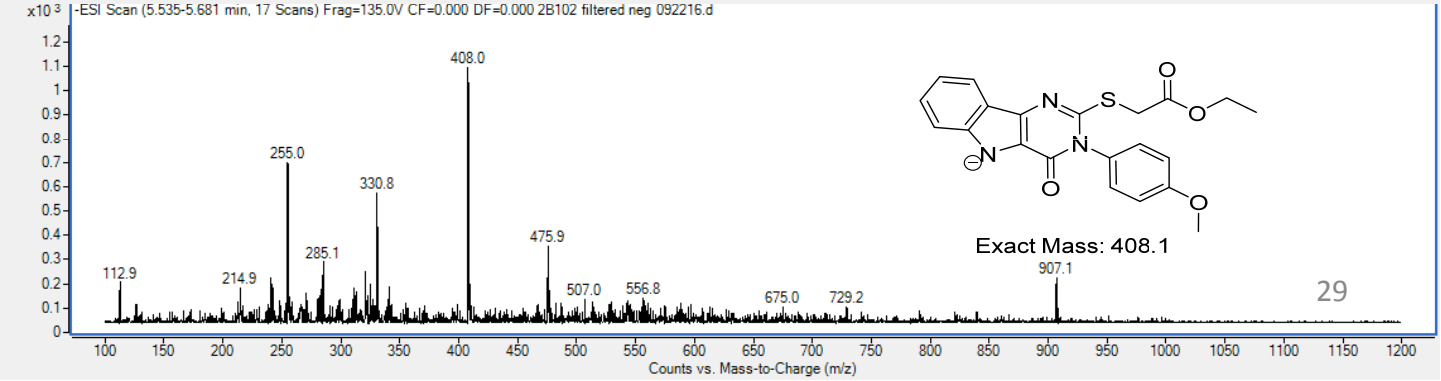
4/19/2017 10:30:04 AM

Acquisition Time (sec)	2.0292	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B102.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16221
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	14.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1967.0524	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.12 (s, 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.47 (t, *J* = 7.60 Hz, 1H), 7.52 (d, *J* = 8.30 Hz, 1H), 7.38 (d, *J* = 7.81 Hz, 2H), 7.25 (t, *J* = 6.80 Hz, 1H), 7.14 (d, *J* = 8.29 Hz, 2H), 4.15 (q, *J* = 6.83 Hz, 2H), 4.00 (s, 2H), 3.87 (s, 3H), 1.22 (t, *J* = 6.83 Hz, 3H)





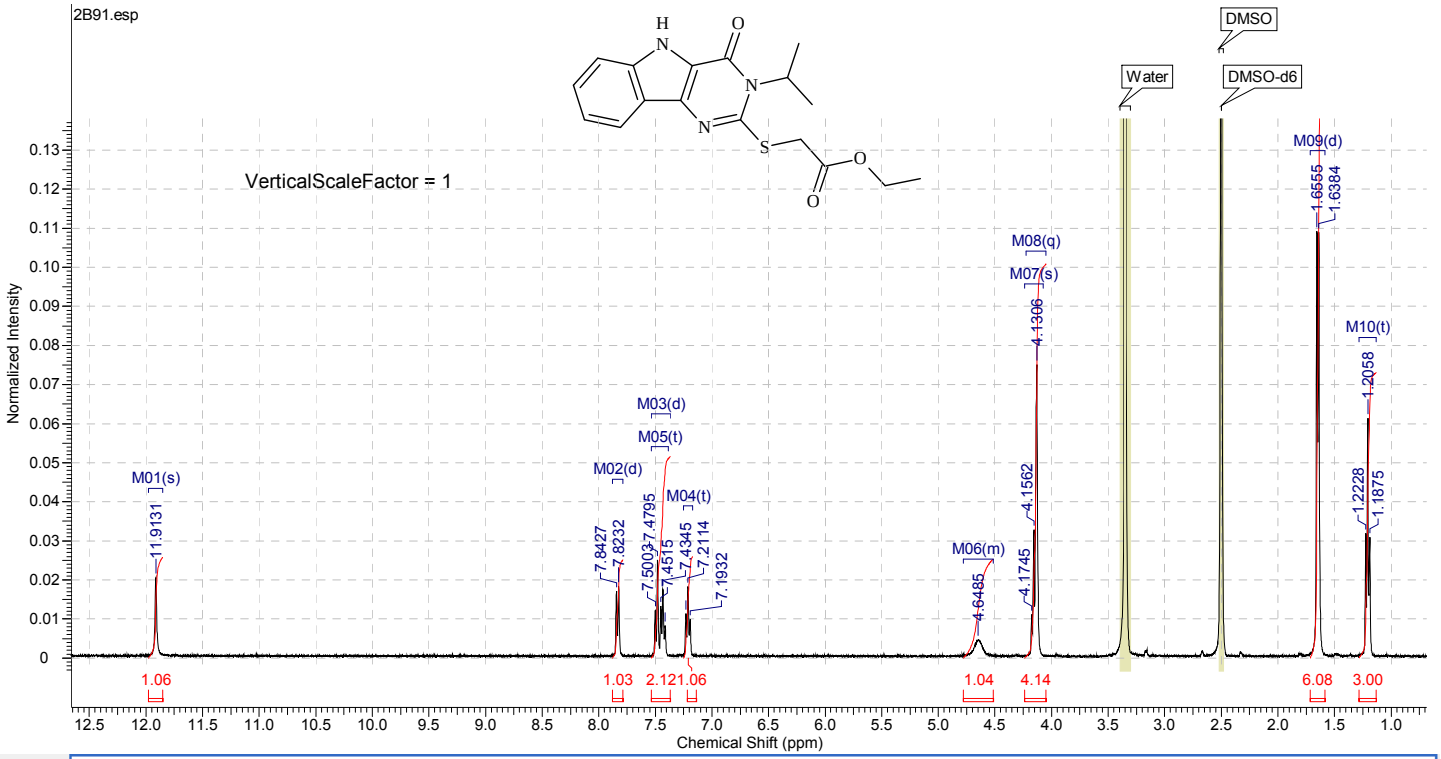


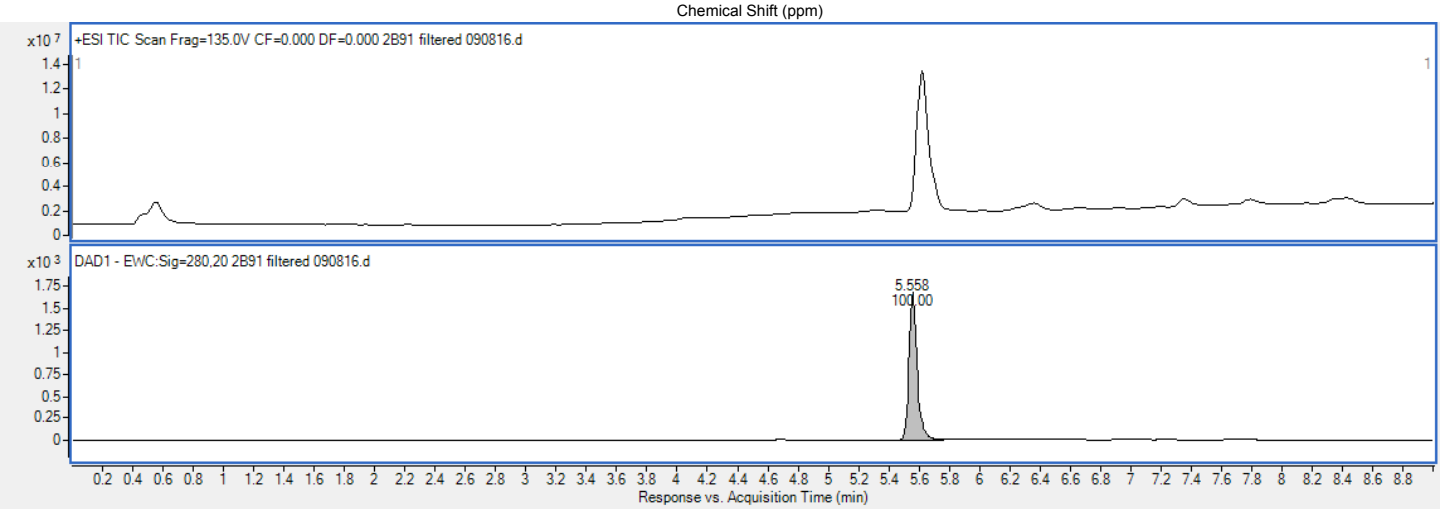
^{1}H NMR, LC-MS **6**{3,2}

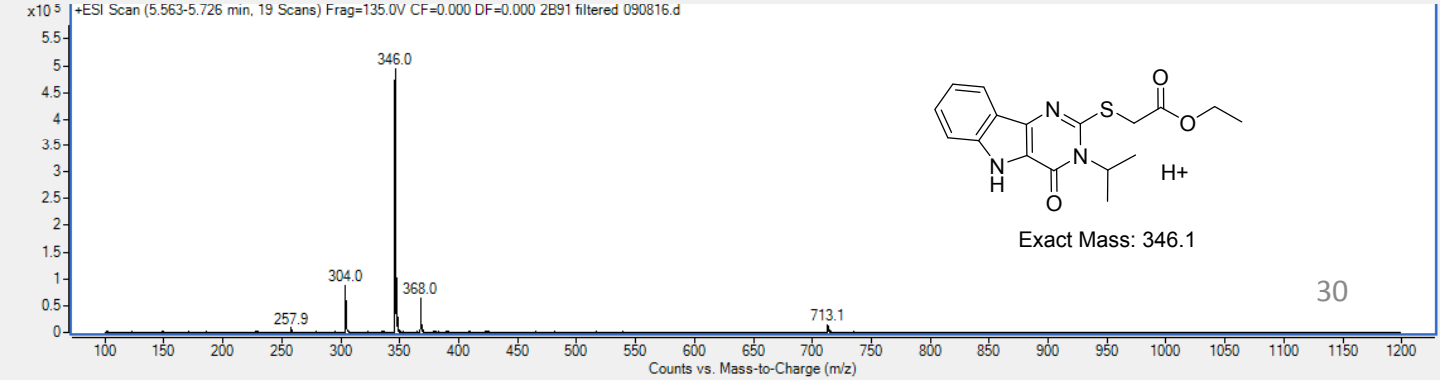
4/19/2017 10:46:23 AM

Acquisition Time (sec)	2.0016	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B91.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	15987
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1965.1851	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7987.22	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.91 (s, 1H), 7.83 (d, *J* = 7.80 Hz, 1H), 7.43 (t, *J* = 7.60 Hz, 1H), 7.49 (d, *J* = 8.30 Hz, 1H), 7.21 (t, *J* = 7.56 Hz, 1H), 4.52 - 4.78 (m, 1H), 4.13 (s, 2H), 4.14 (q, *J* = 7.30 Hz, 2H), 1.65 (d, *J* = 6.83 Hz, 6H), 1.21 (t, *J* = 7.07 Hz, 3H)







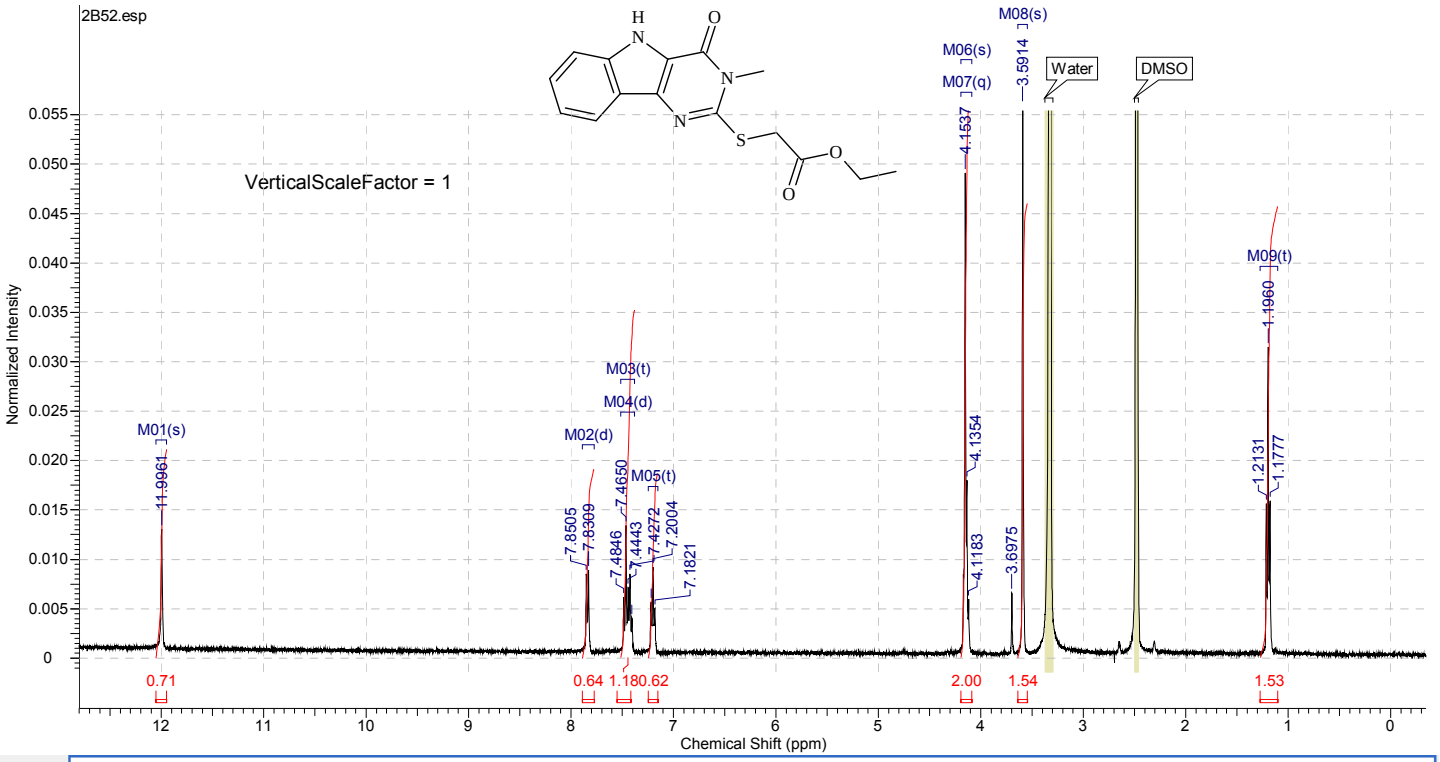
Exact Mass: 346.1

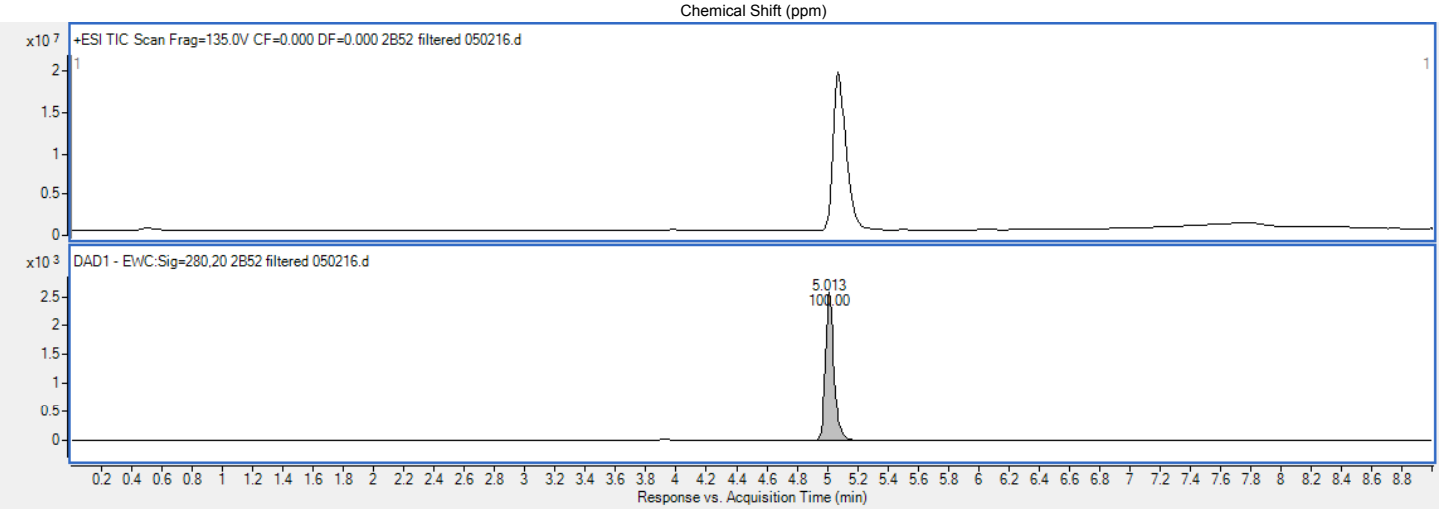
^{1}H NMR, LC-MS **6**{4,2}

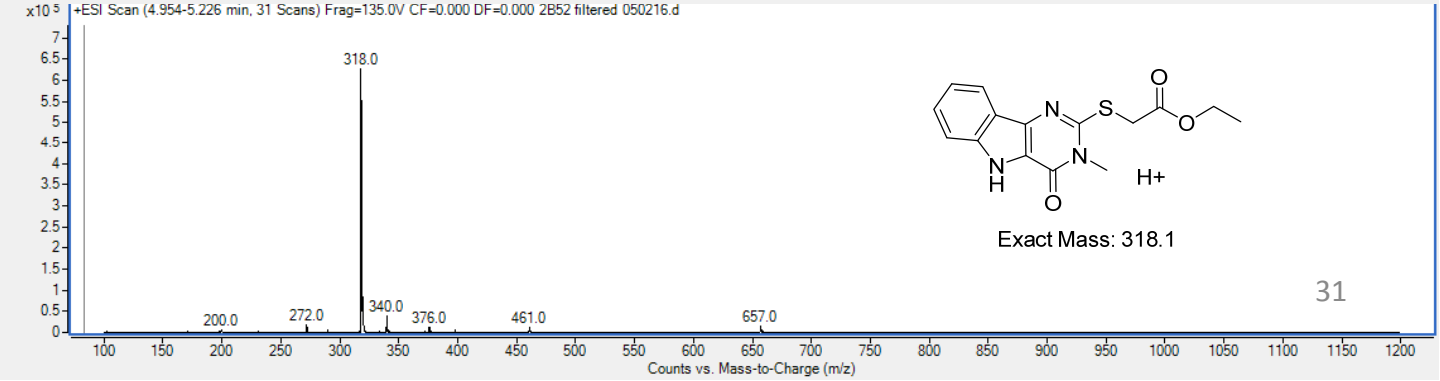
4/19/2017 11:03:45 AM

Acquisition Time (sec)	2.0032	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B52.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16013
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1956.6102	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.84 (d, *J* = 7.81 Hz, 1H), 7.46 (t, *J* = 8.30 Hz, 1H), 7.42 (d, *J* = 8.30 Hz, 1H), 7.20 (t, *J* = 7.60 Hz, 1H), 4.15 (s, 2H), 4.14 (q, *J* = 7.10 Hz, 2H), 3.59 (s, 3H), 1.20 (t, *J* = 7.07 Hz, 3H)







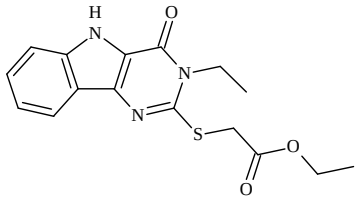
Exact Mass: 318.1

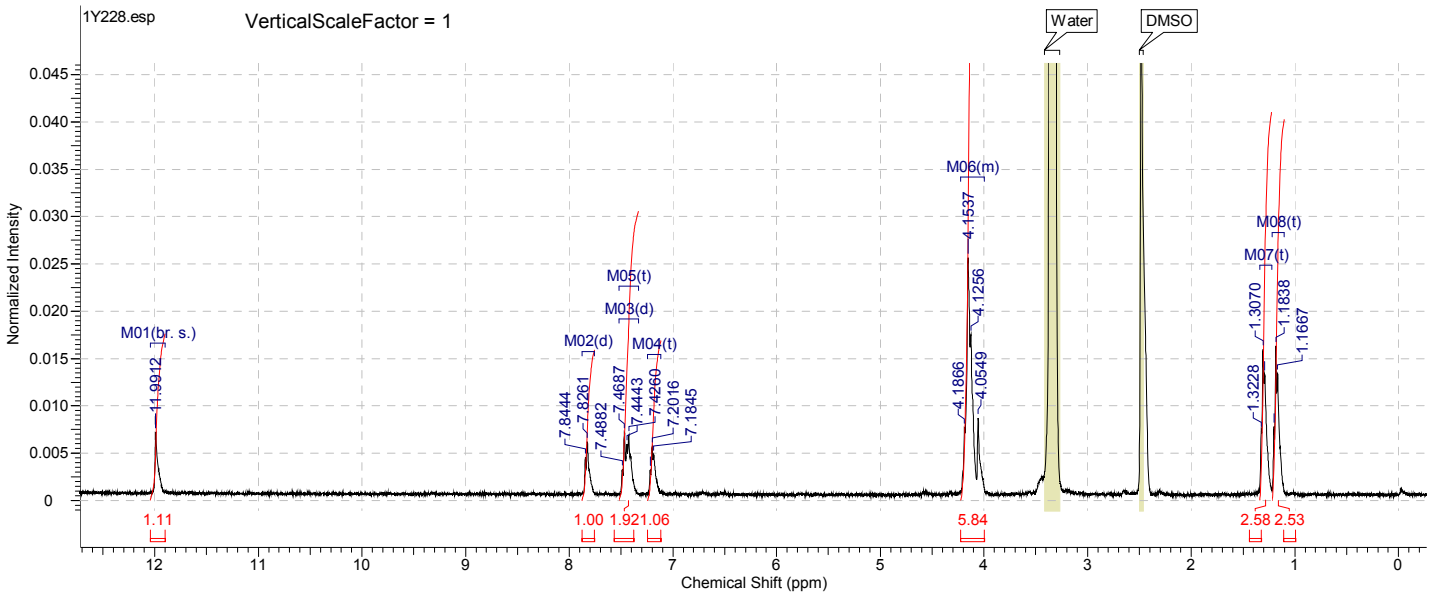
^{1}H NMR, LC-MS **6**{5,2}

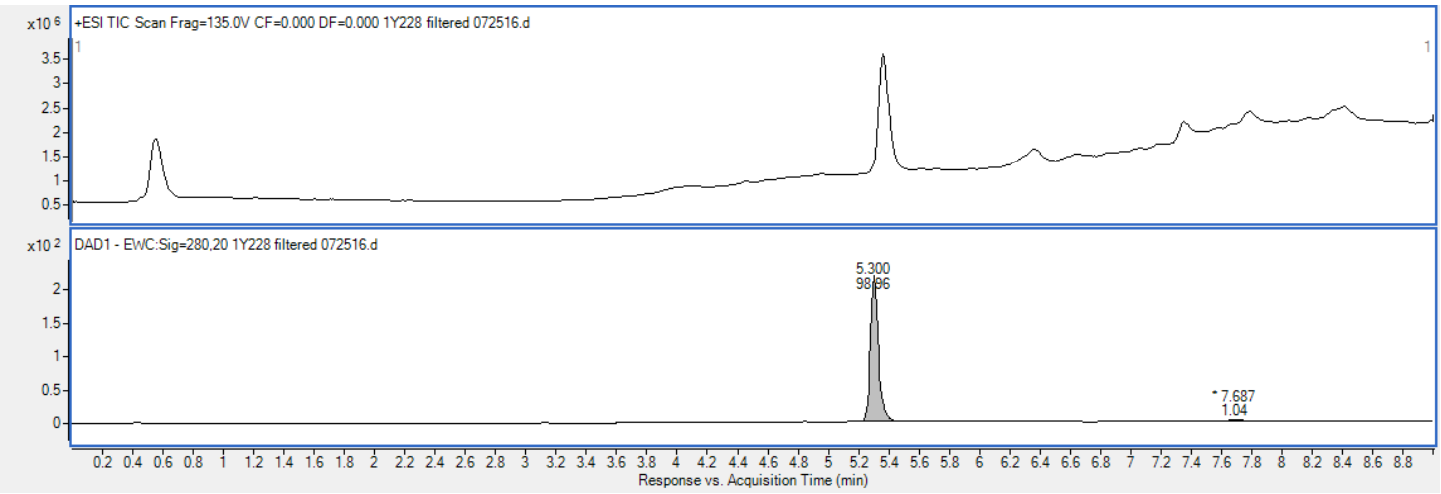
4/19/2017 11:22:14 AM

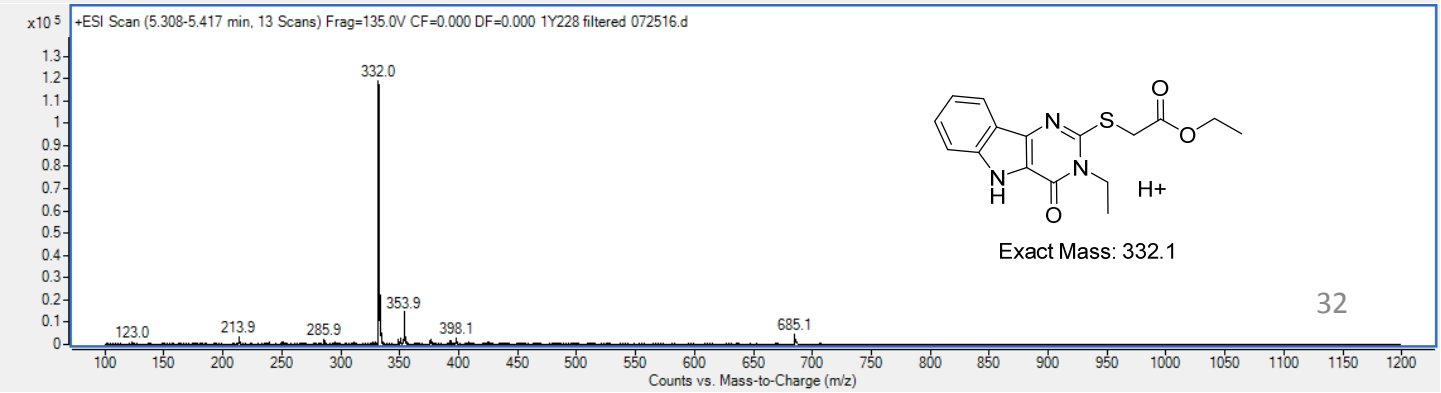
Acquisition Time (sec)	2.0341	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\1Y228.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16260
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	16.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1956.6102	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.99 (br. s., 1H), 7.84 (d, *J* = 7.32 Hz, 1H), 7.43 (t, *J* = 7.30 Hz, 1H), 7.48 (d, *J* = 8.29 Hz, 1H), 7.20 (t, *J* = 6.80 Hz, 1H), 4.00 - 4.22 (m, 6H), 1.31 (t, *J* = 7.30 Hz, 3H), 1.18 (t, *J* = 6.80 Hz, 3H)









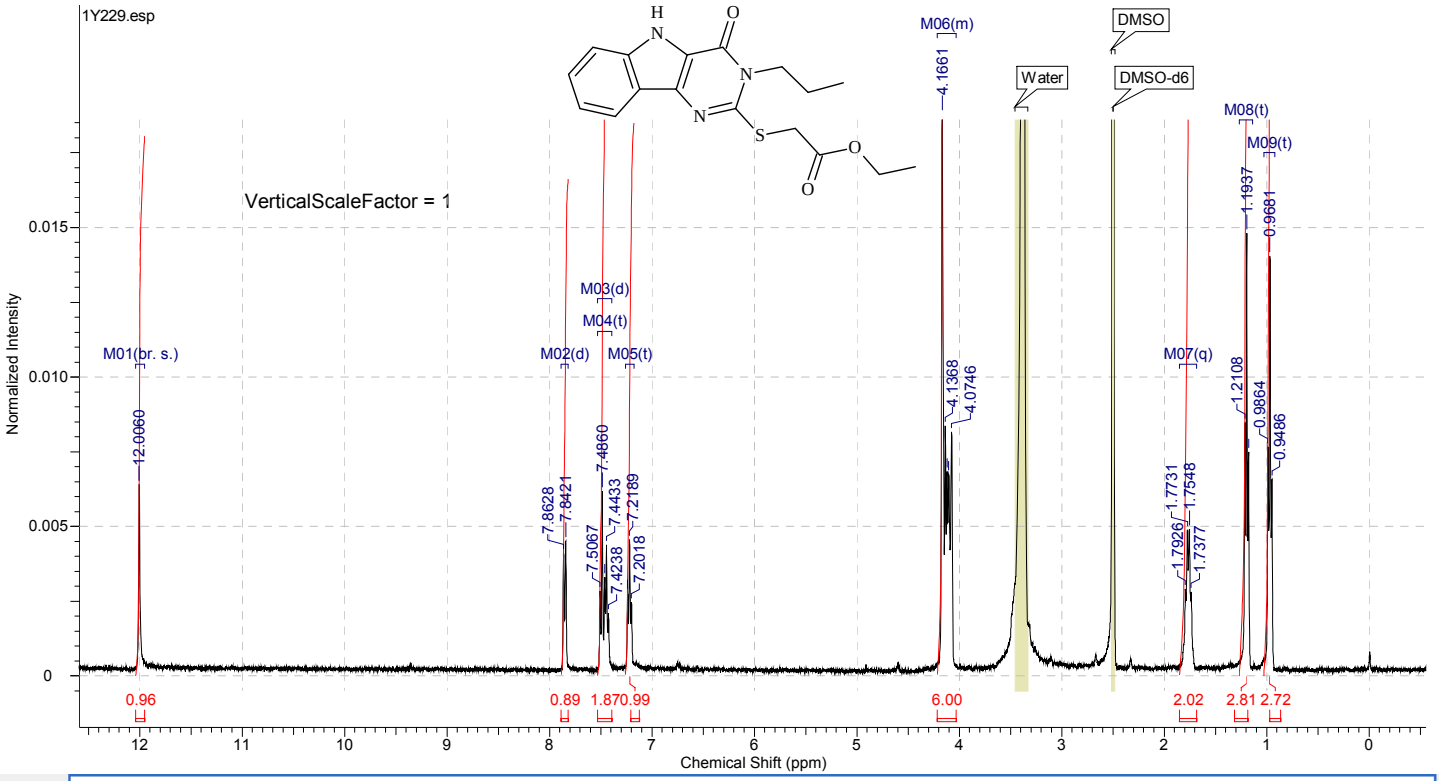
Exact Mass: 332.1

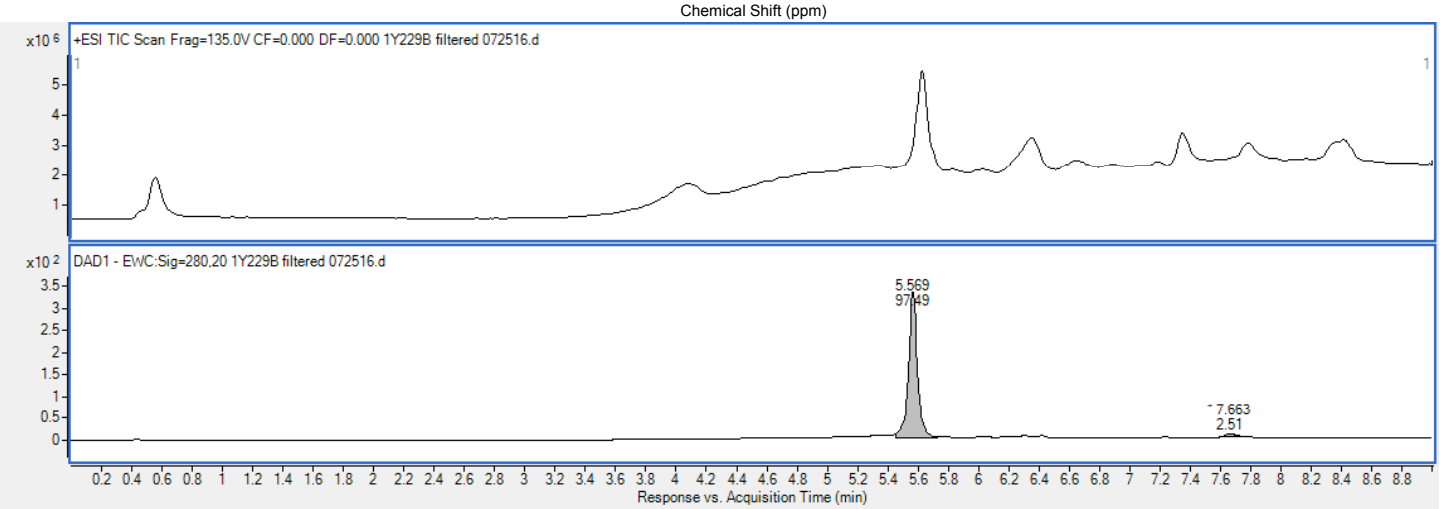
^{1}H NMR, LC-MS **6**{6,2}

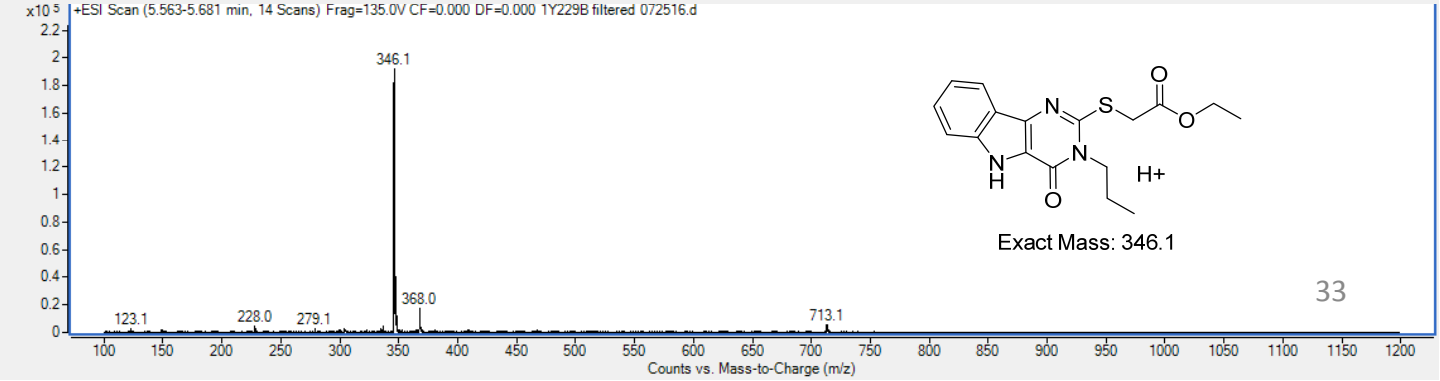
4/19/2017 2:49:23 PM

Acquisition Time (sec)	2.0325	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\1Y229.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16247
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	16.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1964.4928	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.01 (br. s., 1H), 7.85 (d, *J* = 8.29 Hz, 1H), 7.50 (d, *J* = 8.30 Hz, 1H), 7.44 (t, *J* = 7.80 Hz, 1H), 7.22 (t, *J* = 7.07 Hz, 1H), 4.03 - 4.21 (m, 6H), 1.76 (q, *J* = 7.30 Hz, 2H), 1.19 (t, *J* = 7.07 Hz, 1H), 0.97 (t, *J* = 7.56 Hz, 3H)







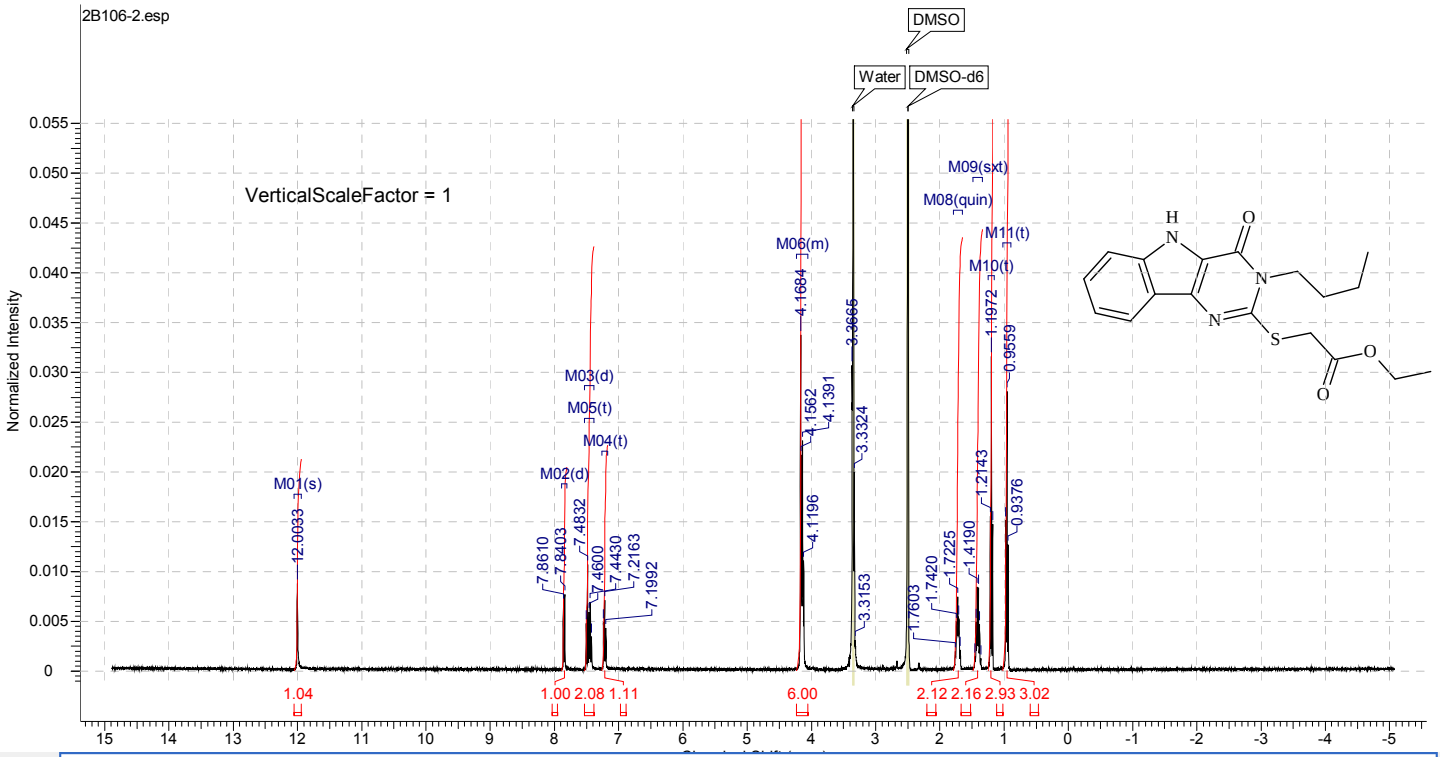
Exact Mass: 346.1

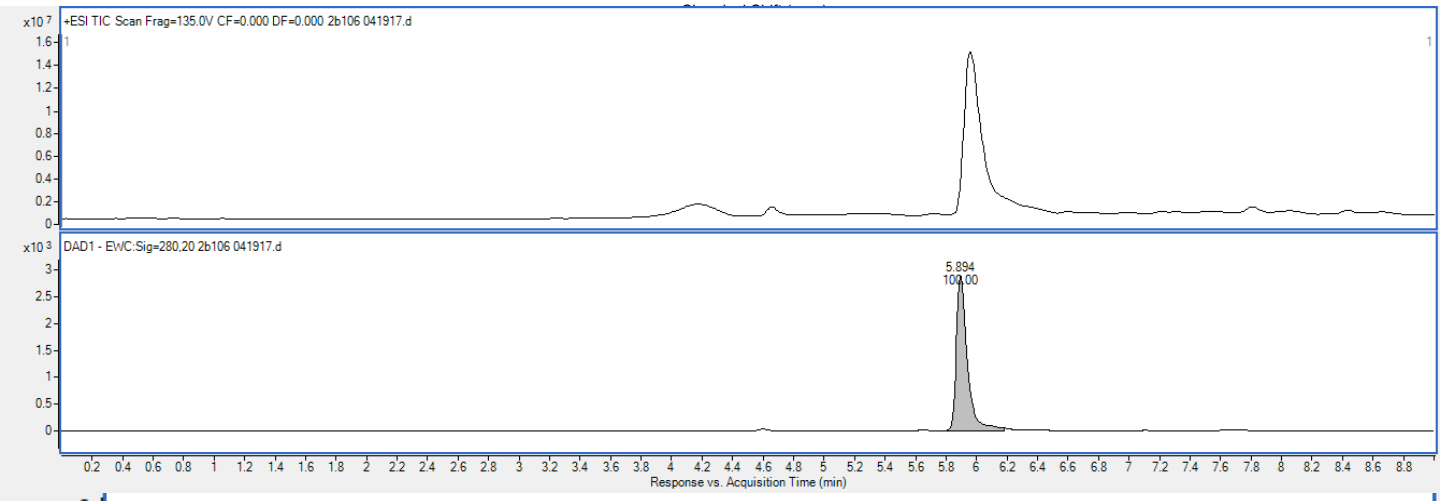
^{1}H NMR, LC-MS **6**{7,2}

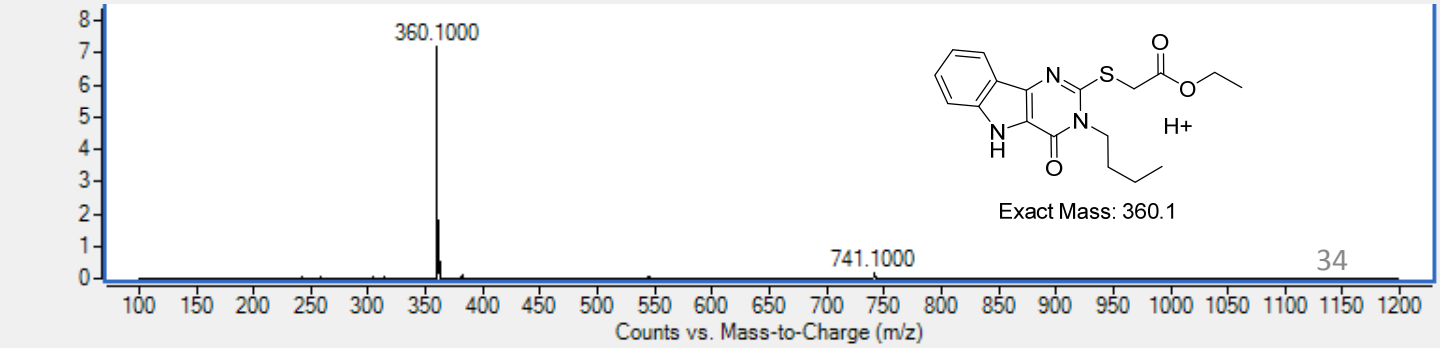
4/19/2017 3:01:50 PM

Acquisition Time (sec)	1.9983	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B106-2.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	15961
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1963.7225	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7987.22	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.85 (d, *J* = 8.29 Hz, 1H), 7.49 (d, *J* = 8.30 Hz, 1H), 7.44 (t, *J* = 8.30 Hz, 1H), 7.22 (t, *J* = 7.56 Hz, 1H), 4.06 - 4.23 (m, 6H), 1.72 (quin, *J* = 7.56 Hz, 2H), 1.41 (sxt, *J* = 7.41 Hz, 2H), 1.20 (t, *J* = 7.07 Hz, 3H), 0.96 (t, *J* = 7.31 Hz, 3H)





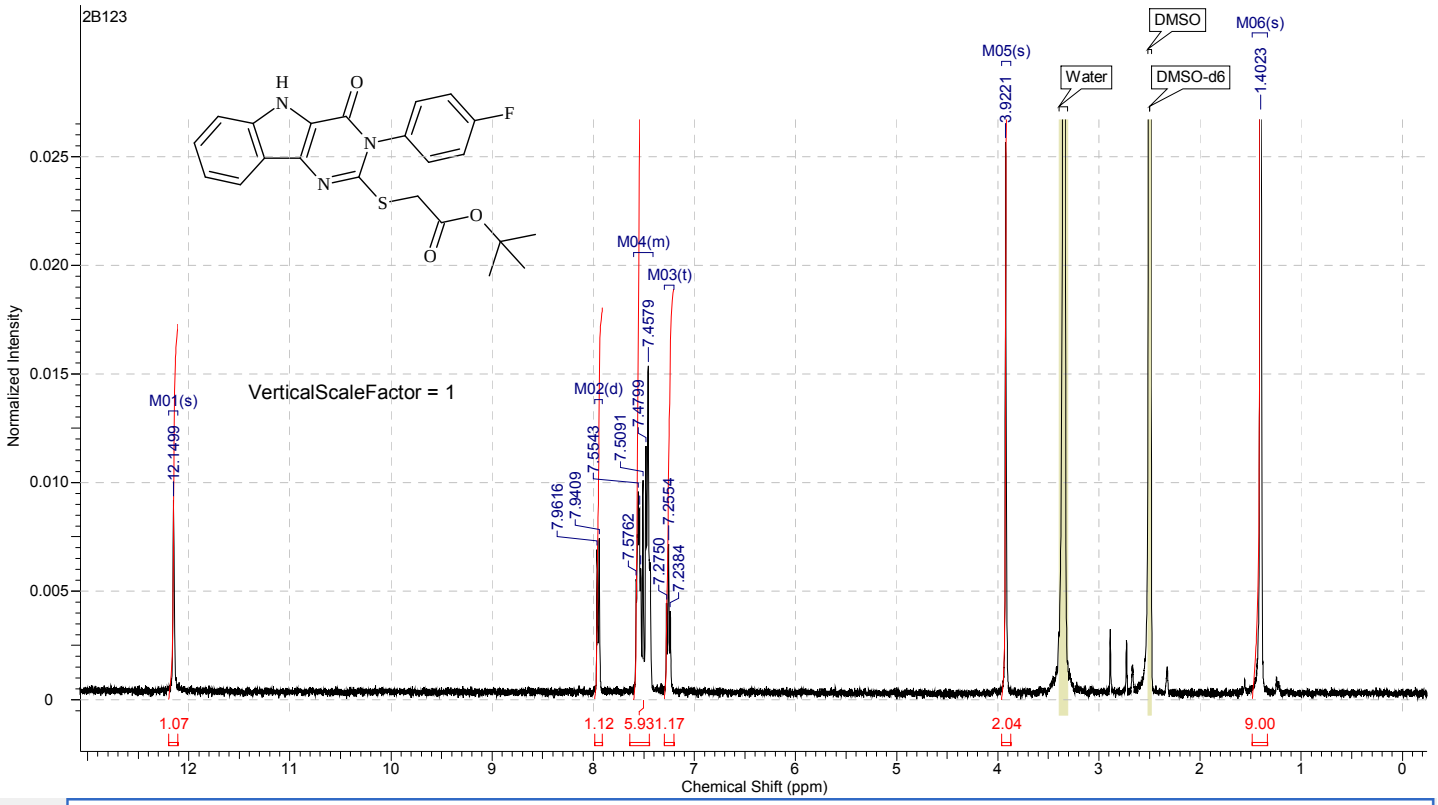


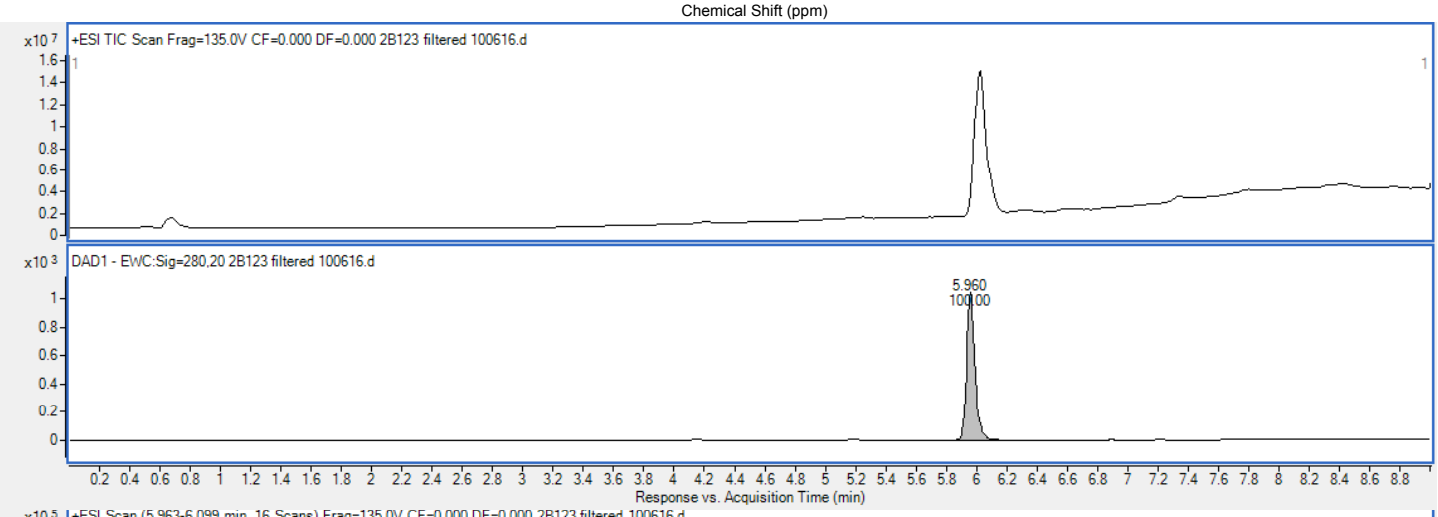
^{1}H NMR, LC-MS **6**{1,3}

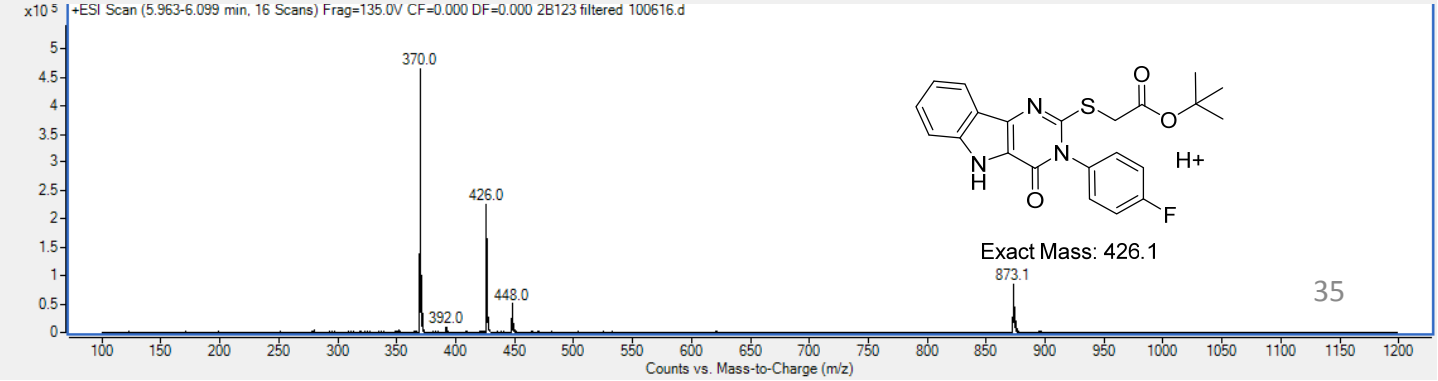
4/19/2017 4:06:17 PM

Acquisition Time (sec)	2.0097	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B123.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16065
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1964.4928	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.15 (s, 1H), 7.95 (d, *J* = 8.29 Hz, 1H), 7.41 - 7.60 (m, 6H), 7.26 (t, *J* = 7.32 Hz, 1H), 3.92 (s, 2H), 1.40 (s, 9H)





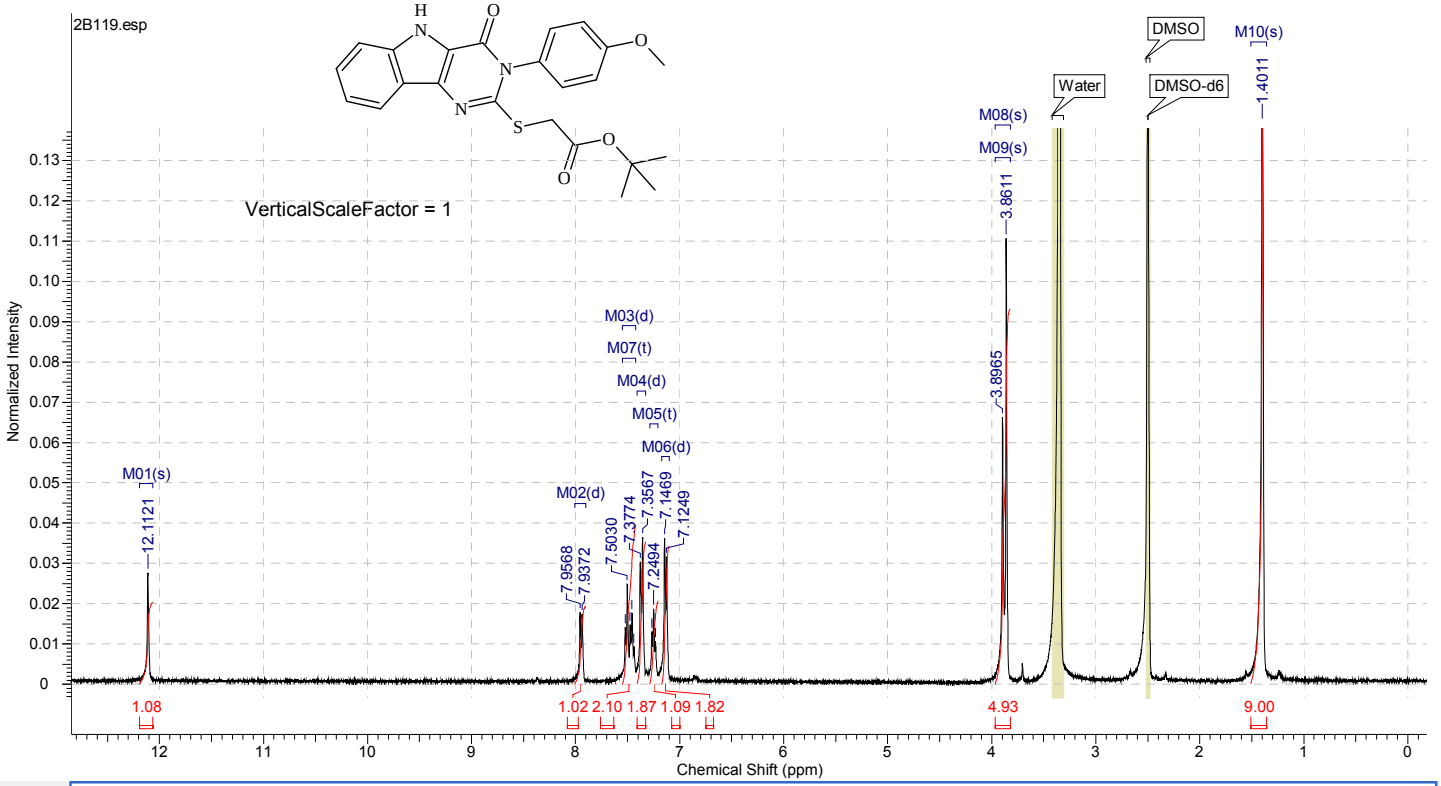


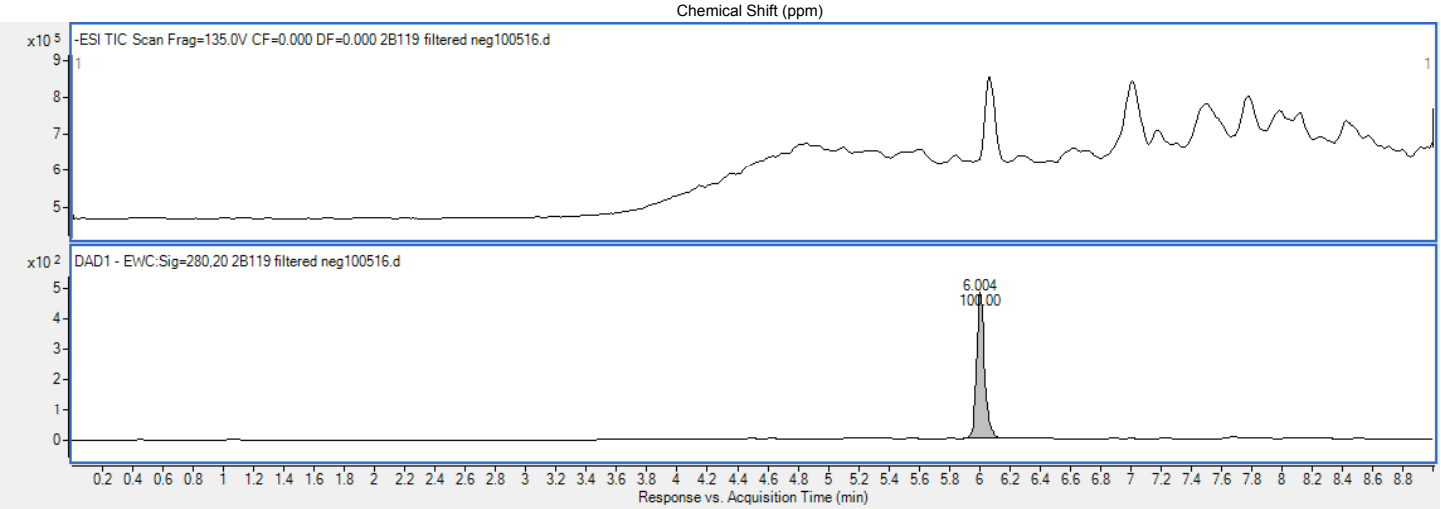
^{1}H NMR, LC-MS **6**{2,3}

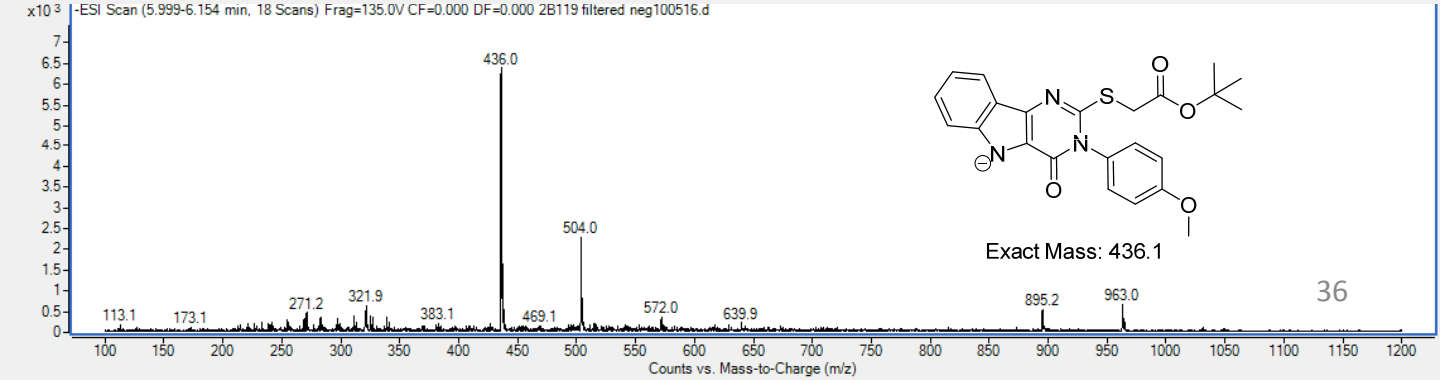
4/20/2017 1:55:15 PM

Acquisition Time (sec)	2.0146	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B119.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16104
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1964.9807	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.11 (s, 1H), 7.95 (d, *J* = 7.81 Hz, 1H), 7.51 (d, *J* = 8.29 Hz, 1H), 7.46 (t, *J* = 7.30 Hz, 1H), 7.37 (d, *J* = 8.29 Hz, 2H), 7.25 (t, *J* = 7.07 Hz, 1H), 7.14 (d, *J* = 8.78 Hz, 2H), 3.90 (s, 2H), 3.86 (s, 3H), 1.40 (s, 9H)







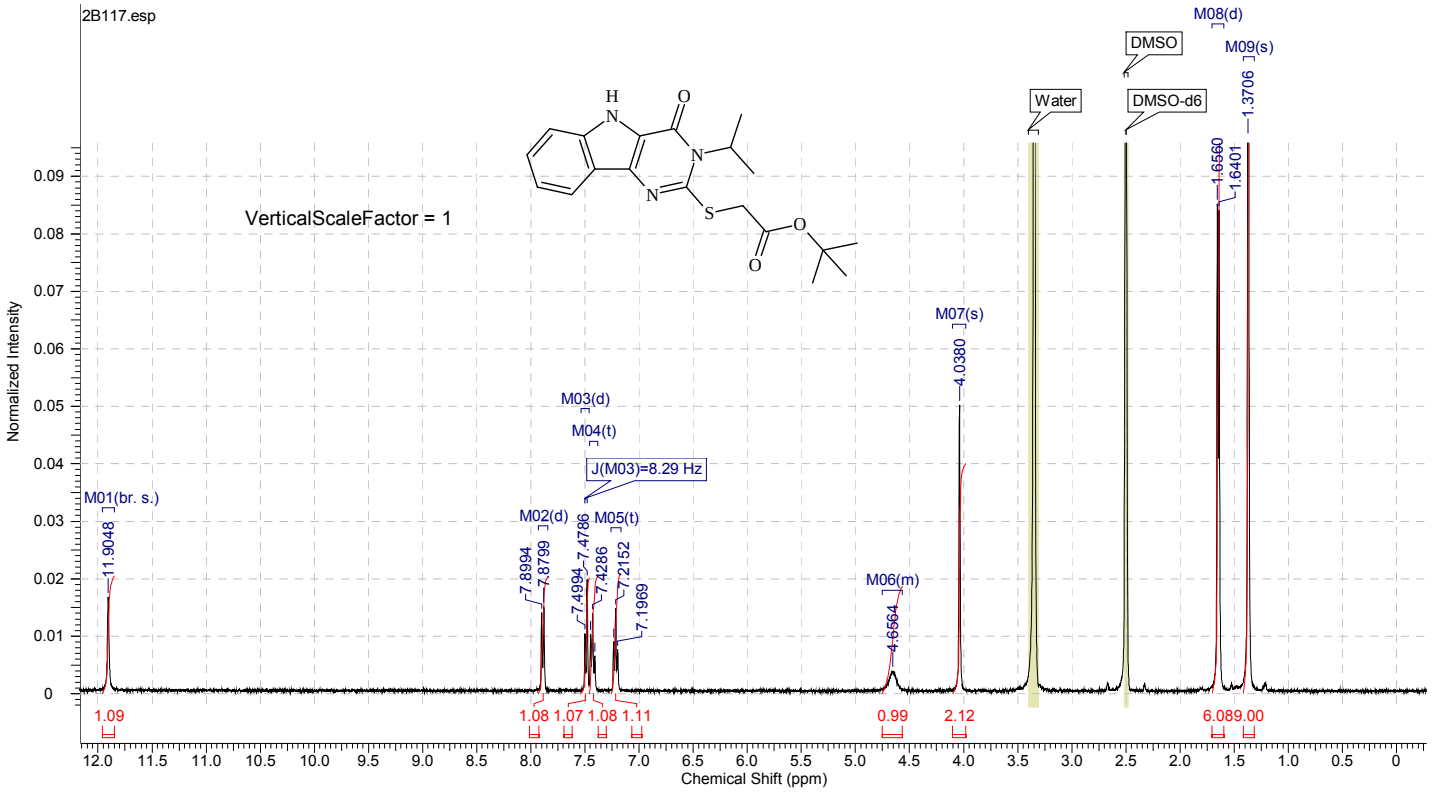
Exact Mass: 436.1

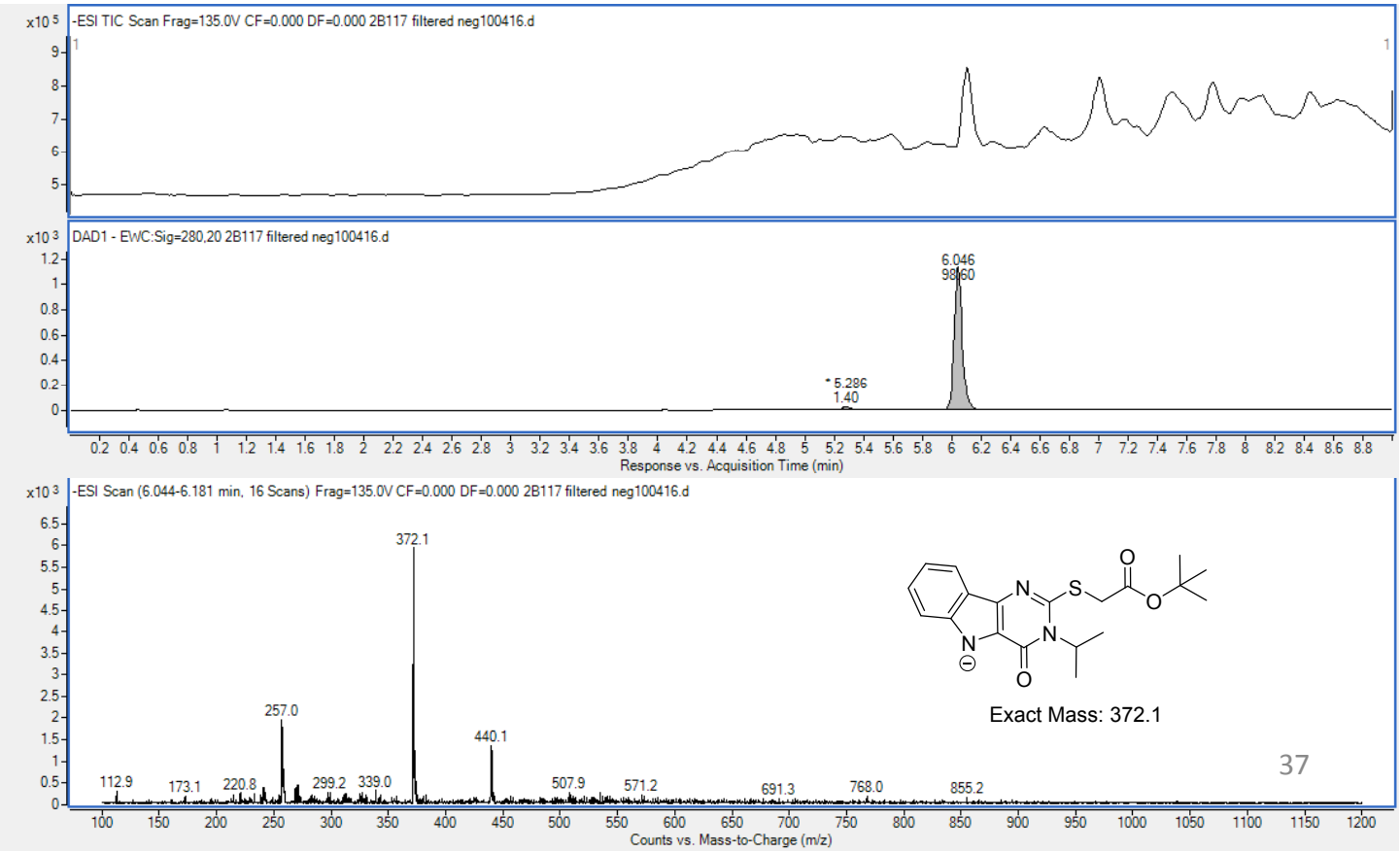
^{1}H NMR, LC-MS **6**{3,3}

4/19/2017 4:11:38 PM

Acquisition Time (sec)	2.0227	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B117.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16169
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1964.9807	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.90 (br. s., 1H), 7.89 (d, *J* = 7.81 Hz, 1H), 7.49 (d, *J* = 8.29 Hz, 1H), 7.43 (t, *J* = 7.80 Hz, 1H), 7.22 (t, *J* = 7.32 Hz, 1H), 4.57 - 4.75 (m, 1H), 4.04 (s, 2H), 1.65 (d, *J* = 6.34 Hz, 6H), 1.37 (s, 9H)





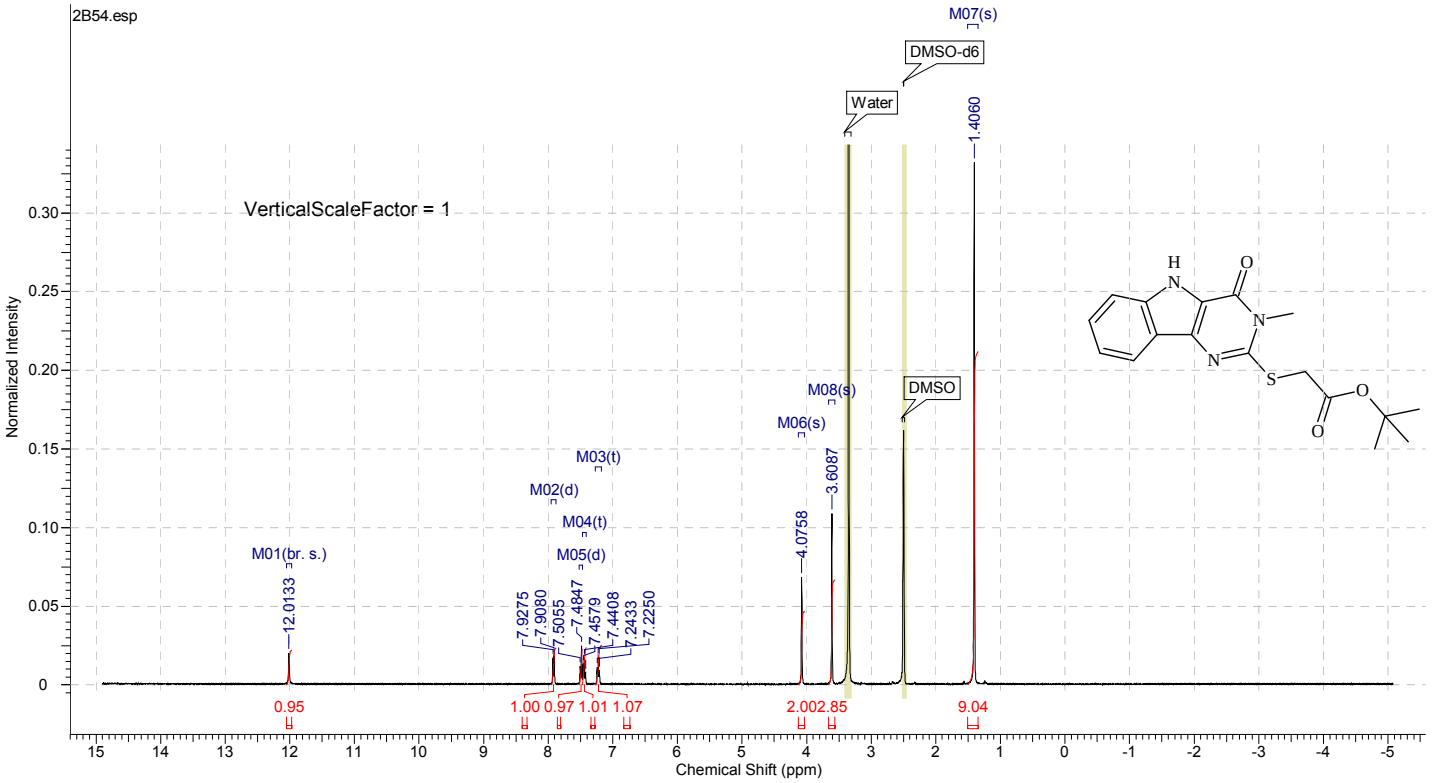
Exact Mass: 372.1

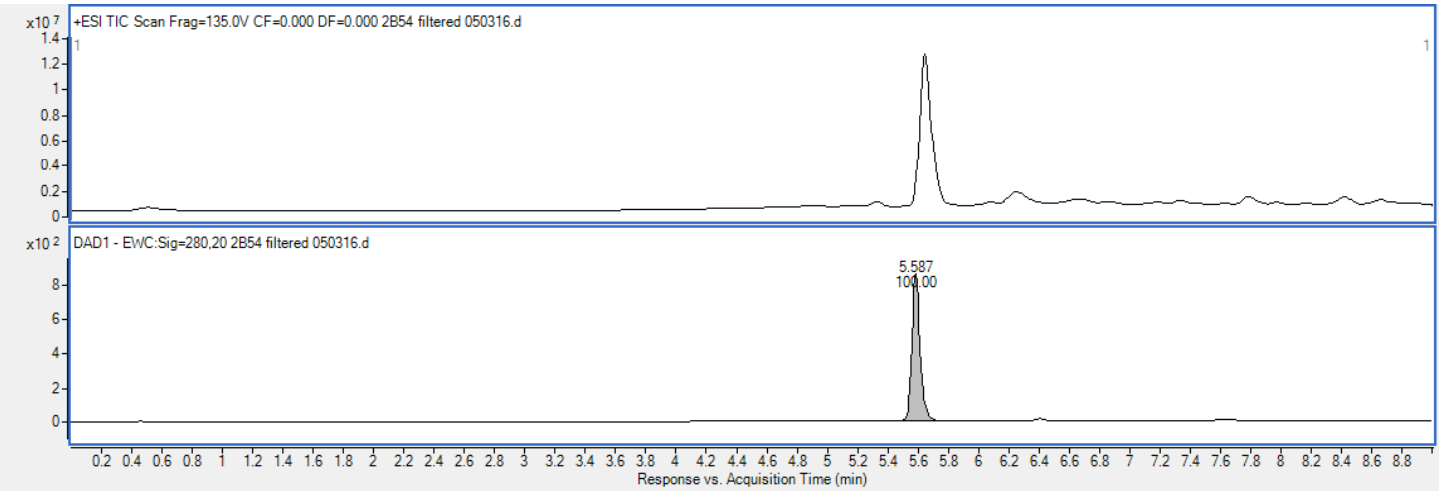
^{1}H NMR, LC-MS **6**{4,3}

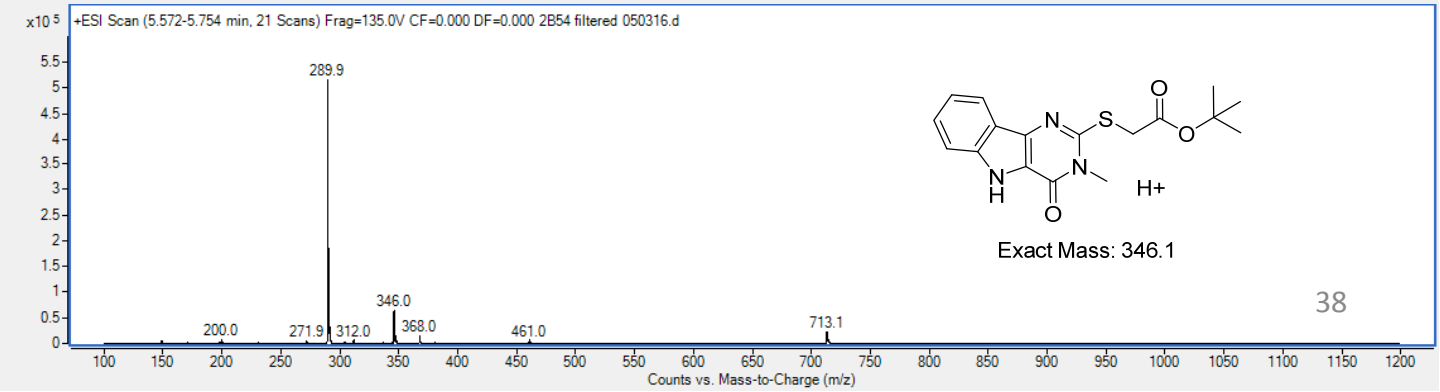
4/20/2017 9:50:55 AM

Acquisition Time (sec)	2.0179	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B54.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16130
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1964.4928	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.01 (br. s., 1H), 7.92 (d, *J* = 7.81 Hz, 1H), 7.49 (d, *J* = 8.30 Hz, 1H), 7.44 (t, *J* = 7.80 Hz, 1H), 7.22 (t, *J* = 7.32 Hz, 1H), 4.08 (s, 2H), 3.61 (s, 3H), 1.41 (s, 9H)





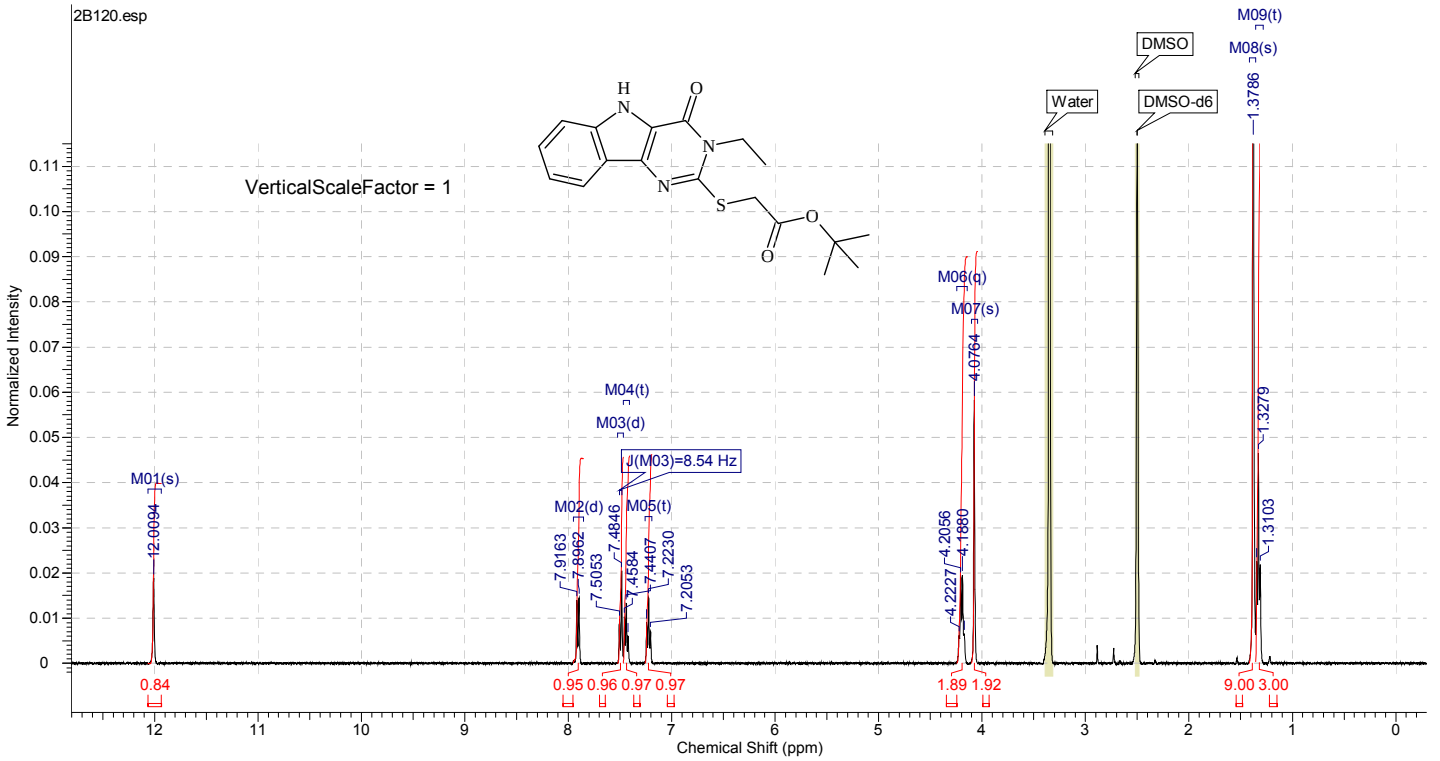


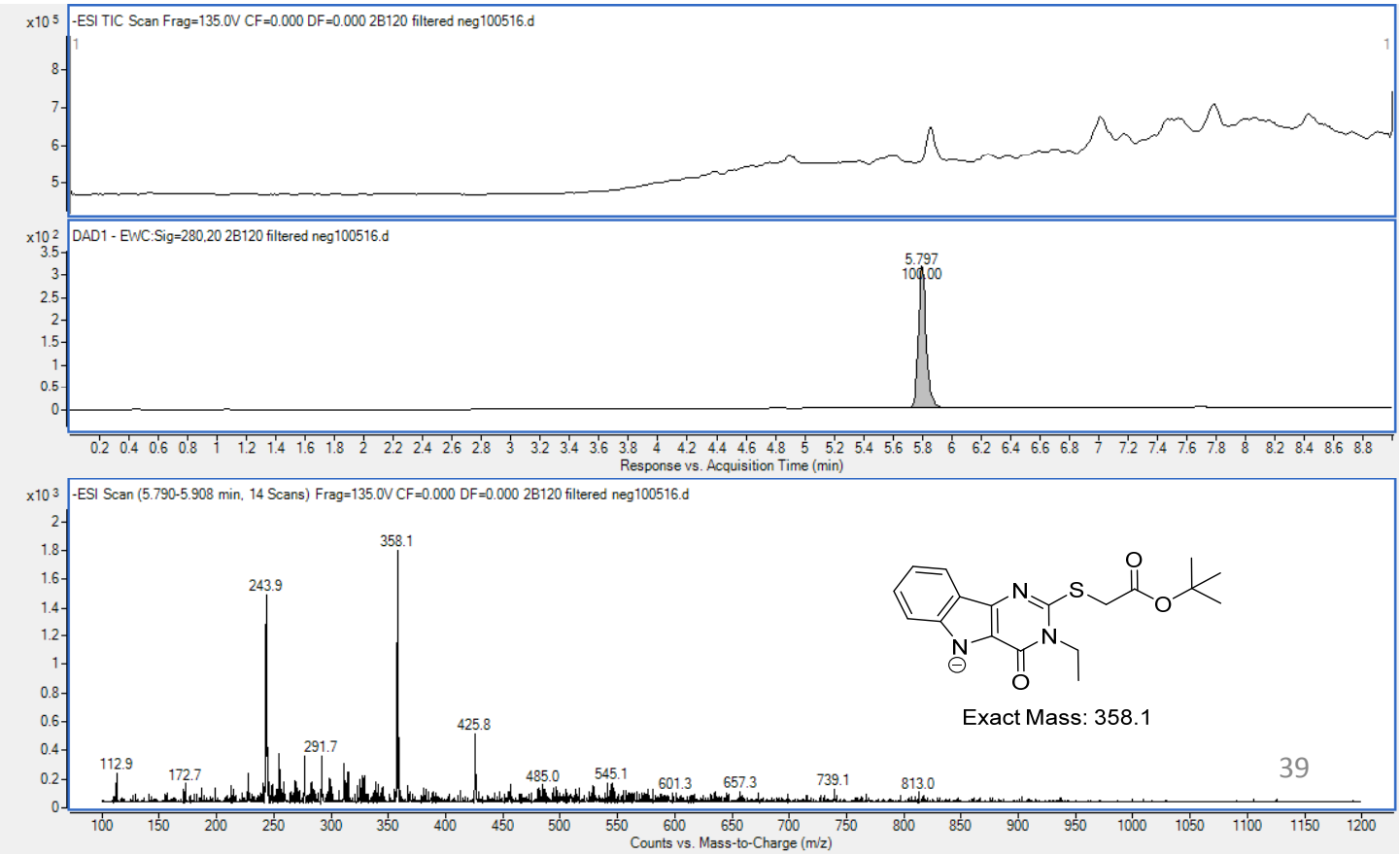
^{1}H NMR, LC-MS **6**{5,3}

4/20/2017 9:56:18 AM

Acquisition Time (sec)	2.0081	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B120.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16052
Points Count	32768	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1964.5853	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.01 (s, 1H), 7.91 (d, J = 8.05 Hz, 1H), 7.49 (d, J = 8.54 Hz, 1H), 7.44 (t, J = 7.80 Hz, 1H), 7.22 (t, J = 7.44 Hz, 1H), 4.20 (q, J = 6.83 Hz, 2H), 4.08 (s, 2H), 1.38 (s, 9H), 1.33 (t, J = 7.07 Hz, 3H)



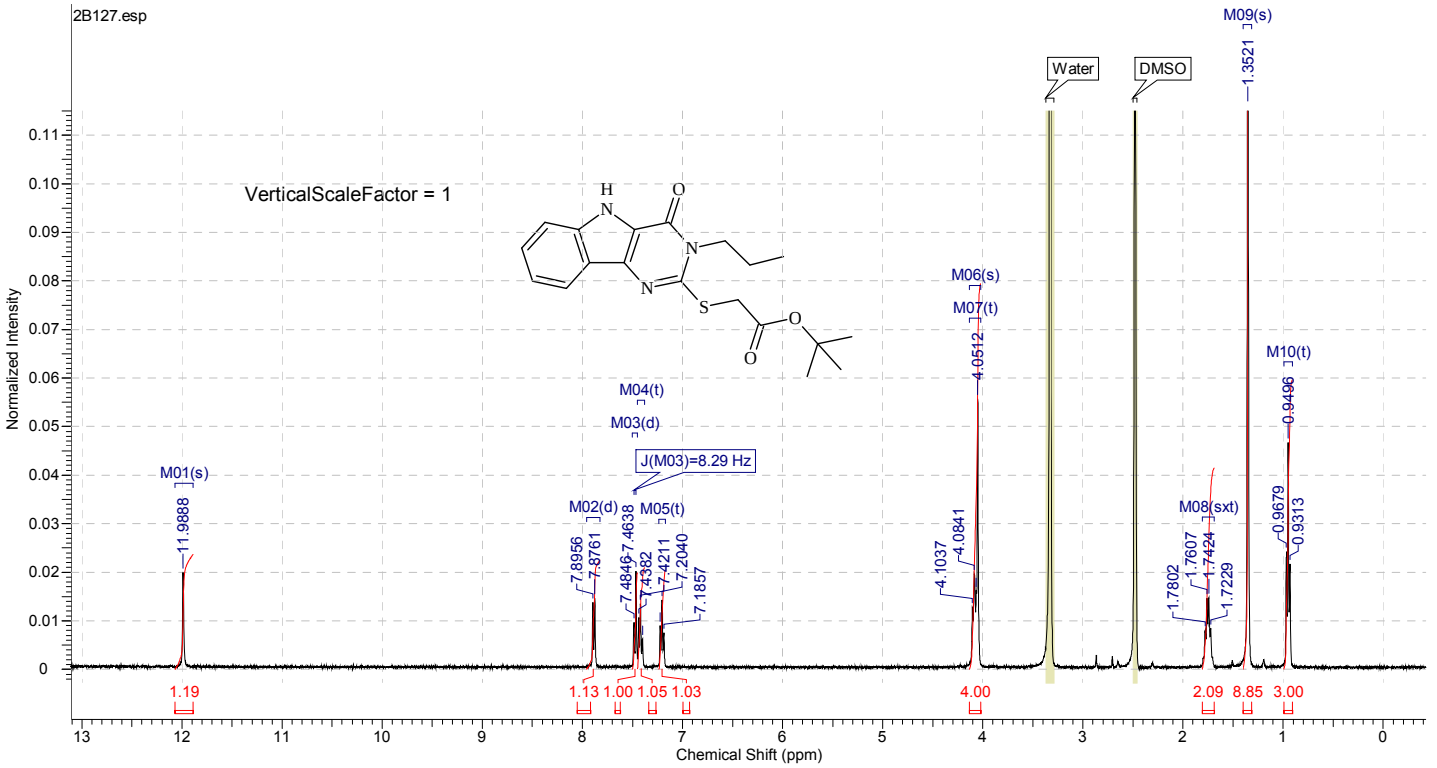


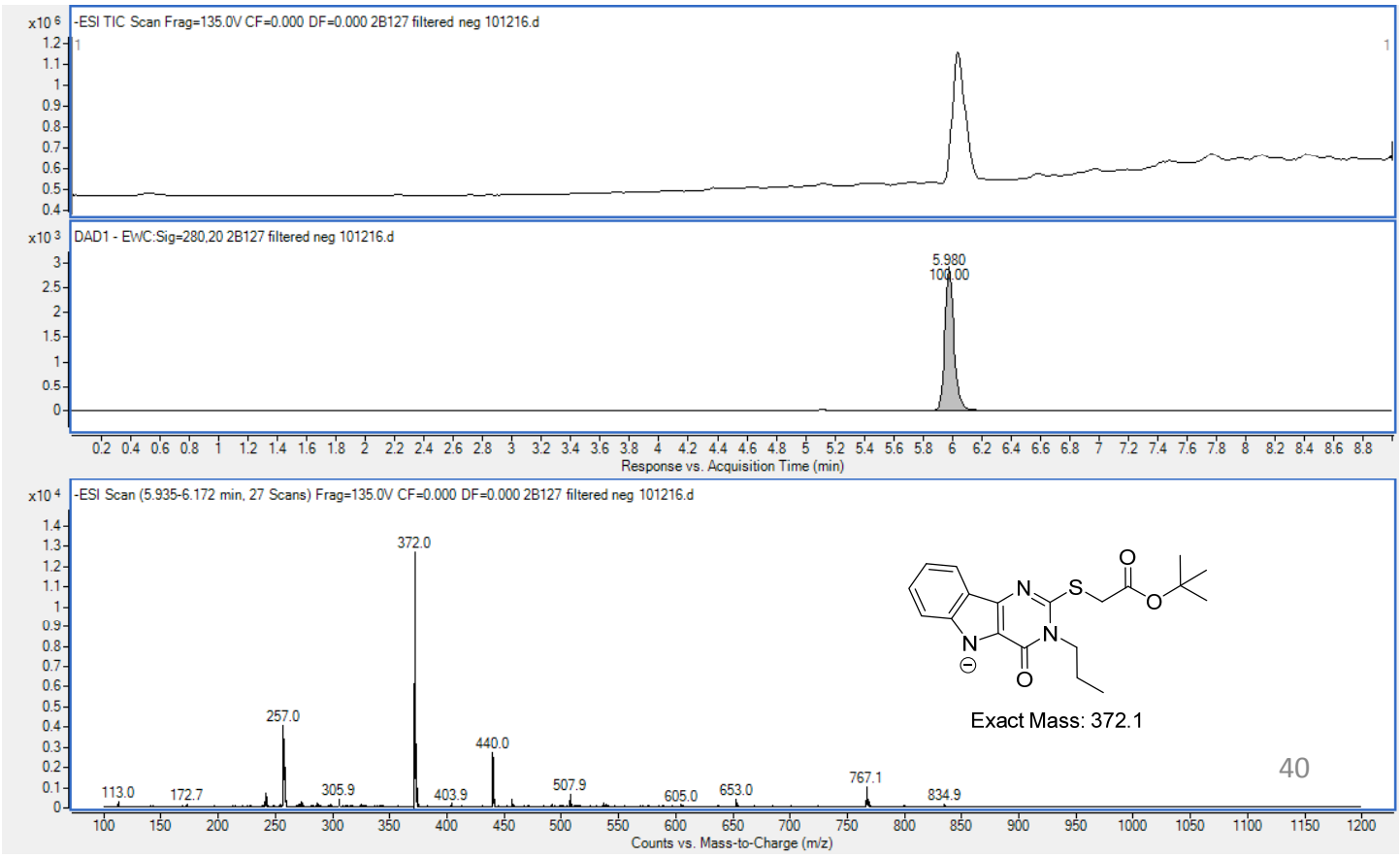
^{1}H NMR, LC-MS **6**{6,3}

4/20/2017 10:02:49 AM

Acquisition Time (sec)	2.0162	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B127.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16117
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1956.6102	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.99 (s, 1H), 7.89 (d, *J* = 7.81 Hz, 1H), 7.47 (d, *J* = 8.29 Hz, 1H), 7.42 (t, *J* = 7.80 Hz, 1H), 7.20 (t, *J* = 7.32 Hz, 1H), 4.05 (s, 2H), 4.08 (t, *J* = 7.80 Hz, 2H), 1.75 (sxt, *J* = 7.30 Hz, 2H), 1.35 (s, 9H), 0.95 (t, *J* = 7.32 Hz, 3H)



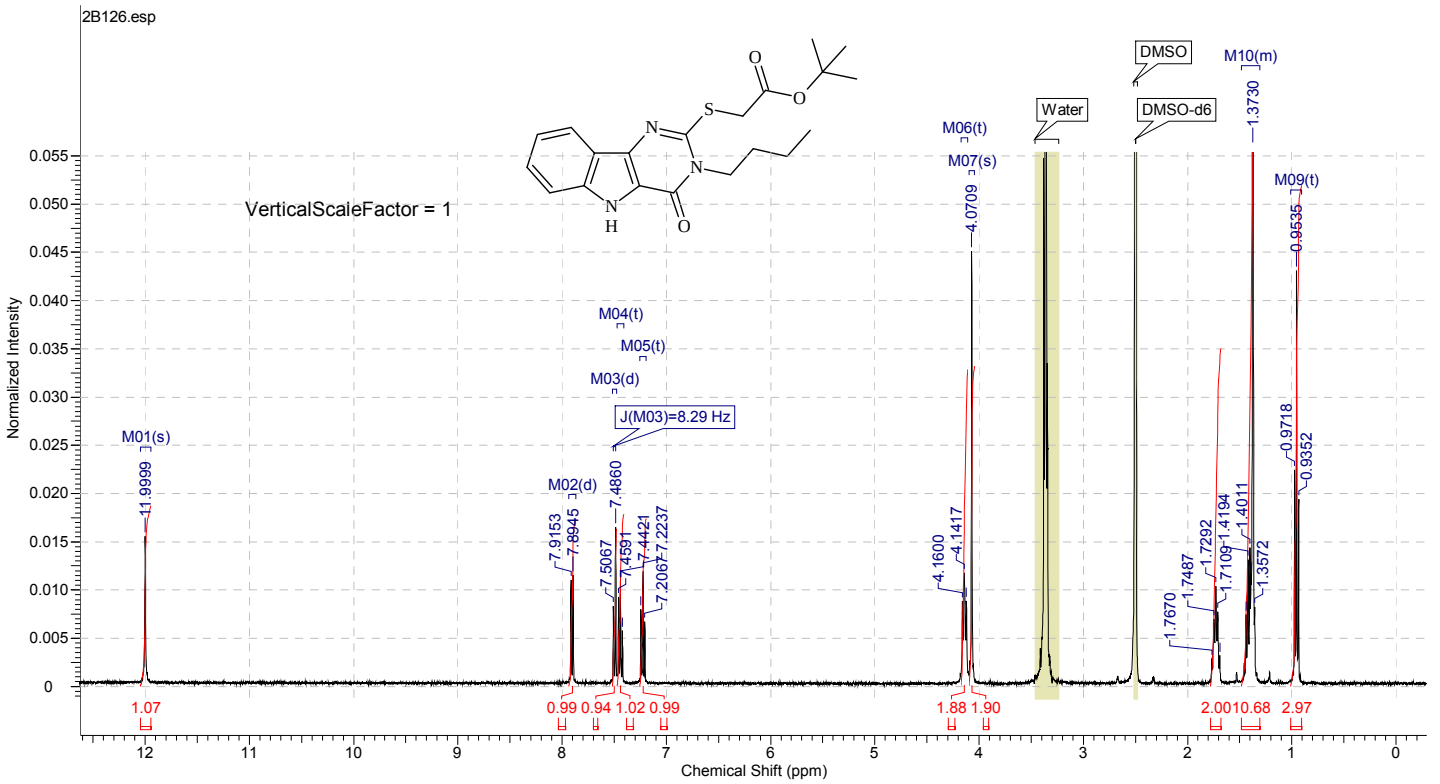


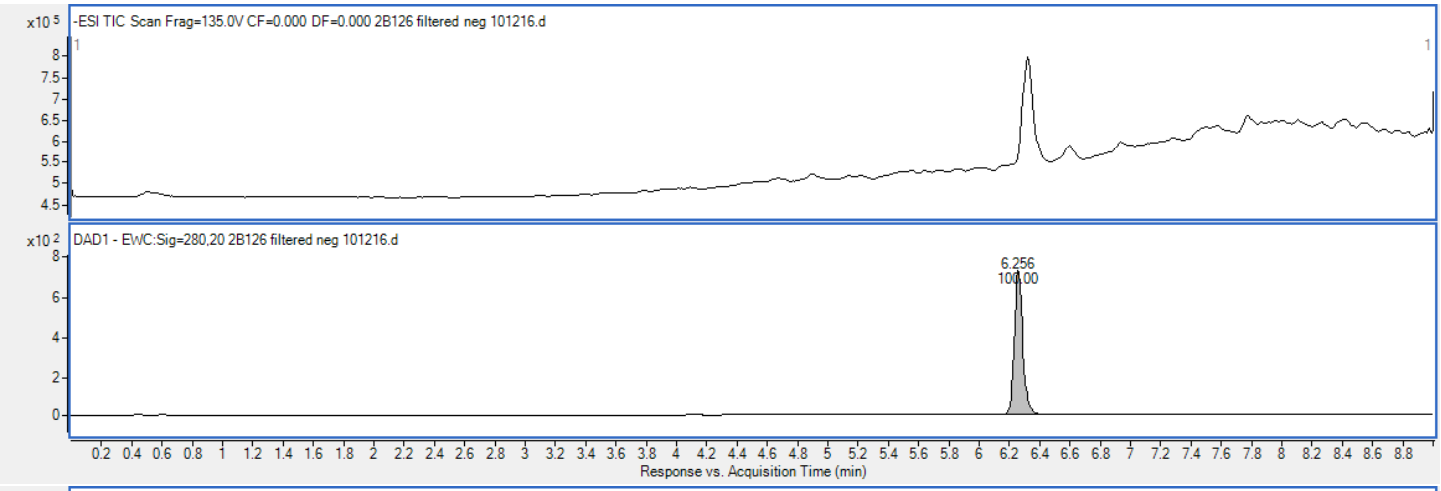
^{1}H NMR, LC-MS **6**{7,3}

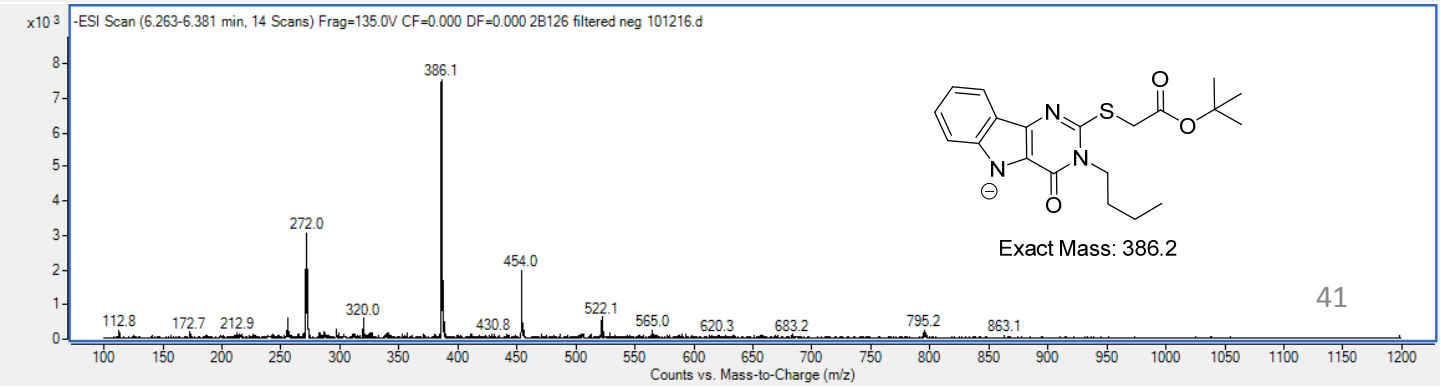
4/20/2017 10:16:16 AM

Acquisition Time (sec)	2.0130	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B126.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16091
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1964.9807	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.90 (d, *J* = 8.29 Hz, 1H), 7.50 (d, *J* = 8.29 Hz, 1H), 7.44 (t, *J* = 7.80 Hz, 1H), 7.22 (t, *J* = 7.32 Hz, 1H), 4.14 (t, *J* = 7.80 Hz, 2H), 4.07 (s, 2H), 1.73 (quin, *J* = 7.70 Hz, 2H), 1.30 - 1.48 (m, 11H), 0.95 (t, *J* = 7.32 Hz, 3H)







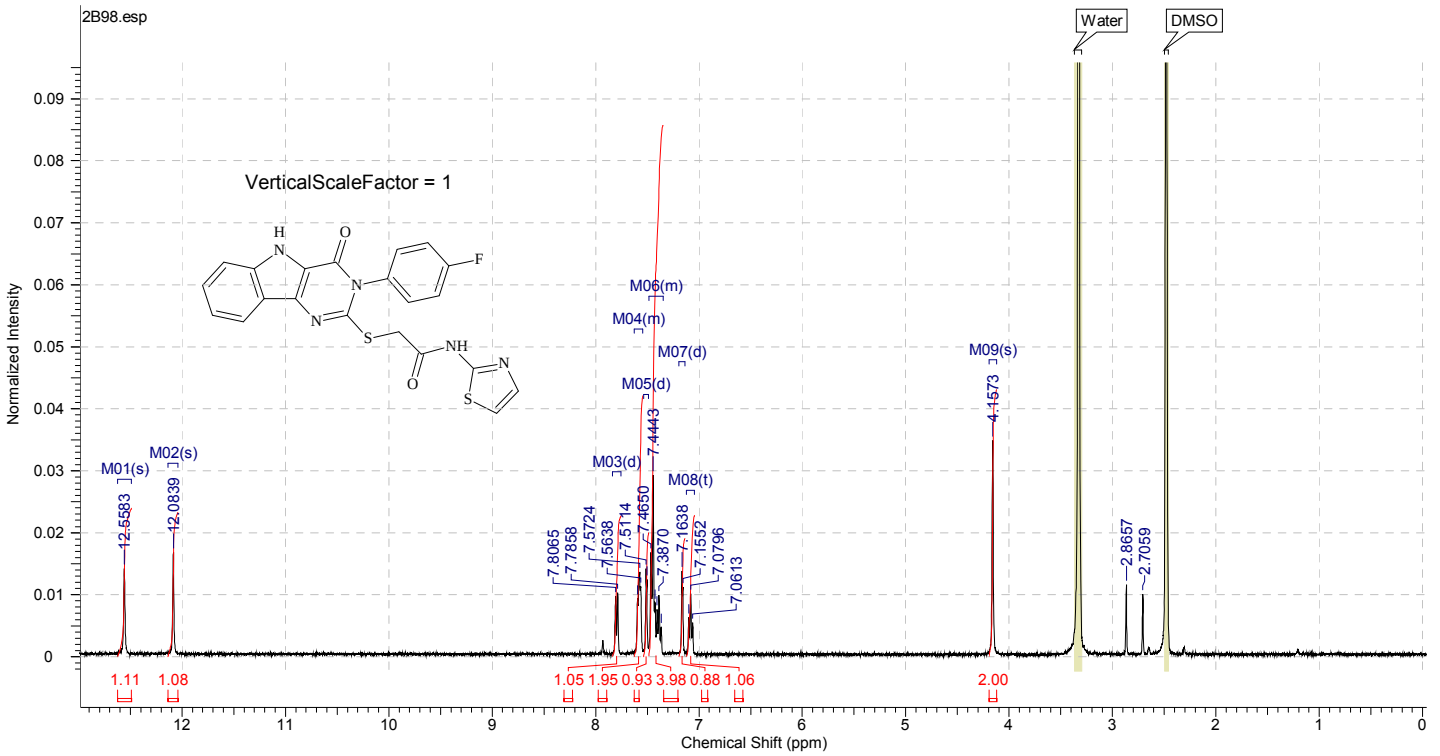
Exact Mass: 386.2

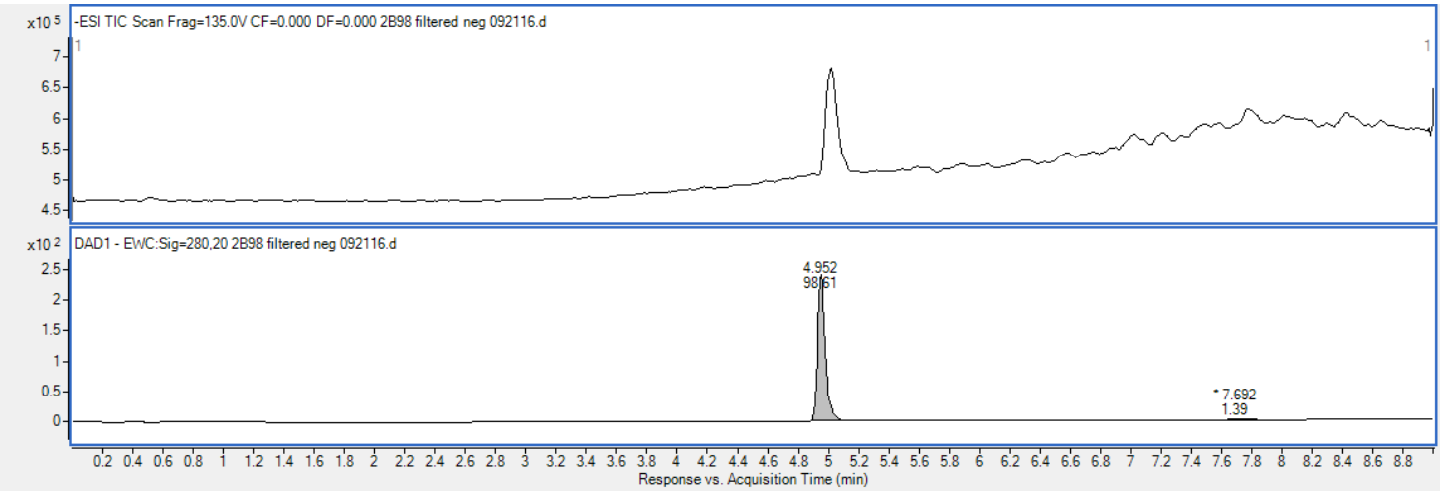
^{1}H NMR, LC-MS **6**{1,4}

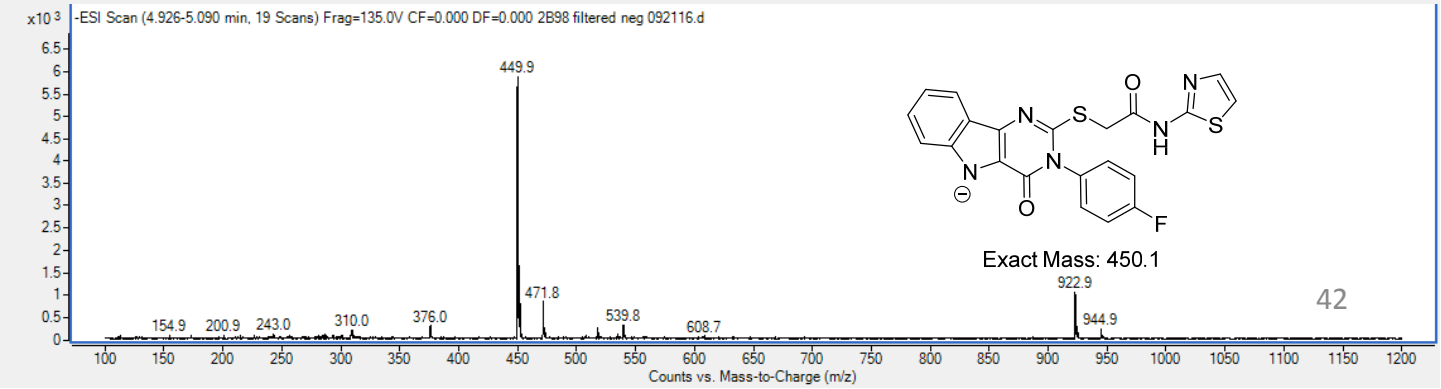
4/20/2017 10:27:57 AM

Acquisition Time (sec)	2.0309	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B98.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16234
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	24.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1956.6102	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.56 (s, 1H), 12.08 (s, 1H), 7.80 (d, *J* = 8.29 Hz, 1H), 7.54 - 7.63 (m, 2H), 7.51 (d, *J* = 3.42 Hz, 1H), 7.35 - 7.48 (m, 4H), 7.16 (d, *J* = 3.42 Hz, 1H), 7.08 (t, *J* = 7.56 Hz, 1H), 4.16 (s, 2H)







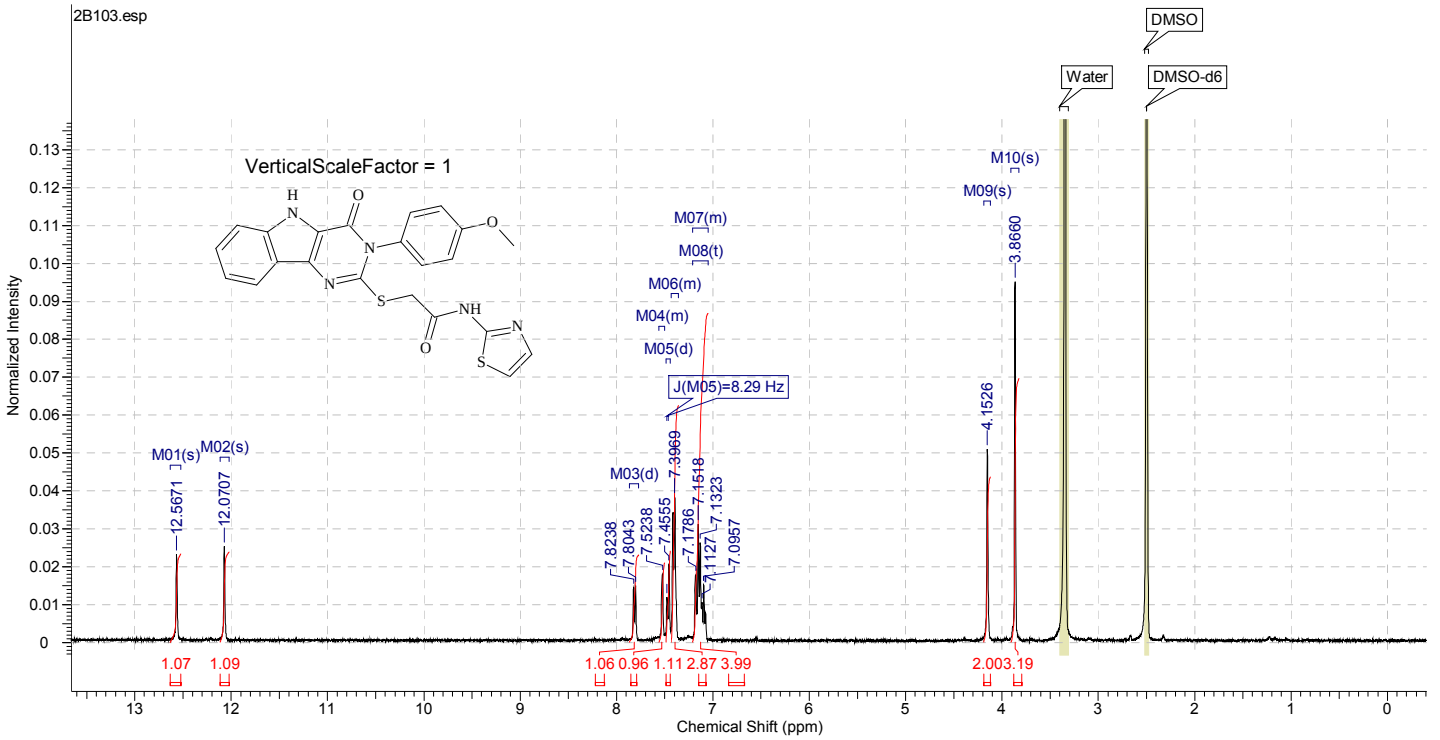
Exact Mass: 450.1

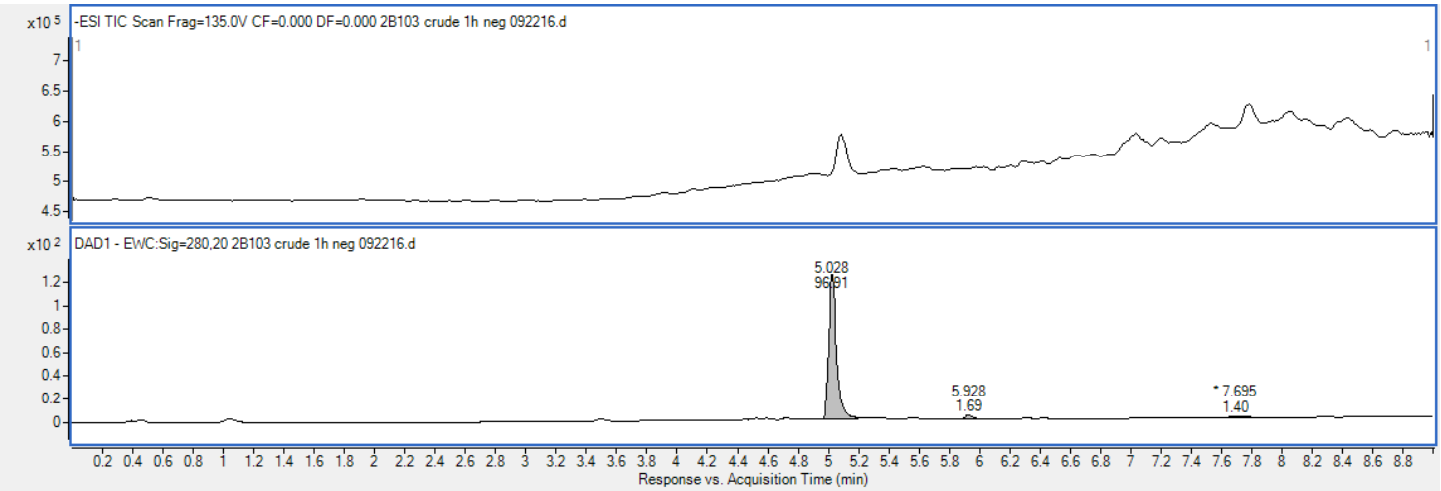
^{1}H NMR, LC-MS **6**{2,4}

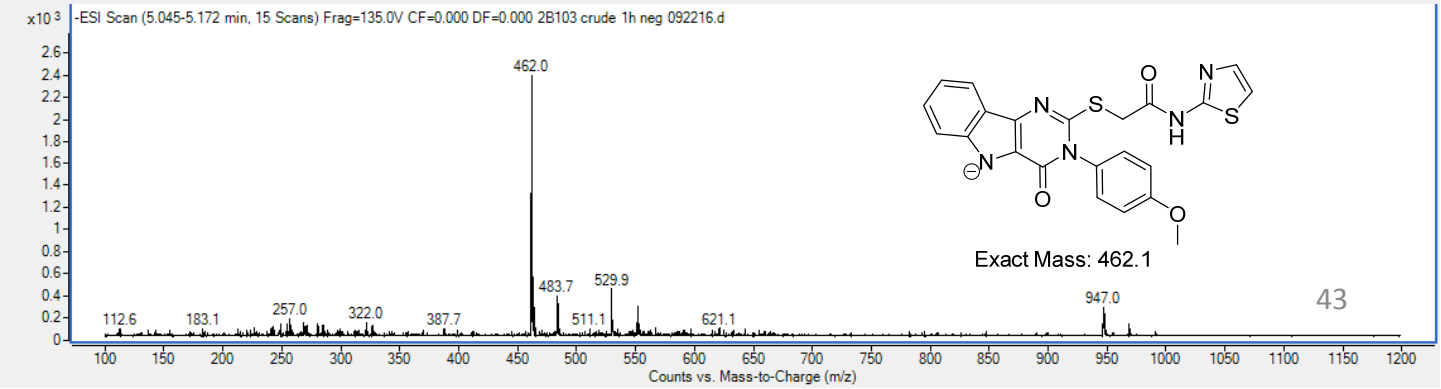
4/20/2017 10:36:32 AM

Acquisition Time (sec)	2.0276	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B103.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16208
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1964.4928	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.57 (s, 1H), 12.07 (s, 1H), 7.81 (d, *J* = 7.81 Hz, 1H), 7.50 - 7.56 (m, 1H), 7.47 (d, *J* = 8.29 Hz, 1H), 7.36 - 7.43 (m, 3H), 7.05 - 7.21 (m, 3H), 7.09 (t, *J* = 7.40 Hz, 1H), 4.15 (s, 2H), 3.87 (s, 3H)





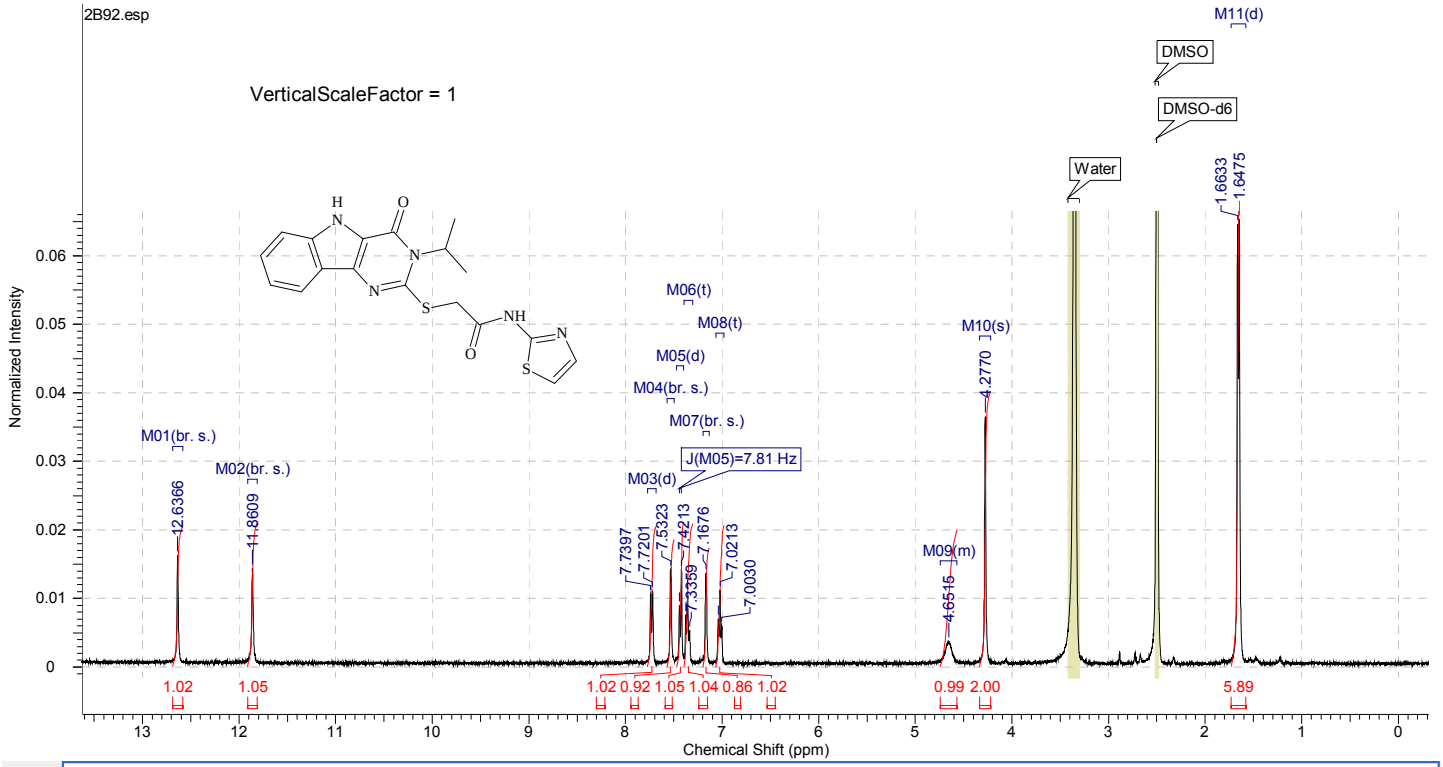


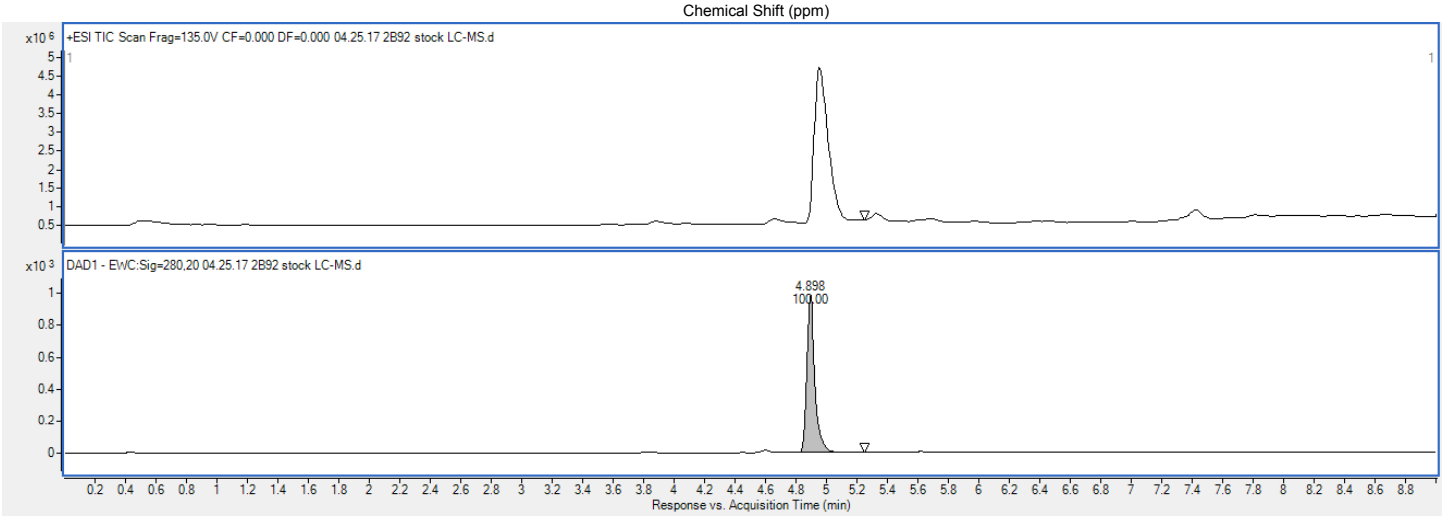
^{1}H NMR, LC-MS **6**{3,4}

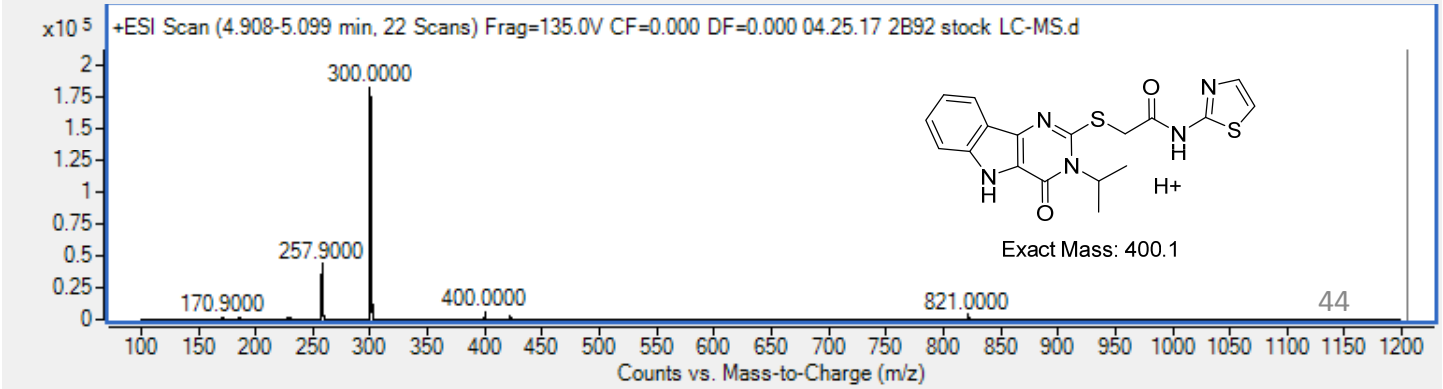
4/20/2017 10:41:21 AM

Acquisition Time (sec)	2.0260	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B92.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16195
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1964.4928	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.64 (br. s., 1H), 11.86 (br. s., 1H), 7.73 (d, *J* = 7.81 Hz, 1H), 7.53 (br. s., 1H), 7.43 (d, *J* = 7.81 Hz, 1H), 7.36 (t, *J* = 7.30 Hz, 1H), 7.17 (br. s., 1H), 7.02 (t, *J* = 7.32 Hz, 1H), 4.57 - 4.74 (m, 1H), 4.28 (s, 2H), 1.66 (d, *J* = 6.34 Hz, 6H)





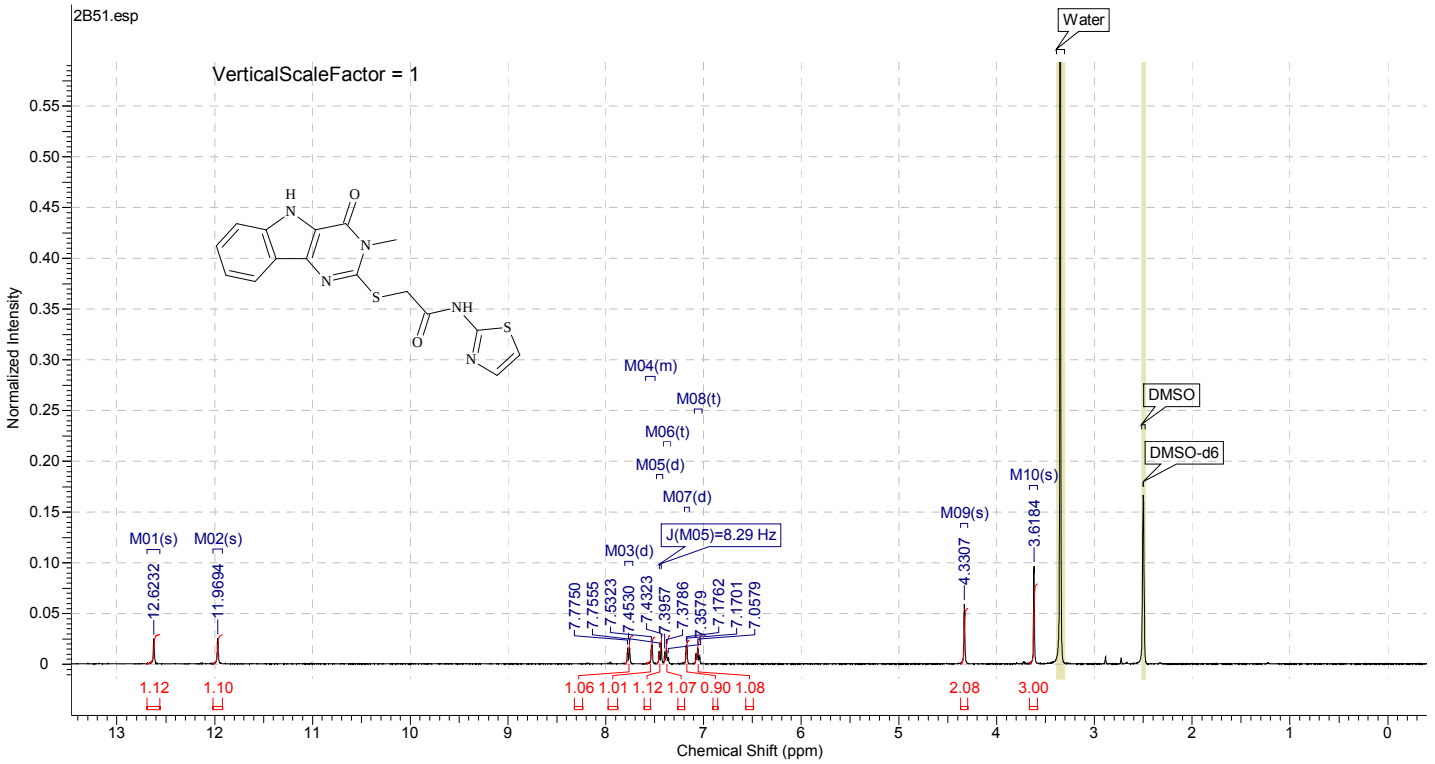


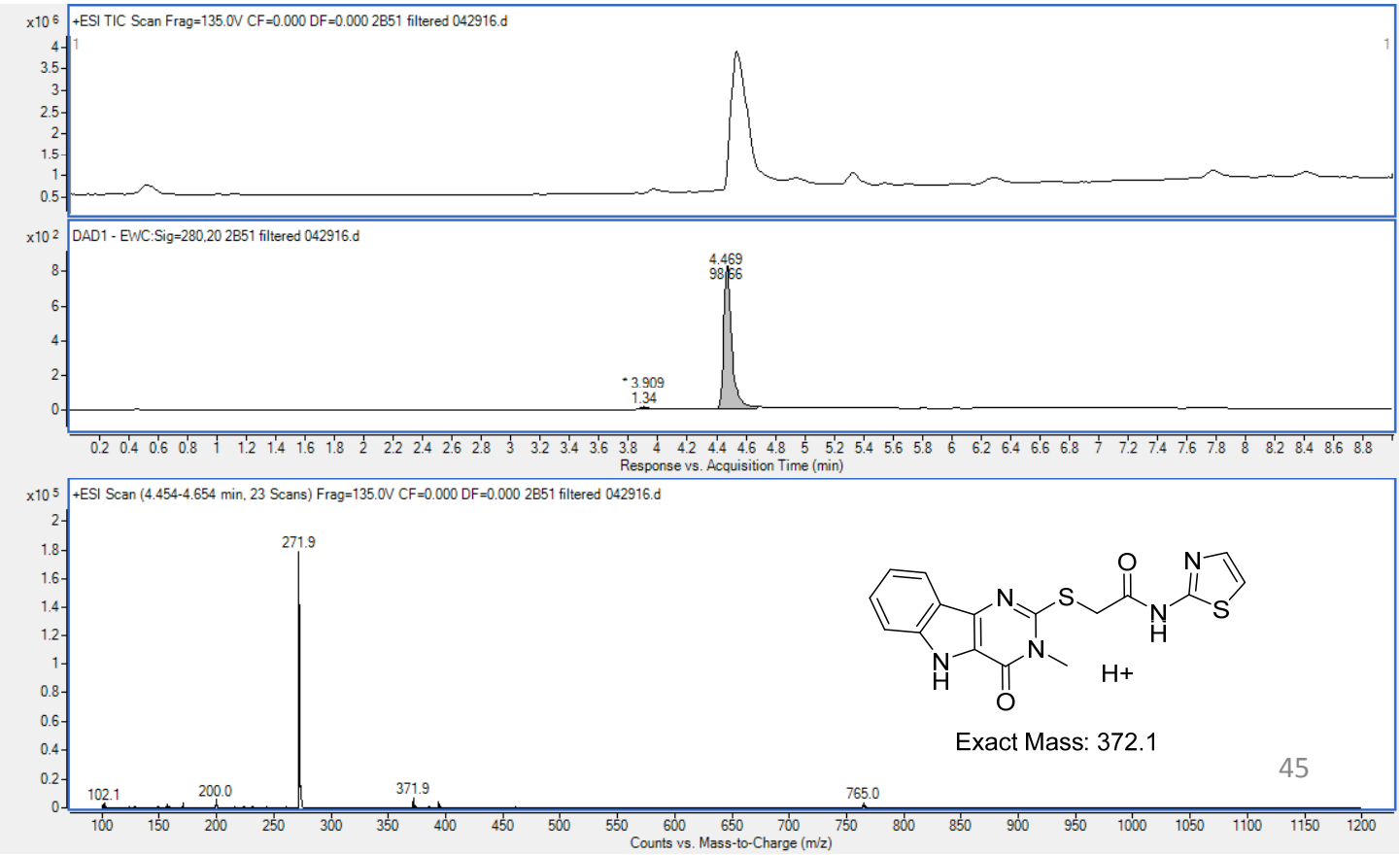
^{1}H NMR, LC-MS **6**{4,4}

4/20/2017 10:46:03 AM

Acquisition Time (sec)	2.0374	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B51.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16286
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	22.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1964.9807	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.62 (s, 1H), 11.97 (s, 1H), 7.77 (d, *J* = 7.81 Hz, 1H), 7.50 - 7.59 (m, 1H), 7.44 (d, *J* = 8.29 Hz, 1H), 7.38 (t, *J* = 7.30 Hz, 1H), 7.17 (d, *J* = 2.44 Hz, 1H), 7.06 (t, *J* = 7.30 Hz, 1H), 4.33 (s, 2H), 3.62 (s, 3H)





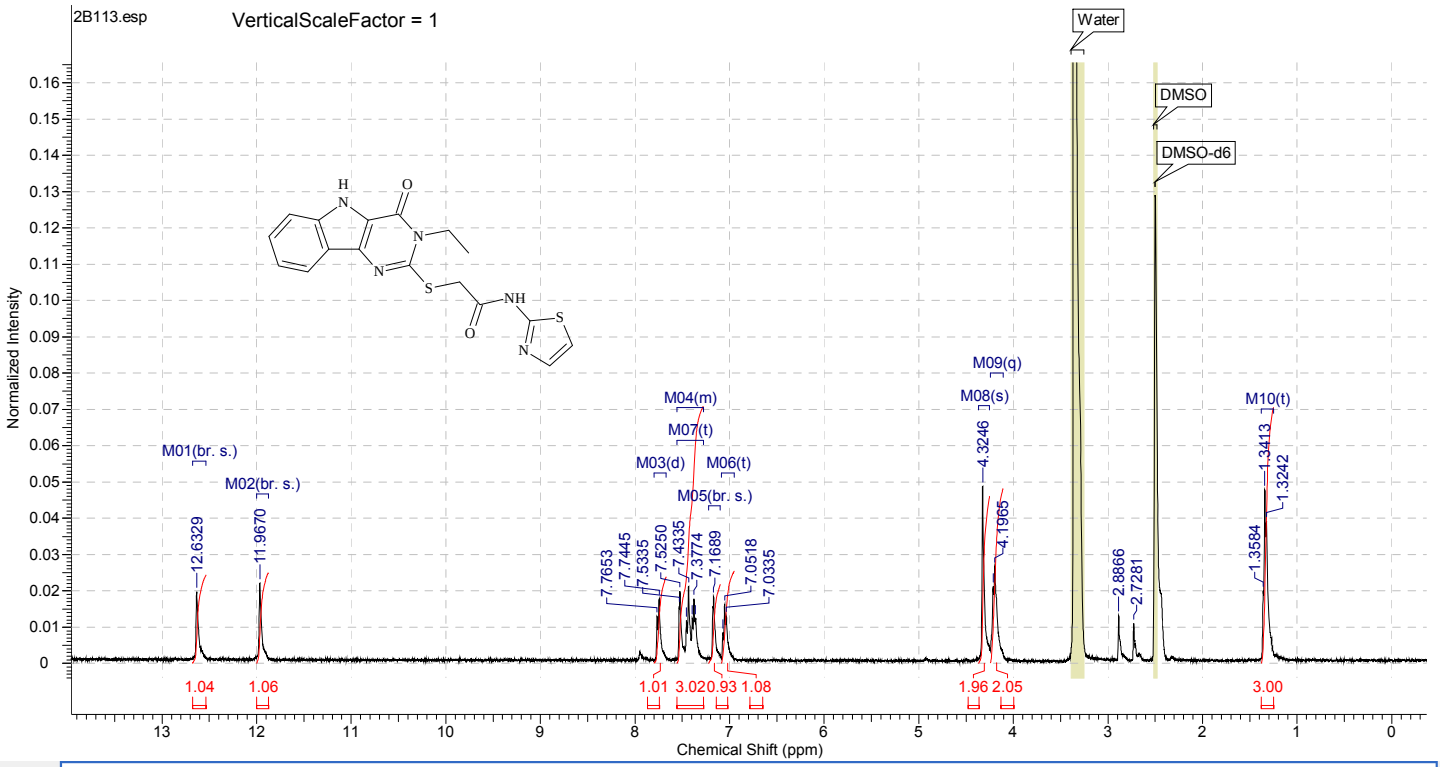
Exact Mass: 372.1

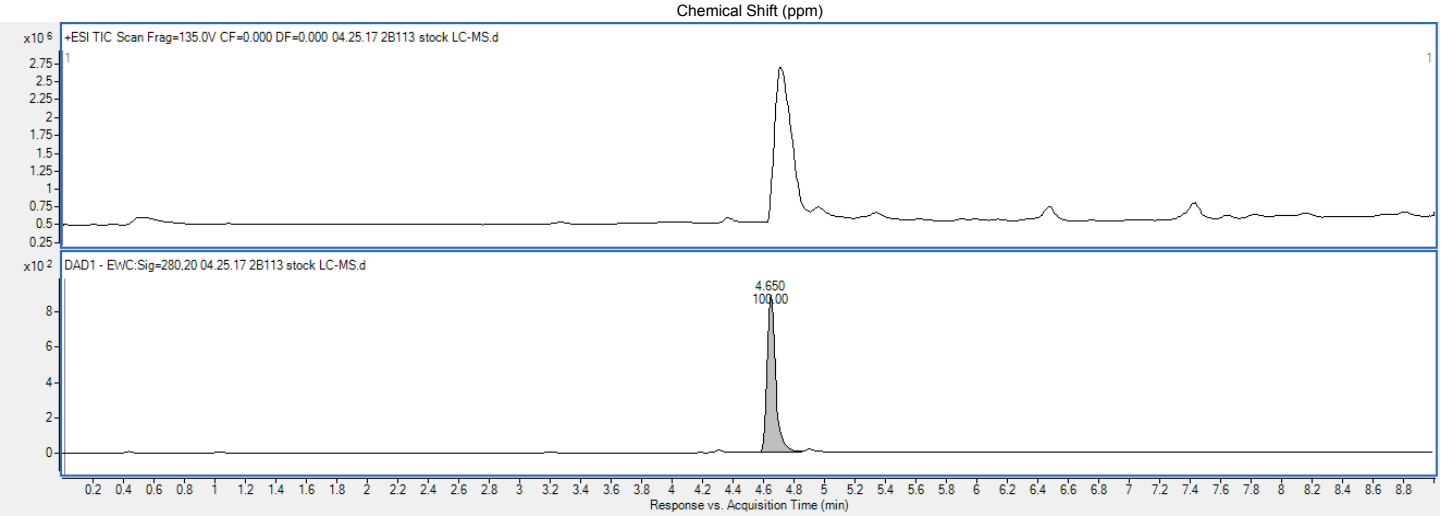
^{1}H NMR, LC-MS **6**{5,4}

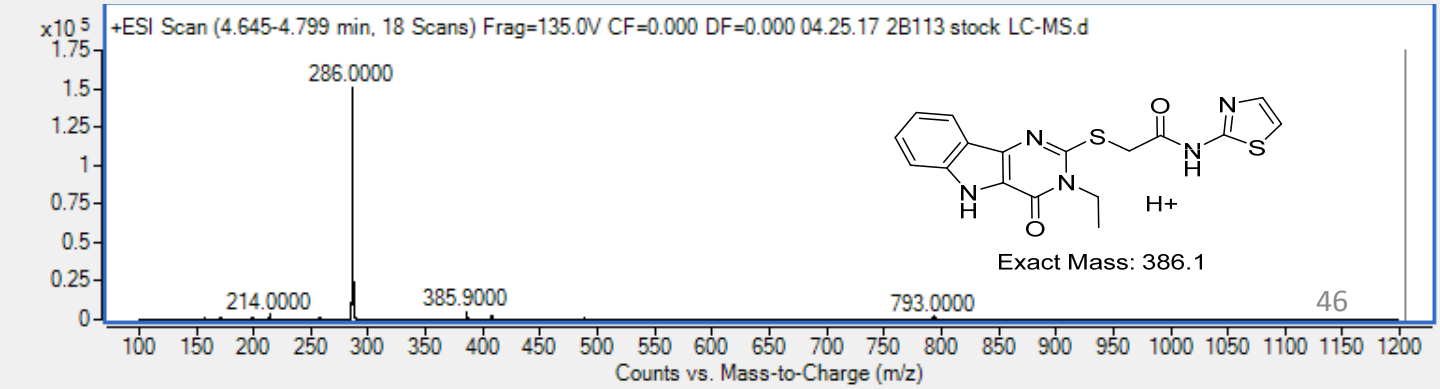
4/20/2017 10:54:06 AM

Acquisition Time (sec)	2.0358	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B113.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16273
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	16.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1964.0049	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.63 (br. s., 1H), 11.97 (br. s., 1H), 7.75 (d, *J* = 8.29 Hz, 1H), 7.28 - 7.56 (m, 2H), 7.38 (t, *J* = 7.00 Hz, 1H), 7.17 (br. s., 1H), 7.05 (t, *J* = 7.30 Hz, 1H), 4.32 (s, 2H), 4.20 (q, *J* = 6.80 Hz, 2H), 1.34 (t, *J* = 6.80 Hz, 3H)





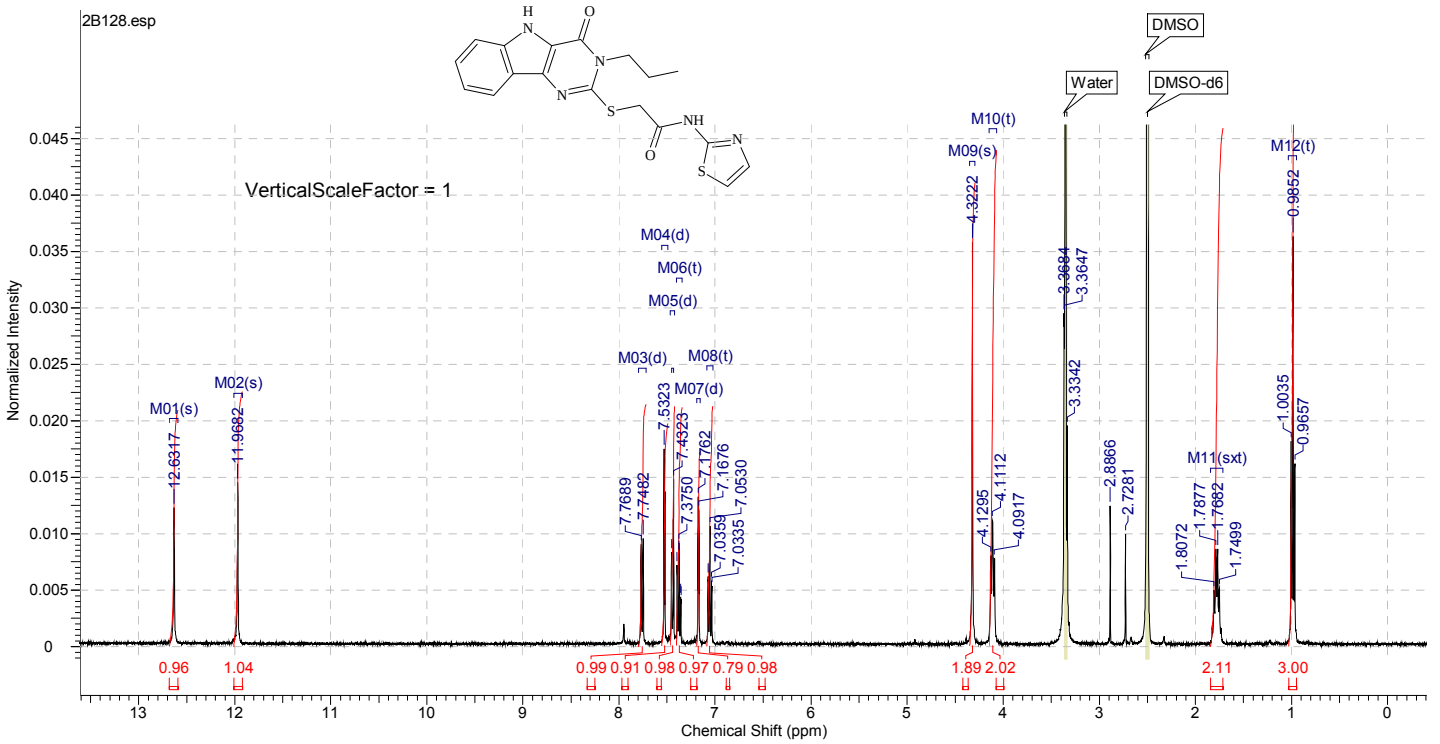


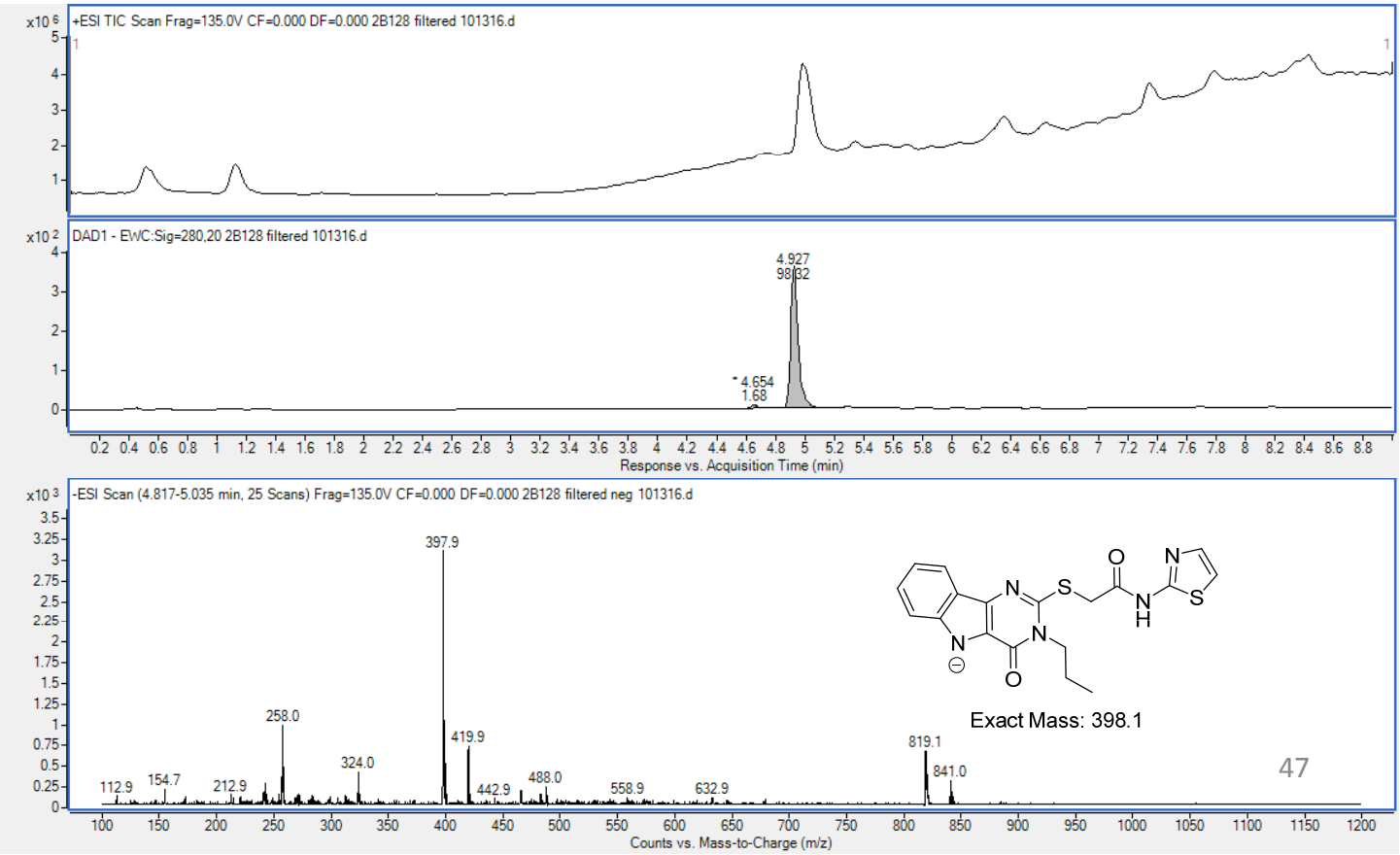
^{1}H NMR, LC-MS **6**{6,4}

4/20/2017 10:59:11 AM

Acquisition Time (sec)	2.0114	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B128.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16078
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1964.4928	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.63 (s, 1H), 11.97 (s, 1H), 7.76 (d, *J* = 8.29 Hz, 1H), 7.53 (d, *J* = 3.90 Hz, 1H), 7.44 (d, *J* = 8.29 Hz, 1H), 7.38 (t, *J* = 7.60 Hz, 1H), 7.17 (d, *J* = 3.42 Hz, 1H), 7.05 (t, *J* = 7.80 Hz, 1H), 4.32 (s, 2H), 4.11 (t, *J* = 7.56 Hz, 2H), 1.78 (sxt, *J* = 7.30 Hz, 2H), 0.98 (t, *J* = 7.56 Hz, 3H)





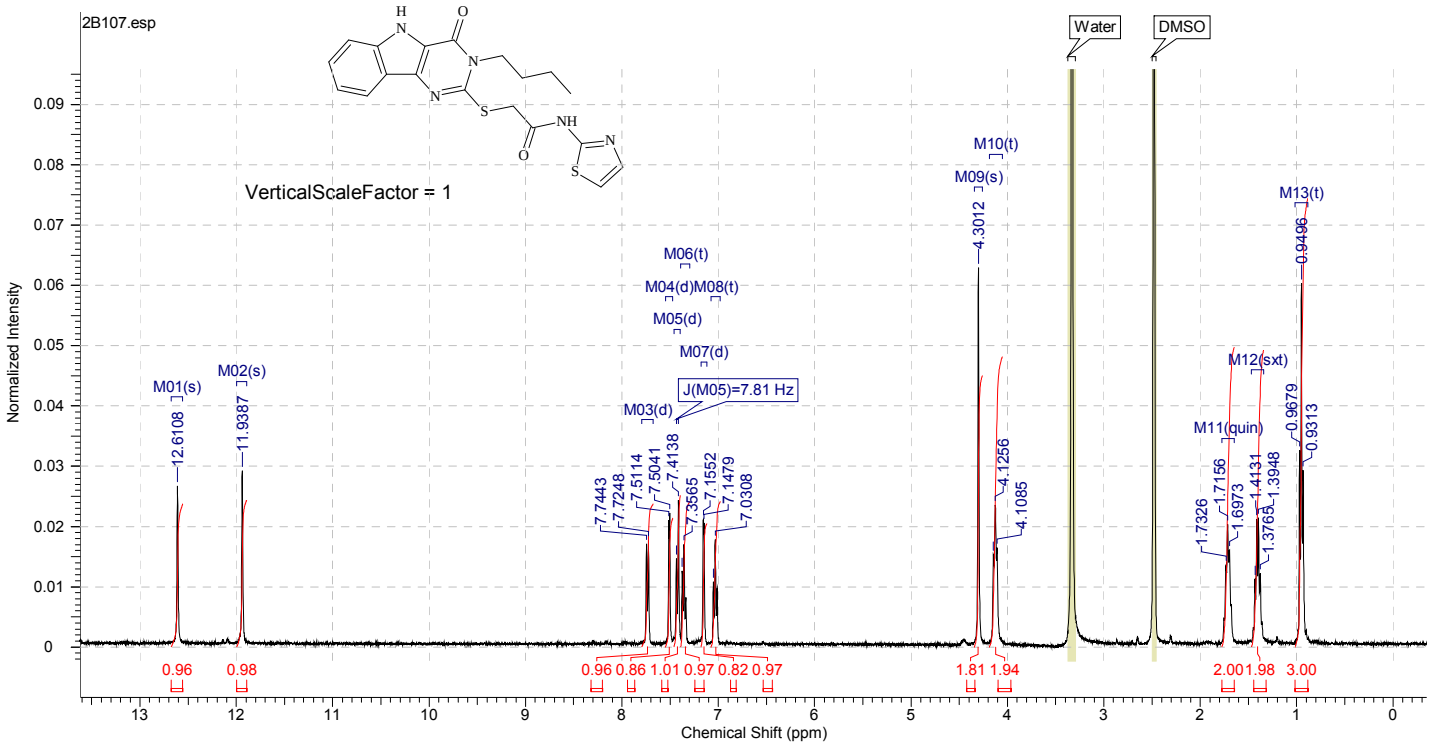
Exact Mass: 398.1

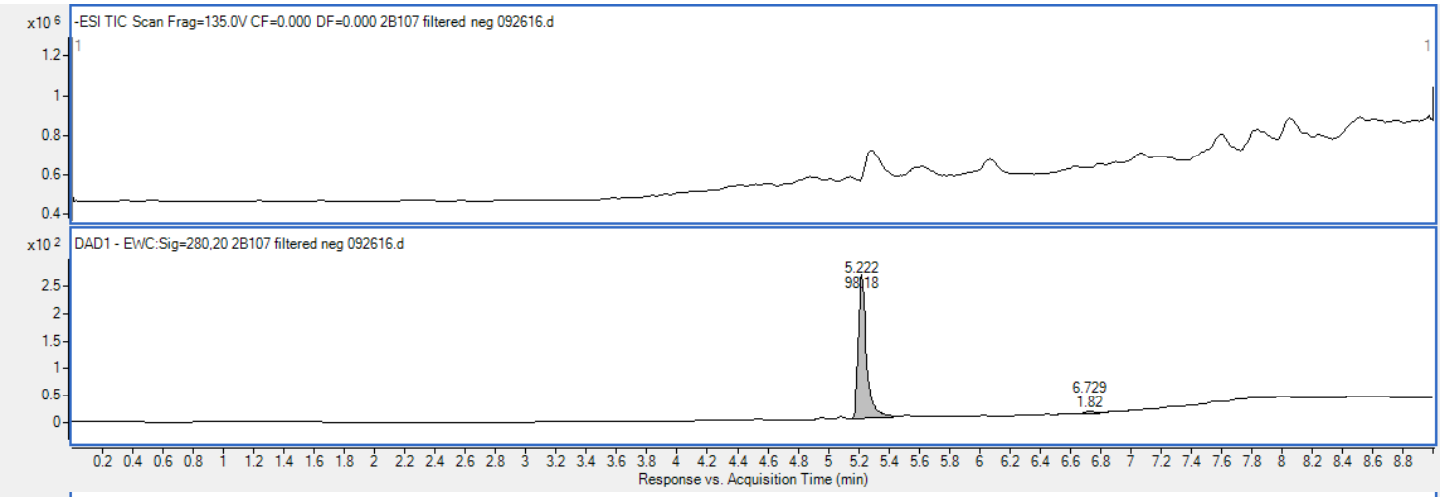
^{1}H NMR, LC-MS **6**{7,4}

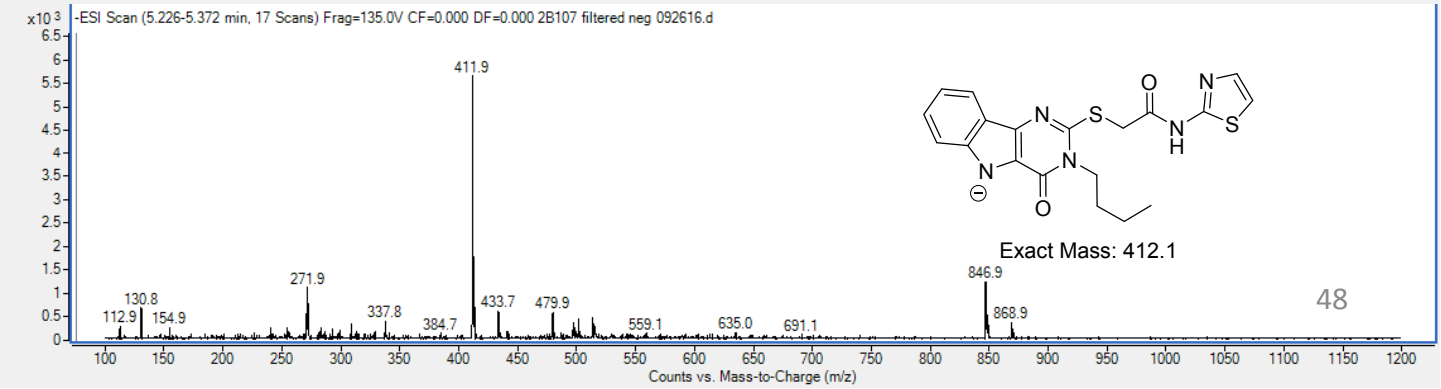
4/20/2017 11:10:54 AM

Acquisition Time (sec)	2.0244	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B107.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16182
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1956.6102	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.61 (s, 1H), 11.94 (s, 1H), 7.73 (d, *J* = 7.81 Hz, 1H), 7.51 (d, *J* = 2.93 Hz, 1H), 7.42 (d, *J* = 7.81 Hz, 1H), 7.36 (t, *J* = 7.80 Hz, 1H), 7.15 (d, *J* = 2.93 Hz, 1H), 7.03 (t, *J* = 7.30 Hz, 1H), 4.30 (s, 2H), 4.13 (t, *J* = 7.32 Hz, 2H), 1.72 (quin, *J* = 7.30 Hz, 2H), 1.40 (sxt, *J* = 7.30 Hz, 2H), 0.95 (t, *J* = 7.32 Hz, 3H)







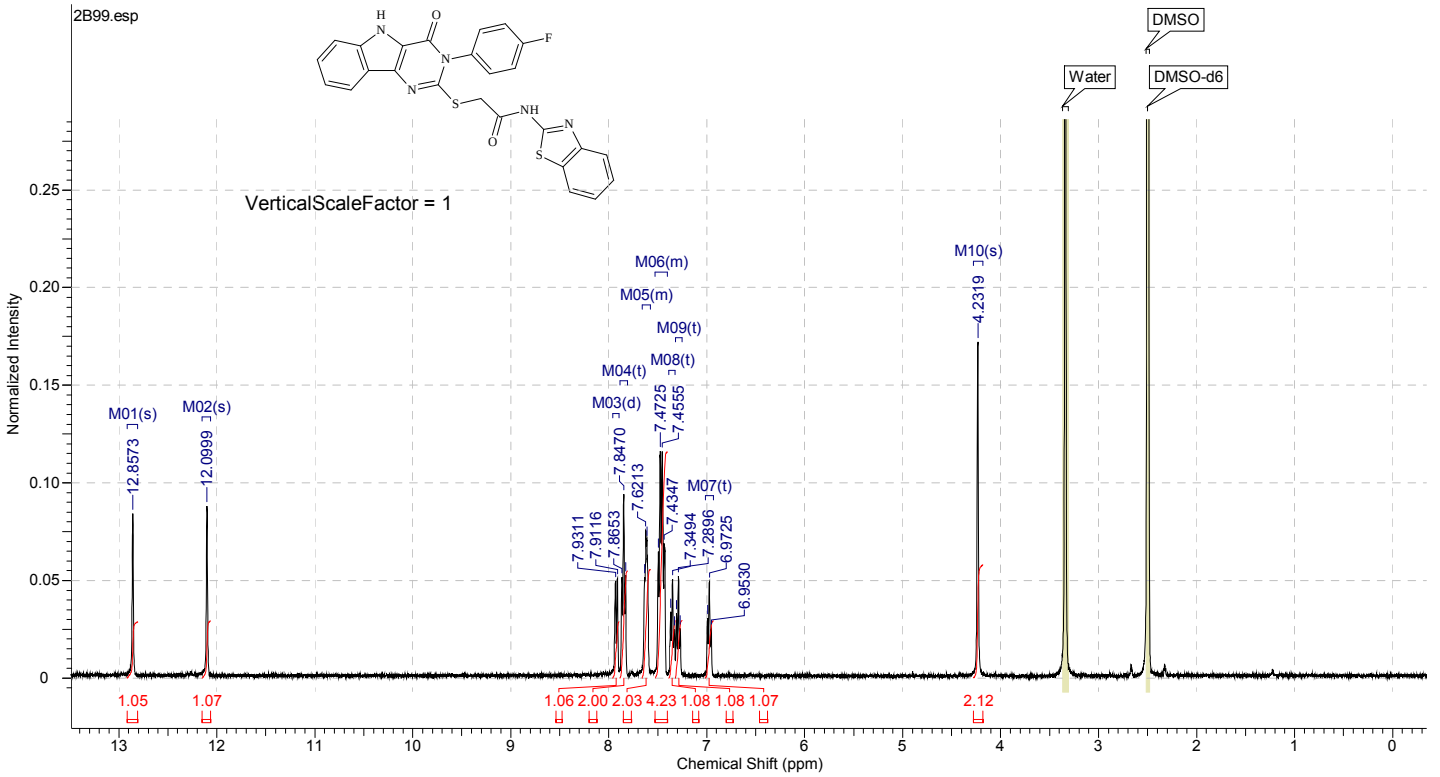
Exact Mass: 412.1

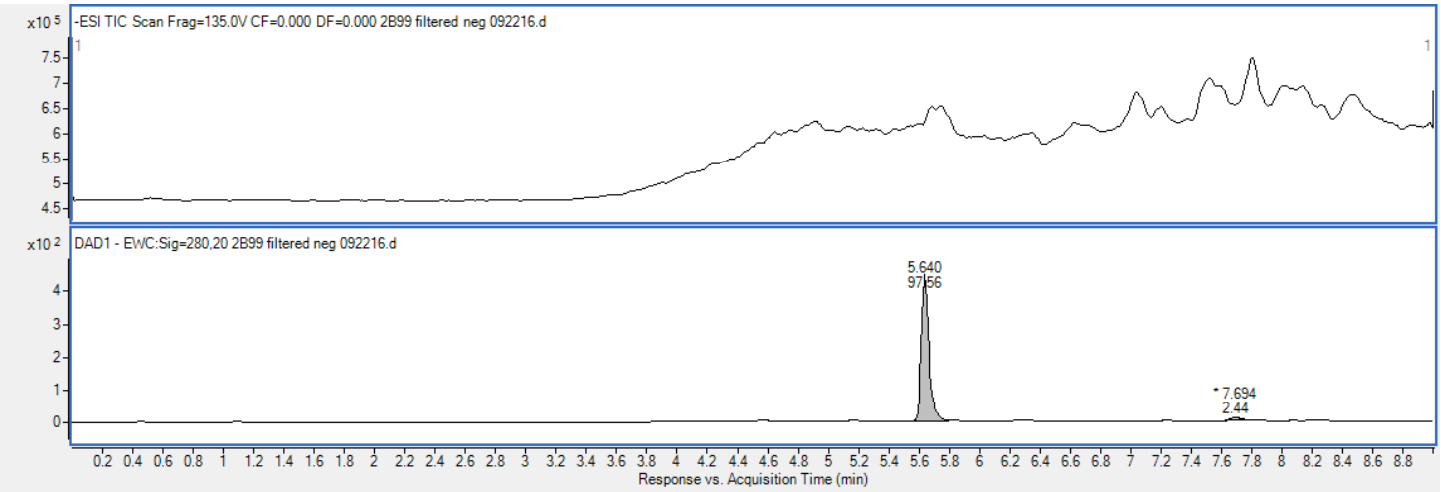
^{1}H NMR, LC-MS **6**{1,5}

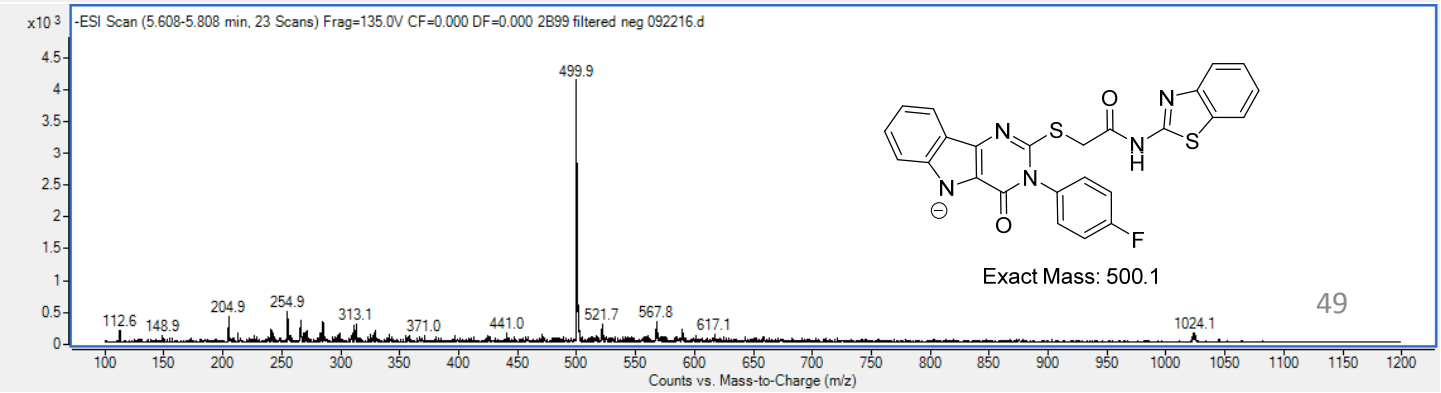
4/20/2017 11:32:20 AM

Acquisition Time (sec)	2.0081	***Comment***	STANDARD 1H OBSERVE			***Date***	Dec 23 2016
Date Stamp	Dec 23 2016	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B99.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16052
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1960.1014	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.86 (s, 1H), 12.10 (s, 1H), 7.92 (d, *J* = 7.81 Hz, 1H), 7.85 (t, *J* = 7.56 Hz, 2H), 7.58 - 7.66 (m, 2H), 7.40 - 7.53 (m, 4H), 7.35 (t, *J* = 7.30 Hz, 1H), 7.29 (t, *J* = 7.80 Hz, 1H), 6.97 (t, *J* = 7.56 Hz, 1H), 4.23 (s, 2H)







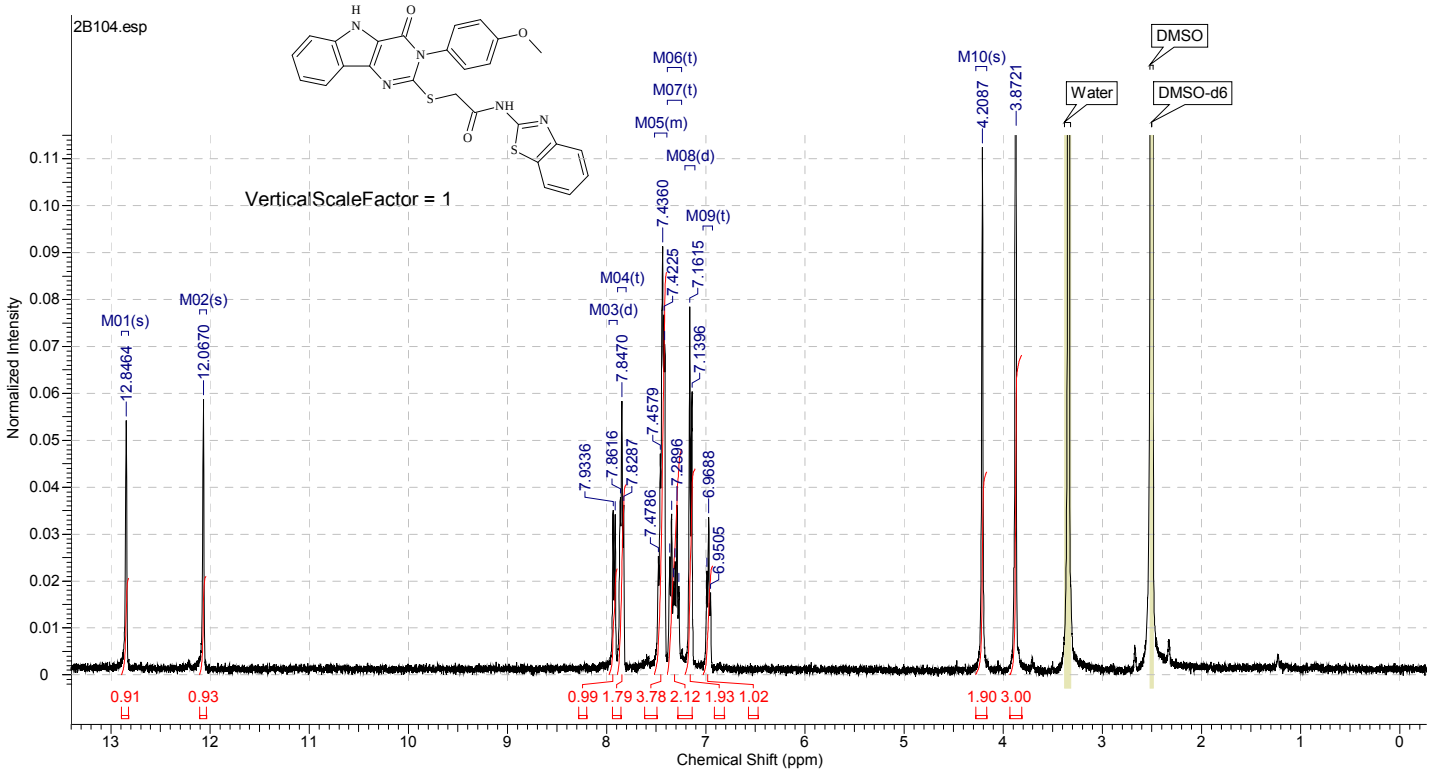
Exact Mass: 500.1

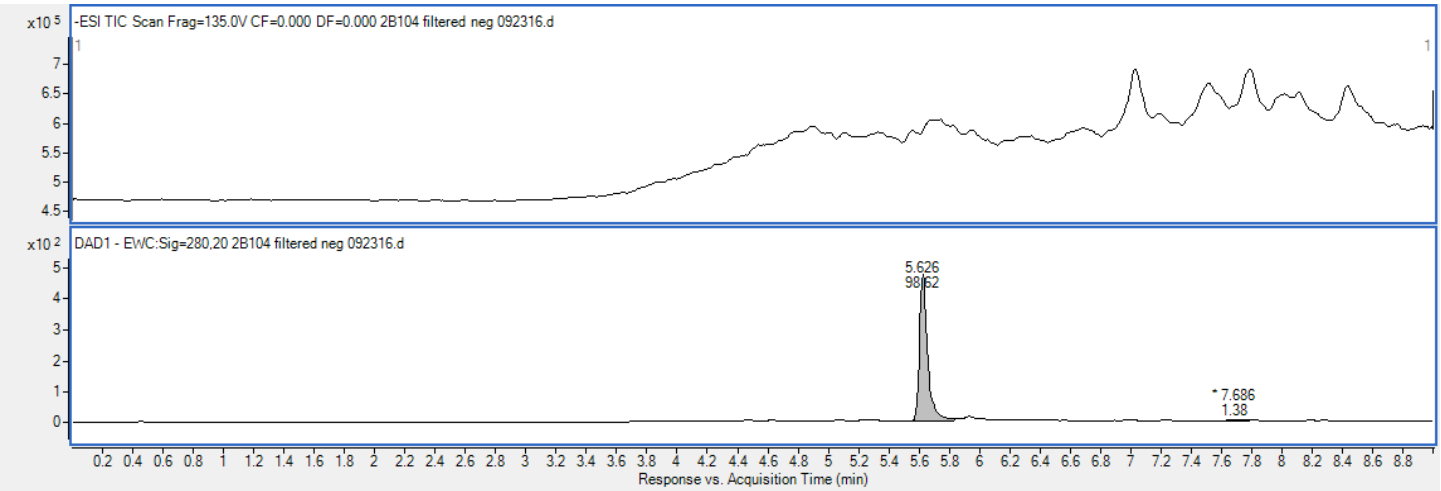
^{1}H NMR, LC-MS **6**{2,5}

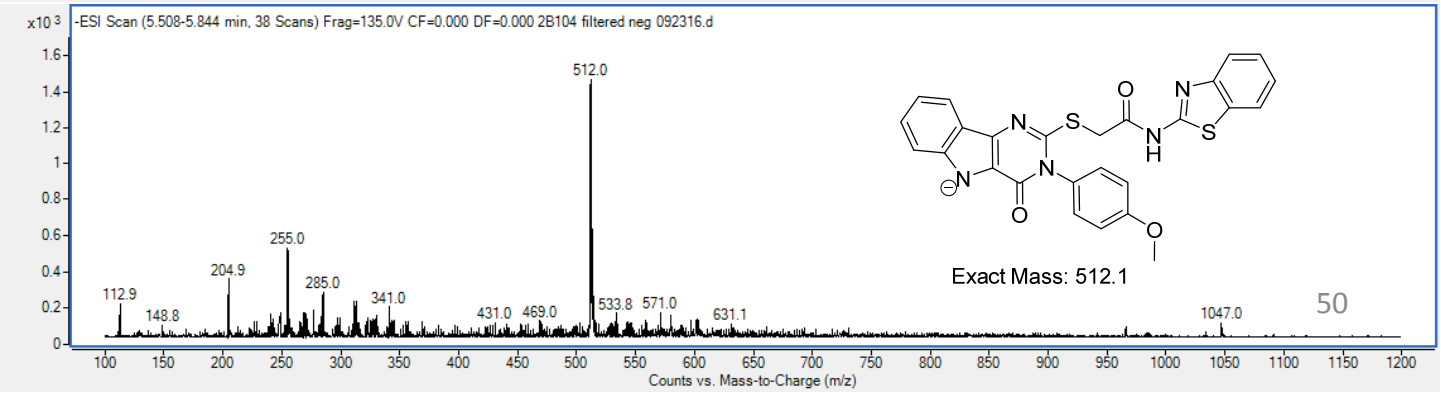
4/20/2017 11:38:18 AM

Acquisition Time (sec)	2.0049	***Comment***	STANDARD 1H OBSERVE			***Date***	Dec 23 2016
Date Stamp	Dec 23 2016	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B104.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16026
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1961.5652	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.85 (s, 1H), 12.07 (s, 1H), 7.92 (d, *J* = 7.81 Hz, 1H), 7.85 (t, *J* = 6.59 Hz, 2H), 7.39 - 7.52 (m, 4H), 7.34 (t, *J* = 7.30 Hz, 1H), 7.29 (t, *J* = 7.30 Hz, 1H), 7.15 (d, *J* = 8.78 Hz, 2H), 6.97 (t, *J* = 7.56 Hz, 1H), 4.21 (s, 2H), 3.87 (s, 3H)







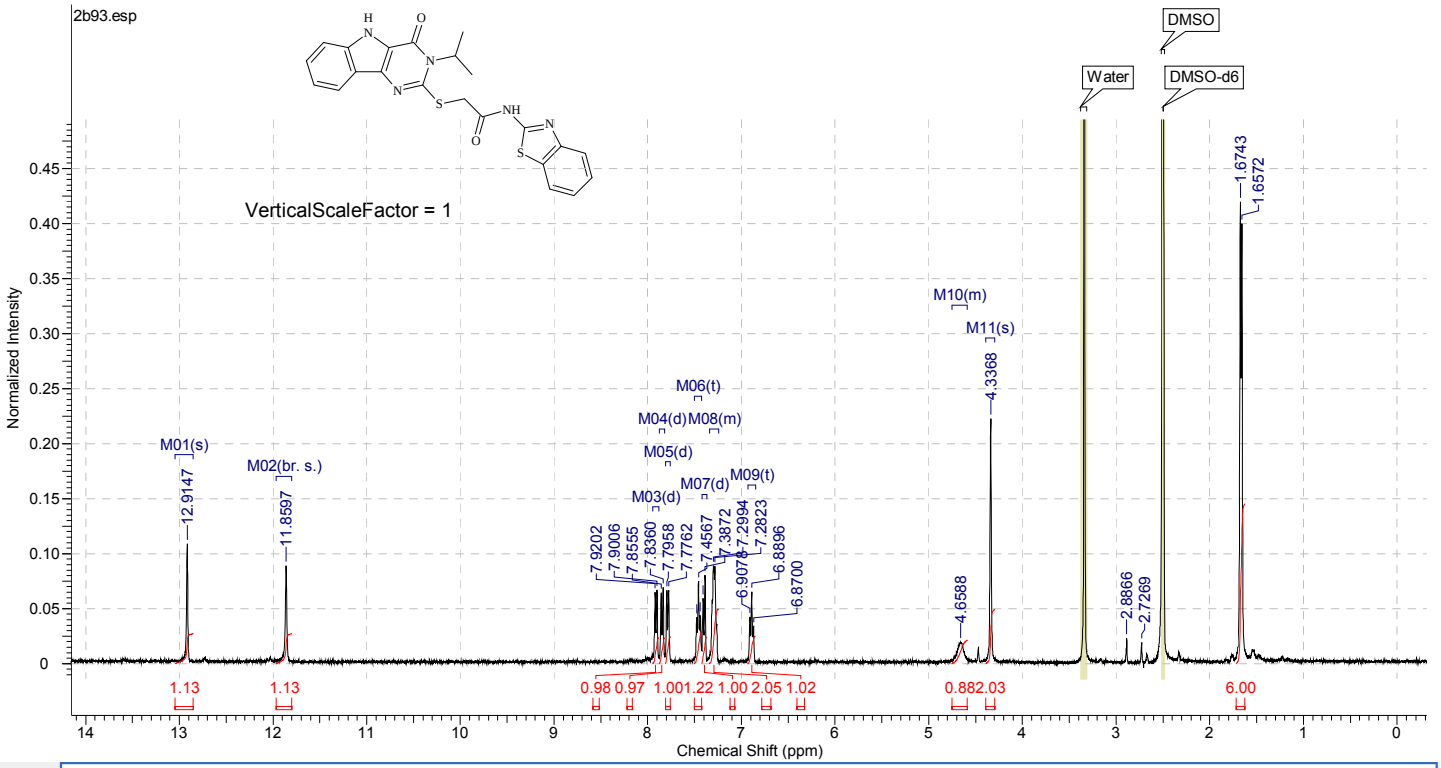
Exact Mass: 512.1

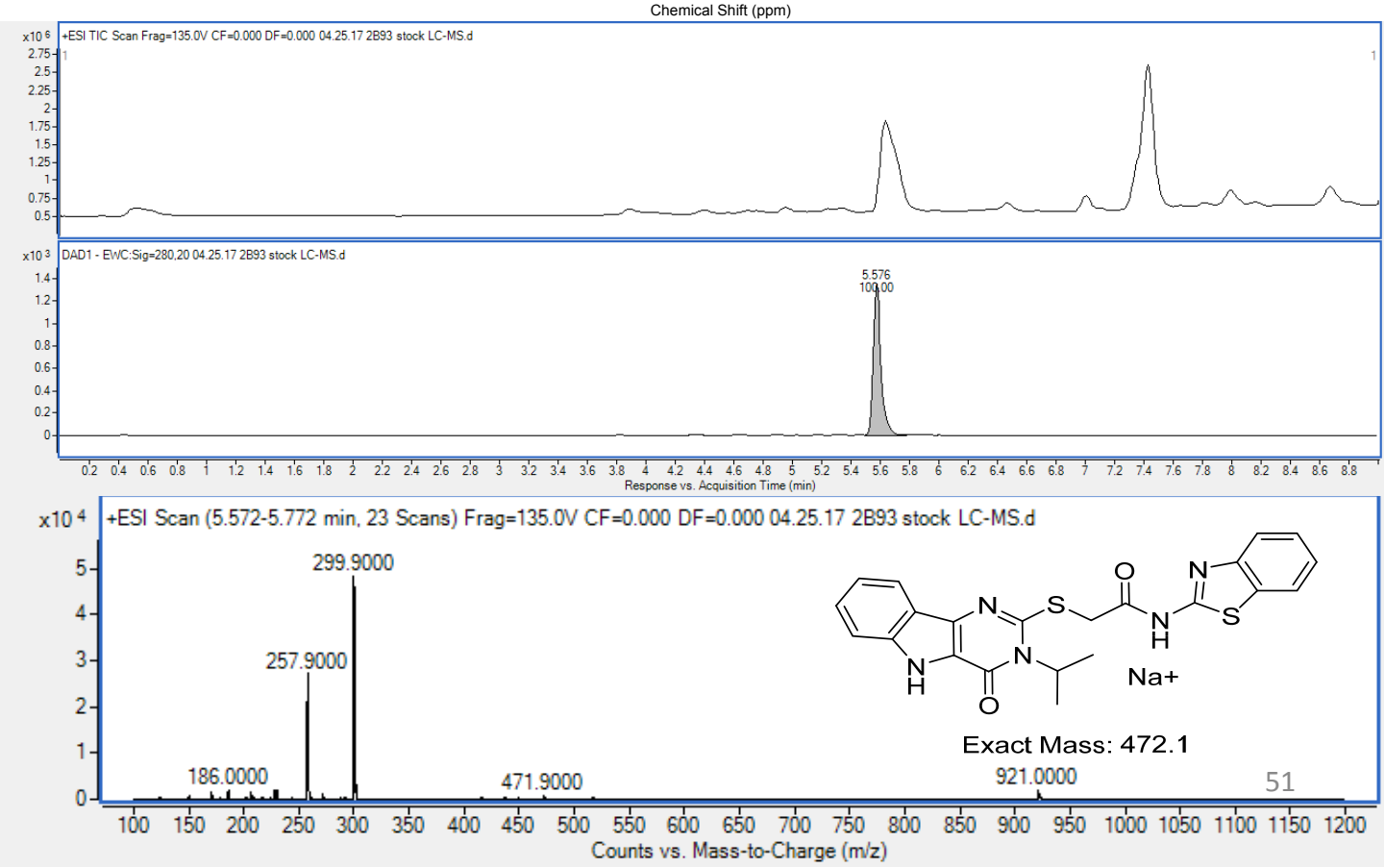
^{1}H NMR, LC-MS **6**{3,5}

4/20/2017 11:44:05 AM

Acquisition Time (sec)	2.0179	***Comment***	STANDARD 1H OBSERVE			***Date***	Dec 23 2016
Date Stamp	Dec 23 2016	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b93.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16130
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1961.0773	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.91 (s, 1H), 11.86 (br. s., 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.85 (d, *J* = 7.81 Hz, 1H), 7.79 (d, *J* = 7.81 Hz, 1H), 7.46 (t, *J* = 7.56 Hz, 1H), 7.40 (d, *J* = 8.29 Hz, 1H), 7.24 - 7.34 (m, *J* = 6.80 Hz, 2H), 6.89 (t, *J* = 7.56 Hz, 1H), 4.59 - 4.75 (m, 1H), 4.34 (s, 2H), 1.67 (d, *J* = 6.83 Hz, 6H)



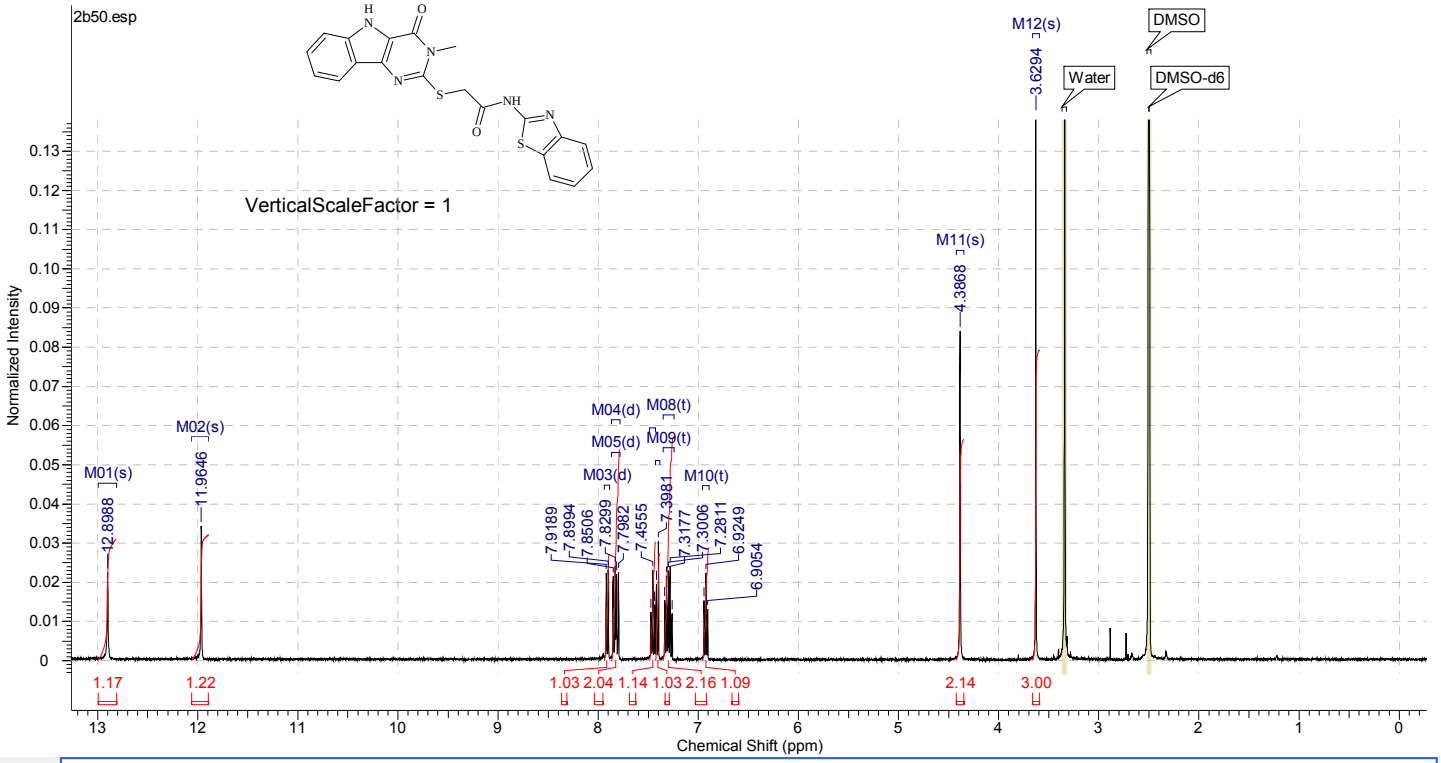


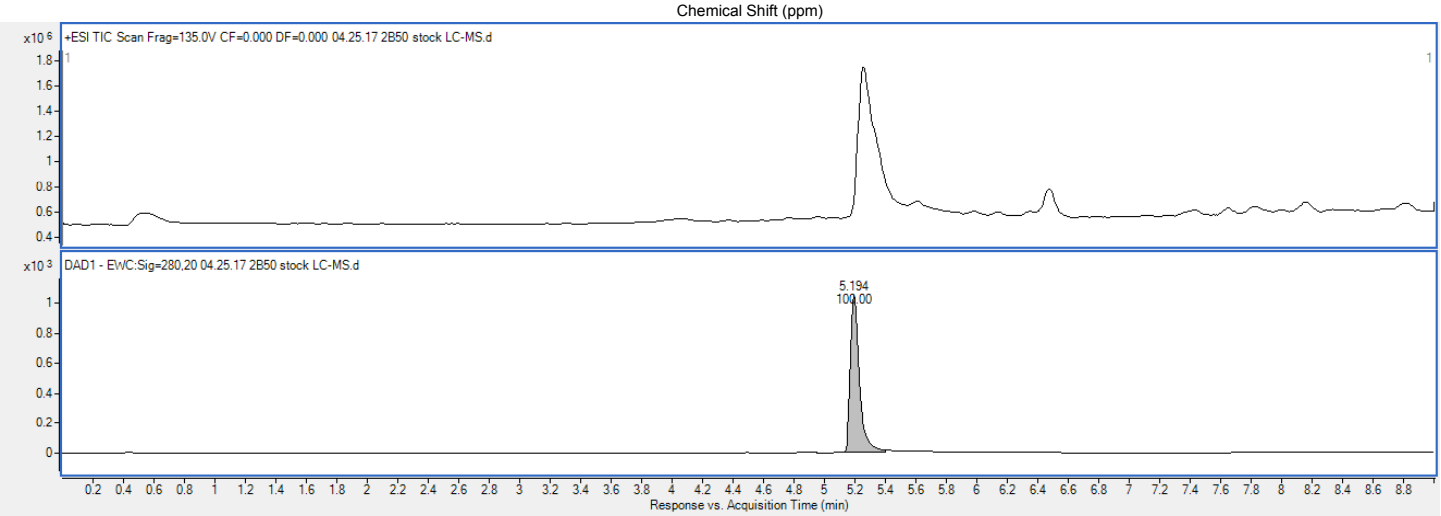
^{1}H NMR, LC-MS **6**{4,5}

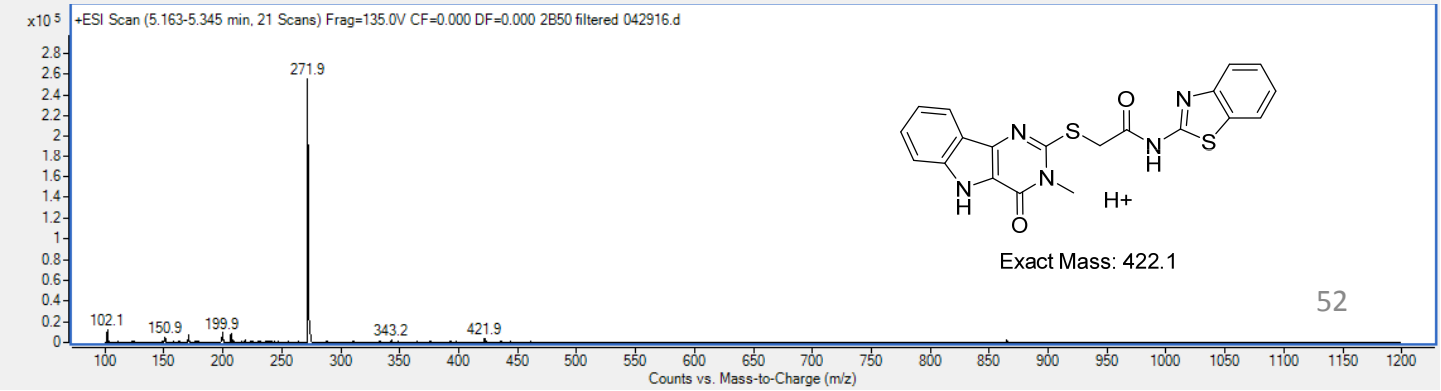
4/20/2017 11:50:06 AM

Acquisition Time (sec)	2.0032	***Comment***	STANDARD 1H OBSERVE			***Date***	Dec 23 2016
Date Stamp	Dec 23 2016	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b50.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16013
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1961.5652	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.90 (s, 1H), 11.96 (s, 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.84 (d, *J* = 8.10 Hz, 1H), 7.81 (d, *J* = 8.10 Hz, 1H), 7.45 (t, *J* = 7.81 Hz, 1H), 7.41 (d, *J* = 8.78 Hz, 1H), 7.32 (t, *J* = 7.30 Hz, 1H), 7.28 (t, *J* = 7.30 Hz, 1H), 6.92 (t, *J* = 7.56 Hz, 1H), 4.39 (s, 2H), 3.63 (s, 3H)







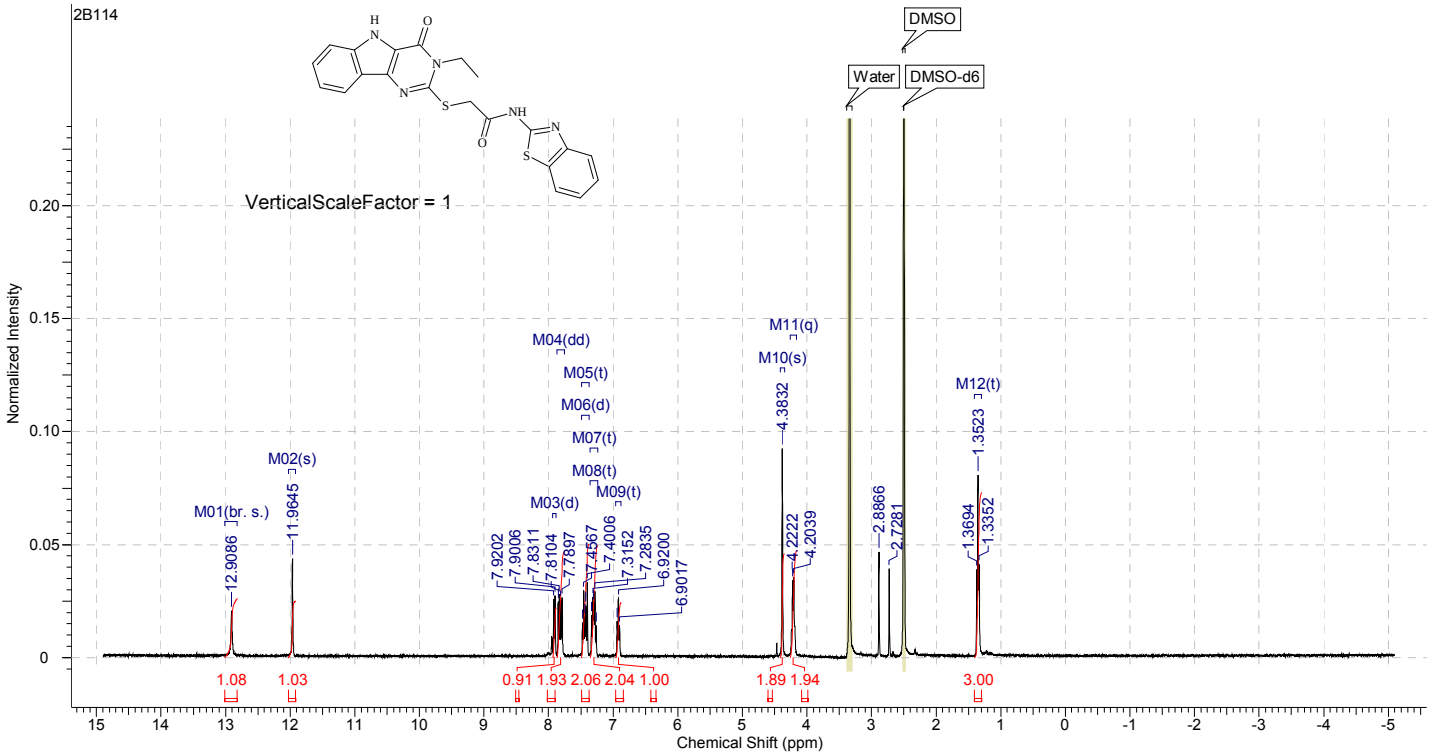
Exact Mass: 422.1

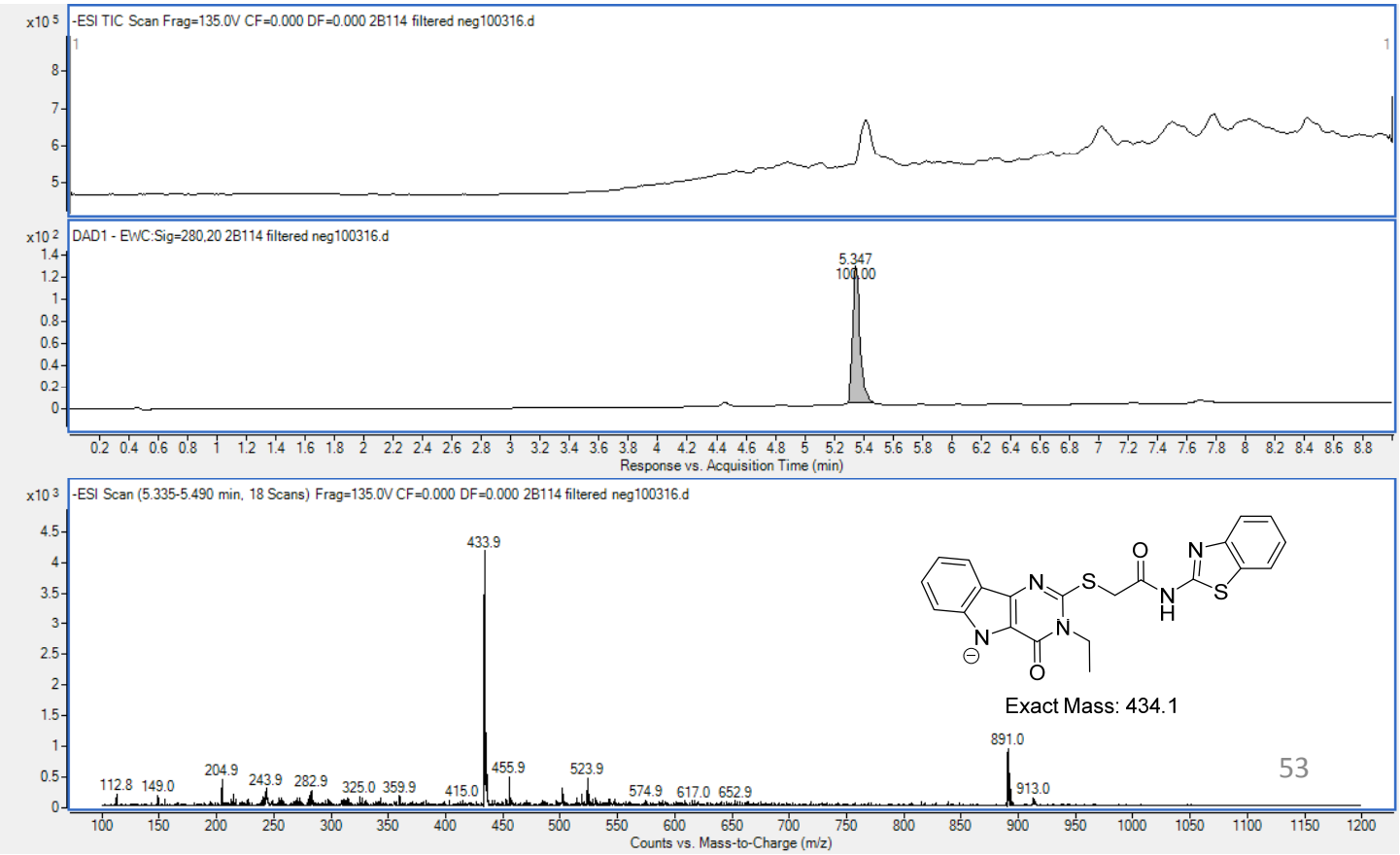
^{1}H NMR, LC-MS **6**{5,5}

4/20/2017 11:59:21 AM

Acquisition Time (sec)	2.0162	***Comment***	STANDARD 1H OBSERVE			***Date***	Dec 23 2016
Date Stamp	Dec 23 2016	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B114.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16117
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1960.5895	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.91 (br. s., 1H), 11.96 (s, 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.82 (dd, *J* = 8.29, 16.59 Hz, 2H), 7.46 (t, *J* = 7.80 Hz, 1H), 7.41 (d, *J* = 8.29 Hz, 1H), 7.32 (t, *J* = 7.40 Hz, 1H), 7.28 (t, *J* = 7.50 Hz, 1H), 6.92 (t, *J* = 7.32 Hz, 1H), 4.38 (s, 2H), 4.21 (q, *J* = 7.30 Hz, 2H), 1.35 (t, *J* = 6.83 Hz, 3H)





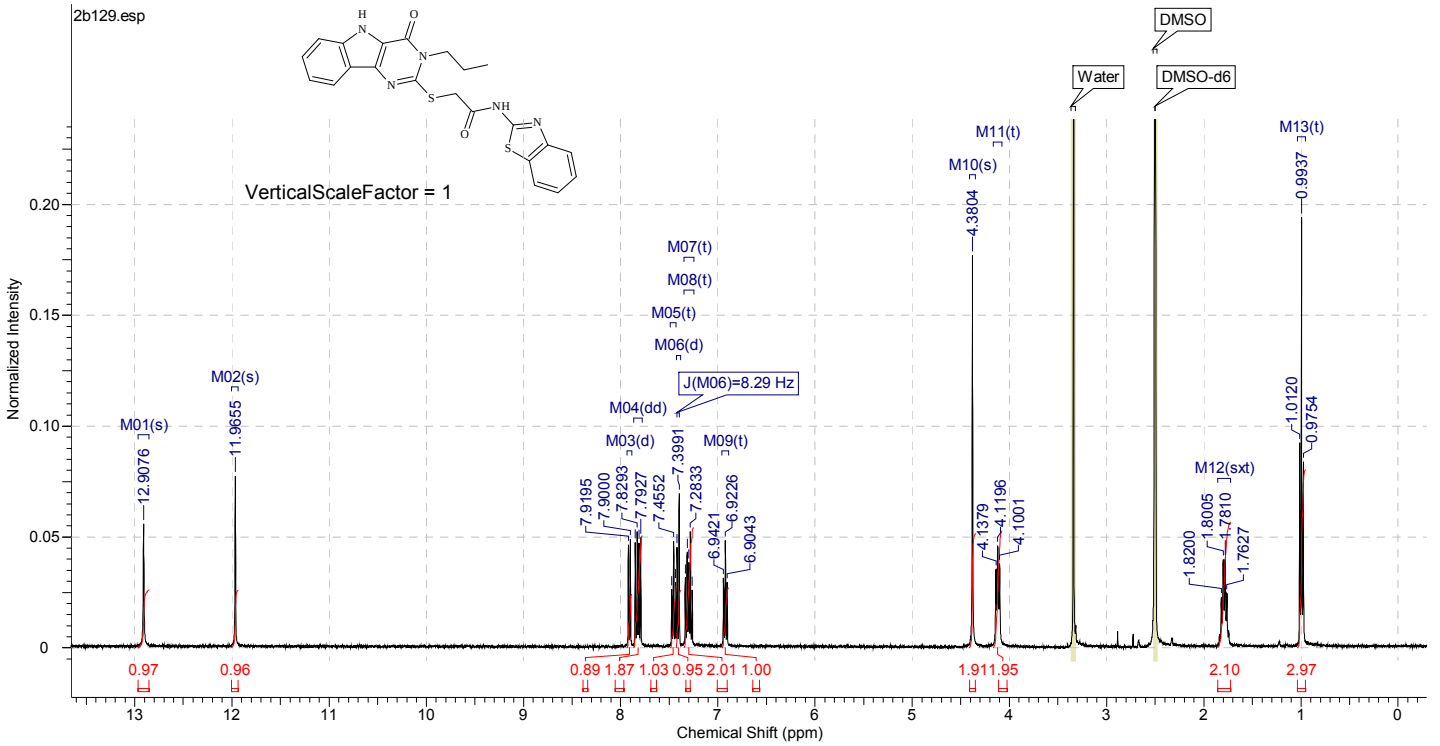
Exact Mass: 434.1

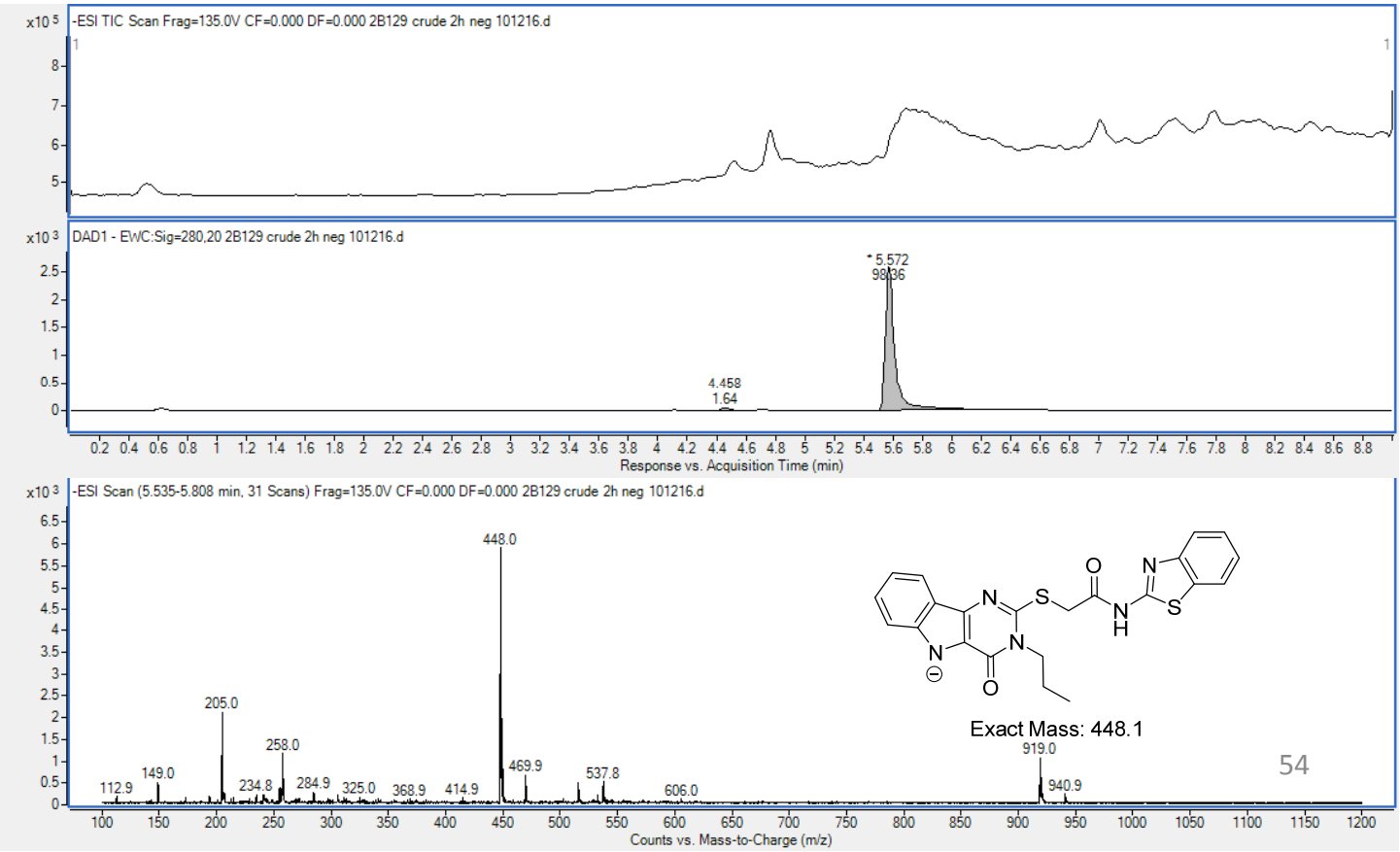
^{1}H NMR, LC-MS **6**{6,5}

4/20/2017 12:14:53 PM

Acquisition Time (sec)	2.0016	***Comment***	STANDARD 1H OBSERVE			***Date***	Dec 23 2016
Date Stamp	Dec 23 2016	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b129.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	15987
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1961.7723	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7987.22	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.91 (s, 1H), 11.97 (s, 1H), 7.91 (d, *J* = 7.80 Hz, 1H), 7.82 (dd, *J* = 8.29, 14.63 Hz, 2H), 7.46 (t, *J* = 7.56 Hz, 1H), 7.41 (d, *J* = 8.29 Hz, 1H), 7.32 (t, *J* = 7.80 Hz, 1H), 7.28 (t, *J* = 7.80 Hz, 1H), 6.92 (t, *J* = 7.56 Hz, 1H), 4.38 (s, 2H), 4.12 (t, *J* = 7.80 Hz, 2H), 1.79 (sxt, *J* = 7.80 Hz, 2H), 0.99 (t, *J* = 7.31 Hz, 3H)



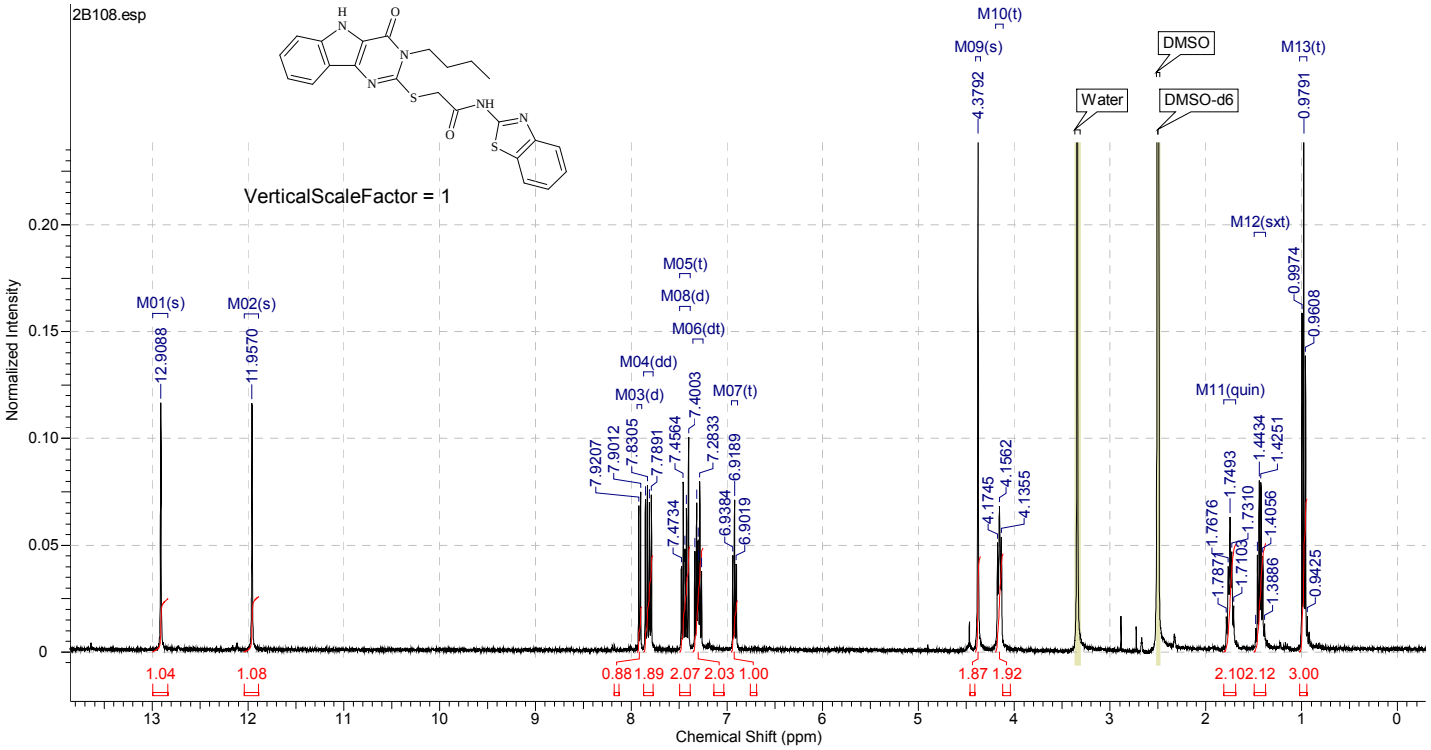


^{1}H, ^{13}C NMR **6**{7,5}

4/20/2017 12:20:47 PM

Acquisition Time (sec)	1.9983	***Comment***	STANDARD 1H OBSERVE			***Date***	Dec 23 2016
Date Stamp	Dec 23 2016	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B108.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	15961
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1961.7723	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7987.22	***Temperature (degree C)***	AMBIENT TEMPERATURE

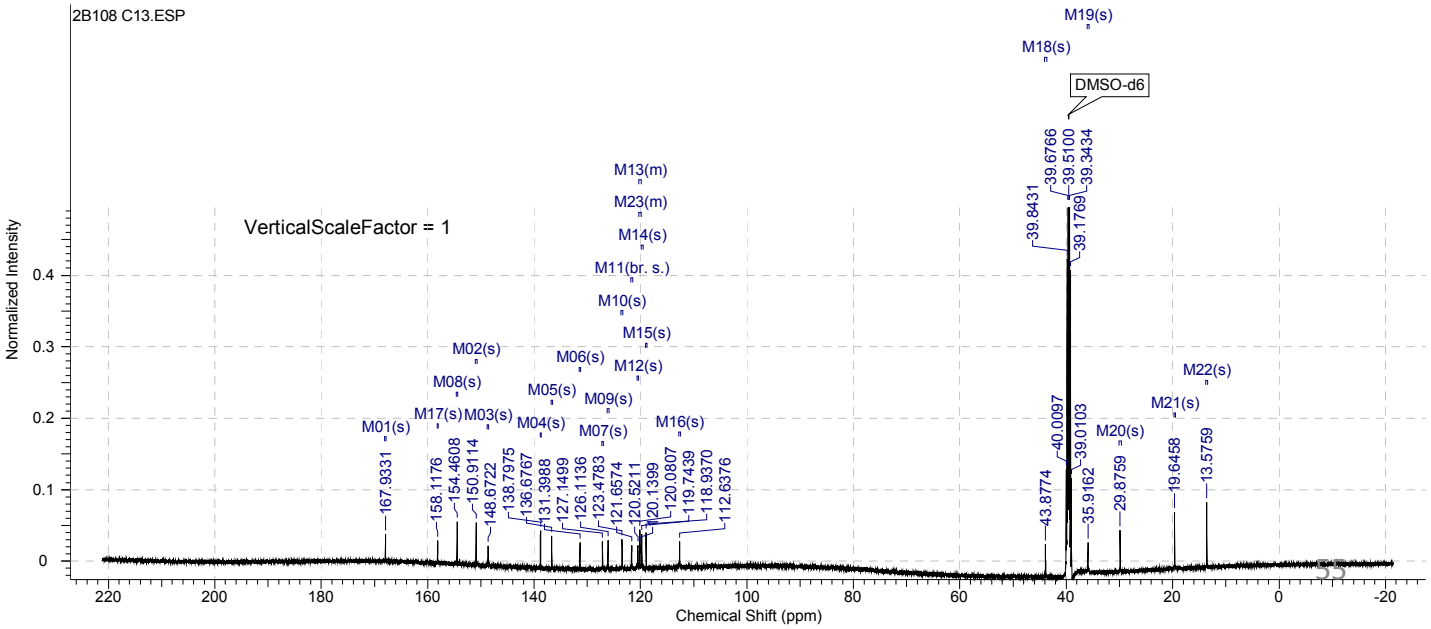
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.91 (s, 1H), 11.96 (s, 1H), 7.91 (d, *J* = 7.80 Hz, 1H), 7.82 (dd, *J* = 8.04, 16.82 Hz, 2H), 7.46 (t, *J* = 7.30 Hz, 1H), 7.41 (d, *J* = 8.29 Hz, 1H), 7.30 (td, *J* = 7.31, 12.68 Hz, 2H), 6.92 (t, *J* = 7.31 Hz, 1H), 4.38 (s, 2H), 4.16 (t, *J* = 7.80 Hz, 2H), 1.75 (quin, *J* = 7.68 Hz, 2H), 1.43 (sxt, *J* = 7.41 Hz, 2H), 0.98 (t, *J* = 7.31 Hz, 3H)



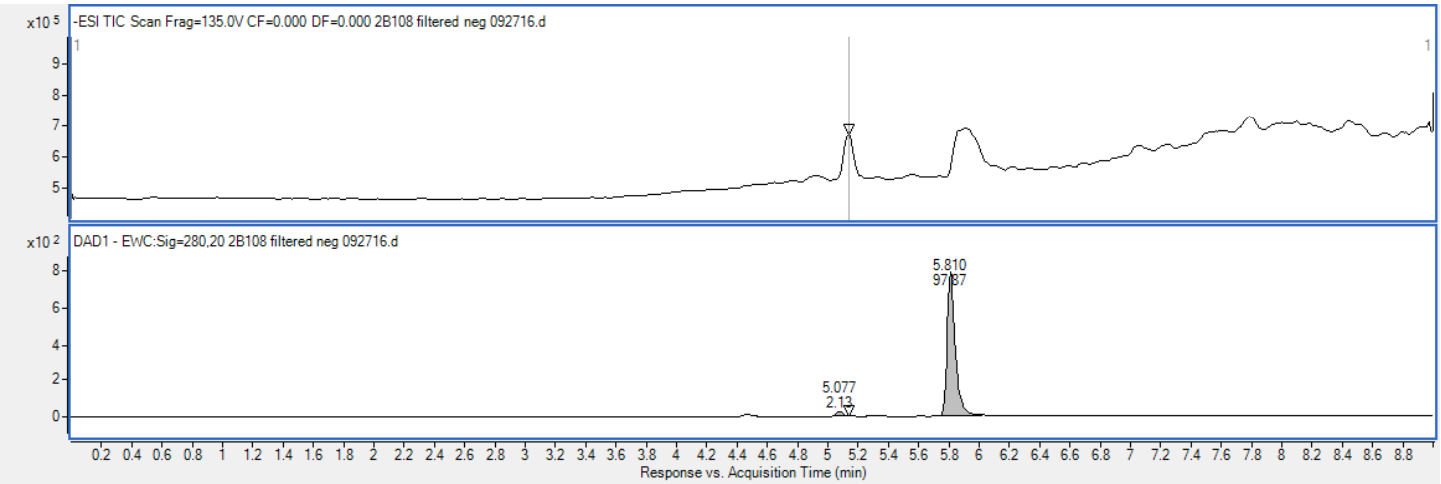
4/21/2017 11:10:53 AM

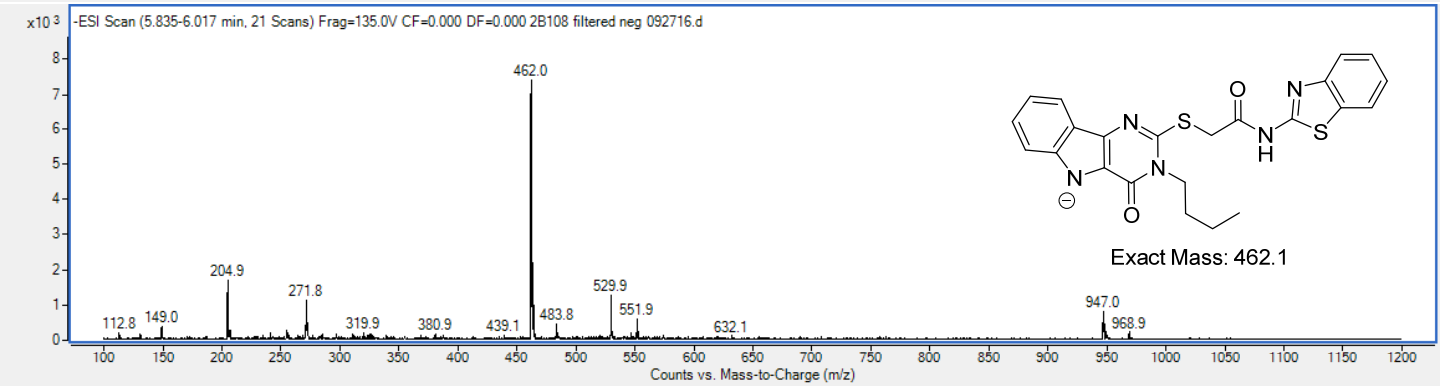
Acquisition Time (sec)	1.3005	***Comment***	Std carbon	***Date***	Apr 6 2017	***Date Stamp***	Apr 6 2017
File Name	C:\Documents and Settings\Mycoahhh\My Documents\NMR\C13 fids\2b108.fid\fid					***Frequency (MHz)***	125.69
Nucleus	13C	***Number of Transients***	32	***Original Points Count***	39649	***Points Count***	65536
Pulse Sequence	s2pul	***Receiver Gain***	60.00	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	12549.8545
Spectrum Type	STANDARD	***Sweep Width (Hz)***	30487.80	***Temperature (degree C)***	35.000		

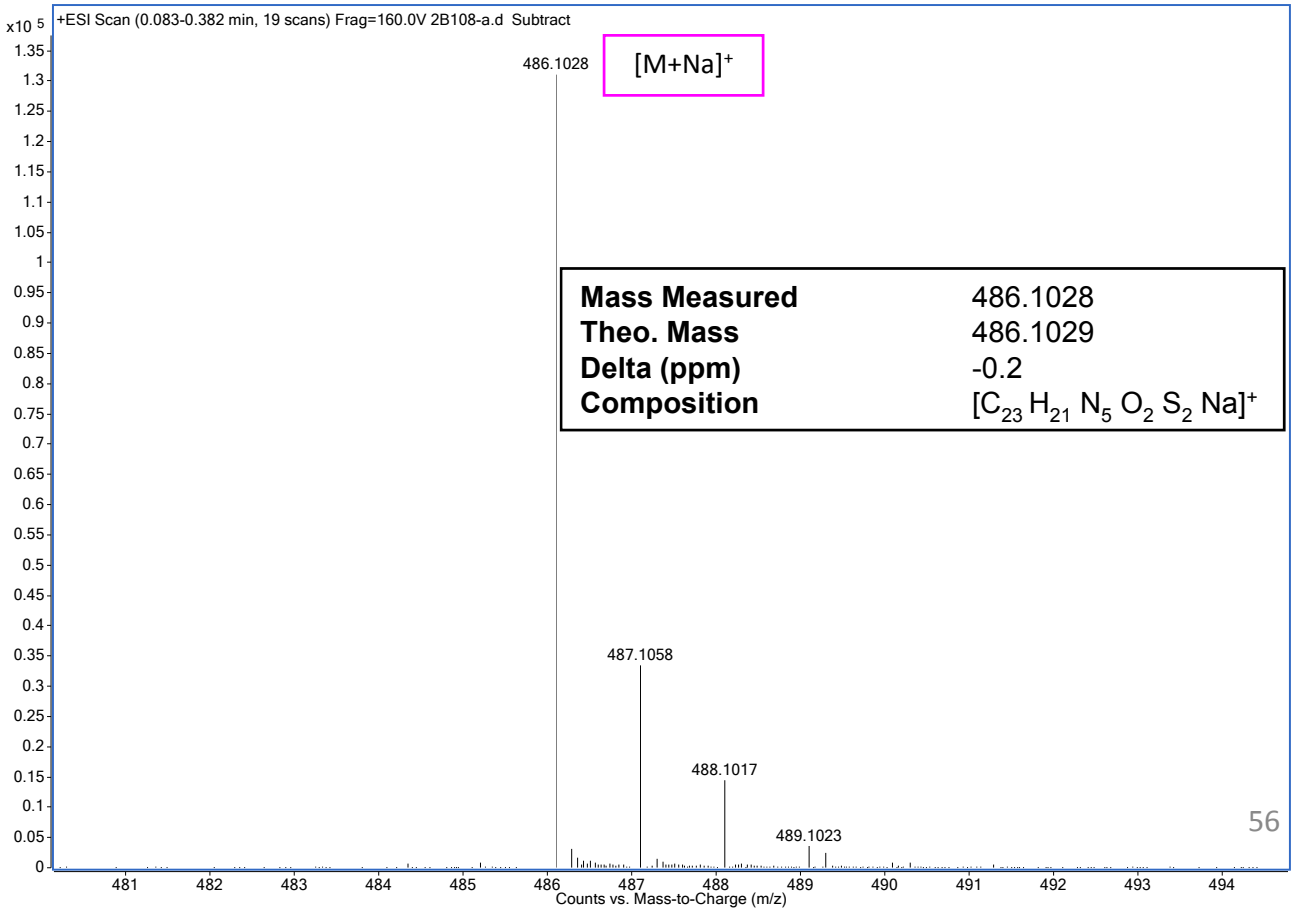
^{13}C NMR (126 MHz, BENZENE-d_6) δ 167.9, 158.1, 154.5, 150.9, 148.7, 138.8, 136.7, 131.4, 127.1, 126.1, 123.5, 121.7, 120.5, 120.1, 120.1, 119.7, 118.9, 112.6, 43.9, 35.9, 29.9, 19.6, 13.6



LC-MS and HRMS **6**{7,5}





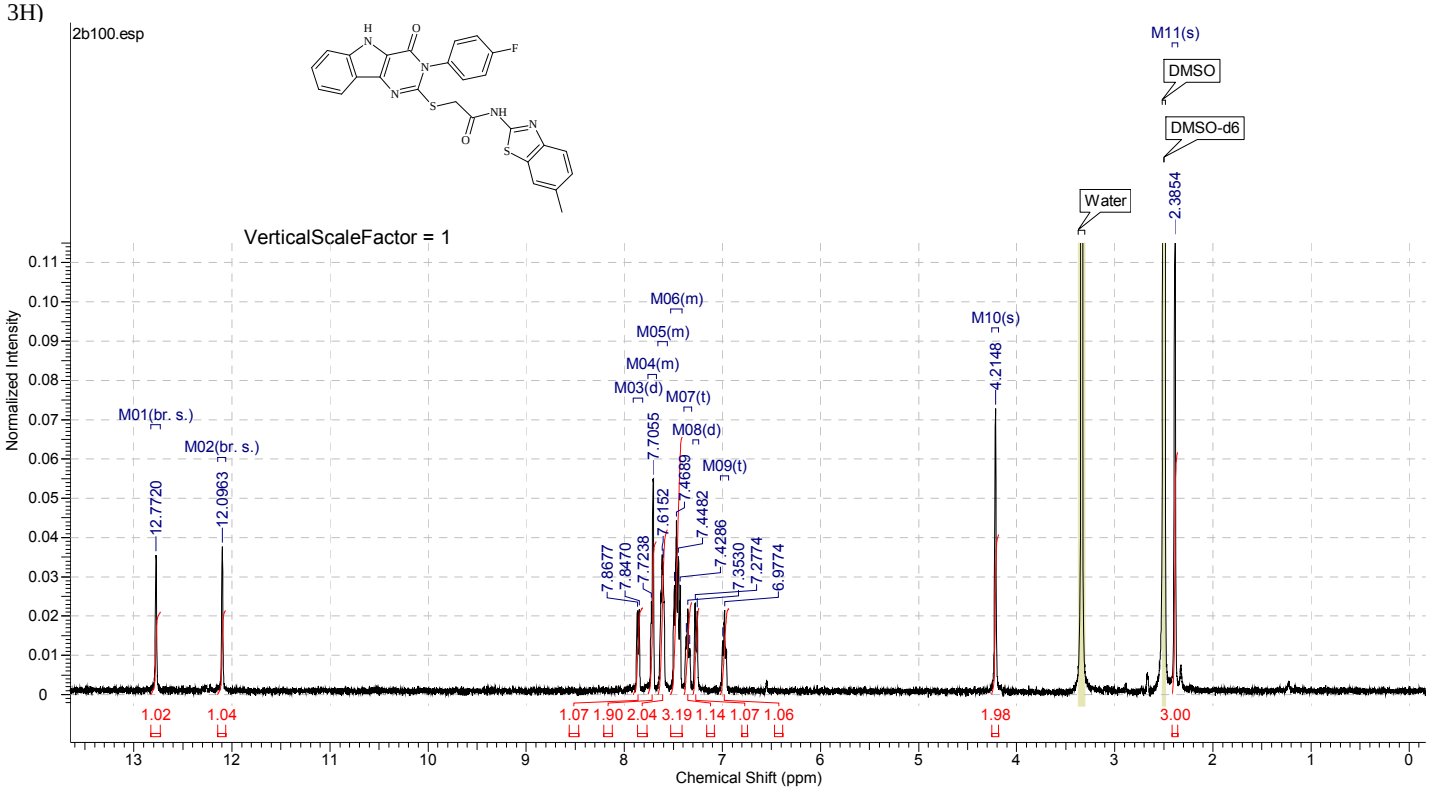


^{1}H, ^{13}C NMR **6**{1,6}

4/20/2017 12:29:28 PM

Acquisition Time (sec)	2.0065	***Comment***	STANDARD 1H OBSERVE			***Date***	Dec 23 2016
Date Stamp	Dec 23 2016	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b100.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16039
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1960.1014	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

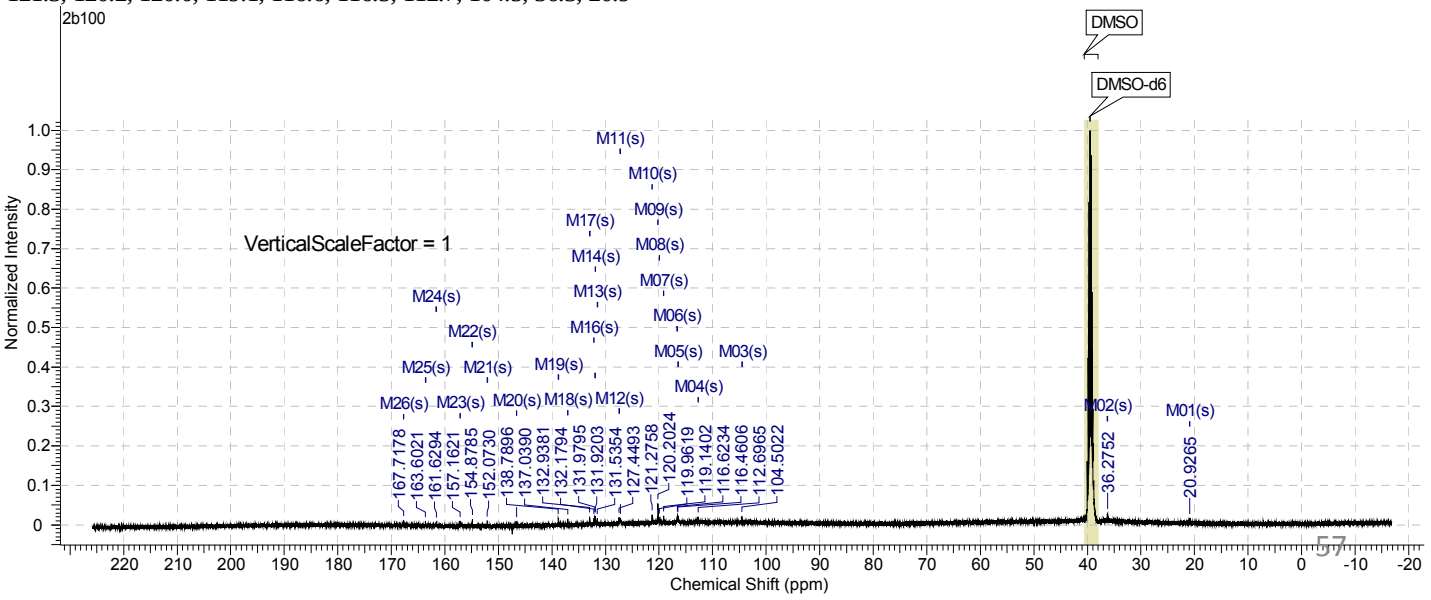
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.77 (br. s., 1H), 12.10 (br. s., 1H), 7.86 (d, *J* = 8.29 Hz, 1H), 7.67 - 7.76 (m, 2H), 7.56 - 7.66 (m, *J* = 3.90 Hz, 2H), 7.41 - 7.53 (m, *J* = 8.30, 16.60 Hz, 3H), 7.35 (t, *J* = 7.40 Hz, 1H), 7.27 (d, *J* = 8.29 Hz, 1H), 6.98 (t, *J* = 7.30 Hz, 1H), 4.22 (s, 2H), 2.39 (s, 3H)



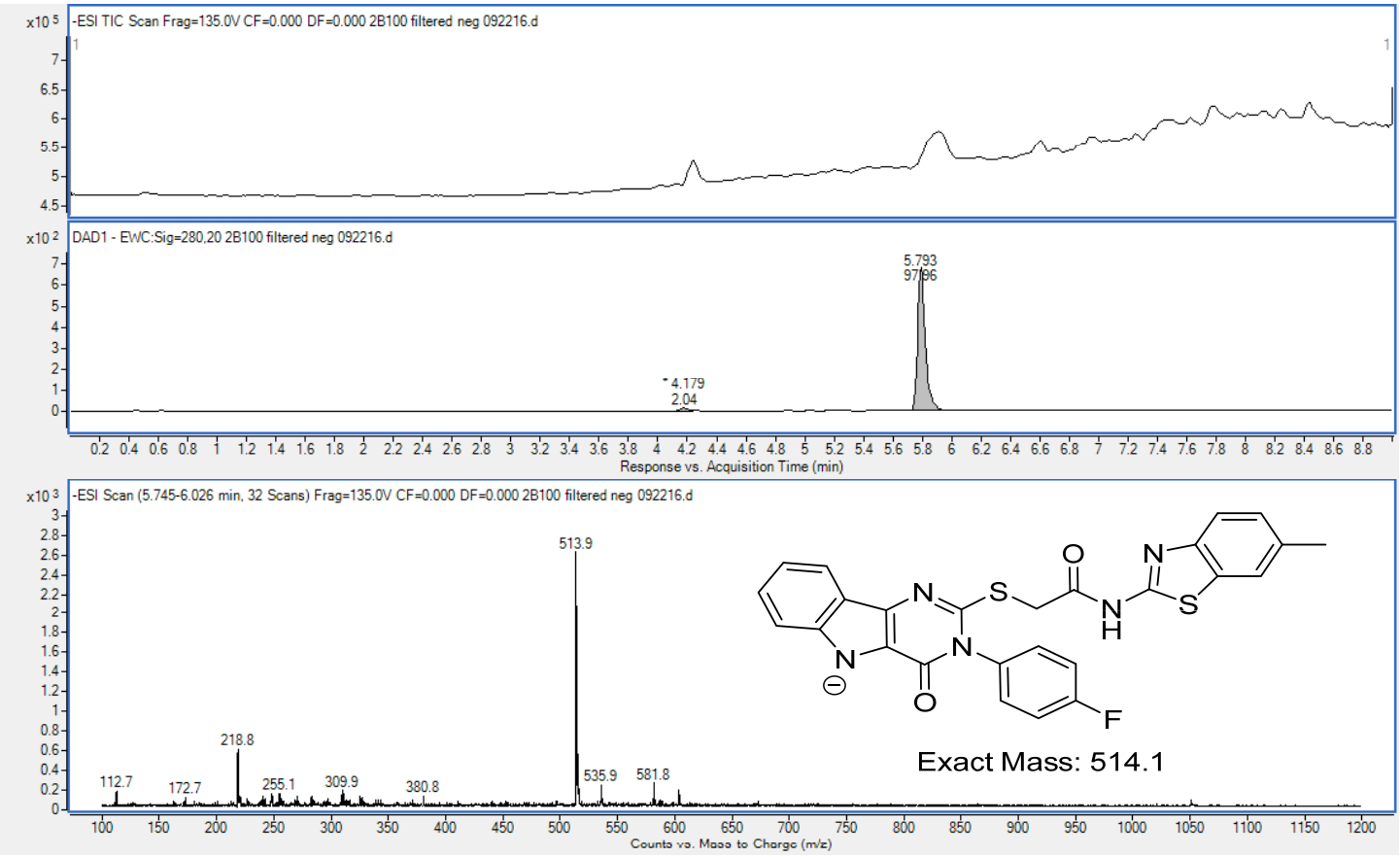
4/24/2017 2:55:19 PM

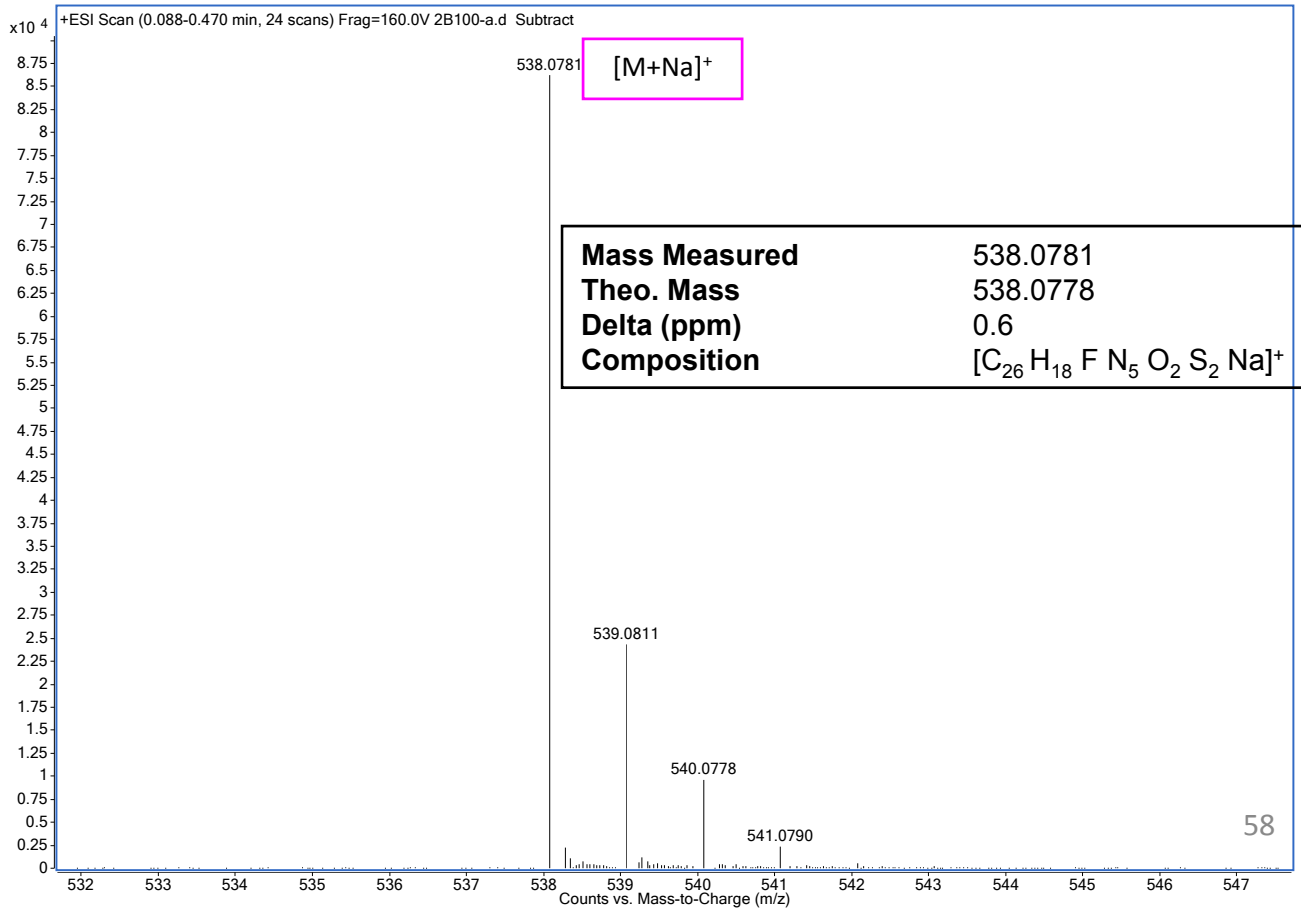
Acquisition Time (sec)	1.3005	***Comment***	Std carbon	***Date***	Apr 24 2017	***Date Stamp***	Apr 24 2017
File Name	C:\Documents and Settings\Mycoahhh\My Documents\NMR\C13 fids\2b100.fid\fid					***Frequency (MHz)***	125.69
Nucleus	13C	***Number of Transients***	128	***Original Points Count***	39649	***Points Count***	65536
Pulse Sequence	s2pul	***Receiver Gain***	56.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	13134.6514
Spectrum Type	STANDARD	***Sweep Width (Hz)***	30487.80	***Temperature (degree C)***	30.000		

^{13}C NMR (126 MHz, DMSO-d_6) δ 167.7, 163.6, 161.6, 157.2, 154.9, 152.1, 146.6, 138.8, 137.0, 132.9, 132.2, 132.0, 131.9, 131.5, 127.4, 127.2, 121.3, 120.2, 120.0, 119.1, 116.6, 116.5, 112.7, 104.5, 36.3, 20.9



LC-MS and HRMS **6**{1,6}





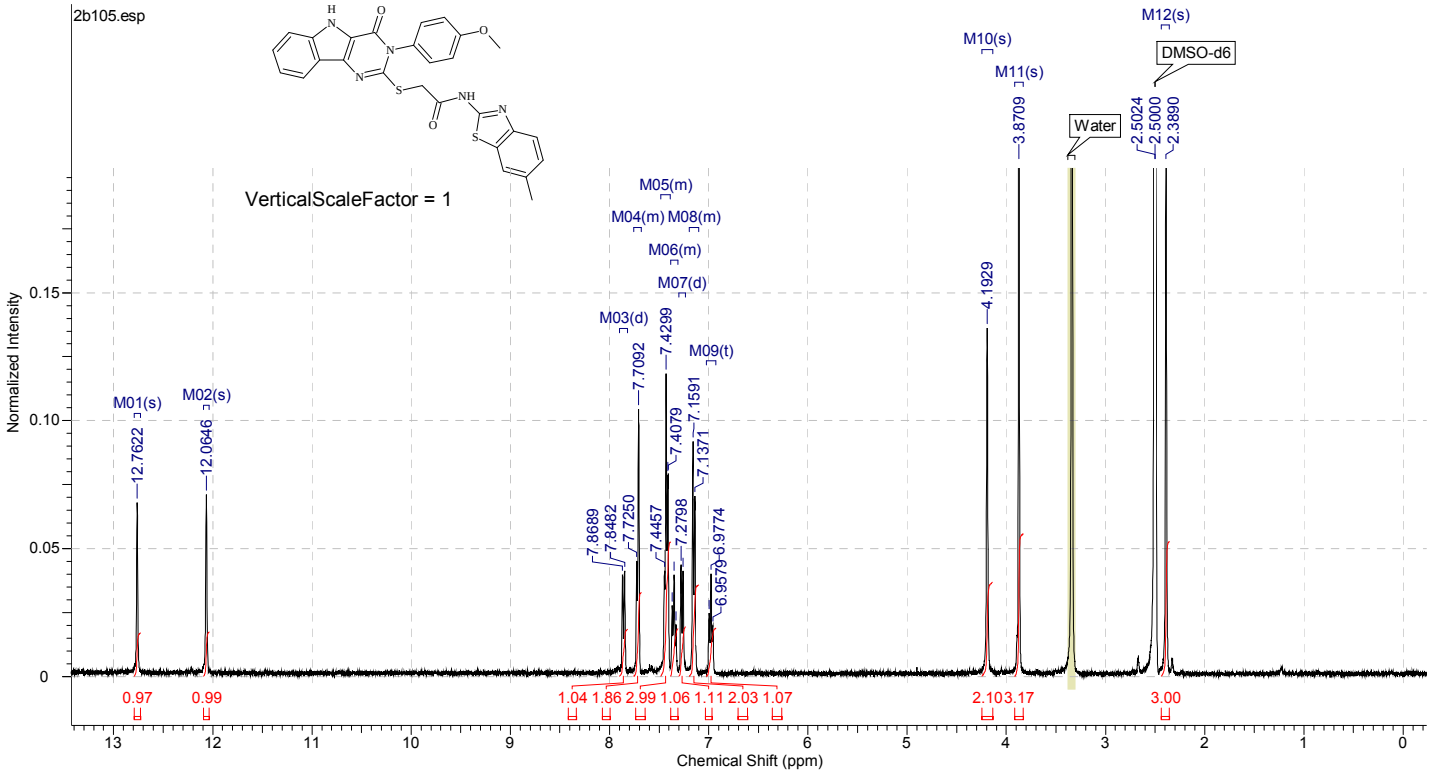
Mass Measured	538.0781
Theo. Mass	538.0778
Delta (ppm)	0.6
Composition	$[C_{26}H_{18}FN_5O_2S_2Na]^+$

^{1}H, ^{13}C NMR **6**{2,6}

4/20/2017 12:33:31 PM

Acquisition Time (sec)	2.0146	***Comment***	STANDARD 1H OBSERVE			***Date***	Dec 23 2016
Date Stamp	Dec 23 2016	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b105.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16104
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1961.0773	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

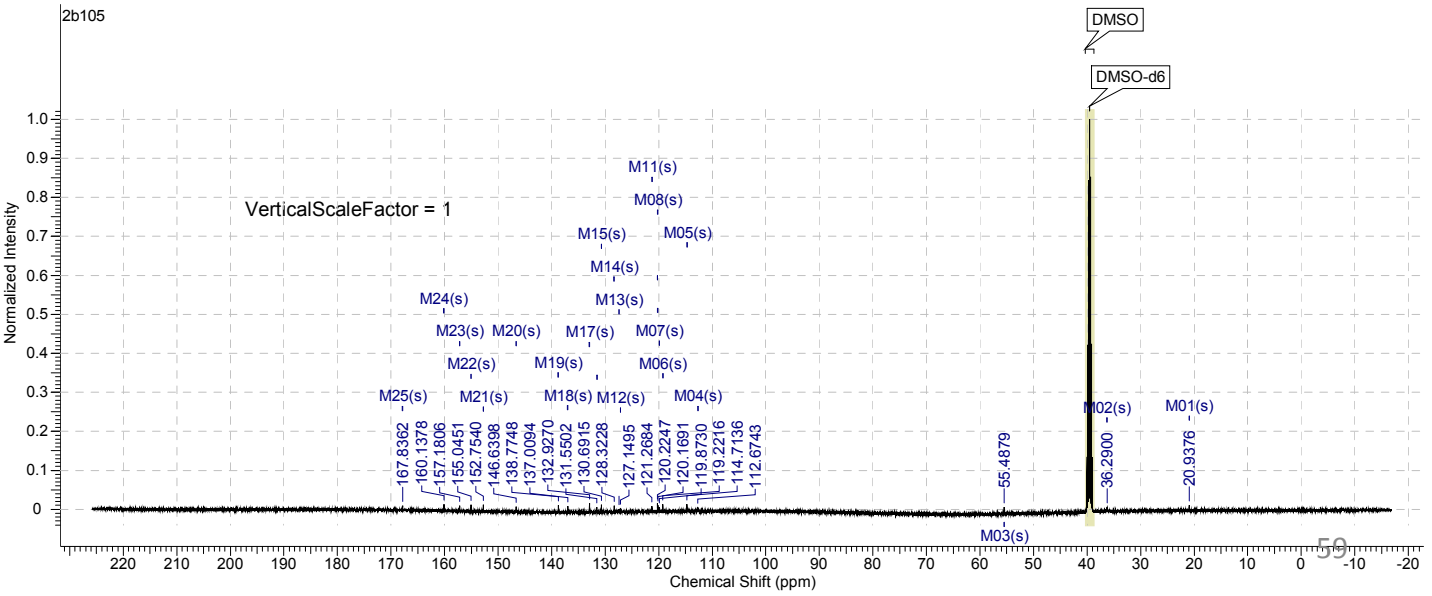
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.76 (s, 1H), 12.06 (s, 1H), 7.86 (d, *J* = 8.29 Hz, 1H), 7.68 - 7.76 (m, 2H), 7.39 - 7.48 (m, 3H), 7.31 - 7.38 (m, 1H), 7.27 (d, *J* = 8.29 Hz, 1H), 7.10 - 7.19 (m, 2H), 6.98 (t, *J* = 7.32 Hz, 1H), 4.19 (s, 2H), 3.87 (s, 3H), 2.39 (s, 3H)



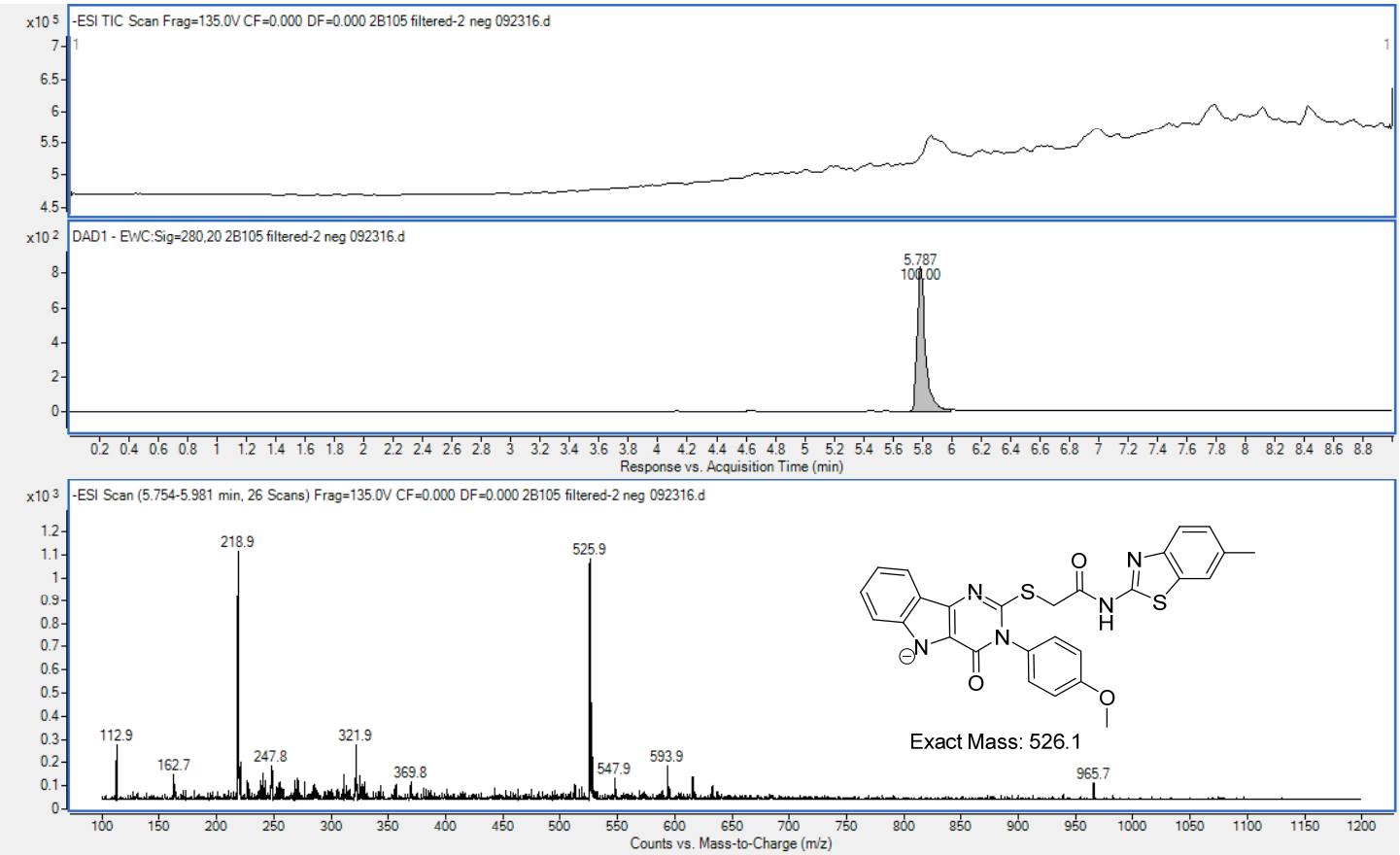
4/24/2017 3:04:03 PM

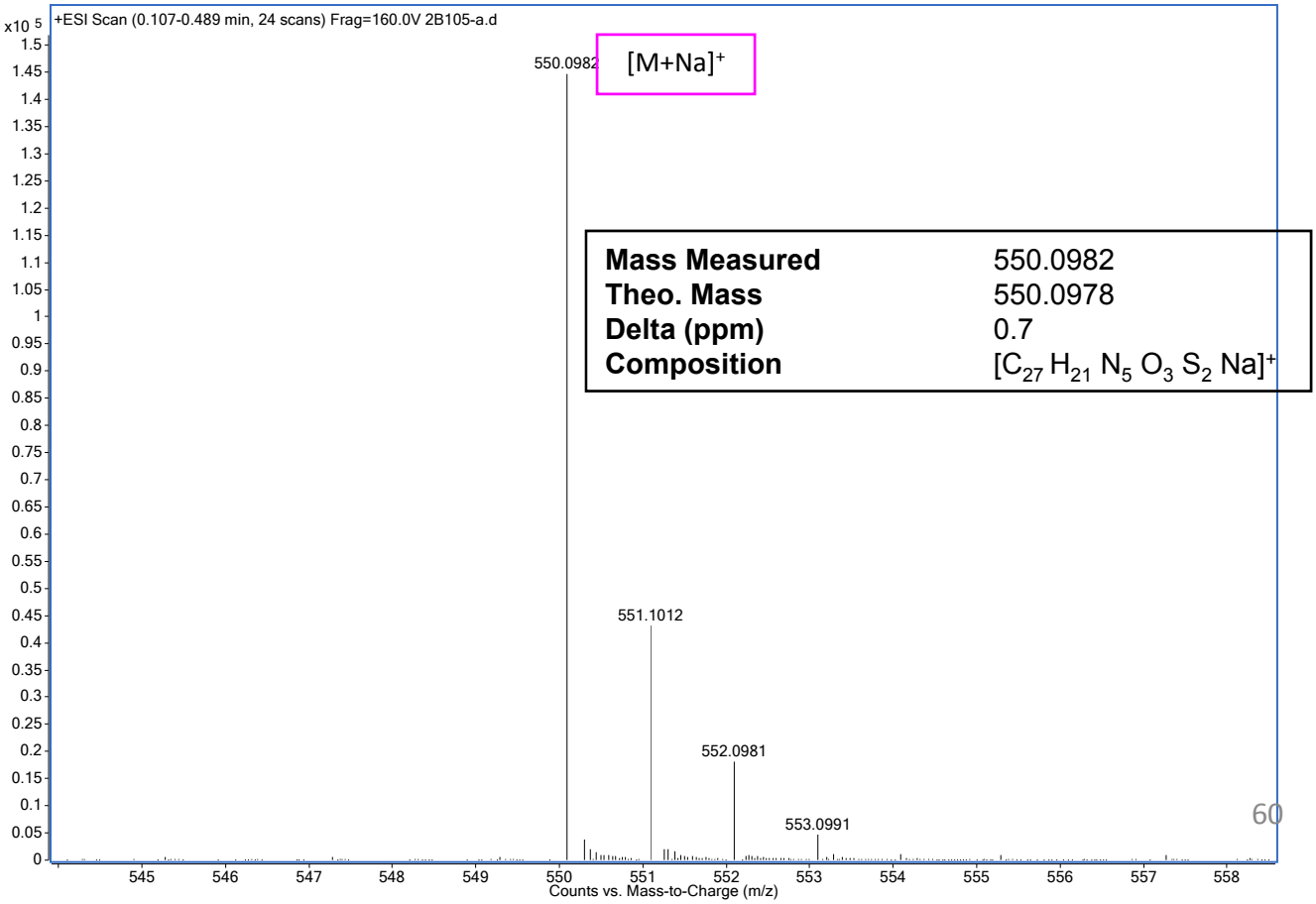
Acquisition Time (sec)	1.3005	***Comment***	Std carbon	***Date***	Apr 24 2017	***Date Stamp***	Apr 24 2017
File Name	C:\Documents and Settings\Mycoahhh\My Documents\NMR\C13 fids\2b105.fid\fid					***Frequency (MHz)***	125.69
Nucleus	13C	***Number of Transients***	128	***Original Points Count***	39649	***Points Count***	65536
Pulse Sequence	s2pul	***Receiver Gain***	58.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	13136.5117
Spectrum Type	STANDARD	***Sweep Width (Hz)***	30487.80	***Temperature (degree C)***	30.000		

^{13}C NMR (126 MHz, DMSO-d_6) δ 167.8, 160.1, 157.2, 155.0, 152.8, 146.6, 138.8, 137.0, 132.9, 131.6, 130.7, 128.3, 127.4, 127.1, 121.3, 120.2, 120.2, 120.2, 119.9, 119.2, 114.7, 112.7, 55.5, 36.3, 20.9



LC-MS and HRMS **6**{2,6}





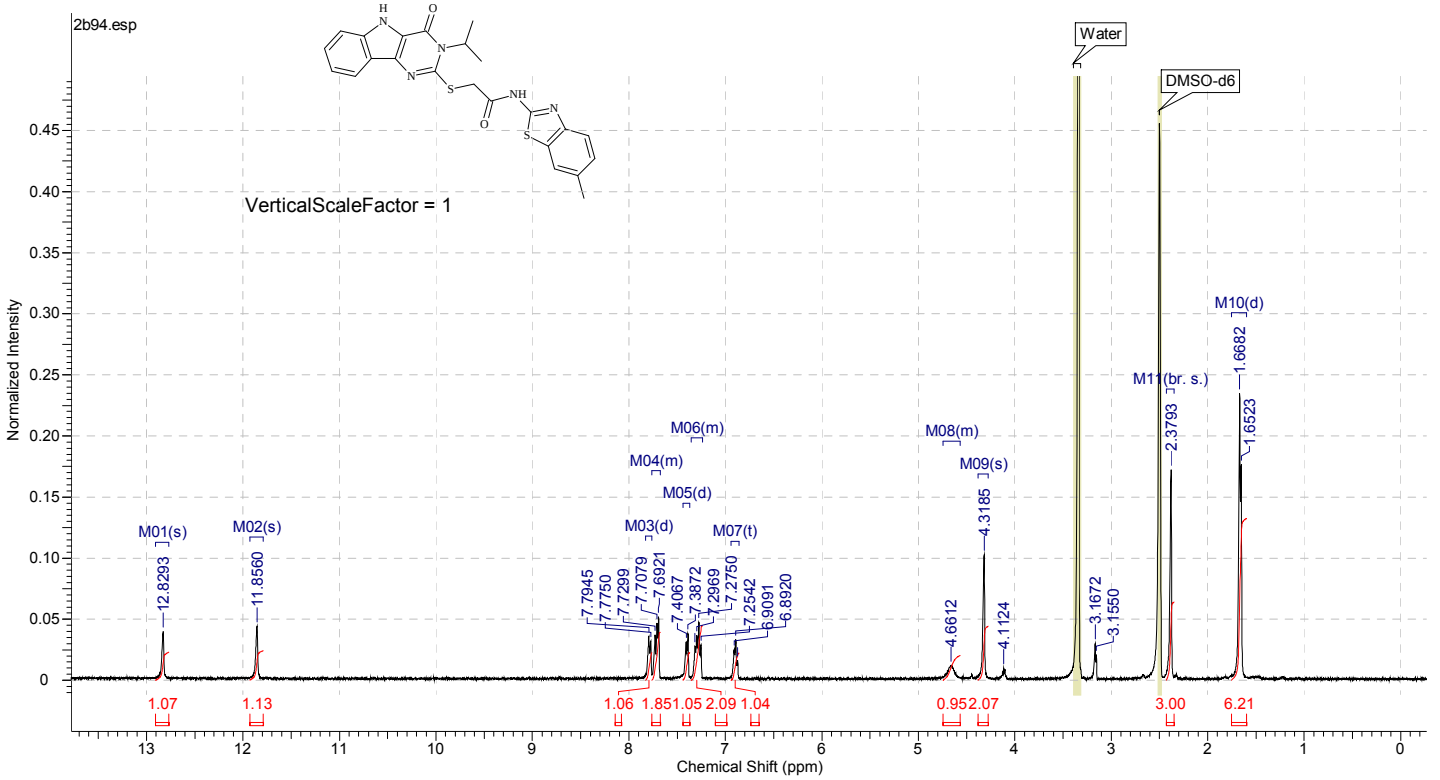
Mass Measured	550.0982
Theo. Mass	550.0978
Delta (ppm)	0.7
Composition	$[C_{27}H_{21}N_5O_3S_2Na]^+$

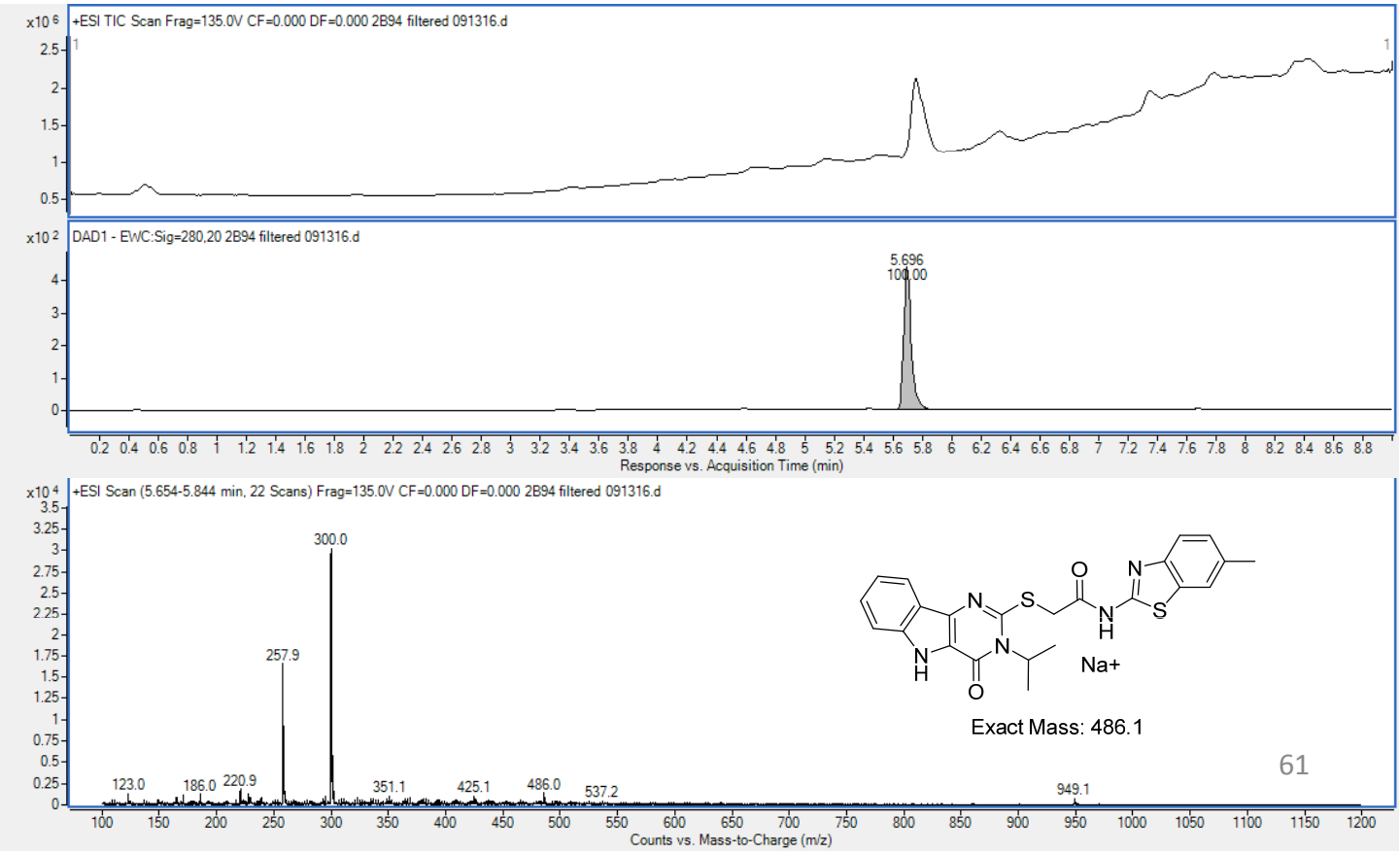
^{1}H NMR, LC-MS **6**{3,6}

4/20/2017 12:40:11 PM

Acquisition Time (sec)	2.0097	***Comment***	STANDARD 1H OBSERVE			***Date***	Dec 23 2016
Date Stamp	Dec 23 2016	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b94.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16065
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1960.5895	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.83 (s, 1H), 11.86 (s, 1H), 7.78 (d, *J* = 7.81 Hz, 1H), 7.67 - 7.76 (m, 2H), 7.40 (d, *J* = 7.81 Hz, 1H), 7.24 - 7.35 (m, 2H), 6.89 (t, *J* = 7.30 Hz, 1H), 4.57 - 4.74 (m, 1H), 4.32 (s, 2H), 2.38 (br. s., 3H), 1.66 (d, *J* = 6.34 Hz, 6H)



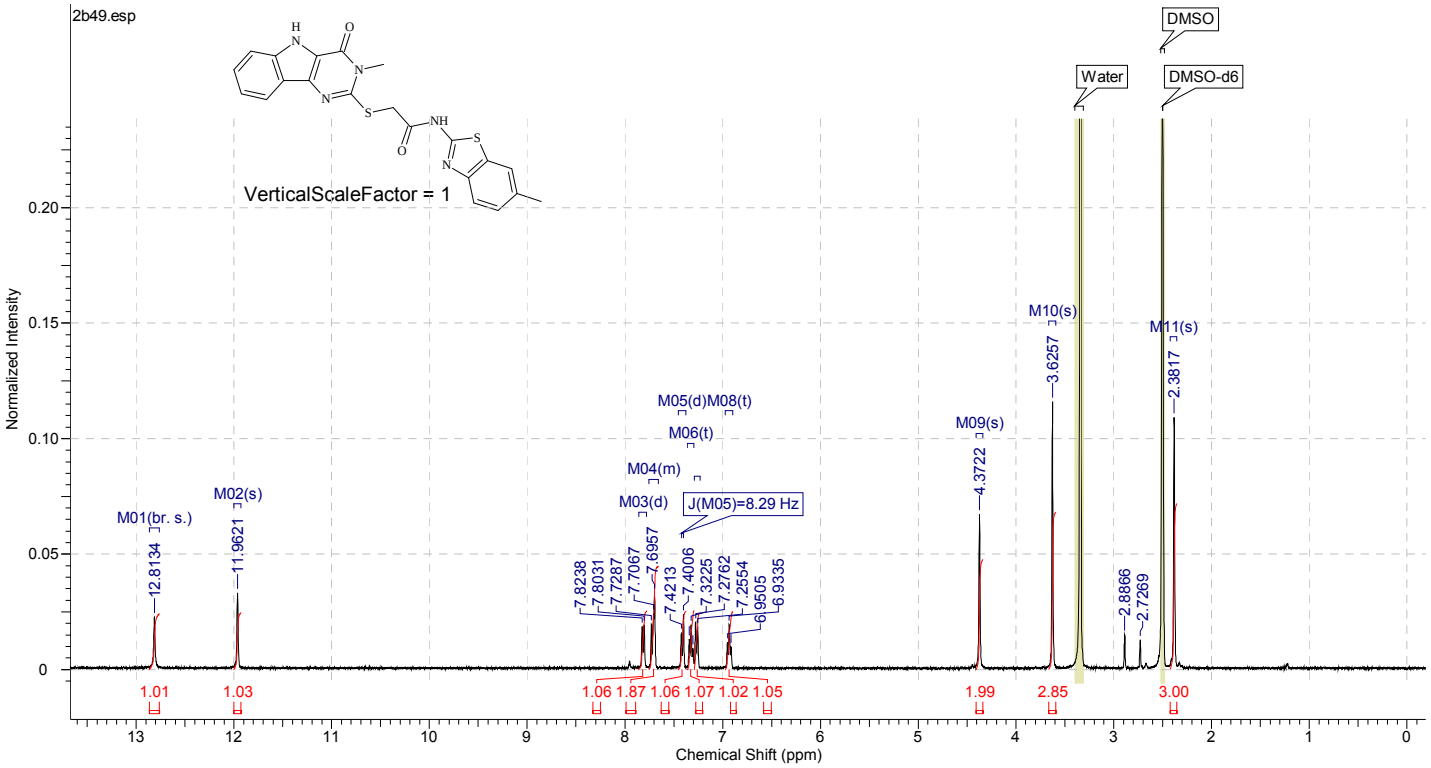


^{1}H, ^{13}C NMR **6**{4,6}

4/20/2017 1:12:10 PM

Acquisition Time (sec)	2.0195	***Comment***	STANDARD 1H OBSERVE			***Date***	Dec 23 2016
Date Stamp	Dec 23 2016	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b49.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16143
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1961.0773	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

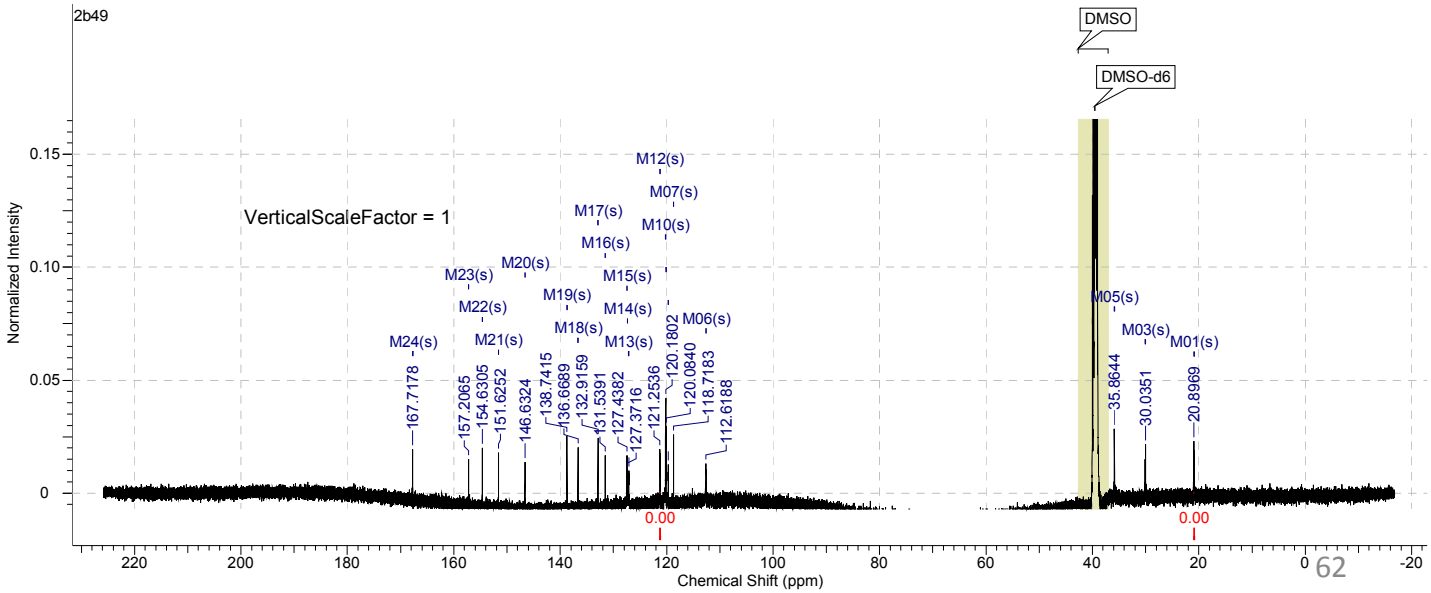
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.81 (br. s., 1H), 11.96 (s, 1H), 7.81 (d, *J* = 8.29 Hz, 1H), 7.66 - 7.75 (m, 2H), 7.41 (d, *J* = 8.29 Hz, 1H), 7.32 (t, *J* = 7.80 Hz, 1H), 7.27 (d, *J* = 8.29 Hz, 1H), 6.93 (t, *J* = 7.32 Hz, 1H), 4.37 (s, 2H), 3.63 (s, 3H), 2.38 (s, 3H)



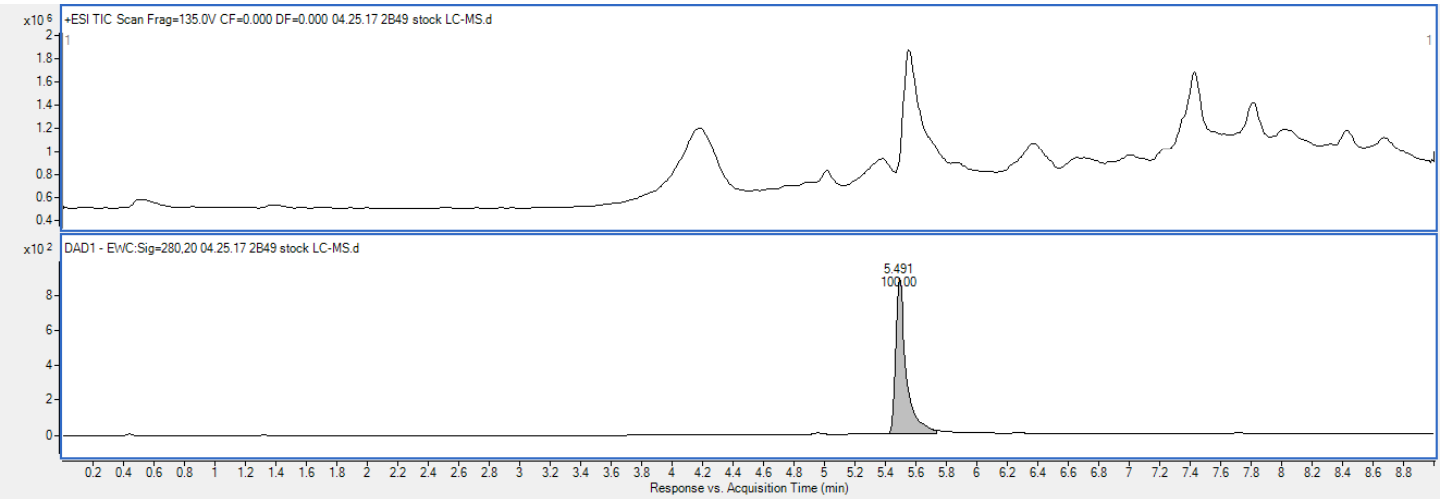
4/24/2017 2:49:06 PM

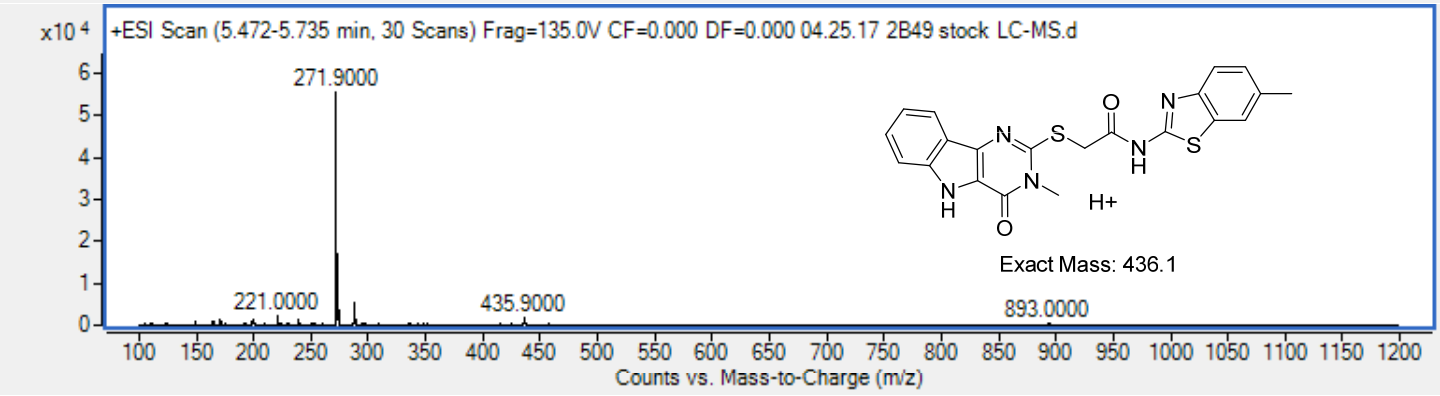
Acquisition Time (sec)	1.3005	***Comment***	Std carbon	***Date***	Apr 24 2017	***Date Stamp***	Apr 24 2017
File Name	C:\Documents and Settings\Mycoahhh\My Documents\NMR\C13 fids\2b49.fid\fid					***Frequency (MHz)***	125.69
Nucleus	13C	***Number of Transients***	128	***Original Points Count***	39649	***Points Count***	65536
Pulse Sequence	s2pul	***Receiver Gain***	56.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	13134.1855
Spectrum Type	STANDARD	***Sweep Width (Hz)***	30487.80	***Temperature (degree C)***	30.000		

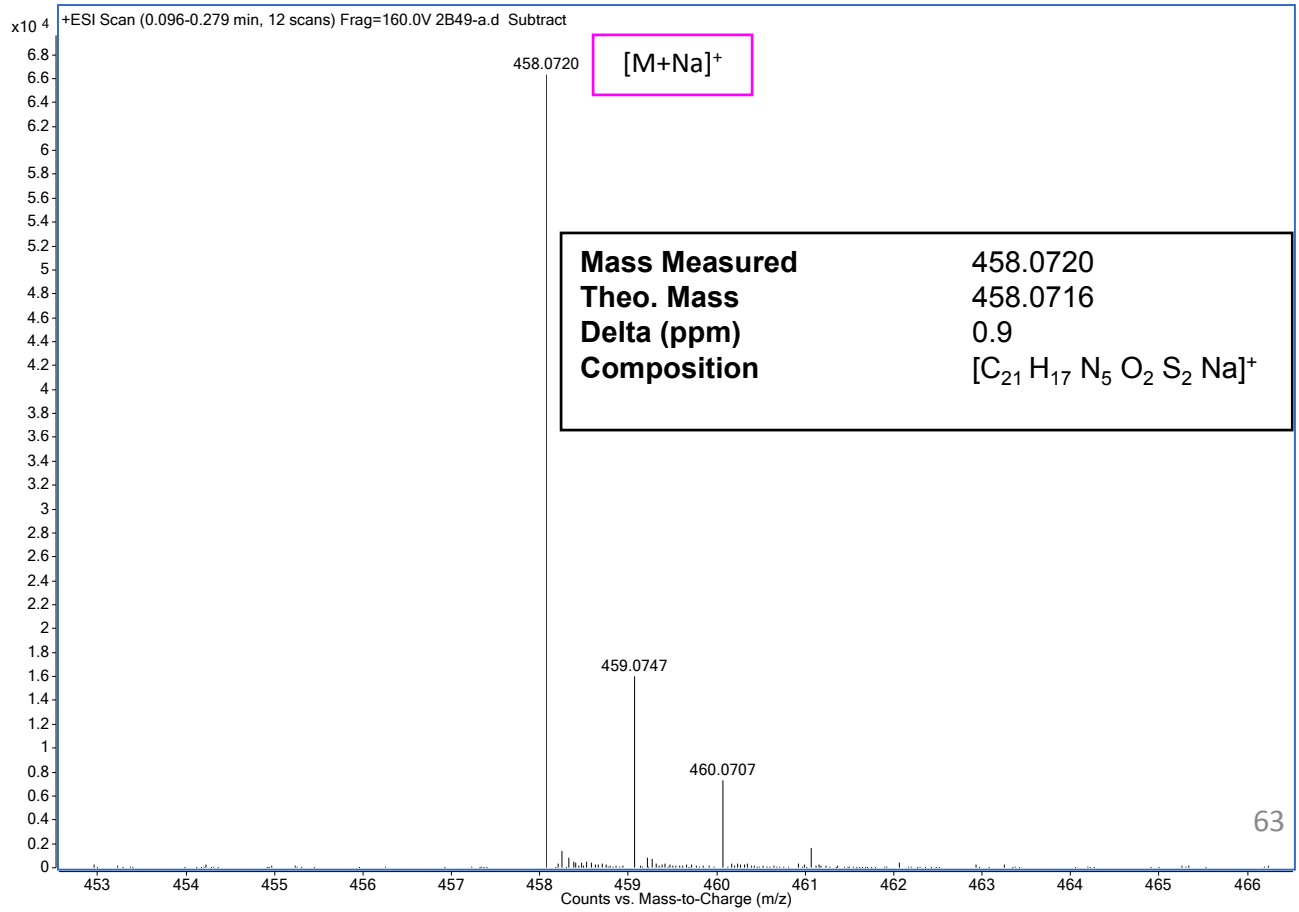
^{13}C NMR (126 MHz, DMSO-d_6) δ 167.7, 157.2, 154.6, 151.6, 146.6, 138.7, 136.7, 132.9, 131.5, 127.4, 127.4, 127.1, 121.3, 120.2, 120.1, 119.7, 118.7, 112.6, 35.9, 30.0, 20.9



LC-MS and HRMS **6**{4,6}





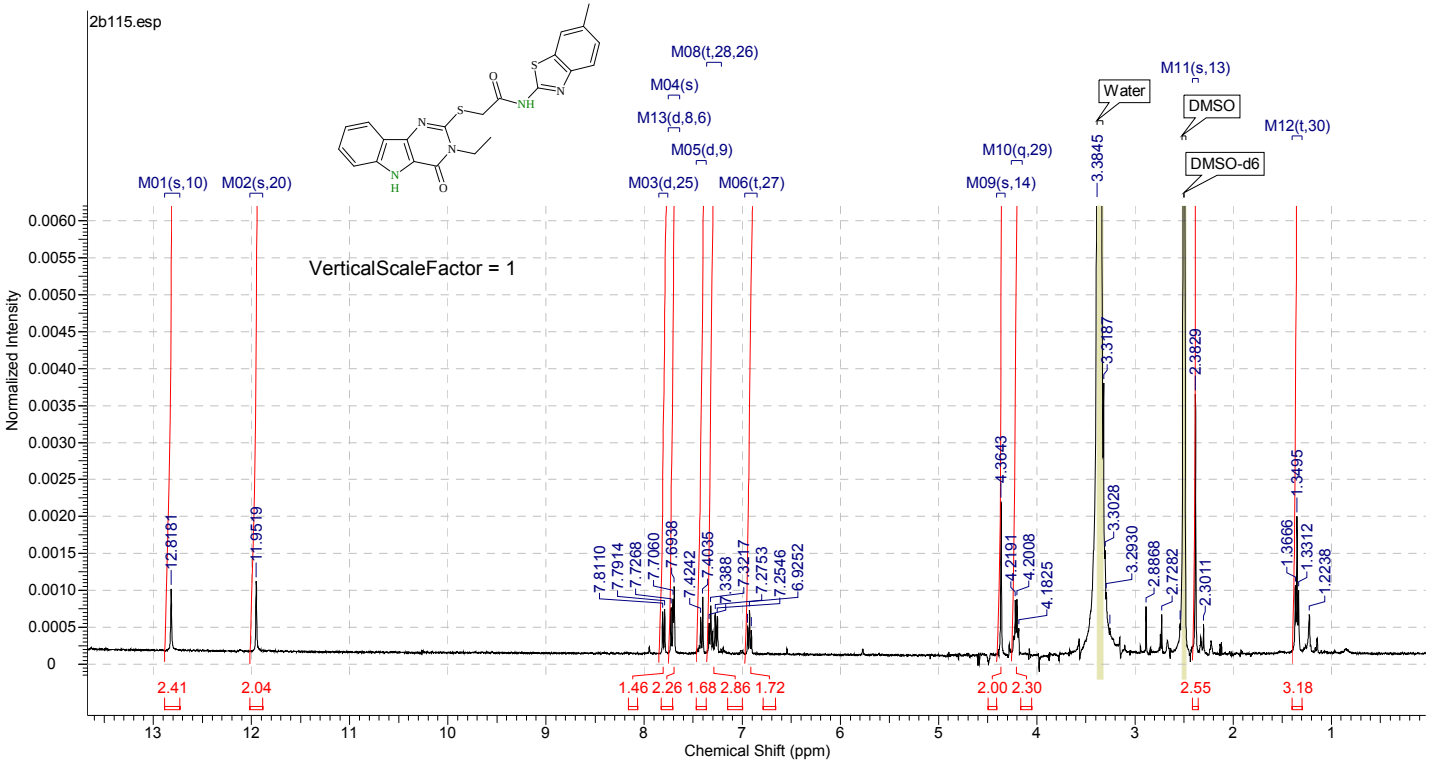


^{1}H, ^{13}C NMR **6**{5,6}

3/29/2017 2:24:35 PM

Acquisition Time (sec)	2.0276	***Comment***	STANDARD 1H OBSERVE			***Date***	Mar 29 2017
Date Stamp	Mar 29 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b115.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	200	***Original Points Count***	16208
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	24.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2033.4424	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

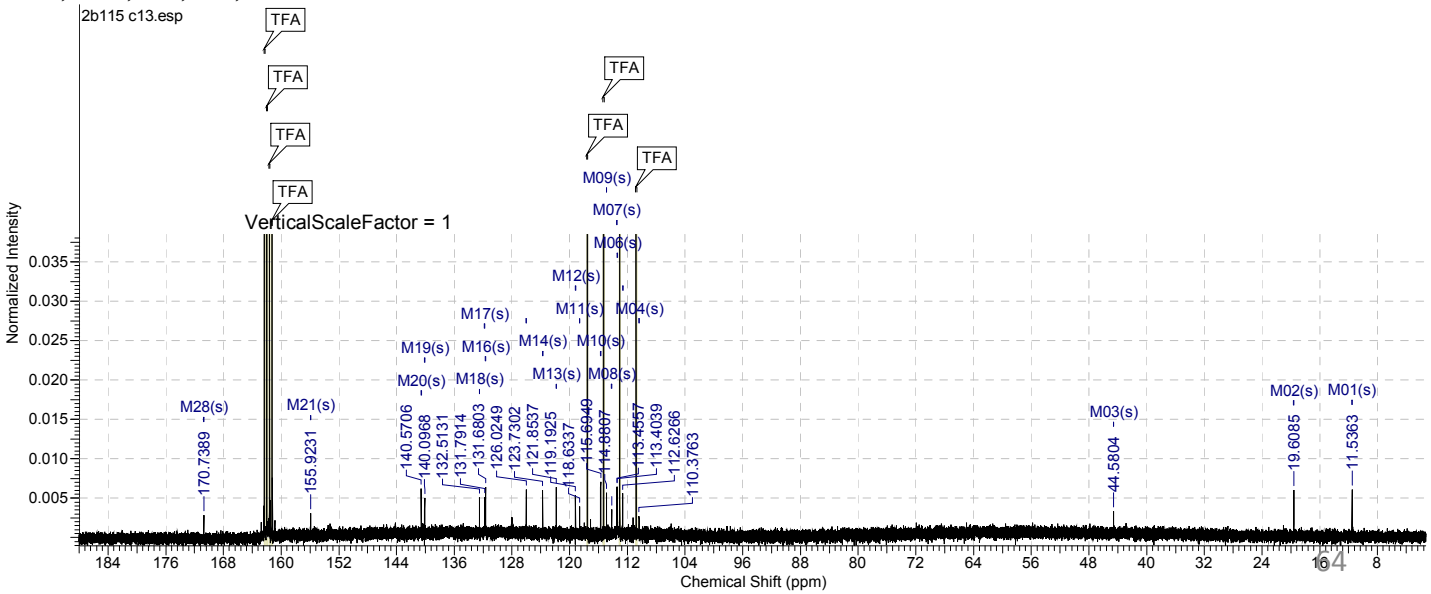
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.82 (s, 1H), 11.95 (s, 1H), 7.80 (d, *J* = 7.81 Hz, 1H), 7.69 (s, 1H), 7.72 (d, *J* = 8.29 Hz, 1H), 7.41 (d, *J* = 8.29 Hz, 1H), 7.26 (d, *J* = 8.29 Hz, 1H), 7.32 (t, *J* = 7.80 Hz, 1H), 6.93 (t, *J* = 7.56 Hz, 1H), 4.36 (s, 2H), 4.21 (q, *J* = 7.32 Hz, 2H), 2.38 (s, 3H), 1.35 (t, *J* = 7.07 Hz, 3H)



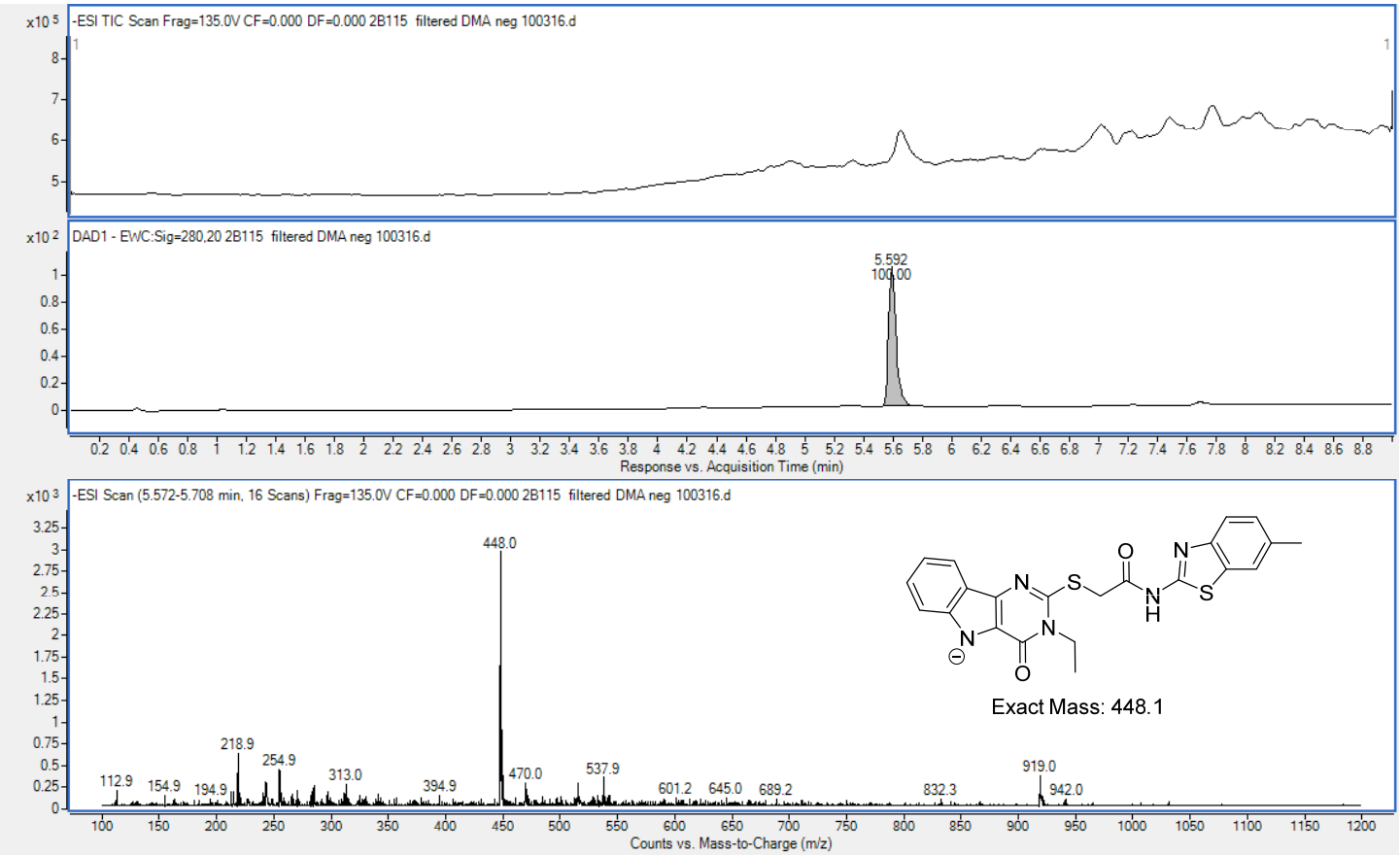
4/25/2017 10:40:55 AM

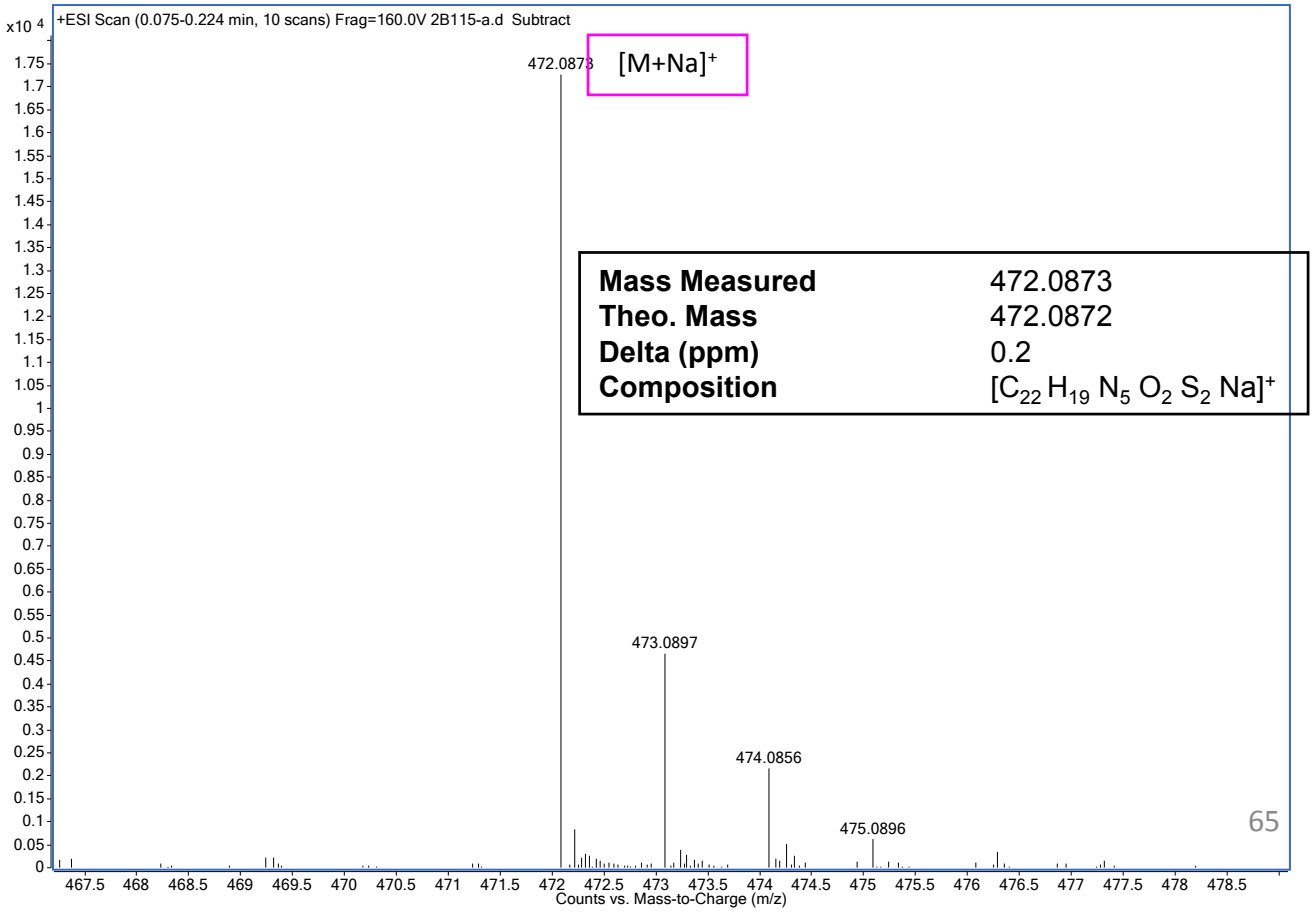
Acquisition Time (sec)	1.3005	***Comment***	Std carbon	***Date***	Apr 24 2017	***Date Stamp***	Apr 24 2017
File Name	C:\Documents and Settings\Mycoahhh\My Documents\NMR\C13 fids\2b115.fid\fid					***Frequency (MHz)***	125.69
Nucleus	13C	***Number of Transients***	32	***Original Points Count***	39649	***Points Count***	65536
Pulse Sequence	s2pul	***Receiver Gain***	58.00	***Solvent***	tfa	***Spectrum Offset (Hz)***	13196.4531
Spectrum Type	STANDARD	***Sweep Width (Hz)***	30487.80	***Temperature (degree C)***	30.000		

^{13}C NMR (126 MHz, tfa) δ 170.7, 155.9, 140.6, 140.1, 132.5, 131.8, 131.7, 126.0, 123.7, 121.9, 119.2, 118.6, 115.7, 114.9, 114.2, 113.5, 113.4, 112.6, 110.4, 44.6, 19.6, 11.5



LC-MS and HRMS **6**{5,6}





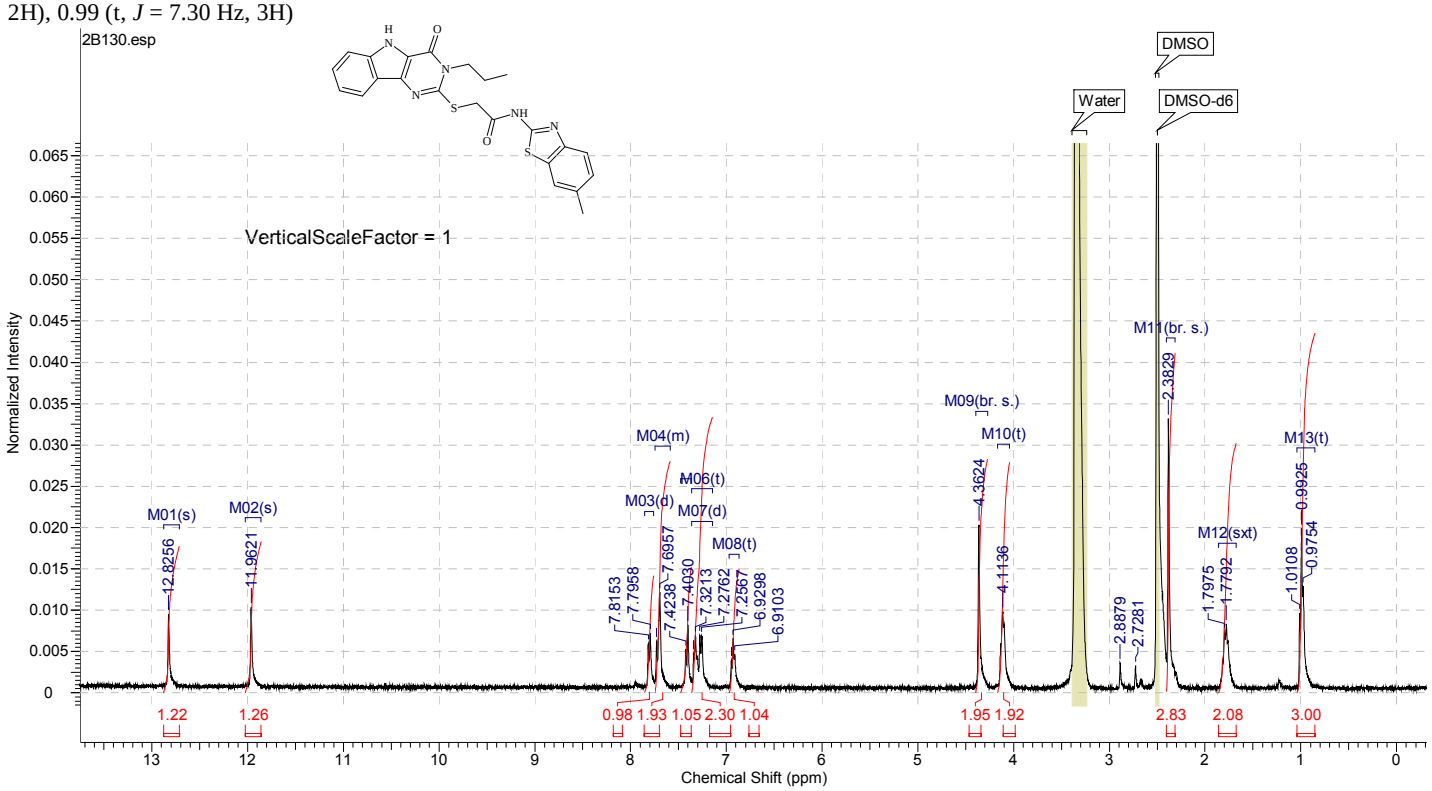
Mass Measured	472.0873
Theo. Mass	472.0872
Delta (ppm)	0.2
Composition	$[C_{22}H_{19}N_5O_2S_2Na]^+$

^{1}H, ^{13}C NMR **6**{6,6}

4/20/2017 1:20:53 PM

Acquisition Time (sec)	2.0211	***Comment***	STANDARD 1H OBSERVE			***Date***	Jan 5 2017
Date Stamp	Jan 5 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B130.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16156
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1964.4928	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

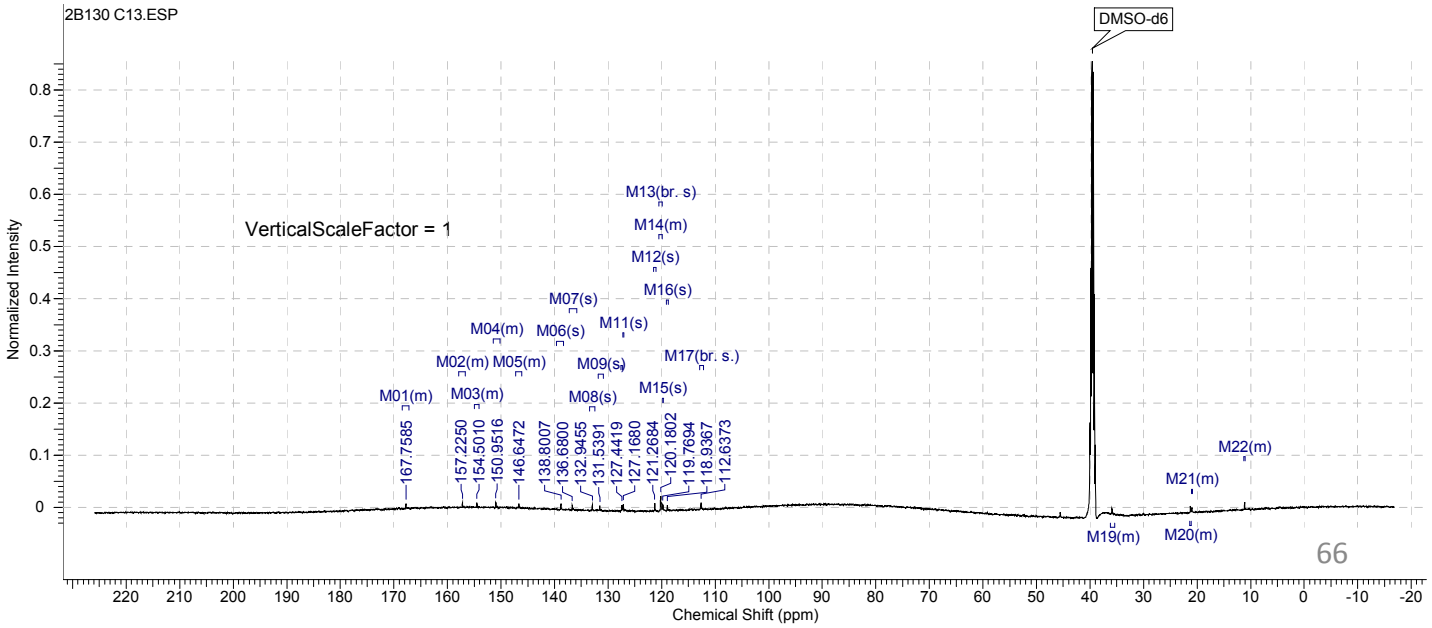
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.83 (s, 1H), 11.96 (s, 1H), 7.81 (d, *J* = 7.81 Hz, 1H), 7.59 - 7.74 (m, 2H), 7.37 - 7.47 (m, 1H), 7.32 (t, *J* = 7.80 Hz, 1H), 7.27 (d, *J* = 8.29 Hz, 1H), 6.93 (t, *J* = 7.56 Hz, 1H), 4.36 (br. s., 2H), 4.11 (t, *J* = 7.80 Hz, 2H), 2.38 (br. s., 3H), 1.79 (sxt, *J* = 7.30 Hz, 2H), 0.99 (t, *J* = 7.30 Hz, 3H)



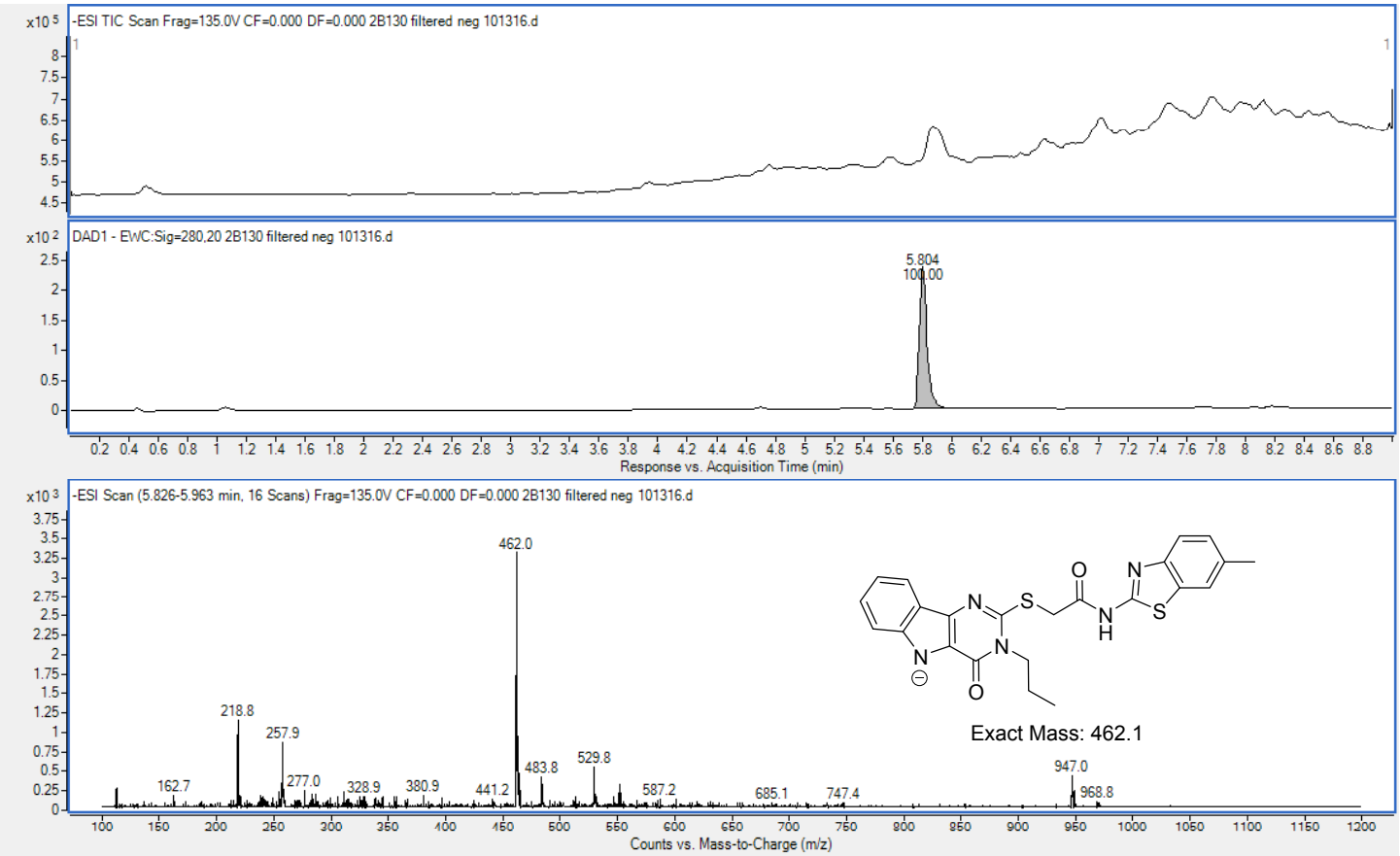
4/21/2017 11:09:16 AM

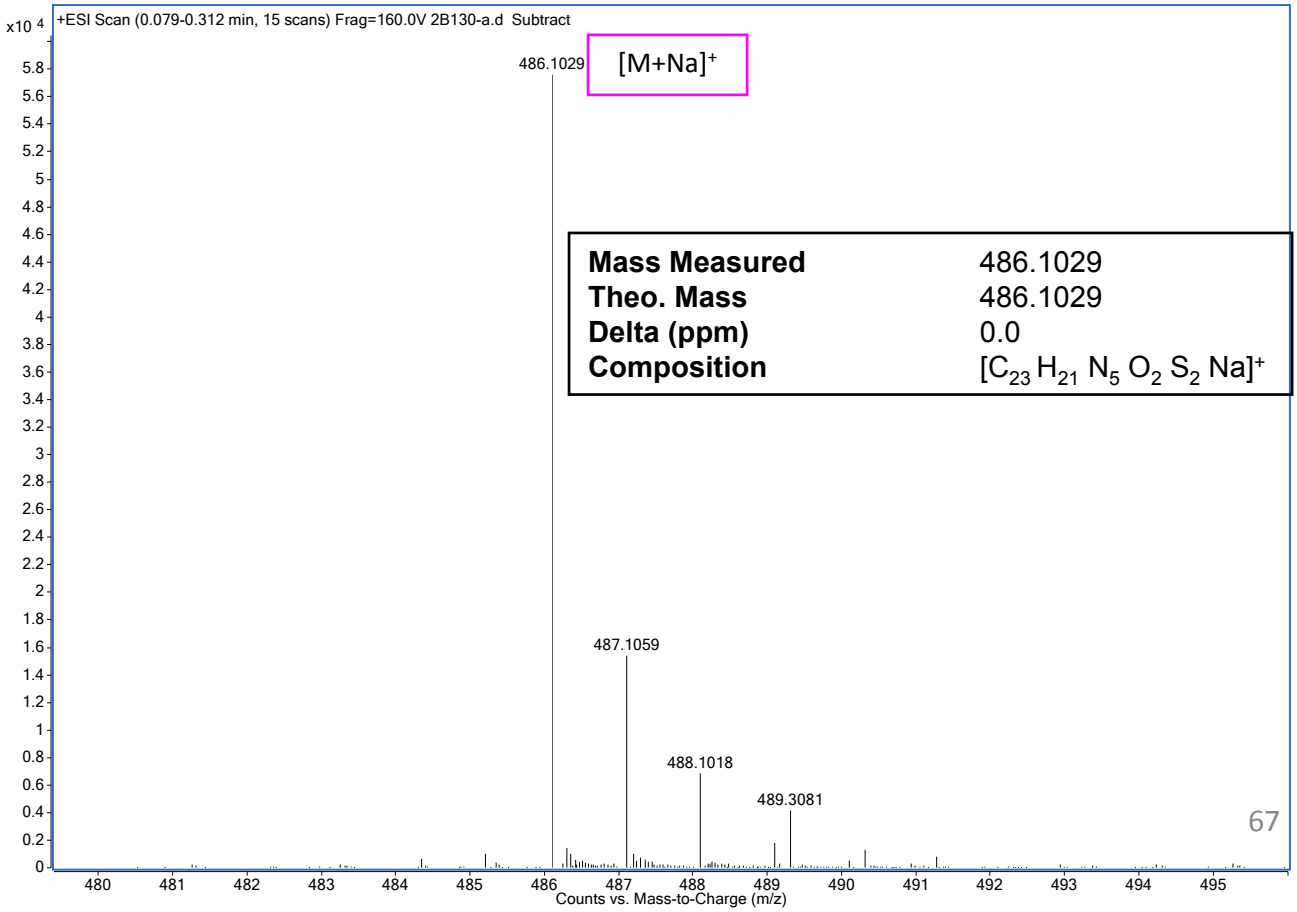
Acquisition Time (sec)	1.3005	***Comment***	Std carbon	***Date***	Apr 6 2017	***Date Stamp***	Apr 6 2017
File Name	C:\Documents and Settings\Mycoahhh\My Documents\NMR\C13 fids\2b130.fid\fid					***Frequency (MHz)***	125.69
Nucleus	13C	***Number of Transients***	32	***Original Points Count***	39649	***Points Count***	65536
Pulse Sequence	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	13137.9072
Spectrum Type	STANDARD	***Sweep Width (Hz)***	30487.80	***Temperature (degree C)***	35.000		

^{13}C NMR (126 MHz, DMSO-d_6) δ 167.8, 157.2, 154.5, 151.0, 146.6, 138.8, 136.7, 132.9, 131.5, 127.4, 127.2, 121.3, 120.2, 120.1, 119.8, 118.9, 112.6, 45.5, 35.9, 21.3, 21.0, 11.1



LC-MS and HRMS **6**{6,6}



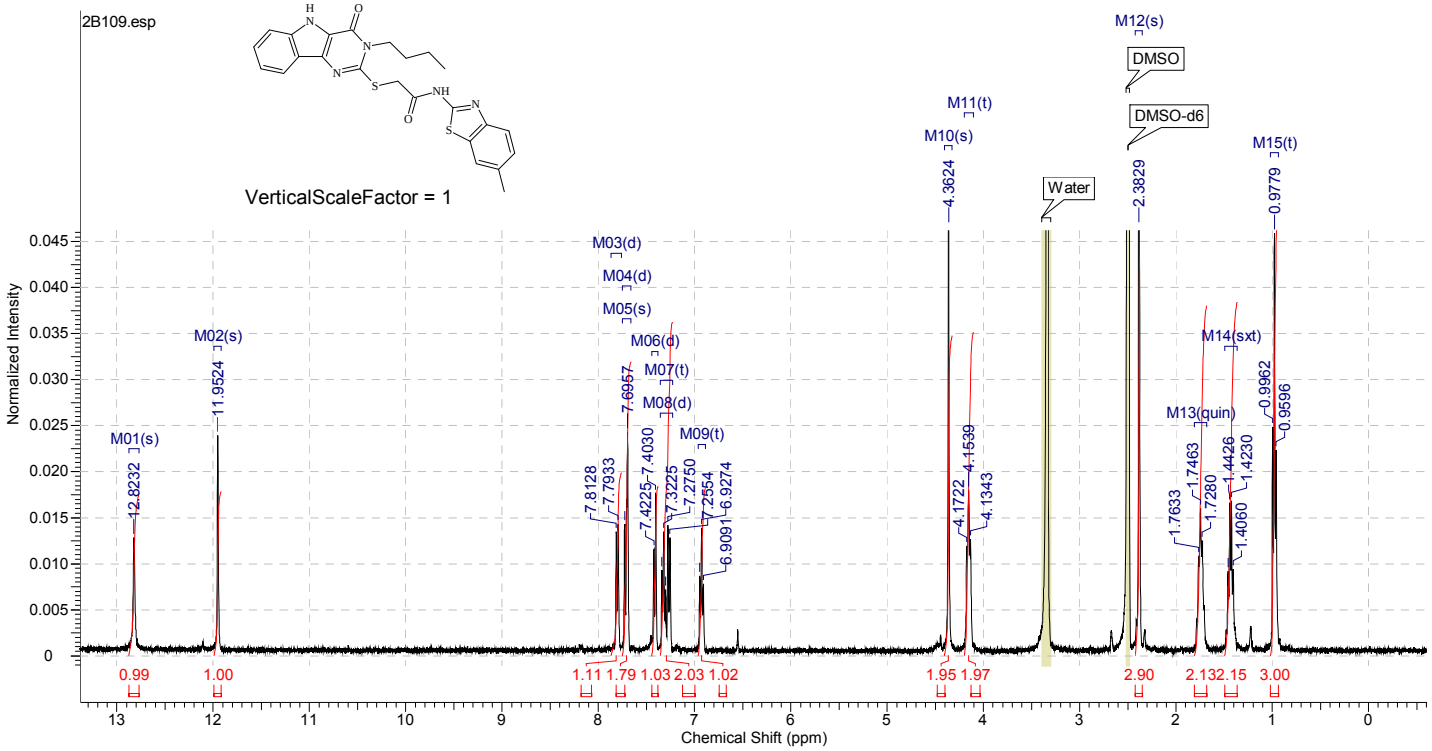


^{1}H, ^{13}C NMR **6**{7,6}

4/20/2017 1:27:13 PM

Acquisition Time (sec)	2.0130	***Comment***	STANDARD 1H OBSERVE			***Date***	Dec 23 2016
Date Stamp	Dec 23 2016	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2B109.fid\fid				
Frequency (MHz)	400.05	***Nucleus***	1H	***Number of Transients***	32	***Original Points Count***	16091
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	20.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	1960.5895	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

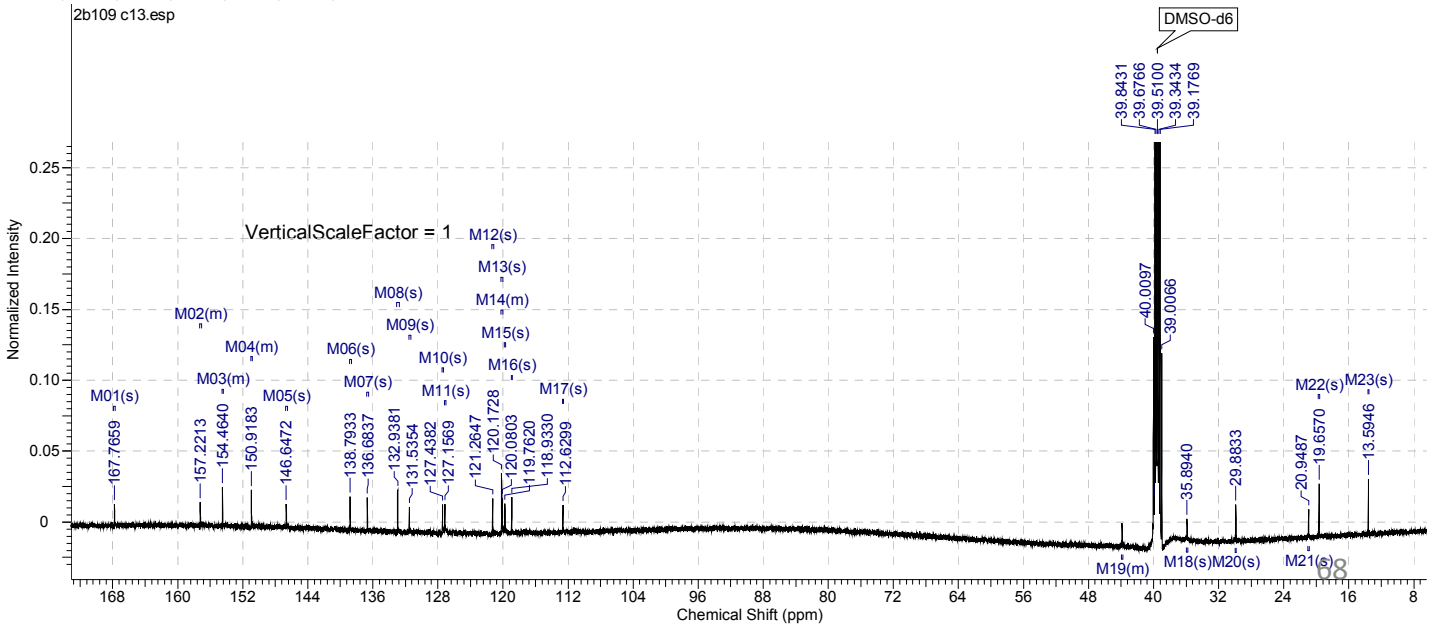
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.82 (s, 1H), 11.95 (s, 1H), 7.80 (d, *J* = 7.81 Hz, 1H), 7.72 (d, *J* = 8.29 Hz, 1H), 7.70 (s, 1H), 7.41 (d, *J* = 7.81 Hz, 1H), 7.32 (t, *J* = 7.40 Hz, 1H), 7.26 (d, *J* = 8.29 Hz, 1H), 6.93 (t, *J* = 7.56 Hz, 1H), 4.36 (s, 2H), 4.15 (t, *J* = 7.56 Hz, 2H), 2.38 (s, 3H), 1.75 (quin, *J* = 7.30 Hz, 2H), 1.43 (sxt, *J* = 7.40 Hz, 2H), 0.98 (t, *J* = 7.32 Hz, 3H)



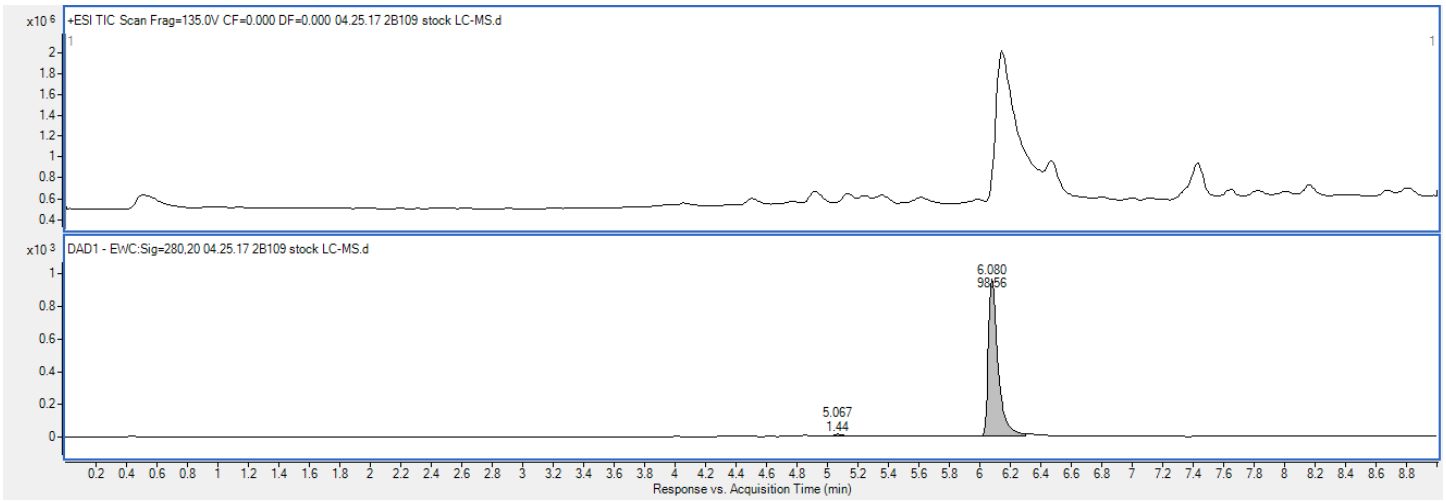
4/25/2017 10:08:42 AM

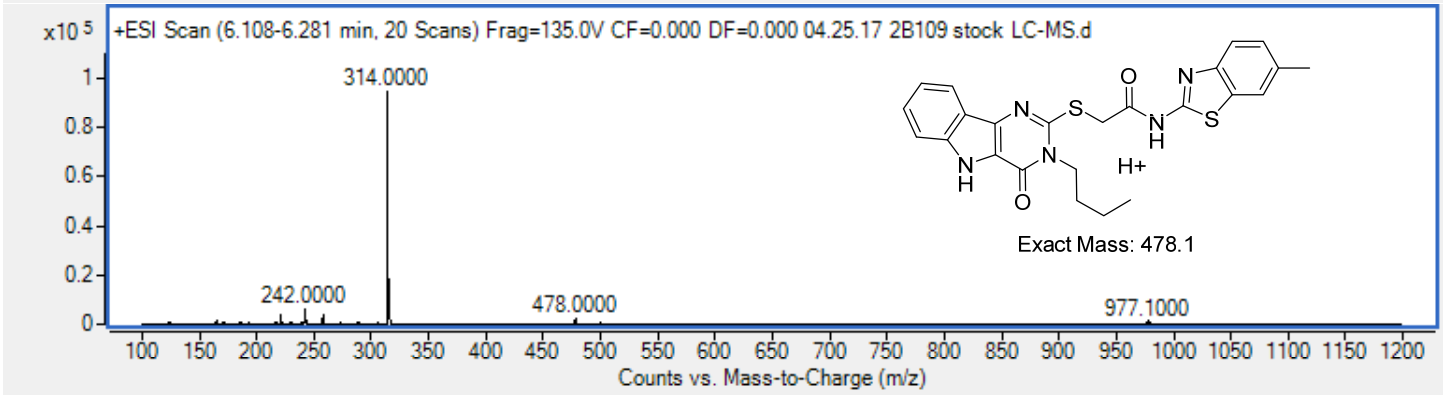
Acquisition Time (sec)	1.3005	***Comment***	Std carbon	***Date***	Apr 6 2017	***Date Stamp***	Apr 6 2017
File Name	C:\Documents and Settings\Mycoahhh\My Documents\NMR\C13 fids\2b109.fid\fid					***Frequency (MHz)***	125.69
Nucleus	13C	***Number of Transients***	32	***Original Points Count***	39649	***Points Count***	65536
Pulse Sequence	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	13136.9775
Spectrum Type	STANDARD	***Sweep Width (Hz)***	30487.80	***Temperature (degree C)***	35.000		

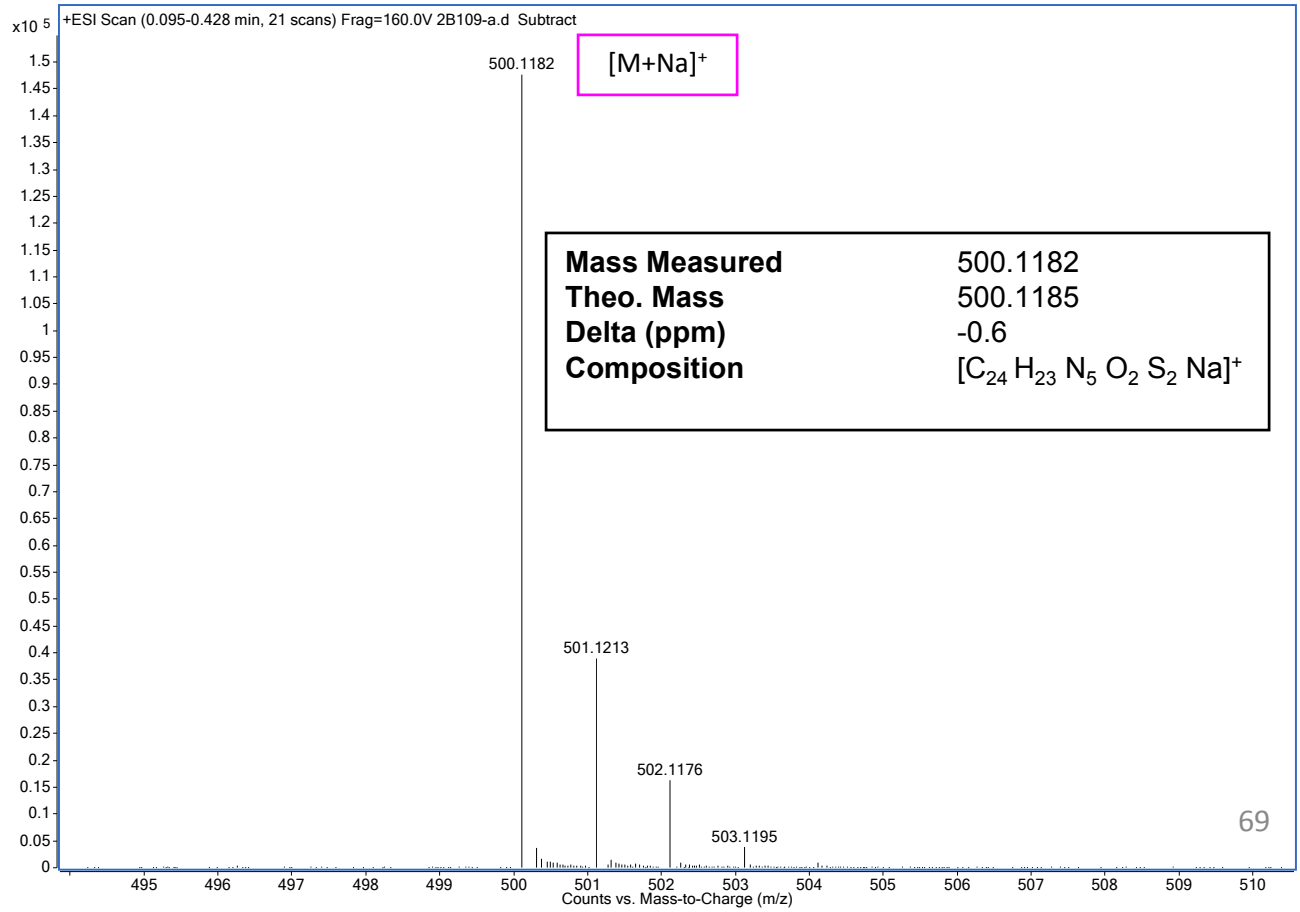
^{13}C NMR (126 MHz, DMSO-d_6) δ 167.8, 157.2, 154.5, 150.9, 146.6, 138.8, 136.7, 132.9, 131.5, 127.4, 127.2, 121.3, 120.2, 120.1, 119.8, 118.9, 112.6, 43.9, 35.9, 29.9, 20.9, 19.7, 13.6



LC-MS and HRMS **6**{7,6}





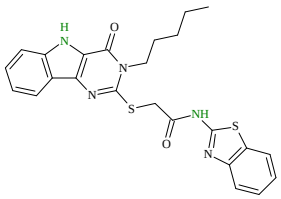


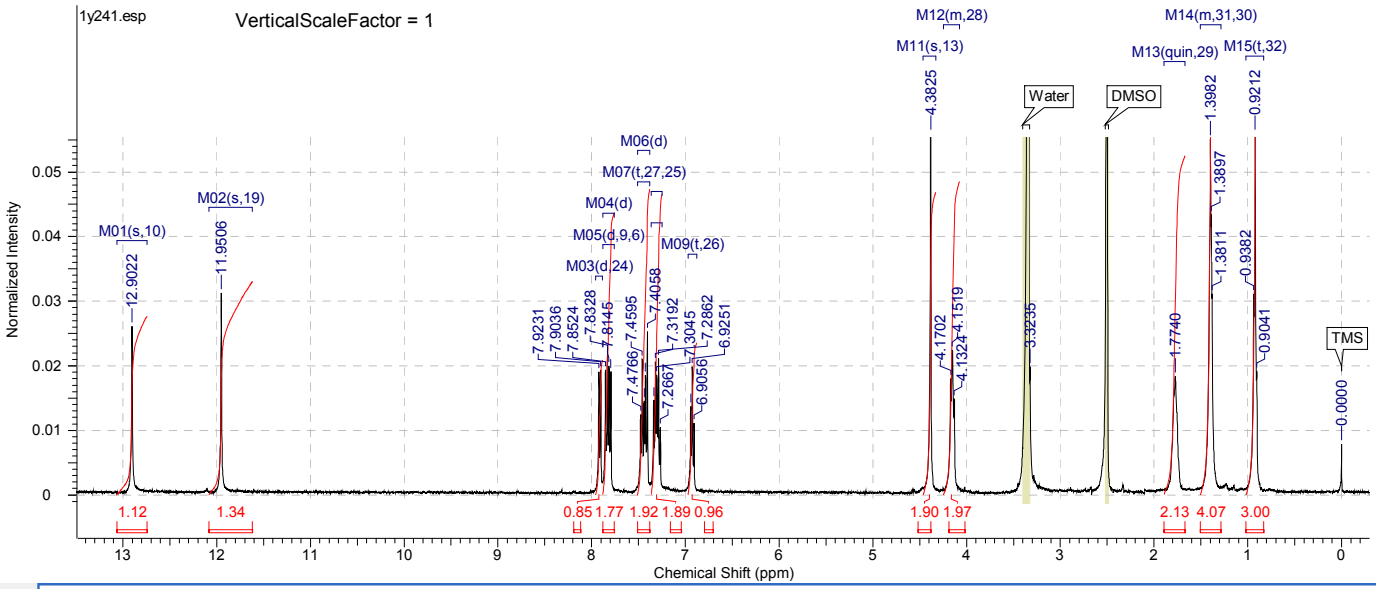
^{1}H NMR, LC-MS **9a**

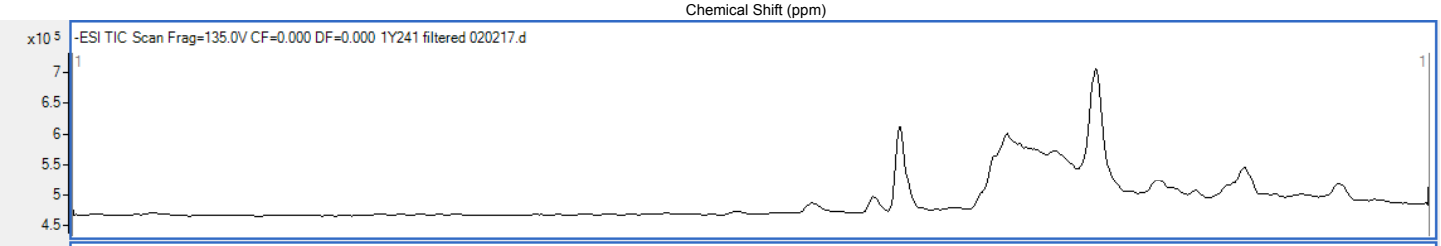
4/21/2017 10:17:08 AM

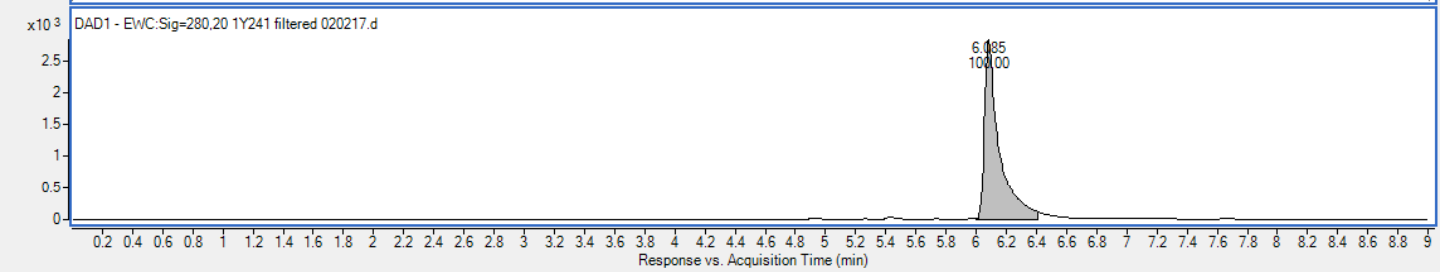
Acquisition Time (sec)	2.0032	***Comment***	STANDARD 1H OBSERVE			***Date***	Mar 24 2017
Date Stamp	Mar 24 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\1y241.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16013
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2030.4821	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

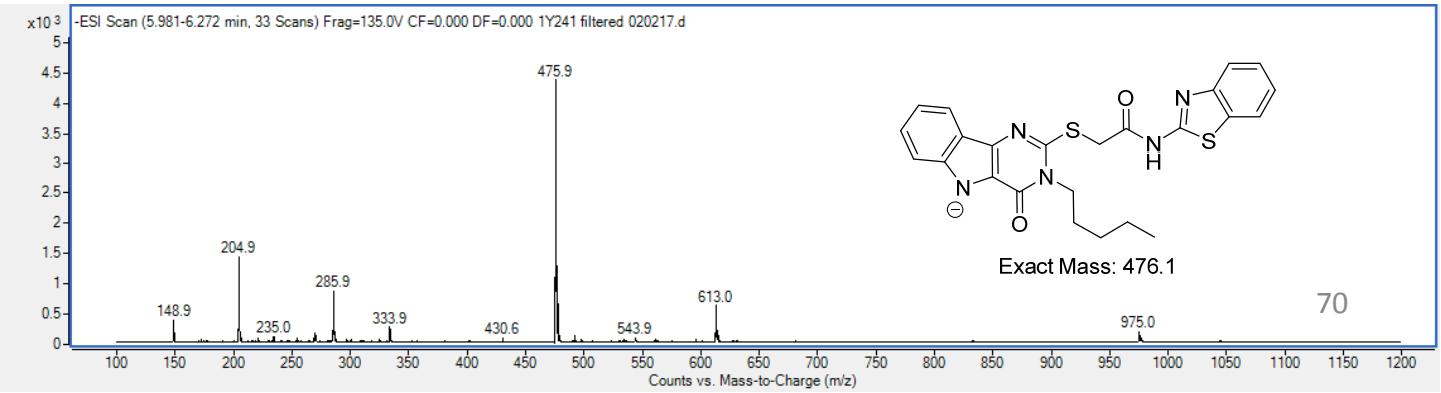
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.90 (s, 1H), 11.95 (s, 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.80 (d, *J* = 7.80 Hz, 1H), 7.84 (d, *J* = 7.80 Hz, 1H), 7.42 (d, *J* = 8.29 Hz, 1H), 7.46 (t, *J* = 7.32 Hz, 1H), 7.32 (t, *J* = 7.30 Hz, 1H), 7.29 (t, *J* = 7.80 Hz, 1H), 6.92 (t, *J* = 7.56 Hz, 1H), 4.38 (s, 2H), 4.08 - 4.25 (m, 2H), 1.77 (quin, *J* = 7.30 Hz, 2H), 1.29 - 1.50 (m, 4H), 0.92 (t, *J* = 7.30 Hz, 3H)











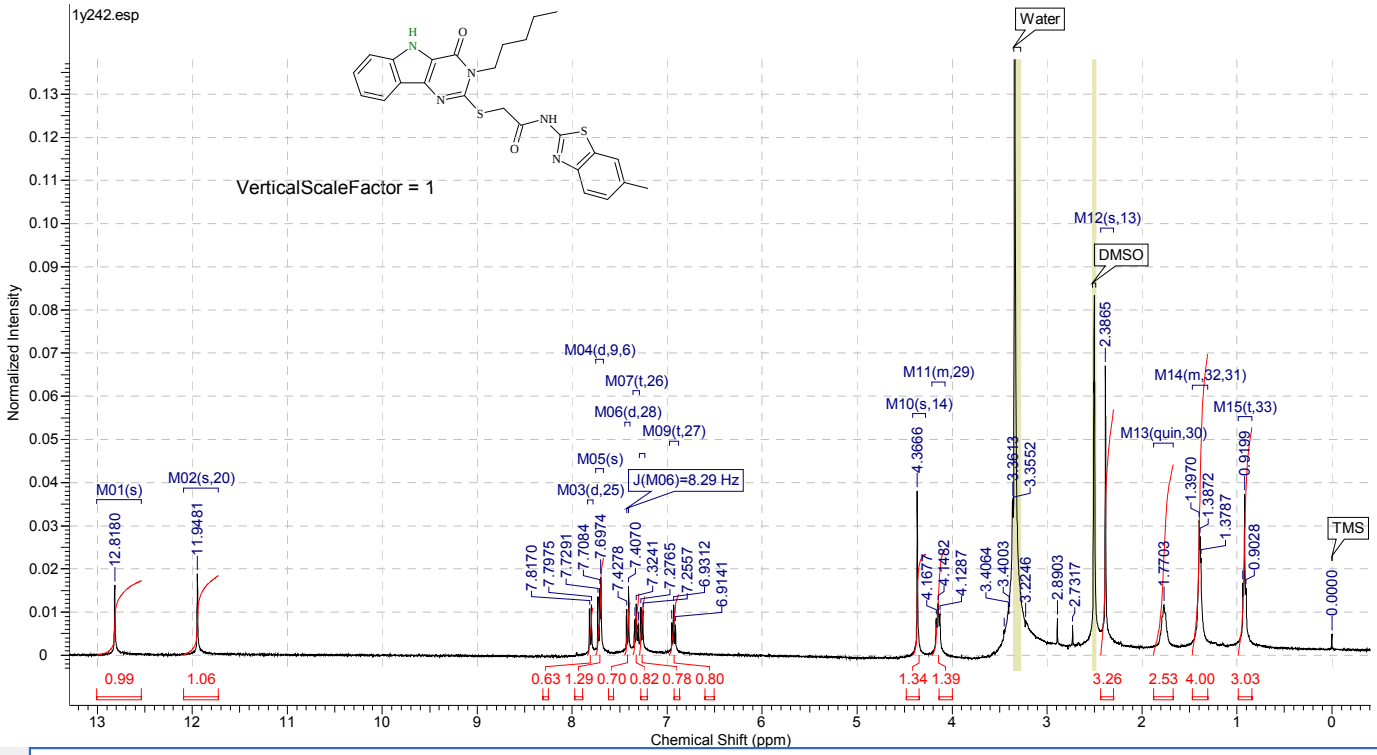
Exact Mass: 476.1

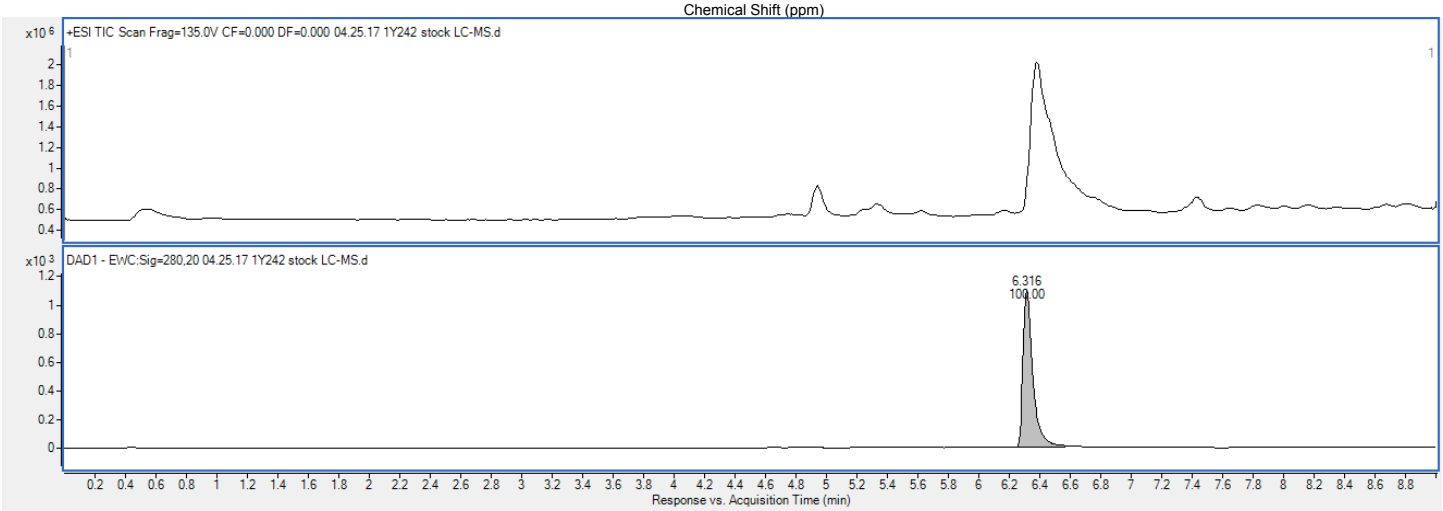
^{1}H NMR, LC-MS **9b**

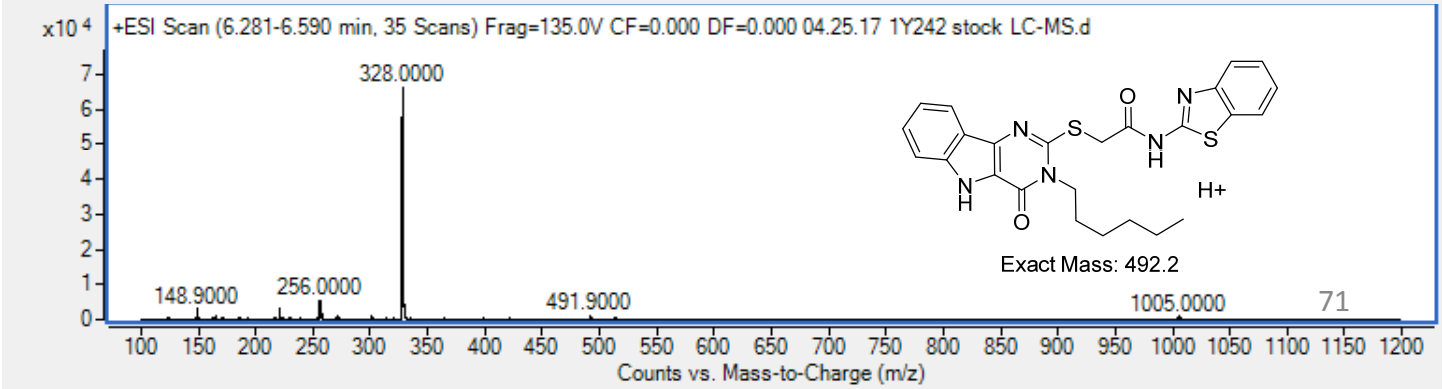
4/21/2017 10:18:12 AM

Acquisition Time (sec)	2.0130	***Comment***	STANDARD 1H OBSERVE			***Date***	Mar 24 2017
Date Stamp	Mar 24 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\1y242.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16091
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2030.4821	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.82 (s, 1H), 11.95 (s, 1H), 7.81 (d, *J* = 7.81 Hz, 1H), 7.70 (s, 1H), 7.72 (d, *J* = 8.29 Hz, 1H), 7.42 (d, *J* = 8.29 Hz, 1H), 7.32 (t, *J* = 7.81 Hz, 1H), 7.27 (d, *J* = 8.29 Hz, 1H), 6.93 (t, *J* = 7.07 Hz, 1H), 4.37 (s, 2H), 4.07 - 4.21 (m, 2H), 2.39 (s, 3H), 1.77 (quin, *J* = 7.30 Hz, 2H), 1.31 - 1.47 (m, 4H), 0.92 (t, *J* = 6.83 Hz, 3H)





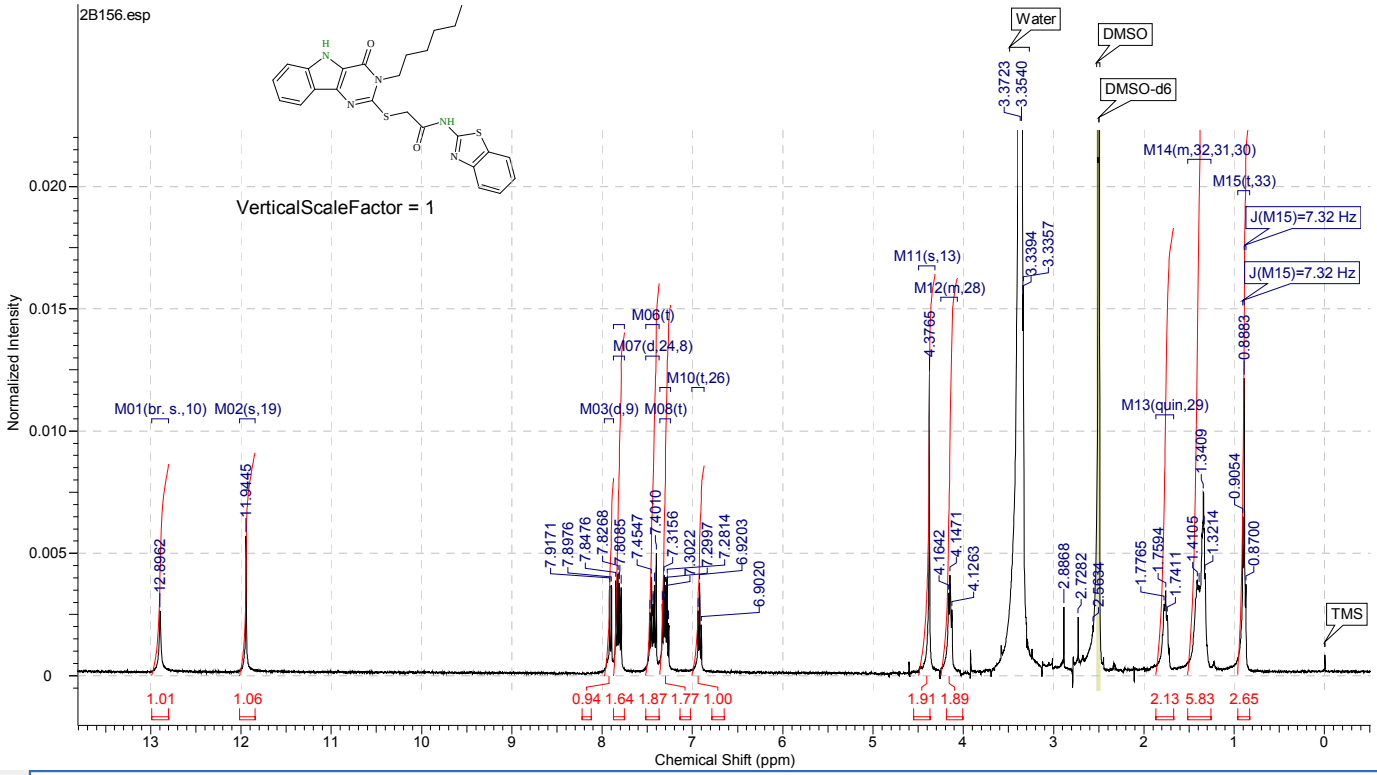


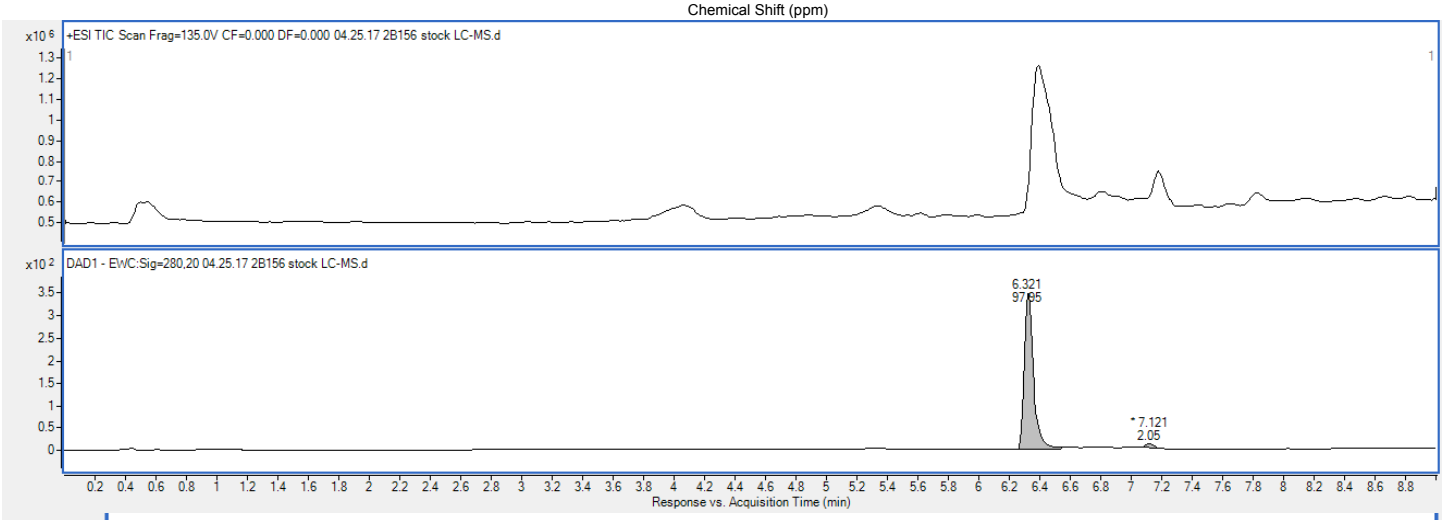
^{1}H NMR, LC-MS **10a**

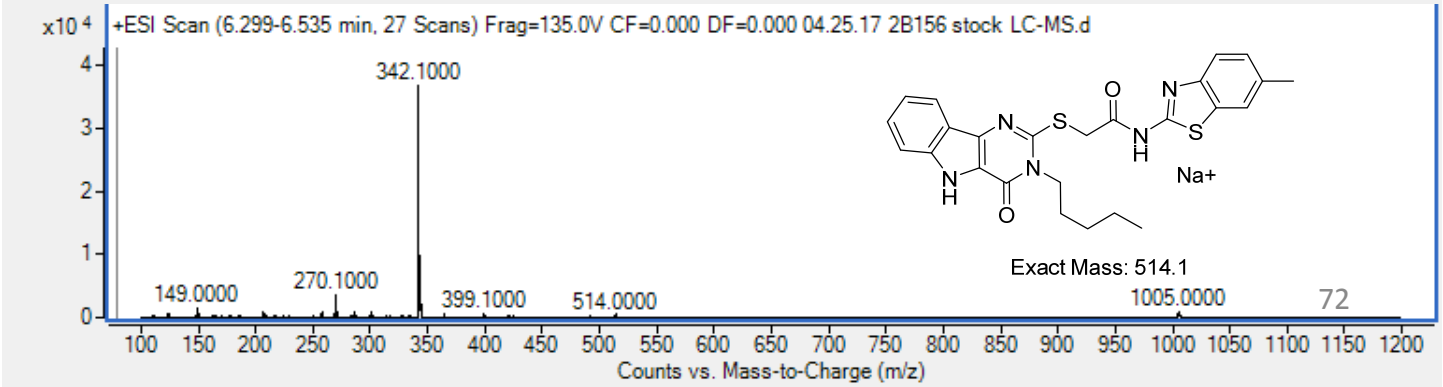
4/21/2017 10:19:57 AM

Acquisition Time (sec)	2.0065	***Comment***	STANDARD 1H OBSERVE			***Date***	Mar 24 2017
Date Stamp	Mar 24 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b156.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16039
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	24.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2029.0510	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.90 (br. s., 1H), 11.94 (s, 1H), 7.91 (d, *J* = 7.81 Hz, 1H), 7.84 (d, *J* = 7.80 Hz, 1H), 7.80 (d, *J* = 7.81 Hz, 1H), 7.45 (t, *J* = 7.81 Hz, 1H), 7.41 (d, *J* = 8.29 Hz, 1H), 7.32 (t, *J* = 7.30 Hz, 1H), 7.28 (t, *J* = 7.80 Hz, 1H), 6.92 (t, *J* = 7.07 Hz, 1H), 4.38 (s, 2H), 4.07 - 4.25 (m, 2H), 1.76 (quin, *J* = 7.30 Hz, 2H), 1.26 - 1.52 (m, 6H), 0.89 (t, *J* = 7.32 Hz, 3H)





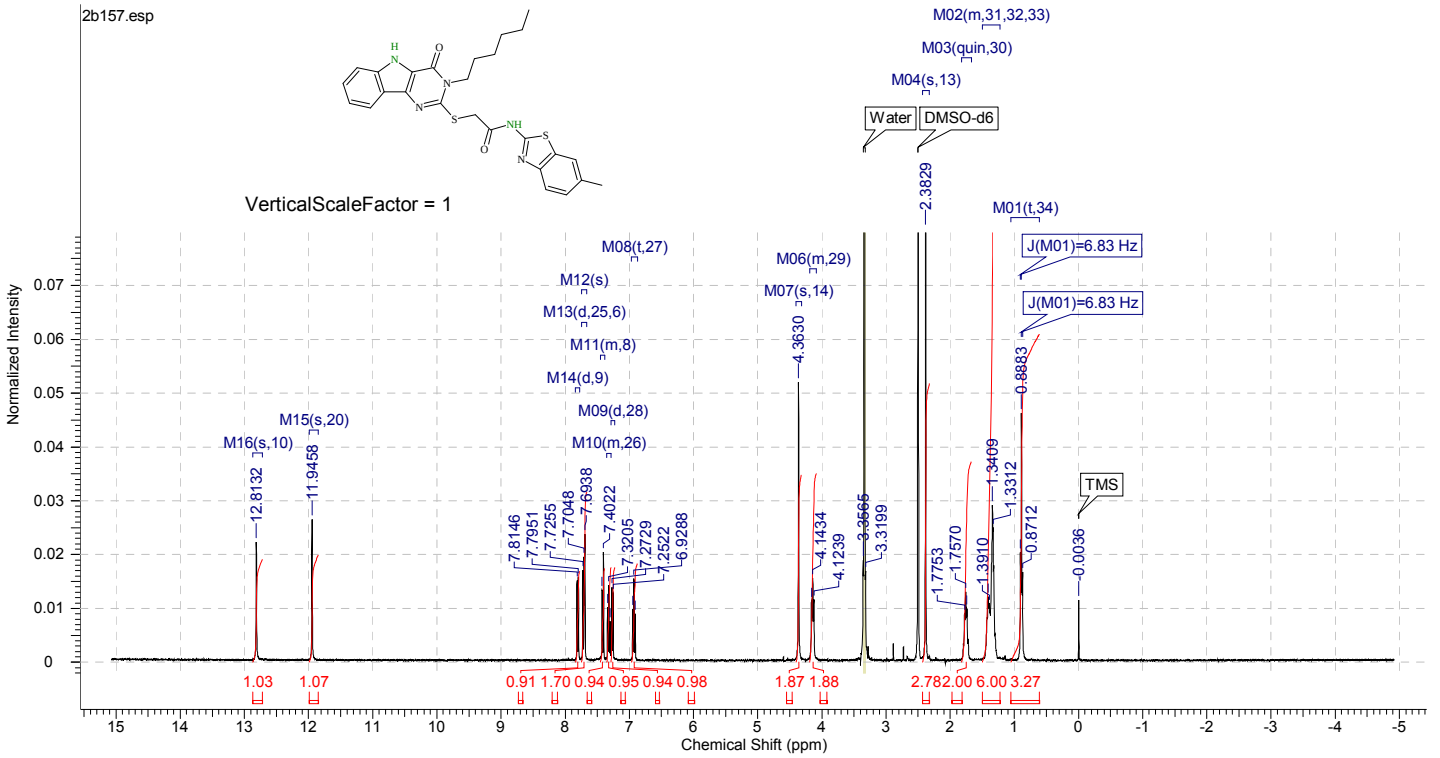


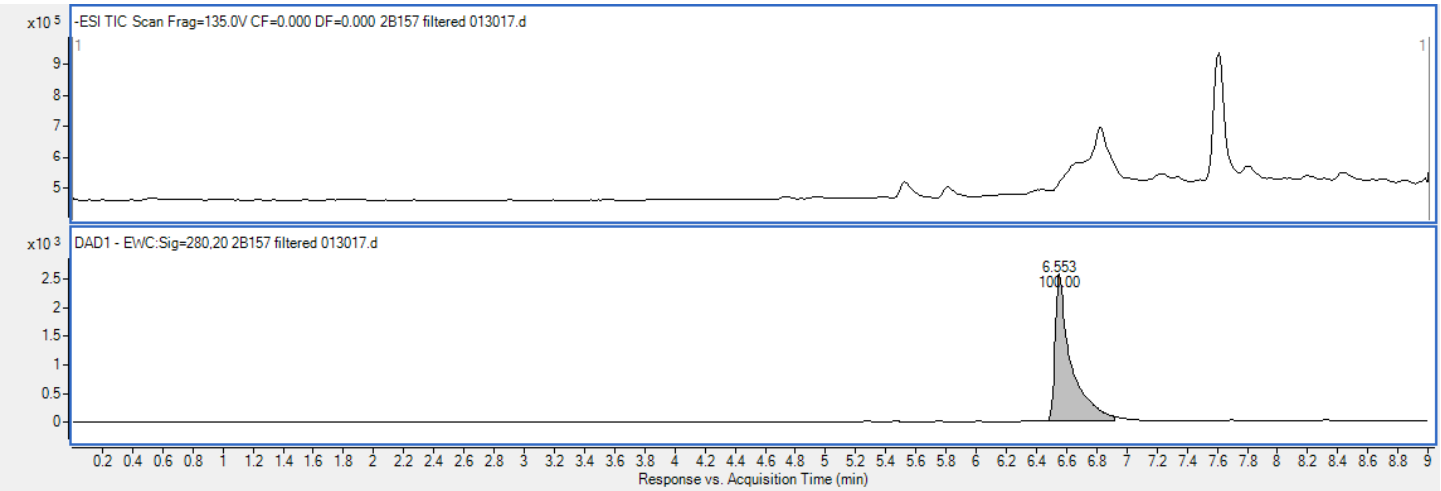
^{1}H NMR, LC-MS **10b**

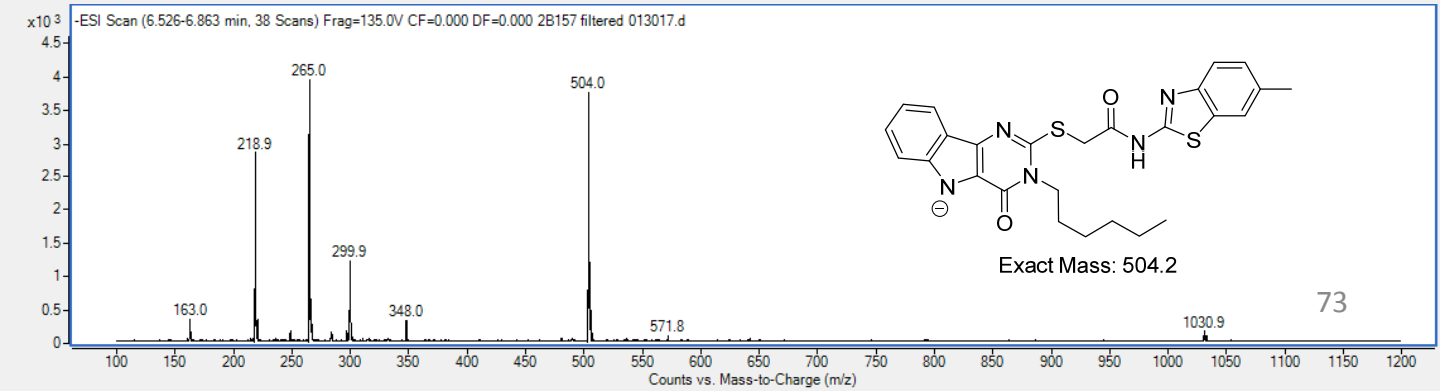
4/20/2017 2:14:44 PM

Acquisition Time (sec)	2.0049	***Comment***	STANDARD 1H OBSERVE			***Date***	Mar 24 2017
Date Stamp	Mar 24 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2b157.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16026
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2028.5632	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.81 (s, 1H), 11.95 (s, 1H), 7.80 (d, *J* = 7.81 Hz, 1H), 7.69 (s, 1H), 7.72 (d, *J* = 7.81 Hz, 1H), 7.39 - 7.45 (m, 1H), 7.29 - 7.35 (m, 1H), 7.26 (d, *J* = 8.29 Hz, 1H), 6.93 (t, *J* = 7.32 Hz, 1H), 4.36 (s, 2H), 4.09 - 4.19 (m, 2H), 2.38 (s, 3H), 1.76 (quin, *J* = 7.80 Hz, 2H), 1.23 - 1.50 (m, 6H), 0.89 (t, *J* = 6.83 Hz, 3H)







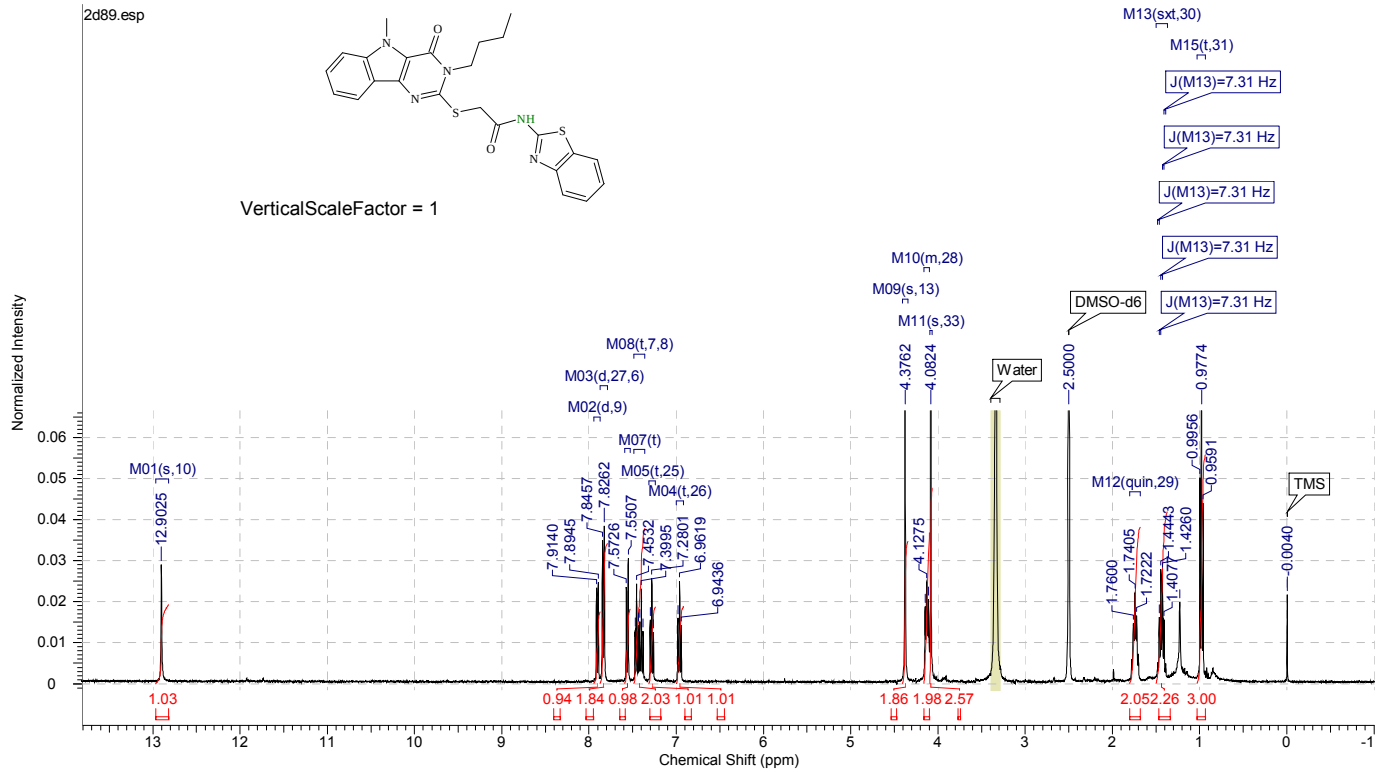
Exact Mass: 504.2

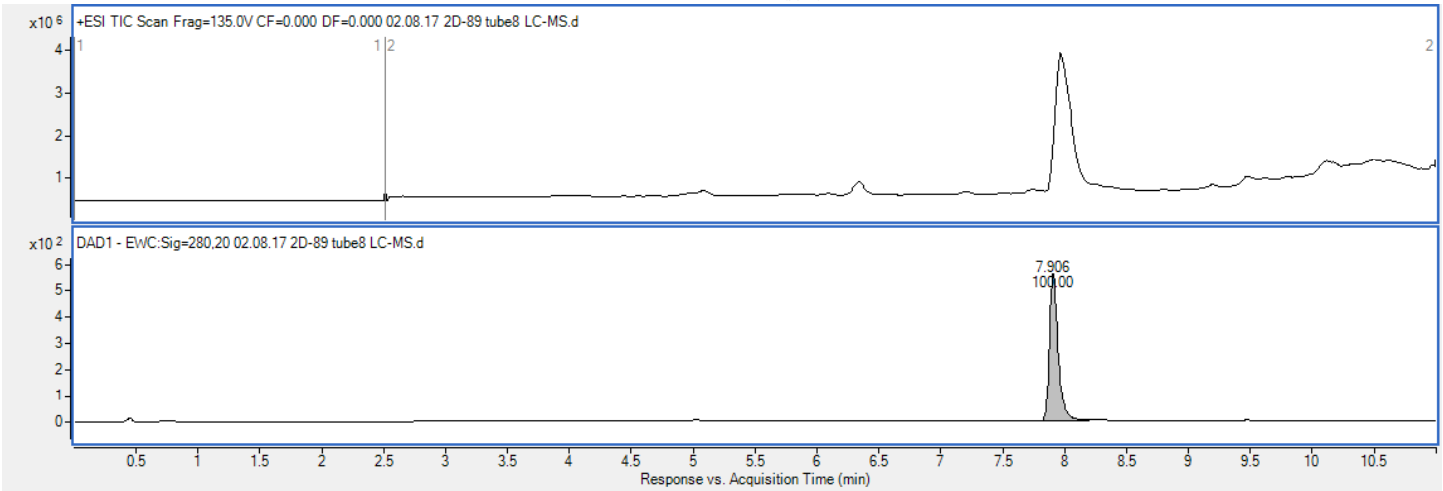
^{1}H NMR, LC-MS **11**

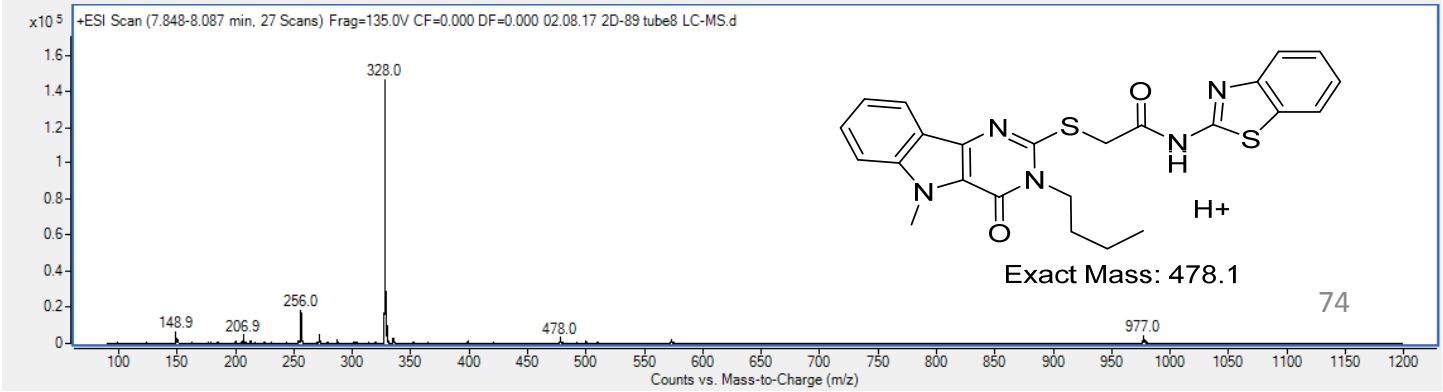
4/21/2017 10:24:10 AM

Acquisition Time (sec)	2.0016	***Comment***	STANDARD 1H OBSERVE			***Date***	Mar 24 2017
Date Stamp	Mar 24 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2d89.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	15987
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2028.2289	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7987.22	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.90 (s, 1H), 7.90 (d, *J* = 7.80 Hz, 1H), 7.84 (d, *J* = 7.80 Hz, 2H), 7.56 (d, *J* = 8.78 Hz, 1H), 7.45 (t, *J* = 7.80 Hz, 1H), 7.40 (t, *J* = 7.30 Hz, 1H), 7.28 (t, *J* = 7.56 Hz, 1H), 6.96 (t, *J* = 7.56 Hz, 1H), 4.38 (s, 2H), 4.10 - 4.16 (m, 2H), 4.08 (s, 3H), 1.74 (quin, *J* = 15.10 Hz, 2H), 1.44 (sxt, *J* = 7.31 Hz, 2H), 0.98 (t, *J* = 7.31 Hz, 3H)







^{1}H NMR, LC-MS **12**

4/21/2017 10:34:02 AM

Acquisition Time (sec)	2.0146	***Comment***	STANDARD 1H OBSERVE			***Date***	Mar 24 2017
Date Stamp	Mar 24 2017	***File Name***	C:\Documents and Settings\Mycoahhh\My Documents\NMR\michan\2d87.fid\fid				
Frequency (MHz)	399.91	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	16104
Points Count	16384	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	2029.5062	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	7993.60	***Temperature (degree C)***	AMBIENT TEMPERATURE

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.82 (s, 1H), 7.84 (d, *J* = 7.81 Hz, 1H), 7.72 (d, *J* = 8.29 Hz, 1H), 7.67 - 7.74 (m, 1H), 7.57 (d, *J* = 8.29 Hz, 1H), 7.41 (t, *J* = 7.81 Hz, 1H), 7.26 (d, *J* = 8.29 Hz, 1H), 6.97 (t, *J* = 7.80 Hz, 1H), 4.36 (s, 2H), 4.09 (s, 3H), 4.13 (t, *J* = 7.80 Hz, 2H), 2.38 (s, 3H), 1.74 (quin, *J* = 7.81 Hz, 2H), 1.44 (sxt, *J* = 7.32 Hz, 2H), 0.98 (t, *J* = 7.32 Hz, 3H)