## **Supporting Information**

Discovery and Biological Evaluation of Nitrofuranyl-Pyrazolopyrimidine Hybrid Conjugates as Potent Antimicrobial Agents Targeting *Staphylococcus aureus* and Methicillin-resistant *Staphylococcus aureus* 

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<sup>†</sup>Equal contribution as first author to this work.

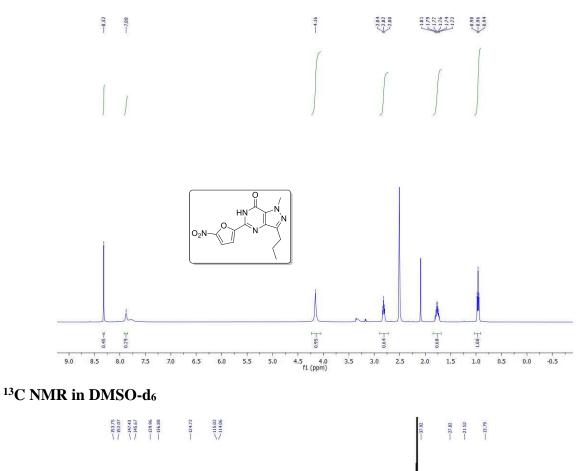
## **Table of Contents**

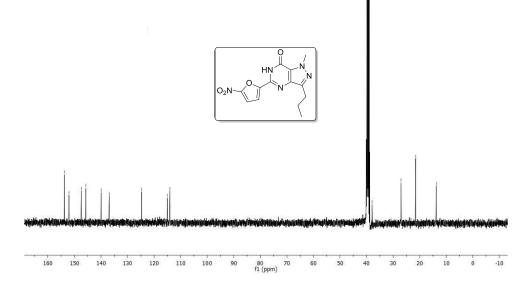
S. No.	Contents	Page Nos.
1.0	Scanned spectra of compounds	\$3-\$116

1.0. Scanned spectra

## Compound (8)

<sup>1</sup>H NMR in DMSO-d<sub>6</sub>

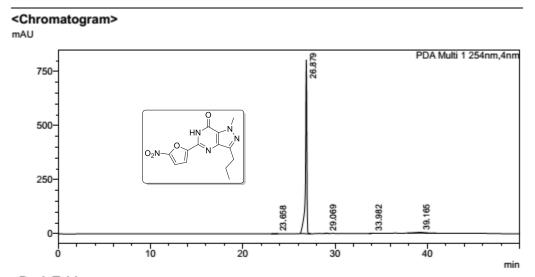




## **Qualitative Compound Report**

Data File Sample <sup>7</sup> Instrum Acq Met IRM Cali Commer Sample (	Type ent Na hod ibrationt	on S		S Ir D S	aily ms00 ample nstrumer DAILY MS Juccess	it 1	Positio User N	ame ed Time 1	6	2 11:41:39 AM		
Compo	und T	abl	e									
											MFG Diff	
	npour	_		RT		Mass	Formu			FG Formula	(ppm)	DB Formula
Сра	30: C	13 H	13 N5 O4	0.2	236 3	03.09682	C13 H13 N	5 04	CI	3 H13 N5 O4	-0.21	C13 H13 N5 O4
Compo	und L	abe	1	m/z		RT	Algorithm		Mas	85		
Cpd 30:				304.1	0409	0.236		ecular Featu		A Constant of the second s		
2 1.5 1 0.5 0	ę., .	150		* 304 10409	C13 H14 N5 04		500 550 vs. Mass-to			50 800 850 900	0 950	
ms spe m/z	ctrun		ak List Abund	E	ormula		Ion					
304.1	0409	1			13 H14 M	N5 04	(M+H)+					
305.1		1		_	13 H14 M		(M+H)+					
306.1		1			13 H14 M		(M+H)+					
307.1		1	5	95.1 C	13 H14 M	N5 04	(M+H)+					
326.0	8634	1	249	63.2 C	13 H13 I	N5 Na O4	(M+Na)	+				
327.0		1				N5 Na O4	(M+Na)					
	0897	1		_		N5 Na O4	(M+Na)					
	5. 7. 1 Cont		e Matc									
Predict		m/z		Calc r		Diff (ppm)	Abund %	Calc Abun	d %	Abund Sum %	Calc Abu	nd Sum %
					4.10403	-0.21	10	0	100	86	.83	84.43
	1	3	04.10409	30	1.10105							
		-	05.10722		5.10671	-1.66	13.3	5	16.2	11	.59	13.68
Predict Isotope	1	3		30							.59	

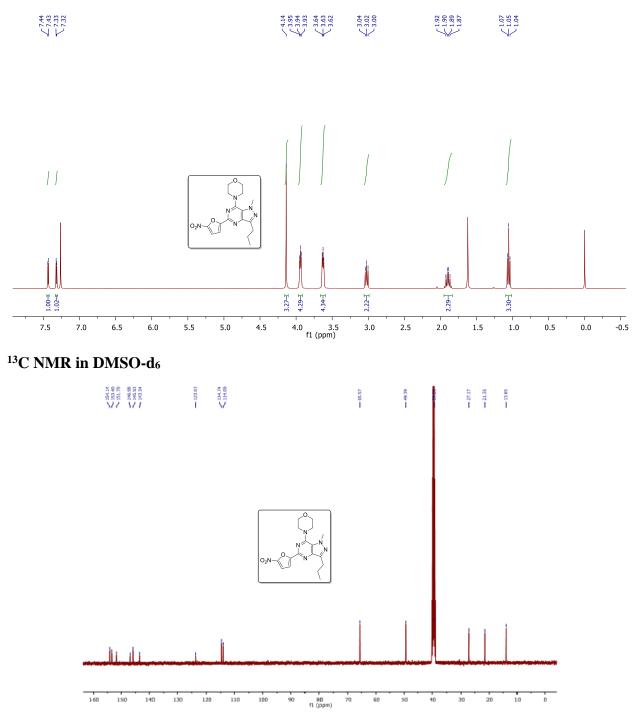
## HPLC



## <Peak Table> PDA Ch1 254nm

PDAC	n1 254nm				
Peak#	Ret. Time	Area	Height	Area%	Height%
1	23.658	9756	861	0.109	0.106
2	26.879	8546397	802561	95.800	98.880
3	29.069	26648	3044	0.299	0.375
4	33.982	18249	1444	0.205	0.178
5	39.165	320040	3739	3.587	0.461
Total		8921091	811649	100.000	100.000

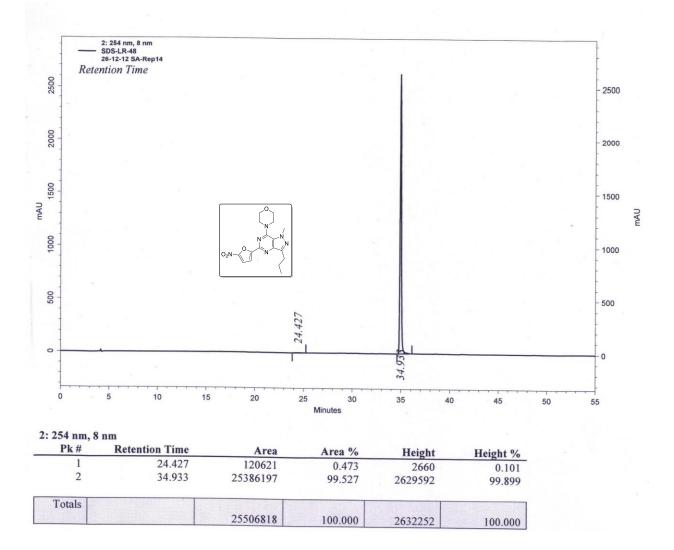
Compound (10) <sup>1</sup>H NMR in CDCl<sub>3</sub>



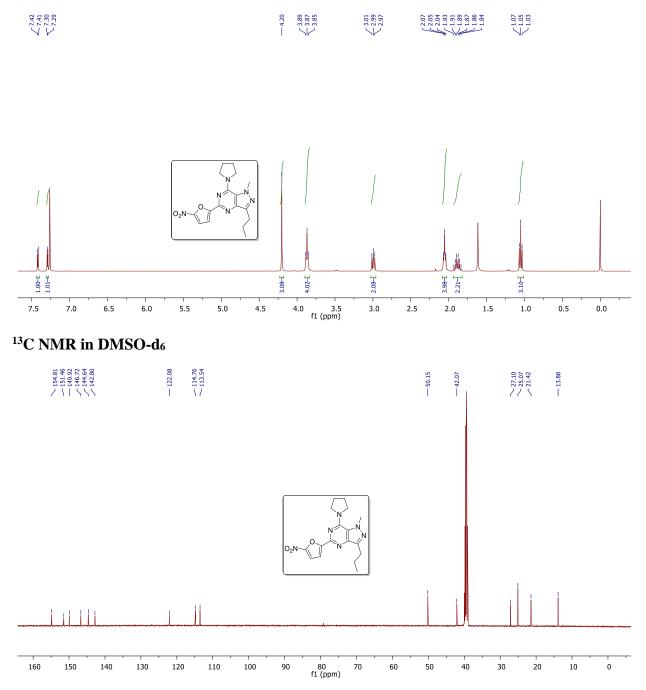
## **Qualitative Compound Report**

Sample Type Instrument I Acq Method IRM Calibrat Comment Sample Grou Compound	Name tion Status up Info	vishal_ Succe	e ment 1 _MS_2507201	2.m	Sample Na Position User Nam Acquired <sup>•</sup> DA Metho	Vial 15 e Time 11/18/	2012 1:01:38 PM			
compound	Table							M	FG Diff	
	und Label	RT	Mass		Formula		MFG Formula	(	ppm)	DB Formula
Cpd 5:	C17 H20 N6 O4	0.172	372.15417	C17	7 H20 N6 O	4	C17 H20 N6 O4		1.15	C17 H20 N6 O4
Compound	Label	m/z	RT	Algo	rithm	M	ass			
Cpd 5: C17 H	120 N6 O4	373.16145	0.13	72 Find	by Molecu	Ilar Feature 3	72.15417			
MFE MS Spect	rum d 5: C17 H20									
2- 1.5- 1-			373.16145 C17 H21 N6 O4				767.29530 C34 H40 N12 Na O8			
0.5	150 200 2	50 300	350 400 Cou			00 650 700 harge (m/z)	750 800 850	900	950	
0	ım Peak List		Cou	unts vs. Ma	ass-to-Ch			900	950	
0 MS Spectru	m Peak List	Form	Cou	unts vs. Ma	ass-to-Ch			900	950	
0 MS Spectru m/z 373.16145	z         Abund           1         2359	Form	Cou ula 21 N6 O4	unts vs. Ma	ass-to-Ch Ion (M+H)+			900	950	
0 MS Spectrum m/z 373.16145 374.16411	z         Abund           1         2359           1         513	Form 73.3 C17 H 44.5 C17 H	Cou ula 21 N6 O4 21 N6 O4	unts vs. Ma	ass-to-Ch <b>Ion</b> (M+H)+ (M+H)+			900	950	
0 MS Spectru <i>m/z</i> 373.16145 374.16411 375.16622	z         Abund           1         2359           1         513           1         68	Form 73.3 C17 H 44.5 C17 H 24.4 C17 H	Cou ula 21 N6 O4 21 N6 O4 21 N6 O4	unts vs. Ma	ass-to-Ch Ion (M+H)+ (M+H)+ (M+H)+			900	950	
0 MS Spectru <i>m/z</i> 373.16145 374.16411 375.16622 376.1728	z         Abund           1         2359           1         513           1         68           1         12	Form 73.3 C17 H 44.5 C17 H 24.4 C17 H 72.5 C17 H	Cou 21 N6 O4 21 N6 O4 21 N6 O4 21 N6 O4 21 N6 O4	11 1 ( ( ( ( ( ( ( ( (	ass-to-Ch (M+H)+ (M+H)+ (M+H)+ (M+H)+			900	950	
0 MS Spectru <i>m/z</i> 373.16145 374.16411 375.16622 376.1728 395.14219	z         Abund           1         2359           1         513           1         68           1         12           1         12           1         12           1         12           1         117	Form 73.3 C17 H 44.5 C17 H 24.4 C17 H 72.5 C17 H 35.8 C17 H	Cou ula 21 N6 O4 21 N6 O4 21 N6 O4 21 N6 O4 21 N6 O4 20 N6 Na O4	1 ( ( ( ( ( ( ( ( ( ( ( ( ( (	ass-to-Ch (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+			900	950	
MS Spectru m/z 373.16145 374.16411 375.16622 376.1728 395.14219 396.14658	z         Abund           1         2359           1         513           1         68           1         12           1         12           1         12           1         12           1         117           1         27	Form 73.3 C17 H 44.5 C17 H 24.4 C17 H 72.5 C17 H 35.8 C17 H 17.6 C17 H	Cou ula 21 N6 O4 21 N6 O4 21 N6 O4 21 N6 O4 21 N6 O4 20 N6 Na O4 20 N6 Na O4	1115 vs. Ma	ass-to-Ch (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+			900	950	
0 MS Spectru <i>m/z</i> 373.16145 374.16411 375.16622 376.1728 395.14219	z         Abund           1         2359           1         513           1         68           1         12           1         12           1         12           1         12           1         12           1         12           1         13           1         13           1         39	Form 73.3 C17 H 44.5 C17 H 24.4 C17 H 72.5 C17 H 35.8 C17 H 17.6 C17 H 62.3 C17 H	Cou 21 N6 04 21 N6 04 21 N6 04 21 N6 04 20 N6 Na 04 20 N6 Na 04 20 N6 Na 04 20 K N6 04	1115 vs. Ma	ass-to-Ch (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+			900	950	
MS Spectru m/z 373.16145 374.16411 375.16622 376.1728 395.14219 396.14658	z         Abund           1         2359           1         513           1         68           1         12           1         12           1         12           1         12           1         12           1         12           1         13           1         13           1         13           1         39	Form 73.3 C17 H 44.5 C17 H 24.4 C17 H 72.5 C17 H 35.8 C17 H 17.6 C17 H 62.3 C17 H	Cou ula 21 N6 O4 21 N6 O4 21 N6 O4 21 N6 O4 21 N6 O4 20 N6 Na O4 20 N6 Na O4	1115 vs. Ma	ass-to-Ch (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+			900	950	
MS Spectru m/z 373.16145 374.16411 375.16622 376.1728 395.14219 396.14658 411.11631	z         Abund           1         2359           1         513           1         68           1         122           1         117           1         27           1         39           1         19	Form 73.3 C17 H 44.5 C17 H 24.4 C17 H 72.5 C17 H 35.8 C17 H 17.6 C17 H 62.3 C17 H 9822 C34 H	Cou 21 N6 04 21 N6 04 21 N6 04 21 N6 04 20 N6 Na 04 20 N6 Na 04 20 N6 Na 04 20 K N6 04	1115 vs. Ma	ass-to-Ch (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+K)+			900	950	
MS Spectru m/z 373.16145 374.16411 375.16622 376.1728 395.14219 396.14658 411.11631 767.2953	z         Abund           1         2359           1         513           1         68           1         12           1         12           1         12           1         12           1         12           1         12           1         12           1         139           1         19           1         94	Form 73.3 C17 H 44.5 C17 H 24.4 C17 H 72.5 C17 H 35.8 C17 H 17.6 C17 H 62.3 C17 H 9822 C34 H 57.8 C34 H	Cou 21 N6 04 21 N6 04 21 N6 04 21 N6 04 20 N6 Na 04 20 N6 Na 04 20 N6 Na 04 20 K N6 04 40 N12 Na 04	1115 vs. Ma	ass-to-Ch (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+K)+ (2M+Na)+			900	950	
MS Spectru m/z 373.16145 374.16411 375.16622 376.1728 395.14219 396.14658 411.11631 767.2953 768.2981 769.30404	z         Abund           1         2359           1         513           1         68           1         12           1         12           1         12           1         12           1         12           1         12           1         12           1         139           1         19           1         94	Form 73.3 C17 H 44.5 C17 H 24.4 C17 H 72.5 C17 H 35.8 C17 H 35.8 C17 H 9822 C34 H 9822 C34 H 985.5 C34 H	Cou 21 N6 O4 21 N6 O4 21 N6 O4 21 N6 O4 20 N6 Na O4 20 N6 Na O4 20 N6 Na O4 20 K N6 O4 40 N12 Na O 40 N12 Na O	1115 vs. Ma	ass-to-Ch (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+K)+ (2M+Na)+ (2M+Na)+			900	950	
MS Spectru m/z 373.16145 374.16411 375.16622 376.1728 395.14219 396.14658 411.11631 767.2953 768.2981 769.30404 Predicted I	Z         Abund           1         2359           1         513           1         68           1         12           1         12           1         12           1         127           1         39           1         139           1         194           1         25	Form 73.3 C17 H 44.5 C17 H 24.4 C17 H 72.5 C17 H 35.8 C17 H 35.8 C17 H 9822 C34 H 9822 C34 H 985.5 C34 H	Cou 21 N6 O4 21 N6 O4 21 N6 O4 21 N6 O4 20 N6 Na O4 20 N6 Na O4 20 N6 Na O4 20 K N6 O4 40 N12 Na O 40 N12 Na O	1 1 1 ( ( ( ( ( ( ( ( ( ( ( ( (	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+K)+           (2M+Na)+           (2M+Na)+           (2M+Na)+				2950 Calc Abund	Sum %
MS Spectru m/z 373.16145 374.16411 375.16622 376.1728 395.14219 396.14658 411.11631 767.2953 768.2981 769.30404 Predicted I	Peak List           z         Abund           1         2359           1         513           1         68           1         122           1         122           1         127           1         39           1         194           1         25           sotope Matcl           m/z	Form 73.3 C17 H 44.5 C17 H 24.4 C17 H 72.5 C17 H 35.8 C17 H 62.3 C17 H 9822 C34 H 9822 C34 H 57.8 C34 H 88.5 C34 H	Cou ula 21 N6 O4 21 N6 O4 21 N6 O4 21 N6 O4 20 N6 Na O4 40 N12 Na O 40 N12	1 1 1 ( ( ( ( ( ( ( ( ( ( ( ( (	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+K)+           (2M+Na)+           (2M+Na)+           (2M+Na)+	Calc Abund %	750 800 850			<b>Sum %</b> 80.52
MS Spectru m/z 373.16145 374.16411 375.16622 376.1728 395.14219 396.14658 411.11631 767.2953 768.2981 769.30404 Predicted I Isotope	Peak List           z         Abund           1         2359           1         513           1         513           1         68           1         122           1         117           1         273           1         11           1         11           1         11           1         11           1         129           1         11           1         129           1         129           1         129           1         129           1         129           1         25           Sotope Matcl           m/z         373.16145	Form 73.3 C17 H 44.5 C17 H 24.4 C17 H 72.5 C17 H 35.8 C17 H 9822 C34 H 57.8 C34 H 57.8 C34 H 88.5 C34 H <b>Table</b> Calc m/z 373.16	Cou ula 21 N6 O4 21 N6 O4 21 N6 O4 21 N6 O4 20 N6 Na O4 20 N6 Na O4 20 N6 Na O4 20 N6 Na O4 20 N12 Na O 40 N12 Na O	1 1 ( ( ( ( ( ( ( ( ( ( ( ( (	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+K)+           (M+K)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (100	Calc Abund %	750 800 850			The second se
MS Spectru m/z 373.16145 374.16411 375.16622 376.1728 395.14219 396.14658 411.11631 767.2953 768.2981 769.30404 Predicted I Isotope	Z         Abund           1         2359           1         513           1         68           1         123           1         68           1         122           1         117           1         27           1         194           1         25           Sotter Per Matcl           m/z         373.16145           374.16411	Form 73.3 C17 H 44.5 C17 H 24.4 C17 H 72.5 C17 H 35.8 C17 H 62.3 C17 H 62.3 C17 H 9822 C34 H 57.8 C34 H 88.5 C34 H h Table Calc m/z	Cou 21 N6 O4 21 N6 O4 21 N6 O4 21 N6 O4 20 N6 Na O4 20 N6 Na O4 20 N6 Na O4 40 N12 Na O 40 N12 Na O 40 N12 Na O 40 N12 Na O 40 N12 Na O	Junts vs. Mi           J           ( <t< td=""><td>Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+K)+           (M+K)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+</td><td>Calc Abund %</td><td>750 800 850</td><td>79.88</td><td></td><td>80.52</td></t<>	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+K)+           (M+K)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+	Calc Abund %	750 800 850	79.88		80.52





Compound (11) <sup>1</sup>H NMR in CDCl<sub>3</sub>

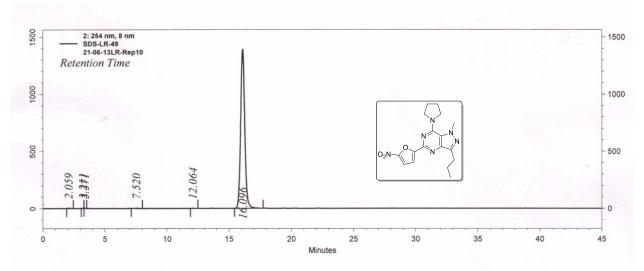


# **Qualitative Compound Report**

ata File ample Type Istrument Nar cq Method RM Calibration omment ample Group	Sta	tus Info.	GLR-4.d Sample Instrumer vishal_MS Success	nt 1 5_25072012.m	Sample Na Position User Name Acquired T	Vial 16 ime 11/18/2012	1:05:08 PM			
ompound Ta	ble							MFG		DB Formula
Compound	Lab	el	RT	Mass	Formula		H20 N6 O3	(pp	0.65	C17 H20 N6 O3
Cpd 5: C1	7 H20	N6 O3	0.172	356.15946	C17 H20 N6 O	3 (1/)	H20 NO 03		0.05	
	-								1	
Compound La	bel	n	1/z	RT	Algorithm	Mass				
Cpd 5: C17 H2		03 3	57.16674	0.172	Find by Molecu	lar Feature 356.1	5946			
5- 4- 3- 2- 1- 0-	150	200 25	0 300 3	5 400 450	500 550 6 vs. Mass-to-C	Cover 2000 2000 000 24 Cover 2000 735,30621 735,30621 06 735,30621 06 735,30621 06 735,30621 06 735,30621 06 735,30621 06 735,30621 735,300000000000000000000000000000000000		900 95	0	
MS Spectrur					-					
m/z	-	Abund	Formu		Ion					
357.16674	1		8.4 C17 H2		(M+H)+ (M+H)+					
358.16916	1		494 C17 H2 945 C17 H2		(M+H)+					
359.17205	1		1.2 C17 H2		(M+H)+					
	1		7.1 C17 H2		(M+K)+					
360.174	1		39.9 C34 H4		(2M+H)+					
395.12085				0 N12 Na O6	(2M+Na)-	F				
395.12085 713.32567	1			0 N12 Na O6	(2M+Na)-					
395.12085	-	1043	94.4 C34 H		(204 ( 010)	+				
395.12085 713.32567 735.30621	1			0 N12 Na O6	(2M+Na)-					
395.12085 713.32567 735.30621 736.30976 737.31306 751.27874	1 1 1	28 14	39.4 C34 H4 25.7	10 N12 Na O6	(2M+Na)- (2M+K)+					
395.12085 713.32567 735.30621 736.30976 737.31306	1 1 1	28 14	39.4 C34 H4 25.7 1 Table		(2M+K)+	Cale Aburd 96	Abund Sum %	10	Calc Abu	nd Sum %
395.12085 713.32567 735.30621 736.30976 737.31306 751.27874 Predicted Is Isotope	1 1 1 soto m/2	28 14 <b>pe Matc</b>	39.4 C34 H4 25.7 Table Calc m/z	Diff (ppm)	(2M+K)+	Calc Abund %	Abund Sum %		Calc Abu	nd Sum % 80.71
395.12085 713.32567 735.30621 736.30976 737.31306 751.27874 Predicted Is Isotope 1	1 1 1 soto m/2 3	28 14 <b>pe Matc</b> 57.16674	39.4 C34 H4 25.7 <b>Table</b> Calc m/z 357.166	<b>Diff (ppm)</b> 97 0.6	(2M+K)+ Abund % 4 100	100		82.56 15	Calc Abu	
395.12085 713.32567 735.30621 736.30976 737.31306 751.27874 Predicted Is Isotope	1 1 1 soto <i>m/2</i> 3	28 14 <b>pe Matc</b>	39.4 C34 H4 25.7 Table Calc m/z	<b>Diff (ppm)</b> 97 0.6 97 1.5	(2M+K)+ Abund % 4 100 1 18.16	100 20.93		82.56	Calc Abu	80.71

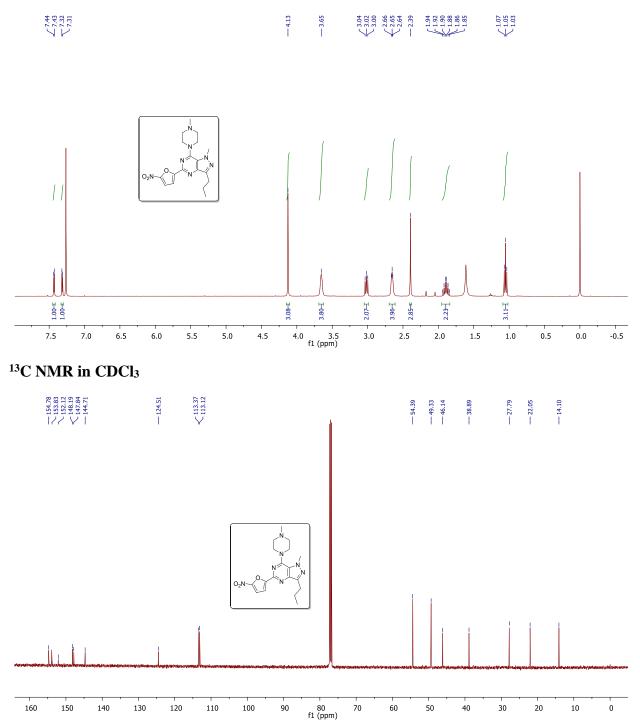


. . .



: 254 nm, 8 Pk #	<b>Retention Time</b>	Area	Area %	Height	Height %
1	2.059	50179	0.156	4345	0.310
2	3.211	11643	0.036	1731	0.124
3	3.371	11268	0.035	1868	0.133
4	7.520	42194	0.131	1902	0.136
5	12.064	11216	0.035	729	0.052
6	16.096	32033014	99.607	1390578	99.245
Totals					
		32159514	100.000	1401153	100.000

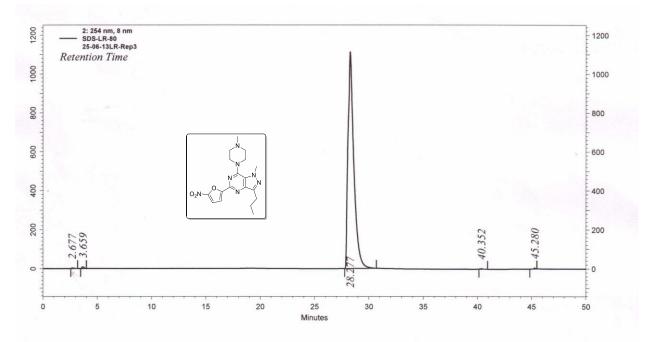
Compound (12) <sup>1</sup>H NMR in CDCl<sub>3</sub>



## **Qualitative Compound Report**

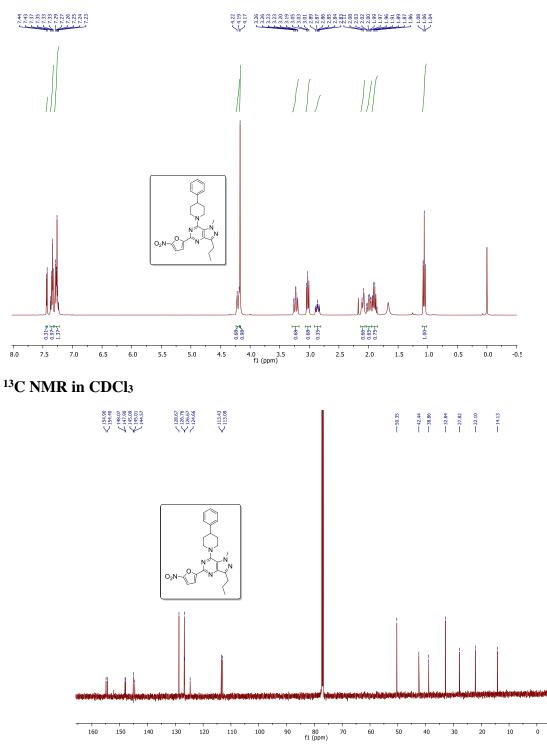
ata File		GLR-5.0	d		Sample N	lame	GLR-5			
ample Type		Sample			Position		Vial 17			
nstrument Na	ame	Instrum	nent 1		User Nam	пе				N
cq Method			MS_25072012	2.m	Acquired	Time	11/18/201	2 1:12:21 PM		N
RM Calibratio	on Status	Succes	S		DA Metho	bd	as.m			O2N NN
omment										
ample Group	) Info	<b>D</b> .								
Compound 1	Table								MFG Diff	
	dishel				Formula		ME	G Formula	(ppm)	DB Formula
Compour		<b>RT</b> 0.173	Mass 385.18543	C	18 H23 N7 (	03		3 H23 N7 O3	2.1	C18 H23 N7 C
Сра 4: С	18 H23 N7 O3	0.175	365.16545	C.	10 1125 117 1	0.5	011			
Compound L	abel	m/z	RT	Algorit	hm		Mass			
pd 4: C18 H		386.1927	0.173	Find by	Molecular	Feature	385.1854	3		
1.4 - 1.2 - 1 - 0.8 - 0.6 - 0.4 - 0.2 - 0 -	150 200	250 300	386.19270 C18 H24 N7 O3	450 50	0 550 6	600 650	0 700 7	793.35889 793.35889 C36 H46 N14 Na O6 C36 H46 N14 Na O6	950	
			Cou	unts vs.	Mass-to-C	harge (	m/z)			
MS Spectru	z Abund	Form	ula		Ion					
386.1927		231.3 C18 H			(M+H)+					
385.1927		957.3 C18 H			(M+H)+					
388.19784		231.9 C18 H			(M+H)+					
408.17537	-	719.9 C18 H			(M+Na)+					
409.17608		923.6 C18 H			(M+Na)+					
424.14983	1	5337 C18 H			(M+K)+					
793.35889			46 N14 Na O	6	(2M+Na)-	+				
794.36056			46 N14 Na O		(2M+Na)					
	-		46 N14 Na O		(2M+Na)					
795 36628		257.5			(2M+K)+					
795.36628					1		A. ME.	18		
809.32941		ch lable				Cale Ab	und %	Abund Sum %	Calc Abu	Ind Sum %
809.32941 Predicted I		Calc m/z	Diff (pp	m) Ab	ound %	Calc AD	unu 70			
809.32941	sotope Mat	Calc m/z		2.1 Ab	100 %		100	77	.29	79.72
809.32941 Predicted Is Isotope	sotope Mat m/z 386.192	Calc m/z           7         386.193	351					77	.29 .94	





Pk #	<b>Retention Time</b>	Area	Area %	Height	Height %
1	2.677	50847	0.122	3231	0.285
2	3.659	120638	0.291	8897	0.786
3	28.277	41262011	99.386	1112491	98.255
4	40.352	42597	0.103	2730	0.241
5	45.280	40967	0.099	4901	0.433
Totals					
		41517060	100.000	1132250	100.000

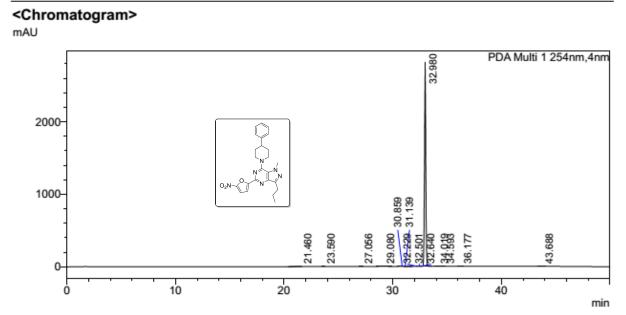
Compound (13) <sup>1</sup>H NMR in CDCl<sub>3</sub>



## **Qualitative Compound Report**

Sample Type Instrument Name Acq Method IRM Calibration Status Comment Sample Group Infe	Succes	e nent 1 MS_25072012.	Sample Na Position User Name M Acquired T	Vial Fime 11/1	19 8/2012 1:19:31 PM			
Compound Table						M	FG Diff	
Compound Label	RT	Mass	Formula		MFG Formula	(	ppm)	DB Formula
Cpd 12: C24 H26 N6 O3	3 0.172	446.20674	C24 H26 N6 O3	3	C24 H26 N6 O3		-0.24	C24 H26 N6 O3
Compound Label	m/z	RT	Algorithm		Mass			
Cpd 12: C24 H26 N6 O3	447.21403		Find by Molecul	lar Feature	and the second se			
6 - 4 -		447.21403	U24 HZ			15.40030 52 N12 Na O		
	250 300 3	350 400 45	1		0 750 800 850	06-015.40030 015.40030 06-015.40030	950	
4 2 0 150 200 2 MS Spectrum Peak List	:	350 400 45 Count	0 500 550 60 s vs. Mass-to-Ch		0 750 800 850	1	950	
4 2 0 150 200 2 MS Spectrum Peak List m/z z Abund	Formu	350 400 45 Count	0 500 550 60 s vs. Mass-to-Cha		0 750 800 850	1	950	
4 2 150 200 2 MS Spectrum Peak List <i>n/z</i> z Abund 447.21403 1 958:	Formu 164.8 C24 H2	350 400 45 Count Ila 17 N6 03	0 500 550 60 s vs. Mass-to-Cha Ion (M+H)+		0 750 800 850	1	950	
4 2 150 200 2 MS Spectrum Peak List <i>n/z</i> z Abund 447.21403 1 958: 448.21645 1 2374	Formu 164.8 C24 H2 876.4 C24 H2	150 400 45 Count 11a 17 N6 03 17 N6 03	0 500 550 60 s vs. Mass-to-Cha (M+H)+ (M+H)+		0 750 800 850	1	950	
4 2 150 200 2 MS Spectrum Peak List <i>n/z</i> z Abund 447.21403 1 958: 448.21645 1 2374 449.21835 1 414	Formu 164.8 C24 H2 876.4 C24 H2 806.9 C24 H2	150 400 45 Count 17 N6 03 17 N6 03 17 N6 03 17 N6 03	0 500 550 60 s vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+		0 750 800 850	1	950	
4 2 150 200 2 MS Spectrum Peak List m/z z Abund 447.21403 1 958: 448.21645 1 2378 449.21835 1 418 450.22169 1 46	Formu 164.8 C24 H2 876.4 C24 H2	160 400 45 Count 7 N6 03 7 N6 03 7 N6 03 7 N6 03 7 N6 03	0 500 550 60 s vs. Mass-to-Cha (M+H)+ (M+H)+		0 750 800 850	1	950	
4 2 150 200 2 MS Spectrum Peak List m/z z Abund 447.21403 1 958: 448.21645 1 2378 449.21835 1 418 450.22169 1 46	Formu 164.8 C24 H2 876.4 C24 H2 806.9 C24 H2 009.4 C24 H2	150 400 45 Count 17 N6 03 17 N6 03 17 N6 03 17 N6 03 17 N6 03 17 N6 03 17 N6 03 16 N6 Na 03	0 500 550 60 s vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+ (M+H)+		0 750 800 850	1	950	
4 2 0 150 200 2 MS Spectrum V=k List m/z z Abund 447.21403 1 958: 448.21645 1 237 449.21835 1 411 450.22169 1 441 450.22169 1 441 450.22169 1 441 450.22169 1 55	Formu 164.8 C24 H2 876.4 C24 H2 806.9 C24 H2 009.4 C24 H2 297.8 C24 H2	150 400 45 Count 7 N6 03 7 N6 03	0 500 550 60 s vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+		0 750 800 850	1	950	
4 2 150 200 2 MS Spectrum V=k List m/z z Abund 447.21403 1 958: 448.21645 1 2371 449.21835 1 411 449.21835 1 411 450.22169 1 441 450.22169 1 441 450.22169 1 641 450.22169 1 641 450.2516 1 641	Formu 164.8 C24 H2 876.4 C24 H2 806.9 C24 H2 009.4 C24 H2 297.8 C24 H2 903.1 C24 H2 056.8 C24 H2	150 400 45 Count 7 N6 03 7 N6 03	0 500 550 60 s vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+		0 750 800 850	1	950	
4 2 150 200 2 MS Spectrum Peak List m/z z Abund 447.21403 1 958: 448.21645 1 2378 449.21835 1 411 450.22169 1 44 450.22169 1 44 450.22169 1 44 450.22169 1 66 915.4003 1 670	Formu 164.8 C24 H2 876.4 C24 H2 806.9 C24 H2 009.4 C24 H2 297.8 C24 H2 903.1 C24 H2 056.8 C24 H2	150 400 45 Count 77 N6 03 77 N6 03 77 N6 03 77 N6 03 77 N6 03 77 N6 03 78 N6 Na 03 76 N6 Na 03	0 500 550 60 s vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+K)+		0 750 800 850	1	950	
4         2           0         150         200         2           MS Spectrum Peak List         m/z         z         Abund           447.21403         1         958:         448.21645         1         2378           449.21835         1         418         469.19481         1         442           459.19481         1         142         469.19481         1         142           470.19727         1         55         485.16837         1         66           915.4003         1         6770         916.40256         1         413           917.40665         1         133         133         133	Formu 164.8 C24 H2 876.4 C24 H2 876.4 C24 H2 909.4 C24 H2 907.8 C24 H2 903.1 C24 H2 903.1 C24 H2 903.1 C24 H2 903.1 C44 H5 161.3 C48 H5 161.3 C48 H5 161.3 C48 H5 161.4 H5 1	150 400 45 Count 77 N6 03 77 N6 03 77 N6 03 77 N6 03 77 N6 03 77 N6 03 78 N6 Na 03 76 N6 Na 03	0 500 550 60 s vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+K)+ (2M+Na)+		0 750 800 850	1	950	
4         2           0         150         200         2           MS Spectrum         Peak List           m/z         z         Abund           447.21403         1         958:           448.21645         1         2374           449.21835         1         418           450.22169         1         447           449.19481         1         143           450.22169         1         460           915.4003         1         677           915.4003         1         677           915.4003         1         677           915.4003         1         677           915.4005         1         133           Predicted Isotope Mato         1         133	Formu 164.8 C24 H2 876.4 C24 H2 876.4 C24 H2 297.8 C24 H2 297.8 C24 H2 093.1 C24 H2 056.8 C24 H2 070.6 C48 H5 161.3 C48	11a 127 N6 03 17 N6 03 17 N6 03 17 N6 03 17 N6 03 17 N6 03 16 N6 Na 03 16 N12 Na 06 12 N12 N12 N12 N12 N12 N12 N12 N12 N12 N	0 500 550 600 s vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+K)+ (2M+Na)+ (2M+Na)+ (2M+Na)+	arge (m/z)		900 9		
4       2         150       200         MS Spectrum Peak List         m/z       z         Abund         447.21403       1         958:         448.21645       1         449.21835       1         449.019481       1         450.22169       1         447.1977       1         485.16837       1         915.4003       1         915.4003       1         917.40665       1         13       Predicted Isotope         m/z	Formu           164.8         C24 H2           876.4         C24 H2           806.9         C24 H2           009.4         C24 H2           903.1         C24 H2           056.8         C24 H2           056.8         C48 H5           161.3         C48 H5           327.1         C48 H5           C41 Table         Calc m/z	350 400 45 Count 7 N6 03 7 N6 03 7 N6 03 7 N6 03 7 N6 03 7 N6 03 6 N6 Na 03 6 N12 Na 06 52 N12 Na 06 52 N12 Na 06 52 N12 Na 06 52 N12 Na 06	0 500 550 60 s vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+	arge (m/z)	6 Abund Sum %	900 9	950 Calc Abunc	
4       2         0       150       200       2 <b>MS Spectrum Perk List</b> <i>m/z</i> <b>z</b> Abund         447.21403       1       958:         448.21645       1       2374         449.21835       1       410         450.22169       1       440         449.19481       1       142         450.1977       1       55         485.16837       1       60         915.4003       1       67         915.4005       1       133         Predicted Isotope <i>m/z</i> 1       447.21403	Formu           164.8         C24 H2           876.4         C24 H2           806.9         C24 H2           009.4         C24 H2           297.8         C24 H2           903.1         C24 H2           055.8         C24 H2           055.8         C48 H5           161.3         C48 H5           327.1         C48 H5           C41 Table         Calc m/z           447.213*         C447.213*	350         400         45           Count         400         45           27         N6         03           27         N6         03           27         N6         03           27         N6         03           26         N6         Na           36         N6         Na           36         N6         Na           37         N6         03           36         N6         Na           37         Na         06           36         N12         Na           32         N12         Na           33         N12         Na           34         Na         Na           35         N12         Na           36         N12         Na           37         Na         Na           38         Na	0 500 550 600 s vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+	arge (m/z)	6 Abund Sum %	900 9		74.79
4       2         0       150       200       2         MS Spectrum P==k List         m/z       z       Abund         447.21403       1       958:         448.21645       1       2374         449.21835       1       410         450.22169       1       440         449.21835       1       410         450.22169       1       440         469.19481       1       142         470.19727       1       59         485.16837       1       607         915.4003       1       67         915.4005       1       133         Predicted Isotope       m/z         1       447.21403         2       448.21645	Formu           164.8         C24 H2           876.4         C24 H2           806.9         C24 H2           009.4         C24 H2           297.8         C24 H2           903.1         C24 H2           0056.8         C24 H2           070.6         C48 H5           161.3         C48 H5           327.7.1         C48 H5           Calc m/z         447.2133           448.2166         448.2166	150 400 45 Count 7 N6 03 7 N6 03 6 N6 Na 03 6 N1 Na 06 2 N12 N12 N12 N12 N12 N12 N12 N12 N12 N1	0 500 550 60 s vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+K)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+	arge (m/z)	6 Abund Sum % 100 8.57	900 9 77.1 19.14		74.79 21.37
4       2         0       150       200       2         MS Spectrum       resk List         m/z       z       Abund         447.21403       1       958:         448.21645       1       2374         449.21835       1       410         450.22169       1       440         449.19481       1       142         445.16837       1       600         915.4003       1       670         915.4003       1       670         915.4005       1       133         Predicted Isotope       m/z         1       447.21403         2       448.21645         3       449.21835	Formu           164.8         C24 H2           876.4         C24 H2           806.9         C24 H2           009.4         C24 H2           297.8         C24 H2           903.1         C24 H2           056.8         C24 H2           056.8         C48 H5           161.3         C48 H5           1	350         400         45           Count         Count           11a	0 500 550 60 s vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)+(2M+Na)+	arge (m/z)	6 Abund Sum % 100 8.57 4.55	900 977.1 19.14 3.36		74.79 21.37 3.41
4       2         0       150       200       2         MS Spectrum P==k List         m/z       z       Abund         447.21403       1       958:         448.21645       1       2374         449.21835       1       410         450.22169       1       440         449.21835       1       410         450.22169       1       440         469.19481       1       142         470.19727       1       59         485.16837       1       607         915.4003       1       67         915.4005       1       133         Predicted Isotope       m/z         1       447.21403         2       448.21645	Formu           164.8         C24 H2           876.4         C24 H2           806.9         C24 H2           009.4         C24 H2           297.8         C24 H2           903.1         C24 H2           0056.8         C24 H2           070.6         C48 H5           161.3         C48 H5           161.3         C48 H5           27.1         C48 H5           247.12         C47.213           4447.213         449.216           450.2220         450.2220	350         400         45           Count         Count           12         7         N6         03           17         N6         03         17           17         N6         03         17           17         N6         03         16           16         N6         Na         03           17         Na         06         12           12         Na         06         12           12         Na         06         0.1           12         O         0.1         10           12         O         0.1         10	0 500 550 60 s vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)+(2M+Na)+ (2M+Na)+(2M+	arge (m/z)	6 Abund Sum % 100 8.57	900 9 77.1 19.14		74.79 21.37

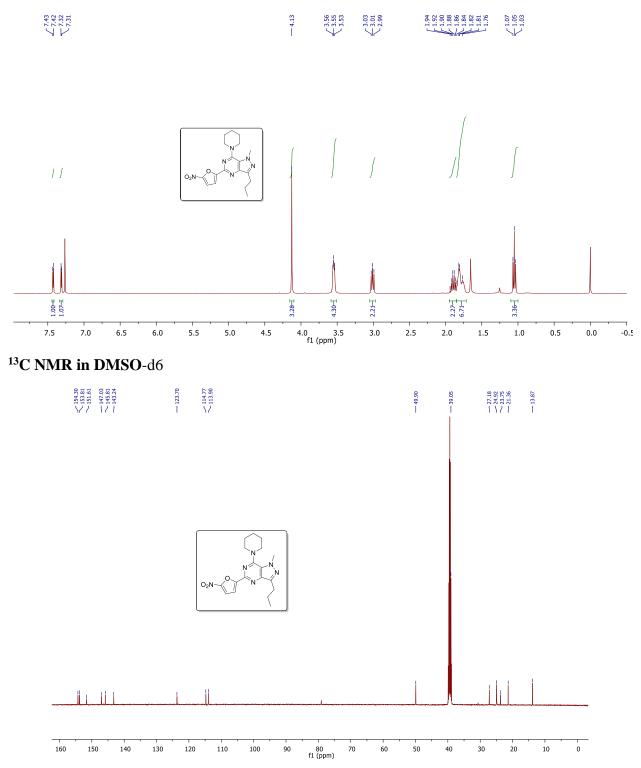
## HPLC



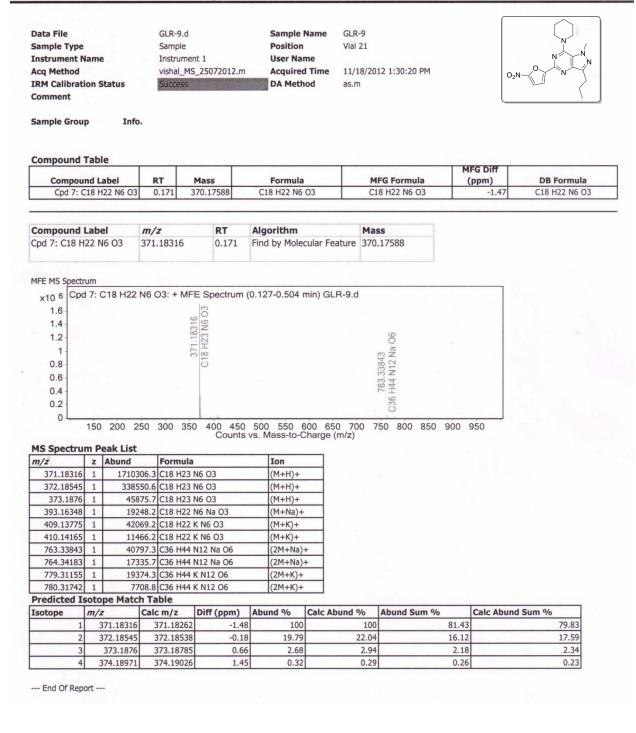
## <Peak Table>

PDA C	h1 254nm					
Peak#	Name	Ret. Time	Area	Height	Area%	Height%
1		21.460	17120	354	0.074	0.013
2		23.590	3788	356	0.016	0.013
3		27.056	2177	175	0.009	0.006
4		29.080	71506	2350	0.309	0.083
5		30.859	20834	979	0.090	0.035
6		31.139	22589	1010	0.098	0.036
7		32.229	6462	617	0.028	0.022
8		32.501	4944	475	0.021	0.017
9		32.640	3442	512	0.015	0.018
10		32.980	22927758	2815679	99.193	99.653
11		34.019	9337	1056	0.040	0.037
12		34.593	7748	740	0.034	0.026
13		36.177	8091	781	0.035	0.028
14		43.688	8557	397	0.037	0.014
Total			23114352	2825481	100.000	100.000

## Compound (14) <sup>1</sup>H NMR in CDCl<sub>3</sub>

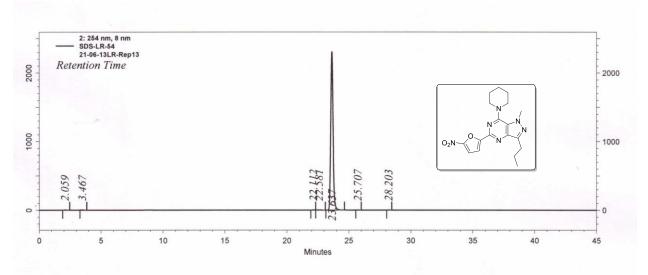


## **Qualitative Compound Report**



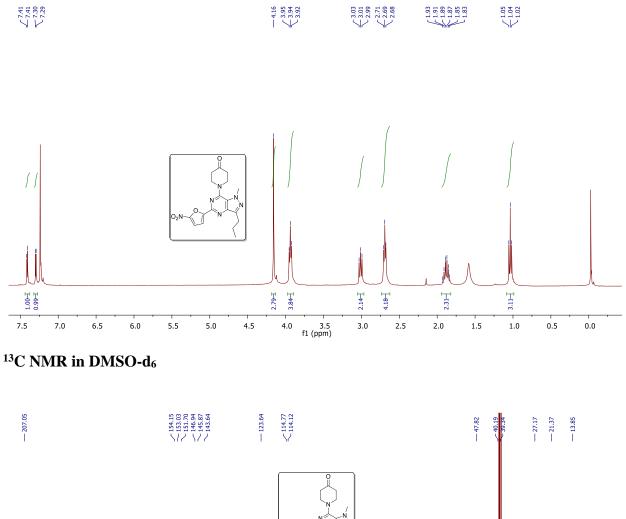


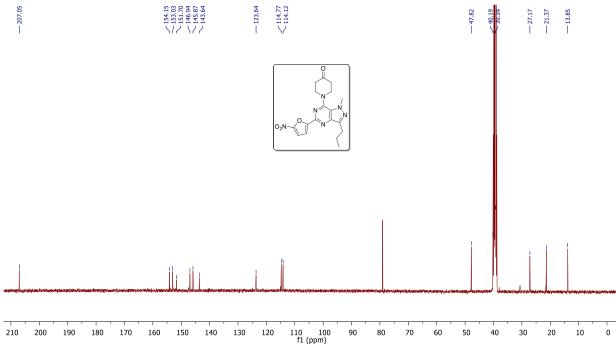
4



Pk #	<b>Retention Time</b>	Area	Area %	Height	Height %
1	2.059	32755	0.110	2637	0.114
2	3.467	35884	0.120	2626	0.113
3	22.112	18641	0.063	1584	0.068
4	22.581	36161	0.121	1764	0.076
5	23.637	29674419	99.500	2306441	99.523
6	25.707	13912	0.047	1267	0.055
7	28.203	11652	0.039	1184	0.051
Totals					
		29823424	100.000	2317503	100.000

Compound (15) <sup>1</sup>H NMR in CDCl<sub>3</sub>



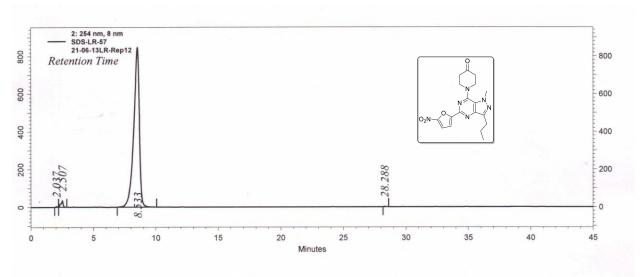


## Qualitative Compound Report

Data File Sample Type Instrument Na Acq Method RM Calibratic Comment Sample Group	on Si	Info.	S Ir V	GLR-4-14.0 ample nstrument ishal_MS_ uccess		Po Us Ac	mple N sition ser Nan quired A Metho	ne Time	GLR-4-14 Vial 13 11/19/201 as.m	2 1:19:16 PM			
Compound 1	abl	e		-					1		MF	G Diff	
Compour	nd La	bel	RT	N	lass	Fo	ormula			G Formula	(1	opm)	DB Formula
Cpd 3: C	18 H	20 N6 O4	0.1	172 38	34.15373	C18 H	120 N6 (	04	C18	3 H20 N6 O4		2.28	C18 H20 N6 O4
Compound I	abe	ł	m/z			orithm			Mass				
Cpd 3: C18 H	20 N	6 04	385.1	.61	0.172 Fin	d by Mo	lecular	Feature	384.1537	3			
0.5 0 MS Spectru	150 m P		50 3	300 350				500 650 Charge (1	0 700 7 m/z)	05 791.29634 06 C36 H40 N12 Na O8 05	900 9	950	
m/z	z	Abund		Formula			on						
385.161	1			C18 H21 I			1+H)+						
386.16381	1			C18 H21			1+H)+						
387.16582	1			C18 H21			1+H)+						
388.16683	1			C18 H21			4+H)+						
407.14279	1			C18 H20 I			4+Na)+						
408.14394	1			C18 H20			1+Na)+ 2M+Na)-						
791.29634	1				N12 Na O8 N12 Na O8		2M+Na)						
792.29832	-				V12 Na O8		2M+Na)						
	1				112 110 00	1(2							
793.29771	SOLO	pe matc	-	m/z	Diff (ppm)	Abund	1 %	Calc Ab	und %	Abund Sum %		Calc Abur	nd Sum %
Predicted Is	m	7				- All all a	- / -						
Predicted Isotope	m/2					7	100		100		79.94		79.66
Predicted Is Isotope		385.161	38	85.16188	2.2				100 22.05		79.94 17.03		
Predicted Isotope			38			7	100 21.31 3.37						79.66

End Of Deport



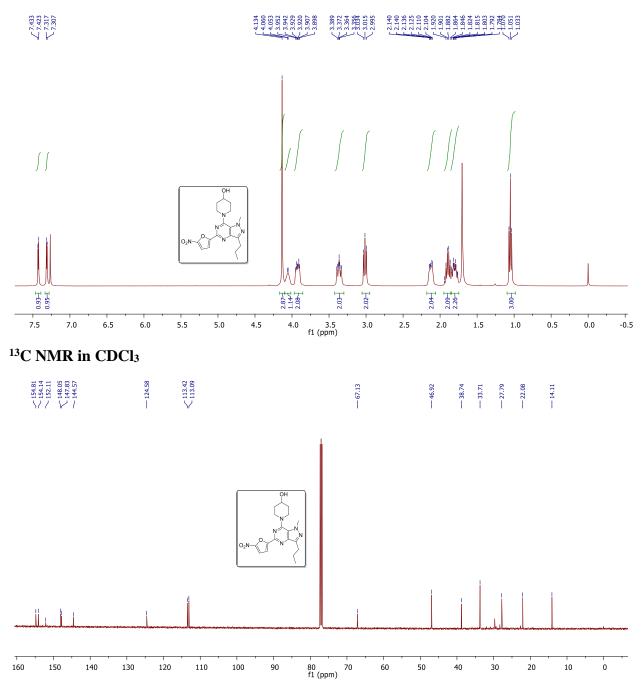


#### 2: 254 nm, 8 nm

2

Pk#	<b>Retention Time</b>	Area	Area %	Height	Height %
1	2.037	25240	0.094	3142	0.354
2	2.507	411832	1.536	34736	3.917
3	8.533	26360654	98.315	847257	95.540
4	28.288	14583	0.054	1671	0.188
Totals	/				
		26812309	100.000	886806	100.000

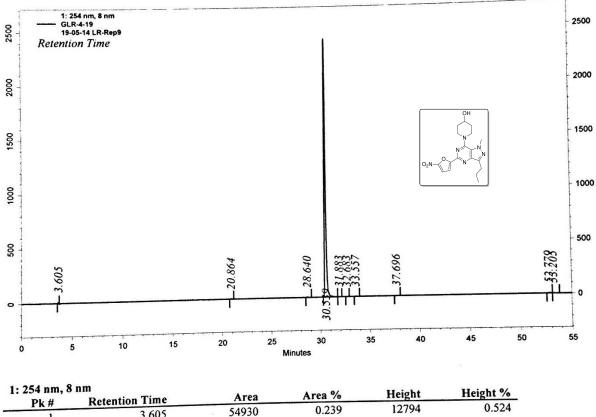
## Compound (16) <sup>1</sup>H NMR in CDCl<sub>3</sub>



## **Qualitative Compound Report**

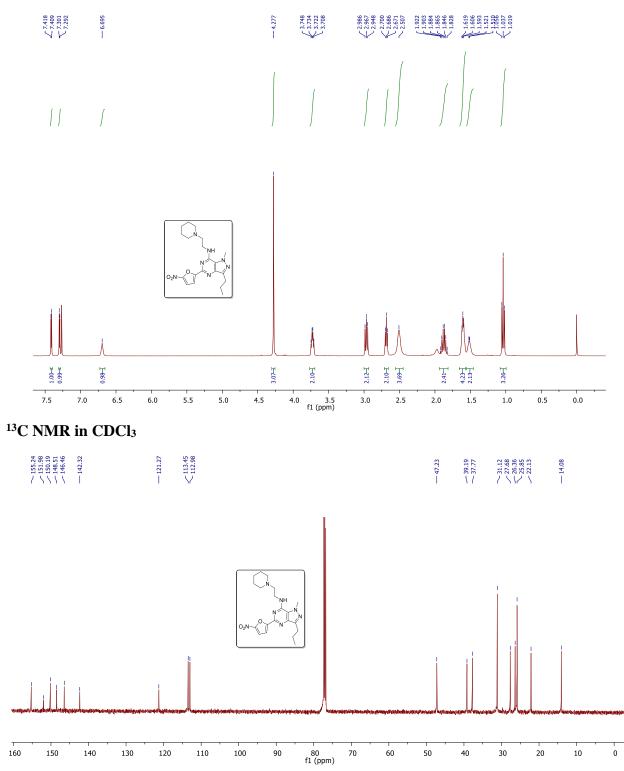
Data File Sample Type			GLR-4- Sample			Sample N Position	lame GLR-4-19 Vial 15			ОН
Instrument N	ame		Instrur			User Nam	ne			
Acq Method	unite				72012.m	Acquired	Time 11/19/201	2 1:29:54 PM		N ./
RM Calibrati	on S	tatus	Succes		1	DA Metho	as.m			
Comment	0.1.0									O2N N
ample Grou	p	Info								
Compound <sup>•</sup>	Tabl	A								
			DT	Mass		Formula	M	-G Formula	MFG Diff (ppm)	DB Formula
Compou		22 N6 O4	<b>RT</b> 0.171	386.1		C18 H22 N6 0		8 H22 N6 O4	1.57	C18 H22 N6 04
Compound	Labo	el	m/z			Algorithm	Mas			
Cpd 4: C18 H	22 N	16 04	387.17693		0.171	Find by Molec	ular Feature 386.	16965		
MFE MS Spectr		C18 H22	N6 04: + I	MFE St	pectrum (	0.121-0.612 n	nin) GLR-4-19.d			
~10		STOTILL								
6				93	16.0			00		
5				176	23 1			0 0		
4 -				387.17693	C18 H23 N6 04			795.32716 C36 H44 N12 Na O8		
3				0	5			5.32 4 N		
2								79 H4		
1-								C30		
0										
	150	200 2	250 300	350 4	00 450	500 550 6 vs. Mass-to-C	600 650 700 T	750 800 850 90	00 950	
MS Spectru	m P	eak List			Counts	vo. mado to o				
m/z	z	Abund	Form	ula		Ion				
387.17693	1		336.8 C18 H			(M+H)+				
388.17937	1		35.9 C18 H			(M+H)+				
389.18176	-		986.6 C18 H			(M+H)+				
409.15852			4909 C18 H			(M+Na)+	-			
410.16204			156.8 C18 H			(M+Na)+				
425.1321		-	910.5 C18 H			(M+K)+ (2M+Na)-	+			
795.32716		-	967.1 C36 H			(2M+Na)-				
		-	136.1 C36 H			(2M+Na)-				
796.3302						(2M+K)+				
797.33364						I				
		ope matc		010	f (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abu	Ind Sum %
797.33364 811.29841			Calc m/z	DIT	(ppin)					
797.33364 811.29841 Predicted I	soto m/				1.56				1.65	79.64
797.33364 811.29841 Predicted I Isotope	soto m/	z	387.17	753		19.47	22.08	1	1.65 15.9 2.21	79.64 17.58 2.51





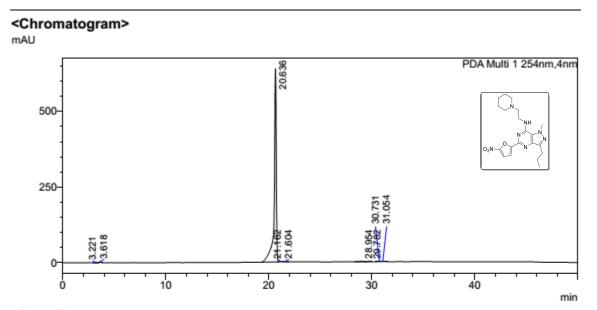
1	3.605	54930	0.239	12794	0.524
	20.864	17134	0.074	1898	0.078
2	the second s	32295	0.140	3312	0.136
3	28.640	22804023	99.052	2413038	98.879
4	30.539	11389	0.049	1313	0.054
5	31.883	10732	0.047	1208	0.050
6	32.683		0.116	2355	0.097
7	33.557	26781	0.056	1076	0.044
8	37.696	12843	0.152	2777	0.114
9	52.779	34955		620	0.025
10	53.205	17108	0.074	820	0.025
Totals	T			0.4.40203	100.000
		23022190	100.000	2440391	100.000

## Compound (17) <sup>1</sup>H NMR in CDCl<sub>3</sub>



			Quali					
Data File Sample Type Instrument N Acq Method IRM Calibrati Comment Sample Grou	lame ion Status	Succes	e ment 1 _MS_25072012.m	Sample Position User Na Acquire DA Met	n Vial 22 ame ed Time 11/18/20	012 1:33:52 PM	0 <sub>2</sub> N-0	
Compound <sup>•</sup>	Table						MFG Diff	
Compou		RT	Mass	Formula		4FG Formula	(ppm)	DB Formu
Cpd 14: 0	20 H27 N7 O3	0.173	413.21772	C20 H27 N7	7 03 C	20 H27 N7 O3	-0.45	C20 H27 N7
x10 5 Cpd				(0.102 0.02)	3 min) GLR-10.d			
6 - 4 - 2 -			414.22501 C20 H28 N7 O3			849.42186 C40 H54 N14 Na O6		
6 - 4 - 2 - 0 -		50 300 3	350 400 450	500 550 vs. Mass-to-(	600 650 700 7 Charge (m/z)	C40	00 950	
6 - 4 - 2 - 0 - IS Spectrur	n Peak List		350 400 450 Counts	vs. Mass-to-(	600 650 700 7 Charge (m/z)	C40	00 950	
6 - 4 - 2 - 0 - S Spectrur	n Peak List z Abund	50 300 3 Formu 386.9 (220 H2	150 400 450 Counts	500 550 vs. Mass-to-( Ion (M+H)+	600 650 700 7 Charge (m/z)	C40	0 950	
6 4 2 0 5 Spectrur ⁄z	m Peak List z Abund 1 9085	Formu	150 400 450 Counts 18 18 18 10 03	vs. Mass-to-0	600 650 700 7 Charge (m/z)	C40	0 950	
6 4 2 0 <b>S Spectrum</b> 1/z 414.22501	z         Abund           1         9085           1         2064	Formu 86.9 C20 H2	150 400 450 Counts 11a 18 N7 03 18 N7 03	vs. Mass-to-0 Ion (M+H)+ (M+H)+	600 650 700 7 Charge (m/z)	C40	0 950	
6 4 2 0 <b>S Spectrum</b> 1/2 414.22501 415.22739	z         Abund           1         9085           1         2064           1         294	Formu 86.9 C20 H2 51.9 C20 H2	150 400 450 Counts 18 N7 03 18 N7 03 18 N7 03	vs. Mass-to-0	600 650 700 7 Charge (m/z)	C40	0 950	
6 - 4 - 2 - 0 - <b>S Spectrur</b> 414.22501 415.22739 416.22999	z         Abund           1         9085           1         2064           1         294           1         294	Formu 86.9 C20 H2 51.9 C20 H2 50.7 C20 H2 57.2 C20 H2	150 400 450 Counts 18 N7 03 18 N7 03 18 N7 03	vs. Mass-to-( Ion (M+H)+ (M+H)+ (M+H)+	Charge (m/z)	C40	0 950	
6 - 4 - 2 - 0 - <b>S Spectrum</b> /z 415.22739 415.22739 415.22739 415.22299	Z         Abund           1         9085           1         2064           1         294           1         29           1         122	Formu 86.9 C20 H2 51.9 C20 H2 50.7 C20 H2 57.2 C20 H2 02.6 C40 H5	150 400 450 Counts 18 N7 03 18 N7 03 18 N7 03 18 N7 03 14 N14 Na O6	vs. Mass-to-( Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+Na)	Charge (m/z)	C40	0 950	
6 - 4 - 2 - 0 - <b>S Spectrum</b> /z 414.22501 415.22739 416.22999 417.23203 849.42186 850.42429	z         Abund           1         9085           1         2064           1         294           1         294           1         229           1         122           1         62	Formu i86.9 C20 H2 i51.9 C20 H2 i50.7 C20 H2 i50.7 C20 H2 i57.2 C20 H2 i20.2 C40 H5 i20.1 C40 H5	10 10 10 10 10 10 10 10 10 10	vs. Mass-to-( Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+Na) (2M+Na)	Charge (m/z)	C40	0 950	
6 - 4 - 2 - 0 - <b>S Spectrum</b> //z 414.22501 415.22739 416.22999 417.2203 849.42186 850.42429 851.42824	z         Abund           1         9085           1         2064           1         294           1         294           1         294           1         294           1         294           1         294           1         294           1         294           1         294           1         122           1         62           1         18	Formu 86.9 C20 H2 51.9 C20 H2 50.7 C20 H2 57.2 C20 H2 02.6 C40 H5 20.1 C40 H5 75.7 C40 H5	150 400 450 Counts 18 N7 03 18 N7 03 18 N7 03 18 N7 03 14 N14 Na 06 14 N14 Na 06 14 N14 Na 06	vs. Mass-to-( Ion (M+H)+ (M+H)+ (M+H)+ (2M+Na) (2M+Na) (2M+Na)	Charge (m/z)	C40	0 950	
6 - 4 - 2 - 0 - 	Peak List           z         Abund           1         9085           1         2064           1         294           1         294           1         229           1         62           1         62           1         18           1         5	Formu 86.9 C20 H2 51.9 C20 H2 50.7 C20 H2 57.2 C20 H2 02.6 C40 H5 20.1 C40 H5 75.7 C40 H5 35.6 C40 H5	10 10 10 10 10 10 10 10 10 10	VS. Mass-to-( Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+Na) (2M+Na) (2M+Na)	Charge (m/z)	C40	0 950	
6 - 4 - 2 - 0 - <b>S Spectrun</b> /z 414.22501 415.22739 416.22999 417.23203 849.42186 850.42429 851.42824 851.42824 851.42824 851.42824 851.42824	Peak List           z         Abund           1         9085           1         2064           1         294           1         294           1         229           1         122           1         62           1         62           1         18           1         5           1         14	Formu 86.9 C20 H2 55.9 C20 H2 55.7 C20 H2 57.2 C20 H2 57.2 C20 H2 57.2 C40 H5 20.1 C40 H5 75.7 C40 H5 35.6 C40 H5 32.2	150 400 450 Counts 18 N7 03 18 N7 03 18 N7 03 18 N7 03 14 N14 Na 06 14 N14 Na 06 14 N14 Na 06	Vs. Mass-to-( Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+Na) (2M+Na) (2M+Na) (2M+Na)	Charge (m/z)	C40	0 950	
6- 4- 2- 0 <b>IS Spectrum</b> 1/2 414.22501 415.22739 416.22999 416.22999 850.42429 851.42824 855.42275 855.39336 865.39336	Peak List           z         Abund           1         9085           1         2064           1         294           1         294           1         229           1         122           1         62           1         62           1         15           1         14           1         13	Formu 86.9 C20 H2 55.9 C20 H2 55.7 C20 H2 57.2 C20 H2 20.1 C40 H5 20.1 C40 H5 35.6 C40 H5 32.2 41.6	150 400 450 Counts 18 N7 03 18 N7 03 18 N7 03 18 N7 03 14 N14 Na 06 14 N14 Na 06 14 N14 Na 06	VS. Mass-to-( Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+Na) (2M+Na) (2M+Na)	Charge (m/z)	C40	0 950	
6 4 2 0 <b>IS Spectrum</b> 1/2 414.22501 415.22739 416.22999 417.23203 849.42186 850.42429 851.42824 855.42275 865.39138 redicted Is	Peak List           z         Abund           1         9085           1         2064           1         229           1         229           1         62           1         122           1         62           1         18           1         5           1         14           1         13           otope Match         Match	Formu 86.9 C20 H2 51.9 C20 H2 50.7 C20 H2 50.7 C20 H2 57.2 C20 H2 20.2.6 C40 H5 20.1 C40 H5 35.6 C40 H5 32.2 41.6 h Table	150 400 450 Counts 18 N7 03 18 N7 03 18 N7 03 18 N7 03 18 N7 03 14 N14 Na 06 14 N14 Na 06 14 N14 Na 06 14 N14 Na 06	Vs. Mass-to-( Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+Na) (2M+Na) (2M+Na) (2M+K)+ (2M+K)+	Charge (m/z)	750 800 850 90		
6 - 4 - 2 - 0 - 414.22501 415.22739 416.22999 417.23203 849.42186 850.42429 851.42824 851.42824 851.42824 852.42775 865.39336 866.39198 redicted Is	Peak List           z         Abund           1         9085           1         2064           1         294           1         294           1         294           1         294           1         122           1         62           1         18           1         13           1         14           1         000tope Matcol           m/z         10	Formu 86.9 C20 H2 51.9 C20 H2 57.7 C20 H2 57.2 C20 H2 57.2 C40 H5 35.6 C40 H5 32.2 44.6 h Table Calc m/z	150 400 450 Counts 18 N7 03 18 N7 03 18 N7 03 18 N7 03 18 N7 03 14 N14 Na 06 14 N14 Na 06	Vs. Mass-to-0 Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+Na) (2	Calc Abund %	750 800 850 90	Calc Abund	
6 - 4 - 2 - 0 - 	Peak List           z         Abund           1         9085           1         2064           1         294           1         294           1         294           1         294           1         122           1         162           1         18           1         55           1         14           1         133           otope Matcomer Matcom	Formu           86.9         C20 H2           51.9         C20 H2           50.7         C20 H2           57.2         C20 H2           02.6         C40 H5           75.7         C40 H5           75.7         C40 H5           75.7         C40 H5           75.7         C40 H5           32.2         I           41.6         I           Table         I           Calc         m/z           414.2248         I	350         400         450           Counts         Counts           18         N7 03           18 N7 03         38           18 N7 03         38           18 N7 03         4           14 N14 Na 06         14           14 N14 Na 06         14           15 Diff (ppm)         31	Vs. Mass-to-0 Ion (M+H)+ (M+H)+ (M+H)+ (2M+Na)	Charge (m/z)	750 800 850 90	Calc Abund	77.81
6 4 2 0 <b>IS Spectrum</b> 1/2 414.22501 415.22739 416.22999 417.23203 849.42186 850.42429 851.42824 851.4284 851	Peak List           z         Abund           1         9085           1         2064           1         294           1         294           1         294           1         294           1         122           1         62           1         18           1         13           otope Matcing         414.22501           415.22739         415.22739	Formu           86.9         C20 H2           51.9         C20 H2           50.7         C20 H2           57.2         C20 H2           20.1         C40 H5           20.1         C40 H5           35.6         C40 H5           32.2         41.6           HTable         Calc m/z           414.224%         415.2275	350         400         450           28         N7         03           4         N14         Na           6         Diff (ppm)         0.46           55         0.39         0.39	Vs. Mass-to-( Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+Na) (	Charge (m/z)	Abund Sum %	Calc Abund 9.18 7.99	77.81 19.16
6 4 2 0 4 4 12 4 15.22739 4 16.22999 4 17.23203 849.42186 850.42429 851.42824 855.424275 855.39336 855.39336 865.39386 865.395.395.395.39566 865.39566 865.39566 865.39566 865.39566 865.3	Peak List           z         Abund           1         9085           1         2064           1         294           1         294           1         294           1         294           1         122           1         162           1         18           1         55           1         14           1         133           otope Matcomer Matcom	Formu           86.9         C20 H2           51.9         C20 H2           50.7         C20 H2           57.2         C20 H2           02.6         C40 H5           75.7         C40 H5           75.7         C40 H5           75.7         C40 H5           75.7         C40 H5           32.2         I           41.6         I           Table         I           Calc         m/z           414.2248         I	350         400         450           200         450         Counts           18         N7         03           14         N14         Na           4         N14         Na           6         14         N14           0         14         N14           0         14         N14           0         14         N14           0         16         16           0         16         0.39           0         0.15         0.15	Vs. Mass-to-( Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+Na) (	Charge (m/z)	Abund Sum %	Calc Abund	77.81

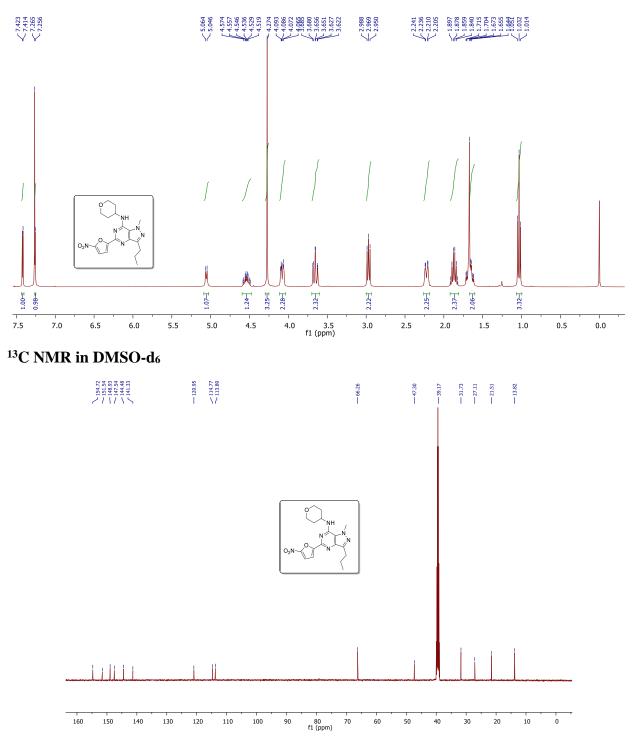




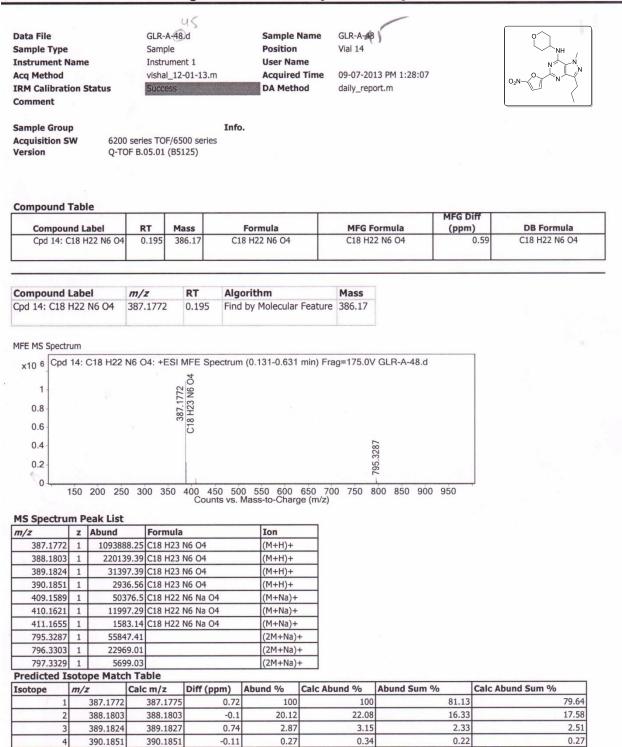
#### <Peak Table>

PDA C	h1 254nm					
Peak#	Name	Ret. Time	Area	Height	Area%	Height%
1		3.221	4892	202	0.053	0.031
2		3.618	30622	4216	0.335	0.649
3		20.636	8993546	639635	98.284	98.493
4		21.162	13128	781	0.143	0.120
5		21.604	20699	1021	0.226	0.157
6		28.954	53571	1766	0.585	0.272
7		29.782	4796	428	0.052	0.066
8		30.731	13181	643	0.144	0.099
9		31.054	16138	732	0.176	0.113
Total			9150573	649423	100.000	100.000

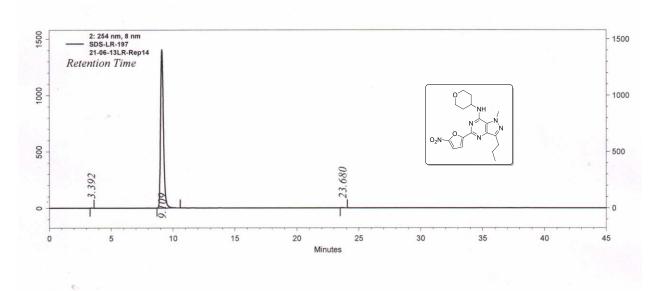
Compound (18) <sup>1</sup>H NMR in CDCl<sub>3</sub>



#### **Qualitative Compound Report**



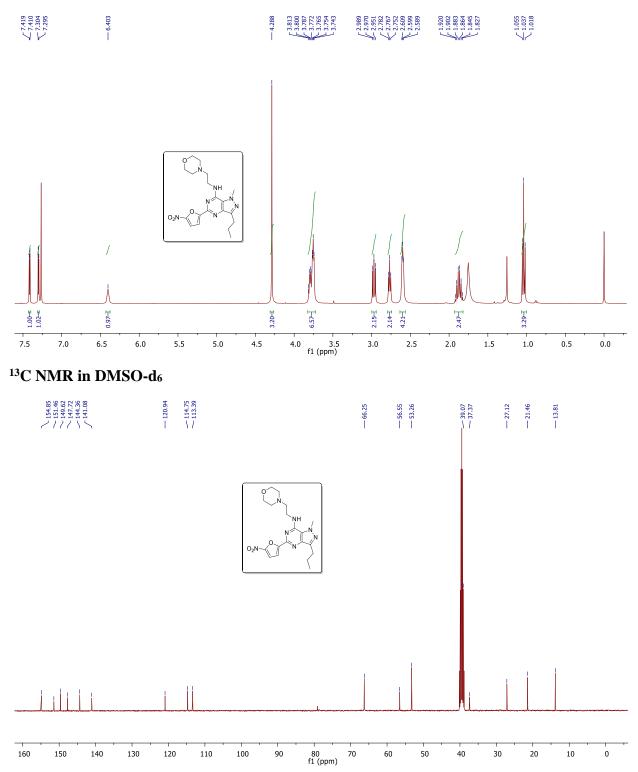




242	an and the		-	
2:	254	nm,	8	nm

Pk #	<b>Retention Time</b>	Area	Area %	Height	Height %
1	3.392	11396	0.050	1609	0.114
2	9.109	22657961	99.867	1404888	99.772
3	23.680	18854	0.083	1603	0.114
Totals					
/		22688211	100.000	1408100	100.000

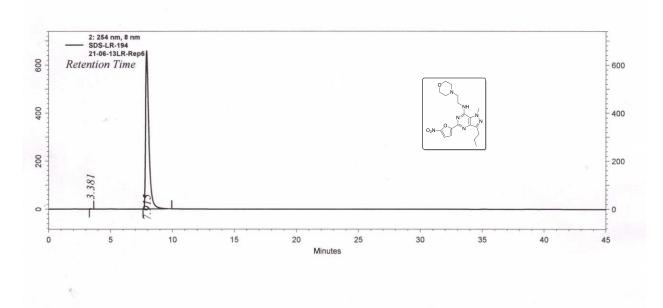
Compound (19) <sup>1</sup>H NMR in CDCl<sub>3</sub>



Qualitative Compound Repo	ort
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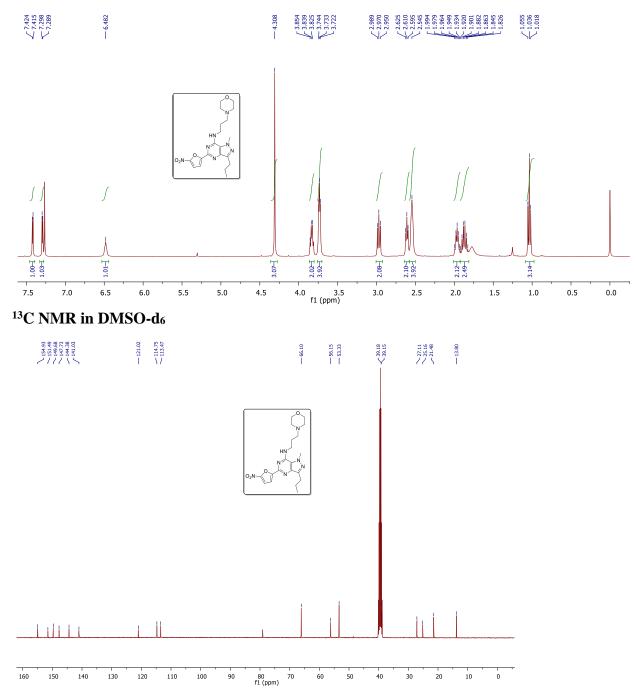
Data File Sample Type Instrument I Acq Method IRM Calibrat Comment	Name		Samp Instru	iment 1 _12-01-13.m	Sample Name Position User Name Acquired Time DA Method	GLR-A Vial 13 09-07-2013 P daily_report.r			0,	NH NN NH NN NH NN
Sample Grou Acquisition S Version Compound	SW	Q-TC	) series TOF DF B.05.01 (	/6500 series (85125)	Info.					
compound	Tabl	C						MF	GDiff	
Compou	_		RT	Mass	Formula	MFG	Formula	and the second	opm)	<b>DB</b> Formula
Cpd 6:	C19 H	25 N7 04	0.196	415.1968	C19 H25 N7 O4	C19 H	25 N7 O4		-0.06	C19 H25 N7 O4
-										
Comnound	Lab			INT			mg			
Compound Cpd 6: C19 F			<i>m/z</i> 416.2041	RT	Algorithm	Mass				
cha 0: C13 l	123 1	17 04	410.2041	0.196	Find by Molecular Featu	ire 415.1968				
5- 4- 3- 2- 1- 0- 1	_	007 C19 H27 N7 O4 C19 H27 N7 O4	300 35		0 500 550 600 650 vs. Mass-to-Charge (m/z	700 750 80	£1333813 0 850 900	950		
<b>IS Spectru</b>			_							
1/Z		Abund	Form		Ion					
208.6055	2			27 N7 O4	(M+2H)+2					
416 2041	1		4.56 C19 H		(M+H)+					
416.2041	1		8.38 C19 H		(M+H)+					
417.2067	1 1		5.35 C19 H2 5.54 C19 H2		(M+H)+					
417.2067 418.2087		234		25 N7 Na O4	(M+H)+					
417.2067 418.2087 419.2121	1	27460		LJ N/ Na 04	(M+Na)+					
417.2067 418.2087 419.2121 438.1859	1			5 N7 Na 04						
417.2067 418.2087 419.2121 438.1859 439.1881	1 1 1	6409	9.97 C19 H2	25 N7 Na O4	(M+Na)+					
417.2067 418.2087 419.2121 438.1859 439.1881 853.3813	1 1 1 1	6409 38166	9.97 C19 H2 5.36	25 N7 Na O4	(2M+Na)+					
417.2067 418.2087 419.2121 438.1859 439.1881 853.3813 854.3845	1 1 1 1 1	6409 38166 17404	9.97 C19 H2 5.36 4.52	25 N7 Na O4	(2M+Na)+ (2M+Na)+					
417.2067 418.2087 419.2121 438.1859 439.1881 853.3813 854.3845 855.3857	1 1 1 1 1 1	6409 38166 17404 4655	9.97 C19 H2 5.36 4.52 5.52	25 N7 Na O4	(2M+Na)+					
417.2067 418.2087 419.2121 438.1859 439.1881 853.3813 854.3845 855.3857 redicted I	1 1 1 1 1 50top	6409 38166 17404 4655 <b>De Match</b>	9.97 C19 H2 5.36 4.52 5.52 1 Table		(2M+Na)+ (2M+Na)+ (2M+Na)+	bund %	ind Sum %		alc Ahund S	um %
417.2067 418.2087 419.2121 438.1859 439.1881 853.3813 854.3845 855.3857 redicted I	1 1 1 1 1 50top <i>m/z</i>	6409 38166 17404 4655 <b>De Match</b>	9.97 C19 H2 5.36 4.52 5.52 <b>1 Table</b> Calc m/z	Diff (ppn	(2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+		ind Sum %		alc Abund S	
417.2067 418.2087 419.2121 438.1859 439.1881 853.3813 854.3845 855.3857 <b>redicted Is</b> sotope	1 1 1 1 1 50top <i>m/z</i>	6409 38166 17404 4655 <b>De Match</b>	9.97 C19 H2 5.36 4.52 5.52 1 Table	Diff (ppn	(2M+Na)+ (2M+Na)+ (2M+Na)+	bund % Abu 100 23.57	ind Sum %	82.34 12.29	alc Abund S	um % 78.71 18.55





Pk #	<b>Retention Time</b>	Area	Area %	Height	Height %
1	3.381	12298	0.100	1764	0.267
2	7.915	12279122	99.900	658213	99.733
Totals					
		12291420	100.000	659977	100.000

Compound (20) <sup>1</sup>H NMR in CDCl<sub>3</sub>

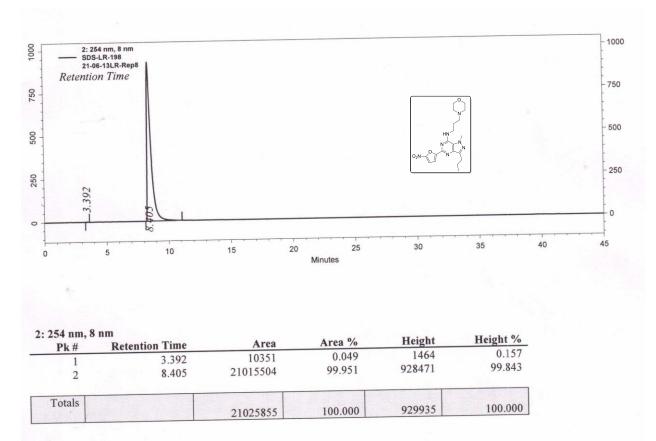


## **Qualitative Compound Report**

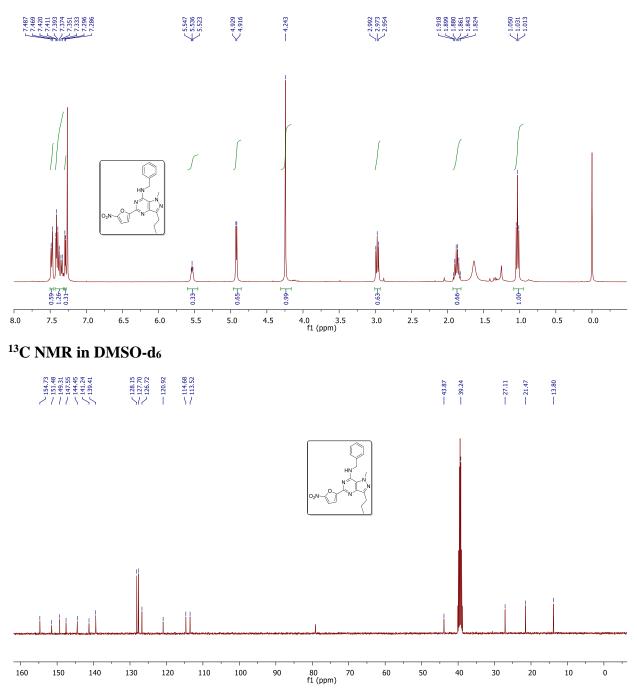
Sample Type			Sam	ple	Position	Vial 2			
Instrument N	Name			rument 1	User Na				HN N
Acq Method			000000000000000000000000000000000000000	al_12-01-13.m	Acquire		13 PM 12:23:54		O2N O N
IRM Calibrati Comment	ion S	tatus	Suc	Cess	DA Meth	od daily_rep	port.m		
Sample Grou	Surger and	600			fo.				
Acquisition S Version	vv		OF B.05.01	F/6500 series (B5125)					
Compound	Tab	le		I I				MFG Diff	
Compou	nd L	abel	RT	Mass	Formula	N	AFG Formula	(ppm)	<b>DB</b> Formula
Cpd 26:	C20 H	127 N7 O4	0.197	429.2126	C20 H27 N7	04 C	20 H27 N7 O4	-0.38	C20 H27 N7 O4
Compound	Lah	al	m/z	RT Algori	thm	Mass	٦		
Cpd 26: C20			and the second	And the second s		ature 429.2126			
MFE MS Spectr	um		I	L			504		
		C20 H27	N7 04. +	ESI MEE Spectru	m (0 102-0 669	min) Frag=175.0	CIR-A-49 d		
~10	20.			States in which the second states and the	111 (0.102-0.000	, min) 1 lag=1/5.01	GEN-A-43.0		
5 -		39		00/10					
4		19 V 61		28 N					
3		215 0 H		0 H 0					
3 -		215.6139 C20 H29 N7 O4		430.2200 C20 H28 N7 04					
3 - 2 -		215 C20 H		430 C20 H.			127		
		215 C20 H		430 C20 H			31.4127		
2 - 1 -		215 C20 H		430 C20 H			- 881,4127		
2	150	-	0 300 3	50 400 450 5	00 550 600	650 700 750 8	820 800 820 900 920 81,4127		
2-1-0		200 25		50 400 450 5	00 550 600 Mass-to-Char	650 700 750 8 ge (m/z)			
2 1 0 MS Spectru	m P	200 25		50 400 450 5 Counts vs	00 550 600 . Mass-to-Char Ion	650 700 750 8 ge (m/z)			
2- 1- 0 MS Spectru <i>m/z</i> 215.6139	<b>m P</b>	200 250 eak List Abund 25262	<b>Form</b> 27.44 C20	50 400 450 5 Counts vs nula H29 N7 O4	. Mass-to-Char	ge (m/z)			
2 1 0 <b>MS Spectru</b> <i>m/z</i> 215.6139 216.1154	<b>m P</b> 2 2	200 250 eak List Abund 25262 6294	Forr 27.44 C20 18.39 C20	50 400 450 5 Counts vs nula H29 N7 O4 H29 N7 O4	. Mass-to-Char Ion (M+2H)+ (M+2H)+	ge (m/z)			
2 1 0 MS Spectru m/z 215.6139 216.1154 216.6168	<b>m P</b> 2 2 2 2	200 250 eak List Abund 25262 6294 1130	Forr 27.44 C20 48.39 C20 03.54 C20	50 400 450 5 Counts vs hula H29 N7 O4 H29 N7 O4 H29 N7 O4 H29 N7 O4	. Mass-to-Char Ion (M+2H)+ (M+2H)+ (M+2H)+	ge (m/z)			
2 1 0 <b>MS Spectru</b> <u>m/z</u> 215.6139 216.1154 216.6168 430.22	<b>m P</b> 2 2 2 1	200 250 eak List Abund 25262 6294 1130 50973	Form 7.44 C20 18.39 C20 13.54 C20 18.03 C20	50 400 450 5 Counts vs hula H29 N7 O4 H29 N7 O4 H29 N7 O4 H28 N7 O4 H28 N7 O4	. Mass-to-Char Ion (M+2H)+ (M+2H)+ (M+2H)+ (M+2H)+ (M+H)+	ge (m/z)			
2 1 0 <b>MS Spectru</b> <u>m/z</u> 215.6139 216.1154 216.6168 430.22 431.2223	<b>m P</b> 2 2 2 1 1	200 250 eak List Abund 25262 6294 1130 50973 11749	Form           27.44         C20           48.39         C20           03.54         C20           48.03         C20           03.54         C20           03.54         C20	50 400 450 5 Counts vs hula H29 N7 O4 H29 N7 O4 H29 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4	Ion           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+H)+           (M+H)+	ge (m/z)			
2 1 0 <b>MS Spectru</b> <u>m/z</u> 215.6139 216.1154 216.6168 430.22 431.2223 432.2247	<b>m P</b> 2 2 2 1 1 1	200 250 eak List Abund 25262 6294 1130 50973 11749 2022	Form           27.44         C20           48.39         C20           48.03         C20           48.03         C20           43.96         C20           54.02         C20	50 400 450 5 Counts vs H129 N7 O4 H29 N7 O4 H29 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4	Ion           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+H)+           (M+H)+           (M+H)+	2 2 2			
2 1 0 <b>MS Spectru</b> <u>m/z</u> 215.6139 216.1154 216.6168 430.22 431.2223 432.2247 452.2012	m P 2 2 2 1 1 1 1 1	200 250 eak List Abund 25262 6294 1130 50973 11749 2022 2196	Form           27.44         C20           18.39         C20           13.54         C20           13.54         C20           13.96         C20           16.92         C20           17.44         C20	50 400 450 5 Counts vs H29 N7 O4 H29 N7 O4 H29 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H27 N7 Na O4	Ion           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+	2 2 2			
2 1 0 <b>MS Spectru</b> <u>m/z</u> 215.6139 216.1154 216.6168 430.22 431.2223 432.2247	<b>P Z 2 2 1 1 1 1 1 1</b>	200 250 eak List Abund 25262 6294 1130 50973 11749 2022 2196	Form           27.44         C20           48.39         C20           03.54         C20           48.03         C20           3.54         C20           3.54         C20           3.60         C20           3.74         C20           3.96         C20           6.92         C20           7.84         C20           00.87         C20	50 400 450 5 Counts vs H129 N7 O4 H29 N7 O4 H29 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4	Ion           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+H)+           (M+H)+           (M+H)+	ge (m/z)			
2 1 0 <b>MS Spectru</b> <i>m/z</i> 215.6139 216.1154 216.6168 430.22 431.2223 432.2247 452.2012 453.2034	<b>P 2 2 2 1 1 1 1 1 1 1</b>	200 250 eak List Abund 25262 6294 1130 50973 11749 2022 2196 719	Form           17.44         C20           18.39         C20           13.54         C20           18.03         C20           13.94         C20           13.94         C20           13.94         C20           13.95         C20           13.94         C20           13.95         C20           13.94         C20           13.95         C20           13.84         C20           13.84         C20	50 400 450 5 Counts vs H29 N7 O4 H29 N7 O4 H29 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H27 N7 Na O4	Ion           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+	ge (m/z)			
2 1 0 MS Spectru m/z 215.6139 216.1154 216.6168 430.222 431.22237 432.2247 432.2247 452.2012 453.2034 881.4127 882.4147 Predicted Is	<b>m P</b> 2 2 2 1 1 1 1 1 1 1 1 1	200 250 eak List Abund 25262 6294 1130 50973 11749 2022 2196 7191 3456 1685	Form           7.7.44         C20           88.39         C20           33.54         C20           36.03         C20           36.04         C20           7.7.84         C20           0.87         C20           3.368         C20	50 400 450 5 Counts vs H29 N7 O4 H29 N7 O4 H29 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H27 N7 Na O4	Ion           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (2M+Na)-	ge (m/z)			
2 1 0 MS Spectru m/z 215.6139 216.1154 216.6168 430.222 431.22237 432.2247 432.2247 452.2012 453.2034 881.4127 882.4147 Predicted Is	<b>m P</b> 2 2 2 1 1 1 1 1 1 1 1 1	200 250 eak List Abund 25262 6294 1130 50973 11749 2022 2196 719 34565 1685 <b>pe Matc</b>	Form           7.44         C20           8.39         C20           3.54         C20           3.96         C20           6.92         C20           7.84         C20           0.87         C20           3.68         6.13           h Table         Calc m/z	50 400 450 5 Counts vs hula H29 N7 O4 H29 N7 O4 H29 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H27 N7 Na O4	Ion           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (2M+Na)-           (2M+Na)-           (2M+Na)-	ge (m/z)		Calc Abund S	Sum %
2 1 0 MS Spectru m/z 215.6139 216.1154 216.6168 430.22 431.2223 432.2247 452.2012 453.2034 881.4127 882.4147 Predicted Is asotope 1	m P z 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	200 250 eak List Abund 25262 6294 1130 50973 11749 2022 2196 719 3456 1685 <b>pe Matc</b> 215.6139	Forr           7.44         C20           8.39         C20           3.54         C20           3.96         C20           3.96         C20           7.84         C20           0.87         C20           3.68         -           6.13         - <b>Data Table Calc m/z</b> 215.6	50 400 450 5 Counts vs hula H29 N7 O4 H29 N7 O4 H29 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H27 N7 Na O4	Ion           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (2M+Na)-           (2M+Na)-           (2M+Na)-           3	ge (m/z) 2 2 2 2 4 + + Calc Abund % 100	Abund Sum %	7	77.61
2 1 0 MS Spectru m/z 215.6139 216.1154 216.6168 430.22 431.2223 432.2247 452.2012 453.2034 453.2034 881.4127 881.4127 Predicted IS sotope 1 2 2	m P z 2 2 1 1 1 1 1 1 1 1 1 5 5000	200 250 eak List Abund 25262 6294 1130 50973 11749 2022 2196 719 3456 1685 <b>pe Matc</b> 215.6139 216.1154	Forr           7.44         C20           8.39         C20           3.54         C20           3.96         C20           3.96         C20           7.84         C20           0.87         C20           3.68         -           6.13         -           h Table         -           Calc m/z         215.0	50 400 450 5 Counts vs hula H29 N7 O4 H29 N7 O4 H29 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H28 N7 O4 H27 N7 Na O4 H27 N7 N2 N7 N7	Ion           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (2M+Na)-           (2M+Na)-           (2M+Na)-           3           100           3           24.92	ge (m/z) 2 2 2 2 4 + + + Calc Abund % 100 24.67	Abund Sum % 76.77 19.13	7	77.61 19.15
2 1 0 MS Spectru m/z 215.6139 216.1154 216.6168 430.22 431.2223 432.2247 452.2012 453.2034 881.4127 882.4147 Predicted Is Isotope 1	m P 2 2 2 1 1 1 1 1 1 1 1 m/z	200 250 eak List Abund 25262 6294 1130 50973 11749 2022 2196 719 3456 1685 <b>pe Matc</b> 215.6139	Forr           7.44         C20           8.39         C20           3.54         C20           3.96         C20           3.96         C20           7.84         C20           0.87         C20           3.68         -           6.13         - <b>Data Table Calc m/z</b> 215.6	50 400 450 5 Counts vs hula H29 N7 04 H29 N7 04 H29 N7 04 H28 N7 04 H28 N7 04 H28 N7 04 H28 N7 04 H27 N7 Na 04	Ion           (M+2H)+           (M+2H)+           (M+2H)+           (M+2H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (2M+Na)-           (3)           (4)           (4)	ge (m/z) 2 2 2 2 4 + + Calc Abund % 100	Abund Sum % 76.77 19.13 3.43	7 3 3	77.61

S37



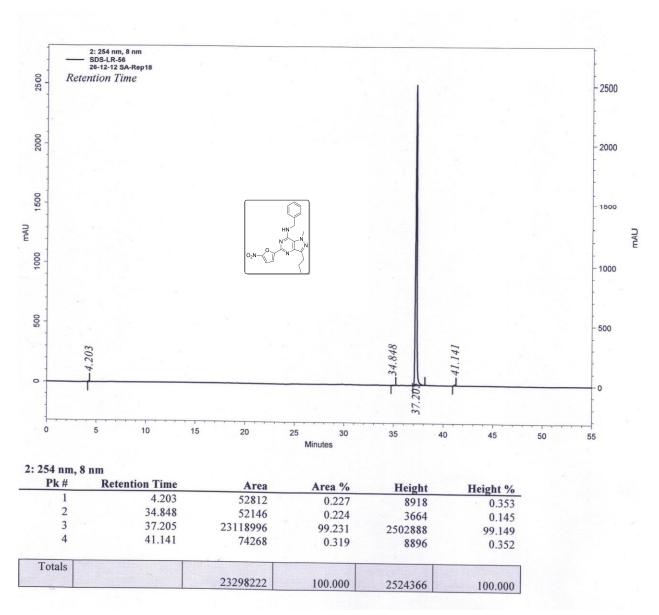


Compound (21) <sup>1</sup>H NMR in CDCl<sub>3</sub>

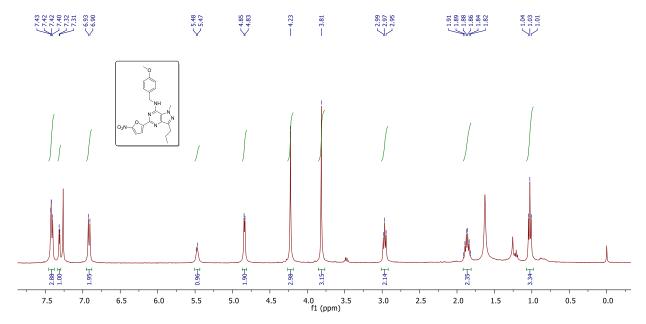


					Qualit	tative (	Compour	nd Report	t			
Data File Sample Type Instrument N Acq Method IRM Calibrati Comment Sample Grou	ion S		San Inst vish Suc	e-11.d nple rrument : al_MS_2 cess	1 25072012.m	Sample   Position User Nar Acquired DA Meth	Vial 23 me 1 Time 11/18/2	2012 1:37:22 PM			H N <sup>2</sup> O <sub>2</sub> N-0	
Compound	Tabl	e							м	FG Diff	. Sala	•
Compou	nd L	abel	RT	Ma	ass	Formula		MFG Formula	(	ppm)	DB Form	nula
Cpd 8: C	20 H	20 N6 O3	0.171	392	2.15963	C20 H20 N6	03 (	C20 H20 N6 O3		0.14	C20 H20 N	16 03
					DT	Algonithm		ass				
Compound Cpd 8: C20 H			<i>m/z</i> 393.166	01	<b>RT</b> 0.171	Algorithm	cular Feature 39	Contraction of the Contraction o				
.pu 0. 020 m	20 1	10 05	595.100	91	0.171	Third by Plote	cular reacure 35	2.13903				
8 - 6 -						0.1210.0001	min) GLR-11.d	05 2 Na O6				
6 - 4 - 2 - 0 -	150	200 2	50 300		233.16891 C20 H21 N6 03 C20 H21 N6 03		500 650 700	807.30605 C40 H40 N12 Na O6	900	950		
6- 4- 2- 0-			50 300		233.16891 C20 H21 N6 03 C20 H21 N6 03	500 550 6	500 650 700	C40	900	950		
6	m Po	eak List Abund	For	350 mula	400 450 Counts	500 550 6 vs. Mass-to-C	500 650 700	C40	900	950		
6 - 4 - 2 - 0	<b>m P</b> z	eak List Abund 9903	For 72.1 C20	350 mula H21 N6	400 450 Counts	500 550 6 vs. Mass-to-C Ion (M+H)+	500 650 700	C40	900	950		
6 - 4 - 2 - 0	<b>m P</b> <b>z</b> 1	eak List Abund 9903 2119	For 72.1 C20 95.5 C20	350 mula H21 N6 H21 N6	400 450 Counts 03 03 03	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+	500 650 700	C40	900	950		
6 - 4 - 2 - 0	<b>m P</b> <b>z</b> 1 1	eak List Abund 9903 2119 301	For 72.1 C20 95.5 C20 76.7 C20	350 <b>mula</b> H21 N6 H21 N6 H21 N6	400 450 Counts 03 03 03 03 03	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+	500 650 700	C40	900	950		
6 - 4 - 2 - 0	m Po z 1 1 1 1	eak List Abund 9903 2119 301 47	For 72.1 C20 95.5 C20 76.7 C20 '38.5 C20	350 <b>mula</b> H21 N6 H21 N6 H21 N6 H21 N6	400 450 Counts 03 03 03 03 03 03 03 03	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+	500 650 700 Charge (m/z)	C40	900	950		
6 - 4 - 2 - 0 - <b>MS Spectru</b> <i>n/z</i> 393.16691 394.16939 395.17143 396.17492 415.14774	m P z 1 1 1 1 1 1	eak List Abund 9903 2119 301 47 151	For 72.1 (20) 95.5 (20) 76.7 (20) 38.5 (20) 20.2 (20)	350 mula H21 N6 H21 N6 H21 N6 H21 N6 H20 N6	400 450 Counts 03 03 03 03 03 03 03 03 03 03 03 03 03	500 550 6 vs. Mass-to-C (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+	500 650 700 Charge (m/z)	C40	900	950		
6 - 4 - 2 - 0	m P z 1 1 1 1 1 1 1 1	eak List Abund 9903 2119 301 47 151	For 72.1 C20 95.5 C20 76.7 C20 38.5 C20 20.2 C20 5045 C20	350 mula H21 N6 H21 N6 H21 N6 H21 N6 H21 N6 H21 N6 H21 N6 H21 N6	400 450 Counts 03 03 03 03 03 03 03 03 03 03 03 03 03	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+	500 650 700 Charge (m/z)	C40	900	950		
6 - 4 - 2 - 0	m Po z 1 1 1 1 1 1 1 1 1 1	eak List Abund 9903 2119 301 47 151	For 72.1 C20 95.5 C20 76.7 C20 38.5 C20 20.2 C20 5045 C20 78.1 C20	350 <b>mula</b> H21 N6 H21 N6 H20 N6 H20 H20 N6 H20 N6 H	400 450 Counts 03 03 03 03 03 03 03 03 03 03 03 03 03	500 550 e vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+K)+	500 650 700 Charge (m/z)	C40	900	950		
6 - 4 - 2 - 0 - MS Spectrum <i>m/z</i> 393.16691 394.16939 395.17143 396.17492 415.14774 416.14941 431.12167 807.30605	m Po z 1 1 1 1 1 1 1 1 1 1 1	eak List Abund 9903 2119 301 47 151 	For 72.1 (20) 95.5 (20) 76.7 (20) 38.5 (20) 20.2 (20) 5045 (20) 78.1 (20) 66.2 (40)	350 H21 N6 H21 N6 H20 N6 H21 N	400 450 Counts 03 03 03 03 03 03 03 03 03 03 03 03 03	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+K)+ (2M+Na)-	500 650 700 Charge (m/z)	C40	900	950		
6 - 4 - 2 - 0 - 393.16691 394.16939 395.17143 396.17492 415.14774 416.14941 431.12167	m Po z 1 1 1 1 1 1 1 1 1 1 1 1 1	eak List Abund 9903 2119 301 47 151 92 92 424 204	For 72.1 C20 95.5 C20 76.7 C20 38.5 C20 20.2 C20 5045 C20 78.1 C20	350 H21 N6 H21 N6 H21 N6 H21 N6 H21 N6 H20 N6 H20 N6 H20 N6 H20 K1 H40 N1	400 450 Counts 03 03 03 03 03 03 03 03 03 03 03 03 03	500 550 e vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+K)+	500 650 700 harge (m/z)	C40	900	950		
6 - 4 - 2 - 0 - <b>MS Spectrum</b> <b>m/z</b> 393.16691 394.16939 395.17143 395.17143 395.17432 395.17442 415.14774 415.14774 415.14774 415.14774 607.30605 808.30886 808.30886 823.28164	m Po z 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	eak List Abund 9903 2119 301 47 151 	For 72.1 (20) 195.5 (20) 76.7 (20) 20.2 (20) 5045 (20) 78.1 (20) 66.2 (40) 48.7 (40) 5097 (40)	350 <b>mula</b> H21 N6 H21 N6 H21 N6 H20 N6 H20 N6 H20 N6 H20 N6 H20 K1 H40 N1 H40 N1	400 450 Counts 03 03 03 03 03 03 03 03 03 03 03 03 03	500 550 6 vs. Mass-to-C <b>Ion</b> (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+K)+ (2M+Na)- (2M+Na)- (2M+Na)-	500 650 700 harge (m/z)	C40	900	950		
6 - 4 - 2 - 2 - 0	m Po z 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	eak List Abund 9903 2119 301 47 151 92 424 204 204 204	For 72.1 (20) 195.5 (20) 76.7 (20) 20.2 (20) 5045 (20) 78.1 (20) 66.2 (40) 48.7 (40) 5097 (40)	350 mula H21 N6 H21 N6 H21 N6 H21 N6 H20 N6 H20 N6 H20 K1 H20 K1 H20 N1 H20 K1 H20 K1	400 450 Counts 03 03 03 03 03 03 03 03 03 03 03 03 03	500 550 6 vs. Mass-to-C <b>Ion</b> (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+K)+ (2M+Na)- (2M+Na)- (2M+Na)-	500 650 700 harge (m/z)	C40	900	950 Calc Abund	Sum %	
6 - 4 - 2 - 2 - 0	m Pa z 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	eak List Abund 9903 2119 301 47 151 92 424 204 204 204	For 72.1 (20) 95.5 (20) 76.7 (20) 38.5 (20) 20.2 (20) 5045 (20) 5045 (20) 5045 (20) 5045 (20) 66.2 (40) 48.7 (40) 5097 (40) <b>h Table</b> <b>Calc m/</b>	350 mula H21 N6 H21 N6 H21 N6 H21 N6 H20 N6 H20 N6 H20 K1 H20 K1 H20 N1 H20 K1 H20 K1	400 450 Counts 400 450 Counts 03 03 03 03 03 03 03 03 03 03	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+K)+ (2M+Na)- (2M+Na)- (2M+K)+	500 650 700 harge (m/z)	750 800 850	80.04		<u>Sum %</u>	15
6 - 4 - 2 - 0	m P( z 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3 3 3 3	eak List Abund 9903 2119 301 47 151 92 424 204 204 93.16691 994.16939	For 72.1 (20) 95.5 (20) 76.7 (20) 20.2 (20) 5045 (20) 78.1 (20) 66.2 (24) 66.2 (44) 5097 (44) <b>h Table</b> <b>Calc m/</b> 393.1 394.1	350 mula H21 N6 H21 N6 H21 N6 H21 N6 H20 H20 H20 N6 H20 N6	400 450 Counts 400 450 Counts 03 03 03 03 03 03 03 03 03 03 03 03 03	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+K)+ (2M+Na)- (2M+Na)- (2M+Na)- (2M+Na)- (2M+K)+ (2M+K)+ (2M+K)+ (2M+K)+	200 650 700 harge (m/z) + + + + Calc Abund % 10 24.1	750 800 850 Abund Sum % 10 8	<u>80.04</u> 17.13	Calc Abund	78.1 18	.9
6 4 2 0 <b>MS Spectru</b> <i>m/z</i> 393.16691 394.16939 395.17143 396.17492 415.14774 416.14941 431.12167 807.30605 808.30886 823.28164 <b>Predicted Is</b> <b>Isotope</b> 1	m P( z 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3 3 3 3	eak List Abund 9903 2119 301 477 151 92 92 4224 204 <b>pe Matc</b> 93.16691	For 72.1 (20) 95.5 (20) 76.7 (20) 20.2 (20) 5045 (20) 78.1 (20) 66.2 (24) 66.2 (24) 66.2 (24) 66.2 (24) 66.2 (24) 78.1 (20) 66.2 (24) 66.2 (24) 78.1 (20) 66.2 (24) 78.1 (20) 78.1 (	350 <b>mula</b> H21 N6 H21 N6 H21 N6 H21 N6 H20 N6 H20 N6 H20 N1 H40 N1 H40 N1 H40 N1 H40 N1	400 450 Counts 400 450 Counts 03 03 03 03 03 03 03 03 03 03 03 03 03	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+K)+ (2M+Na)- (2M+Na)- (2M+Na)- (2M+Na)- (2M+K)+ (2M+K)+ (2M+K)+ (2M+K)+	500 650 700 harge (m/z) + + +	Abund Sum %	80.04	Calc Abund	78.1	.9 57

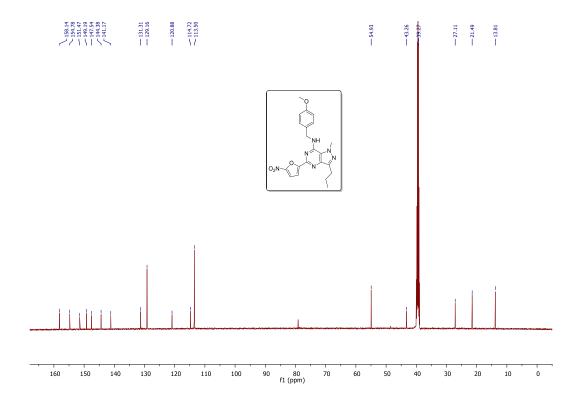




Compound (22) <sup>1</sup>H NMR in CDCl<sub>3</sub>



## <sup>13</sup>C NMR in DMSO-d<sub>6</sub>

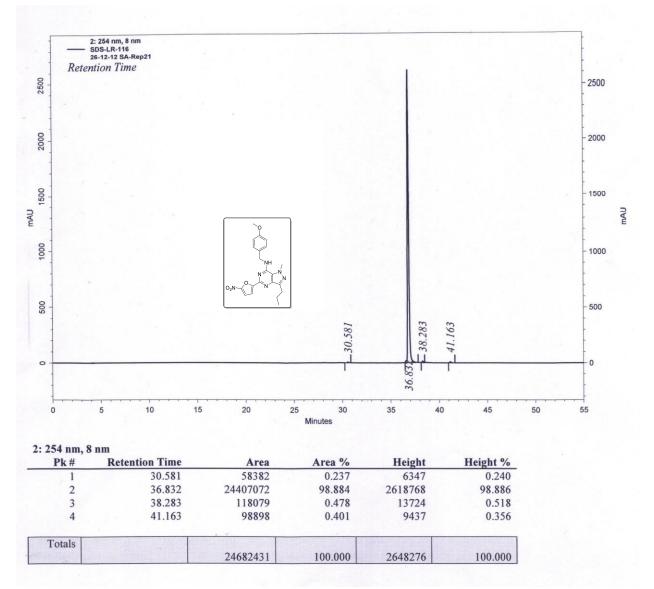


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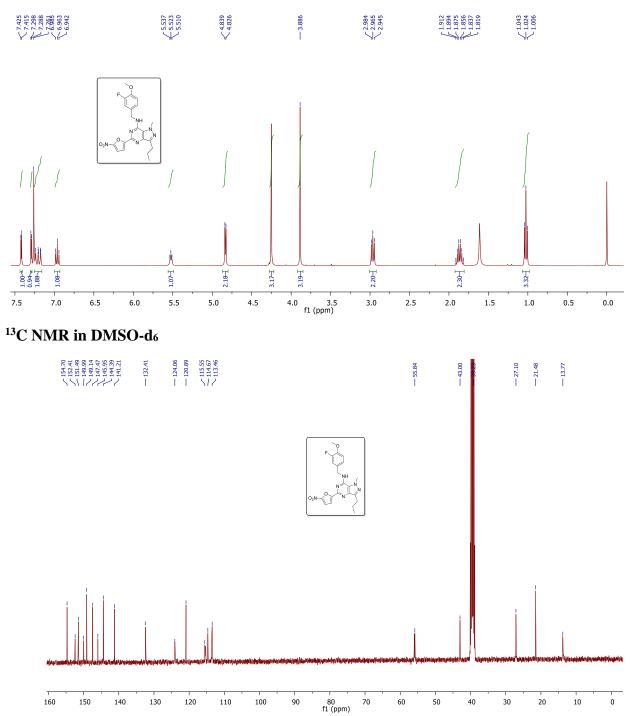
# **Qualitative Compound Report**

ata File		G	LR-4-37.d		Sample Name	GLR-4	-37				
ample Type		Sa	ample		Position	Vial 8					
strument Nar	ne	In	strument 1		User Name			-0.00 PM			Ň
cg Method		vi	shal_MS_2	5072012.m	Acquired Time		/2012 12:5	58:00 PM			$\bigcirc$
RM Calibration	Status	S	uccess		DA Method	as.m					Ľ.
omment			Decentration of the local decentration of th								
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ample Group	I	Info.								Ľ	
Compound Ta	able					-			MFG Di		
Compound	ladel	RT	Ma	ISS	Formula		MFG Fo		(ppm)		DB Formula C21 H22 N6 O4
Cpd 3: C2				.16984	C21 H22 N6 O4		C21 H22	N6 04	(	0.97	C21 H22 NO 04
сри 5. С2	1 1122 110	011 011									
					a		Mass				
Compound La	abel	m/z		RT	Algorithm			4			
Cpd 3: C21 H2	2 N6 O4	423.1	17712	0.172	Find by Molecular Fo	eature	722.1098				
3-2-				423.17712 C21 H23 N6 04				867.32815 C42 H44 N12 Na O8			
			300 350	400 450 Counts	500 550 600 6 vs. Mass-to-Charge	650 70 e (m/z)	00 750	800 850 90	00 950	_	
MS Spectru	m Peak	List	300 350	400 450 Counts	500 550 600 6 vs. Mass-to-Charge	650 70 e (m/z)	00 750	800 850 94	00 950	_	
MS Spectrum	m Peak z Abu	List	Formula	Counts	vs. Mass-to-Charge	550 70 e (m/z)	00 750	800 850 90	00 950		
0	r Peak	List und 466922.1	Formula C21 H23 N	Counts	vs. Mass-to-Charge	650 70 e (m/z)	00 750	800 850 90	0 950		
MS Spectrum m/z 423.17712 424.17976	m Peak z Abu 1	List and 466922.1 122132.7	Formula C21 H23 N C21 H23 N	Counts 16 04	Ion (M+H)+	550 70 e (m/z)	00 750	800 850 90	00 950		
MS Spectrum m/z 423.17712 424.17976 425.18177	r Peak	List 466922.1 122132.7 18589.5	Formula C21 H23 N C21 H23 N C21 H23 N	Counts 1 16 04 16 04 16 04	Ion (M+H)+ (M+H)+	550 70 e (m/z)	00 750	800 850 94	00 950		
0 MS Spectrui <i>m/z</i> 423.17712 424.17976 425.18177 445.15869	m Peak z Abu 1 1 1 1	List and 466922.1 122132.7 18589.5 15127.3	Formula C21 H23 N C21 H23 N C21 H23 N C21 H22 N	Counts 1 16 04 16 04 16 04 16 04 16 Na 04	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+	650 70 e (m/z)	00 750	800 850 94	00 950		
0 <b>MS Spectrui</b> <i>m/z</i> 423.17712 424.17976 425.18177 445.15869 446.16148	m Peak z Abu 1 1 1 1 1 1 1 1	List 466922.1 122132.7 18589.5 15127.3 5373.9	Formula C21 H23 N C21 H23 N C21 H23 N C21 H22 N C21 H22 N	Counts 1 16 04 16 04 16 04 16 04 16 Na 04 16 Na 04	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+	650 70 e (m/z)	00 750	800 850 94	00 950		
MS Spectrui m/z 423.17712 424.17976 425.18177 445.15869 446.16148 461.13245	z         Abu           1	List 466922.1 122132.7 18589.5 15127.3 5373.9 5001.9	Formula C21 H23 N C21 H23 N C21 H23 N C21 H22 N C21 H22 N C21 H22 N	Counts 16 04 16 04 16 04 16 04 16 04 16 Na 04 16 Na 04 16 Na 04 16 Na 04	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+	650 70 e (m/z)	00 750	800 850 94	00 950		
MS Spectrui m/z 423.17712 424.17976 425.18177 445.15869 446.16148 461.13245 867.32815	m Peak z Abu 1 1 1 1 1 1 1 1 1 1 1 1 1 1	List 466922.1 122132.7 18589.5 15127.3 5373.9 5001.9 37016.4	Formula C21 H23 N C21 H23 N C21 H23 N C21 H22 N C21 H22 N C21 H22 N C21 H22 K	Counts 16 04 16 04 16 04 16 04 16 Na 04 16 Na 04 16 Na 04 16 Na 04 17 Na 08	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+K)+	650 70 e (m/z)	0 750	800 850 94	00 950		
MS Spectrut m/z 423.17712 424.17976 425.18177 445.15869 446.16148 461.13245 867.32815 868.33036	z         Abu           1	List 466922.1 122132.7 18589.5 15127.3 5373.9 5001.9 37016.4 18324.1	Formula C21 H23 N C21 H23 N C21 H23 N C21 H22 N C21 H22 N C21 H22 N C21 H22 K C21 H22 K C21 H22 K C21 H24 N	Counts 16 04 16 04 16 04 16 Na 04 16 Na 04 16 Na 04 10 Na 04 112 Na 08 112 Na 08	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+K)+           (2M+Na)+	550 70 e (m/z)	0 750	800 850 94	00 950	_	
MS Spectrum m/z 423.17712 424.17976 425.18177 445.15869 446.16148 461.13245 867.32815 868.33036 869.33289	m Peak z Abu 1	List 466922.1 122132.7 18589.5 15127.3 5373.9 5001.9 37016.4 18324.1 6392.2	Formula           C21 H23 N           C21 H23 N           C21 H23 N           C21 H23 N           C21 H22 N           C21 H24 N           C42 H44 N           C42 H44 N	Counts 16 04 16 04 16 04 16 Na 04 16 Na 04 16 Na 04 112 Na 08 112 Na 08 112 Na 08	Ion           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+K)+           (2M+Na)+           (2M+Na)+	650 70 e (m/z)	0 750	800 850 94	0 950		
MS Spectrum m/z 423.17712 424.17976 425.18177 445.15869 446.16148 461.13245 867.32815 868.33036 869.33289 883.30209	Peak           z         Abu           1	List 466922.1 122132.7 18589.5 15127.3 5373.9 5001.9 37016.4 18324.1 6392.2 3364	Formula           C21 H23 N           C21 H23 N           C21 H23 N           C21 H23 N           C21 H22 N           C21 H24 N           C42 H44 N           C42 H44 N           C42 H44 N           C42 H44 N	Counts 16 04 16 04 16 04 16 Na 04 16 Na 04 16 Na 04 112 Na 08 112 Na 08 112 Na 08	Ion           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+K)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+	650 70 e (m/z)					
MS Spectrum m/z 423.17712 424.17976 425.18177 445.15869 446.16148 461.13245 866.33036 869.33289 883.30209 Predicted I	m Peak z Abu 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 5000pe	List 466922.1 122132.7 18589.5 15127.3 5373.9 5001.9 37016.4 18324.1 6392.2 3364 Match Ta	Formula           C21 H23 N           C21 H23 N           C21 H23 N           C21 H22 N           C21 H24 N           C42 H44 N	Counts 16 04 16 04 16 04 16 Na 04 16 Na 04 112 Na 08 112 Na	Ion           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+K)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+	650 70 € (m/z)		und Sum %	Са	Ic Abund S	
MS Spectrum m/z 423.17712 424.17976 425.18177 445.15869 446.16148 461.13245 867.32815 868.33036 869.33289 883.30209 Predicted I Isotope	m         Peak           z         Abu           1	List 466922.1 122132.7 18589.5 15127.3 5373.9 5001.9 37016.4 18324.1 6392.2 3364 Match Ta Cal	Formula           C21 H23 N           C21 H23 N           C21 H23 N           C21 H22 N           C21 H24 N           C42 H44 N	Counts 16 04 16 04 16 04 16 Na 04 16 Na 04 16 Na 04 112 Na 08 112 Na 08 112 Na 08	Ion           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+K)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+K)+	e (m/z)	% Ab 100	und Sum %	Ca 76.61	Ic Abund 1	77.12
MS Spectrum           #/z           423.17712           424.17976           425.18177           445.15869           446.16148           461.13245           867.32815           868.33036           869.33289           883.30209           Predicted I           Isotope           1	Peak           z         Abu           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         2           sotope         m/z           423.         423.	List 466922.1 122132.7 18589.5 15127.3 5373.9 5001.9 37016.4 18324.1 6392.2 3364 Match Ta Cal 17712	Formula           C21 H23 N           C21 H23 N           C21 H23 N           C21 H22 N           C21 H24 N           C42 H44 N           C	Counts 16 04 16 04 16 04 16 04 16 04 16 04 16 04 112 Na 04 112 Na 08 112 Na 08	Ion           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+K)+           (M+K)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+K)+           5           100	e (m/z)	% Ab	und Sum %	76.61 20.04	Ic Abund S	77.12 19.53
MS Spectrum m/z 423.17712 424.17976 425.18177 445.15869 446.16148 461.13245 867.32815 868.33036 869.33289 883.30209 Predicted I Isotope	m         Peak           z         Abu           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         423.           2         424.	List 466922.1 122132.7 18589.5 15127.3 5373.9 5001.9 37016.4 18324.1 63922.3 3364 Match Ti Cal 17712 17976	Formula           C21 H23 N           C21 H23 N           C21 H23 N           C21 H22 N           C21 H24 N           C42 H44 N	Counts 16 04 16 04 16 04 16 Na 04 16 Na 04 16 Na 04 16 Na 04 12 Na 08 112 Na 08	Ion           (M+H)+           (M+Na)+           (M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+K)+           Abund %         Calc           5         100           5         26.16	e (m/z)	% Ab 100	und Sum %	Ca 76.61	Ic Abund S	77.12





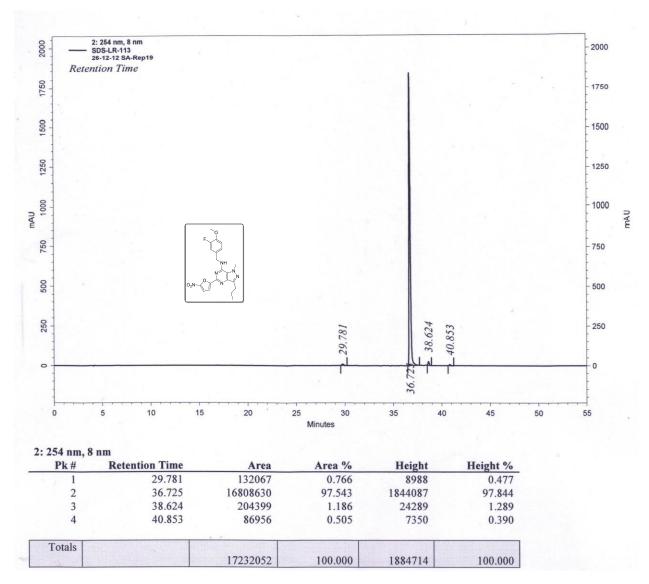
Compound (23) <sup>1</sup>H NMR in CDCl<sub>3</sub>



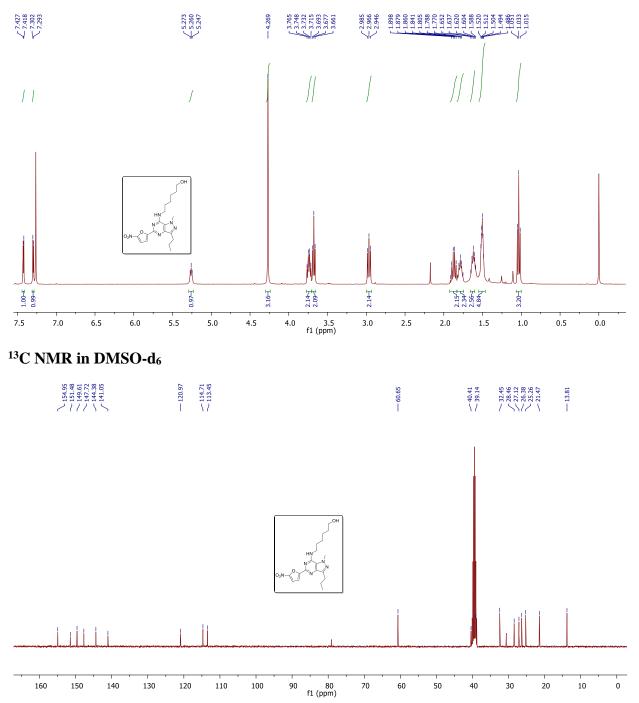
## **Qualitative Compound Report**

Data File Sample Type Instrument I Acq Method IRM Calibrat Comment Sample Grou	Name tion Statu	s Info.	GLR-4-3 Sample Instrume vishal_M Success		Sample N Position User Nam 2.m Acquired DA Metho	Vial 5 ne Time 11/19			0,N-0-N-
Compound	Table							MFG Diff	
	nd Label		<b>RT</b> 0.172	Mass 440.16055	Formula C21 H21 F N6	04	MFG Formula C21 H21 F N6 O4	(ppm) 0.65	DB Formula C21 H21 F N6 O4
Compound Cpd 7: C21 H		<b>m</b> / 04 441	/ <i>z</i> 1.16783	<b>RT</b> 0.17	Algorithm 2 Find by Molect		Mass 440.16055		
2								nin .	
1-0-	150 20 m Peak		300 3		450 500 550 nts vs. Mass-to-Cl		00 750 800 85	056 006 00 C42 H42 F2 N12 Na 08	
1 0 IS Spectru		List	300 3	Cou			00 750 800 85		
1 0 IS Spectru 1/z 441.16783	r Peak	<b>List</b> nd 612374.8	Formula C21 H22	Cou a F N6 O4	nts vs. Mass-to-Cl Ion (M+H)+		00 750 800 85		
1- 0- <b>15 Spectru</b> <b>1/z</b> 441.16783 442.17029	m Peak z Abu 1	List nd 612374.8 143914	Formula C21 H22 C21 H22	Cou F N6 04 F N6 04	Ion (M+H)+ (M+H)+		00 750 800 85		
1-0 <b>15 Spectru</b> <b>1/2</b> 441.16783 442.17029 443.17311	m Peak	List nd 612374.8 143914 21446.9	Formula 3 C21 H22 4 C21 H22 9 C21 H22	Cou F N6 04 F N6 04 F N6 04	Ion (M+H)+ (M+H)+ (M+H)+		00 750 800 85		
1- 0 <b>45 Spectru</b> <b><i>n/z</i></b> 441.16783 442.17029 443.17311 444.17514	z         Abu           1         1           1         1           1         1           1         1	List nd 612374.8 143914 21446.9	Formula C21 H22 C21 H22	Cou F N6 04 F N6 04 F N6 04	Ion (M+H)+ (M+H)+		00 750 800 85		
1- 0 <b>MS Spectru</b> <i>m/z</i> 441.16783 442.17029 443.17311	z         Abu           1         1           1         1           1         1           1         1	List nd 612374.8 143914 21446.9 3302.3	Formula 3 C21 H22 4 C21 H22 9 C21 H22 3 C21 H22 3 C21 H22	Cou F N6 04 F N6 04 F N6 04	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+		00 750 800 85		
1- 0 <b>MS Spectru</b> <i>n/z</i> 441.16783 442.17029 443.17311 444.17514	<b>m Peak z Abu</b> 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	List nd 612374.8 143914 21446.9 3302.3 12489.3	Formula           C21 H22	Cou F N6 04 F N6 04 F N6 04 F N6 04 F N6 04	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+		00 750 800 85		
1 - 0	z         Abu           1         1           1         1           1         1           1         1           1         1           1         1           1         1	List nd 612374.8 143914 21446.9 3302.3 12489.3 5574.6	Formula 3 C21 H22 4 C21 H22 3 C21 H22 3 C21 H22 3 C21 H22 4 C21 H22 3 C21 H21 5 C21 H21	Cou F N6 O4 F N6 O4 F N6 O4 F N6 O4 F N6 O4 F N6 Na O4 F K N6 O4	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+K)+	harge (m/z)	00 750 800 85		
1 - 0 - <b>MS Spectru</b> <i>m/z</i> 441.16783 442.17029 443.17311 444.17514 463.14834	z         Abu           1         1           1         1           1         1           1         1           1         1           1         1           1         1	List nd 612374.8 143914 21446.9 3302.3 12489.3 5574.6	Formula 3 C21 H22 4 C21 H22 3 C21 H22 3 C21 H22 3 C21 H22 4 C21 H22 3 C21 H21 5 C21 H21	Cou F N6 O4 F N6 O4 F N6 O4 F N6 O4 F N6 O4 F N6 Na O4	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+K)+	harge (m/z)	00 750 800 85		
1 - 0	Peak           z         Abu           1	List nd 612374.8 143914 21446.9 3302.3 12489.3 5574.6 26851.2	Formul:           C21 H22           C21 H21	Cou F N6 O4 F N6 O4 F N6 O4 F N6 O4 F N6 O4 F N6 Na O4 F K N6 O4	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+K)+           (M+K)+           (08           (2M+Na)+	harge (m/z)	00 750 800 85		
1 - 0 - <b>MS Spectru</b> <i>m/z</i> 441.16783 442.17029 443.17311 444.17514 463.14834 479.12258 903.30928	m Peak z Abu 1 1 1 1 1 1 1 1 1 1 1	List nd 612374.8 143914 21446.9 3302.3 12489.3 5574.6 26851.2 13429.6	Formula           221 H22           221 H21           221 H22           221 H21           222 H21           233 C21 H21           244 H21	Cou F N6 04 F N6 04 F N6 04 F N6 04 F N6 Na 04 F K N6 04 FZ N12 Na	Ion           (M+H)+           (M+K)+           (M+K)+           08         (2M+Na)+           08         (2M+Na)+	harge (m/z)	00 750 800 85		
1- 0 <b>MS Spectru</b> <i>m/z</i> 441.16783 442.17029 443.17311 444.17514 463.14834 479.12258 903.30928 904.30993	z         Abu           1         -           1         -           1         -           1         -           1         -           1         -           1         -           1         -           1         -           1         -           1         -           1         -           1         -           1         -           1         -           1         -           1         -           1         -	List nd 612374.8 143914 21446.9 3302.3 12489.3 5574.6 26851.2 13429.6	Formul:           3 (21 H22           4 (21 H22           2 (21 H22           2 (21 H22           3 (21 H22           4 (21 H22           5 (21 H22           6 (24 H42           6 (24 H42           6 (24 H42	Cou F N6 O4 F N6 O4 F N6 O4 F N6 O4 F N6 Na O4 F N6 Na O4 F X N6 O4 F2 N12 Na F2 N12 Na	Ion           (M+H)+           (M+K)+           (M+K)+           08         (2M+Na)+           08         (2M+Na)+	harge (m/z)	00 750 800 85		
1 - 0	z         Abu           1	List nd 612374.6 143914 21446.9 3302.3 12489.3 5574.6 26851.2 13429.6 3559.8 3761.6	Formul:           C21 H22           C42 H42           C42 H42           C42 H42	Cou F N6 O4 F N6 O4 F N6 O4 F N6 O4 F N6 Na O4 F N6 Na O4 F X N6 O4 F2 N12 Na F2 N12 Na	Ion           (M+H)+           (M+K)+           08         (2M+Na)+           08         (2M+Na)+           08         (2M+Na)+	harge (m/z)	00 750 800 85		
1 - 0 - MS Spectru m/z 441.16783 442.17029 443.17311 444.17514 463.14834 479.12258 903.30928 904.30993 904.30993 905.31342 919.28295 Predicted I	z         Abu           1	List nd 612374.6 143914 21446.9 3302.3 12489.3 5574.6 26851.2 13429.6 3559.8 3761.6 <b>1atch T</b>	Formul:           C21 H22           C42 H42           C42 H42           C42 H42	Cou F N6 O4 F N6 O4 F N6 O4 F N6 O4 F N6 Na O4 F N6 Na O4 F X N6 O4 F2 N12 Na F2 N12 Na	Ion           (M+H)+           (M+K)+           08         (2M+Na)+           08         (2M+Na)+           (2M+Na)+         (2M+Na)+           08         (2M+Na)+           (2M+K)+         (2M+K)+	harge (m/z)		50 900 950	d Sum %
1 - 0 - MS Spectru m/z 441.16783 442.17029 443.17311 444.17514 463.14834 479.12258 903.30928 904.30993 904.30993 905.31342 919.28295 Predicted I	Image: Peak         Z         Abu           1         1         1           1         1         1           1         1         1           1         1         1           1         1         1           1         1         1           1         1         1           1         1         1           1         1         1           1         1         1           1         1         1           1         1         1           1         1         1	List nd 612374.8 143914 21446.9 3302.3 12489.3 5574.6 26851.2 13429.6 3559.8 3761.6 1atch Ta Cal	Formul:           C21 H22           C42 H42           C42 H42           C42 H42           C42 H42	Cou F N6 O4 F N6 O4 F N6 O4 F N6 O4 F N6 O4 F N6 Na O4 F X N6 O4 F2 N12 Na F2 N12 Na F2 N12 Na F2 N12 Na	Ion           (M+H)+           (M+K)+           08         (2M+Na)+           08         (2M+Na)+           (2M+Na)+         (2M+Na)+           08         (2M+Na)+           (2M+K)+         (2M+K)+	Calc Abund %		50 900 950	d Sum % 77.13
1 - 0	Implementation         Peak           z         Abu           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         441.1	List nd 612374.8 143914 21446.9 3302.3 12489.3 5574.6 26851.2 13429.6 3559.8 3761.6 1atch Ta Cal 6783	Formul:           C21 H22           C42 H42           C42 H42           C42 H42           C42 H42           DEDE           C42 H42	Cou F N6 04 F N6 04 F N6 04 F N6 04 F N6 04 F N6 Na 04 F N6 Na 04 F X N6 04 F2 N12 Na F2 N12 Na F2 N12 Na F2 N12 Na F2 N12 Na	Ion           (M+H)+           (M+K)+           08         (2M+Na)+           08         (2M+Na)+           08         (2M+Na)+           (2M+K)+         (2M+K)+           (D)         Abund %	harge (m/z)	Abund Sum %	60 900 950 Calc Abun	
1 - 0 - MS Spectrum m/z 441.16783 442.17029 443.17311 444.17514 463.14834 479.12258 903.30928 904.30993 905.31342 919.28295 Predicted I Isotope 1	Implementation         Peak           z         Abu           1         1           1	List nd 612374.8 143914 21446.9 3302.3 12489.3 5574.6 26851.2 13429.6 3559.8 3761.6 13429.	Formula           2 C21 H22           2 C42 H42           2 C42 H42           3 C42 H42           4 C42 H42           5 C42 H42           6 C42 H42           6 C42 H42	Cou F N6 04 F N6 04 F N6 04 F N6 04 F N6 04 F N6 Na 04 F N6 Na 04 F X N6 04 F2 N12 Na F2 N12 Na F2 N12 Na F2 N12 Na F2 N12 Na	Ion           (M+H)+           (M+K)+           08         (2M+Na)+           08         (2M+Na)+           (2M+Na)+         (2M+Na)+           08         (2M+Na)+           08         (2M+Na)+           09         (2M+Na)+           004         100	harge (m/z)	<ul> <li>Abund Sum %</li> <li>100</li> </ul>	50 900 950	77.13





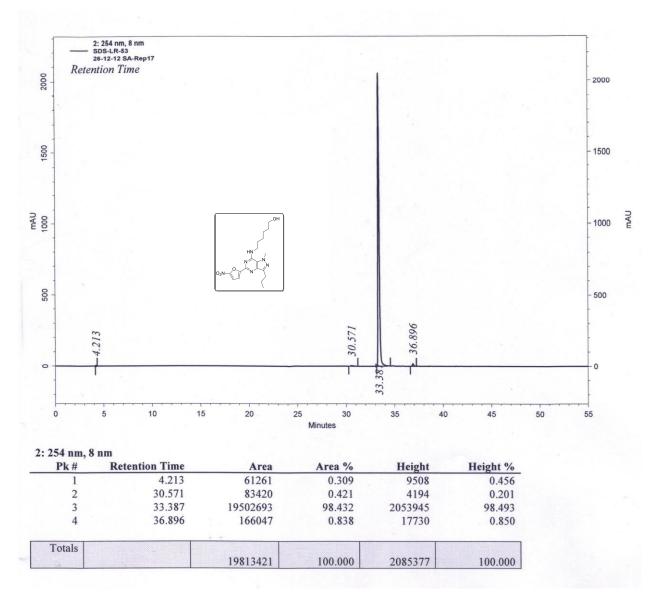
Compound (24) <sup>1</sup>H NMR in CDCl<sub>3</sub>



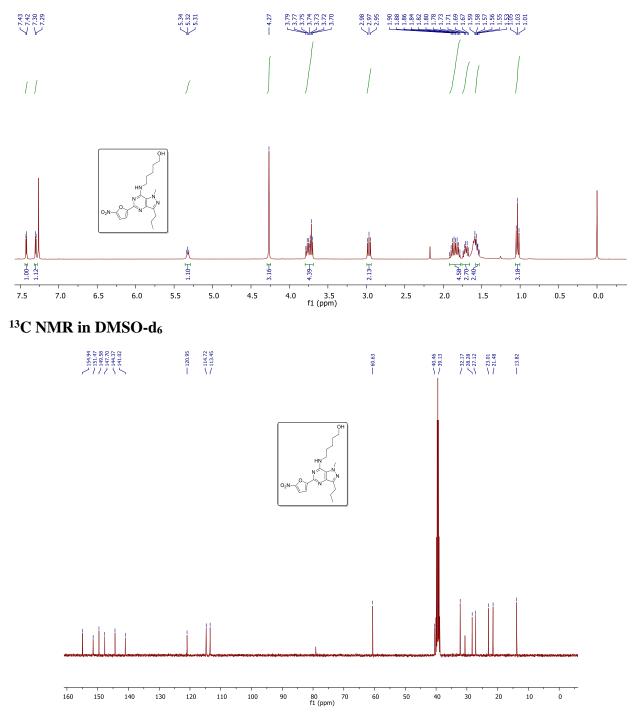
## Qualitative Compound Report

Sample Type Instrument N Acq Method IRM Calibrati Comment Sample Group Compound 1	on S	Status Info	I V	Sample nstrument 1 rishal_MS_25 Success	072012.m	Position User Na Acquired DA Meth	me d Time 11/18	) /2012 1:26:45	F PM		HN N N N O2N O
										FG Diff	
Compour			RT			Formula		MFG Formu		(ppm)	DB Formula
Cpd 4: C	19 H	26 N6 O4	0.1	172 402.	20115	C19 H26 N6	04	C19 H26 N6	04	1.01	C19 H26 N6 O4
Compound I	Labe	el	m/z		RT	Algorithm	1	lass			
Cpd 4: C19 H	26 N	16 04	403.2	20843	0.172	Find by Mole	cular Feature	02.20115			
2 - 1.5 - 1 - 0.5 - 0 -					C19 H27 N6 O4			827.38945	C38		
	150	200 2	250 3	00 350 4		500 550 6 vs. Mass-to-C	600 650 700 Charge (m/z)	750 800	850 900	950	
MS Spectru	-										
m/z	Z	Abund		Formula		Ion					
403.20843	1			C19 H27 N6 (		(M+H)+					
404.21069	1			C19 H27 N6 (		(M+H)+					
405.21287	1			C19 H27 N6 (		(M+H)+					
425.18996	1			C19 H26 N6 I C19 H26 N6 I		(M+Na)+ (M+Na)+					
426.19267	1					(M+Na)+ (M+K)+					
441.16296	-			C19 H26 K N							
827.38945	1			C38 H52 N12		(2M+Na)					
828.39343	1			C38 H52 N12		(2M+Na)					
020 20744	1			C38 H52 N12		(2M+Na)					
829.39711	1			C38 H52 K N	12 08	(2M+K)+					
843.3663	oto		11 1 00	ne on		Abund %	Calc Abund %	Abund S	um %	Calc Abund Su	um %
843.3663 Predicted Is	-		1	m/z Did	f(nnm)					I work house of	
843.3663 Predicted Is Isotope	m/2		Calc		ff (ppm)						
843.3663 Predicted Is Isotope	m/2	03.20843	Calc 40	3.20883	0.99	100		100	78.17		78.75
843.3663 Predicted Is Isotope	<i>m/2</i>		<b>Calc</b> 40			100 23.68	2				

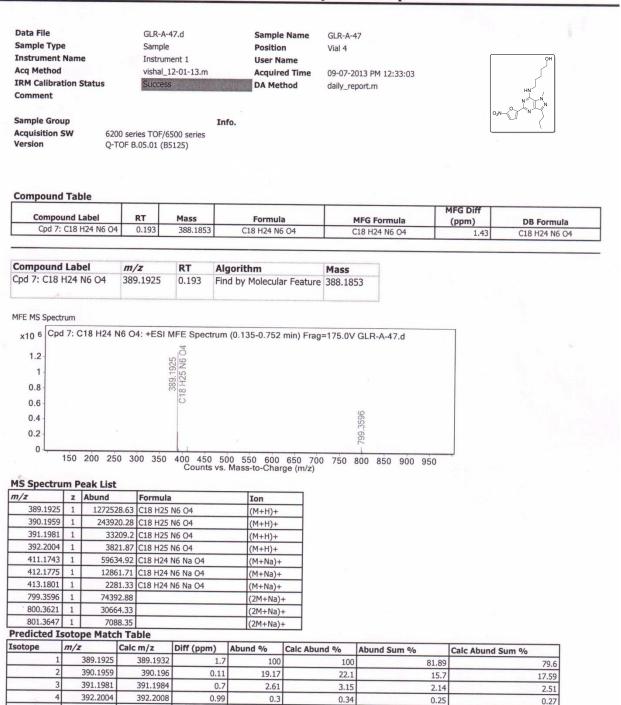




Compound (25) <sup>1</sup>H NMR in CDCl<sub>3</sub>



### **Qualitative Compound Report**



--- End Of Report ---

5

393.2003

393.2031

7.07

0.03

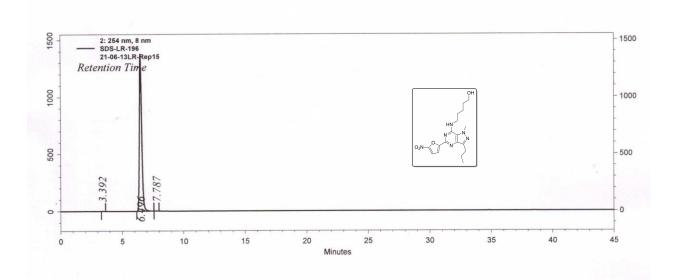
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0.02

0.03

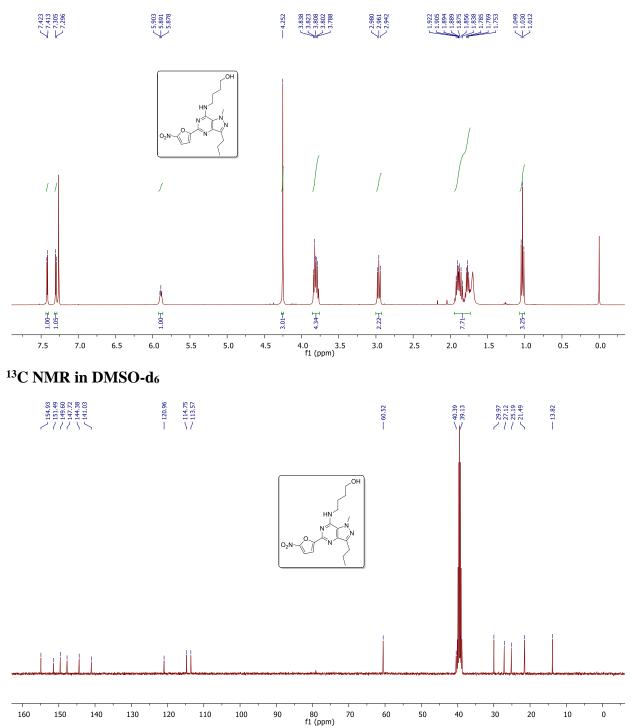


5



Pk #	<b>Retention Time</b>	Area	Area %	Height	Height %
1	3.392	10279	0.056	1484	0.107
2	6.496	18300925	99.867	1378069	99.799
3	7.787	14146	0.077	1290	0.093
Totals					
		18325350	100.000	1380843	100.000

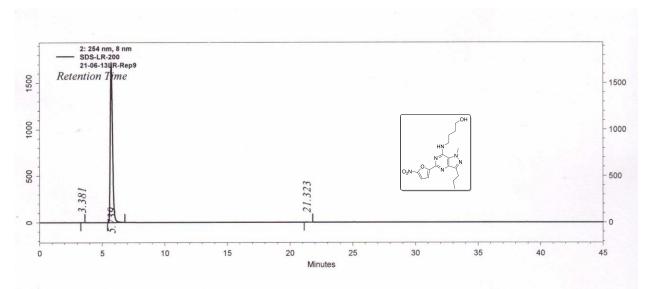
Compound (26) <sup>1</sup>H NMR in CDCl<sub>3</sub>



## **Qualitative Compound Report**

ample Type Instrument Na Acq Method RM Calibratic Comment			e ment 1 _12-01-13.n	١	Sample Na Position User Name Acquired T DA Method	Vial 5 ime 09-07-201	3 PM 12:40:36 rt.m			
Sample Group Acquisition SV Version	<b>V</b> 620	0 series TOF OF B.05.01	6500 serie: (85125)	Info. S						
Compound T	able									
Compour	dlabol	RT	Mass	F	ormula	MFG Fo	rmula	MFG Di (ppm)		DB Formula
Compoun Cpd 18: C:	17 H22 N6 O4		374.17		H22 N6 O4	C17 H22				C17 H22 N6 O4
Compound L Cpd 18: C17 H		<i>m/z</i> 375.1771	<b>RT</b> 0.195	Algor Find b	www.enders.com/a	Mass eature 374.17				
2 - 1.5 - 1 - 0.5 -			000	50 500	550 600 6	9825 50 700 750 8	00 850 900	950		
0 - 1	50 200 25	50 300 3		110 10. 111						
0 4					5					
0	n Peak List				Ion					
0	n Peak List z Abund	t	nula			Ξ				
0 1 MS Spectrur m/z	n Peak List z Abund 1 2258	Form	<b>1ula</b> 123 N6 O4		Ion					
0 <b>MS Spectrum</b> <i>m/z</i> 375.1771	m Peak List z Abund 1 2258 1 4336	Forn 091.5 C17	nula 123 N6 O4 123 N6 O4		<b>Ion</b> (M+H)+					
0 1 <b>MS Spectrum</b> <i>m/z</i> 375.1771 376.1806	Z         Abund           1         2258           1         4336           1         507           1         48	Form 091.5 C17 1 39.53 C17 1 26.54 C17 1 20.64 C17 1	123 N6 O4 123 N6 O4 123 N6 O4 123 N6 O4 123 N6 O4		Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+					
0 1 <b>MS Spectrum</b> <i>m/z</i> 375.1771 376.1806 377.1828 378.1847 397.159	Peak List           z         Abund           1         2258           1         4336           1         507           1         48           1         723	Form 091.5 C17 1 39.53 C17 1 26.54 C17 1 20.64 C17 1 42.15 C17	nula 123 N6 O4 123 N6 O4 123 N6 O4 123 N6 O4 122 N6 Na C		Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+					
01 <b>MS Spectrum</b> <i>m/z</i> 375.1771 376.1806 377.1828 378.1847 397.159 398.1619	z         Abund           1         2258           1         4336           1         507           1         48           1         723           1         153	Form 091.5 C17 39.53 C17 26.54 C17 20.64 C17 42.15 C17 900.32 C17	nula 123 N6 O4 123 N6 O4 123 N6 O4 123 N6 O4 122 N6 Na ( 122 N6 Na (	04	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+					
0 m/z 375.1771 376.1806 377.1828 378.1847 397.159 398.1619 399.164	Abund           1         2258           1         4336           1         507           1         48           1         723           1         153           1         222	Form           091.5         C17           39.53         C17           26.54         C17           20.64         C17           42.15         C17           190.32         C17           33.592         C17	nula 123 N6 O4 123 N6 O4 123 N6 O4 123 N6 O4 122 N6 Na C	04	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+Na)+					
0 <b>MS Spectrum</b> <i>m/z</i> 375.1771 376.1806 377.1828 378.1847 397.159 398.1619 399.164 771.3286	Abund           1         2258           1         4336           1         507           1         48           1         723           1         153           1         222           1         947	Form           091.5         C17           39.53         C17           26.54         C17           20.64         C17           42.15         C17           90.32         C17           35.92         C17           78.48         C17	nula 123 N6 O4 123 N6 O4 123 N6 O4 123 N6 O4 122 N6 Na ( 122 N6 Na (	04	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+Na)+           (M+Na)+           (2M+Na)+					
0 <b>MS Spectrum</b> <i>m/z</i> 375.1771 376.1806 377.1828 378.1847 397.159 398.1619 399.164 771.3286 772.3307	z         Abund           1         2258           1         4336           1         507           1         507           1         723           1         153           1         222           1         947           1         947           1         403	Form           091.5         C17           39.53         C17           26.54         C17           20.64         C17           42.15         C17           90.32         C17           78.48         70.81	nula 123 N6 O4 123 N6 O4 123 N6 O4 123 N6 O4 122 N6 Na ( 122 N6 Na (	04	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+Na)+           (2M+Na)+           (2M+Na)+					
0 MS Spectrum <i>m/z</i> 375.1771 376.1806 377.1828 378.1847 397.159 399.164 771.3286 772.3307 773.3338	z         Abund           1         2258           1         4336           1         507           1         48           1         723           1         153           1         222           1         947           1         403           1         96	Form           091.5         C17           39.53         C17           26.54         C17           20.64         C17           20.62         C17           90.32         C17           33.592         C17           78.48         20.81           20.64         64	nula 123 N6 O4 123 N6 O4 123 N6 O4 123 N6 O4 122 N6 Na ( 122 N6 Na (	04	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+Na)+           (M+Na)+           (2M+Na)+					
0 MS Spectrum m/z 375.1771 376.1806 377.1828 378.1847 397.159 398.1619 399.164 771.3286 772.3307 773.3338 Predicted Is	z         Abund           1         2258           1         4336           1         507           1         48           1         723           1         153           1         225           1         48           1         723           1         153           1         225           1         947           1         403           1         96           50000pe Mate         500	Form           091.5         C17           39.53         C17           26.54         C17           20.64         C17           39.53         C17           39.53         C17           30.64         C17           30.75         C17           30.93         C17           35.92         C17           35.92         C17           70.84         C17           39.406         C           64.06         C	123 N6 04 123 N6 04 123 N6 04 123 N6 04 123 N6 04 122 N6 Na ( 122 N6 Na ( 122 N6 Na (	04	Ion (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+		Abund Sum 94		Calc Abum	d Sum %
0 MS Spectrur <i>m/z</i> 375.1771 376.1806 377.1828 378.1847 397.159 398.1619 399.164 771.3286 772.3307 773.3338 Predicted Is Isotope	n         Peak List           z         Abund           1         2258           1         4336           1         507           1         48           1         723           1         153           1         222           1         947           1         947           1         946           5000         947           1         947           1         947           1         947           1         947           1         947	Form           091.5         C17           39.53         C17           20.54         C17           20.54         C17           42.15         C17           190.32         C17           135.92         C17           78.48            94.06            CH         Table           Q4.05	123 NG 04 123 NG 04 123 NG 04 123 NG 04 123 NG 04 122 NG NG 04 124 NG 04	04 04 09 <b>pm)</b>	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+	Calc Abund %	Abund Sum %		Calc Abune	
0 MS Spectrur <i>m/z</i> 375.1771 376.1806 377.1828 378.1847 397.159 398.1619 399.164 771.3286 771.3286 771.32307 773.3338 Predicted IS Isotope 1	m Peak List z Abund 1 2258 1 4336 1 507 1 48 1 723 1 153 1 222 1 947 1 403 1 947 1 403 1 965 505 → Pattern Materna m/z	Form           091.5         C17           39.53         C17           26.54         C17           42.15         C17           42.15         C17           90.32         C17           35.92         C17           78.48	123 N6 04           122 N6 Na 04           123 N6           124 N6           125 N6           125 N6           126 N6           127 N6	04 04 09 09 09 09 09 09 09 09 09 09 09 09 09	Ion (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)+(2M+Na)+ (2M+Na)+(2M+Na)	Calc Abund %	Abund Sum %	82.18	Calc Abund	80.48
0 MS Spectrum <i>m/z</i> 375.1771 376.1806 377.1828 378.1847 399.159 399.164 771.3286 772.3307 773.3338 Predicted Is Isotope 1 2	m Peak List           z         Abund           1         2258           1         4336           1         507           1         48           1         723           1         153           1         222           1         947           1         947           1         940           1         960           sotope Matte         m/z           375.177         376.180	Form           091.5         C17           39.53         C17           20.54         C17           20.54         C17           30.53         C17           42.55         C17           90.32         C17           33.592         C17           78.48            70.81            994.06         Calc m/2           1         Calc m/2           1         3756           6         3767	123 NG 04 123 NG 04 123 NG 04 123 NG 04 123 NG 04 122 NG NG 04 123 NG 04 122 NG NG 04 123 NG 0	04 04 09 09 09 09 09 00 04 00 04 00 04 00 04 00 04 00 04 00 04 00 04 00 04 00 04	Ion (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)+	Calc Abund % 100 21	Abund Sum %	82.18 15.78	Calc Abune	80.48 16.9
0 MS Spectrur <i>m/z</i> 375.1771 376.1806 377.1828 378.1847 397.159 398.1619 399.164 771.3286 777.3307 773.3338 Predicted IS Isotope 1	m Peak List z Abund 1 2258 1 4336 1 507 1 48 1 723 1 153 1 222 1 947 1 403 1 947 1 403 1 965 505 → Pattern Materna m/z	b 091.5 C17 39.53 C17 26.54 C17 20.64 C17 90.22 C17 35.92 C17 35.92 C17 78.48 70.81 70.81 78.48 C17	123 NG 04 123 NG 04 123 NG 04 123 NG 04 123 NG 04 122 NG NG 04 123 NG 04 122 NG NG 04 123 NG 0	04 04 09 09 09 09 09 09 09 09 09 09 09 09 09	Ion (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)+(2M+Na)+ (2M+Na)+(2M+Na)	Calc Abund %	Abund Sum %	82.18	Calc Abune	80.48



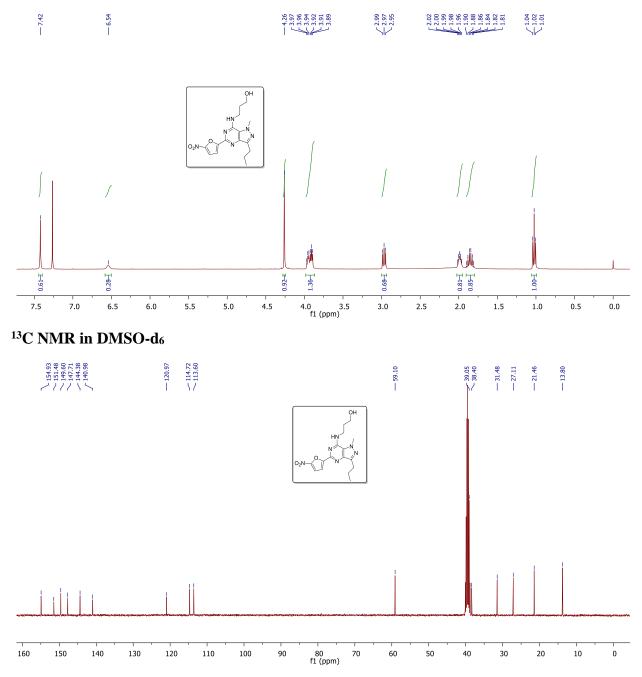


2: 254 nm, 8 nm	2:	254	nm,	8	nm	
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5

Pk#	<b>Retention Time</b>	Area	Area %	Height	Height %
1	3.381	10594	0.050	1547	0.090
2	5.739	21345161	99.844	1721036	99.815
3	21.323	22860	0.107	1641	0.095
Totals					-
· /=		21378615	100.000	1724224	100.000

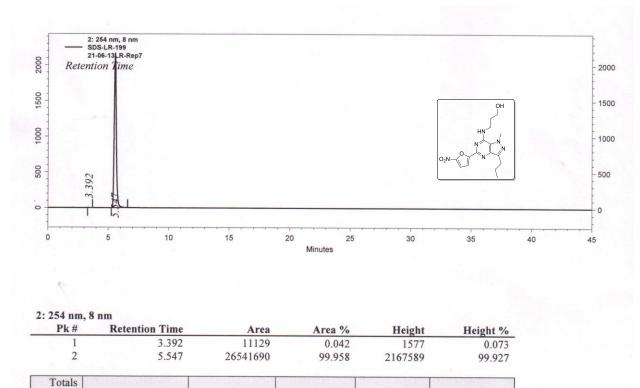
## Compound (27) <sup>1</sup>H NMR in CDCl<sub>3</sub>



## **Qualitative Compound Report**

Data File Sample Type Instrument Na Acq Method RM Calibration Comment		tus	Sai Ins vis	R-A-50.d mple strument : shal_12-01 iccess			Sample Nan Position User Name Acquired Ti DA Method	ime (	GLR-A-50 /ial 6 09-07-2013 daily_report.	PM 12:42:09 .m		c		
Sample Group Acquisition SW /ersion	1			TOF/6500 01 (B5125		fo.								
Compound T	able										MFG	Diff		-
Compoun	dla	hel	RT	M	ass		Formula		MF	G Formula	(p	pm)		rmula
Cpd 4: C			0.19		60.1547	C1	16 H20 N6 O4	4	C16	H20 N6 O4		-0.33	C16 H2	0 N6 O4
Compound L Cpd 4: C16 H	20 N		<b>m/z</b> 361.16	and the second		Igorith nd by I	Molecular F	Feature	360.1547					
x10 6 Cpd	4: C1	6 H20 N	6 04:		E Spectrur	m (0.14	45-0.645 mi	in) Frag=	=175.0V G	LR-A-50.d				
0.8 0.6 0.4 0.2	4: C1	6 H20 N	6 O4: ·	361.1620 C16 H21 N6 O4										
	150	200 25	0 300	361.1620 C16 H21 N6 O4	400 450	500 5	45-0.645 mi 550 600 ( ss-to-Charg	650 70		LR-A-50.d	950			
0.8 0.6 0.4 0.2 0 MS Spectru	150 m Pe	200 25 eak List	0 300	361.1620 C16 H21 N6 O4	400 450	500 5	550 600 ( ss-to-Charg	650 70			950			
0.8 0.6 0.4 0.2 0 MS Spectru	150 m Pe	200 25 eak List Abund	0 300 F	361.1620 320 C16 H21 N6 O4	400 450 Counts v	500 5	550 600 ( ss-to-Chargo Ion	650 70			950			
0.8 0.6 0.4 0.2 0 <b>MS Spectru</b> <i>m/z</i> 361.162	50 <b>m Pe</b> 1	200 25 <b>ak List</b> <b>Abund</b> 93460	0 300 F 14.69 C	0 350 4 Formula C16 H21 N	400 450 Counts v 16 04	500 5	550 600 ( ss-to-Charge <b>Ion</b> (M+H)+	650 70			950			
0.8 0.6 0.4 0.2 0 <b>MS Spectru</b> <i>m/z</i> 361.162 362.1648	150 m Pe z 1 1	200 25 <b>ak List</b> <b>Abund</b> 93460 16143	0 300 14.69 C	0 350 4 Formula C16 H21 NC C16 H21 NC C16 H21 NC	400 450 Counts v 16 04 16 04	500 5	550 600 ( ss-to-Charge (M+H)+ (M+H)+	650 70			950			
0.8 0.6 0.4 0.2 0 <b>MS Spectru</b> <i>m/z</i> 361.162 362.1648 363.1666	50 <b>m Pe</b> <b>z</b> 1 1 1	200 25 <b>ak List</b> <b>Abund</b> 93460 16141 21:	0 300 <b>F</b> 14.69 C 17.45 C 325.7 C	0 350 4 Formula C16 H21 N	400 450 Counts v 16 04 16 04	500 5	550 600 ( ss-to-Charge <b>Ion</b> (M+H)+	650 70			950			
0.8 0.6 0.4 0.2 0 <b>MS Spectru</b> <i>m/z</i> 361.162 362.1648 363.1666 364.1688	150 <b>z</b> 1 1 1 1	200 25 <b>ak List</b> <b>Abund</b> 93460 16141 21: 21:	0 300 14.69 C 17.45 C 325.7 C 35.81 C	361.1620 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200 361.162000 361.16200 361.16200 361.16200 361.16200 361.162	400 450 Counts v 16 04 16 04 16 04	500 5	550 600 ( ss-to-Charge (M+H)+ (M+H)+ (M+H)+	650 70			950			
0.8 0.6 0.4 0.2 0 <b>MS Spectru</b> <i>m/z</i> 361.162 362.1648 363.1666	150 <b>z</b> 1 1 1 1	200 25 <b>ak List</b> <b>Abund</b> 93460 16141 21: 629	0 300 14.69 C 225.7 C 144.37 C	361.1620 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200 361.16200	400 450 Counts v 16 04 16 04 16 04 16 04 16 Na 04	500 5	550 600 ( ss-to-Charge (M+H)+ (M+H)+ (M+H)+ (M+H)+	650 70			950			
0.8 0.6 0.4 0.2 0 <b>MS Spectru</b> <i>m/z</i> 361.162 362.1648 363.1666 364.1688 383.1436	150 <b>z</b> 1 1 1 1 1 1	200 255 <b>Abund</b> 93460 16143 211 211 211 212 212 212 212 21	0 300 44.69 C 325.7 C 335.81 C 44.37 C 41.51 C	3911620 3911600 3911600 3911600 3911600 39116000000000000000000000000000000000	400 450 Counts v 16 04 16 04 16 04 16 04 16 Na 04	500 5	550 600 ( ss-to-Charge (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+	650 700 e (m/z)			950			
0.8 0.6 0.4 0.2 0 <b>MS Spectru</b> <i>m/z</i> 361.162 362.1648 363.1666 364.1688 383.1436	<b>1</b> 50 <b>2</b> 1 1 1 1 1 1 1 1 1 1	200 25 ak List Abund 93460 16141 211 212 629 1255 177 573	0 300 44.69 C 325.7 C 325.81 C 44.37 C 41.51 C 01.56 C 76.84 C	Formula 190 350 4 Formula 190 350 4 Formula 190 350 4 Formula 190 350 4 190 350 4 190 10 190	400 450 Counts v 16 04 16 04 16 04 16 Na 04 16 Na 04 16 Na 04 11 Na 08	500 5	550 600 ( ss-to-Charge (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)+	650 700 e (m/z)			950			
0.8 0.6 0.4 0.2 0 <b>MS Spectrui</b> <i>m/z</i> 361.162 362.1648 363.1666 364.1688 383.1436 384.1464	150 <b>z</b> 1 1 1 1 1 1 1 1 1 1 1 1 1 1	200 25 eak List Abund 93460 16141 211 211 6299 1255 177 573 214	0 300 44.69 C 35.81 C 44.37 C 41.51 C 11.56 C 76.84 C 01.39 C	Formula 10291:198 0 350 4 Formula 116 H21 N 116 H2	400 450 Counts v 16 04 16 04 16 04 16 Na 04 16 Na 04 16 Na 04 112 Na 08 112 Na 08	500 5	550 600 ( ss-to-Charg) (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)+ (2M+Na)+	650 700 e (m/z)			950			
0.8 0.6 0.4 0.2 0 <b>MS Spectru</b> <i>m/z</i> 361.162 362.1648 363.1666 364.1688 383.1436 384.1464 385.1486 743.2978 744.2997 745.3023	150 <b>z</b> 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	200 25 eak List Abund 93460 16141 211 212 125 177 573 214 52	0 300 44.69 C 35.81 C 41.51 C 01.56 C 6.84 ( 01.39 C 49.12 C	<b>Formula</b> <b>C16</b> H21 N <b>C16</b> H20 N <b>C17</b> H0 H	400 450 Counts v 16 04 16 04 16 04 16 Na 04 16 Na 04 16 Na 04 11 Na 08	500 5	550 600 ( ss-to-Charge (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)+	650 700 e (m/z)			950			
0.8 0.6 0.4 0.2 0 <b>MS Spectru</b> <i>m/z</i> 361.162 362.1648 363.1666 364.1688 383.1436 384.1464 385.1486 743.2978 744.2997 745.3023 <b>Predicted I</b>	150 <b>m</b> Pe <b>z</b> 1 1 1 1 1 1 1 1 1 1 1 1 1	200 25 ak List Abund 93460 16141 211 211 629 125 177 573 214 52 pe Mate	0 300 44.69 C 35.81 C 44.37 C 44.37 C 41.51 C 76.84 ( 01.39 C 49.12 C <b>ch Tat</b>	50 350 4 50 100 100 100 100 100 100 100 100 100 1	400 450 Counts v 16 04 16 04 16 04 16 Na 04 112 Na 08 112 Na 08 112 Na 08	500 5 s. Mas	550 600 ( ss-to-Charge (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+	650 701 e (m/z)	0 05- 05- 05- 05 05 05 05 05 05 05 05 05 05 05 05 05	0 850 900 9	950	Calc Abu	nd Sum %	
0.8 0.6 0.4 0.2 0 <b>MS Spectrui</b> <i>m/z</i> 361.162 362.1648 363.1666 364.1688 383.1436 384.1464 385.1486 743.2978 745.3023 <b>Predicted I</b> Isotope	150 <b>z</b> 1 1 1 1 1 1 1 1 1 1 1 1 1	200 25 eak List Abund 93460 1614; 21; 6294 125; 17; 573; 21;4 522 pe Mate	0         300           14.69         C           35.81         C           45.92         C           35.81         C           41.51         C           50         C           51         C           52         C           52         C           52         C           53         C           54         C           54         C           55         C           56         C           57         C           58         C           59         C           50         C           50         C           57         C           58         C           59	00000000000000000000000000000000000000	6 04 6 04 6 04 6 04 6 04 16 04 16 04 16 Na 04 112 Na 08 112 Na 08 112 Na 08 112 Na 08	500 5 s. Mas	550 600 ( ss-to-Charge (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+ (2M+Na)+	650 700 e (m/z)	% pun 98 052 0 98 055 0 98 055 0 98 055 0 98 055 0 98 055 0 98 055 0 99 055 0 99 055 0 90 0 90			Calc Abu	nd Sum %	81.37
0.8 0.6 0.4 0.2 0 <b>MS Spectru</b> <i>m/z</i> 361.162 362.1648 363.1666 364.1688 383.1436 384.1464 385.1486 743.2978 744.2997 745.3023 <b>Predicted I</b> <b>Isotope</b> 1	50 <b>z</b> 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	200 25 eak List Abund 93460 16141 211 229 125 177 573 214 525 525 525 525 525 525 525 52	0         300           44.69         C           525.7         C           55.81         C           44.51         C           64.51         C           70.56         C           70.139         C           49.12         C           Ch Tat         Calc	00000000000000000000000000000000000000	400 450 Counts v 604 604 604 604 604 604 604 604 604 604	500 5 s. Mas	550 600 ( ss-to-Charge (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (2M+Na)+(2M+Na)+ (2M+Na)+	650 701 e (m/z)	743.2978 98 052. 0 98 052. 0 99 001	0 850 900 9	83.45	Calc Abu	nd Sum %	<u>81.37</u> 16.19
0.8 0.6 0.4 0.2 0 <b>MS Spectru</b> <i>m/z</i> 361.162 362.1648 363.1666 364.1688 383.1436 384.1464 385.1486 743.2978 744.2997 745.3023 <b>Predicted I</b> Isotope 1 2	50 <b>z</b> 1 1 1 1 1 1 1 1 1 1 1 1 1	200 25 ack List Abund 93460 16141 21: 22: 170 573 214 52 pe Matr 361.162 362.1648	0         3000           #4.69         C           225.7         C           35.81         C           41.51         C           01.56         C           01.39         C           49.12         C           Calc         C	Formula           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         16         10           0         16         10           0         16         10           0         16         10           0         16         10           0         16         10           0         16         10           0         16	400 450 Counts v 6 04 6 04 6 04 6 04 6 04 6 04 16 Na 04 16 Na 04 112 Na 08 112 Na 08 112 Na 08 112 Na 08 112 Na 08 112 Na 08	500 5 s. Mas 0.34 0.56	550         600         6           Ion         (M+H)+         (M+H)+           (M+H)+         (M+H)+         (M+H)+           (M+H)+         (M+Na)+         (M+Na)+           (M+Na)+         (M+Na)+         (M+Na)+           (M+Na)+         (2M+Na)+         (2M+Na)+           (2M+Na)+         (2M+Na)+         (2M+Na)+           (100)         17.27         100	650 701 e (m/z)	743.2978 743.2978 08 052 0 100 108 108 108 108 108 108 108 108 10	0 850 900 9	83.45 14.41	Calc Abu	nd Sum %	
0.8 0.6 0.4 0.2 0 <b>MS Spectru</b> <i>m/z</i> 361.162 362.1648 363.1666 364.1688 363.1666 364.1688 383.1436 384.1464 385.1486 743.2978 744.2997 745.3023 <b>Predicted I</b> Isotope 1 2 3	50 <b>z</b> 1 1 1 1 1 1 1 1 1 1 1 1 1	200 250 ak List Abund 93460 16141 21: 629 1250 177 573 214 52 pe Mate 361.162 362.1648 363.1666	0 300 →4.69 C 7.7.45 C →5.81 C ↓4.37 C ↓4.	Formula           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         16         12           0         16         120           0         16         140           0         16         140           0         16         16           0         16         16           0         16         16           0         16	400 450 Counts v 6 04 6 04 16 04 16 04 16 Na 04 16 Na 04 112 Na 08 112 Na 08	500 5 /s. Mas /.34 /.56 /s.95	550 600 ( ss-to-Charge (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)	650 701 e (m/z)	243.2978 743.2978 7440 N12 Na 08 762 0 762 0 763 763 763 763 763 763 763 763 763 763	00 850 900 9	83.45 14.41 1.9	Caic Abu	nd Sum %	16.19
0.8 0.6 0.4 0.2 0 <b>MS Spectru</b> <i>m/z</i> 361.162 362.1648 363.1666 364.1688 383.1436 384.1464 385.1486 743.2978 744.2997 745.3023 <b>Predicted I</b> Isotope 1 2	50 <b>2</b> 1 1 1 1 1 1 1 1 1 1 1 1 1	200 25 ack List Abund 93460 16141 21: 22: 170 573 214 52 pe Matr 361.162 362.1648	0 300 4.69 C 225.7 C 225.7 C 225.7 C 25.81 C 25.81 C 25.81 C 25.81 C 25.81 C 25.81 C 25.81 C 25.81 C 41.51 C 1.52 C 1.52 C 2.52 C 2.5	Formula           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         350         4           0         16         10           0         16         10           0         16         10           0         16         10           0         16         10           0         16         10           0         16         10           0         16	400 450 Counts v 66 04 16 04 16 04 16 04 16 Na 04 16 Na 04 112 Na 08 112 Na	500 5 s. Mas 0.34 0.56	550         600         6           Ion         (M+H)+         (M+H)+           (M+H)+         (M+H)+         (M+H)+           (M+H)+         (M+Na)+         (M+Na)+           (M+Na)+         (M+Na)+         (M+Na)+           (M+Na)+         (2M+Na)+         (2M+Na)+           (2M+Na)+         (2M+Na)+         (2M+Na)+           (100)         17.27         100	650 70 e (m/z)	743.2978 743.2978 08 052 0 100 108 108 108 108 108 108 108 108 10	00 850 900 9	83.45 14.41	Calc Abu	nd Sum %	16.19 2.2





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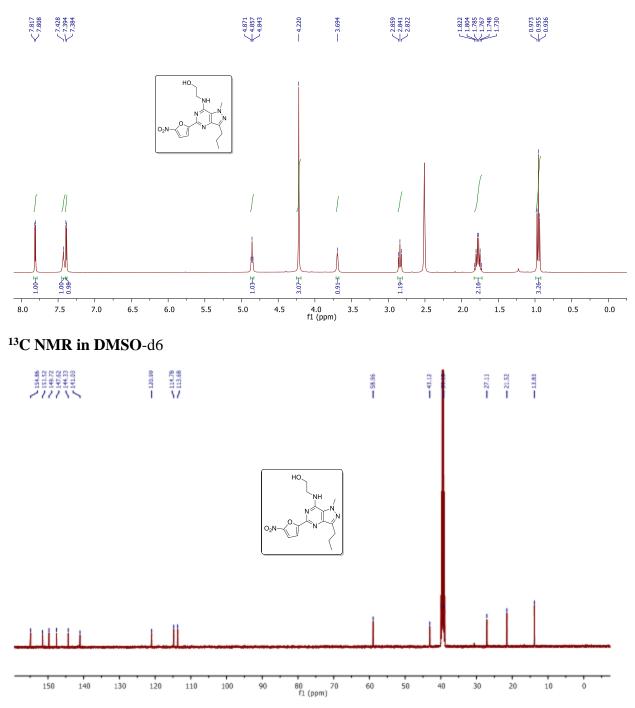
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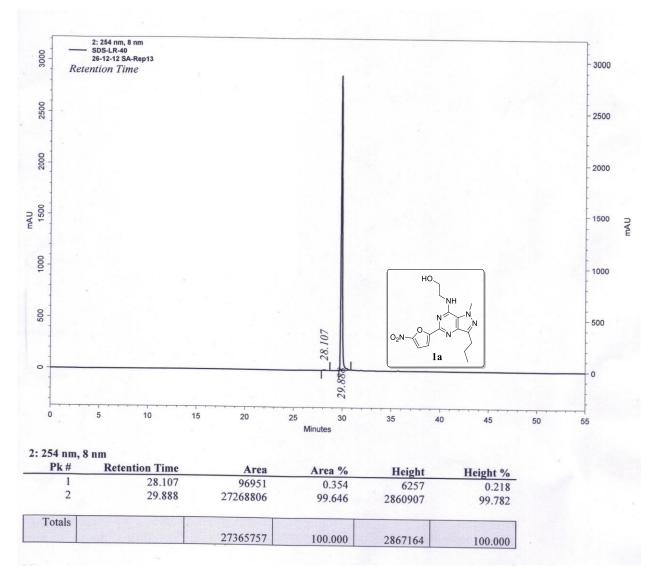
Compound (28)

<sup>1</sup>H NMR in DMSO-d6

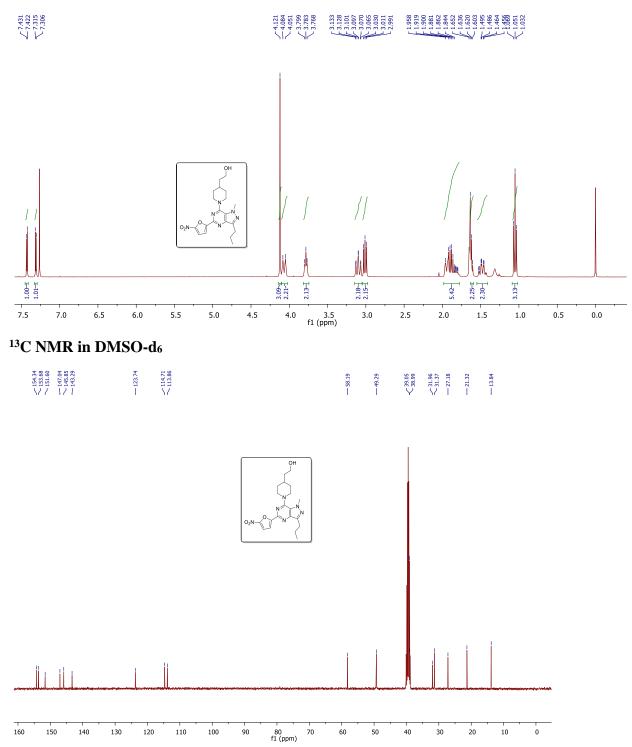


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ata File ample Type nstrument Na	me		le Iment 1	Sample Name Position User Name	GLR-1 Vial 14	50-04 DM	O <sub>2</sub> N-	
cq Method		000000000000000000000000000000000000000	_MS_25072012.m	And an and a second descent	11/18/2012 12:	58:04 PM	0211	T.
RM Calibratio	n Status	Succe	ISS	DA Method	as.m			1a \
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ample Group	Info							
ompound T	able					M	FG Diff	
Compoun	d Label	RT	Mass	Formula	MFG Fo		ppm)	DB Formul
Cpd 5: C1	5 H18 N6 O4	0.17	346.13848	C15 H18 N6 O4	C15 H18	3 N6 O4	1.38	C15 H18 N6
omnound	ahel	m/z	RT	Algorithm	Mass			
ompound L pd 5: C15 H1		347.1457	and the second se	Find by Molecular F		8		
pu 5. C15 111	0 10 04	547.1457	5 0.17	This by Holecaldr I				
2			200					
		250 300	347.14575 347.14575 C15 H19 N6 O4 247.14575 Cont	0 500 550 600 6 s vs. Mass-to-Charge	(z) 005 002 002 C30 H36 N12 Na 08 C30 H36 N12 Na 08	800 850 900 1	950	
1 0.5 0 45 Spectrum	n Peak List	250 300	350 400 454 Count	s vs. Mass-to-Charge	50 700 750	800 850 900 1	950	
1 - 0.5 - 0	r Peak List	250 300	350 400 45 Count	s vs. Mass-to-Charge	50 700 750	800 850 900 1	950	
1- 0.5- 0 <b>15 Spectrum</b> <i>n/z</i> 347.14575	<b>Peak List</b> <b>z Abund</b> 1 2255	250 300 Form 247.6 C15 I	350 400 45 Count H19 N6 04	s vs. Mass-to-Charge	50 700 750	800 850 900 1	950	
1 - 0.5 - 0 - <b>15 Spectrum</b> <i>n/z</i> 347.14575 348.14846	Peak List           z         Abund           1         2255           1         465	<b>Form</b> 247.6 C15 I 517.4 C15 I	350 400 45 Count H19 N6 04 H19 N6 04	s vs. Mass-to-Charge	50 700 750	800 850 900 1	950	
1 - 0.5 - 0 - <b>15 Spectrum</b> <i>n/z</i> 347.14575 348.14846 349.15045	z         Abund           1         2255           1         465           1         55	<b>Form</b> 247.6 C15 I 517.4 C15 I 888.2 C15 I	350 400 45 Count H19 N6 04 H19 N6 04	Ion           (M+H)+           (M+H)+	50 700 750	800 850 900 1	950	
1 - 0.5 - 0 - <b>15 Spectrum</b> <i>n/z</i> 347.14575 348.14846 349.15045 369.12753	z         Abund           1         2253           1         463           1         55	250 300 Form 247.6 C15 517.4 C15 888.2 C15 064.4 C15	350 400 454 Count H19 N6 04 H19 N6 04 H19 N6 04 H19 N6 04	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+	50 700 750	800 850 900 1	950	
1 - 0.5 - 0 - <b>15 Spectrum</b> 7/z 347.14575 348.14846 349.15045 369.12753 370.13073	z         Abund           1         2255           1         465           1         55           1         196           1         196	250 300 Form 247.6 C15 1 517.4 C15 1 888.2 C15 1 064.4 C15 1 3624 C15 1	350 400 454 Count 119 N6 04 119 N6 04 119 N6 04 119 N6 04 118 N6 Na 04 118 N6 Na 04	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+	50 700 750	800 850 900 9	950	
1 - 0.5 - 0 - <b>IS Spectrum</b> 1/z 347.14575 348.14846 349.15045 369.12753 370.13073 371.13112	z         Abund           1         2253           1         463           1         533           1         199           1         119           1         119           1         119           1         119	250 300 Form 247.6 C15 1 517.4 C15 1 888.2 C15 1 064.4 C15 1 3624 C15 1 3624 C15 1 3624 C15 1	350 400 454 Count 119 N6 04 119 N6 04 119 N6 04 119 N6 04 118 N6 Na 04 118 N6 Na 04 118 N6 Na 04	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+	50 700 750	800 850 900 9	950	
1 - 0.5 - 0 - <b>AS Spectrum</b> <i>n/z</i> 347.14575 348.14846 349.15045 369.12753 370.13073 371.13112 385.10281	z         Abund           1         2253           1         463           1         56           1         190           1         191           1         113           1         133	250 300 Form 247.6 C15 1 517.4 C15 1 888.2 C15 1 064.4 C15 1 3624 C15 1 3624 C15 1 3625 C15 1 3627 C15 1 357.7 C	350 400 456 Count 19 N6 04 19 N6 04 19 N6 04 19 N6 04 19 N6 04 118 N6 Na 04 118 N6 Na 04 118 N6 Na 04 118 K N6 04	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+Na)+           (M+Na)+	50 700 750	800 850 900 9	950	
1 - 0.5 - 0 - <b>15 Spectrum</b> <i>m/z</i> 347.14575 348.14846 349.15045 369.12753 370.13073 370.13073 371.13112 385.10281 715.26527	z         Abund           1         2253           1         463           1         56           1         190           1         191           1         113           1         33           1         223	Form           247.6         C15           517.4         C15           888.2         C15           064.4         C15           3624         C15           591.5         C15           357.7         C15           254.8         C30	350 400 45 Count 119 N6 04 119 N6 04 119 N6 04 119 N6 04 118 N6 Na 04 118 N6 Na 04 118 N6 Na 04 118 N6 Na 04 118 K N6 04 118 K N6 04 136 N12 Na 08	Ion           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+Na)+           (M+K)+           (M+K)+           (2M+Na)+	50 700 750	800 850 900 9	950	
1 - 0.5 - 0 <b>4S Spectrum</b> <i>m/z</i> 347.14575 348.14846 349.15045 369.12753 370.13073 370.13073 371.13112 385.10281 715.26527 716.26916	Peak List           z         Abund           1         2253           1         463           1         59           1         199           1         191           1         11           1         13           1         222           1         222           1         222           1         88	550         300           Form         247.6         C15           517.4         C15         15           3624         C15         3624         C15           3624         C15         15         15         15           591.5         C15         254.8         C30         1439.9         C30	350 400 45 Count 119 N6 04 119 N6 04 119 N6 04 119 N6 04 118 N6 Na 04 118 N6 Na 04 118 N6 Na 04 118 K N6 04 118 K N6 04 118 K N6 04 118 K N6 04 136 K 12 Na 08	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+Na)+           (M+Na)+           (M+K)+	50 700 750	800 850 900 9	950	
1 - 0.5 - 0 - <b>15 Spectrum</b> <i>n/z</i> 347.14575 348.14846 349.15045 369.12753 370.13073 370.13073 371.13112 385.10281 715.26527 716.26916 717.27129	z         Abund           1         2255           1         466           1         551           1         199           1         191           1         11           1         11           1         1222           1         1333           1         2222           1         88           1         112	250 300 Form 247.6 C15 517.4 C15 388.2 C15 3624 C15 3626 C15	350 400 45 Count 119 N6 04 119 N6 04 119 N6 04 119 N6 04 118 N6 Na 04 118 N6 Na 04 118 N6 Na 04 118 N6 Na 04 118 K N6 04 118 K N6 04 136 N12 Na 08	Ion           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+Na)+           (M+K)+           (2M+Na)+           (2M+Na)+	50 700 750	800 850 900 9	950	
1 - 0.5 - 0 - <b>15 Spectrum</b> <i>n/z</i> 347.14575 348.14846 349.15045 369.12753 370.13073 371.13112 385.10281 715.26527 716.26916 717.27129 <b>Predicted Is</b>	z         Abund           1         2255           1         466           1         56           1         199           1         199           1         119           1         199           1         222           1         88           1         119           1         222           1         88           1         119           1         222           1         88           1         119           1         88           1         119	250 300 Form 247.6 C15 517.4 C15 388.2 C15 3624 C15 3625 C15 3626 C15	350 400 45 Count H19 N6 04 H19 N6 04 H19 N6 04 H19 N6 04 H18 N6 Na 04 H18 N6 Na 04 H18 N6 Na 04 H18 N6 04 H18 N6 04 H18 K 06 04 H36 N12 Na 08 H36 N12 Na 08 H36 N12 Na 08	Ion           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (QM+Na)+           (2M+Na)+           (2M+Na)+	50 700 750 (m/z)	800 850 900 1	950 Calc Abunc	1 Sum %
1 - 0.5 - 0 <b>15 Spectrum</b> <i>n/z</i> 347.14575 348.14846 349.15045 369.12753 370.13073 371.13112 385.10281 715.26527 716.26916 717.27129 <b>Predicted Is</b> <b>sotope</b>	z         Abund           1         2255           1         466           1         551           1         199           1         199           1         119           1         199           1	250 300 247.6 C15 517.4 C15 388.2 C15 3624	350 400 45 Count H19 N6 04 H19 N6 04 H19 N6 04 H19 N6 04 H18 N6 Na 04 H18 N6 Na 04 H18 N6 Na 04 H18 N6 O4 H18 N6 04 H18 N6	Ion           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+Na)+           (M+K)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+	50 700 750 (m/z)		Calc Abunc	<b>d Sum %</b> 82.45
1 - 0.5 - 0 - <b>15 Spectrum</b> <i>n/z</i> 347.14575 348.14846 349.15045 369.12753 370.13073 371.13112 385.10281 715.26527 716.26916 717.27129 <b>Predicted Is</b>	z         Abund           1         2255           1         466           1         56           1         199           1         199           1         119           1         199           1         222           1         88           1         119           1         222           1         88           1         119           1         222           1         88           1         119           1         88           1         119	Form           247.6         C15           517.4         C15           3624         C15           357.7         C15           254.8         C30           908.5         C30           ch Table         Calc m/z           347.14         Calc m/z	350 400 45 Count H19 N6 04 H19 N6 04 H19 N6 04 H19 N6 04 H18 N6 Na 04 H18 N6 Na 04 H18 N6 Na 04 H18 N6 Na 04 H18 N6 04 H18 N6 04 H36 N12 Na 08 H36 N12 Na 08 H36 N12 Na 08 H36 N12 Na 08 H36 N12 Na 08	Ion           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+Na)+           (M+Na)+           (M+K)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+	50 700 750 (m/z)	nd Sum %	Calc Abunc	

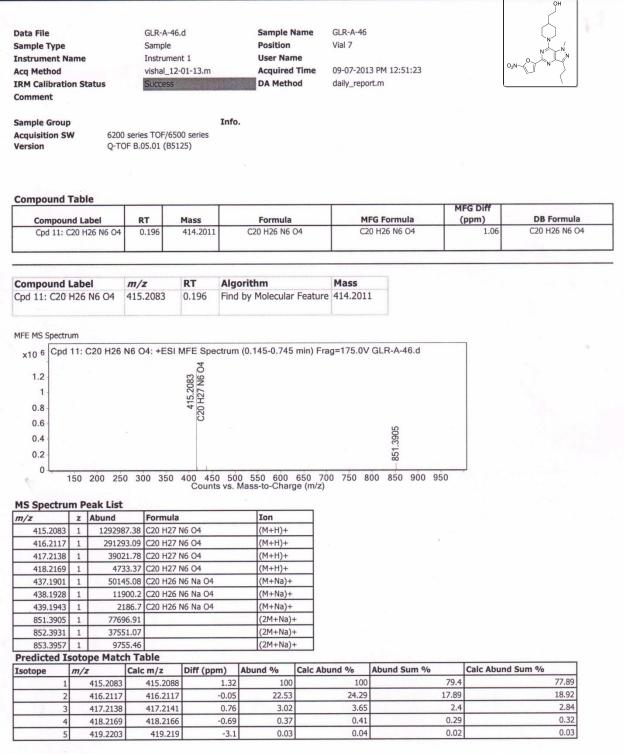




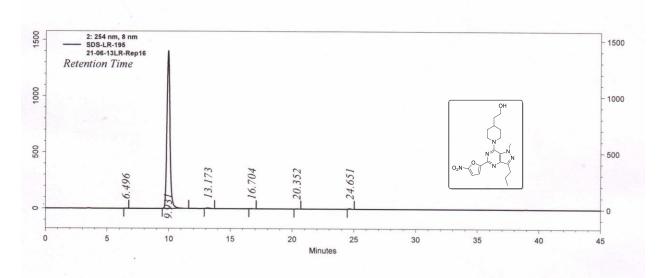
Compound (29) <sup>1</sup>H NMR in CDCl<sub>3</sub>



#### **Qualitative Compound Report**

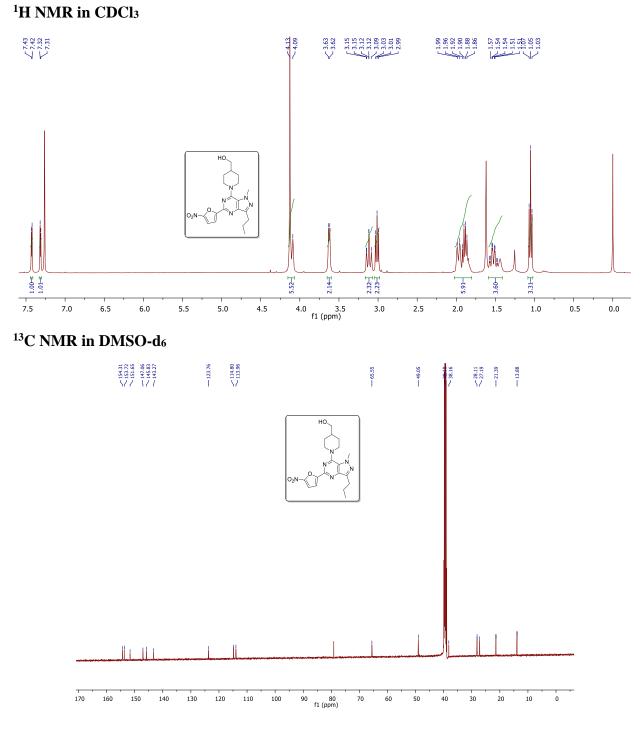






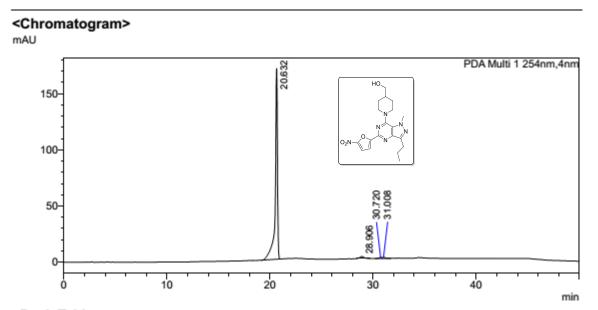
Pk #	<b>Retention Time</b>	Area	Area %	Height	Height %
1	6.496	10741	0.044	967	0.068
2	9.931	24200097	99.287	1403390	99.16
3	13.173	85912	0.352	4511	0.319
4	16.704	11043	0.045	671	0.04
5	20.352	16214	0.067	1096	0.07
6	24.651	49770	0.204	4535	0.320
Totals					
		24373777	100.000	1415170	100.00

Compound (30)



#### **Qualitative Compound Report** Sample Name GLR-4-36 GLR-4-36.d Data File HO. Vial 7 Sample Position Sample Type User Name Instrument 1 Instrument Name 11/19/2012 12:50:56 PM vishal MS 25072012.m Acquired Time Acq Method **DA Method** as.m **IRM Calibration Status** Comment Info. Sample Group **Compound Table** MFG Diff **DB** Formula Formula **MFG Formula** (ppm) RT Mass **Compound Label** C19 H24 N6 O4 C19 H24 N6 O4 2.1 Cpd 6: C19 H24 N6 O4 400.18506 C19 H24 N6 O4 0.172 RT Algorithm Mass m/z **Compound Label** Find by Molecular Feature 400.18506 Cpd 6: C19 H24 N6 O4 401.19234 0.172 MFE MS Spectrum x10 5 Cpd 6: C19 H24 N6 O4: + MFE Spectrum (0.133-0.460 min) GLR-4-36.d 401.19234 C19 H25 N6 O4 2.5 823.35836 C38 H48 N12 Na O8 2 1.5 1 0.5 0 400 450 500 550 600 650 700 750 800 850 900 950 Counts vs. Mass-to-Charge (m/z) 150 200 250 300 350 **MS Spectrum Peak List** Formula Ion m/z z Abund (M+H)+ 282970.2 C19 H25 N6 O4 401.19234 1 (M+H)+ 67367.8 C19 H25 N6 O4 402.19526 1 (M+H)+ 11081.3 C19 H25 N6 O4 403.19781 1 (M+Na)+ 423.17484 7723.5 C19 H24 N6 Na O4 1 (M+K)+ 7726.5 C19 H24 K N6 O4 439.14864 1 2042 C19 H24 K N6 O4 (M+K)+ 440.15073 1 (2M+Na)+ 823.35836 26678.9 C38 H48 N12 Na O8 1 12483.3 C38 H48 N12 Na O8 (2M+Na)+ 824.36126 1 (2M+Na)+ 3587.6 C38 H48 N12 Na O8 825.36353 1 2868.5 C38 H48 K N12 O8 (2M+K)+ 839.33337 1 Predicted Isotope Match Table Calc Abund Sum % Abund % Calc Abund % Abund Sum % Calc m/z Diff (ppm) Isotope m/z 78.77 77.93 100 100 401.19318 2.1 401.19234 18.26 23.18 18.55 23.81 402.19598 1.78 402.19526 2 2.67 3.05 3.39 1.54 3.92 403.19781 403.19843 3 0.29 0.37 0.46 404.20084 1.84 0.59 4 404.2001

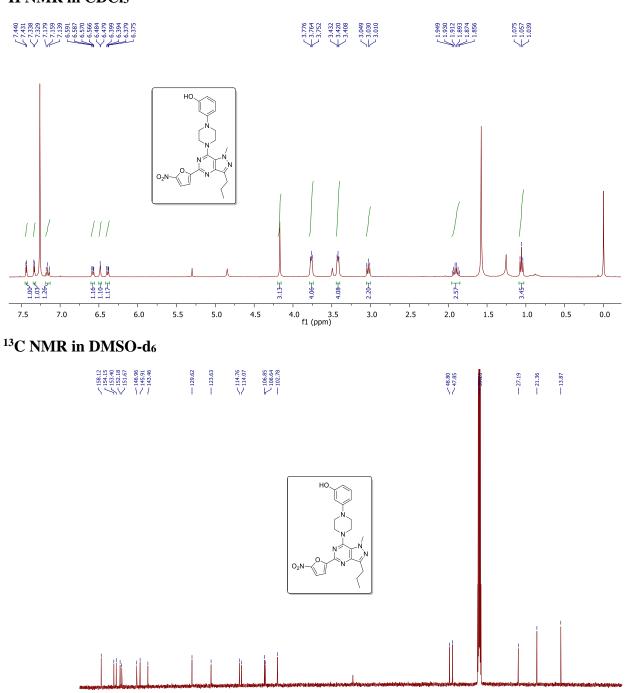




#### <Peak Table>

PDA Ch1 254nm											
Peak#	Name	Ret. Time	Area	Height	Area%	Height%					
1		20.632	2551608	169677	96.403	97.966					
2		28.906	56197	1832	2.123	1.058					
3		30.720	15467	789	0.584	0.455					
4		31.008	23540	902	0.889	0.521					
Total			2646813	173199	100.000	100.000					

Compound (31) <sup>1</sup>H NMR in CDCl<sub>3</sub>

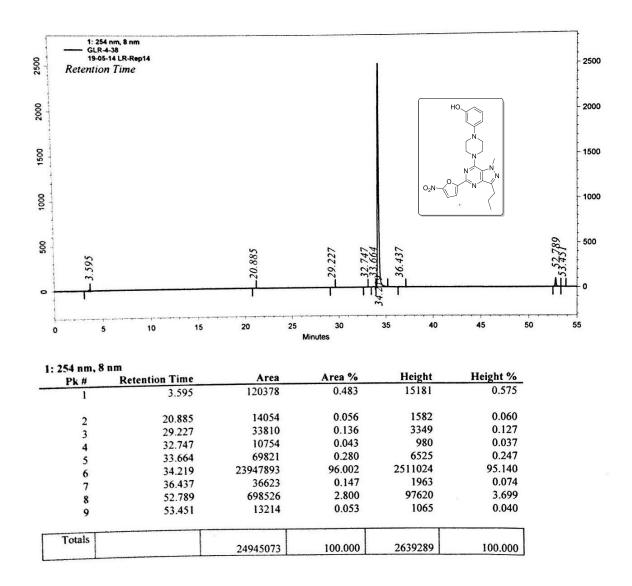


. 150 . 140 f1 (ppm) , 70 . 40 

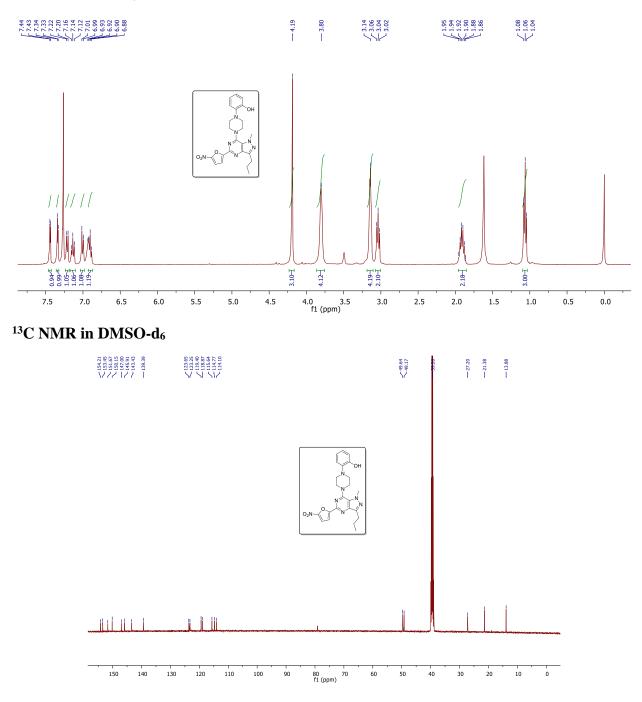
			- Vi	anta	cive con					
Data File Sample Type Instrument Name Acq Method IRM Calibration Status Comment Sample Group Inf		Sample Instrument 1 vishal_MS_25072012.m		Sample Name Position User Name Acquired Time DA Method	Vial 14	1:26:20 PM	$ \begin{array}{c} HO \\ HO \\ HO \\ N \\ $			
Compound T	able							MFG	Diff	
Compound Label Cpd 9: C23 H25 N7 O4		<b>RT Mass</b> 4 0.172 463.19602			Formula	MF	G Formula	(pp	m)	DB Formula
				02 (			H25 N7 O4		1.68	C23 H25 N7 O4
				-	aorithm	Mag				
Compound Label         m/z           Cpd 9: C23 H25 N7 O4         464.20331		RT Algorithm 0.172 Find by Molecula		Feature 463.19602						
2.5 2 1.5 1 0.5				464.20331 C23 H26 N7 O4					- 444.5/950	
						and the second sec			50	
0			350 40		500 550 600 . Mass-to-Charg		50 800 850	900 9		
0 MS Spectrur		:					50 800 850	900 9		
0 MS Spectrur	n Peak List z Abund	For			. Mass-to-Charg Ion (M+H)+		50 800 850	900 9		
MS Spectrum	z         Abund           1         388           1         120	For 142.2 C23 954.3 C23	mula H26 N7 O4 H26 N7 O4	Counts vs	. Mass-to-Charg Ion (M+H)+ (M+H)+		50 800 850	900 9		
0 MS Spectrum m/z 464.20331	n Peak List z Abund 1 388 1 120 1	For 142.2 C23 954.3 C23 19834 C23	mula H26 N7 O4 H26 N7 O4 H26 N7 O4	Counts vs	. Mass-to-Charg Ion (M+H)+ (M+H)+ (M+H)+		50 800 850	900 9		
0 <b>MS Spectrum</b> <i>m/z</i> 464.20331 465.20582	n Peak List z Abund 1 388 1 120 1 1 1 2	For 142.2 C23 954.3 C23 19834 C23 581.2 C23	mula H26 N7 O4 H26 N7 O4	Counts vs	. Mass-to-Charg Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+		50 800 850	900 9		
MS Spectrum m/z 464.20331 465.20582 466.20898 467.21078 949.37935	n Peak List z Abund 1 388 1 120 1 1 1 2 1 2	For 142.2 C23 954.3 C23 19834 C23 19834 C23 499.6	mula H26 N7 O4 H26 N7 O4 H26 N7 O4	Counts vs	Ion           (M+H)+		50 800 850	900 9		
MS Spectrum m/z 464.20331 465.20582 466.20898 467.21078	Peak List           z         Abund           1         388           1         120           1         1           1         2           1         2           1         2           1         3	For           142.2         C23           954.3         C23           19834         C23           581.2         C23           499.6         5277.5	mula H26 N7 O4 H26 N7 O4 H26 N7 O4	Counts vs	. Mass-to-Charg (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+Na)+ (2M+Na)+		50 800 850	900 9		
MS Spectrum m/z 464.20331 465.20582 466.20898 467.21078 949.37935 950.38136 951.38441	Peak List           z         Abund           1         388           1         120           1         2           1         2           1         2           1         3           1         3           1         3           1         3	For 142.2 C23 954.3 C23 19834 C23 581.2 C23 499.6 2277.5 .005.2	mula H26 N7 04 H26 N7 04 H26 N7 04 H26 N7 04	Counts vs	Ion           (M+H)+		50 800 850	300 3		
MS Spectrum m/z 466.20331 465.20582 466.20898 467.21078 949.37935 950.38136	Peak List           z         Abund           1         388           1         120           1         2           1         2           1         2           1         2           1         2           1         2           1         2           1         2           1         3           50         50	For 142.2 C23 1954.3 C23 19834 C23 581.2 C23 499.6 5277.5 .005.2 ch Table	mula H26 N7 04 H26 N7 04 H26 N7 04 H26 N7 04	Counts vs	Ion           (M+H)+           (2M+Na)+           (2M+Na)+	ge (m/z)			alc Ahund 4	Sum %
MS Spectrum m/z 464.20331 465.20582 466.20898 467.21078 949.37935 950.38136 951.38441	Peak List           z         Abund           1         388           1         120           1         2           1         2           1         3           1         3           1         3           1         3           1         3           1         3           1         3           1         3           1         3           1         3           1         3           1         3	t 142.2 C23 1954.3 C23 19834	mula H26 N7 04 H26 N7 04 H26 N7 04 H26 N7 04 Z Diff	Counts vs	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+	ge (m/z)	50 800 850 Abund Sum %		Calc Abund S	
MS Spectrum m/z 464.20331 465.20582 466.20898 467.21078 949.37935 950.38136 951.38441 Predicted Is Isotope 1	Peak List           z         Abund           1         388           1         120           1         21           1         22           1         23           1         24           1         25           1         26           1         27           464.2033         464.2033	For 142.2 C23 954.3 C23 19834 C23 581.2 C23 581.2 C23 499.6 277.5 005.2 Ct Table Calc m/ 1 464.2	mula H26 N7 04 H26 N7 04 H26 N7 04 H26 N7 04 H26 N7 04 Z0408	Counts vs (ppm) A 1.66	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (bund %           100	ge (m/z)		73.03	Calc Abund S	75.18
MS Spectrum m/z 464.20331 465.20582 466.20898 467.21078 949.37935 950.38136 951.38441 Predicted Is Isotope 1 2	Peak List           z         Abund           1         388           1         120           1         1           1         2           1         3           1         3           1         3           1         3           1         3           1         4           1         3           464.2033         465.2058	For           142.2         C23           9954.3         C23           19834         C23           2581.2         C23           277.5         005.2           Cch Table         Calc m/           1         464.2           2         465.3	mula H26 N7 O4 H26 N7 O4 H26 N7 O4 H26 N7 O4 H26 N7 O4 Z0408 20689	(ppm) A 1.66 2.3	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           100           31.16	c Abund % 100 27.88		73.03 22.76	Calc Abund S	
MS Spectrum m/z 464.20331 465.20582 466.20898 467.21078 949.37935 950.38136 951.38441 Predicted Is Isotope 1	Peak List           z         Abund           1         388           1         120           1         21           1         22           1         23           1         24           1         25           1         26           1         27           464.2033         464.2033	For           142.2         C23           954.3         C23           19834         C23           2581.2         C23           277.5         005.2           Cch         Table           2         Calc m/           1         464.3           2         465.3           8         466.3	mula H26 N7 04 H26 N7 04 H26 N7 04 H26 N7 04 H26 N7 04 Z0408	Counts vs (ppm) A 1.66	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (bund %           100	ge (m/z)		73.03	Calc Abund S	75.18 20.96

HPLC

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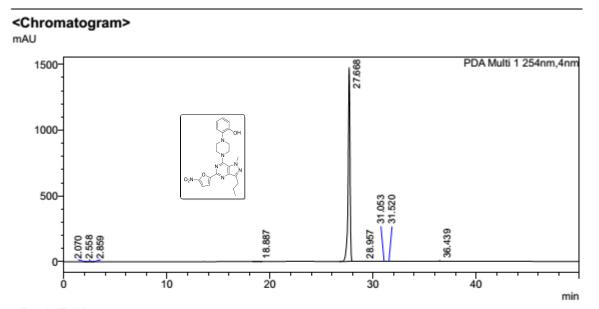


Compound (32) <sup>1</sup>H NMR in CDCl<sub>3</sub>



#### **Qualitative Compound Report** GLR-4-39 Sample Name GLR-4-39.d Vial 9 Position Data File Sample Sample Type User Name 11/19/2012 1:01:32 PM Instrument 1 Acquired Time Instrument Name vishal\_MS\_25072012.m as.m DA Method Acq Method Succes **IRM** Calibration Status Comment Info. Sample Group MFG Diff **DB** Formula Compound Table (ppm) MFG Formula C23 H25 N7 O4 Formula 0.87 C23 H25 N7 O4 Mass RT **Compound Label** C23 H25 N7 O4 463.1964 Cpd 4: C23 H25 N7 O4 0.171 Mass Algorithm RT Find by Molecular Feature 463.1964 m/z **Compound Label** 0.171 464.20368 Cpd 4: C23 H25 N7 O4 Cpd 4: C23 H25 N7 O4: + MFE Spectrum (0.130-0.572 min) GLR-4-39.d MFE MS Spectrum x10 5 04 464.20368 C23 H26 N7 O 4 3 2 1 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 Counts vs. Mass-to-Charge (m/z) 0 **MS Spectrum Peak List** Ion Formula z Abund m/z (M+H)+ 436361 C23 H26 N7 O4 464.20368 1 (M+H)+ 116429.5 C23 H26 N7 O4 465.20611 1 (M+H)+ 16902.8 C23 H26 N7 O4 466.20809 1 (M+H)+ 2940.3 C23 H26 N7 O4 467.21058 1 (M+Na)+ 3394.2 C23 H25 N7 Na O4 486.18616 1 (M+Na)+ 509.1 C23 H25 N7 Na O4 487.18794 1 Calc Abund Sum % Abund Sum % Predicted Isotope Match Table Calc Abund % 75.18 Diff (ppm) Abund % 76.2 Calc m/z 100 m/z 100 20.96 Isotope 20.33 0.85 464.20408 464.20368 27.88 3.44 26.68 1.68 2.95 465.20611 465.20689 4.57 0.42 3.87 2.89 0.51 466.20943 0.55 466.20809 3 0.67 2.83 467.2119 467.21058 4

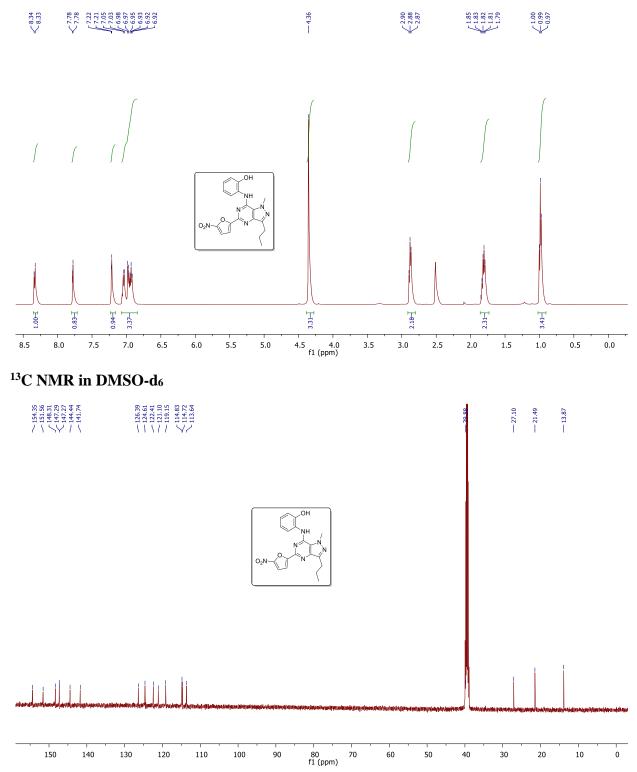




#### <Peak Table>

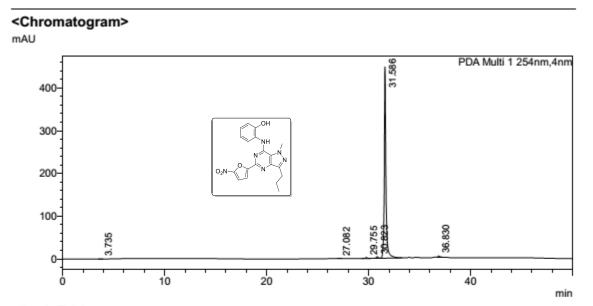
PDA C	h1 254nm					
Peak#	Name	Ret. Time	Area	Height	Area%	Height%
1		2.070	3052	423	0.016	0.028
2		2.558	58737	2872	0.308	0.193
3		2.859	3296	954	0.017	0.064
4		18.887	25108	1232	0.132	0.083
5		27.668	18875450	1473646	98.993	99.203
6		28.957	56933	1733	0.299	0.117
7		31.053	4307	275	0.023	0.019
8		31.520	201	37	0.001	0.002
9		36.439	40407	4320	0.212	0.291
Total			19067491	1485490	100.000	100.000

## Compound (33) <sup>1</sup>H NMR in DMSO-d<sub>6</sub>



						mpound Re		
Data File Sample Type Instrument Na Acq Method IRM Calibratic Comment		Sam Inst vish	t-4-33.d nple rument : al_12-01 cess		Sample Name Position User Name Acquired Time DA Method	Vial 2		
Sample Group				Info.				
Acquisition SV Version		00 series TO FOF B.05.01						
Compound 1	Fable	1	-				MFG Di	ff
Compoun	d Label	RT	M	ass	Formula	MFG Form	ula (ppm)	
Cpd 12: C	19 H18 N6 O	4 0.266		394.138 C	19 H18 N6 O4	C19 H18 N6	04	2.54 C19 H18 N6 O4
							1	
Compound L Cpd 12: C19 H		m/z 395.145		and the second se	orithm	Mass Feature 394.138		
		8 N6 O4: +	ESI MI	E Spectrum (0.	193-0.744 min)	Frag=135.0V GCR-4-3	33.d	
x10 4 Cpd 8 6 4 2 0	12: C19 H1 75 100	125 150		00 225 250		3350 375 400 425		
x10 4 Cpd 8 6 4 2 0 MS Spectru m/z	12: C19 H1 75 100 m Peak Li z Abund	125 150 st	175 2 rmula	00 225 250 Counts vs. Ma:	275 300 325 ss-to-Charge (m	3350 375 400 425		
x10 4 Cpd 8 6 4 2 0 MS Spectru m/z 395.1453	12: C19 H1 75 100 m Peak Li z Abund 1 88	125 150 st 1725.32 C19	175 2 mula 9 H19 N6	00 225 250 Counts vs. Ma:	275 300 325 ss-to-Charge (m Ion (M+H)+	3350 375 400 425		
8 6 4 2 0 <b>MS Spectru</b> <i>m/z</i> 395.1453 396.1479	12: C19 H1 75 100 m Peak Li 2 Abund 1 88 1 1 1	125 150 st 1725.32 C19 19502.1 C19	175 2 mula 9 H19 N6 9 H19 N6	00 225 250 Counts vs. Ma:	275 300 325 ss-to-Charge (m Ion (M+H)+ (M+H)+	3350 375 400 425		
x10 4 Cpd 8 6 4 2 0 MS Spectru <i>m/z</i> 395.1453 396.1479 397.1506	12: C19 H1 75 100 m Peak Li 2 Abund 1 88 1 1 2	125 150 st 1725.32 C19 9502.1 C19 1852.16 C19	175 2 mula 9 H19 N6 9 H19 N6 9 H19 N6	00 225 250 Counts vs. Ma:	275 300 325 ss-to-Charge (m (M+H)+ (M+H)+ (M+H)+	3350 375 400 425		
x10 4 Cpd 8 6 4 2 0 MS Spectru <i>m/z</i> 395.1453 396.1479 397.1506 398.143	75 100 m Peak Li z Abund 1 81 1 2 1 2	125 150 st 1725.32 [15] 9502.1 [15] 852.16 [15] 373.73 [15]	175 2 mula 9 H19 N6 9 H19 N6 9 H19 N6 9 H19 N6	00 225 250 Counts vs. Ma:	275 300 325 ss-to-Charge (m Ion (M+H)+ (M+H)+	3350 375 400 425		
x10 4 Cpd 8 6 4 2 0 MS Spectru <i>m/z</i> 395.1453 396.1479 397.1506 398.143 Predicted Is	75 100 m Peak Li z Abund 1 80 1 2 1 2 1 3 5000pe Ma	125 150 st 7725.32 (19 9502.1 (19 8852.16 (19 373.73 (19 tch Table	175 2 9 H19 NG 9 H19 NG 9 H19 NG 9 H19 NG 9 H19 NG 9 H19 NG	00 225 250 Counts vs. Ma: 04 04 04 04 04	275 300 325 s-to-Charge (m (M+H)+ (M+H)+ (M+H)+ (M+H)+	*0 9N 61H 61: 350 375 400 425	450 475	Calc Abund Sum %
x10 4 Cpd 8 6 4 2 0 MS Spectru <i>m/z</i> 395.1453 396.1479 397.1506 398.143	75 100 m Peak Li z Abund 1 81 1 2 1 2	125 150 st For 1725.32 C19 9502.1 C19 852.16 C19 373.73 C19 tch Table Calc m/	175 2 9 H19 NG 9 H19 NG 9 H19 NG 9 H19 NG 9 H19 NG 9 H19 NG	00 225 250 Counts vs. Ma:	275 300 325 ss-to-Charge (m (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+	3350 375 400 425	450 475	Calc Abund Sum %
x10 4 Cpd 8 6 4 2 0 MS Spectru <i>m/z</i> 395.1453 396.1479 397.1506 398.143 Predicted Is Isotope	12: C19 H1 75 100 m Peak Li 2 Abund 1 88 1 1 1 2 1 1 50tope Ma m/z	125 150 st For 1725.32 C19 9502.1 C19 852.16 C19 373.73 C19 tch Table Calc m/ 33 395	175 2 9 H19 N6 9 H19 N6 9 H19 N6 9 H19 N6 9 H19 N6 9 H19 N6 1 H19 H19 N6 1 H19 N6 1 H19 H19 H19 H19 H19 H19 H19 H19 H19 H1	00 225 250 Counts vs. Ma: 04 04 04 04 04 04 04 04 04 04 04 04	275 300 325 ss-to-Charge (m (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+	*0 9N 61H 61 350 375 400 425 //Z) Calc Abund %	450 475 Abund Sum % 79	
x10 4 Cpd 8 6 4 2 0 MS Spectru <i>m/z</i> 395.1453 396.1479 397.1506 398.143 Predicted IS Isotope 1	12: C19 H1 75 100 m Peak Li z Abund 1 88 1 1 1 2 1 sotope Ma m/z 395.14	125 150 st For 1725.32 C19 9502.1 C19 1852.16 C19 373.73 C19 Calc m/ 33 395 79 39	175 2 mula 9 H19 N6 9 H19 N6 9 H19 H19 H19 H19 H19 H19 H19 H19 H19 H	00 225 250 Counts vs. Ma: 004 004 004 004 004 004 004 004 004 00	275 300 325 ss-to-Charge (m (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+	*0 9N 61 565 565 565 565 565 565 565 5	450 475 Abund Sum % 79	.61 78.8

### HPLC

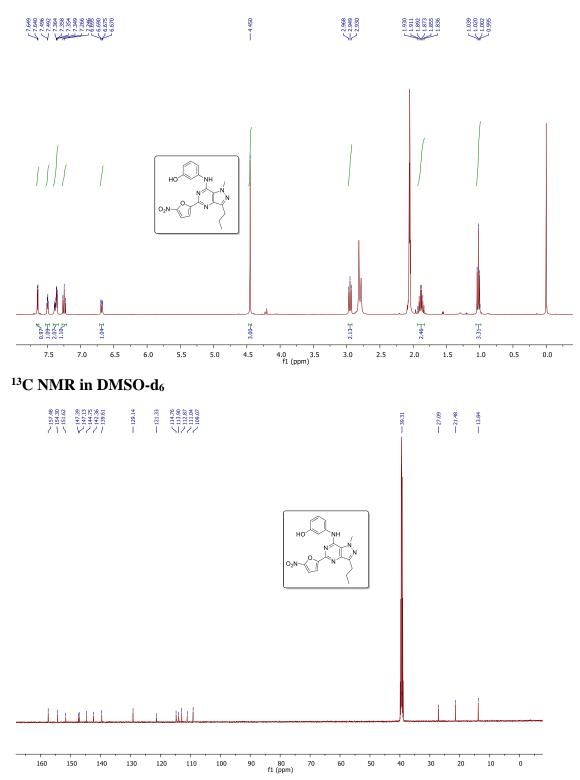


# <Peak Table>

PDA C	h1 254nm				
Peak#	Ret. Time	Area	Height	Area%	Height%
1	3.735	3233	275	0.061	0.060
2	27.082	2253	261	0.042	0.057
3	29.755	34028	2442	0.639	0.533
4	30.823	57222	4195	1.075	0.915
5	31.586	5165122	447714	97.060	97.667
6	36.830	59705	3521	1.122	0.768
Total		5321563	458408	100.000	100.000

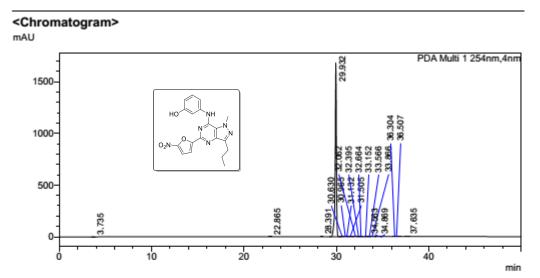
### Compound (34)

<sup>1</sup>H NMR in Acetone-d<sub>6</sub>



#### **Qualitative Compound Report** GLR-4-27.d Sample Name GLR-4-27 **Data File** Sample Type Sample Position 1 Instrument 1 **User Name** Instrument Name Acq Method 29\_may\_positive.m **Acquired Time** 6/4/2012 1:15:01 PM **DA Method IRM Calibration Status** as.m Comment Sample Group Info. **Compound Table** MFG Diff **MFG Formula DB** Formula **Compound Label** RT Mass Formula (ppm) C19 H18 N6 O4 C19 H18 N6 O4 C19 H18 N6 O4 394.13826 1.75 Cpd 34: C19 H18 N6 O4 0.32 **Compound Label** m/z RT Algorithm Mass Find by Molecular Feature 394.13826 Cpd 34: C19 H18 N6 O4 395.14553 0.32 MFE MS Spectrum x10 5 Cpd 34: C19 H18 N6 O4: + MFE Spectrum (0.236-0.720 min) GLR-4-27.d 395.14553 C19 H19 N6 O4 5 811.26614 C38 H36 N12 Na O8 4 3 2 1 0 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 Counts vs. Mass-to-Charge (m/z) **MS Spectrum Peak List** z Abund Formula Ion m/z 544598.1 C19 H19 N6 O4 (M+H)+ 395.14553 1 117609 C19 H19 N6 O4 396.14906 (M+H)+ 1 397.15002 18189 C19 H19 N6 O4 (M+H)+ 1 417.1278 28855.3 C19 H18 N6 Na O4 (M+Na)+ 1 34032.1 C19 H18 K N6 O4 (M+K)+ 433.10154 1 434.1044 1 8206 C19 H18 K N6 O4 (M+K)+ 26655.5 C38 H36 N12 Na O8 (2M+Na)+ 811.26614 1 812.26847 1 13316.7 C38 H36 N12 Na O8 (2M+Na)+ 25617.8 C38 H36 K N12 O8 (2M+K)+ 827.23687 1 11309 C38 H36 K N12 O8 (2M+K)+ 828.2422 1 Predicted Isotope Match Table Calc Abund Sum % Isotope Calc m/z Diff (ppm) Abund % Calc Abund % Abund Sum % m/z 395.14623 100 100 79.74 78.83 395.14553 1.76 17.22 23.11 18.22 2 396.14906 396,14902 -0.11 21.6 3 397.15002 397.15146 3.62 3.34 3.38 2.66 2.66 0.29 0.47 0.37 0.37 4 398.15323 398.15386 1.6





### <Peak Table>

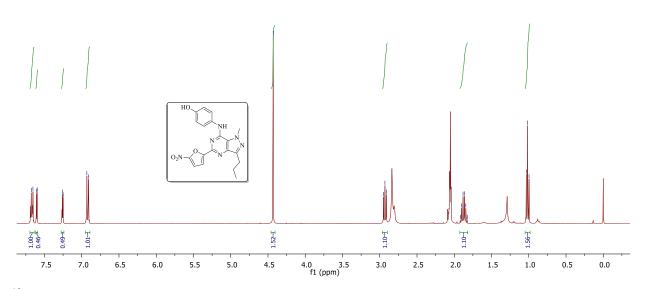
PDA C	h1 254nm				
Peak#	Ret. Time	Area	Height	Area%	Height%
1	3.735	3618	307	0.023	0.018
2	22.865	3566	302	0.023	0.018
3	28.391	4146	452	0.026	0.027
4	29.932	15639625	1681682	98.810	99.038
5	30.630	14365	1007	0.091	0.059
6	30.965	14933	1391	0.094	0.082
7	31.132	8188	849	0.052	0.050
8	31.505	14036	1015	0.089	0.060
9	32.062	31640	2973	0.200	0.175
10	32.395	1271	150	0.008	0.009
11	32.664	4994	513	0.032	0.030
12	33.152	1621	123	0.010	0.007
13	33.566	1240	170	0.008	0.010
14	33.866	30674	2208	0.194	0.130
15	34.563	24599	2097	0.155	0.124
16	34.869	2705	308	0.017	0.018
17	36.304	4339	530	0.027	0.031
18	36.507	17486	1566	0.110	0.092
19	37.635	4918	383	0.031	0.023
Total		15827965	1698025	100.000	100.000

### Compound (35)

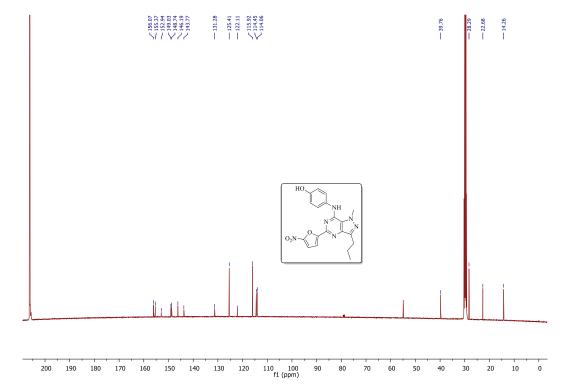
<sup>1</sup>H NMR in Acetone- d6



# -4.43 -4.



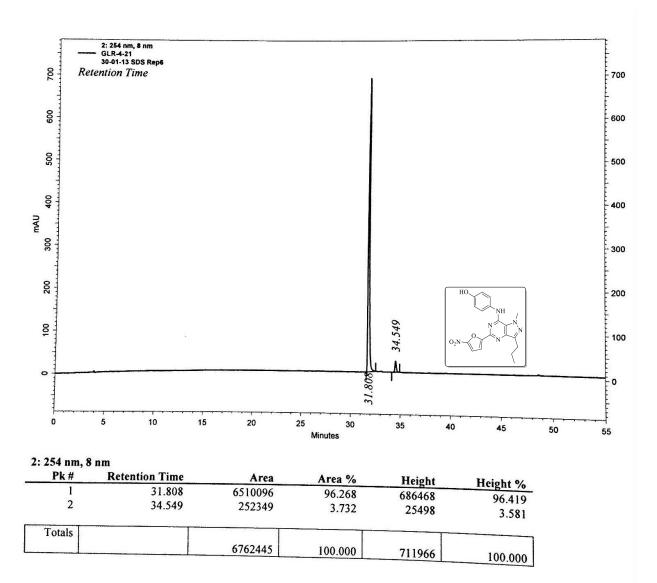
### <sup>13</sup>C NMR in Acetone –d6



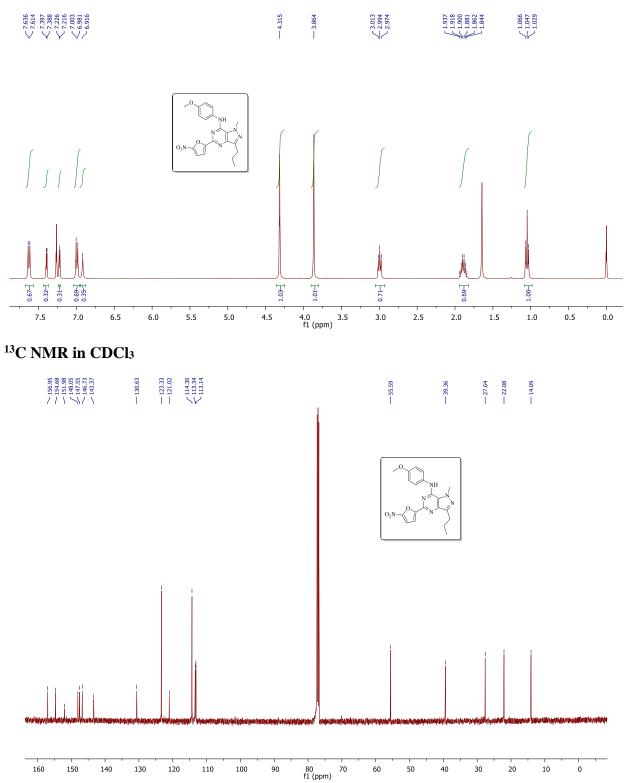
### **Qualitative Compound Report**

Sample Type	B	SDS- Samp	LR-59.d ble		Sample Position		SDS-LR-5 Vial 9	9			HONNH
Instrument I	Name	Instr	ument 1		User Na	me					
Acq Method		visha	l_12-01-13.	n	Acquire	d Time	09-07-20	13 PM 1:00:32			
IRM Calibrat	tion Status	Succ	ess	-	DA Meth	bon	daily_rep	ort.m		C	$D_2N \rightarrow N \rightarrow N$
Comment											
Sample Grou	up			Info						_	
Acquisition S			F/6500 serie	S							
Version	Q-T	OF B.05.01	(B5125)								
Compound	Table										
Compou	und Label	RT	Mass		Formula		MEG E	ormula	MFG D (ppm		DB Formula
	C19 H18 N6 O4		394.139	C1	9 H18 N6 O4		C19 H18 N6 O4			-0.07	C19 H18 N6 O4
Compound	Label	m/z	RT	Alg	orithm		Mass				
Cpd 9: C19 H		395.1463	0.196	and the second	by Molecular	Feature	394.139				
MFE MS Spect	rum										
	9: C19 H18 M	N6 04: +E	SI MFE Spe	ctrum	(0.139-0.506 )	min) Frag=	175.0V	SDS-LR-59.d		1	
			24								
3-			95.1463 H19 N6 O4								
2.5			395.1463 2 H19 N6								
2			m (m)								
1.5			Ö							1. 24	
1								65(			
0.5								811.2650		1.1.1	
								00		-	
0	150 200 25	0 300 3		50 50	0 550 600 Mass-to-Charg	650 700	750 8	00 850 900	950	-	
MS Spectru	ım Peak List		000	10 10.1		go (m/2)					
is specia	z Abund	Form	nula	2	Ion						
m/z			119 N6 O4		(M+H)+						
<i>m/z</i> 395.1463	1 30788	36.81 C19 H	115 110 01		((11+11)+						
		36.81 C19 H			(M+H)+						
395.1463	1 696		119 N6 O4	_		_					
395.1463 396.1487 397.1511 398.1521	1 696 1 105 1 12	51.94 C19 H 27.27 C19 H 16.98 C19 H	119 N6 O4 119 N6 O4 119 N6 O4		(M+H)+						
395.1463 396.1487 397.1511 398.1521 417.1277	1         696!           1         1052           1         122           1         392	51.94 C19 H 27.27 C19 H 16.98 C19 H 788.2 C19 H	119 N6 O4 119 N6 O4 119 N6 O4 119 N6 O4 118 N6 Na C		(M+H)+ (M+H)+ (M+H)+ (M+Na)+						
395.1463 396.1487 397.1511 398.1521 417.1277 418.1314	1         696           1         105           1         122           1         395           1         84	51.94 C19 H 27.27 C19 H 16.98 C19 H 788.2 C19 H 19.64 C19 H	119 N6 O4 119 N6 O4 119 N6 O4 118 N6 Na C 118 N6 Na C	4	(M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+						
395.1463 396.1487 397.1511 398.1521 417.1277 418.1314 419.1316	1         696!           1         105           1         12:           1         39:           1         84:           1         16	51.94 C19 F 27.27 C19 F 16.98 C19 F 788.2 C19 F 19.64 C19 F 543.5 C19 F	119 N6 O4 119 N6 O4 119 N6 O4 119 N6 O4 118 N6 Na C	4	(M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+						
395.1463 396.1487 397.1511 398.1521 417.1277 418.1314 419.1316 -811.265	1         696!           1         105?           1         12?           1         39?           1         84?           1         10           1         251?	51.94 C19 H 27.27 C19 H 16.98 C19 H 788.2 C19 H 19.64 C19 H 543.5 C19 H 12.88	119 N6 O4 119 N6 O4 119 N6 O4 118 N6 Na C 118 N6 Na C	4	(M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)	+					
395.1463 396.1487 397.1511 398.1521 417.1277 418.1314 419.1316 -811.265 812.2685	1         696!           1         1057           1         127           1         397           1         847           1         16           1         2517           1         1157	51.94 C19 H 27.27 C19 H 16.98 C19 H 788.2 C19 H 19.64 C19 H 543.5 C19 H 12.88 25.41	119 N6 O4 119 N6 O4 119 N6 O4 118 N6 Na C 118 N6 Na C	4	(M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)- (2M+Na)-	+ +					
395.1463 396.1487 397.1511 398.1521 417.1277 418.1314 '419.1316 	1         6963           1         1055           1         122           1         397           1         842           1         16           1         2511           1         1551           1         311	51.94 C19 H 27.27 C19 H 16.98 C19 H 788.2 C19 H 19.64 C19 H 543.5 C19 H 12.88 25.41 34.63	119 N6 O4 119 N6 O4 119 N6 O4 118 N6 Na C 118 N6 Na C	4	(M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)	+ +					
395.1463 396.1487 397.1511 398.1521 417.1277 418.1314 419.1316 -811.265 812.2685 813.2712 Predicted I	1         696!           1         1057           1         127           1         397           1         847           1         16           1         2517           1         1157	51.94 C19 H 27.27 C19 H 16.98 C19 H 788.2 C19 H 19.64 C19 H 543.5 C19 H 12.88 25.41 34.63	119 N6 O4 119 N6 O4 119 N6 O4 118 N6 Na C 118 N6 Na C 118 N6 Na C	4	(M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)- (2M+Na)-	+ +	nd %	Abund Sum %	0	Calc Ab	ound Sum %
395.1463 396.1487 397.1511 398.1521 417.1277 418.1314 419.1316 -811.265 812.2685 813.2712 Predicted I	1 696: 1 1057 1 122: 1 399: 1 84: 1 14: 1 15: 1 31: sotope Matc m/z	51.94 C19 F 27.27 C19 F 16.98 C19 F 788.2 C19 F 19.64 C19 F 543.5 C19 F 12.88 25.41 34.63 <b>C19 F</b> 12.88 <b>C19 F</b> 12.88 <b>C19 F</b> <b>C10 F</b>	119 N6 04 119 N6 04 119 N6 04 118 N6 Na 0 118 N6 Na 0 118 N6 Na 0 118 N6 Na 0	4	(M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)- (2M+Na)- (2M+Na)-	+ + + + +	<b>nd %</b> 100		o 79.09	Calc Ab	ound Sum % 78.83
395.1463 396.1487 397.1511 398.1521 417.1277 418.1314 419.1316 811.265 812.2685 813.2712 Predicted In Isotope	1         6963           1         1057           1         122           1         397           1         844           1         16           1         2512           1         1155           1         312           sotope Matc         m/z           395.1463         395.1463	51.94 C19 F 27.27 C19 F 16.98 C19 F 788.2 C19 F 19.64 C19 F 543.5 C19 F 12.88 25.41 34.63 34.63 Ch Table Calc m/z 395.1	119 N6 04 119 N6 04 119 N6 04 118 N6 Na 0 118 N6 Na 0	4 4 pm)	(M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)- (2M+Na)- (2M+Na)- (2M+Na)-	+ + + + +				Calc Ab	78.83 18.22
396.1487 397.1511 398.1521 417.1277 418.1314 419.1316 811.265 812.2685 813.2712 Predicted I Isotope	1         6963           1         1057           1         122           1         397           1         844           1         164           1         157           1         1157           1         313           sotope Matter         M/z           395.1463         396.1487	51.94         C19 H           27.27         C19 H           16.98         C19 H           788.2         C19 H           19.64         C19 H           543.5         C19 H           12.88         25.41           34.63	119 N6 04 119 N6 04 119 N6 04 119 N6 04 118 N6 Na 0 118 N6 Na 0	4 4 pm) -0.29	(M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)- (2M)- (2M+Na)- (2M)	+ + + + +	100		79.09	Calc Ab	78.83





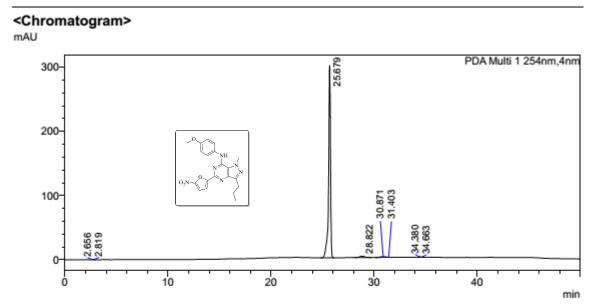
Compound (36) <sup>1</sup>H NMR in CDCl<sub>3</sub>



### **Qualitative Compound Report**

Data File Sample Type Instrument Na Acq Method IRM Calibratic Comment Sample Group	on Si		Samp Instru visha Succe	ument 1 I_MS_250720	12.m	Sample N Position User Nam Acquired DA Metho	Vial 4 ne Time 11/19/20	12 12:36:43 PM			
Compound T	abl	e							M	G Diff	
Compoun	dLa	hel	RT	Mass		Formula	M	FG Formula		ppm)	DB Formula
Cpd 6: C2			0.172	408.15402	2	C20 H20 N6 0		0 H20 N6 O4		1.43	C20 H20 N6 O4
		-	_								
Compound L	abe	1	m/z	RT	Algori	ithm	Mass				
Cpd 6: C20 H2			409.1613	and the second sec			Feature 408.154	02			
4 - 3 - 2 - 1 - 0 -	150	200 2	50 300	409.16130 C20 H21 N6 04	1.	00 550 6	00 650 700 7	00- 00- 00- 01- 01- 01- 01- 01- 01- 01-	900	950	
			50 500	Co	unts vs.	Mass-to-Cl	harge (m/z)	00 000 000	000		
MS Spectrun		Abund	Form	ula		Ion	_				
	1			121 N6 O4		(M+H)+	_				
	1			121 N6 04		(M+H)+					
410.16397	-			121 N6 O4	1.1	(M+H)+					
	1	260	80.6 C20 H	120 N6 Na O4		(M+Na)+					
410.16397 411.16613	1	209									
410.16397 411.16613 431.14238	-		96.8 C20 I	120 N6 Na O4		(M+Na)+					
410.16397 411.16613 431.14238 432.14612	1	65		120 N6 Na O4 120 K N6 O4		(M+Na)+ (M+K)+	_				
410.16397 411.16613 431.14238 432.14612 447.11766 839.29676	1	65 157 33	01.7 C20 H 3978 C40 H	120 K N6 O4 140 N12 Na C	8	(M+K)+ (2M+Na)+					
410.16397 411.16613 431.14238 432.14612 447.11766 839.29676 840.29929	1 1 1 1	65 157 33 157	01.7 C20 H 3978 C40 H 86.4 C40 H	120 K N6 O4 140 N12 Na C 140 N12 Na C	)8 )8	(M+K)+ (2M+Na)+ (2M+Na)+					
410.16397 411.16613 431.14238 432.14612 447.11766 839.29676 840.29929 855.27026	1 1 1 1 1 1	65 157 33 157 167	01.7 C20 H 3978 C40 H 86.4 C40 H 01.6 C40 H	120 K N6 O4 140 N12 Na C 140 N12 Na C 140 K N12 O8	)8 )8	(M+K)+ (2M+Na)+ (2M+Na)+ (2M+K)+					
410.16397 411.16613 431.14238 432.14612 447.11766 839.29676 840.29929 855.27026 856.27436	1 1 1 1 1 1 1 1	65 157 3: 157 167 66	01.7 C20 H 3978 C40 H 86.4 C40 H 01.6 C40 H 08.2 C40 H	120 K N6 O4 140 N12 Na C 140 N12 Na C	)8 )8	(M+K)+ (2M+Na)+ (2M+Na)+					
410.16397 411.16613 431.14238 432.14612 447.11766 839.29676 840.29929 855.27026 856.27436 <b>Predicted Is</b>	1 1 1 1 1 1 1 1 0 top	65 157 3: 157 167 66 <b>De Matc</b>	01.7 C20 F 3978 C40 F 86.4 C40 F 01.6 C40 F 08.2 C40 F h Table	120 K N6 O4 140 N12 Na C 140 N12 Na C 140 K N12 O8 140 K N12 O8	18	(M+K)+ (2M+Na)+ (2M+Na)+ (2M+K)+ (2M+K)+		Abund Sum %		Calc Abund	Sum %
410.16397 411.16613 431.14238 432.14612 447.11766 839.29676 840.29929 855.27026 856.27436 Predicted Ise Isotope	1 1 1 1 1 1 1 0 top	65 157 33 157 167 66 <b>De Matc</b>	01.7 C20 H 3978 C40 H 86.4 C40 H 01.6 C40 H 08.2 C40 H h Table Calc m/z	120 K N6 O4 140 N12 Na C 140 N12 Na C 140 K N12 O8 140 K N12 O8 140 K N12 O8	98 98 98 98 98 98 98 98 98 98 98 98 98 9	(M+K)+ (2M+Na)+ (2M+Na)+ (2M+K)+ (2M+K)+ (2M+K)+	Calc Abund %	Abund Sum %	79.45	Calc Abund	
410.16397 411.16613 431.14238 432.14612 447.11766 839.29676 840.29929 855.27026 855.27036 856.27436 Predicted Iss Isotope 1 1	1 1 1 1 1 1 1 1 0 top	65 157 3: 157 167 66 <b>De Matc</b> 409.1613	01.7 C20 H 8978 C40 H 86.4 C40 H 01.6 C40 H 08.2 C40 H <b>h Table</b> Calc m/z 409.16	120 K N6 O4 140 N12 Na O 140 N12 Na O 140 K N12 O8 140 K N12 O8 140 K N12 O8 Diff (pp 188	08 08 08 08 08 00 00 00 00 00 00 00 00 0	(M+K)+ (2M+Na)+ (2M+Na)+ (2M+K)+ (2M+K)+ (2M+K)+ bund % 100			79.45	Calc Abund	Sum % 77.97 18.88
410.16397 411.16613 431.14238 432.14612 447.11766 839.29676 840.29929 855.27026 856.27436 Predicted Ise Isotope	1 1 1 1 1 1 1 1 0 top m/z 4	65 157 33 157 167 66 <b>De Matc</b>	01.7 C20 H 3978 C40 H 86.4 C40 H 01.6 C40 H 08.2 C40 H h Table Calc m/z	120 K NG O4 140 N12 Na O 140 N12 Na O 140 K N12 O8 140 K N12 O8 140 K N12 O8 0	98 98 98 98 98 98 98 98 98 98 98 98 98 9	(M+K)+ (2M+Na)+ (2M+Na)+ (2M+K)+ (2M+K)+ (2M+K)+	Calc Abund %		79.45 17.65 2.48	Calc Abund	77.97

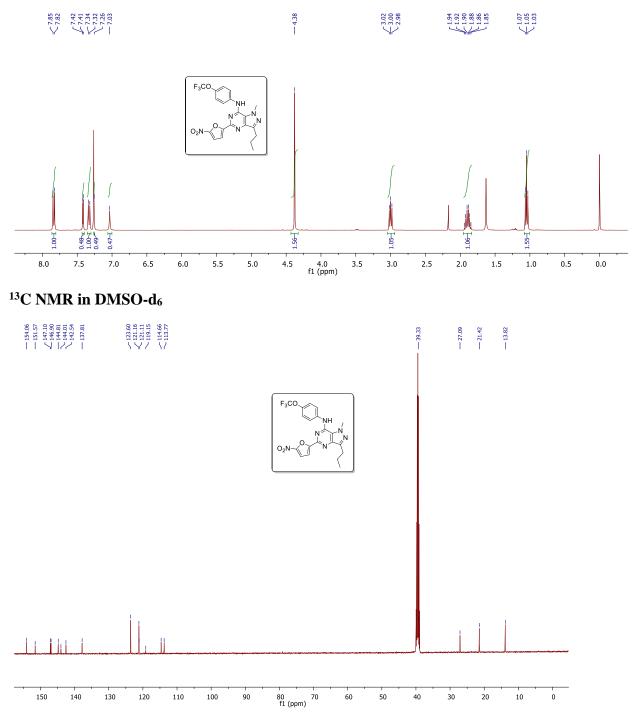
HPL	C
	$\mathbf{v}$



#### <Peak Table>

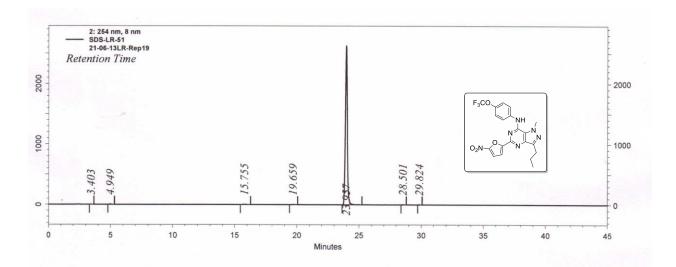
PDA C	h1 254nm					
Peak#	Name	Ret. Time	Area	Height	Area%	Height%
1		2.656	1244	193	0.031	0.063
2		2.819	3413	469	0.085	0.154
3		25.679	3867286	299855	96.247	98.190
4		28.822	81184	2126	2.020	0.696
5		30.871	47681	1146	1.187	0.375
6		31.403	3952	397	0.098	0.130
7		34.380	8786	785	0.219	0.257
8		34.663	4528	410	0.113	0.134
Total			4018072	305382	100.000	100.000

### Compound (37) <sup>1</sup>H NMR in CDCl<sub>3</sub>



### **Qualitative Compound Report**

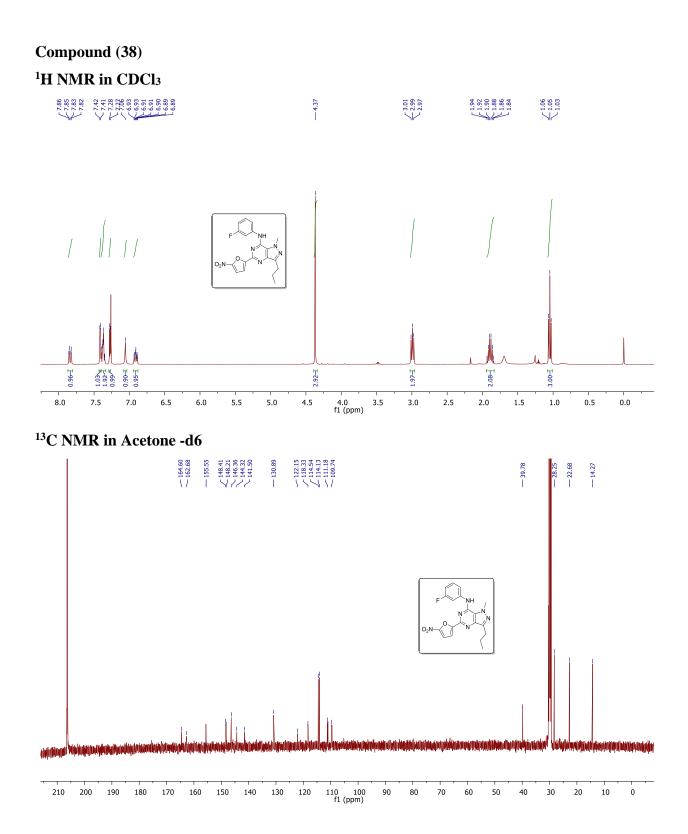
Sample Typ Instrument Acq Method IRM Calibra Comment	Name I Intion Status	GLR-6. Sample Instrur vishal_ Succes	e nent 1 MS_25072012.	Positio User N	ame ed Time 11/18/2	2012 1:15:54 PM		
Sample Gro		D.						
Compo	und Label	RT	Mass				MFG Diff	
	0 H17 F3 N6 O4		462.12592	C20 H17 F3		MFG Formula 20 H17 F3 N6 O4	(ppm) 0.91	DB Formula C20 H17 F3 N6 O4
Compound	l <b>Label</b> H17 F3 N6 O4	<i>m/z</i>		Igorithm	Mass			22
Cpu 4: C20 i	n17 F3 No 04	463.1332	0.172 Fi	nd by Molecula	r Feature 462.12	592		
MFE MS Spect	trum							
3			4	10			N11	
2-1-0	150 200 2	50 300 3	50 400 450	C20 H18 F3 N6 04 C20 H18 F3 N6 04 C20 H18 F3 N6 04	600 650 700 Charge (m/z)	750 800 850 900	6 C40 H34 F6 N12 Na O8	
2 1 0 MS Spectru	m Peak List		50 400 450 Counts	0 500 550 s vs. Mass-to-(	600 650 700 Charge (m/z)			
2 1 0 MS Spectru <i>m/z</i>	m Peak List	Formul	50 400 45 Count	0 500 550 s vs. Mass-to- <b>Ion</b>	600 650 700 Charge (m/z)			
2 - 1 - 0 - <b>MS Spectru</b> <i>m/z</i> 463.1332	<b>z Abund</b>	Formul 08.3 C20 H18	50 400 450 Counts <b>Ia</b> 3 F3 N6 O4	0 500 550 s vs. Mass-to-( <b>Ion</b> (M+H)+	600 650 700 Charge (m/z)			
2 - 1 - 0 - MS Spectru <i>m/z</i> 463.1332 464.13579	z         Abund           1         5688           1         1318	Formul 08.3 C20 H18 93.8 C20 H18	50 400 456 Counts 3 F3 N6 04 3 F3 N6 04	0 500 550 s vs. Mass-to-( (M+H)+ (M+H)+	600 650 700 Charge (m/z)			
2 - 1 - 0 - MS Spectru <i>m/z</i> 463.1332 464.13579 465.13886	z         Abund           1         5688           1         1318           1         201	Formul 08.3 C20 H18 93.8 C20 H18 75.6 C20 H18	50 400 45 Counts 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04	0 500 550 s vs. Mass-to-( (M+H)+ (M+H)+ (M+H)+	600 650 700 Charge (m/z)			
2 - 1 - 0 - MS Spectru <i>m/z</i> 463.1332 464.13579	z         Abund           1         5688           1         1318           1         201           1         293	Formul 08.3 C20 H18 93.8 C20 H18 75.6 C20 H18 32.9 C20 H18	50 400 45 Count 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04	0 500 550 s vs. Mass-to-( (M+H)+ (M+H)+ (M+H)+ (M+H)+	600 650 700 Charge (m/z)			
2 - 1 - 0 - MS Spectru <i>m/z</i> 463.1332 464.13579 465.13886 466.1372	z         Abund           1         5688           1         1318           1         201           1         291           1         601	Formul 08.3 C20 H18 93.8 C20 H18 75.6 C20 H18 32.9 C20 H18 53.9 C20 H17	50 400 45 Count 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04	0 500 550 s vs. Mass-to- (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+K)+	600 650 700 Charge (m/z)			
2 - 1 - 0 - <b>MS Spectru</b> <i>m/z</i> 463.1332 464.13579 465.13886 466.1372 501.08746	z         Abund           1         5688           1         1318           1         201           1         201           1         60           1         130	Formul 08.3 C20 H18 93.8 C20 H18 75.6 C20 H18 32.9 C20 H18 53.9 C20 H17 64.8 C20 H17	50 400 45 Counts 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 7 F3 K N6 04	0 500 550 s vs. Mass-to-( (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+K)+ (M+K)+	Charge (m/z)			
2 - 1 - 0 - MS Spectrum m/z 463.1332 465.13886 466.1372 501.08746 502.09058	z         Abund           1         5688           1         1318           1         201           1         291           1         600           1         130           1         1420	Formul 08.3 C20 H18 93.8 C20 H18 75.6 C20 H18 32.9 C20 H18 53.9 C20 H17 54.8 C20 H17 32.7 C40 H34	50         400         450           Counts         Counts           8         F3 N6 O4           8         F3 N6 O4           8         F3 N6 O4           8         F3 N6 O4           7         F3 K N6 O4           7         F3 K N6 O4           7         F3 K N6 O4	0 500 550 s vs. Mass-to-( (M+H)+ (M+H)+ (M+H)+ (M+K)+ (M+K)+ (M+K)+ 3 (2M+Na)	Charge (m/z)			
2 - 1 - 0 - <b>MS Spectru</b> <i>4</i> 63.1332 464.13579 465.13886 466.1372 501.08746 502.09058 947.23844	z         Abund           1         5688           1         1318           1         201           1         291           1         600           1         134           1         142           1         655	Formul           08.3         C20 H18           93.8         C20 H18           75.6         C20 H18           32.9         C20 H17           53.9         C20 H17           54.8         C20 H34           32.7         C40 H34           14.4         C40 H34	50 400 450 Count: 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 7 F3 K N6 04 7 F3 K N6 04 4 F6 N12 Na 08	0 500 550 s vs. Mass-to-( (M+H)+ (M+H)+ (M+H)+ (M+K)+ (M+K)+ (M+K)+ (M+K)+ 3 (2M+Na) 3 (2M+Na)	Charge (m/z)			
2 - 1 - 0 - <b>MS Spectru</b> <i>m/z</i> 463.1332 465.13886 466.1372 501.08746 502.09058 947.23844 948.24204 949.24633 963.21522	z         Abund           1         5688           1         1318           1         201           1         201           1         600           1         1348           1         1422           1         653           1         199           1         155           1         155	Formul           08.3         C20 H18           93.8         C20 H18           32.9         C20 H18           53.9         C20 H17           54.8         C20 H134           14.4         C40 H34           90.3         C40 H34           11.5         C40 H34	50 400 450 Count: 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 7 F3 K N6 04 7 F3 K N6 04 4 F6 N12 Na 08	0 500 550 s vs. Mass-to-( (M+H)+ (M+H)+ (M+H)+ (M+K)+ (M+K)+ (M+K)+ (M+K)+ 3 (2M+Na) 3 (2M+Na)	Charge (m/z)			
2 - 1 - 0 - <b>MS Spectru</b> <i>m/z</i> 463.1332 464.13579 465.13886 466.1372 501.08746 502.09058 947.23844 948.24204 948.24204 949.24633 963.21522 <b>Predicted Is</b>	z         Abund           1         5688           1         1318           1         201           1         299           1         600           1         1338           1         1422           1         653           1         1422           1         653           1         199           1         153           sotope Match         Match	Formul           08.3         C20 H18           93.8         C20 H18           32.9         C20 H18           32.9         C20 H18           33.9         C20 H17           54.8         C20 H17           32.7         C40 H34           14.4         C40 H34           00.3         C40 H34           11.5         C40 H34	50 400 45 Counts B F3 N6 04 B F3 N6 04 B F3 N6 04 B F3 N6 04 F5 K N6 04 F6 N12 Na 08 F6 N12 Na 08 F6 N12 Na 08 F6 K N12 Na 08	0 500 550 s vs. Mass-to-( (M+H)+ (M+H)+ (M+H)+ (M+K)+ (M+K)+ (M+K)+ (M+K)+ 3 (2M+Na) 3 (2M+Na)	Charge (m/z)			
2 - 1 - 0 - <b>MS Spectru</b> <i>m/z</i> 463.1332 465.13886 466.1372 501.08746 502.09058 947.23844 948.24204 949.24633 963.21522	z         Abund           1         5688           1         1318           1         201           1         202           1         600           1         133           1         1422           1         655           1         199           1         155           sootope Match         m/z	Formul           08.3         C20 H18           93.8         C20 H18           93.8         C20 H18           32.9         C20 H18           32.9         C20 H17           32.7         C40 H34           14.4         C40 H34           90.3         C40 H34           11.5         C40 H34	50 400 45 Count: 8 F3 N6 04 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 7 F3 K N6 04 7 F3 K N6 04 4 F6 N12 Na 08 4 F6 N12 Na 08 4 F6 N12 Na 08 5 F6 K N12 08 0 Ff (ppm)	0 500 550 vs. Mass-to-( (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+K)+ (M+K)+ (M+K)+ 3 (2M+Na) 3 (2M+Na) 4 (2M+Na) 4 (2M+Na) 5 (2M+Na) 6 (2M+Na)	Charge (m/z)			um %
2 - 1 - 0 - <b>MS Spectru</b> <i>m/z</i> 463.1332 464.13579 465.13886 466.1372 501.08746 502.09058 947.23844 948.24204 949.24633 963.21522 <b>Predicted Is</b> <b>Isotope</b> 1	z         Abund           1         5688           1         1318           1         201           1         291           1         600           1         1330           1         1422           1         655           1         199           1         155           sotope Match         m/z           463.1332         463.1332	Formul           08.3         C20 H18           93.8         C20 H18           75.6         C20 H18           53.9         C20 H17           54.8         C20 H17           54.8         C20 H17           54.8         C20 H17           54.8         C40 H34           14.4         C40 H34           90.3         C40 H34           11.5         C40 H34           11.5         C40 H34           12.5         C40 H34           13.5         C40 H34           14.4         C40 H34	50 400 45 Count: 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 7 F3 K N6 04 4 F6 N12 Na 08 4 F6 N12 Na 08 4 F6 N12 Na 08 4 F6 N12 Na 08 4 F6 N12 Na 08 1 F6 K N12 08	0 500 550 s vs. Mass-to-( (M+H)+ (M+H)+ (M+H)+ (M+K)+ (M+K)+ 3 (2M+Na) 3 (2M+Na) 4 (2M+Na) 4 (2M+Na) 5 (2M+Na) 6 (2M+Na) 7 (2M+K)+ 6 (2M+Na) 7 (2M+K)+ 7 (2M+K)+	Charge (m/z)	750 800 850 900	950 Calc Abund St	<b>um %</b> 77.99
2 - 1 - 0 - <b>MS Spectru</b> <i>m/z</i> 463.1332 464.13579 465.13886 466.1372 501.08746 502.09058 947.23844 948.24204 948.24204 949.24633 963.21522 <b>Predicted Is</b>	z         Abund           1         5688           1         1318           1         201           1         201           1         201           1         1318           1         1422           1         1422           1         1422           1         155           sootope Match         Match           m/z         463.1332           464.13579         464.13579	Formul           08.3         C20 H18           93.8         C20 H18           93.8         C20 H18           32.9         C20 H18           32.9         C20 H17           32.7         C40 H34           14.4         C40 H34           90.3         C40 H34           11.5         C40 H34	50 400 450 Count: 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 3 F3 N6 04 7 F3 K N6 04 4 F6 N12 Na 08 4 F6 N12 Na 08 4 F6 N12 Na 08 4 F6 K12 Na 08 5 F6 K12 Na 0	0 500 550 s vs. Mass-to-( (M+H)+ (M+H)+ (M+H)+ (M+K)+ (M+K)+ (M+K)+ 3 (2M+Na) 3 (2M+Na) 3 (2M+Na) 3 (2M+Na) 4 (2M+Na) 3 (2M+Na) 5 (2M+Na) 6 23.19	Charge (m/z)	Abund Sum %           3         18.22	950 Calc Abund Si	



Pk #	<b>Retention Time</b>	Area	Area %	Height	Height %
1	3.403	10275	0.035	1422	0.054
2	4.949	43431	0.148	4175	0.158
3	15.755	41166	0.140	1944	0.074
4	19.659	44427	0.151	2542	0.096
5	23.957	29155654	99.387	2628026	99.422
6	28.501	28367	0.097	3582	0.136
7	29.824	12104	0.041	1610	0.061
Totals					
		29335424	100.000	2643301	100.000

4

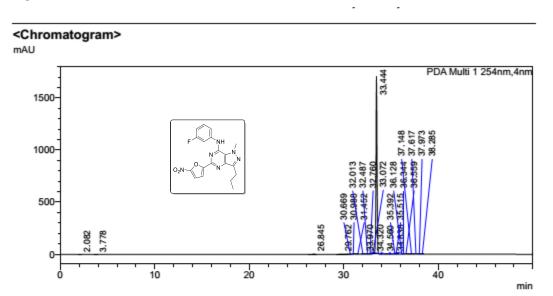
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## Qualitative Compound Report

Statistica - Statistica												
ata File		GI	LR-4-22.d		Sample N	ame GLR-	4-22					
ample Type		Sa	ample		Position	23					F	NH ,
nstrument Na	ame		strument	1	User Name Acquired Time	ie					Ņ	NN N
cq Method				oositive.m		Time 6/4/2	2012 2	:56:52 PM			02N-0-1	
RM Calibratio	n Status		Tons Mis	contraction in the	DA Metho	d as.m				32.2		2
Comment	Jil Status			and the second second								
omment												
Sample Group	Info											
Compound T	able								MF	G Diff		
Compoun	I abol	RT	N	lass	Formula		MF	G Formula	(	opm)		ormula
	H17 F N6 O3			6.13447	C19 H17 F N6	03	C19	H17 F N6 O3		0.38	C19 H17	F N6 03
Compound L	abel	m/z		RT	Algorithm		Mass					
Cpd 91: C19 H		397.1	4174	0.331	Find by Molec	ular Feature	396.1	.3447				
3.5 - 3 - 2.5 -					m (0.213-0.70	04 min) GLR∙	-4-22.					
3 - 2.5 - 1.5 - 1 - 0.5 -			•	397.14174 C19 H18 F N6 O3				793.27598 C38 H35 F2 N12 O6	900 \$	250		
3 2.5 1.5 1- 0.5 0		250 3	•	397.14174 009 019 H18 F N6 03	500 550 6 vs. Mass-to-C	00 650 70		793.27598 C38 H35 F2 N12 O6	900 \$	50		
3 2.5 2 1.5 1 0.5 0 MS Spectru		250 3	•	397.14174 009 019 H18 F N6 03	500 550 6	00 650 70		793.27598 C38 H35 F2 N12 O6	900 \$	950		
3 2.5 2 1.5 1 0.5 0 <b>MS Spectrum</b> <i>m/z</i>	m Peak List	250 3	00 350 Formula	397.14174 Conte 2007 00 700 03 700 03 70000000000	500 550 6 vs. Mass-to-C	00 650 70		793.27598 C38 H35 F2 N12 O6	900 \$	950		
3 2.5 2 1.5 1 0.5 0 <b>MS Spectrum</b> <i>m/z</i> 397.14174	m Peak List z Abund 1 363	250 3	00 350	200 400 450 200 450 200 200 450 200 200 450 200 200 200 200 200 200 200 200 200 2	500 550 6 vs. Mass-to-C Ion	00 650 70		793.27598 C38 H35 F2 N12 O6	900 \$	950		
3 2.5 2 1.5 1 0.5 0 <b>MS Spectrum</b> <i>m/z</i> 397.14174 398.1453	m Peak List z Abund 1 363 1 79	250 3	00 350 Formula C19 H18 F C19 H18 F	200 400 450 200 400 450 200 400 450 200 400 450 200 800 200 800 200 200 800 200 200 800 200 200 200 200 200 200 200 200 200	500 550 6 vs. Mass-to-C Ion (M+H)+	00 650 70		793.27598 C38 H35 F2 N12 O6	900 \$			
3 2.5 2 1.5 1 0.5 0 <b>MS Spectrum</b> <i>m/z</i> 399.14174 399.14803	z         Abund           1         363           1         79           1         1	250 3	00 350 Formula C19 H18 F C19 H18 F C19 H18 F C19 H18 F	397.14174 397.14174 397.14174 397.14174 397.00 397.14174 397.00 307.04 3	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+	00 650 70 harge (m/z)		793.27598 C38 H35 F2 N12 O6	900 \$	550		
3 2.5 2 1.5 1 0.5 0 MS Spectrum <i>m/z</i> 397.14174 398.1453 399.14803 793.27598	z         Abund           1         363           1         79           1         1           1         2	250 3 797.2 0 824.5 0 11748 0 116.4 0	Formula C19 H18 F C19 H18 F C19 H18 F C19 H18 F C19 H18 F C19 H18 F C19 H18 F	232.11114 232.111114 232.111114 232.111114 232.111111114 232.1111111111111111111111111	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (2M+H)+	00 650 70 harge (m/z)		793.27598 C38 H35 F2 N12 O6	900 \$	250		
3 2.5 2 1.5 1 0.5 0 MS Spectrum <i>m/z</i> 397.14174 398.1453 399.14803 793.27598 794.27897	z         Abund           1         363           1         79           1         1           1         2           1         1           1         1	250 3 797.2 0 824.5 0 11748 0 116.4 0 080.9 0	Formula C19 H18 F C19 H18 F C19 H18 F C19 H18 F C19 H18 F C19 H18 F C38 H35 F C38 H35 F	232.11114 232.111114 232.111114 232.111114 232.111111114 232.1111111111111111111111111	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (2M+H)+ (2M+H)+	500 650 70 Charge (m/z)		793.27598 C38 H35 F2 N12 O6	900 \$	950		
3 - 2.5 - 2 - 1.5 - 1 - 0.5 - 0 - <b>MS Spectrum</b> <i>m/z</i> 399.1474 399.14803 793.27598 794.27897 795.28384	Peak List           z         Abund           1         363           1         79           1         2           1         2           1         1           1         2           1         1           1         2           1         1	250 3 797.2 ( 11748 ( 116.4 ( 080.9 ( 800.5 (	Formula C19 H18 F C19 H18 F C19 H18 F C19 H18 F C19 H18 F C38 H35 F C38 H35 F C38 H35 F	232.11114 232.111114 232.111114 232.111114 232.111111114 232.1111111111111111111111111	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (2M+H)+	500 650 70 Charge (m/z)		793.27598 C38 H35 F2 N12 O6	900 \$	950		
3 - 2.5 - 2 - 1.5 - 1 - 0.5 - 0	z         Abund           1         363           1         79           1         1           1         2           1         1           1         2           1         1           1         2           1         1           1         2           1         1           1         1	250 3 797.2 ( 824.5 ( 116.4 ( 080.9 ( 800.5 ( <b>ch Tat</b>	Formula C19 H18 F C19 H18 F C19 H18 F C19 H18 F C19 H18 F C38 H35 F C38 H35 F C38 H35 F C38 H35 F	200 450 200 450 2010 450 2010 2010 450 2010 2010 2010 2010 2010 20	500 550 6 vs. Mass-to-C <b>Ion</b> (M+H)+ (M+H)+ (M+H)+ (2M+H)+ (2M+H)+ (2M+H)+	500 650 70 harge (m/z)	00 75	00- 03.27598 00- 038 H35 F2 N12 O6 058 05- 058 05- 058 05- 058 05- 058 05- 058 05- 058 05- 05- 05- 05- 05- 05- 05- 05- 05- 05-	900 \$		nd Sum %	
3 - 2.5 - 2 - 1.5 - 1 - 0.5 - 0	z         Abund           1         363           1         79           1         1           1         2           1         1           1         2           1         1           1         2           1         1           1         2           1         1           1         2           1         1           1         2           1         1	110.4 ( 080.9 ( 800.5 ( 080.5 ( 080.5 ( 0800.5 (	Formula Formula C19 H18 F C19 H18 F C18 H35 F C18	2 NE 03 2 NE 03 2 NE 03 2 NE 03 2 NE 06 2 NI2 06	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+	650 70 harge (m/z)	00 75	793.27598 C38 H35 F2 N12 O6			nd Sum %	79.22
3 - 2.5 - 2 - 1.5 - 1 - 0.5 - 0	z         Abund           1         363           1         79           1         1           1         2           1         1           1         2           1         1           1         2           1         1           1         2           1         397.14174	<b>1</b> 797.2 ( 824.5 ( 1116.4 ( 080.9 ( 800.5 ( <b>ch Tat</b> <b>Calc</b> <b>4</b> 35	Formula C19 H18 F C19 H18 F C19 H18 F C19 H18 F C19 H18 F C19 H18 F C18 H35 F C38 H35 F C38 H35 F C38 H35 F DIE m/z 97.14189	<ul> <li>10 400 450</li> <li>10 400 450</li></ul>	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+	00 650 70 harge (m/z)	00 75 % 100	00- 03.27598 00- 038 H35 F2 N12 O6 058 05- 058 05- 058 05- 058 05- 058 05- 058 05- 058 05- 05- 05- 05- 05- 05- 05- 05- 05- 05-	79.89		nd Sum %	79.22
3 - 2.5 - 2 - 1.5 - 1 - 0.5 - 0	z         Abund           1         363           1         79           1         1           1         2           1         1           1         2           1         1           1         2           1         1           1         397.14174           398.1452         398.1452	1797.2 ( 824.5 ( 11748 ( 11748 ( 116.4 ( 800.9 ( 800.5 ( <b>ch Tat</b> <b>Calc</b> 4 35 3 3 55	Formula Formula C19 H18 F C19 H18 F C18 H35 F C18	2 NE 03 2 NE 06 2 N	500 550 6 vs. Mass-to-C Ion (M+H)+ (M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+	500 650 70 Charge (m/z)	00 75	00- 03.27598 00- 038 H35 F2 N12 O6 058 05- 058 05- 058 05- 058 05- 058 05- 058 05- 058 05- 05- 05- 05- 05- 05- 05- 05- 05- 05-			nd Sum %	79.22

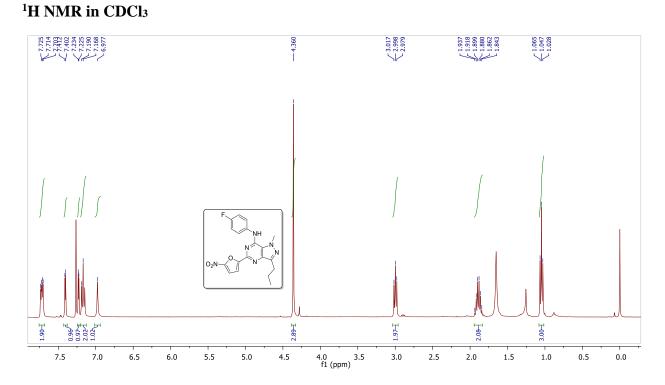
LIDI	C
ΠΓL	<i>i</i>



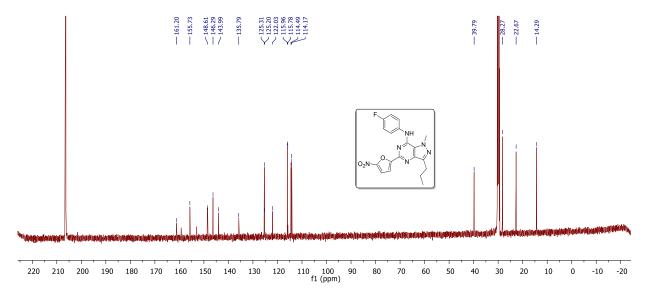
#### <Peak Table> PDA Ch1 254nm

PDAC					
Peak#		Area	Height	Area%	Height%
1	2.082	3740	436	0.027	0.025
2	3.778	2496	243	0.018	0.014
3	26.845	40589	3569	0.297	0.206
4	29.762	39430	2519	0.288	0.145
5	30.669	13659	971	0.100	0.056
6	30.988	7765	519	0.057	0.030
7	31.452	6511	448	0.048	0.026
8	32.013	3547	297	0.026	0.017
9	32.487	4100	445	0.030	0.026
10	32.760	7253	797	0.053	0.046
11	33.072	63081	7307	0.461	0.421
12	33.444	13378635	1705861	97.816	98.400
13	33.970	20411	1637	0.149	0.094
14	34.320	7807	843	0.057	0.049
15	34.560	2871	277	0.021	0.016
16	34.838	6431	423	0.047	0.024
17	35.392	7765	919	0.057	0.053
18	35.515	10210	1183	0.075	0.068
19	36.128	1154	145	0.008	0.008
20	36.344	5597	654	0.041	0.038
21	36.559	20371	1652	0.149	0.095
22	37.148	3433	405	0.025	0.023

# Compound (39)

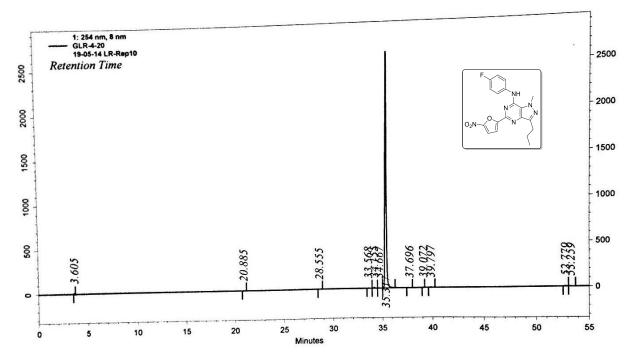


<sup>13</sup>C NMR in Acetone-d<sub>6</sub>



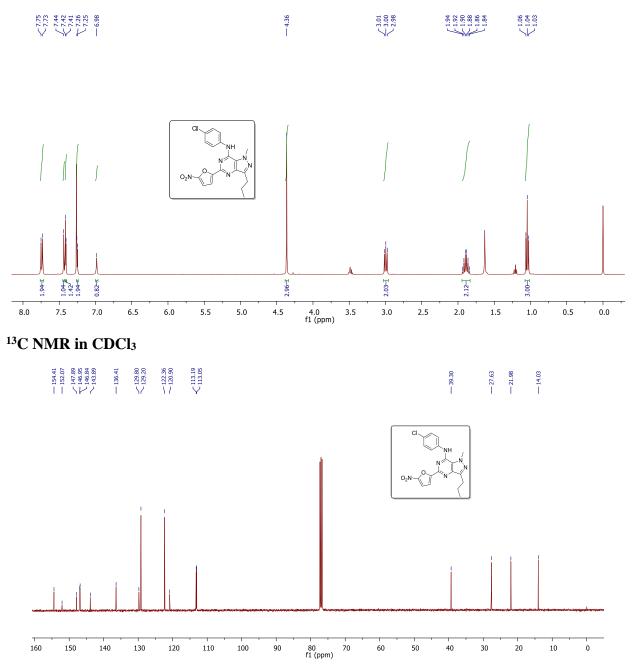
Data File			GLR-A-20	.d	Sample I	Name GLR-A-20		F	
Sample Type			Sample		Position	Vial 10			
Instrument N	lame		Instrumer	nt 1	User Nar	me			NH /
Acq Method			vishal_12-	01-13.m	Acquired	I Time 09-07-203	13 PM 1:05:11		N N
RM Calibrati	on Statu	s	Success		DA Meth	od daily_repo	ort.m	O2N V	N
comment									
Sample Group	n			Info					
cquisition S		6200 serie	es TOF/650						
ersion		Q-TOF B.	05.01 (B51	25)					
	Table								
Compound	Table						M	FG Diff	
Compou	nd Labe	I F	RT	Mass	Formula	M	IFG Formula	(ppm) I	DB Formula
Cpd 9: C1	9 H17 F	N6 O3 (	0.193	396.1344	C19 H17 F N6	03 C1	9 H17 F N6 O3	0.66 C1	9 H17 F N6 (
				-		- states			
Compound	Label	m/.	'z	RT Alg	orithm	Mass			
Cpd 9: C19 H		011111001110001110000				Feature 396.134	4		
x10 6 Cpd 1.2 - 1 -	9: C19	H17 F N6		203	m (0.137-0.77	1 min) Frag=175.0'	V GLR-A-20.d	]	
1.2 - 1 - 0.8 - 0.6 - 0.4 -	9: C19	H17 F N6		N6 03	m (0.137-0.77 <sup>-</sup>	1 min) Frag=175.0'			
1.2 - 1 - 0.8 - 0.6 - 0.4 - 0.2 -	9: C19	H17 F N6		H18 F N6 03	m (0.137-0.77	1 min) Frag=175.0'	V GLR-A-20.d		
1.2 1 0.8 0.6 0.4 0.2 0				CO 9N J 8LH 6LO 400 450 50	00 550 600	650 700 750 8			
1.2 - 1 - 0.8 - 0.6 - 0.4 - 0.2 - 0 -	150 20	0 250 30		CO 9N J 8LH 6LO 400 450 50		650 700 750 8	- 815.2568		
1.2 1 0.8 0.6 0.4 0.2 0 <b>IS Spectru</b>	150 20 <b>m Peal</b>	0 250 30 <b>k List</b>	00 350	CO 9N J 8LH 6LO 400 450 50	10 550 600 Mass-to-Charg	650 700 750 8	- 815.2568		
1.2 1.2 1. 0.8 0.6 0.4 0.2 0 15 Spectru	150 20 m Peal z Ab	0 250 3( k List	00 350	CON 281H 610 CI-HI / Sec 400 450 50 Counts vs.	0 550 600 Mass-to-Charg <b>Ion</b>	650 700 750 8	- 815.2568		
1.2 1.2 1. 0.8 0.6 0.4 0.2 0 <b>IS Spectru</b> <i>n/z</i> 397.1415	150 20 m Peal z Ab	0 250 3( <b>k List</b> 1264502.5	00 350 Formula C19 H18 F	CONVERSE CITATION 400 450 50 Counts vs.	0 550 600 Mass-to-Charo Ion (M+H)+	650 700 750 8	- 815.2568		
1.2 1.2 1. 0.8 0.6 0.4 0.2 0 MS Spectru m/z 397.1415 398.1448	150 20 m Peal z Ab	0 250 30 k List 1264502.5 263032.88	00 350 Formula C19 H18 F C19 H18 F	COUNTS VS.	0 550 600 Mass-to-Charg Ion (M+H)+ (M+H)+	650 700 750 8	- 815.2568		
1.2 1.2 1. 0.8 0.6 0.4 0.2 0 <b>IS Spectru</b> <b>n/z</b> 397.1415 398.1448 399.1468	150 20 m Peal z Ab 1 1 1	0 250 30 k List 1264502.5 263032.88 35780.83	00 350 Formula C19 H18 F C19 H18 F C19 H18 F	COUNTRY SECOND	0 550 600 Mass-to-Charg (M+H)+ (M+H)+ (M+H)+	650 700 750 8	- 815.2568		
1.2 1.2 1. 0.8 0.6 0.4 0.2 0 MS Spectru m/z 397.1415 398.1448	150 20 m Peal 1 1 1 1	0 250 30 <b>k List</b> 1264502.5 263032.88 35780.83 3477	<b>Formula</b> C19 H18 F C19 H18 F C19 H18 F C19 H18 F C19 H18 F	COUNTRY SECOND	0 550 600 Mass-to-Charg Ion (M+H)+ (M+H)+	650 700 750 8	- 815.2568		
1.2 - 1.2 - 1.3 - 0.8 - 0.6 - 0.4 - 0.2 - 0 - 15 Spectru n/z 397.1415 398.1448 399.1468 400.1491	150 20 m Peal 1 1 1 1 1	0 250 30 <b>k List</b> 1264502.5 263032.88 35780.83 3477 33089	Formula           C19 H18 f           C19 H17 f	CO 9N 4 81 H 61 J 400 450 50 Counts vs. N6 03 N6 03 N6 03 N6 03	0 550 600 Mass-to-Charg (M+H)+ (M+H)+ (M+H)+ (M+H)+	650 700 750 8 ge (m/z)	- 815.2568		
1.2 - 1.2 - 1.3 - 0.8 - 0.6 - 0.4 - 0.2 - 0 - 15 Spectru n/z 397.1415 398.1448 399.1468 400.1491 419.1237	150 20 m Peal 1 1 1 1 1	0 250 30 <b>k List</b> <b>jund</b> 1264502.5 263032.88 35780.83 3477 33089 8806.8	Formula           C19 H18 f           C19 H17 f           C19 H17 f           C19 H17 f	COUNTS VS. CUITE / X00 400 400 400 450 50 Counts VS. 16 16 10 10 10 10 10 10 10 10 10 10	0 550 600 Mass-to-Charg (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+	650 700 750 8 ge (m/z)	- 815.2568		
1.2 1.2 1. 0.8 0.6 0.4 0.2 0 <b>AS Spectru</b> <i>n/z</i> 397.1415 398.1448 399.1468 400.1491 419.1237 420.126	150 20 m Peal 2 Ab 1 1 1 1 1 1 1 1	0 250 30 <b>k List</b> <b>jund</b> 1264502.5 263032.88 35780.83 3477 33089 8806.8	Formula           C19 H18 f           C19 H17 f           C19 H17 f           C19 H17 f	COUNTS VS. 0 99N 481H 660 400 450 50 Counts vs. N6 03 N6 03	00 550 600 Mass-to-Charg (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+	650 700 750 8 ge (m/z)	- 815.2568		
1.2 - 1.2 - 1.3 - 0.8 - 0.6 - 0.4 - 0.2 - 0 - <b>1S Spectru</b> <b>n/z</b> 397.1415 398.1448 399.1468 400.1491 419.1237 420.1267 421.1289 815.2568 816.2599	150 20 m Peal 1 1 1 1 1 1 1 1 1 1 1 1 1	0 250 30 <b>k List</b> 1264502.5 263032.88 35780.83 3477 33089 8806.8 1259.4 23681.71 11912.44	600         350           Formula         C19 H18 F           C19 H18 F         C19 H18 F           C19 H18 F         C19 H18 F           C19 H18 F         C19 H17 F           C19 H17 F         C19 H17 F           C19 H17 F         C19 H17 F	COUNTS VS. 0 99N 481H 660 400 450 50 Counts vs. N6 03 N6 03	0 550 600 Mass-to-Charg (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)- (2M+Na)-	650 700 750 8 ge (m/z)	- 815.2568		
1.2 1.2 1. 0.8 0.6 0.4 0.2 0 <b>4S Spectru</b> <i>m/z</i> 397.1415 398.1448 399.1468 400.1491 419.1237 420.126 421.1289 815.2568 816.2599 817.2607	150 20 m Peal 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0 250 30 k List 1264502.5 263032.88 35780.83 3477 33089 8806.8 1259.4 23681.71 11912.44 3235.56	Formula           C19 H18 f           C19 H17 f	COUNTS VS. 0 99N 481H 660 400 450 50 Counts vs. N6 03 N6 03	0 550 600 Mass-to-Char (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+	650 700 750 8 ge (m/z)	- 815.2568		
1.2 1.2 1. 0.8 0.6 0.4 0.2 0 <b>15 Spectru</b> <i>n/z</i> 397.1415 398.1448 399.1468 400.1491 419.1237 420.126 421.1289 815.2568 816.2599 817.2607 <b>Predicted I</b>	150         20           m         Peal           z         Ab           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1	0 250 30 k List 1264502.5 263032.88 35780.83 3477 33089 8806.8 1259.4 23681.71 11912.44 3235.56 Match Ta	Formula C19 H18 F C19 H18 F C19 H18 F C19 H18 F C19 H18 F C19 H17 F C19 H18 F C19 H17 F C1	COULT (1970) CULTURE (1970) CULTURE (1970) COULT (1970) COULTURE (1970	0 550 600 Mass-to-Charg (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)- (2M+Na)- (2M+Na)-	650 700 750 8 ge (m/z)	8127598 000 850 900 950		
1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2	150 20 m Peal 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0 250 30 k List 1264502.5 263032.88 35780.83 3477 33089 8806.8 1259.4 23681.71 11912.44 3235.56 Match Ta Calc	Formula           C19 H18 f           C19 H17 f           C	COULT 100 100 100 100 100 100 100 100 100 10	0 550 600 Mass-to-Charg (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)- (2M+Na)- (2M+Na)-	650 700 750 8 ge (m/z) + + + +	899 200 850 900 950 Abund Sum %	Calc Abund Sum	
1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2	150 20 m Peal 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0 250 30 k List 1264502.5 263032.88 35780.83 3477 33089 8806.8 1259.4 23681.71 11912.44 3235.56 Match Ta Calc 7.1415	Formula           C19 H18 f           C19 H17 f           C	COULT 100 100 100 100 100 100 100 100 100 10	0 550 600 Mass-to-Charg (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)- (2M)-(2M+Na)- (2M)-(2M+Na)- (2M)-(2M+Na)- (2M)-(2M+Na)-(2M+	650 700 750 8 ge (m/z) + + + + + + - - 	89 90 90 850 900 950 Abund Sum % 80.71		79.02
1.2 1.2 1. 0.8 0.6 0.4 0.2 0 MS Spectru m/z 397.1415 398.1448 399.1468 400.1491 419.1237 420.126 421.1289 815.2568 816.2599 817.2607 Predicted Is sotope	150 20 m Peal 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0 250 30 k List 1264502.5 263032.88 35780.83 3477 33089 8806.8 1259.4 23681.71 11912.44 3235.56 Match Ta Calc	Formula           C19 H18 f           C19 H17 f           C	COULT 100 100 100 100 100 100 100 100 100 10	0 550 600 Mass-to-Charg (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (2M+Na)- (2M+NA)- (2M+NA)- (2M+NA)- (2M+NA)- (2M+NA)- (2M+NA	650 700 750 8 ge (m/z) + + + +	Abund Sum % 80.71 16.79		





nm Retention Time	Area	Area %	Height	Height %
3.605	53859	0.224	12696	0.476
20.885	17322	0.072	1864	0.070
28.555	11566	0.048	1126	0.042
33.568	26433	0.110	2320	0.087
34.155	84278	0.350	9090	0.34
34.667	30599	0.127	3001	0.112
35.317	23700456	98.533	2627329	98.47
37.696	20651	0.086	1311	0.04
39.072	12697	0.053	1826	0.06
39.797	38574	0.160	3617	0.13
52.779	35728	0.149	2961	0.11
53.259	21219	0.088	918	0.03
	24052282	100.000	2660046	100.00
	Retention Time           3.605           20.885           28.555           33.568           34.155           34.667           35.317           37.696           39.072           39.797           52.779	Retention TimeArea3.6055385920.8851732228.5551156633.5682643334.1558427834.6673059935.3172370045637.6962065139.0721269739.7973857452.77935728	Retention Time         Area         Area %           3.605         53859         0.224           20.885         17322         0.072           28.555         11566         0.048           33.568         26433         0.110           34.155         84278         0.350           34.667         30599         0.127           35.317         23700456         98.533           37.696         20651         0.086           39.072         12697         0.053           39.797         38574         0.160           52.779         35728         0.149           53.259         21219         0.088	Area         Area         Area         Area         Height           3.605         53859         0.224         12696           20.885         17322         0.072         1864           28.555         11566         0.048         1126           33.568         26433         0.110         2320           34.155         84278         0.350         9090           34.667         30599         0.127         3001           35.317         23700456         98.533         2627329           37.696         20651         0.086         1311           39.072         12697         0.053         1826           39.797         38574         0.160         3617           52.779         35728         0.149         2961           53.259         21219         0.088         918

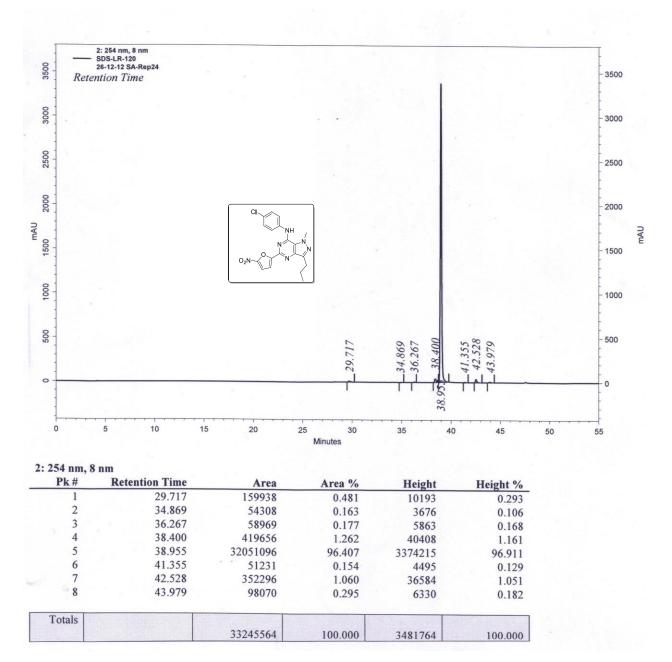
Compound (40) <sup>1</sup>H NMR in CDCl<sub>3</sub>



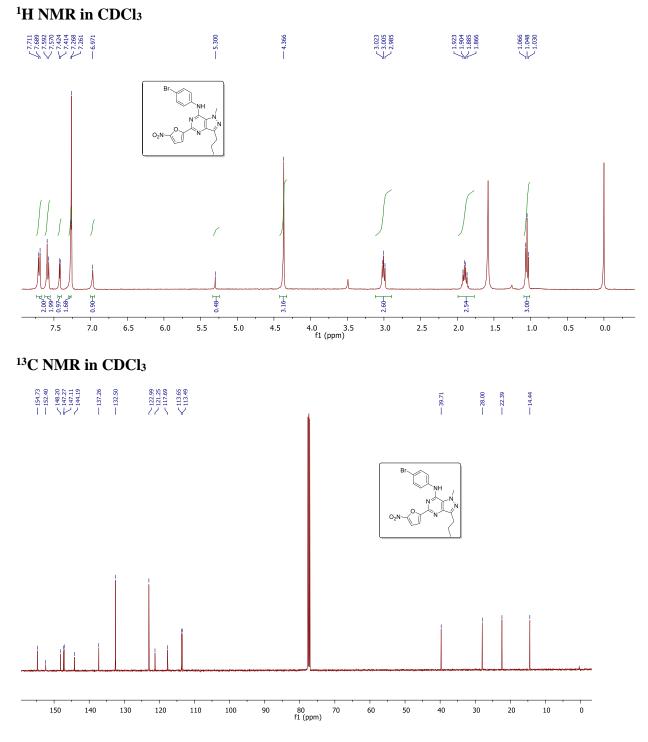
Oualitative	Compound	Report
Ollalitative	Compound	

ata File iample Type nstrument Nan Acq Method IRM Calibration Comment Sample Group		tus Info.	San Ins vist	R-4-41.d nple trument 1 hal_MS_250 ccess	72012.m	Sample Name Position User Name Acquired Time DA Method	GLR-4-41 Vial 11 a 11/19/2012 as.m	1:12:13 PM		0 <sub>2</sub> N-(	
Compound Ta	ble								MFG	Diff	
			RT	Mas	s	Formula		G Formula	(ppr	n) 1.05	DB Formula C19 H17 Cl N6 O3
Compound Cpd 5: C19 H	117 C	I N6 O3	0.17		10463 C1	9 H17 CI N6 O3	C19	H17 CI N6 O3		1.05	
Compound La Cpd 5: C19 H1	abel 7 Cl	N6 O3	<i>m/z</i> 413.1	1194	<b>RT AI</b> 0.172 Fir	<b>gorithm</b> nd by Molecular	Mas r Feature 412.				
					413.11194 19 H18 CI N6			119711 110 N10			
2- 1- 0-	150	200	250	300 350	451.06774	500 550 600 5. Mass-to-Cha	0 650 700 arge (m/z)	008 847.19711 974 Con Llad CJ2 N12 Na O6		50	
1-				300 350	451.0677	s. Mass-to-Cha	0 650 700 arge (m/z)	4		50	
1	m P	eak Lis	t	Formula	400 450 Counts vs	Ion	0 650 700 arge (m/z)	4		50	
1- 0 MS Spectru	<b>m P</b>	Abund	t 3276.4	Formula C19 H18 Cl	400 450 Counts vs N6 03	Ion (M+H)+	0 650 700 arge (m/z)	4		50	
1 0 MS Spectru <u><i>m/z</i></u> 413.11194 414.11451	m Po	Abund 438	t 3276.4 03107	Formula C19 H18 Cl C19 H18 Cl	400 450 Counts vs N6 03 N6 03	Ion (M+H)+ (M+H)+	0 650 700 arge (m/z)	4		50	
1 0 MS Spectru <u><i>m</i>/z</u> 413.11194 414.11451 415.10911	m Po	eak List Abund 438 1	t 3276.4 03107 5445.3	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl	400 450 Counts vs N6 03 N6 03 N6 03	Ion (M+H)+ (M+H)+ (M+H)+	0 650 700 arge (m/z)	4		50	
1 0 MS Spectru 413.11194 414.11451 415.10911 416.112	m Po	<b>Abund</b> 438 155	t 3276.4 03107 5445.3 3909.6	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl	400 450 Counts vs N6 03 N6 03 N6 03 N6 03	Ion (M+H)+ (M+H)+	0 650 700 arge (m/z)	4		50	
1 0 MS Spectru 413.11194 414.11451 415.10911 416.112 435.0923	m P z 1 1 1 1 1 1 1	Abund           438           1           155           33           10	t 3276.4 03107 5445.3 3909.6 0911.2	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl	400 450 Counts vs N6 03 N6 03 N6 03 N6 03	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+	0 650 700 arge (m/z)	4		50	
1 0 MS Spectru 413.11194 414.11451 415.10911 416.112	m P z 1 1 1 1 1 1 1	Abund           438           1           155           33           10	t 3276.4 03107 5445.3 3909.6	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl	400 450 Counts vs N6 03 N6 03 N6 03 N6 03	Ion           (M+H)+           (M+Na)+	0 650 700 arge (m/z)	4		50	
<b>MS Spectru</b> <b>MS Spectru</b> <u>m/z</u> <u>413.11194</u> 414.11451 <u>415.10911</u> <u>415.0923</u> <u>451.06774</u>	m Pe	Abund           438           1           155           3:           11	t 3276.4 03107 5445.3 3909.6 0911.2 4673.1	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H17 Cl	400 450 Counts vs N6 03 N6 03 N6 03 N6 03 N6 03 N6 03 N6 03	Ion           (M+H)+           (M+Na)+	0 650 700 arge (m/z)	4		50	
1 0 MS Spectru 413.11194 414.11451 415.10911 416.112 435.0923	m Pe	Abund           438           1           155           33           10           1	t 3276.4 03107 5445.3 3909.6 0911.2 4673.1 4619.5	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H17 Cl C19 H17 Cl C18 H34 Cl	400 450 Counts vs N6 03 N6 N6 N	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+K)+           (2M+Na)+	0 650 700 arge (m/z)	4		50	
1 0 MS Spectru 413.11194 414.11451 415.10911 416.112 435.0923 451.06774 847.19711	m Po	Abund           438           1           155           33           10           1	t 3276.4 03107 5445.3 3909.6 0911.2 4673.1 4619.5	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H17 Cl C19 H17 Cl C18 H34 Cl	400 450 Counts vs N6 03 N6 N6 N	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+K)+	0 650 700 arge (m/z)	4		50	
<b>MS Spectru</b> <b>MS Spectru</b> <u>m/z</u> <u>413.11194</u> 414.11451 <u>415.10911</u> <u>415.0923</u> <u>451.06774</u>	m Po	eak List	t 3276.4 03107 5445.3 3909.6 0911.2 4673.1 4619.5 7708.6	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H17 Cl C38 H34 Cl C38 H34 Cl C38 H34 Cl	400 450 Counts vs N6 03 N6 N6 N	Ion           (M+H)+           (M+K)+           (2M+Na)+           (2M+Na)+	0 650 700 arge (m/z)	4		50	
1 0 MS Spectru 413.11194 414.11451 415.10911 416.112 435.0923 451.06774 847.19711	m Pe	Abund           438           1           15!           3:           10           1	t 3276.4 03107 5445.3 3909.6 0911.2 4673.1 4619.5 7708.6	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H17 Cl C38 H34 Cl C38 H34 Cl C38 H34 Cl	400 450 Counts vs N6 03 N6 N6 N	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+Na)+           (M+K)+           (2M+Na)+	0 650 700 arge (m/z)	4		50	
1 0 MS Spectru 413.11194 414.11451 415.10911 416.112 435.0923 451.06774 847.19711 848.20076	m Pe	Abund           438           1           15!           3:           10           1	t 3276.4 03107 5445.3 3909.6 0911.2 4673.1 4619.5 7708.6	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H17 Cl C19 H17 Cl C19 H17 Cl C18 H34 Cl C38 H34 Cl C38 H34 Cl C38 H34 Cl	400 450 Counts vs N6 03 N6 N2 06 N6 03 N6 N2 06 N6 N2 06 N6 N2 0 N2 N12 N2	Ion           (M+H)+           (M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+		h.		50	
1 0 MS Spectru <i>m/z</i> 413.11194 414.11451 415.10911 416.112 435.0923 451.06774 847.19711 848.20076 849.19455 850.1964	<b>P</b> <b>Z</b> 1 1 1 1 1 1 1 5 1 5 1 3 1	eak List Abund 438 1 155 33 10 1 1	t 3276.4 03107 5445.3 3909.6 0911.2 4673.1 4619.5 7708.6 1221.8	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H17 Cl C19 H17 Cl C19 H17 Cl C19 H17 Cl C19 H18 Cl C19 H17 Cl C19 H18 Cl C19 H17 Cl C18 H34 Cl C38 H34 Cl S C38 H	400 450 Counts vs N6 03 N6 N6 N	Ion           (M+H)+           (M+K)+           (2M+Na)+           (2M+Na)+		h.			
1 0 MS Spectru <i>m/z</i> 413.11194 414.11451 415.10911 416.112 435.0923 451.06774 847.19711 848.20076 849.19455 850.1964	<b>P</b> <b>Z</b> 1 1 1 1 1 1 1 5 1 5 1 3 1	eak List Abund 438 1 155 33 10 1 1	t 3276.4 03107 5445.3 3909.6 0911.2 4673.1 4619.5 7708.6 1221.8 5989.8 tch T	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H17 Cl C19 H17 Cl C19 H17 Cl C38 H34 Cl C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	400 450 Counts vs N6 03 N6 N2 06 N2 N12 N2 N3 06	Ion           (M+H)+           (M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+		750 800 85	0 900 9		ound Sum %
1 0 MS Spectru 413.11194 414.11451 415.10911 416.112 435.0923 451.06774 847.19711 848.20076 849.19455	<b>P</b> <b>Z</b> 1 1 1 1 1 1 1 5 1 5 1 3 1	eak List Abund 438 1 155 33 10 1 1 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0	t 3276.4 03107 5445.3 3909.6 0911.2 4673.1 4619.5 7708.6 1221.8 5989.8 tch T	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H17 Cl C19 H17 Cl C19 H17 Cl C19 H17 Cl C38 H34 Cl C19 H18 Cl C19 H17 C	400 450 Counts vs N6 03 N6 N2 03 N2 N12 N2	Ion           (M+H)+           (M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+	Calc Abund %	750 800 85	0 900 9	Calc Ab	59.9
1 0 MS Spectru <i>m/z</i> 413.11194 414.11451 415.10911 416.112 435.0923 451.06774 847.19711 848.20076 849.19455 850.1964 Predicted Isotope	m Per 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	eak List Abund 438 1 155 33 10 1 1 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0	t 3276.4 03107 5445.3 3909.6 0911.2 4673.1 4619.5 7708.6 1221.8 5989.8 1221.8 5989.8	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H17 Cl C19 H17 Cl C19 H17 Cl C19 H17 Cl C38 H34 Cl C19 H17 Cl Cl C19 H17 Cl Cl C19 H17 Cl Cl C19 H17 Cl Cl C19 H17 Cl Cl C19 H17 Cl Cl Cl C19 H17 Cl Cl C19 H17 Cl Cl Cl C19 H17 Cl Cl Cl Cl Cl Cl Cl Cl Cl Cl	400 450 Counts vs N6 03 N6	Ion           (M+H)+           (M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+	Calc Abund %	750 800 85	<u>90909</u>	Calc Ab	59.9 13.81
1 0 MS Spectru <i>m/z</i> 413.11194 414.11451 415.10911 416.112 435.0923 451.06774 847.19711 848.20076 849.19455 850.1964 Predicted Isotope	m Po z 1 1 1 1 1 1 1 1 1 1 1 1 1	eak List Abund 438 1 155 3. 10 1 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0	t 3276.4 03107 5445.3 3909.6 0911.2 4673.1 4619.5 7708.6 11221.8 5989.6 tch T Cai 994	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H17 Cl C19 H17 Cl C19 H17 Cl C18 H34 Cl C38 H34 Cl C19 H17 Cl Cl C19 H17 Cl Cl C19 H17 Cl Cl Cl C19 H17 Cl Cl Cl Cl Cl Cl Cl Cl Cl Cl	400 450 Counts vs N6 03 N6 N6 03 N6 N6 03 N6 N6 N6 03 N6 N	Ion           (M+H)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+	Calc Abund %	750 800 85	<u>%</u> 59.69	Calc Ab	59.9 13.81 21.06
1 0 MS Spectru <i>m/z</i> 413.11194 414.11451 415.10911 416.112 435.0923 451.06774 847.19711 848.20076 849.19455 850.1964 Predicted Isotope	m Po z 1 1 1 1 1 1 1 1 1 1 1 5 1 5 1 5 1 I I I I I I I I I I I I I	eak List Abund 438 1 155 3 10 1 1 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0	t 3276.4 03107 6445.3 3990.6 3991.2 4673.1 4619.5 7708.6 11221.8 5989.6 11221.8 5989.6 5989.6 1221.8 5989.6 1221.8 5989.6 5989.6 1221.8 5989.6 5989.6 5989.6 5989.6 5989.6 5989.6 5989.6 5989.6 5989.6 5989.6 5989.6 5989.6 5989.6 5999.6 5989.6 59990.6 5999.6 5999.6 5999.6 5999.6 5999.6 5999.6 5999.6 5999.6 5999.	Formula C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H18 Cl C19 H17 Cl C19 H17 Cl C19 H17 Cl C19 H17 Cl C38 H34 Cl C19 H17 Cl Cl C19 H17 Cl Cl C19 H17 Cl Cl C19 H17 Cl Cl C19 H17 Cl Cl C19 H17 Cl Cl Cl C19 H17 Cl Cl C19 H17 Cl Cl Cl C19 H17 Cl Cl Cl Cl Cl Cl Cl Cl Cl Cl	400 450 Counts vs N6 03 N6 03 N2 N12 N8 06	Ion           (M+H)+           (M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+           (2M+Na)+	Calc Abund %	750 800 85	% 59.69 14.04	Calc Ab	59.9 13.81



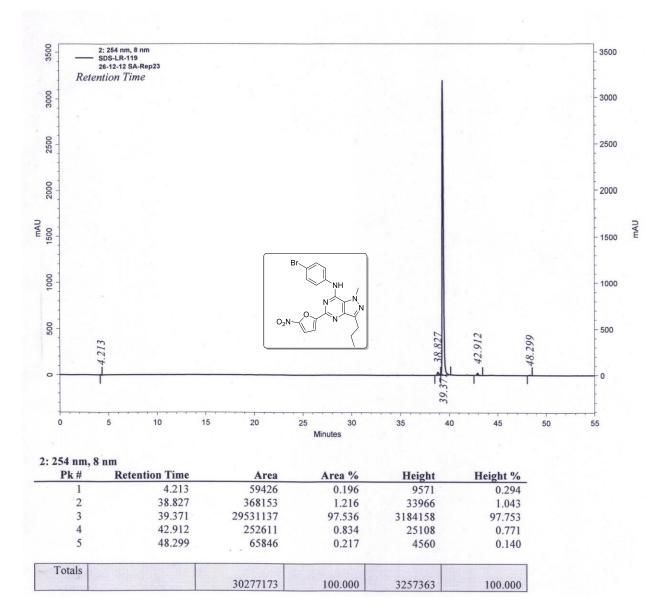


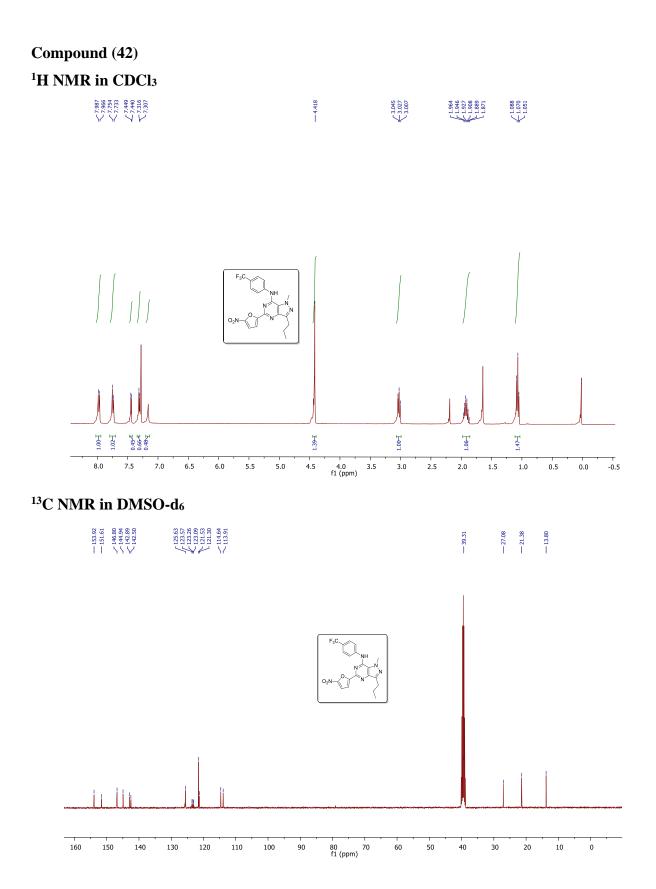
Compound (41)



#### **Qualitative Compound Report** GLR-4-40 Data File GLR-4-40.d Sample Name Position Vial 10 Br Sample Type Sample **Instrument Name** Instrument 1 User Name Acq Method vishal\_MS\_25072012.m **Acquired Time** 11/19/2012 1:05:07 PM **IRM Calibration Status DA Method** as.m Comment Sample Group Info. **Compound Table** MFG Diff **Compound Label** Formula **MFG Formula DB** Formula RT Mass (ppm) C19 H17 Br N6 O3 C19 H17 Br N6 O3 C19 H17 Br N6 O3 Cpd 5: C19 H17 Br N6 O3 0.173 456.05368 1.91 **Compound Label** m/z RT Algorithm Mass Cpd 5: C19 H17 Br N6 O3 457.06101 0.173 Find by Molecular Feature 456.05368 MFE MS Spectrum Cpd 5: C19 H17 Br N6 O3: + MFE Spectrum (0.123-0.451 min) GLR-4-40.d x10 4 457.06101 C19 H18 Br N6 O3 3.5 3 2.5 .09482 2 1.5 937. 495.01677 1 0.5 0 400 450 500 550 600 650 700 750 800 850 900 950 Counts vs. Mass-to-Charge (m/z) 150 200 250 300 350 **MS Spectrum Peak List** m/z z Abund Formula Ion 457.06101 1 160124.5 C19 H18 Br N6 O3 (M+H)+ 38239.7 C19 H18 Br N6 O3 (M+H)+ 458.06399 1 157646.4 C19 H18 Br N6 O3 459.05908 1 (M+H)+ 35501.4 C19 H18 Br N6 O3 (M+H)+ 460.06201 1 461.06331 5224.2 C19 H18 Br N6 O3 (M+H)+ 1 5088.1 C19 H17 Br N6 Na O3 481.03964 1 (M+Na)+ 935.09612 1 4998.8 (2M+Na)+ 937.09482 1 10595 (2M+Na)+ 938.09518 4493.5 (2M+Na)+ 1 939.09344 1 4989.1 (2M+Na)+ **Predicted Isotope Match Table** Calc m/z Diff (ppm) Abund % Calc Abund % Abund Sum % Calc Abund Sum % Isotope m/z 457.06183 40.05 99.56 40.29 457.06101 1.78 100 458.06461 1.37 23.88 22.96 9.62 9.24 458.06399 98.45 40.23 459.05908 459.06001 2.04 100 39.67 2 9.11 460.06201 460.06266 1.43 22.17 22.66 8.93 4 5 461.06331 461.06512 3.94 3.26 3.09 1.31 1.24 0.31 0.17 0.13 462.06645 462.06753 2.34 0.41 6







S102

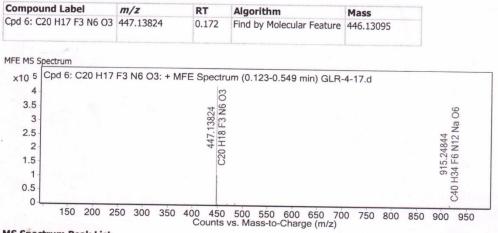
## **Qualitative Compound Report**

Data File	GLR-4-17.d	Sample Name	GLR-4-17	
Sample Type	Sample	Position	Vial 3	
Instrument Name	Instrument 1	User Name		F <sub>3</sub> C
Acq Method	vishal_MS_25072012.m	Acquired Time	11/19/2012 12:33:11 PM	NH /
<b>IRM Calibration Status</b>	Success	DA Method	as.m	N N
Comment			43.11	O2N N

Sample Group Info.

#### **Compound Table**

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C20 H17 F3 N6 O3	0.172	446.13095	C20 H17 F3 N6 O3	C20 H17 F3 N6 O3	1.05	C20 H17 F3 N6 O3



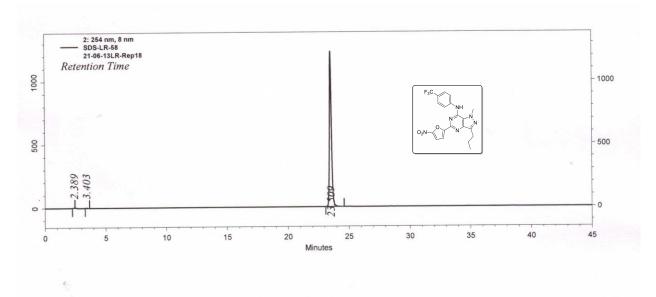
#### MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
447.13824	1	427502.1	C20 H18 F3 N6 O3	(M+H)+
448.14049	1	106718	C20 H18 F3 N6 O3	(M+H)+
449.14344	1	15102.1	C20 H18 F3 N6 O3	(M+H)+
450.14326	1	1907.9	C20 H18 F3 N6 O3	(M+H)+
469.11917	1	5028.1	C20 H17 F3 N6 Na O3	(M+Na)+
485.09308	1	6205.8	C20 H17 F3 K N6 O3	(M+K)+
486.09766	1	2048.1	C20 H17 F3 K N6 O3	(M+K)+
915.24844	1	9625.8	C40 H34 F6 N12 Na O6	(2M+Na)+
916.25487	1	4850.3	C40 H34 F6 N12 Na O6	(2M+Na)+
931.22519	1	1870.5	C40 H34 F6 K N12 O6	(2M+K)+

#### Predicted Isotope Match Table

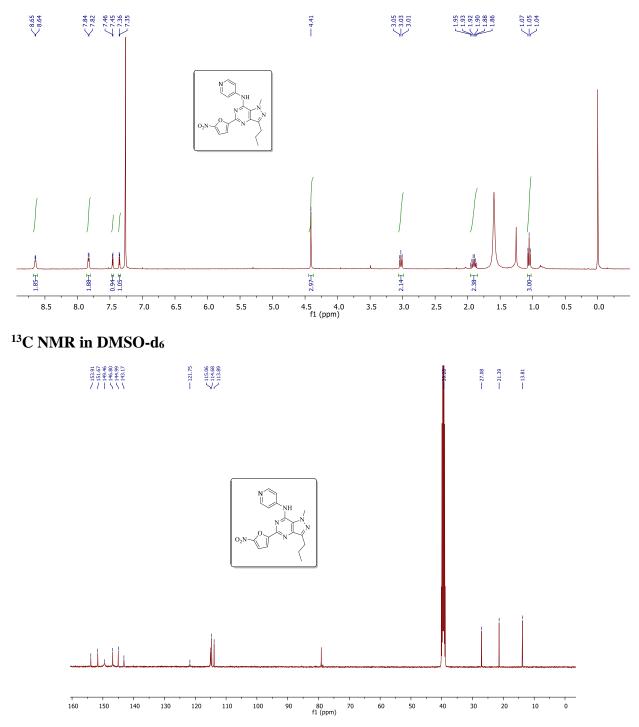
	Calc m		Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
382	824 44	387	1.03	100	100		
404	049 448	151	2.27	24.96	24.14		70110
134	344 449	405	1.34	3.53			10100
132	326 45	465	7.21	0.45			LIUT
132	520 45	405	7.21	0.45		0.35	0.35 0.35





Pk#	<b>Retention Time</b>	Area	Area %	Height	Height %
1	2.389	11776	0.082	1483	0.120
2	3.403	17683	0.124	2485	0.201
3	23.509	14268912	99.794	1230948	99.679
Totals		14298371	100.000	1234916	100.000

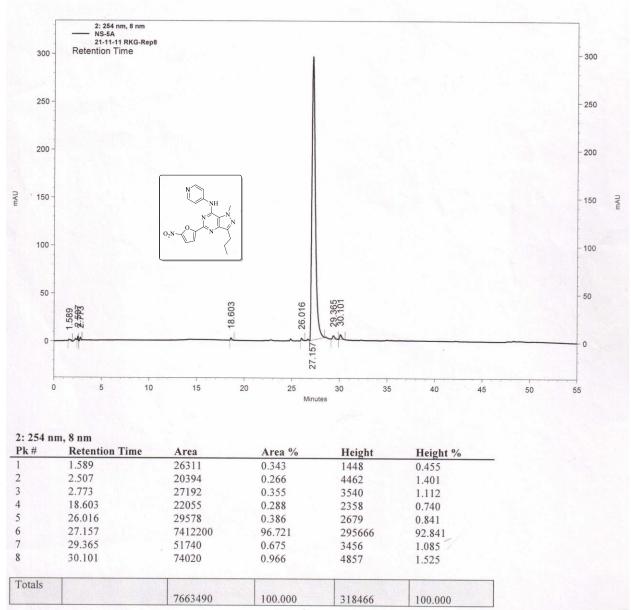
### Compound (43) <sup>1</sup>H NMR in CDCl<sub>3</sub>



Qualitative	Compound	Report
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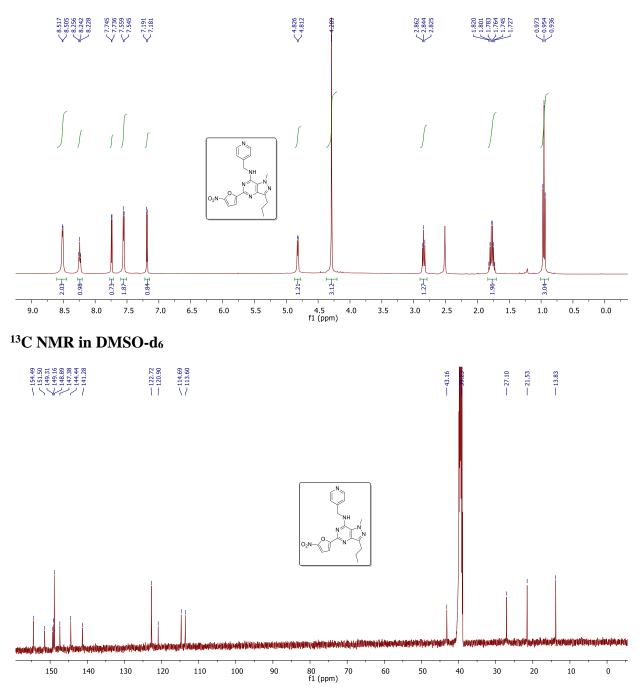
Data File Sample Type Instrument N Acq Method IRM Calibrati Comment	on s		Sam Instr visha Succ	ument		Sample Position User Na Acquired DA Meth	me d Time 11/1	19/201	2 12:47:24 PM				
Sample Group													
											FG Diff		
Compou	0.00		RT		9.13889	Formula C18 H17 N7			FG Formula 8 H17 N7 O3	(	(ppm) 1.05		7 N7 O3
Сра 7: С	18 F	117 N7 O3	0.173	3/	9.13889	C18 H17 N7	03	CIG	B H1/ N/ U3		1.05	C10 H1.	/ 11/ 03
Compound I Cpd 7: C18 H			<i>m/z</i> 380.146		<b>RT</b> 0.173	Algorithm	cular Feature	Mas					
6 - 5 - 4 -				220 14617									
5-	150	200 2	250 300		400 450		600 650 70	00 7	028 008 02, 781.26482	900	950		
5 - 4 - 3 - 2 - 1 - 0 <b>MS Spectru</b>	m P	eak List		350	400 450	vs. Mass-to-0		00 7		900	950		
5 - 4 - 3 - 2 - 1 - 0	m P z	eak List Abund	For	350 nula	400 450 Counts	vs. Mass-to-0		00 7		900	950		
5 - 4 - 3 - 2 - 1 - 0 - <b>MS Spectrum</b> <i>m/z</i> 380.14617	m P z	eak List Abund 6895	<b>For</b>	350 <b>mula</b> H18 N	400 450 Counts	vs. Mass-to-0		00 7		900	950		
5 - 4 - 3 - 2 - 1 - 0 - <b>MS Spectrum</b> <i>m/z</i> 380.14617 381.14848	m P z 1	eak List Abund 6895 1374	Forr 556.9 C18 191.3 C18	350 <b>nula</b> H18 N H18 N	400 450 Counts 7 03 7 03	Vs. Mass-to-0		00 7		900	950		
5 - 4 - 3 - 2 - 1 - 0 - <b>MS Spectrum</b> <i>m/z</i> 380.14617 381.14848 382.15117	m P z 1 1 1	eak List Abund 6895 1374 175	For 556.9 C18 191.3 C18 561.8 C18	350 <b>nula</b> H18 N H18 N H18 N	400 450 Counts 7 03 7 03 7 03 7 03	Vs. Mass-to-0 Ion (M+H)+ (M+H)+ (M+H)+		00 7		900	950		
5 - 4 - 3 - 2 - 1 - 0 - 	m P z 1 1 1 1	eak List Abund 6895 1374 175 23	<b>Form</b> 556.9 C18 491.3 C18 561.8 C18 329.3 C18	350 <b>nula</b> H18 N H18 N H18 N H18 N	400 450 Counts 7 03 7 03 7 03 7 03 7 03 7 03	Vs. Mass-to-0 Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+	Charge (m/z)	00 7		900	950		
5 - 4 - 3 - 2 - 1 - 0 - 	m P z 1 1 1 1 1 1	eak List Abund 6895 1374 175 23 15	Forr 556.9 C18 191.3 C18 561.8 C18 529.3 C18 510.2 C18	350 nula H18 N H18 N H18 N H18 N H18 N H17 N	400 450 Counts 7 03 7 03 7 03 7 03 7 03 7 03 7 03 7 03	Vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+	Charge (m/z)	00 7		900	950		
5- 4- 3- 2- 1- 0 <b>MS Spectrum</b> <i>m/z</i> 380.14617 381.14848 382.15117 383.15339 402.12775 418.1014	m P z 1 1 1 1 1 1 1 1	eak List Abund 6895 1374 175 23 15 13	Forr 556.9 C18 491.3 C18 561.8 C18 329.3 C18 510.2 C18 363.8 C18	350 nula H18 N H18 N H18 N H18 N H18 N H17 N	400 450 Counts 7 03 7 03 7 03 7 03 7 03 7 03 7 03 7 03	Vs. Mass-to-0	Charge (m/z)	00 7		900	950		
5 - 4 - 3 - 2 - 1 - 0 - <b>MS Spectrum</b> <i>m/z</i> 380.14617 383.14848 382.15117 383.15339 402.12775 418.1014 781.26482	m P z 1 1 1 1 1 1 1 1 1 1	eak List Abund 6895 1374 175 23 15 13 13	Forr 556.9 C18 491.3 C18 561.8 C18 329.3 C18 329.3 C18 363.8 C18 389.7	350 nula H18 N H18 N H18 N H18 N H18 N H17 N	400 450 Counts 7 03 7 03 7 03 7 03 7 03 7 03 7 03 7 03	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+K)+           (M+K)+           (2M+Na)	Charge (m/z)	00 7		900	950		
5 - 4 - 3 - 2 - 1 - 0 - <b>MS Spectru</b> <i>m/z</i> 380.14617 381.14848 382.15117 383.15339 402.12775 418.1014 781.26482 782.26457	m P z 1 1 1 1 1 1 1 1 1 1 1	eak List Abund 6895 1374 175 23 15 13 13 13 9	Forr 556.9 C18 491.3 C18 561.8 C18 329.3 C18 510.2 C18 363.8 C18 389.7 910.2	350 nula H18 N H18 N H18 N H18 N H18 N H17 N	400 450 Counts 7 03 7 03 7 03 7 03 7 03 7 03 7 03 7 03	Vs. Mass-to-0	Charge (m/z)	00 7		900	950		
5 - 4 - 3 - 2 - 1 - 0 - <b>MS Spectru</b> <i>m/z</i> 380.14617 381.14848 382.15117 383.15339 402.12775 418.1014 781.26482 782.26457 <b>Predicted Is</b>	m P z 1 1 1 1 1 1 1 1 1 1 1	eak List Abund 6895 1374 175 23 15 13 13 13 9	<b>Forr</b> 556.9 C18 191.3 C18 561.8 C18 329.3 C18 510.2 C18 363.8 C18 389.7 910.2 <b>h Table</b>	350 nula H18 N H18 N H18 N H18 N H17 N H17 N H17 K	400 450 Counts 7 03 7 03 7 03 7 03 7 03 7 03 7 03 7 Na 03 N7 03	VS. Mass-to-( Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+K)+ (2M+Na) (2M+Na)	Charge (m/z)		50 800 850	900			
5 - 4 - 3 - 2 - 1 - 0 - <b>MS Spectru</b> <i>m/z</i> 380.14617 381.14848 382.15117 383.15339 402.12775 418.1014 781.26482 782.26457 <b>Predicted Is</b>	m P z 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	eak List Abund 6895 1374 175 23 15 13 13 13 9 9 pe Matc	Forn 556.9 C18 191.3 C18 561.8 C18 329.3 C18 510.2 C18 363.8 C18 389.7 910.2 th Table Calc m/z	350 nula H18 N H18 N H18 N H17 N H17 K H17 K	400 450 Counts 7 03 7 03 7 03 7 03 7 03 7 Na 03 N7 03 Diff (ppm)	Vs. Mass-to-( Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+N+)+ (M+K)+ (2M+Na) (2M+Na) Abund %	Charge (m/z)	2%			Calc Abund		
5 - 4 - 3 - 2 - 1 - 0 - MS Spectrum <i>m/z</i> 380.14617 381.14848 382.15117 383.15339 402.12775 418.1014 782.26457 Predicted Is Isotope 1	m P z 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	eak List Abund 6895 1374 175 23 15 13 13 13 9 9 pe Matco 880.14617	Form           556.9         C18           191.3         C18           561.8         C18           322.3         C18           510.2         C18           363.8         C18           397.7         10.2           10.2         Table           Calc m/z         380.1	350 nula H18 N H18 N H18 N H17 N H17 K H17 K	400 450 Counts 7 03 7 03 7 03 7 03 7 03 7 03 7 03 7 03	Vs. Mass-to-( Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+K)+ (2M+Na) (2M+Na) Abund % 100	Charge (m/z)	<b>2%</b> 100	50 800 850	81.42	Calc Abund	7	9.59
5- 4- 3- 2- 1- 0 <b>MS Spectru</b> <i>m/z</i> 380.14617 381.14848 382.15117 383.15339 402.12775 418.1014 782.26457 <b>Predicted Is</b> <b>Isotope</b> 1 2	m P z 1 1 1 1 1 1 1 1 1 1 1 1 5000 m/2	eak List Abund 6895 1374 175 23 15 13 13 13 9 9 <b>pe Matc</b> 880.14617 881.14848	Form           556.9         C18           191.3         C18           561.8         C18           510.2         C18           363.8         C18           89.7         10.2           101.2         Table           Calc m/2         380.1           381.1         381.1	350 nula H18 N H18 N H18 N H18 N H17 N H17 K H17 K 4656 4923	400 450 Counts 7 03 7 03 7 03 7 03 7 03 7 03 7 03 7 Na 03 N7 03 Diff (ppm) 1.04 1.95	Vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+K)+ (M+K)+ (2M+Na) (2M+Na) (2M+Na) Abund % 100 19.94	Charge (m/z)	% 100 22.35	50 800 850	<u>81.42</u> 16.23	Calc Abund	7	7.79
5 - 4 - 3 - 2 - 1 - 0 - MS Spectrum <i>m/z</i> 380.14617 381.14848 382.15117 383.15339 402.12775 418.1014 782.26457 Predicted Is Isotope 1	m P z 1 1 1 1 1 1 1 1 1 1 1 1 5000 m/2	eak List Abund 6895 1374 175 23 15 13 13 13 9 9 pe Matco 880.14617	Form           556.9         C18           191.3         C18           561.8         C18           510.2         C18           363.8         C18           89.7         10.2           101.2         Table           Calc m/2         380.1           381.1         381.1	350 nula H18 N H18 N H18 N H18 N H17 N H17 K H17 K 4656 4923	400 450 Counts 7 03 7 03 7 03 7 03 7 03 7 03 7 03 7 03	Vs. Mass-to-C Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+K)+ (M+K)+ (2M+Na) (2M+Na) (2M+Na) Abund % 100 19.94	Charge (m/z)	<b>2%</b> 100	50 800 850	81.42	Calc Abund	7	

HPLC



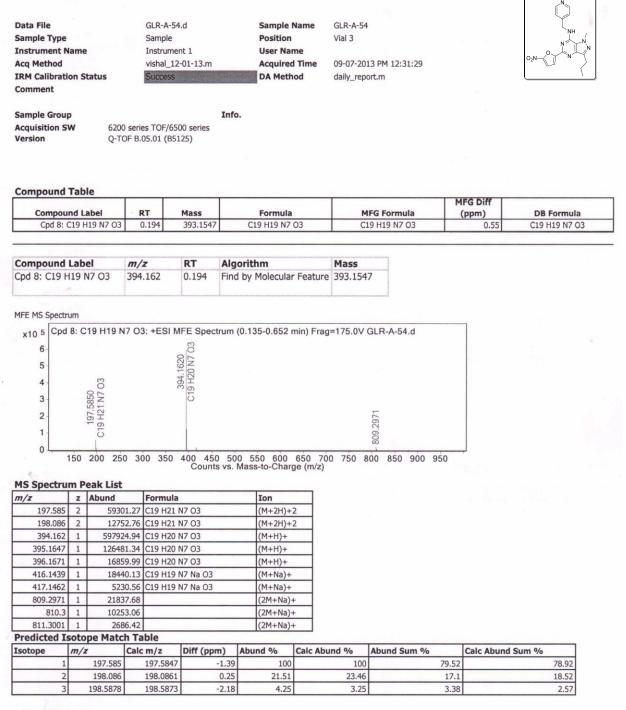
## Compound (44)

<sup>1</sup>H NMR in DMSO-d<sub>6</sub>



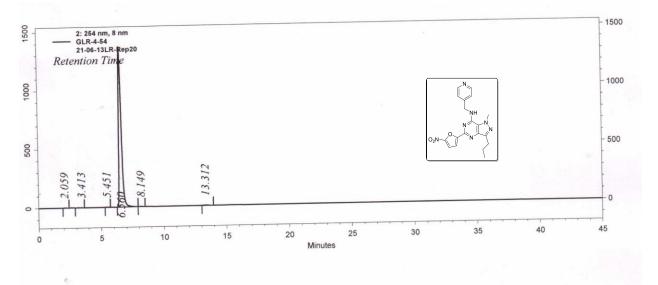
## HRMS

## **Qualitative Compound Report**



--- End Of Report ---

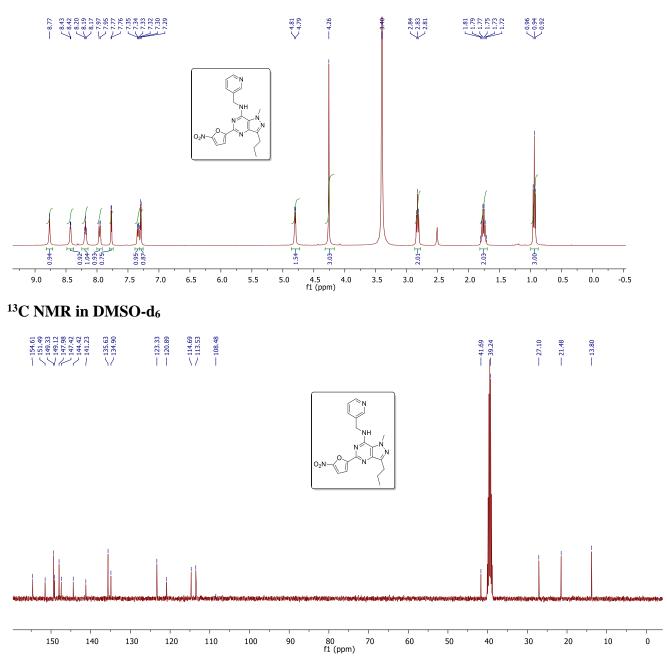




	Area	Area %	Height	Height %
etention Time		0.066	1088	0.079
			1318	0.096
			1856	0.135
- Bernard Barner		99.371	1369377	99.410
		0.121	1627	0.118
13.312	52458	0.270	2245	0.163
		100.000	1277511	100.000
	2.059 3.413 5.451 6.560 8.149 13.312	3.413136765.451197456.560193139118.14923537	2.039       11/10         3.413       13676       0.070         5.451       19745       0.102         6.560       19313911       99.371         8.149       23537       0.121         13.312       52458       0.270	2.059       12750       0.000         3.413       13676       0.070       1318         5.451       19745       0.102       1856         6.560       19313911       99.371       1369377         8.149       23537       0.121       1627         13.312       52458       0.270       2245

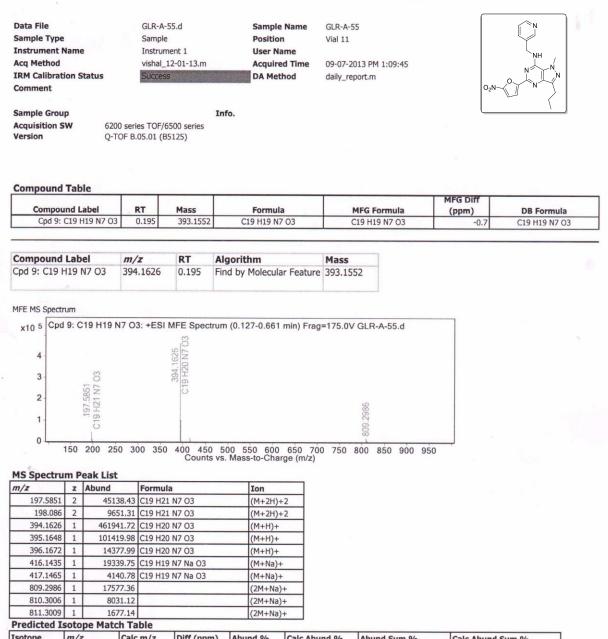
Compound (45)

<sup>1</sup>H NMR in DMSO-d<sub>6</sub>



## HRMS

# **Qualitative Compound Report**

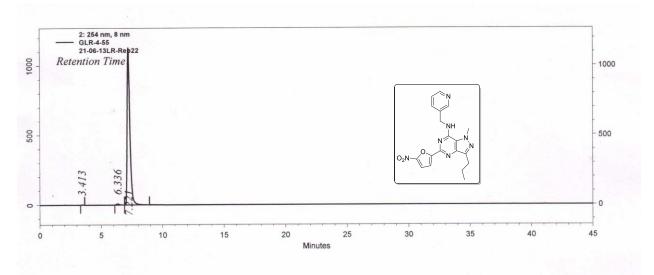


Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	197.5851	197.5847	-1.7	100	100	80.59	78.92
2	198.086	198.0861	0.24	21.38	23.46	17.23	18.52
3	198.5871	198.5873	0.98	2.71	3.25	2.18	2.57

--- End Of Report ---

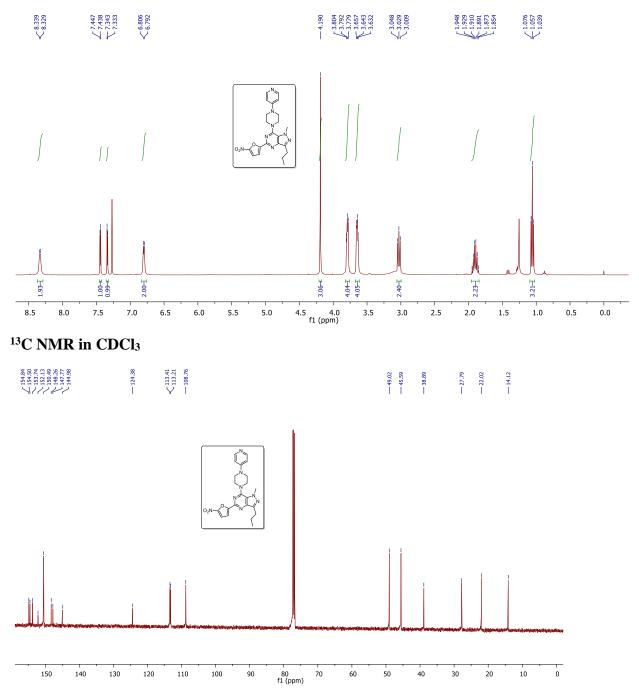


1



Pk #	<b>Retention Time</b>	Area	Area %	Height	Height %
1	3.413	12013	0.069	1712	0.150
2	6.336	124836	0.718	7744	0.680
3	7.221	17260308	99.213	1129344	99.170
Totals .					
		17397157	100.000	1138800	100.000

# Compound (46) <sup>1</sup>H NMR in CDCl<sub>3</sub>



## HRMS

3

4

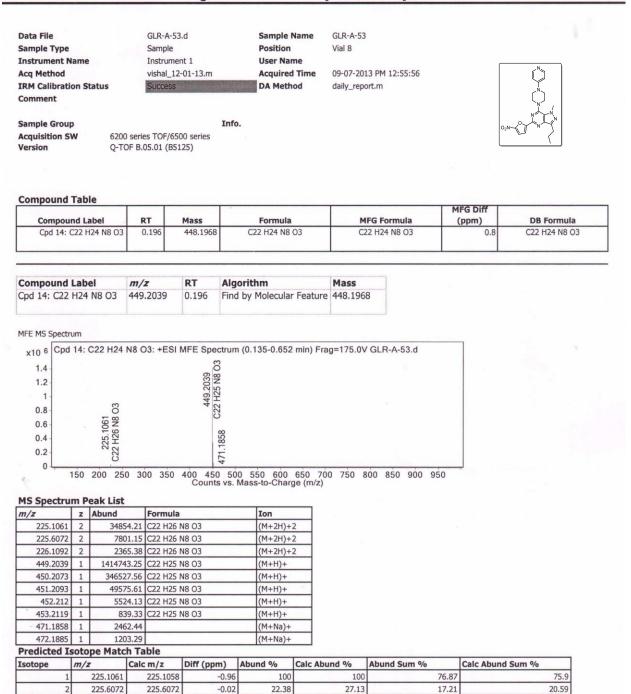
226.1092

226.6073

226.1085

226.6097

## **Qualitative Compound Report**



4.16

0.46

6.79

0.92

5.22

0.71

3.16

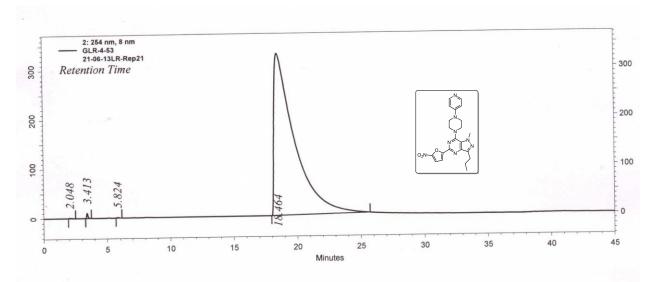
0.35

-3.08

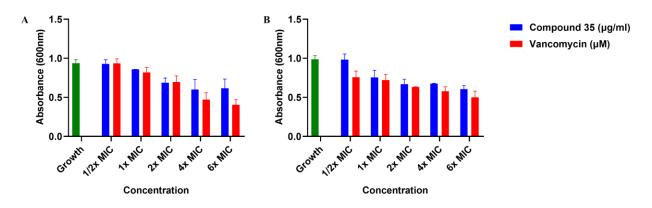
10.61



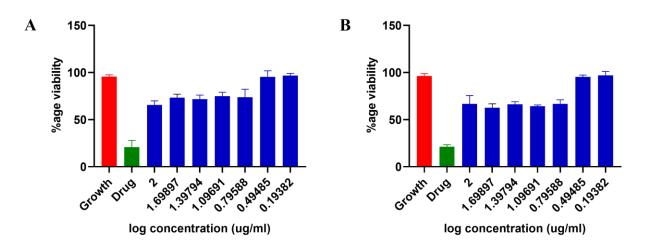
 $\tilde{\tau}_{i}$ 



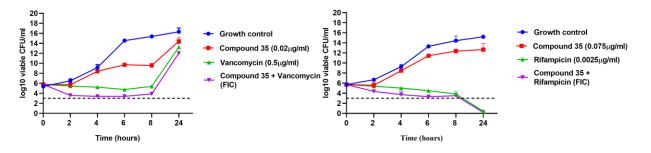
Pk #	<b>Retention Time</b>	Area	Area %	Height	Height %
1	2.048	15484	0.042	863	0.252
2	3.413	75574	0.204	10325	3.017
2 3 4	5.824 18.464	10940 36973719	0.030 99.725	966 330017	0.282 96.448



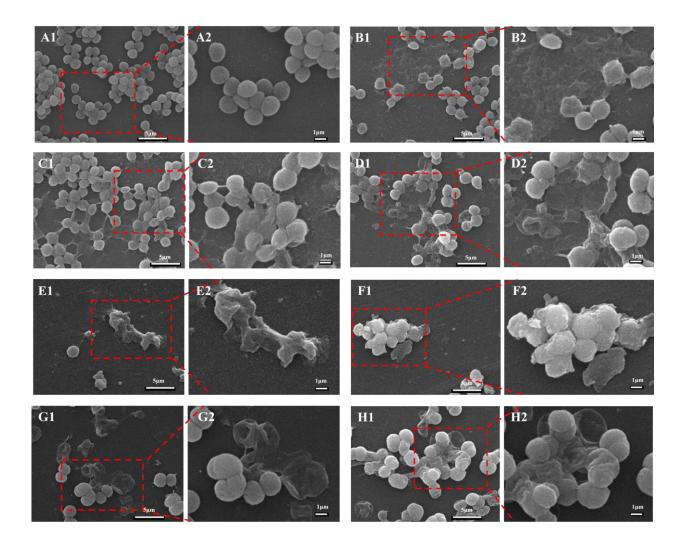
**Figure S1.** The graph represents the preformed biofilm disruption at different concentrations of the compound **35** (1/2x, 1x, 2x, 4x and 6x MIC) while vancomycin is used as drug control at respective concentrations. The untreated cells or growth control in (A) *S. aureus* and (B) MRSA show the biofilm formation ability. In (A) *S. aureus*, compound **35** exhibits the potency of disrupting biofilm at 4x and 6x of MIC (maximum 30%) while the drug control vancomycin shows 40-50% disruption ability at 4x and 6x of MIC. In (B) MRSA, compound 35 exhibits similar ability at 4x and 6x of MIC compared to the drug control vancomycin. The figure is representative of three experiments.



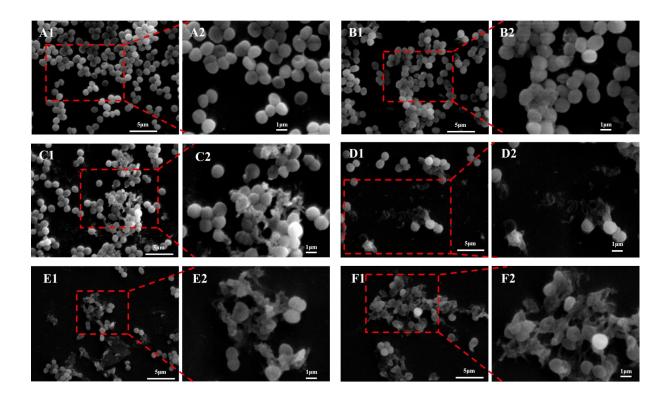
**Figure S2.** The compound **35** (blue bars) shows >50% growth of macrophage cells RAW264.7 at all concentrations ranging from  $100\mu$ g/ml to  $1.5\mu$ g/ml when exposed for A) 48 h and B) 72 h. The untreated cells (red) act as growth control. Drug control (green), Doxorubicin was used at a concentration of  $10\mu$ M which showed a greater reduction in the growth of cells.



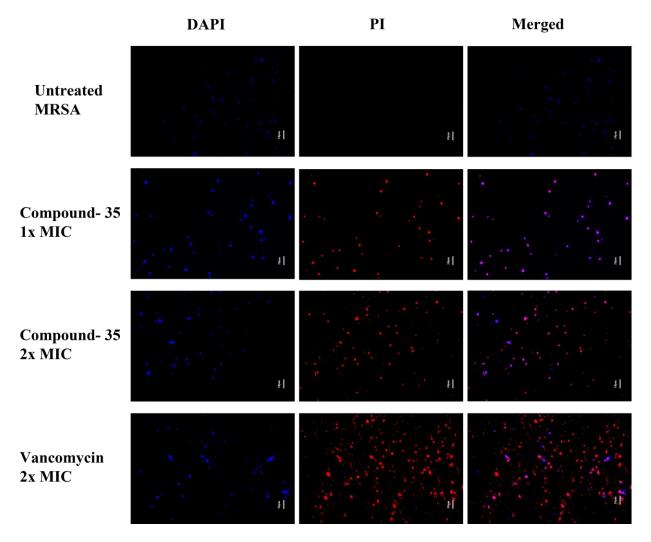
**Figure S3.** Killing efficacy of synergistic combinations of (A) compound **35** with vancomycin in *S. aureus and (B)* compound **35** with rifampicin in MRSA strains. Sub-inhibitory concentrations of vancomycin  $(0.5\mu g/ml)$ , and compound 35  $(0.02\mu g/ml)$  in *S. aureus* and rifampicin  $(0.0025\mu g/ml)$  and compound 35  $(0.075\mu g/ml)$  in MRSA were used. The untreated growth control was used to compare the data.



**Figure S4.** Scanning electron micrographs of MRSA at 2 hours of incubation with compound **35**, including images at  $5\mu$ m and  $1\mu$ m scales, with the  $1\mu$ m scale image providing a magnified view of a portion of the  $5\mu$ m scale image. Panels A1 and A2 depict the morphology of untreated cells, which appear in clusters. The treated samples with compound **35** at 1x MIC (B1, B2), 2x MIC (C1, C2), and 4x MIC (D1, D2) exhibit concentration-dependent morphological disruption. The drug controls vancomycin 1x MIC (E1, E2), 2x MIC (F1, F2) and daptomycin 1x MIC (G1, G2), 2x MIC (H1, H2) were used which demonstrated significant disruption at both concentrations.



**Figure S5.** Scanning electron micrographs of MRSA at 6 hours of incubation with compound **35**, including images at  $5\mu$ m and  $1\mu$ m scales, with the  $1\mu$ m scale image providing a magnified view of a portion of the  $5\mu$ m scale image. Panels A1 and A2 depict the morphology of untreated cells, which appear in clusters. The treated samples with compound **35** at 1x MIC (B1, B2), 2x MIC (C1, C2), and 4x MIC (D1, D2) exhibit concentration-dependent morphological disruption. The vancomycin control demonstrates significant disruption at both concentrations, 1x MIC (E1, E2) and 2x MIC (F1, F2).



**Figure S6.** Fluorescence micrographs of MRSA stained with DAPI and PI after treatment with compound **35** at 1X and 2X MIC. Vancomycin, at 2X MIC, served as a positive control. In the blank control (untreated bacteria), DAPI staining was present without PI staining, signifying intact bacterial membranes. Conversely, treatment with compound **35** showed intense blue (DAPI) and red (PI) fluorescence, indicating a compromise in bacterial cell wall integrity. Scale bar: 10 µm.