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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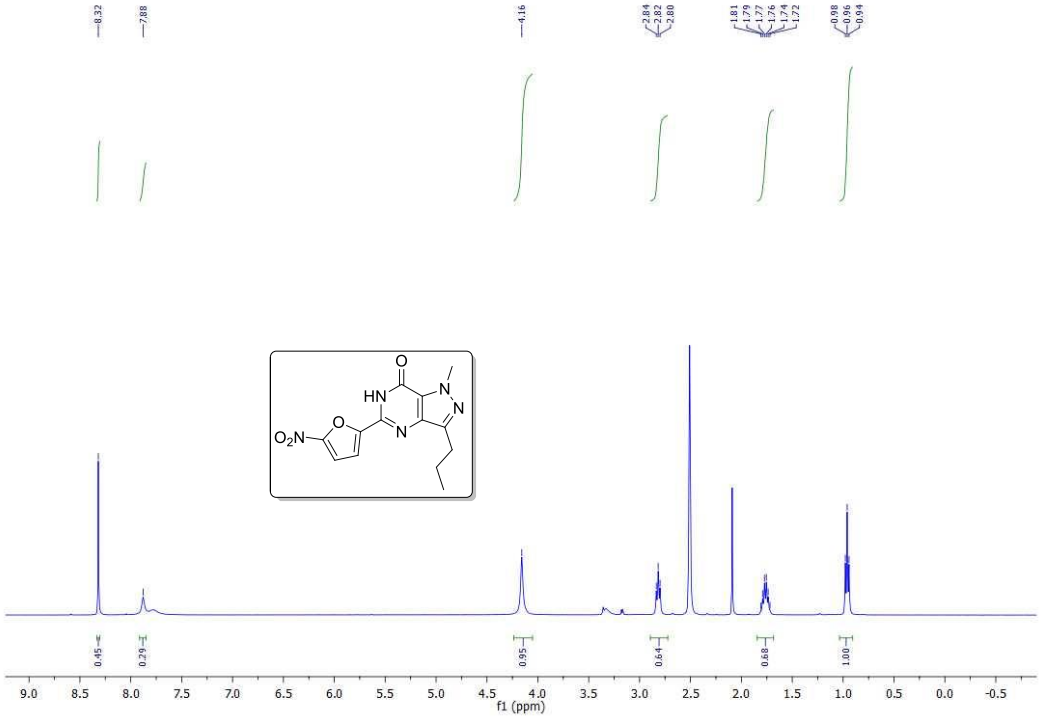
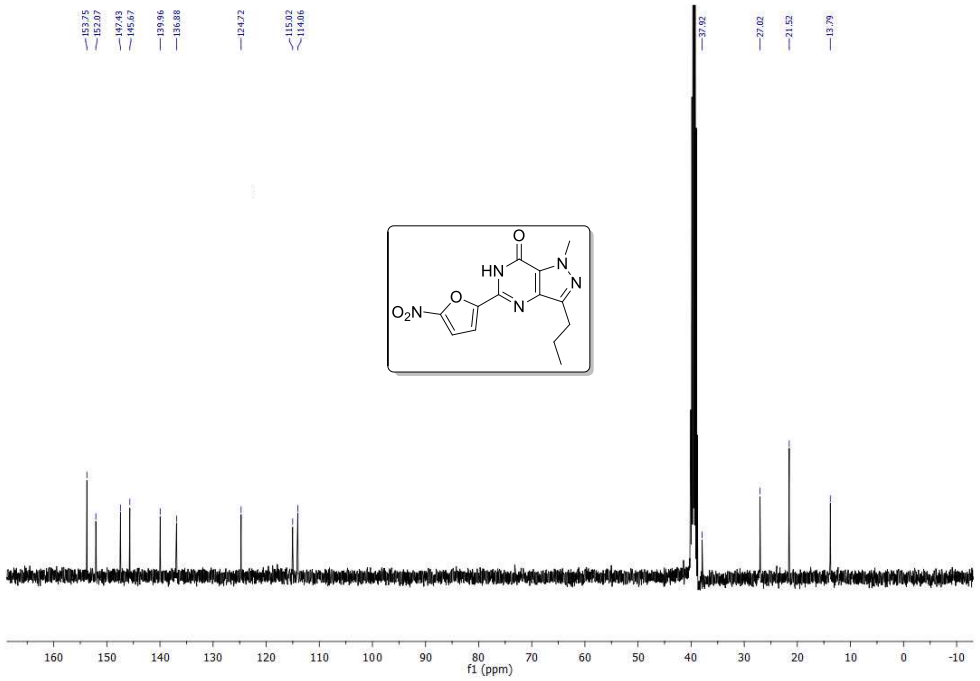
1.0. Scanned spectra

Compound (8)

^{1}H NMR in DMSO-d$_6$



^{13}C NMR in DMSO-d$_6$



HRMS

Qualitative Compound Report

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IRM Calibration Status	Success	**DA Method**	as.m
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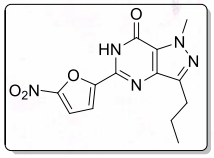


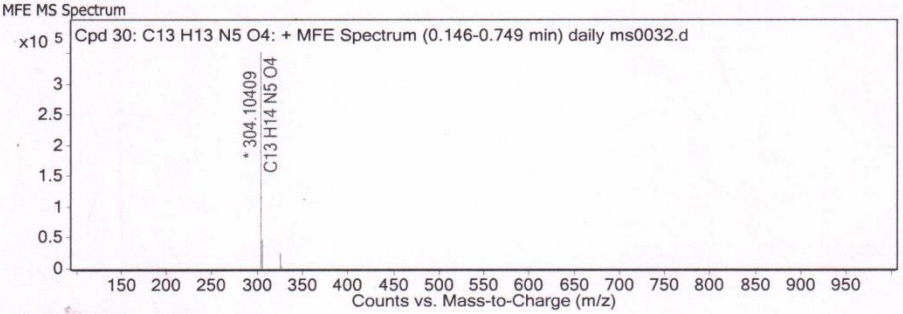
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 30: C13 H13 N5 O4	0.236	303.09682	C13 H13 N5 O4	C13 H13 N5 O4	-0.21	C13 H13 N5 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 30: C13 H13 N5 O4	304.10409	0.236	Find by Molecular Feature	303.09682

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
304.10409	1	352052.5	C13 H14 N5 O4	(M+H)+
305.10722	1	46982.8	C13 H14 N5 O4	(M+H)+
306.10937	1	5822.5	C13 H14 N5 O4	(M+H)+
307.11129	1	595.1	C13 H14 N5 O4	(M+H)+
326.08634	1	24963.2	C13 H13 N5 Na O4	(M+Na)+
327.08911	1	3812.6	C13 H13 N5 Na O4	(M+Na)+
328.0897	1	744	C13 H13 N5 Na O4	(M+Na)+

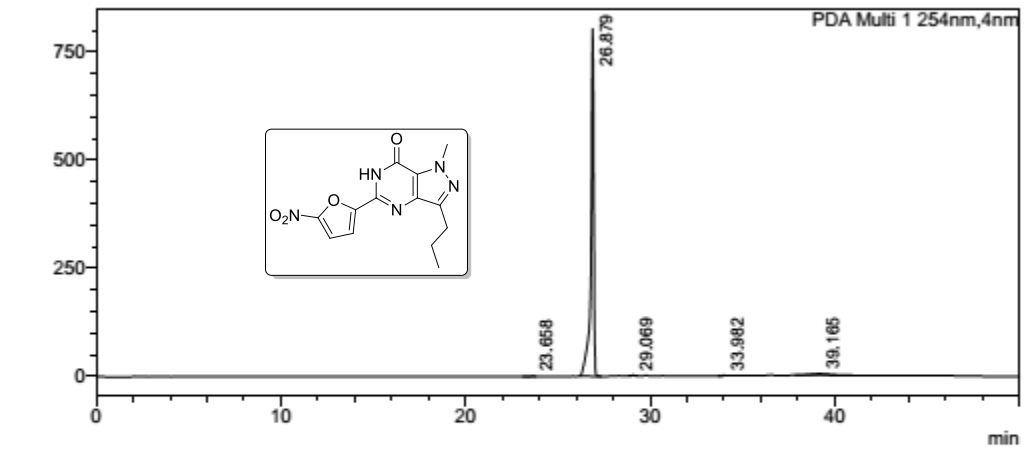
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	304.10409	304.10403	-0.21	100	100	86.83	84.43
2	305.10722	305.10671	-1.66	13.35	16.2	11.59	13.68
3	306.10937	306.10891	-1.48	1.65	2.05	1.44	1.73
4	307.11129	307.11124	-0.16	0.17	0.19	0.15	0.16

--- End Of Report ---

HPLC

<Chromatogram>



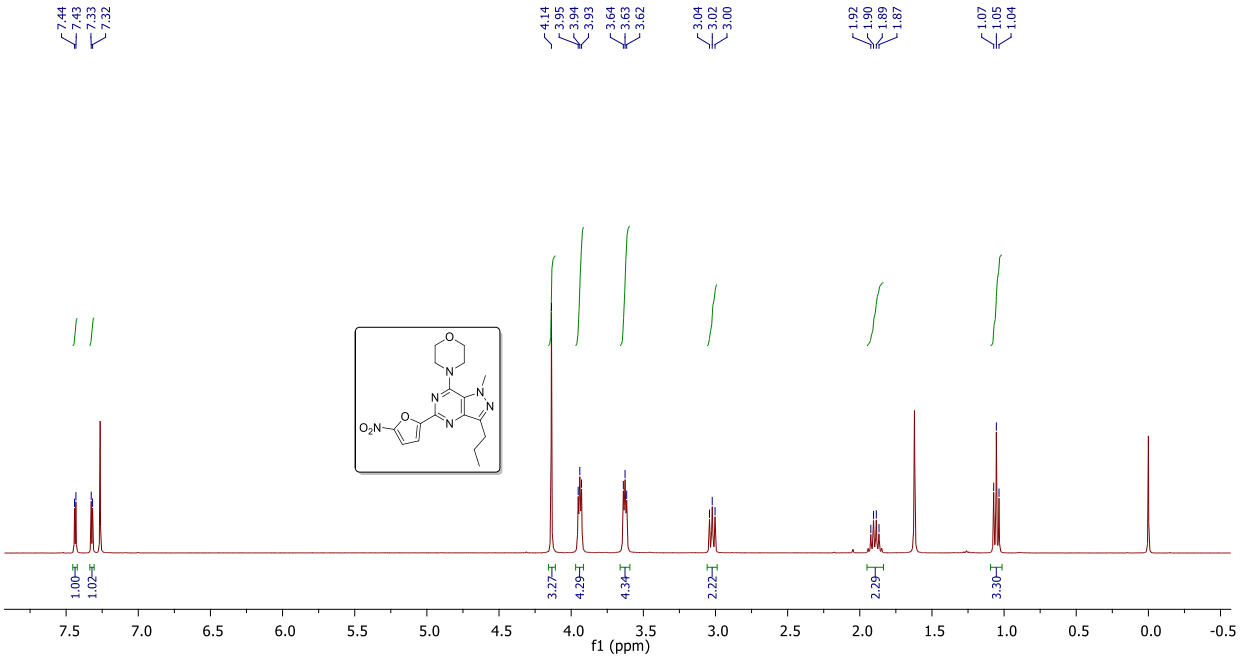
<Peak Table>

PDA Ch1 254nm

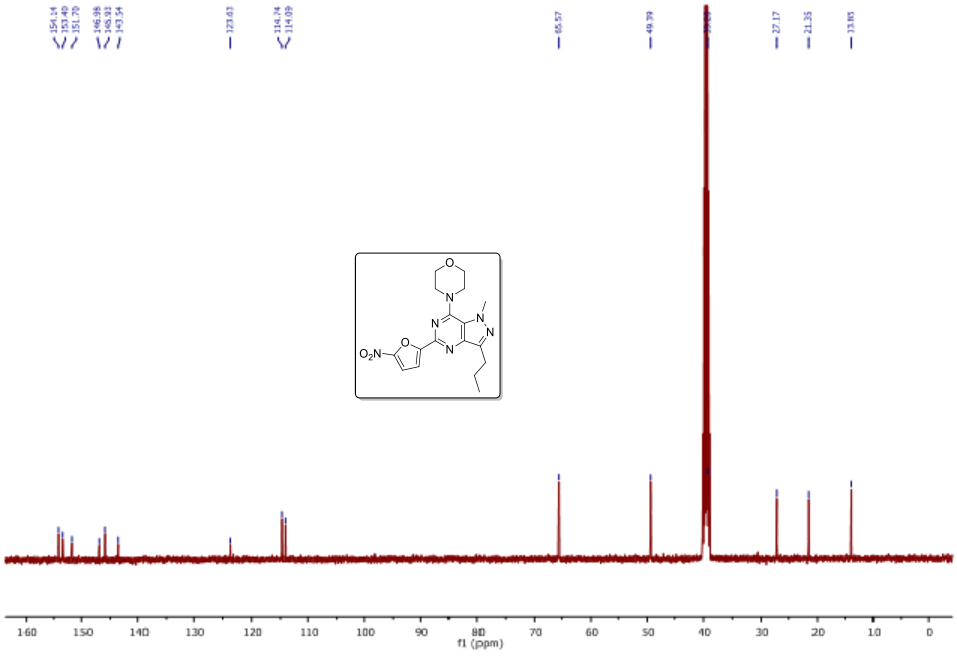
Peak#	Ret. Time	Area	Height	Area%	Height%
1	23.658	9756	861	0.109	0.106
2	26.879	8546397	802561	95.800	98.880
3	29.069	26648	3044	0.299	0.375
4	33.982	18249	1444	0.205	0.178
5	39.165	320040	3739	3.587	0.461
Total		8921091	811649	100.000	100.000

Compound (10)

^{1}H NMR in $CDCl_3$

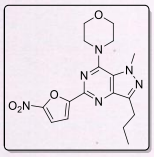


^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report



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Sample Type	Sample	**Position**	Vial 15
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/18/2012 1:01:38 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

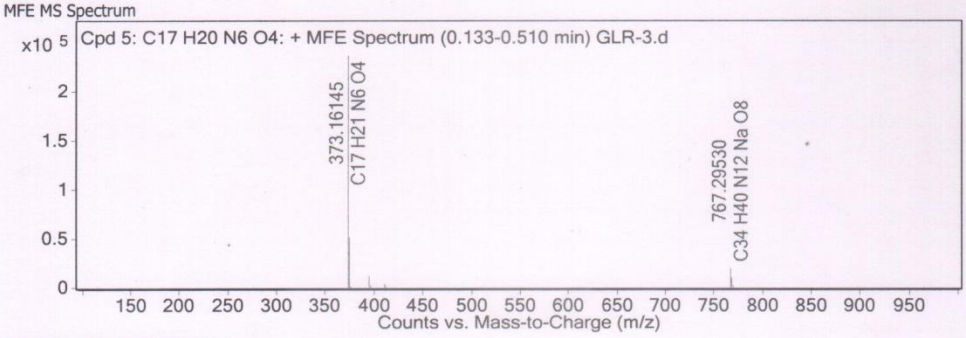
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C17 H20 N6 O4	0.172	372.15417	C17 H20 N6 O4	C17 H20 N6 O4	1.15	C17 H20 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C17 H20 N6 O4	373.16145	0.172	Find by Molecular Feature	372.15417

MFE MS Spectrum



MS Spectrum Peak List

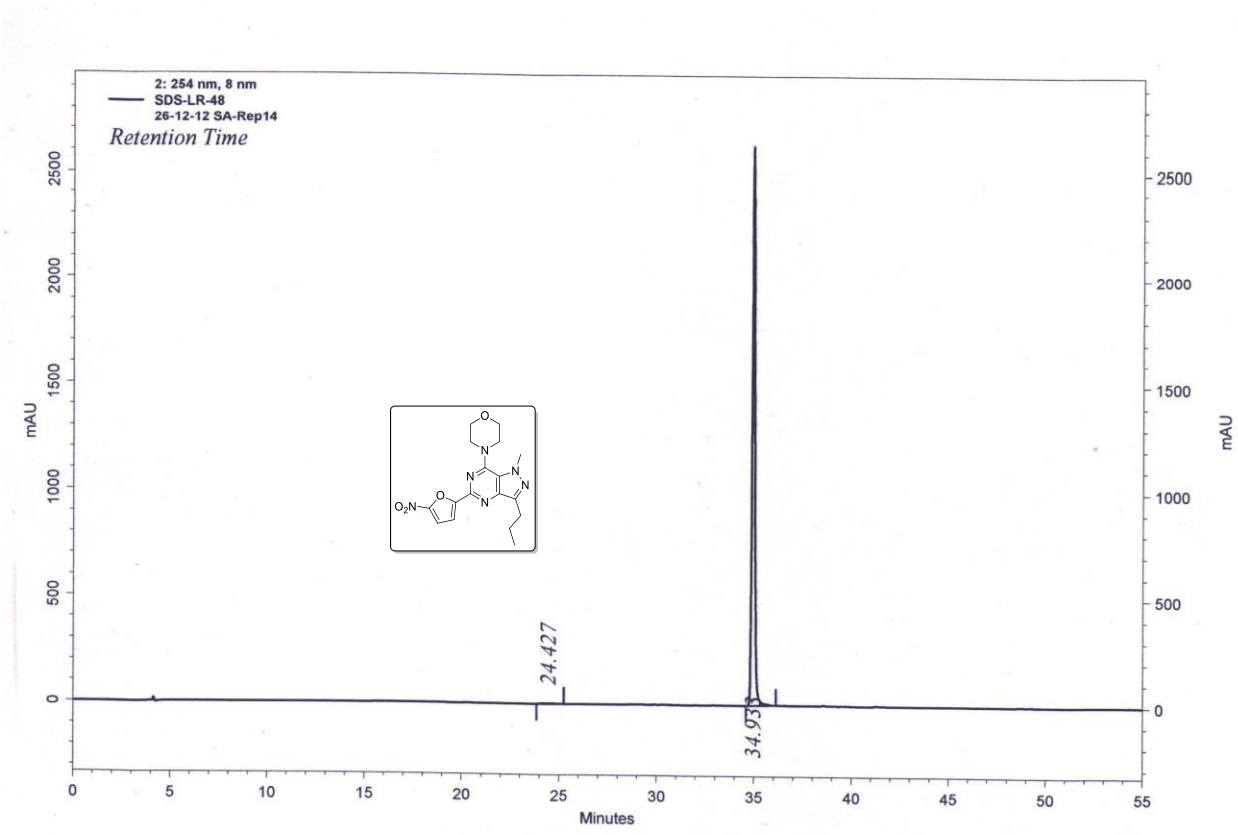
m/z	z	Abund	Formula	Ion
373.16145	1	235973.3	C17 H21 N6 O4	(M+H)+
374.16411	1	51344.5	C17 H21 N6 O4	(M+H)+
375.16622	1	6824.4	C17 H21 N6 O4	(M+H)+
376.1728	1	1272.5	C17 H21 N6 O4	(M+H)+
395.14219	1	11735.8	C17 H20 N6 Na O4	(M+Na)+
396.14658	1	2717.6	C17 H20 N6 Na O4	(M+Na)+
411.11631	1	3962.3	C17 H20 K N6 O4	(M+K)+
767.2953	1	19822	C34 H40 N12 Na O8	(2M+Na)+
768.2981	1	9457.8	C34 H40 N12 Na O8	(2M+Na)+
769.30404	1	2588.5	C34 H40 N12 Na O8	(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	373.16145	373.16188	1.15	100	100	79.88	80.52
2	374.16411	374.16461	1.35	21.76	20.97	17.38	16.89
3	375.16622	375.16698	2.02	2.89	2.92	2.31	2.35
4	376.1728	376.16934	-9.19	0.54	0.3	0.43	0.25

--- End Of Report ---

HPLC

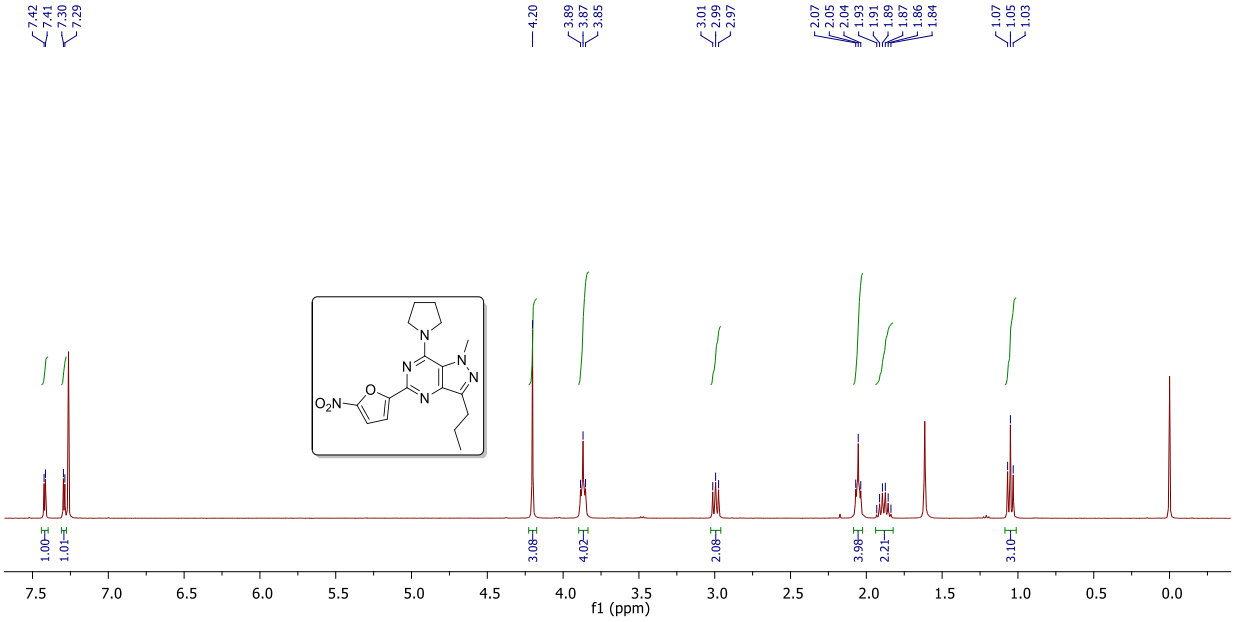


2: 254 nm, 8 nm

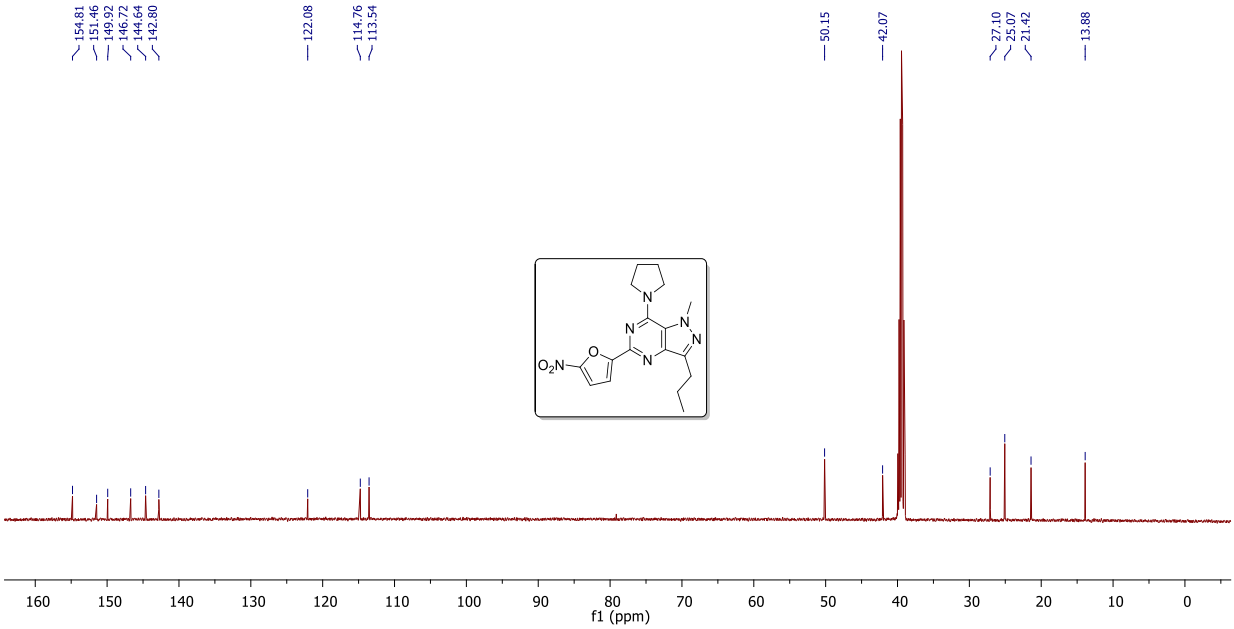
Pk #	Retention Time	Area	Area %	Height	Height %
1	24.427	120621	0.473	2660	0.101
2	34.933	25386197	99.527	2629592	99.899
Totals		25506818	100.000	2632252	100.000

Compound (11)

^{1}H NMR in $CDCl_3$

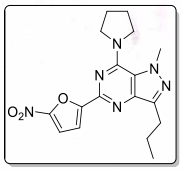


^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report



Data File	GLR-4.d	**Sample Name**	GLR-4
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Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/18/2012 1:05:08 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

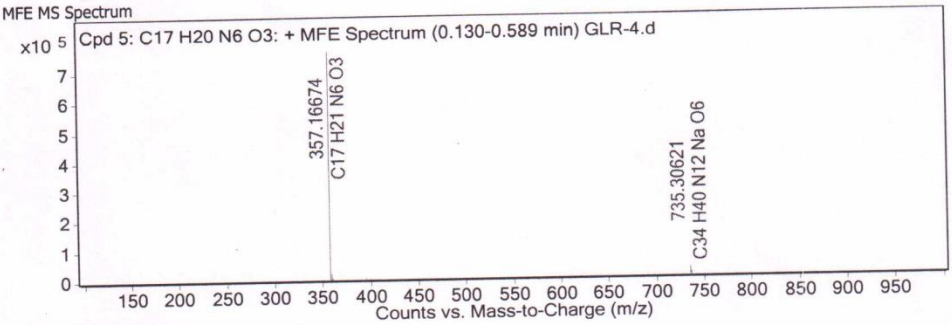
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C17 H20 N6 O3	0.172	356.15946	C17 H20 N6 O3	C17 H20 N6 O3	0.65	C17 H20 N6 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C17 H20 N6 O3	357.16674	0.172	Find by Molecular Feature	356.15946

MFE MS Spectrum



MS Spectrum Peak List

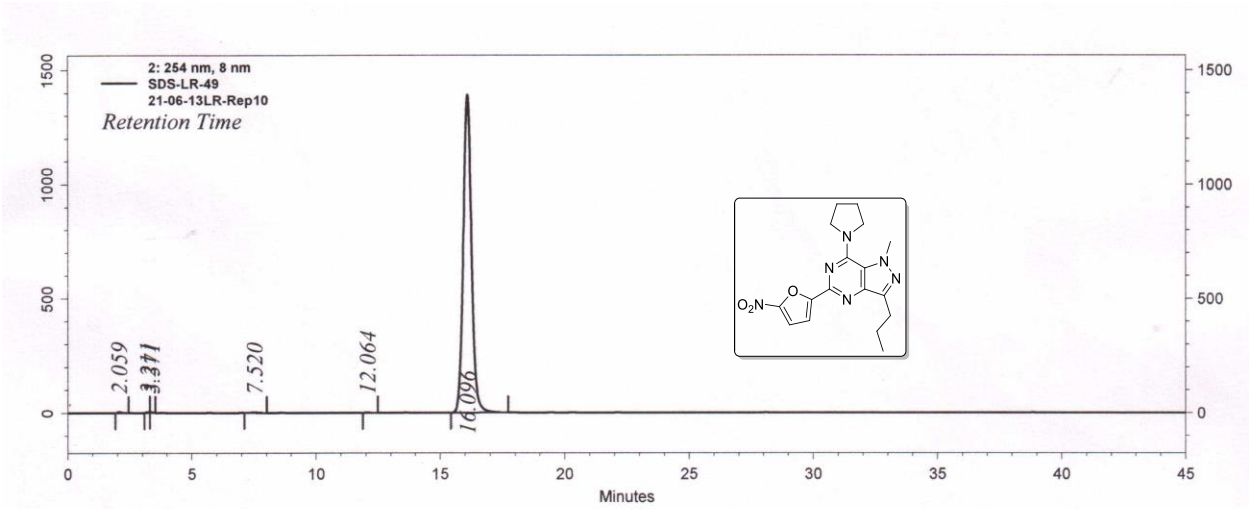
m/z	z	Abund	Formula	Ion
357.16674	1	768028.4	C17 H21 N6 O3	(M+H)+
358.16916	1	139494	C17 H21 N6 O3	(M+H)+
359.17205	1	19945	C17 H21 N6 O3	(M+H)+
360.174	1	2781.2	C17 H21 N6 O3	(M+H)+
395.12085	1	3667.1	C17 H20 K N6 O3	(M+K)+
713.32567	1	1339.9	C34 H41 N12 O6	(2M+H)+
735.30621	1	25984.2	C34 H40 N12 Na O6	(2M+Na)+
736.30976	1	10434.4	C34 H40 N12 Na O6	(2M+Na)+
737.31306	1	2889.4	C34 H40 N12 Na O6	(2M+Na)+
751.27874	1	1425.7		(2M+K)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	357.16674	357.16697	0.64	100	100	82.56	80.71
2	358.16916	358.1697	1.51	18.16	20.93	15	16.9
3	359.17205	359.17212	0.19	2.6	2.7	2.14	2.18
4	360.174	360.1745	1.39	0.36	0.26	0.3	0.21

--- End Of Report ---

HPLC

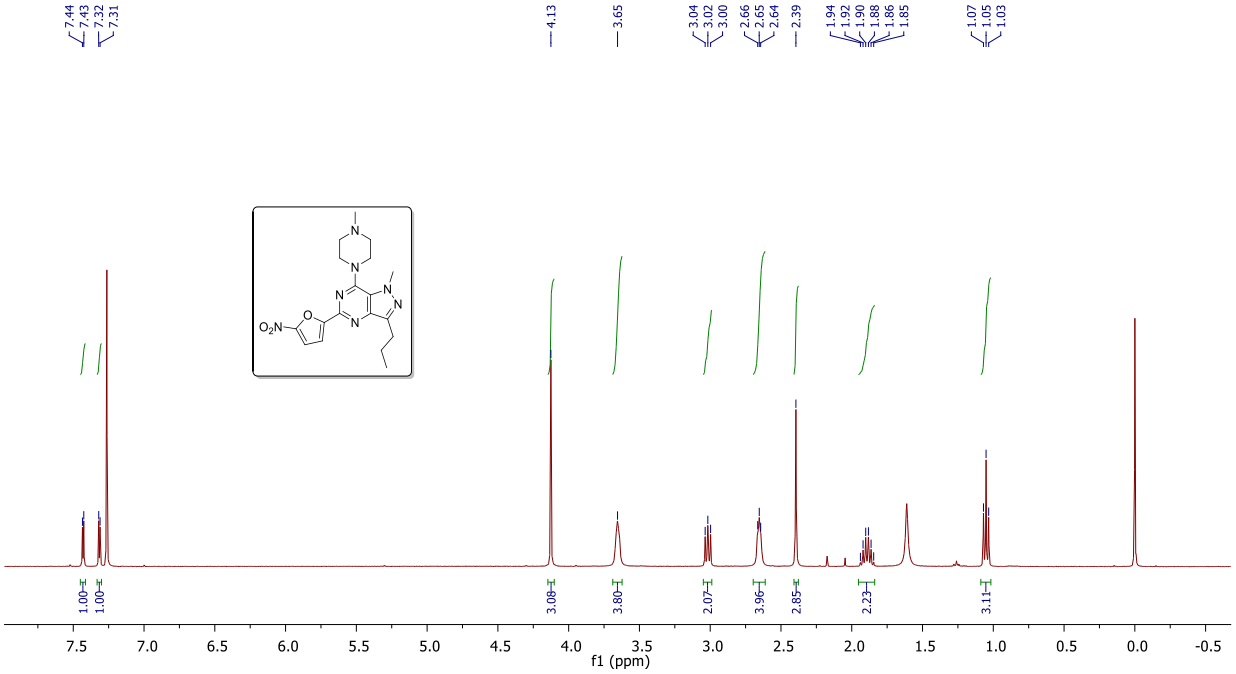


2: 254 nm, 8 nm

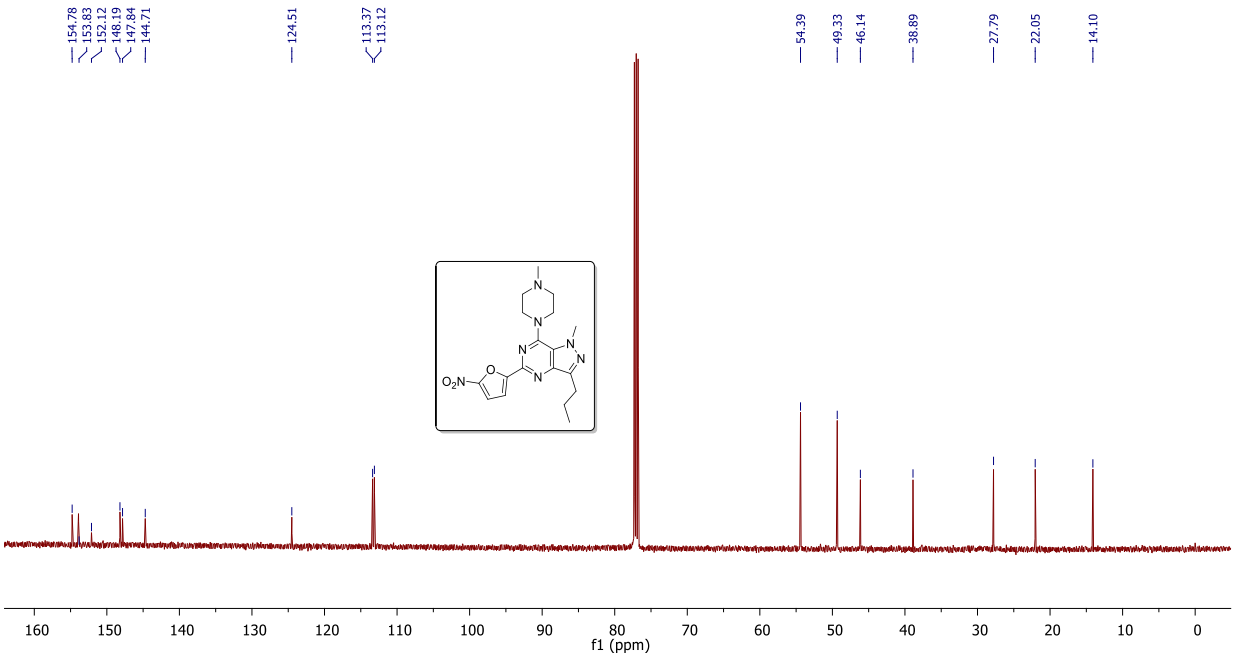
Pk #	Retention Time	Area	Area %	Height	Height %
1	2.059	50179	0.156	4345	0.310
2	3.211	11643	0.036	1731	0.124
3	3.371	11268	0.035	1868	0.133
4	7.520	42194	0.131	1902	0.136
5	12.064	11216	0.035	729	0.052
6	16.096	32033014	99.607	1390578	99.245
Totals		32159514	100.000	1401153	100.000

Compound (12)

^{1}H NMR in $CDCl_3$



^{13}C NMR in $CDCl_3$



HRMS

Qualitative Compound Report

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Sample Type	Sample	**Position**	Vial 17
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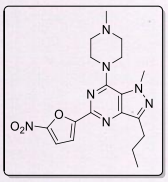
Comment			



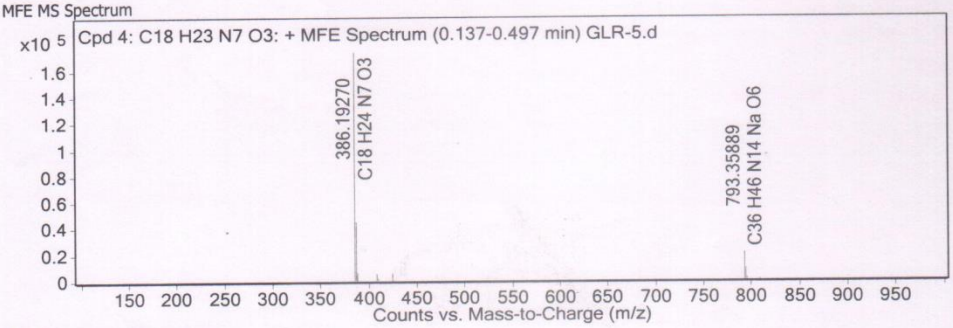
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C18 H23 N7 O3	0.173	385.18543	C18 H23 N7 O3	C18 H23 N7 O3	2.1	C18 H23 N7 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C18 H23 N7 O3	386.1927	0.173	Find by Molecular Feature	385.18543

MFE MS Spectrum



MS Spectrum Peak List

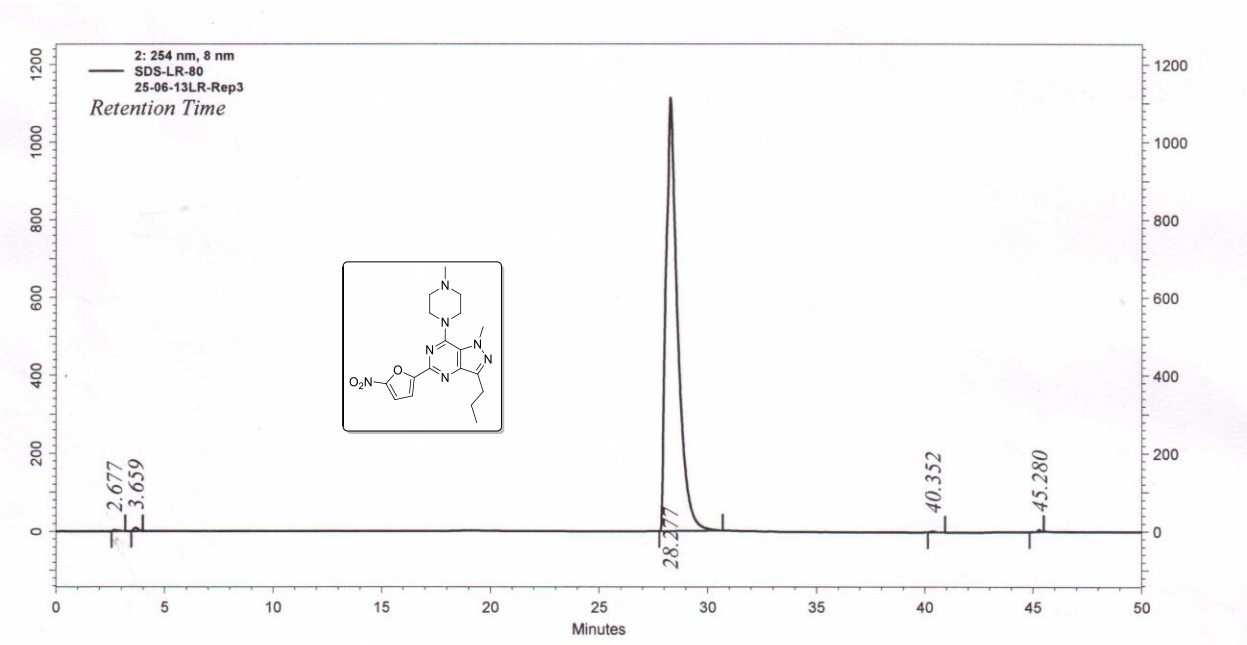
m/z	z	Abund	Formula	Ion
386.1927	1	174231.3	C18 H24 N7 O3	(M+H)+
387.19537	1	44957.3	C18 H24 N7 O3	(M+H)+
388.19784	1	6231.9	C18 H24 N7 O3	(M+H)+
408.17537	1	5719.9	C18 H23 N7 Na O3	(M+Na)+
409.17608	1	1923.6	C18 H23 N7 Na O3	(M+Na)+
424.14983	1	5337	C18 H23 K N7 O3	(M+K)+
793.35889	1	20263.4	C36 H46 N14 Na O6	(2M+Na)+
794.36056	1	8667.9	C36 H46 N14 Na O6	(2M+Na)+
795.36628	1	1957.3	C36 H46 N14 Na O6	(2M+Na)+
809.32941	1	1257.5		(2M+K)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	386.1927	386.19351	2.1	100	100	77.29	79.72
2	387.19537	387.19619	2.11	25.8	22.42	19.94	17.87
3	388.19784	388.19861	1.99	3.58	3.02	2.76	2.41

--- End Of Report ---

HPLC

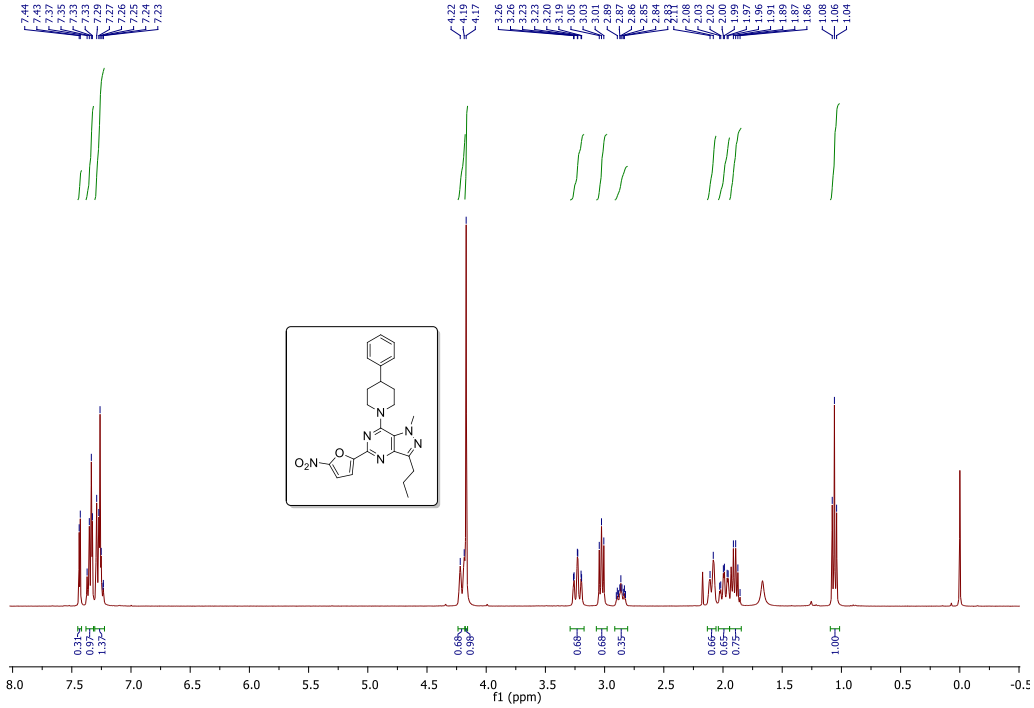


2: 254 nm, 8 nm

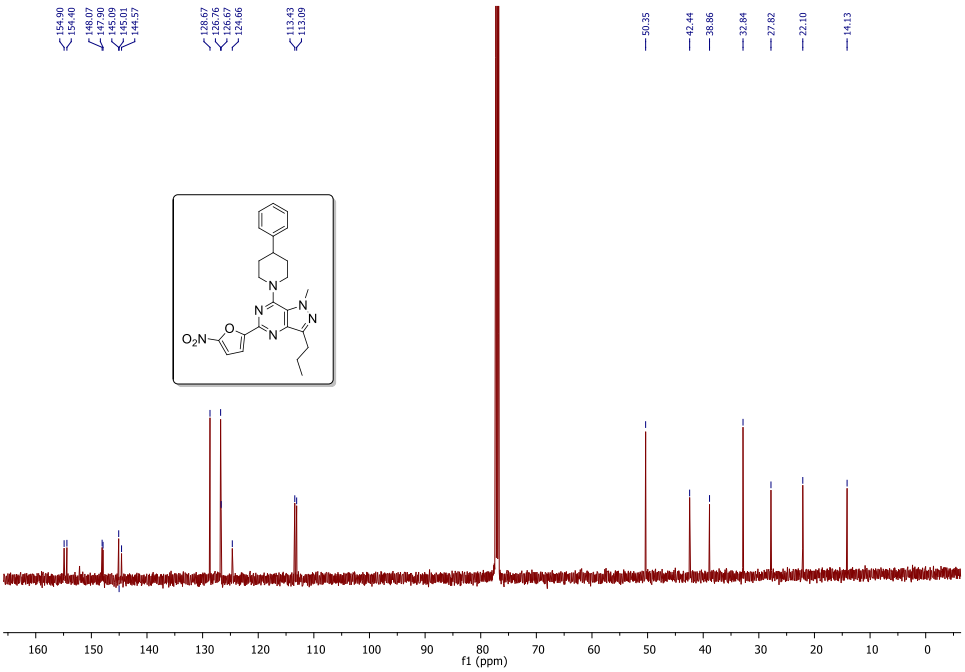
Pk #	Retention Time	Area	Area %	Height	Height %
1	2.677	50847	0.122	3231	0.285
2	3.659	120638	0.291	8897	0.786
3	28.277	41262011	99.386	1112491	98.255
4	40.352	42597	0.103	2730	0.241
5	45.280	40967	0.099	4901	0.433
Totals		41517060	100.000	1132250	100.000

Compound (13)

^{1}H NMR in $CDCl_3$



^{13}C NMR in $CDCl_3$



HRMS

Qualitative Compound Report

Data File	GLR-7.d	**Sample Name**	GLR-7
Sample Type	Sample	**Position**	Vial 19
Instrument Name	Instrument 1	**User Name**	
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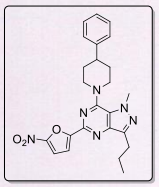
IRM Calibration Status	Success	**DA Method**	as.m
Comment			



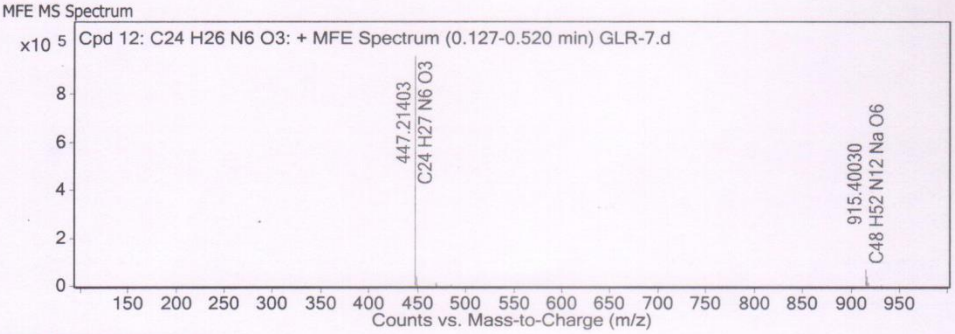
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 12: C24 H26 N6 O3	0.172	446.20674	C24 H26 N6 O3	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	0.172	Find by Molecular Feature	446.20674

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
447.21403	1	958164.8	C24 H27 N6 O3	(M+H)+
448.21645	1	237876.4	C24 H27 N6 O3	(M+H)+
449.21835	1	41806.9	C24 H27 N6 O3	(M+H)+
450.22169	1	4009.4	C24 H27 N6 O3	(M+H)+
469.19481	1	14297.8	C24 H26 N6 Na O3	(M+Na)+
470.19727	1	5903.1	C24 H26 N6 Na O3	(M+Na)+
485.16837	1	6056.8	C24 H26 K N6 O3	(M+K)+
915.4003	1	67070.6	C48 H52 N12 Na O6	(2M+Na)+
916.40256	1	41161.3	C48 H52 N12 Na O6	(2M+Na)+
917.40665	1	13327.1	C48 H52 N12 Na O6	(2M+Na)+

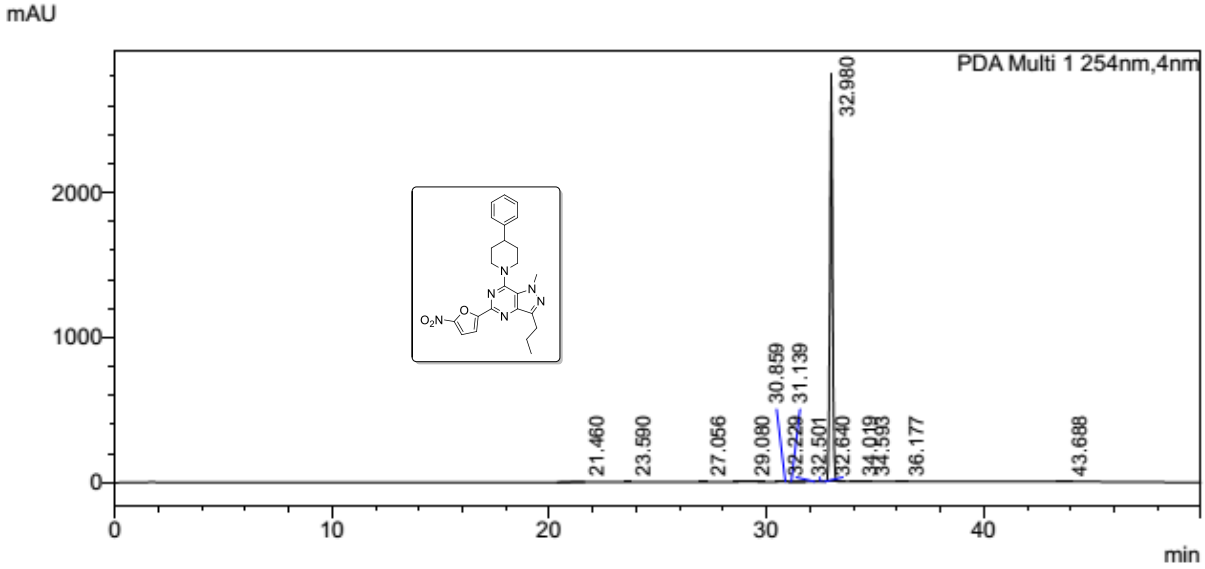
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	447.21403	447.21392	-0.25	100	100	77.1	74.79
2	448.21645	448.21682	0.84	24.83	28.57	19.14	21.37
3	449.21835	449.2195	2.54	4.36	4.55	3.36	3.41
4	450.22169	450.22206	0.82	0.42	0.52	0.32	0.39
5	451.2252	451.22459	-1.34	0.1	0.05	0.08	0.04

--- End Of Report ---

HPLC

<Chromatogram>



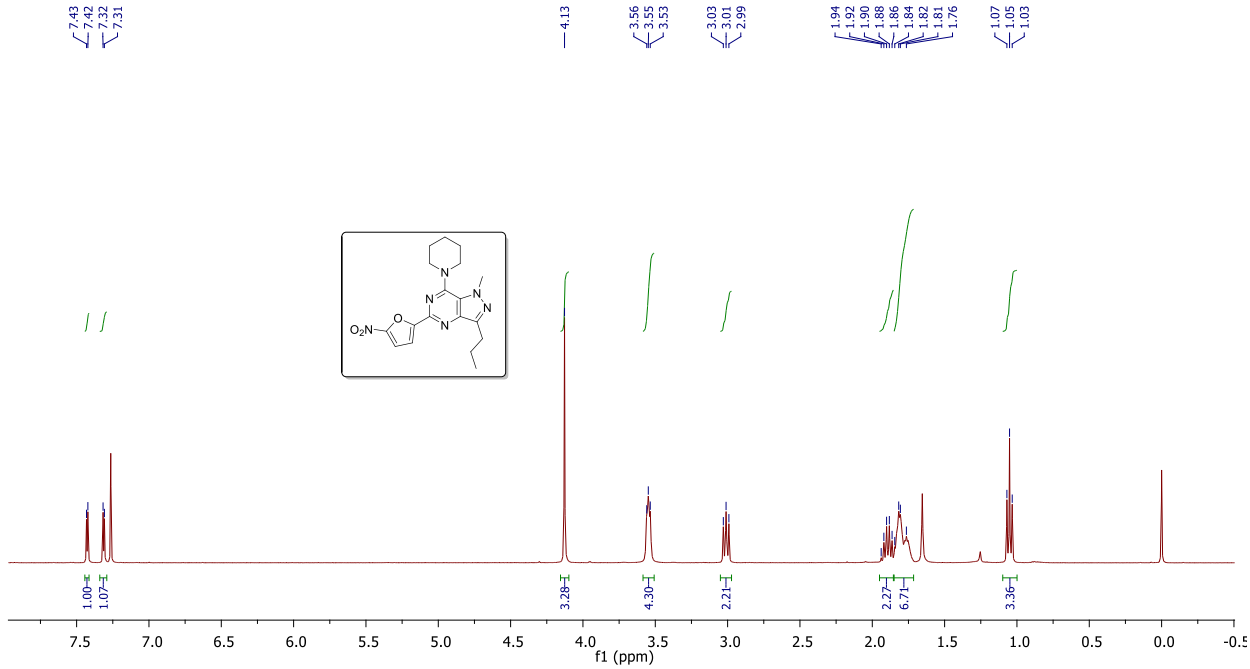
<Peak Table>

PDA Ch1 254nm

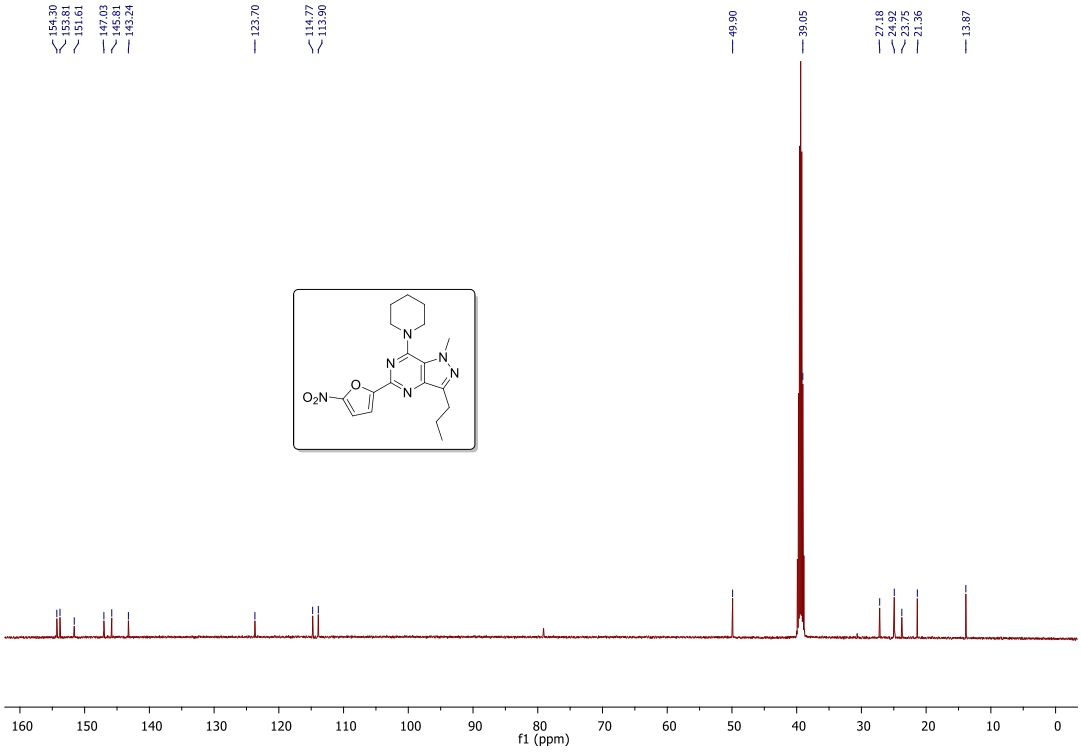
Peak#	Name	Ret. Time	Area	Height	Area%	Height%
1		21.460	17120	354	0.074	0.013
2		23.590	3788	356	0.016	0.013
3		27.056	2177	175	0.009	0.006
4		29.080	71506	2350	0.309	0.083
5		30.859	20834	979	0.090	0.035
6		31.139	22589	1010	0.098	0.036
7		32.229	6462	617	0.028	0.022
8		32.501	4944	475	0.021	0.017
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)

^{1}H NMR in $CDCl_3$

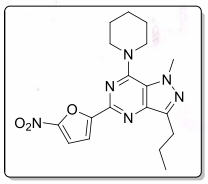


^{13}C NMR in DMSO-d6



Qualitative Compound Report

Data File	GLR-9.d	**Sample Name**	GLR-9
Sample Type	Sample	**Position**	Vial 21
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/18/2012 1:30:20 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			



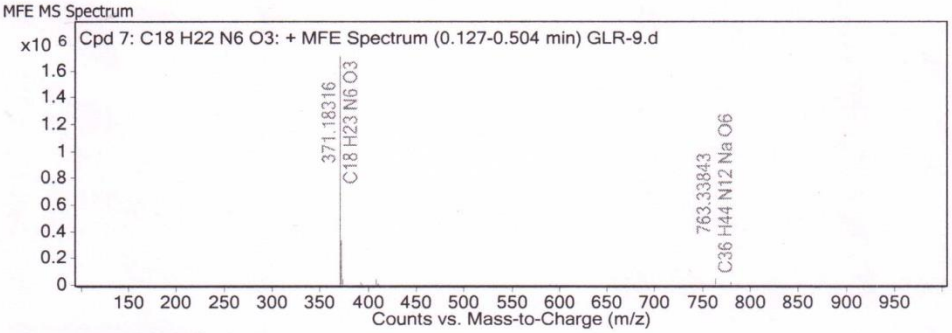
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C18 H22 N6 O3	0.171	370.17588	C18 H22 N6 O3	C18 H22 N6 O3	-1.47	C18 H22 N6 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C18 H22 N6 O3	371.18316	0.171	Find by Molecular Feature	370.17588

MFE MS Spectrum



MS Spectrum Peak List

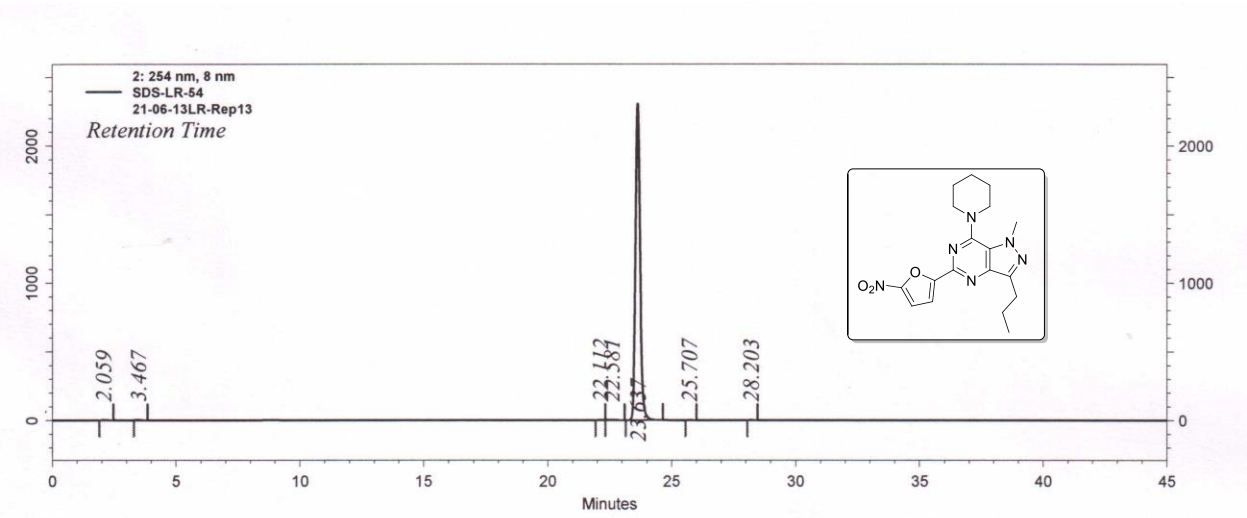
m/z	z	Abund	Formula	Ion
371.18316	1	1710306.3	C18 H23 N6 O3	(M+H)+
372.18545	1	338550.6	C18 H23 N6 O3	(M+H)+
373.1876	1	45875.7	C18 H23 N6 O3	(M+H)+
393.16348	1	19248.2	C18 H22 N6 Na O3	(M+Na)+
409.13775	1	42069.2	C18 H22 K N6 O3	(M+K)+
410.14165	1	11466.2	C18 H22 K N6 O3	(M+K)+
763.33843	1	40797.3	C36 H44 N12 Na O6	(2M+Na)+
764.34183	1	17335.7	C36 H44 N12 Na O6	(2M+Na)+
779.31155	1	19374.3	C36 H44 K N12 O6	(2M+K)+
780.31742	1	7708.8	C36 H44 K N12 O6	(2M+K)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	371.18316	371.18262	-1.48	100	100	81.43	79.83
2	372.18545	372.18538	-0.18	19.79	22.04	16.12	17.59
3	373.1876	373.18785	0.66	2.68	2.94	2.18	2.34
4	374.18971	374.19026	1.45	0.32	0.29	0.26	0.23

--- End Of Report ---

HPLC

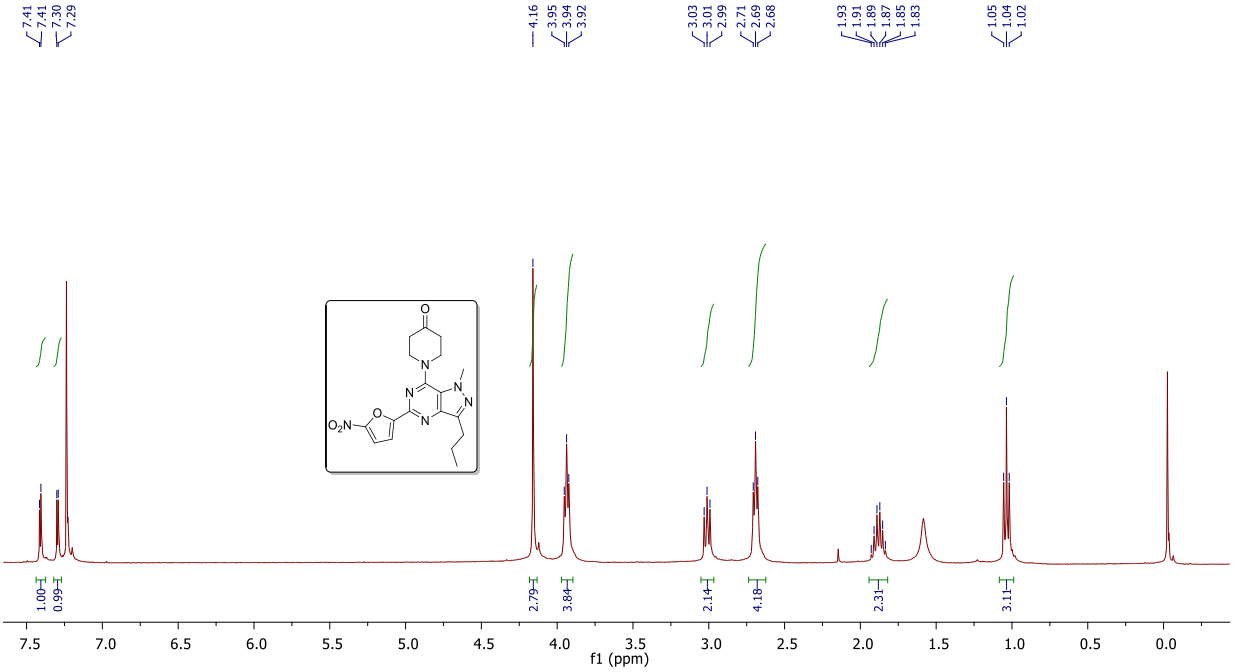


2: 254 nm, 8 nm

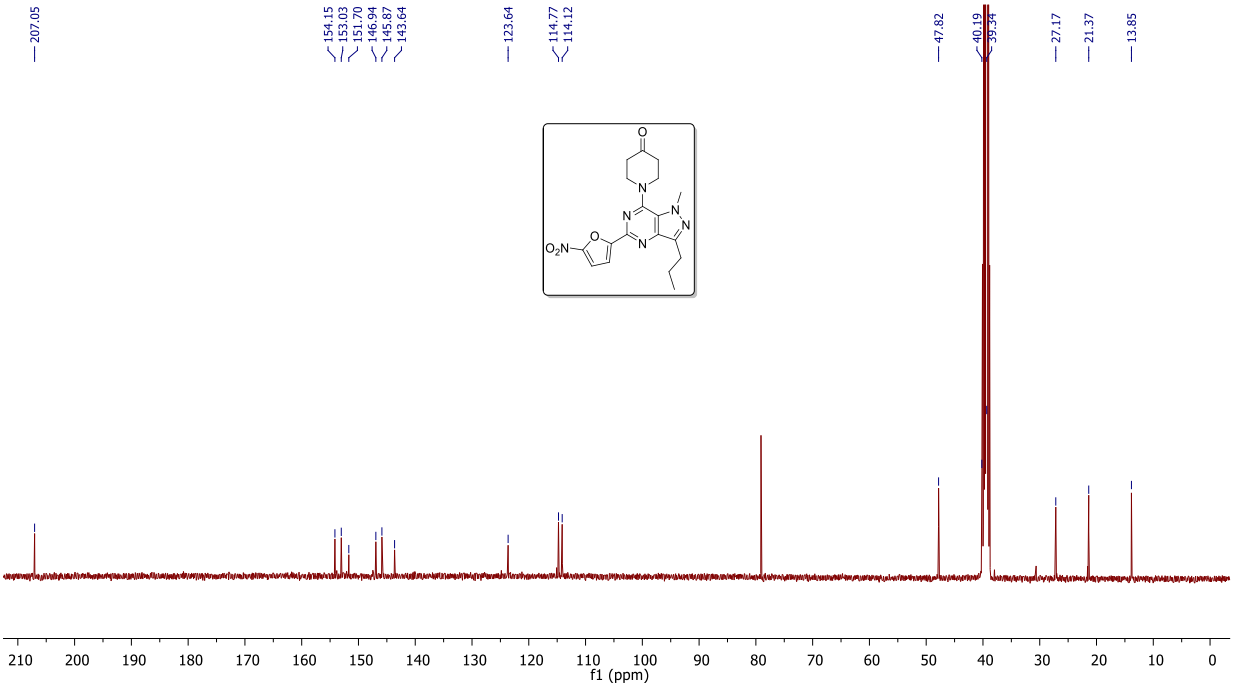
Pk #	Retention Time	Area	Area %	Height	Height %
1	2.059	32755	0.110	2637	0.114
2	3.467	35884	0.120	2626	0.113
3	22.112	18641	0.063	1584	0.068
4	22.581	36161	0.121	1764	0.076
5	23.637	29674419	99.500	2306441	99.523
6	25.707	13912	0.047	1267	0.055
7	28.203	11652	0.039	1184	0.051
Totals		29823424	100.000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

Compound (15)

^{1}H NMR in $CDCl_3$

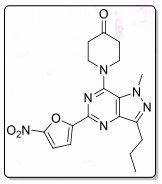


^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report



Data File	GLR-4-14.d	**Sample Name**	GLR-4-14
Sample Type	Sample	**Position**	Vial 13
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/19/2012 1:19:16 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

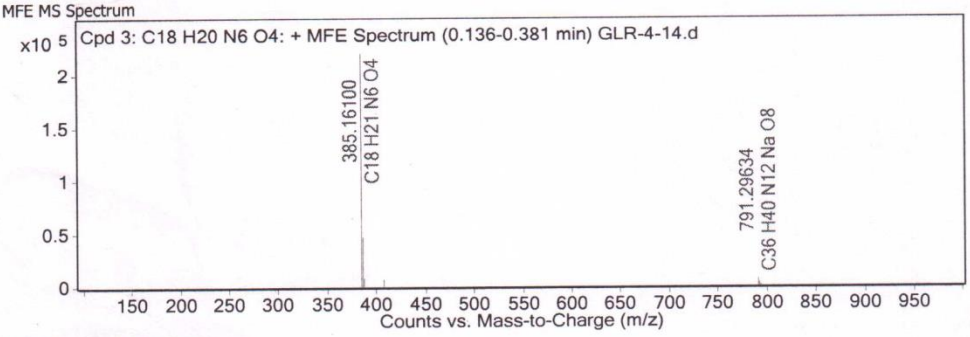
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C18 H20 N6 O4	0.172	384.15373	C18 H20 N6 O4	C18 H20 N6 O4	2.28	C18 H20 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C18 H20 N6 O4	385.161	0.172	Find by Molecular Feature	384.15373

MFE MS Spectrum



MS Spectrum Peak List

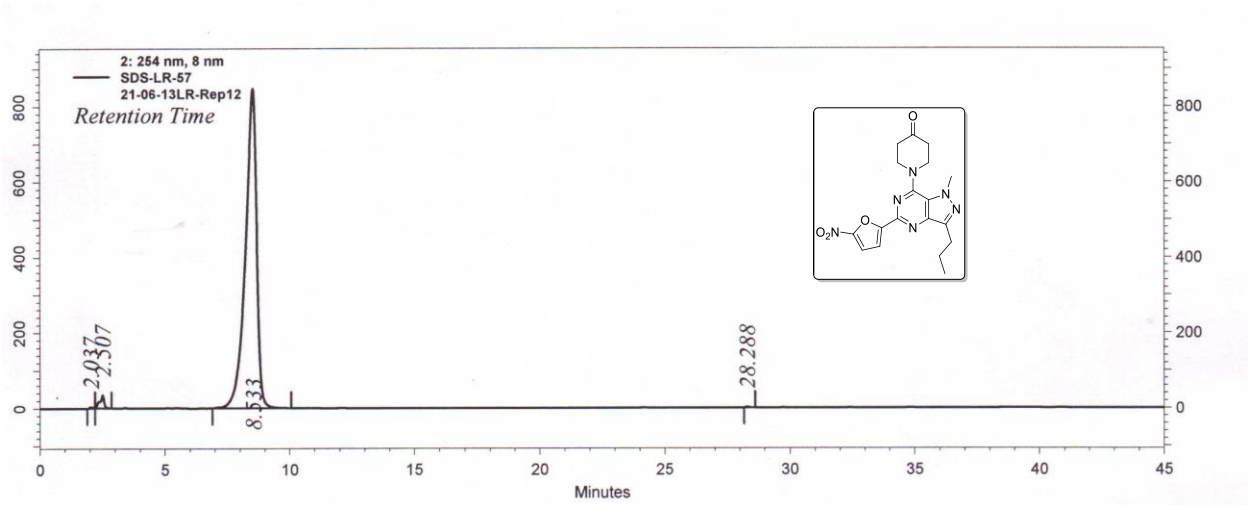
m/z	z	Abund	Formula	Ion
385.161	1	219860.1	C18 H21 N6 O4	(M+H)+
386.16381	1	46843.7	C18 H21 N6 O4	(M+H)+
387.16582	1	7415.2	C18 H21 N6 O4	(M+H)+
388.16683	1	926.5	C18 H21 N6 O4	(M+H)+
407.14279	1	7253.8	C18 H20 N6 Na O4	(M+Na)+
408.14394	1	1536.1	C18 H20 N6 Na O4	(M+Na)+
791.29634	1	6643.8	C36 H40 N12 Na O8	(2M+Na)+
792.29832	1	3234.9	C36 H40 N12 Na O8	(2M+Na)+
793.29771	1	761.9	C36 H40 N12 Na O8	(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	385.161	385.16188	2.27	100	100	79.94	79.66
2	386.16381	386.16464	2.17	21.31	22.05	17.03	17.57
3	387.16582	387.16705	3.18	3.37	3.14	2.7	2.5
4	388.16683	388.16943	6.71	0.42	0.34	0.34	0.27

End Of Report

HPLC

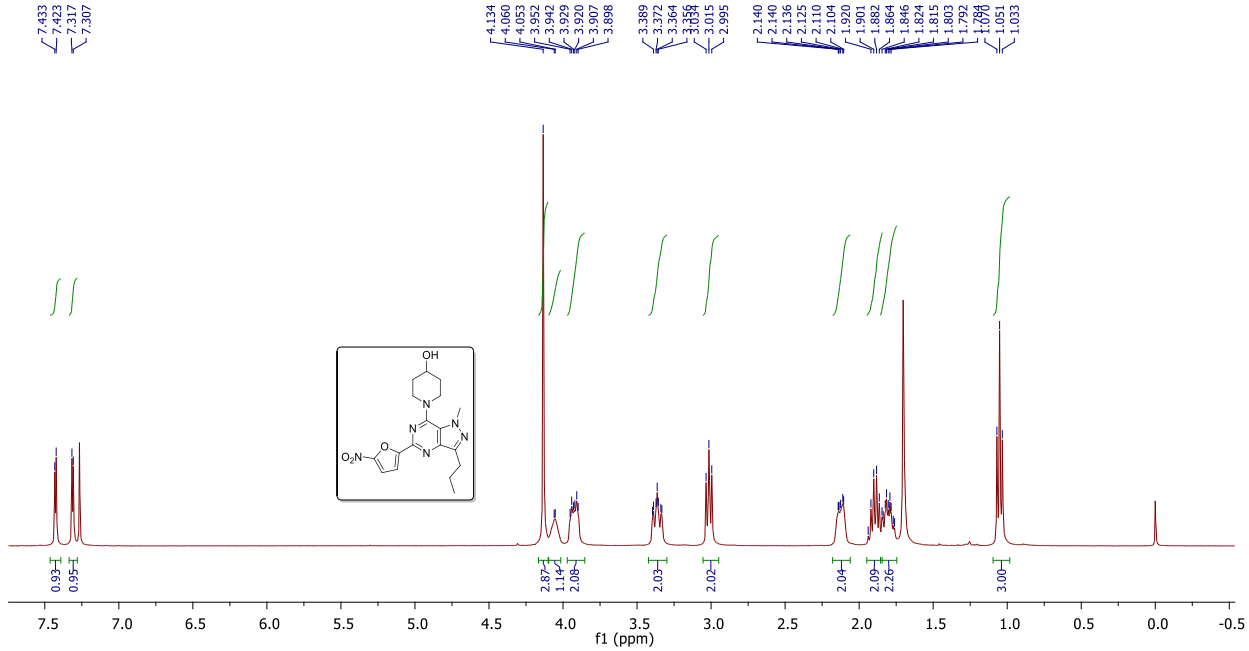


2: 254 nm, 8 nm

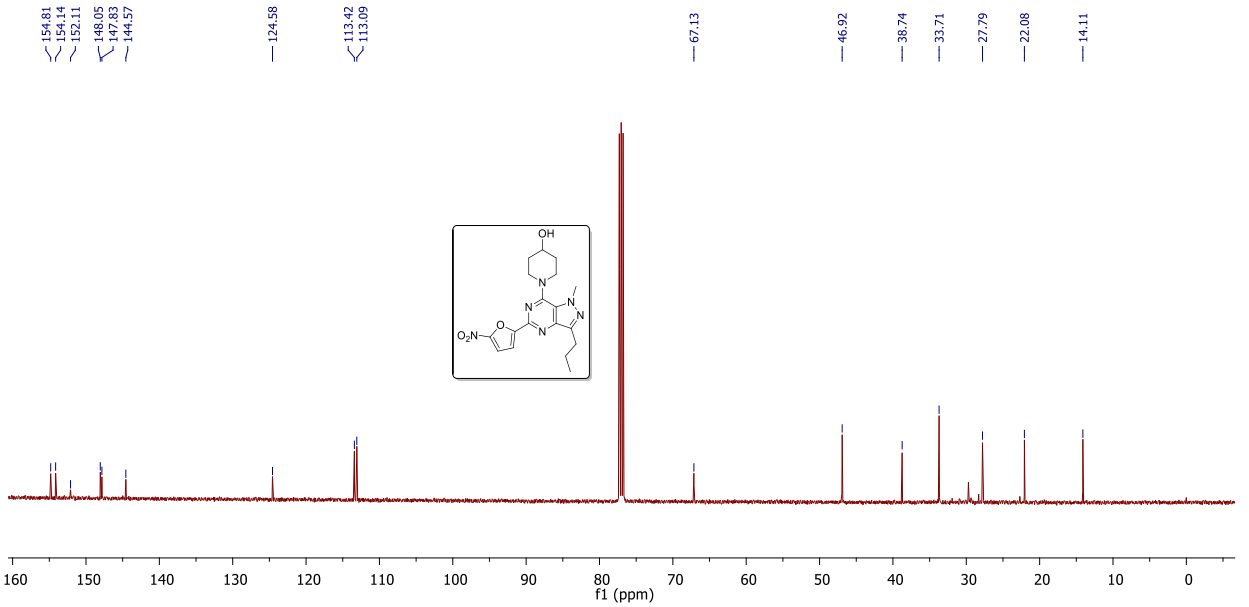
Pk #	Retention Time	Area	Area %	Height	Height %
1	2.037	25240	0.094	3142	0.354
2	2.507	411832	1.536	34736	3.917
3	8.533	26360654	98.315	847257	95.540
4	28.288	14583	0.054	1671	0.188
Totals		26812309	100.000	886806	100.000

Compound (16)

^{1}H NMR in $CDCl_3$



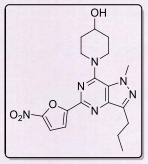
^{13}C NMR in $CDCl_3$



HRMS

Qualitative Compound Report

Data File	GLR-4-19.d	**Sample Name**	GLR-4-19
Sample Type	Sample	**Position**	Vial 15
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/19/2012 1:29:54 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			



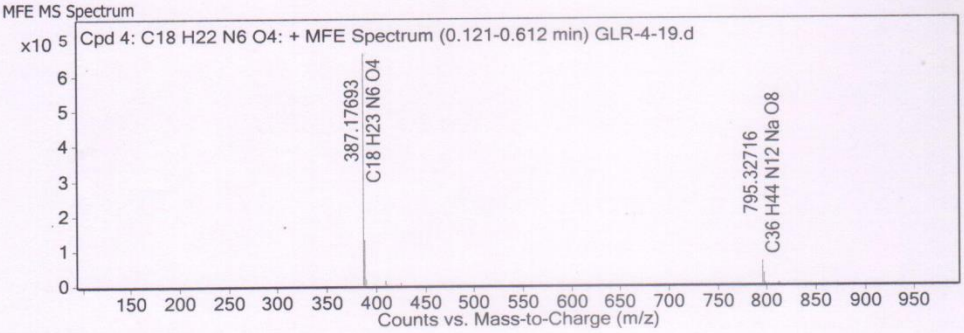
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C18 H22 N6 O4	0.171	386.16965	C18 H22 N6 O4	C18 H22 N6 O4	1.57	C18 H22 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C18 H22 N6 O4	387.17693	0.171	Find by Molecular Feature	386.16965

MFE MS Spectrum



MS Spectrum Peak List

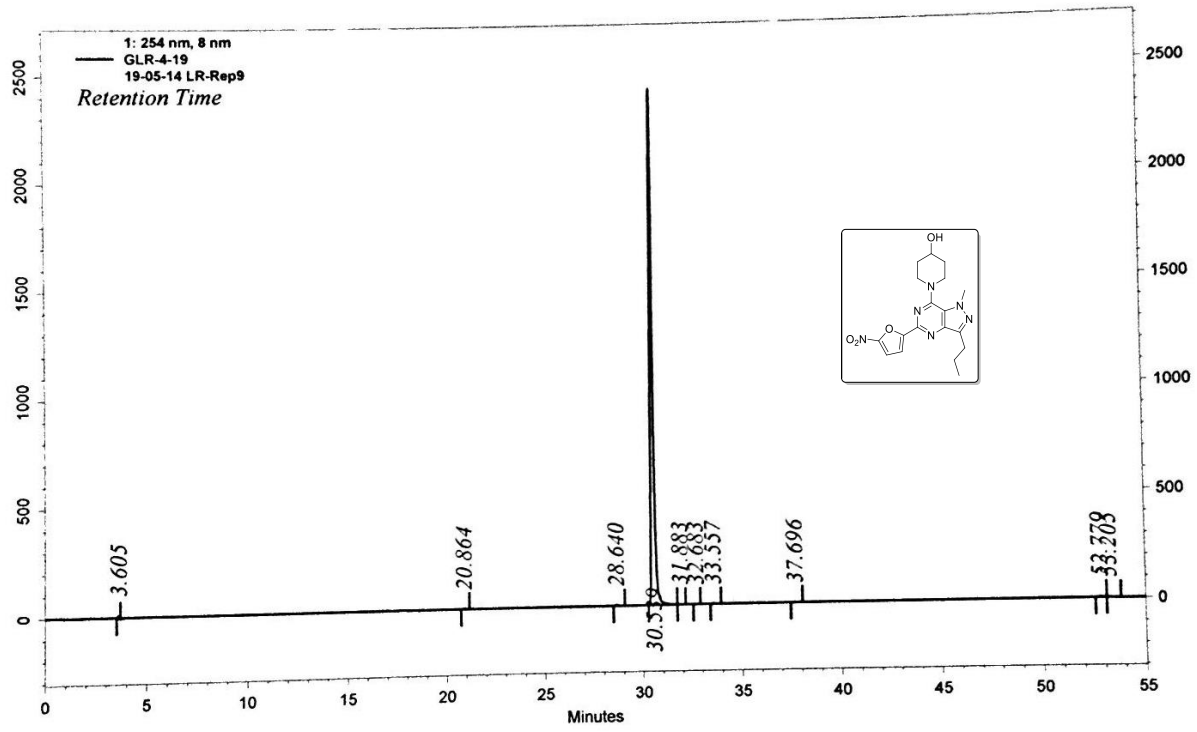
m/z	z	Abund	Formula	Ion
387.17693	1	665836.8	C18 H23 N6 O4	(M+H)+
388.17937	1	129635.9	C18 H23 N6 O4	(M+H)+
389.18176	1	17986.6	C18 H23 N6 O4	(M+H)+
409.15852	1	14909	C18 H22 N6 Na O4	(M+Na)+
410.16204	1	4156.8	C18 H22 N6 Na O4	(M+Na)+
425.1321	1	7910.5	C18 H22 K N6 O4	(M+K)+
795.32716	1	65967.1	C36 H44 N12 Na O8	(2M+Na)+
796.3302	1	30962.9	C36 H44 N12 Na O8	(2M+Na)+
797.33364	1	9136.1	C36 H44 N12 Na O8	(2M+Na)+
811.29841	1	2967		(2M+K)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	387.17693	387.17753	1.56	100	100	81.65	79.64
2	388.17937	388.1803	2.4	19.47	22.08	15.9	17.58
3	389.18176	389.1827	2.43	2.7	3.15	2.21	2.51
4	390.18225	390.18509	7.28	0.3	0.34	0.25	0.27

--- End Of Report ---

HPLC

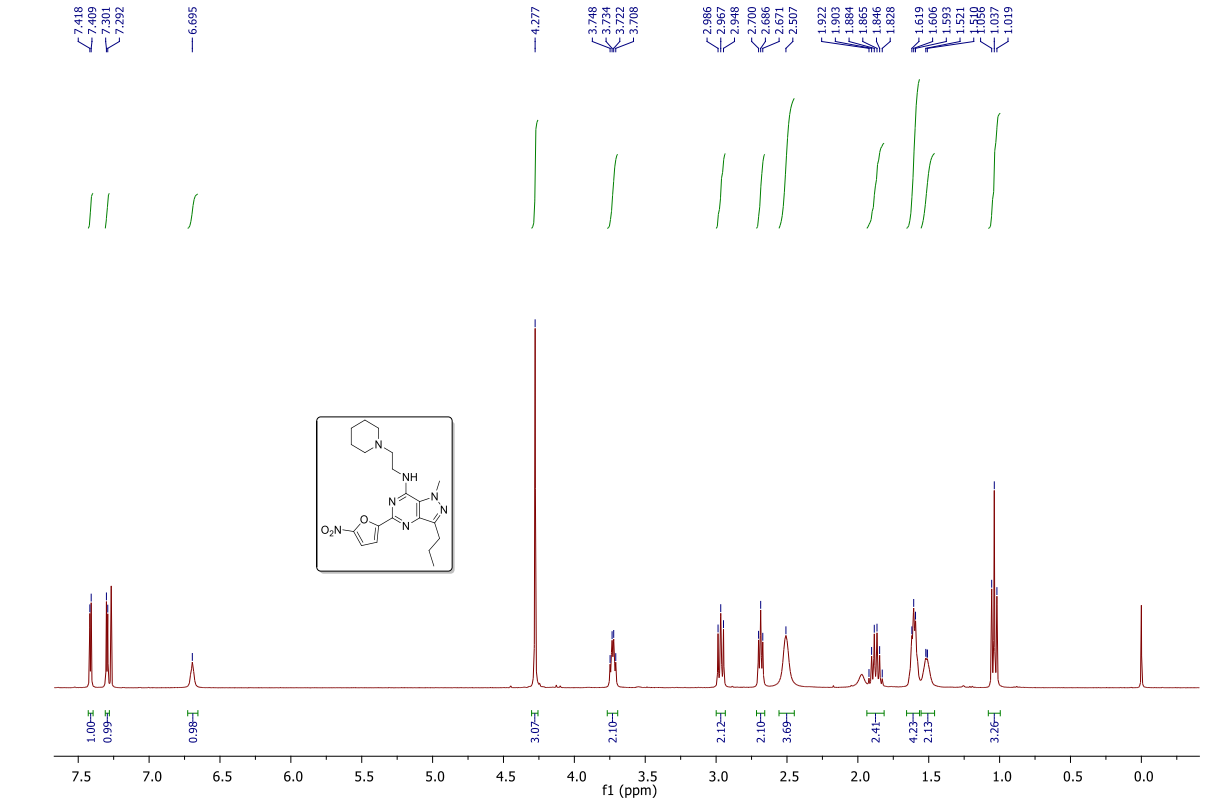


1: 254 nm, 8 nm

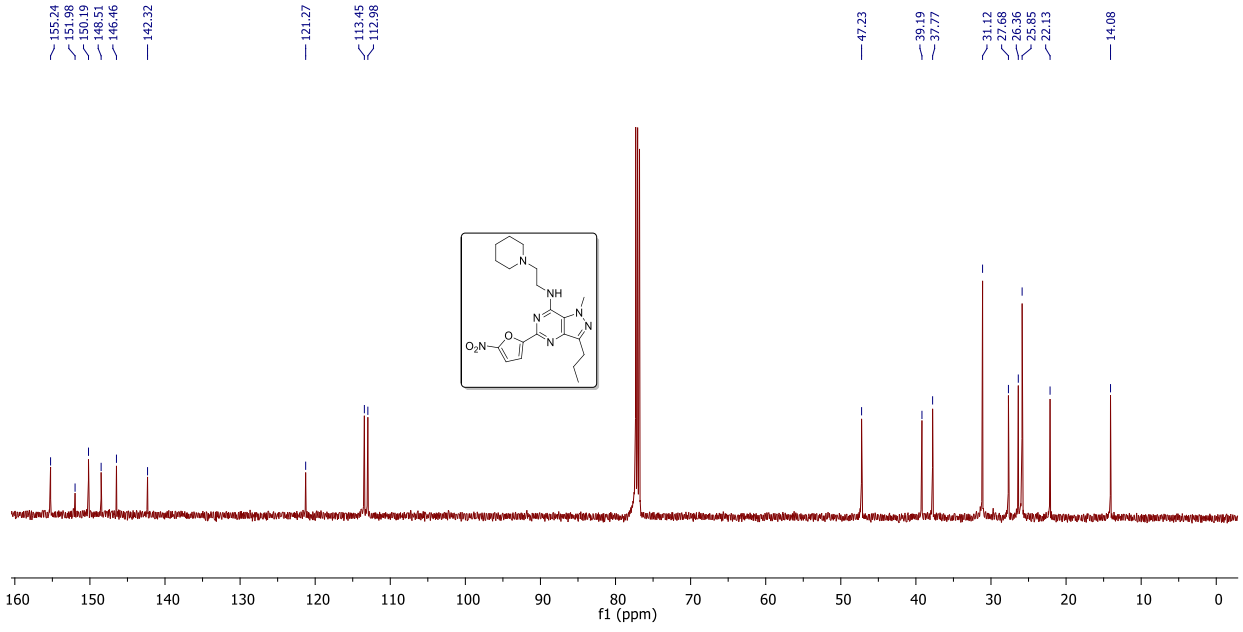
Pk #	Retention Time	Area	Area %	Height	Height %
1	3.605	54930	0.239	12794	0.524
2	20.864	17134	0.074	1898	0.078
3	28.640	32295	0.140	3312	0.136
4	30.539	22804023	99.052	2413038	98.879
5	31.883	11389	0.049	1313	0.054
6	32.683	10732	0.047	1208	0.050
7	33.557	26781	0.116	2355	0.097
8	37.696	12843	0.056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

Compound (17)

^{1}H NMR in $CDCl_3$



^{13}C NMR in $CDCl_3$

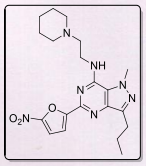


HRMS

Qualitative Compound Report

Data File	GLR-10.d	**Sample Name**	GLR-10
Sample Type	Sample	**Position**	Vial 22
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/18/2012 1:33:52 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

Sample Group **Info.**

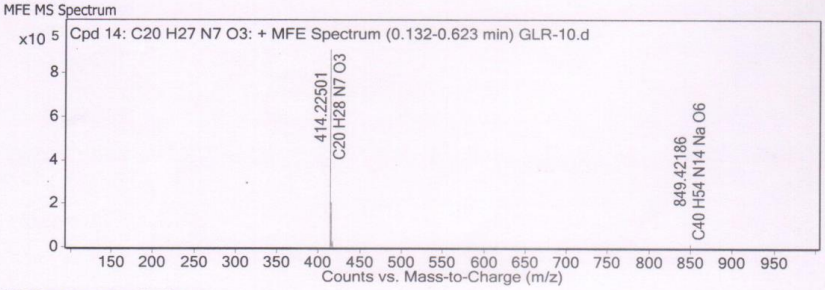


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 14: C20 H27 N7 O3	0.173	413.21772	C20 H27 N7 O3	C20 H27 N7 O3	-0.45	C20 H27 N7 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 14: C20 H27 N7 O3	414.22501	0.173	Find by Molecular Feature	413.21772

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
414.22501	1	908586.9	C20 H28 N7 O3	(M+H)+
415.22739	1	206451.9	C20 H28 N7 O3	(M+H)+
416.22999	1	29450.7	C20 H28 N7 O3	(M+H)+
417.23203	1	2957.2	C20 H28 N7 O3	(M+H)+
849.42186	1	12202.6	C40 H54 N14 Na O6	(2M+Na)+
850.42429	1	6220.1	C40 H54 N14 Na O6	(2M+Na)+
851.42824	1	1875.7	C40 H54 N14 Na O6	(2M+Na)+
852.42775	1	535.6	C40 H54 N14 Na O6	(2M+Na)+
865.39336	1	1432.2		(2M+K)+
866.39198	1	1341.6		(2M+K)+

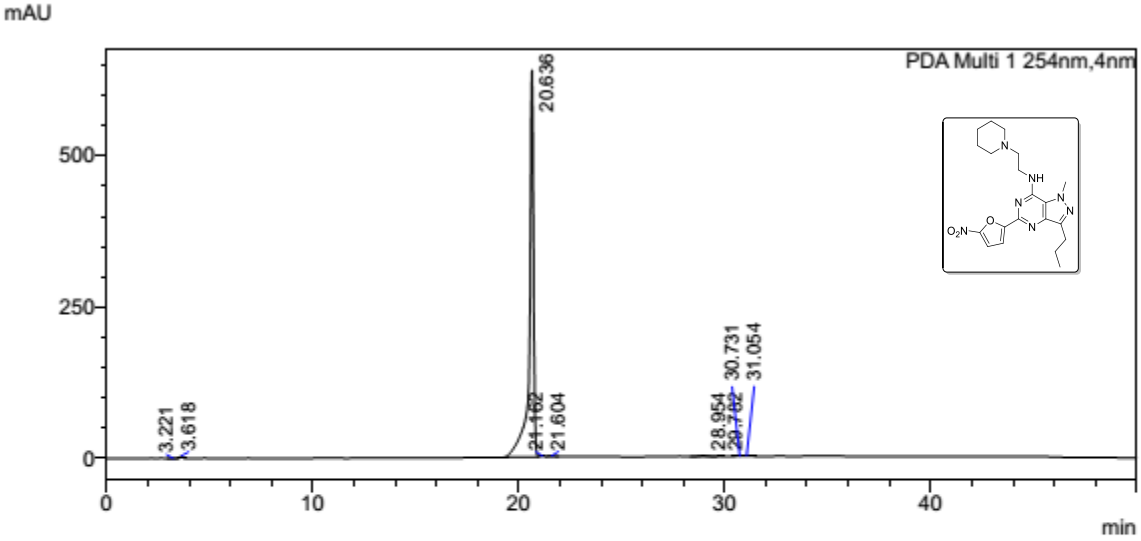
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	414.22501	414.22481	-0.46	100	100	79.18	77.81
2	415.22739	415.22755	0.39	22.72	24.63	17.99	19.16
3	416.22999	416.23005	0.15	3.24	3.53	2.57	2.74
4	417.23203	417.23247	1.06	0.33	0.37	0.26	0.29

--- End Of Report ---

HPLC

<Chromatogram>



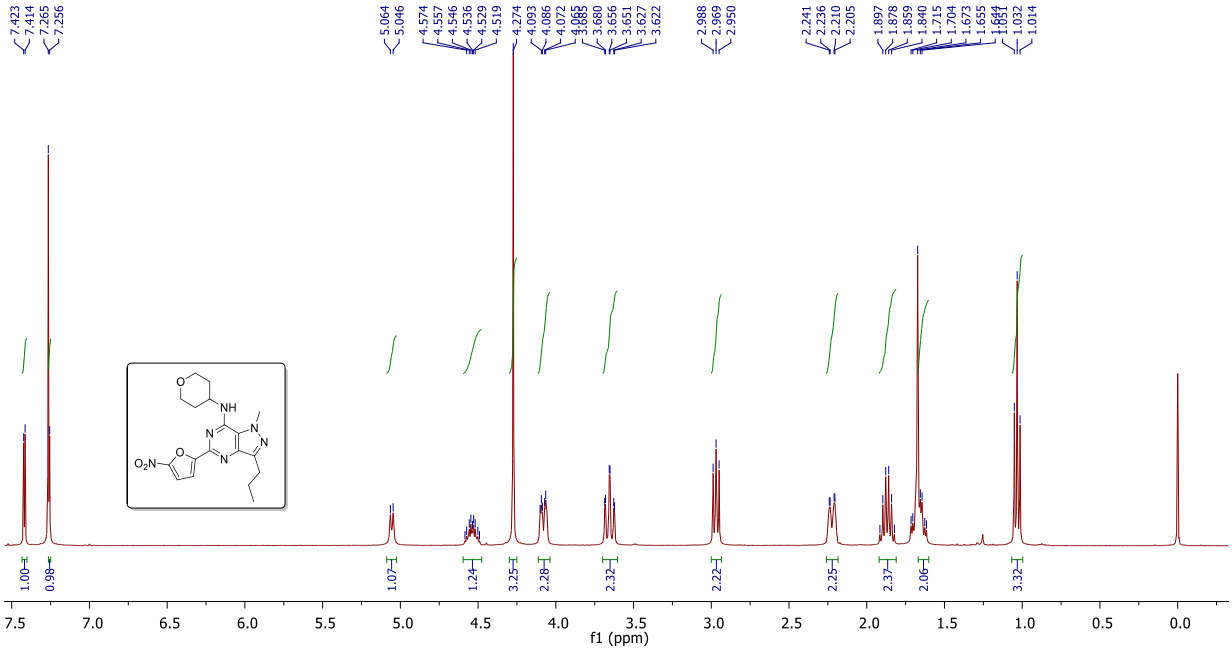
<Peak Table>

PDA Ch1 254nm

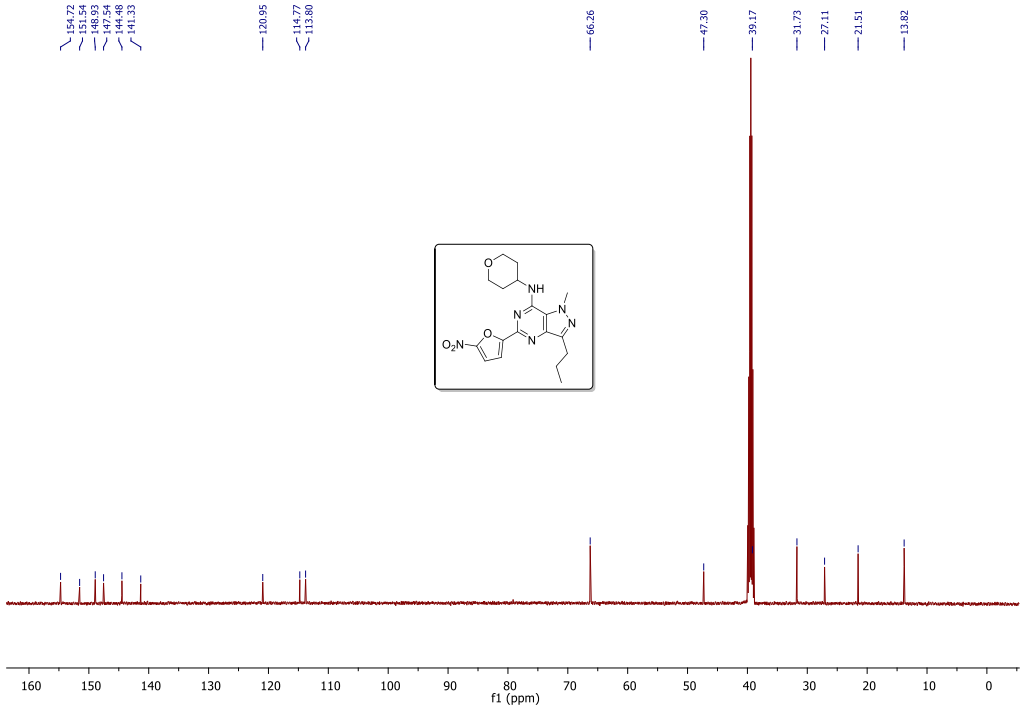
Peak#	Name	Ret. Time	Area	Height	Area%	Height%
1		3.221	4892	202	0.053	0.031
2		3.618	30622	4216	0.335	0.649
3		20.636	8993546	639635	98.284	98.493
4		21.162	13128	781	0.143	0.120
5		21.604	20699	1021	0.226	0.157
6		28.954	53571	1766	0.585	0.272
7		29.782	4796	428	0.052	0.066
8		30.731	13181	643	0.144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

Compound (18)

^{1}H NMR in $CDCl_3$



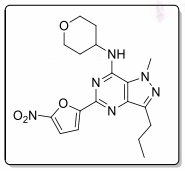
^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report

Data File	GLR-A-48.d	**Sample Name**	GLR-A-48
Sample Type	Sample	**Position**	Vial 14
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-07-2013 PM 1:28:07
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



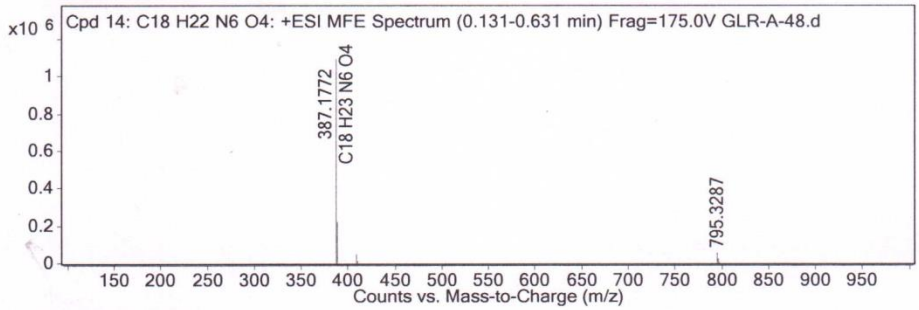
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 14: C18 H22 N6 O4	0.195	386.17	C18 H22 N6 O4	C18 H22 N6 O4	0.59	C18 H22 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 14: C18 H22 N6 O4	387.1772	0.195	Find by Molecular Feature	386.17

MFE MS Spectrum



MS Spectrum Peak List

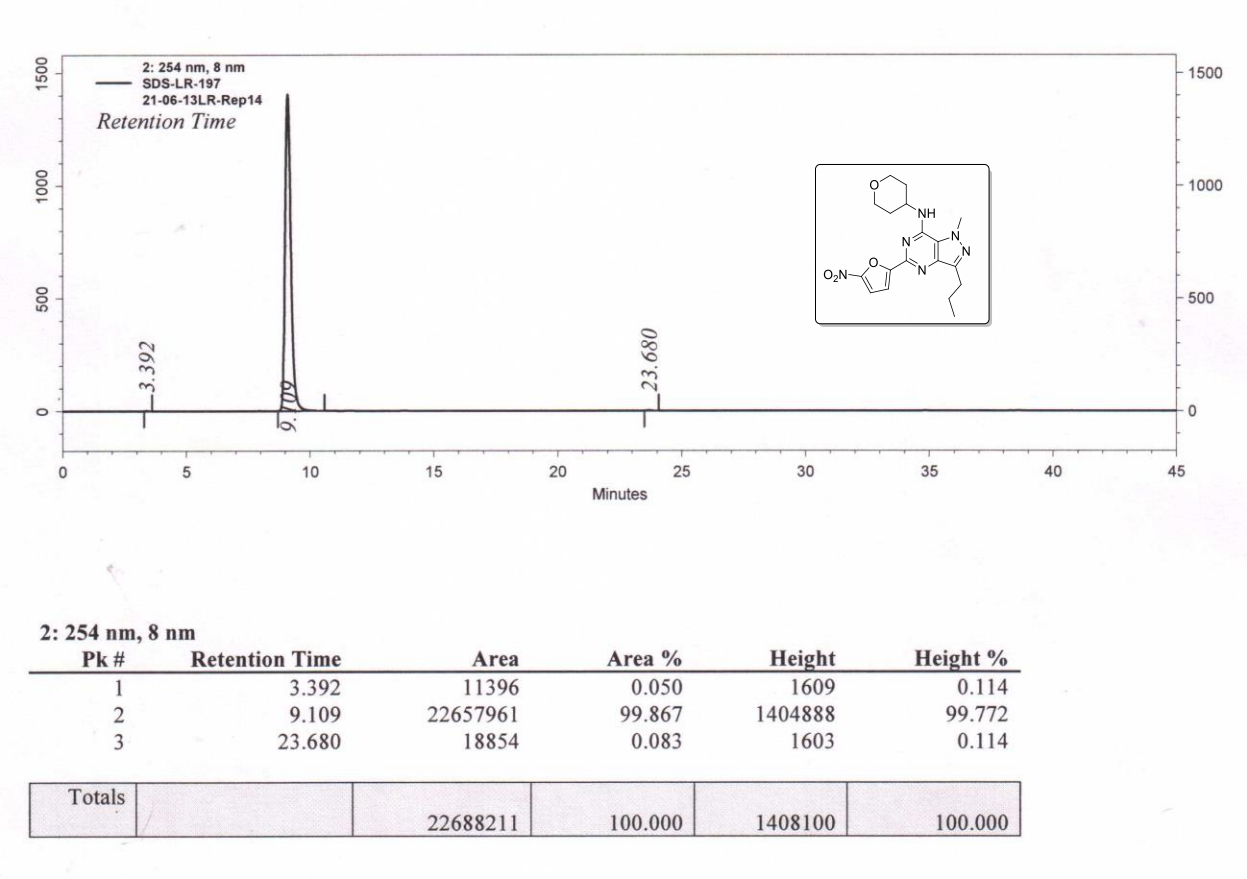
m/z	z	Abund	Formula	Ion
387.1772	1	1093888.25	C18 H23 N6 O4	(M+H)+
388.1803	1	220139.39	C18 H23 N6 O4	(M+H)+
389.1824	1	31397.39	C18 H23 N6 O4	(M+H)+
390.1851	1	2936.56	C18 H23 N6 O4	(M+H)+
409.1589	1	50376.5	C18 H22 N6 Na O4	(M+Na)+
410.1621	1	11997.29	C18 H22 N6 Na O4	(M+Na)+
411.1655	1	1583.14	C18 H22 N6 Na O4	(M+Na)+
795.3287	1	55847.41		(2M+Na)+
796.3303	1	22969.01		(2M+Na)+
797.3329	1	5699.03		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	387.1772	387.1775	0.72	100	100	81.13	79.64
2	388.1803	388.1803	-0.1	20.12	22.08	16.33	17.58
3	389.1824	389.1827	0.74	2.87	3.15	2.33	2.51
4	390.1851	390.1851	-0.11	0.27	0.34	0.22	0.27

--- End Of Report ---

HPLC

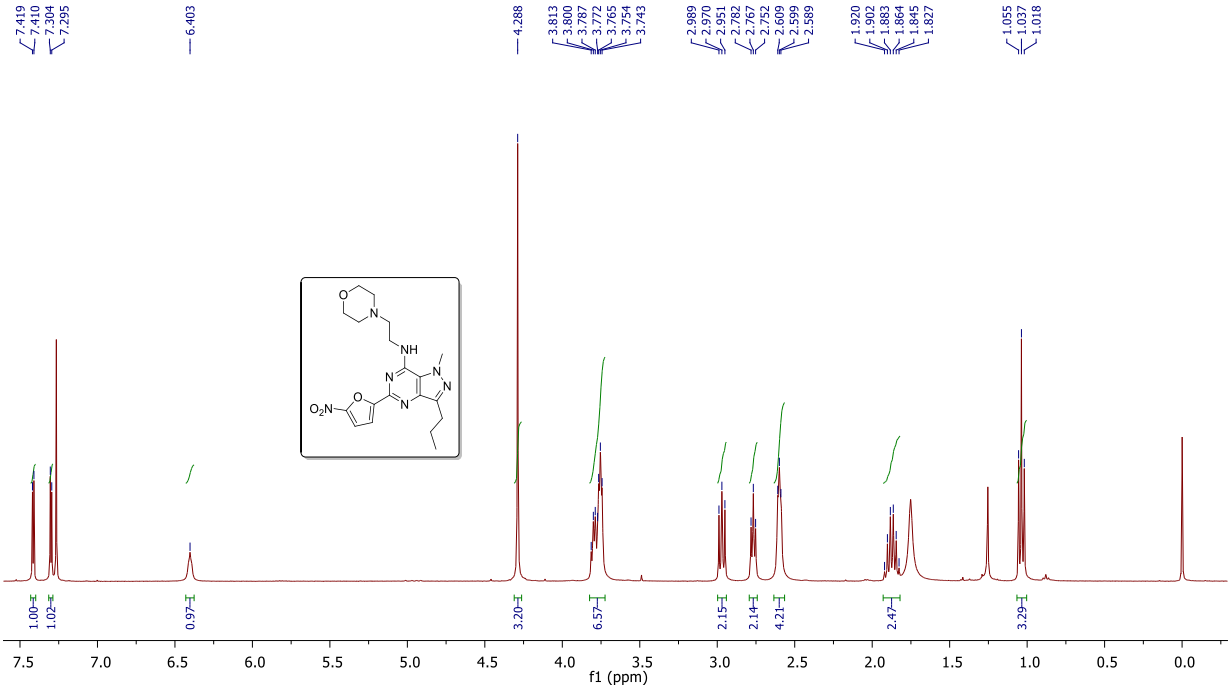


2: 254 nm, 8 nm

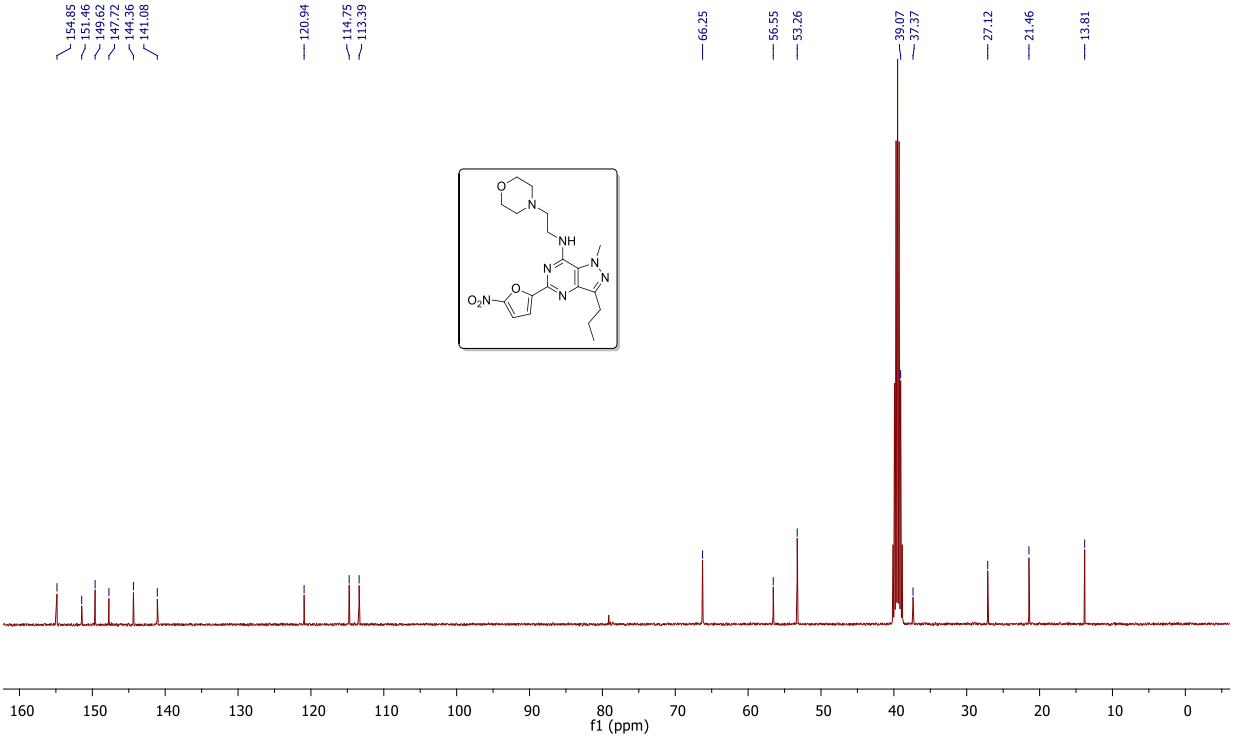
Pk #	Retention Time	Area	Area %	Height	Height %
1	3.392	11396	0.050	1609	0.114
2	9.109	22657961	99.867	1404888	99.772
3	23.680	18854	0.083	1603	0.114
Totals		22688211	100.000	1408100	100.000

Compound (19)

^{1}H NMR in $CDCl_3$



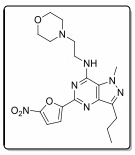
^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report

Data File	GLR-A-45.d	**Sample Name**	GLR-A-45
Sample Type	Sample	**Position**	Vial 13
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-07-2013 PM 1:23:34
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



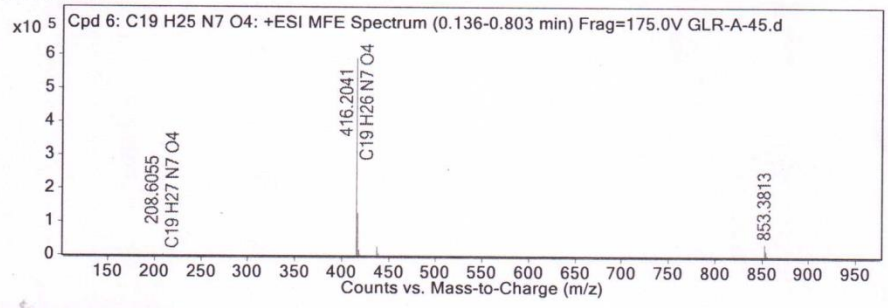
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C19 H25 N7 O4	0.196	415.1968	C19 H25 N7 O4	C19 H25 N7 O4	-0.06	C19 H25 N7 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C19 H25 N7 O4	416.2041	0.196	Find by Molecular Feature	415.1968

MFE MS Spectrum



MS Spectrum Peak List

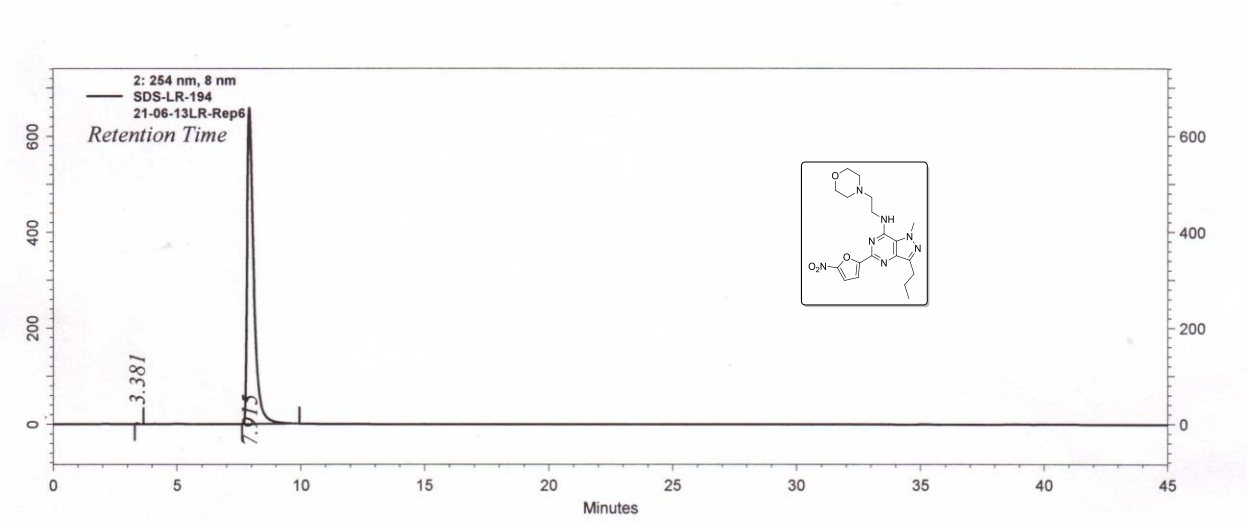
m/z	z	Abund	Formula	Ion
208.6055	2	4185.32	C19 H27 N7 O4	(M+2H)+2
416.2041	1	590204.56	C19 H26 N7 O4	(M+H)+
417.2067	1	126948.38	C19 H26 N7 O4	(M+H)+
418.2087	1	17805.35	C19 H26 N7 O4	(M+H)+
419.2121	1	2345.54	C19 H26 N7 O4	(M+H)+
438.1859	1	27460.32	C19 H25 N7 Na O4	(M+Na)+
439.1881	1	6409.97	C19 H25 N7 Na O4	(M+Na)+
853.3813	1	38166.36		(2M+Na)+
854.3845	1	17404.52		(2M+Na)+
855.3857	1	4655.52		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	208.6055	208.6057	1.06	100	100	82.34	78.71
2	209.1079	209.107	-4.35	14.93	23.57	12.29	18.55
3	209.6045	209.6082	17.69	6.52	3.48	5.37	2.74

--- End Of Report ---

HPLC

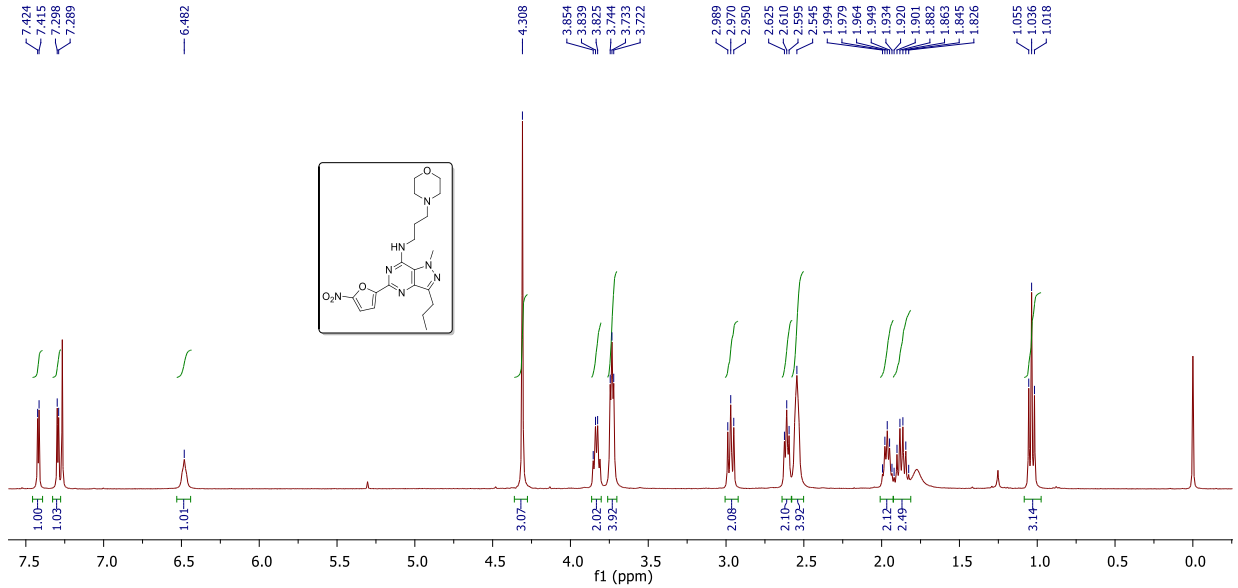


2: 254 nm, 8 nm

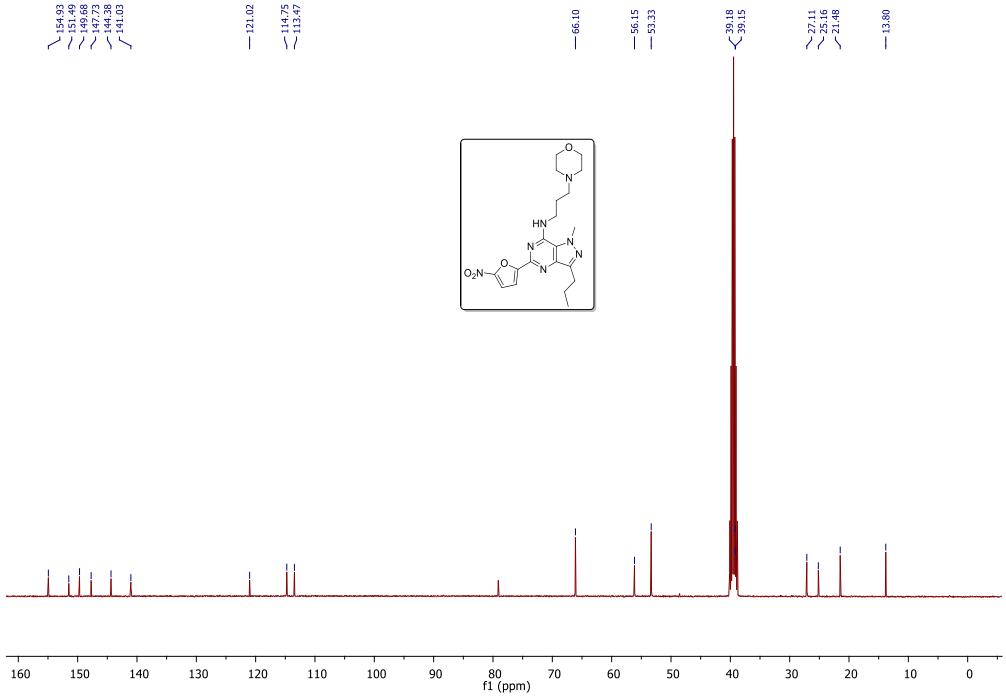
Pk #	Retention Time	Area	Area %	Height	Height %
1	3.381	12298	0.100	1764	0.267
2	7.915	12279122	99.900	658213	99.733
Totals		12291420	100.000	659977	100.000

Compound (20)

^{1}H NMR in $CDCl_3$



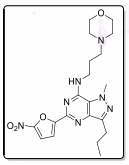
^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report

Data File	GLR-A-49.d	**Sample Name**	GLR-A-49
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-07-2013 PM 12:23:54
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



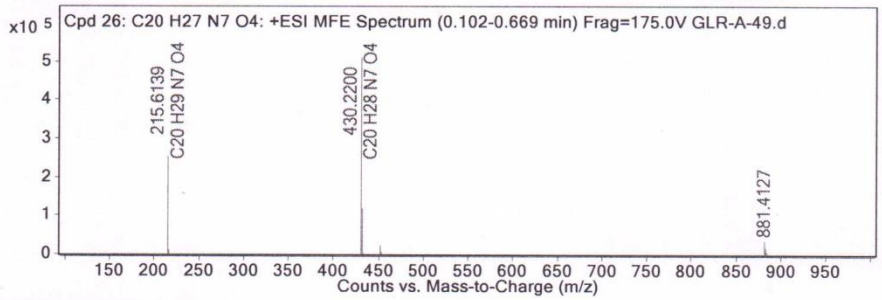
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 26: C20 H27 N7 O4	0.197	429.2126	C20 H27 N7 O4	C20 H27 N7 O4	-0.38	C20 H27 N7 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 26: C20 H27 N7 O4	430.22	0.197	Find by Molecular Feature	429.2126

MFE MS Spectrum



MS Spectrum Peak List

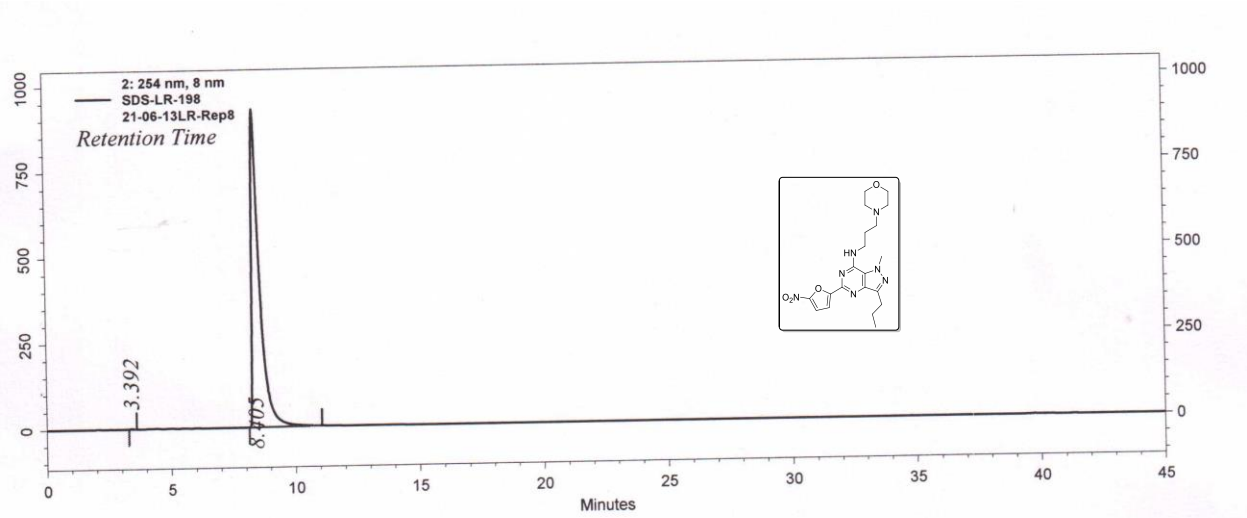
m/z	z	Abund	Formula	Ion
215.6139	2	252627.44	C20 H29 N7 O4	(M+2H)+2
216.1154	2	62948.39	C20 H29 N7 O4	(M+2H)+2
216.6168	2	11303.54	C20 H29 N7 O4	(M+2H)+2
430.22	1	509738.03	C20 H28 N7 O4	(M+H)+
431.2223	1	117493.96	C20 H28 N7 O4	(M+H)+
432.2247	1	20226.92	C20 H28 N7 O4	(M+H)+
452.2012	1	21967.84	C20 H27 N7 Na O4	(M+Na)+
453.2034	1	7190.87	C20 H27 N7 Na O4	(M+Na)+
881.4127	1	34563.68		(2M+Na)+
882.4147	1	16856.13		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	215.6139	215.6135	-1.93	100	100	76.77	77.61
2	216.1154	216.1149	-2.3	24.92	24.67	19.13	19.15
3	216.6168	216.6161	-3.39	4.47	3.74	3.43	2.91
4	217.1172	217.1173	0.42	0.87	0.42	0.67	0.33

--- End Of Report ---

HPLC

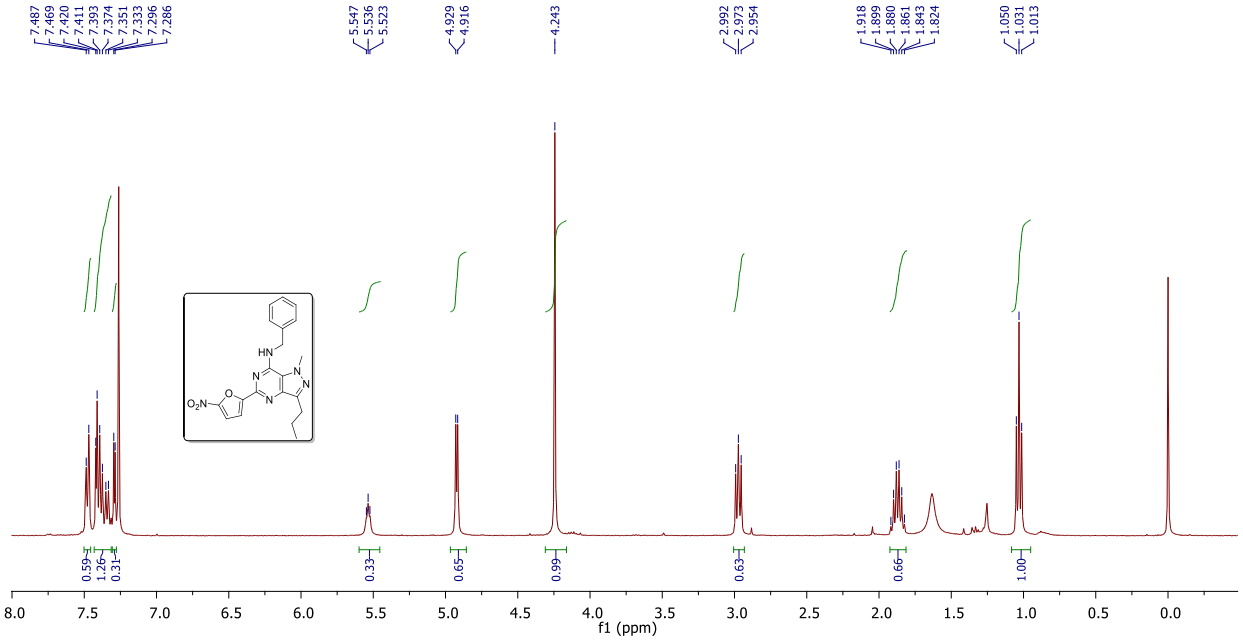


2: 254 nm, 8 nm

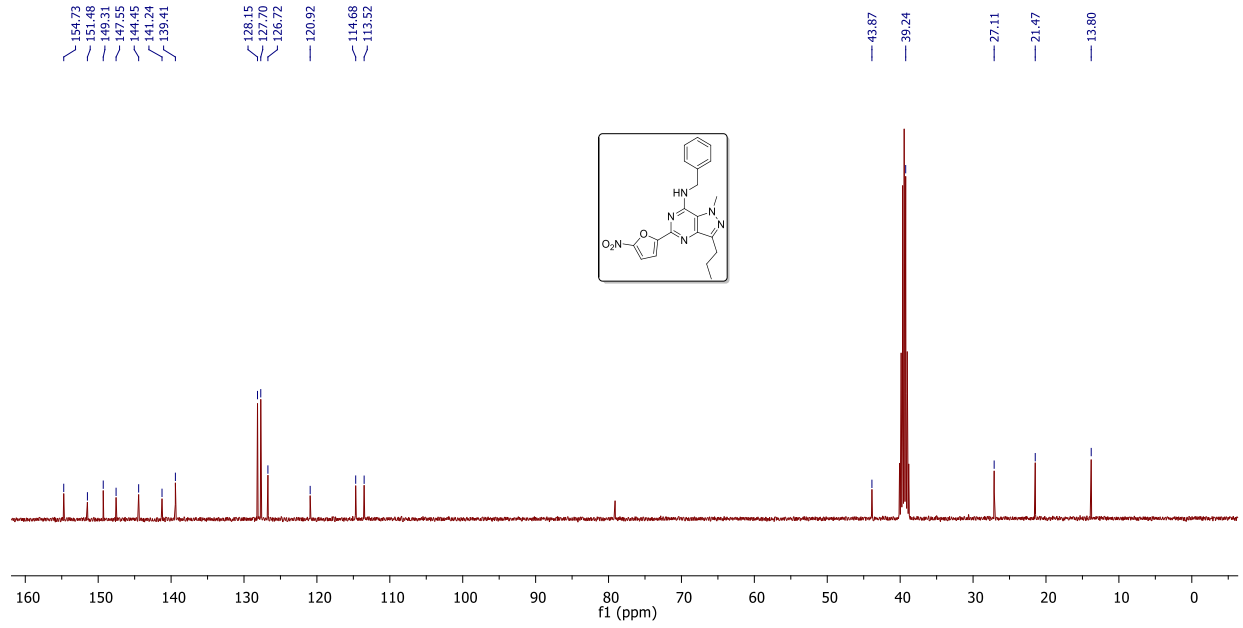
Pk #	Retention Time	Area	Area %	Height	Height %
1	3.392	10351	0.049	1464	0.157
2	8.405	21015504	99.951	928471	99.843
Totals		21025855	100.000	929935	100.000

Compound (21)

^{1}H NMR in $CDCl_3$

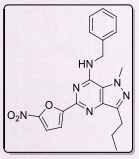


^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report



Data File	GLR-11.d	**Sample Name**	GLR-11
Sample Type	Sample	**Position**	Vial 23
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/18/2012 1:37:22 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

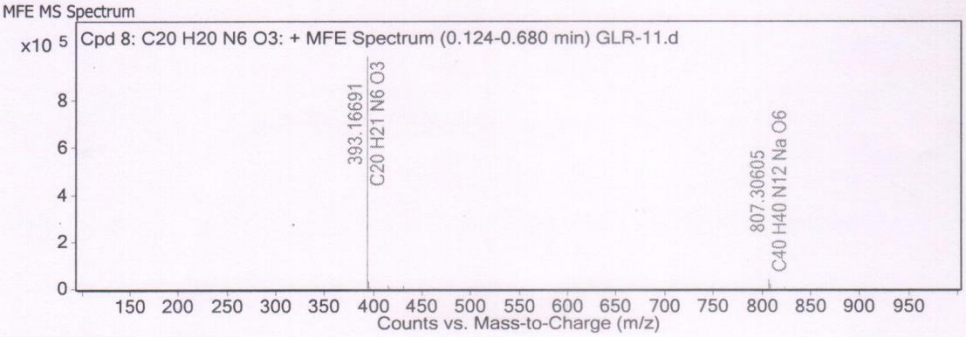
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C20 H20 N6 O3	0.171	392.15963	C20 H20 N6 O3	C20 H20 N6 O3	0.14	C20 H20 N6 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C20 H20 N6 O3	393.16691	0.171	Find by Molecular Feature	392.15963

MFE MS Spectrum



MS Spectrum Peak List

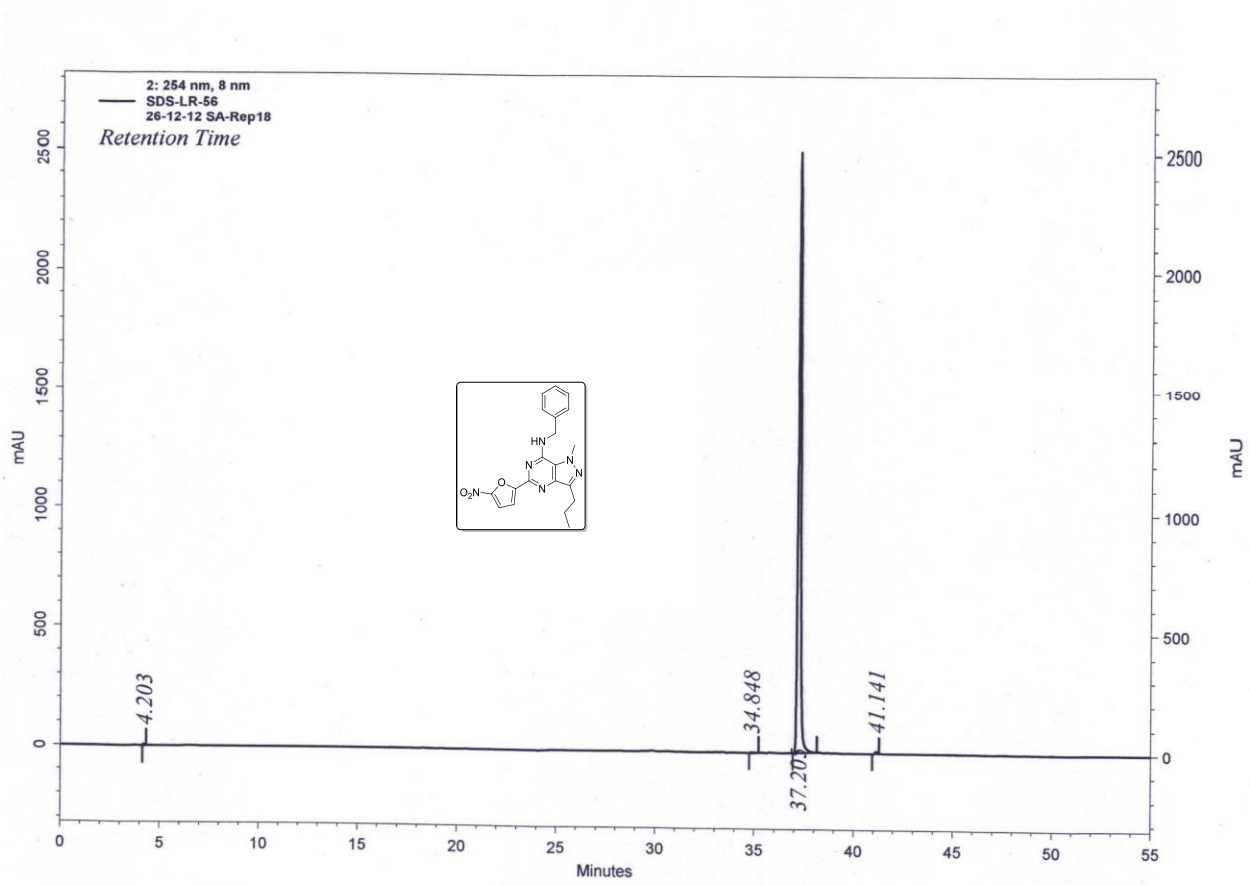
m/z	z	Abund	Formula	Ion
393.16691	1	990372.1	C20 H21 N6 O3	(M+H)+
394.16939	1	211995.5	C20 H21 N6 O3	(M+H)+
395.17143	1	30176.7	C20 H21 N6 O3	(M+H)+
396.17492	1	4738.5	C20 H21 N6 O3	(M+H)+
415.14774	1	15120.2	C20 H20 N6 Na O3	(M+Na)+
416.14941	1	5045	C20 H20 N6 Na O3	(M+Na)+
431.12167	1	9278.1	C20 H20 K N6 O3	(M+K)+
807.30605	1	42466.2	C40 H40 N12 Na O6	(2M+Na)+
808.30886	1	20448.7	C40 H40 N12 Na O6	(2M+Na)+
823.28164	1	5097	C40 H40 K N12 O6	(2M+K)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	393.16691	393.16697	0.13	100	100	80.04	78.15
2	394.16939	394.16978	1	21.41	24.18	17.13	18.9
3	395.17143	395.17232	2.25	3.05	3.42	2.44	2.67
4	396.17492	396.17478	-0.35	0.48	0.36	0.38	0.28

--- End Of Report ---

HPLC

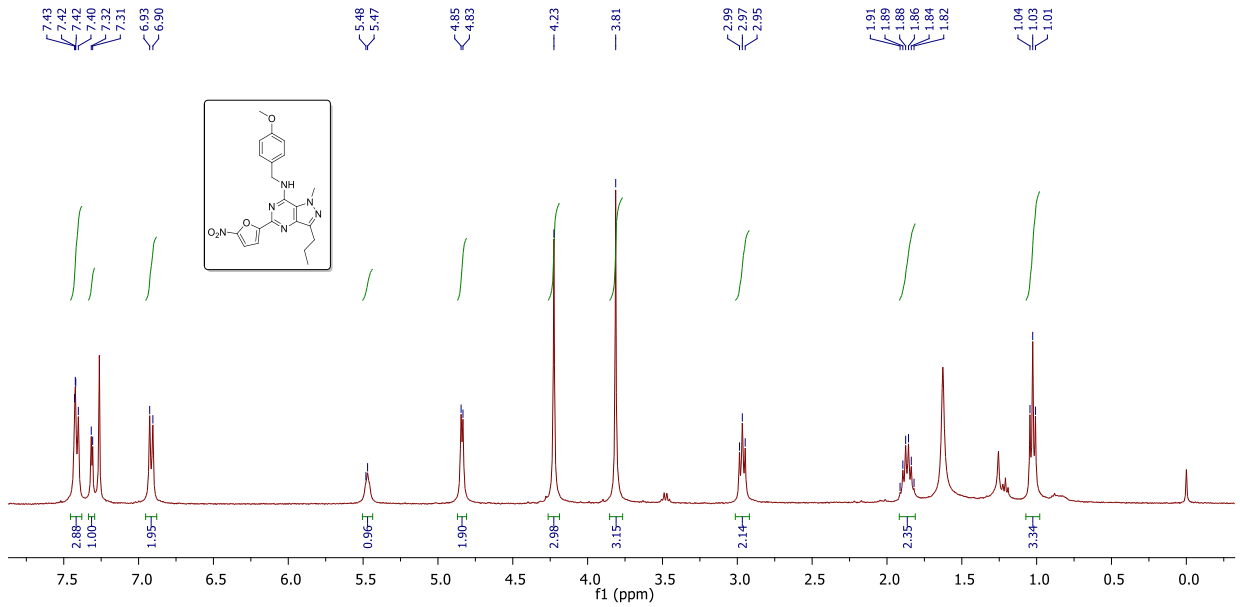


2: 254 nm, 8 nm

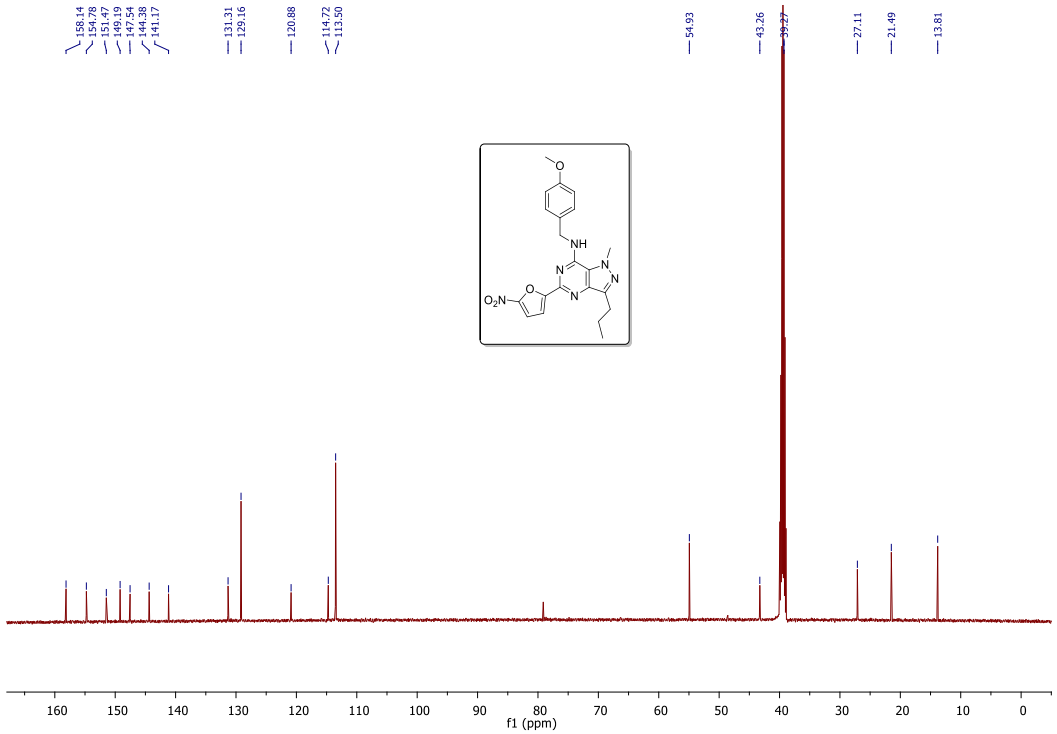
Pk #	Retention Time	Area	Area %	Height	Height %
1	4.203	52812	0.227	8918	0.353
2	34.848	52146	0.224	3664	0.145
3	37.205	23118996	99.231	2502888	99.149
4	41.141	74268	0.319	8896	0.352
Totals		23298222	100.000	2524366	100.000

Compound (22)

^{1}H NMR in $CDCl_3$



^{13}C NMR in DMSO-d_6

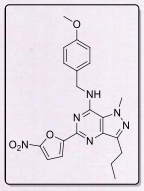


HRMS

Qualitative Compound Report

Data File	GLR-4-37.d	**Sample Name**	GLR-4-37
Sample Type	Sample	**Position**	Vial 8
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/19/2012 12:58:00 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

Sample Group **Info.**

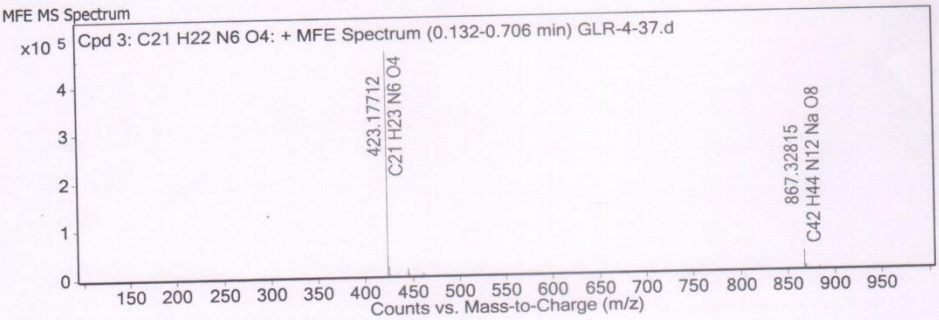


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C21 H22 N6 O4	0.172	422.16984	C21 H22 N6 O4	C21 H22 N6 O4	0.97	C21 H22 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C21 H22 N6 O4	423.17712	0.172	Find by Molecular Feature	422.16984

MFE MS Spectrum



MS Spectrum Peak List

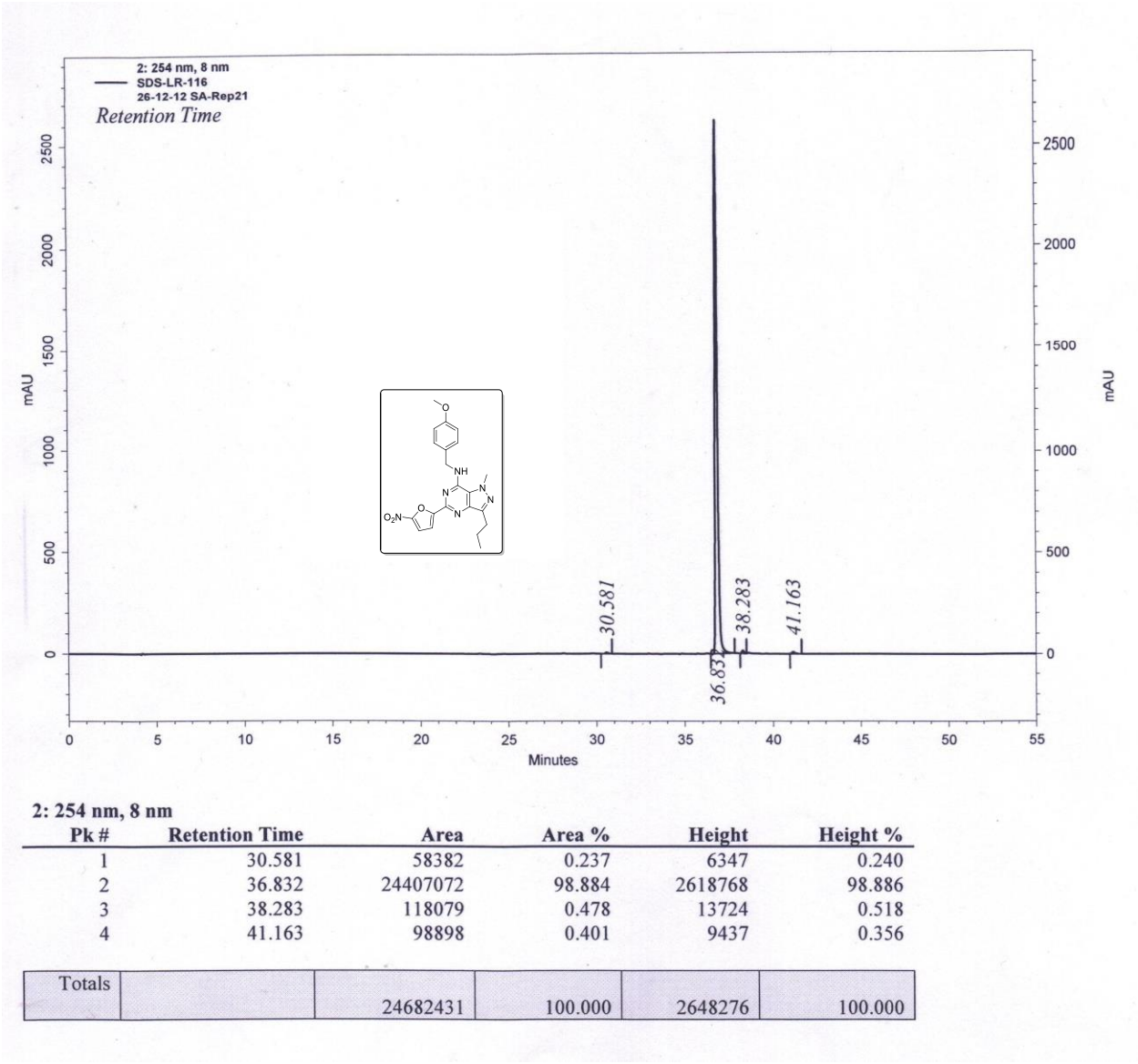
m/z	z	Abund	Formula	Ion
423.17712	1	466922.1	C21 H23 N6 O4	(M+H)+
424.17976	1	122132.7	C21 H23 N6 O4	(M+H)+
425.18177	1	18589.5	C21 H23 N6 O4	(M+H)+
445.15869	1	15127.3	C21 H22 N6 Na O4	(M+Na)+
446.16148	1	5373.9	C21 H22 N6 Na O4	(M+Na)+
461.13245	1	5001.9	C21 H22 K N6 O4	(M+K)+
867.32815	1	37016.4	C42 H44 N12 Na O8	(2M+Na)+
868.33036	1	18324.1	C42 H44 N12 Na O8	(2M+Na)+
869.33289	1	6392.2	C42 H44 N12 Na O8	(2M+Na)+
883.30209	1	3364	C42 H44 K N12 O8	(2M+K)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	423.17712	423.17753	0.96	100	100	76.61	77.12
2	424.17976	424.18037	1.46	26.16	25.32	20.04	19.53
3	425.18177	425.18289	2.65	3.98	3.9	3.05	3.01
4	426.18753	426.18535	-5.11	0.4	0.45	0.3	0.34

--- End Of Report ---

HPLC

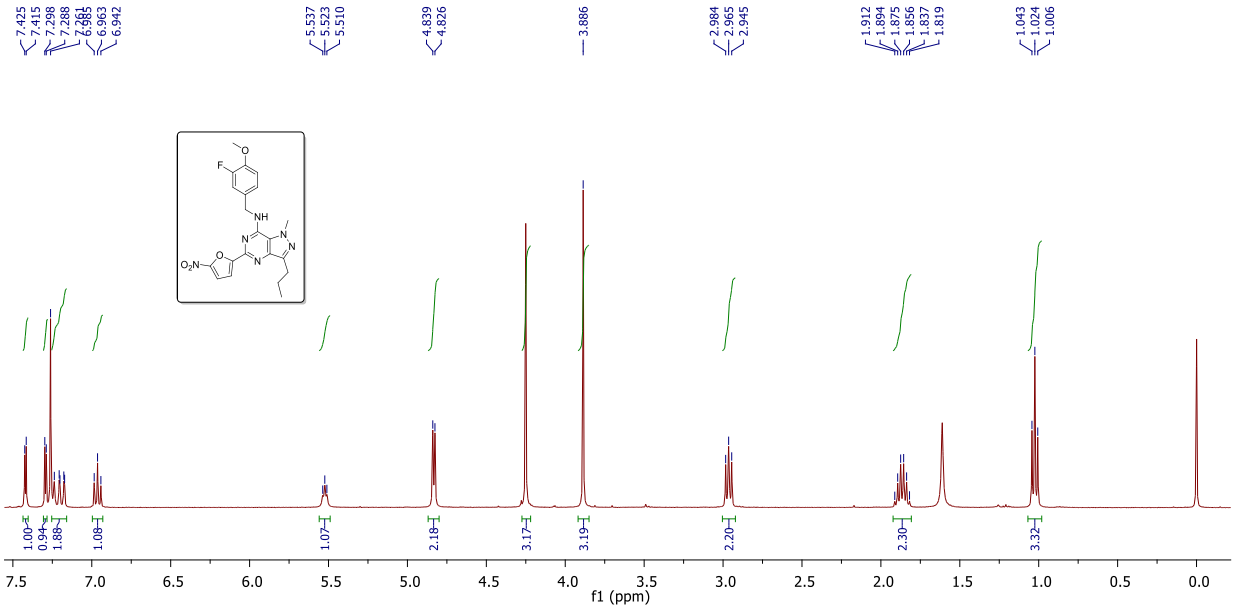


2: 254 nm, 8 nm

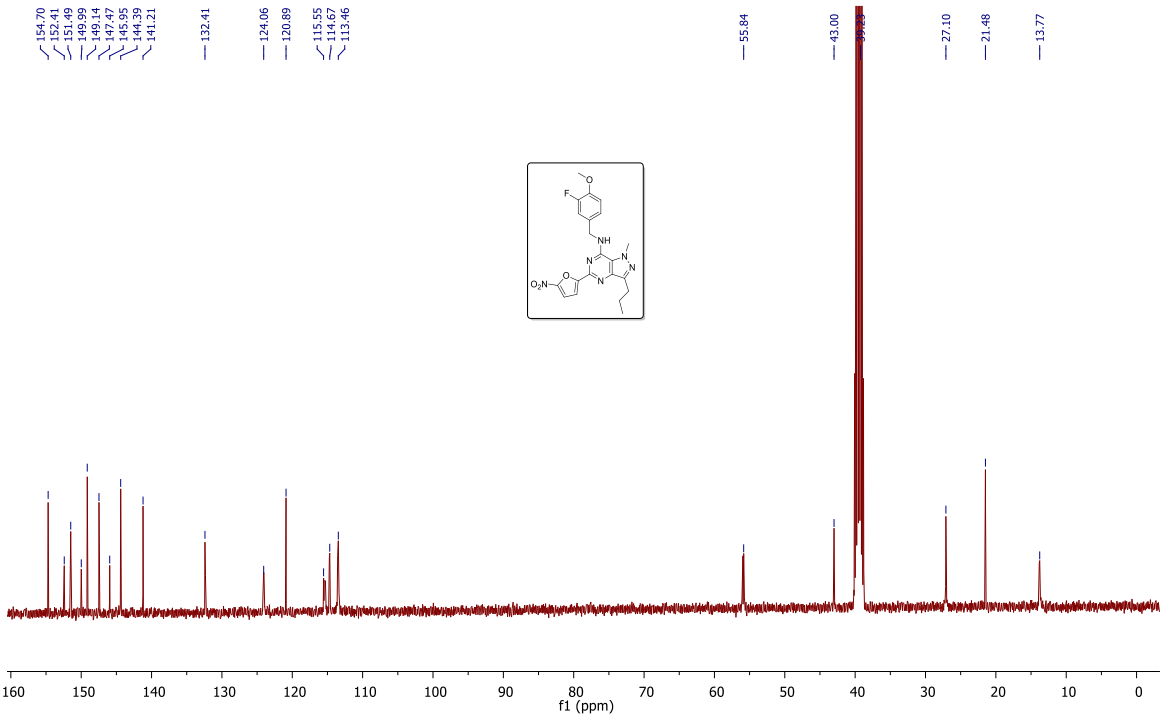
Pk #	Retention Time	Area	Area %	Height	Height %
1	30.581	58382	0.237	6347	0.240
2	36.832	24407072	98.884	2618768	98.886
3	38.283	118079	0.478	13724	0.518
4	41.163	98898	0.401	9437	0.356
Totals		24682431	100.000	2648276	100.000

Compound (23)

^{1}H NMR in $CDCl_3$

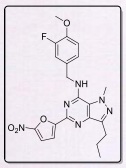


^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report



Data File	GLR-4-34.d	**Sample Name**	GLR-4-34
Sample Type	Sample	**Position**	Vial 5
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/19/2012 12:43:51 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

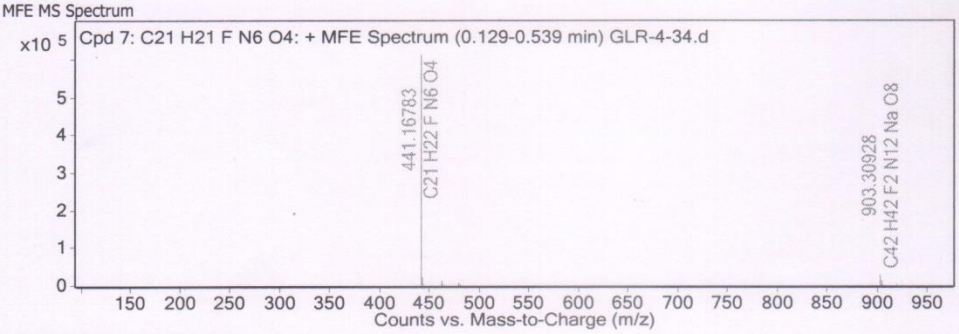
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C21 H21 F N6 O4	0.172	440.16055	C21 H21 F N6 O4	C21 H21 F N6 O4	0.65	C21 H21 F N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C21 H21 F N6 O4	441.16783	0.172	Find by Molecular Feature	440.16055

MFE MS Spectrum



MS Spectrum Peak List

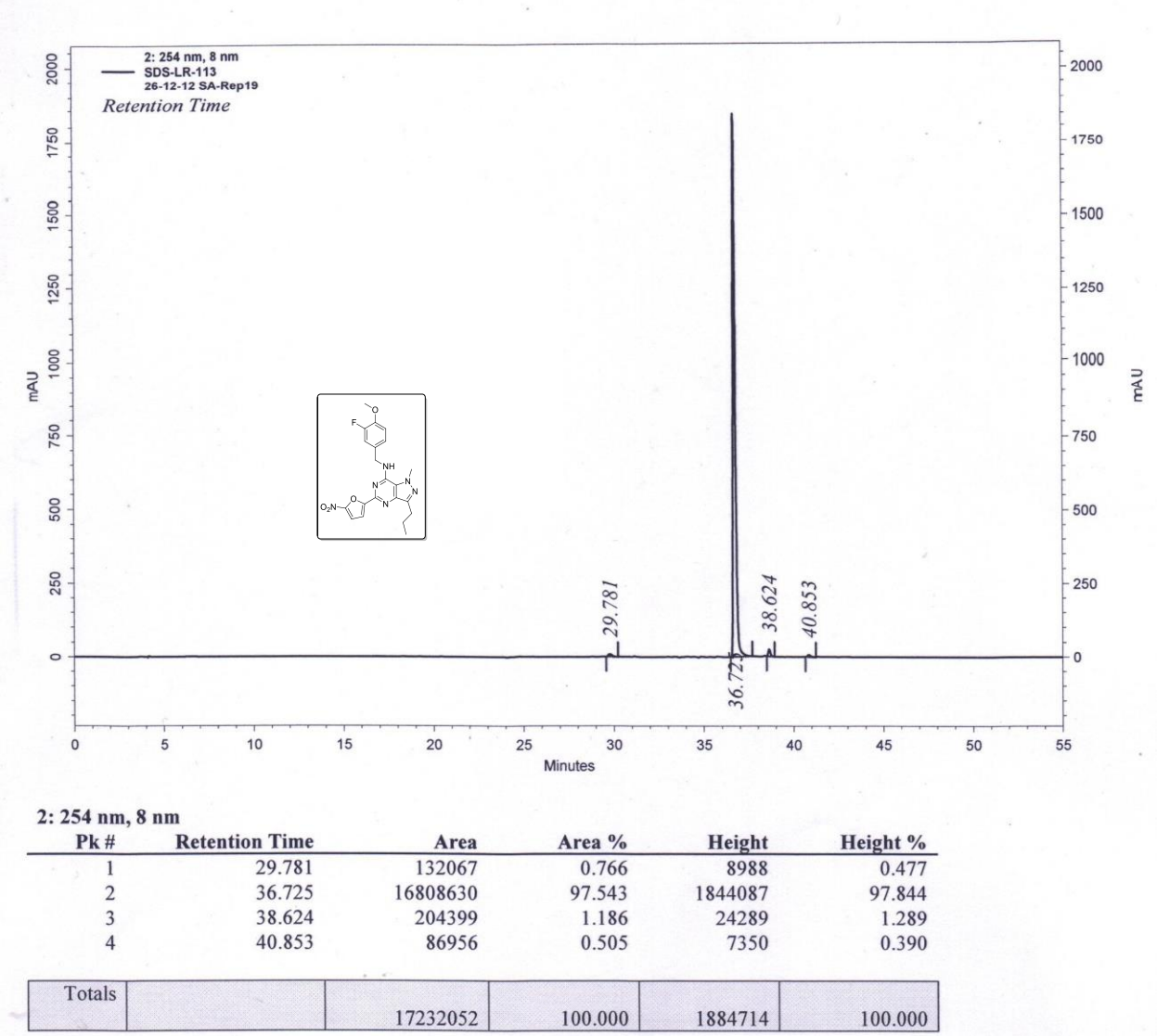
m/z	z	Abund	Formula	Ion
441.16783	1	612374.8	C21 H22 F N6 O4	(M+H)+
442.17029	1	143914	C21 H22 F N6 O4	(M+H)+
443.17311	1	21446.9	C21 H22 F N6 O4	(M+H)+
444.17514	1	3302.3	C21 H22 F N6 O4	(M+H)+
463.14834	1	12489.3	C21 H21 F N6 Na O4	(M+Na)+
479.12258	1	5574.6	C21 H21 F K N6 O4	(M+K)+
903.30928	1	26851.2	C42 H42 F2 N12 Na O8	(2M+Na)+
904.30993	1	13429.6	C42 H42 F2 N12 Na O8	(2M+Na)+
905.31342	1	3559.8	C42 H42 F2 N12 Na O8	(2M+Na)+
919.28295	1	3761.6		(2M+K)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	441.16783	441.16811	0.64	100	100	78.41	77.13
2	442.17029	442.17095	1.49	23.5	25.31	18.43	19.52
3	443.17311	443.17347	0.8	3.5	3.9	2.75	3.01
4	444.17514	444.17592	1.75	0.54	0.45	0.42	0.34

--- End Of Report ---

HPLC

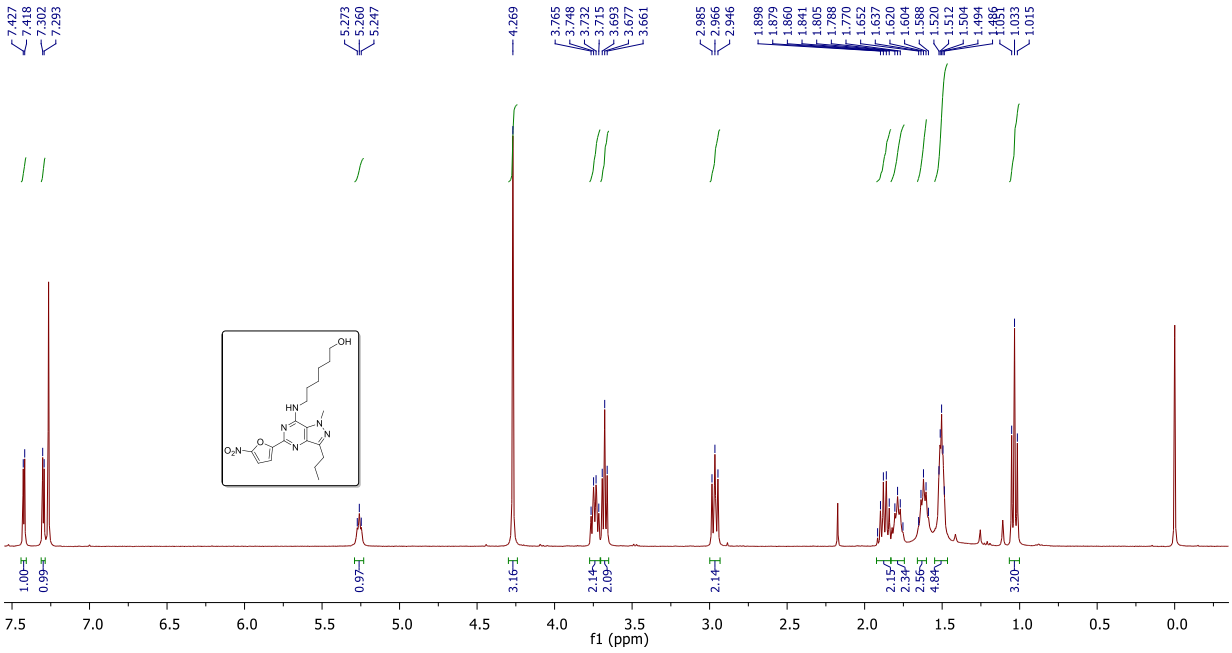


2: 254 nm, 8 nm

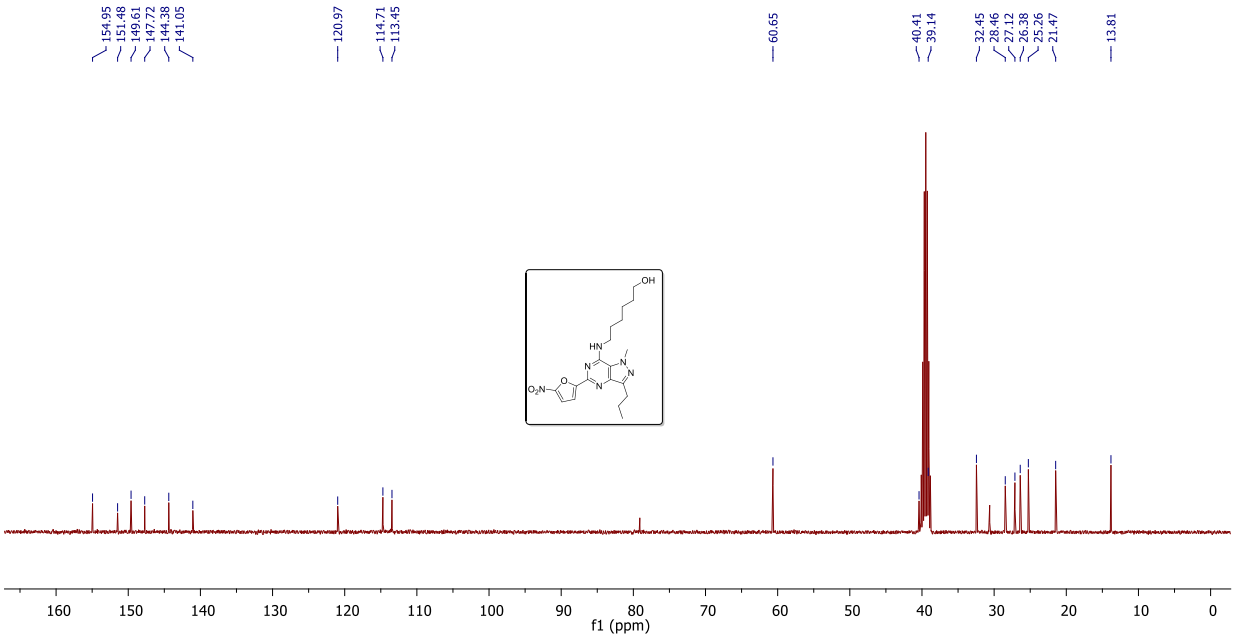
Pk #	Retention Time	Area	Area %	Height	Height %
1	29.781	132067	0.766	8988	0.477
2	36.725	16808630	97.543	1844087	97.844
3	38.624	204399	1.186	24289	1.289
4	40.853	86956	0.505	7350	0.390
Totals		17232052	100.000	1884714	100.000

Compound (24)

^{1}H NMR in $CDCl_3$



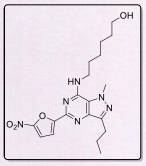
^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report

Data File	GLR-8.d	**Sample Name**	GLR-8
Sample Type	Sample	**Position**	Vial 20
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/18/2012 1:26:45 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			



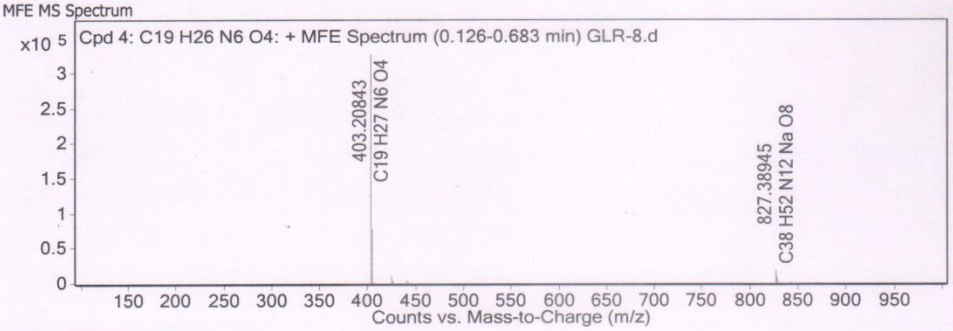
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C19 H26 N6 O4	0.172	402.20115	C19 H26 N6 O4	C19 H26 N6 O4	1.01	C19 H26 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C19 H26 N6 O4	403.20843	0.172	Find by Molecular Feature	402.20115

MFE MS Spectrum



MS Spectrum Peak List

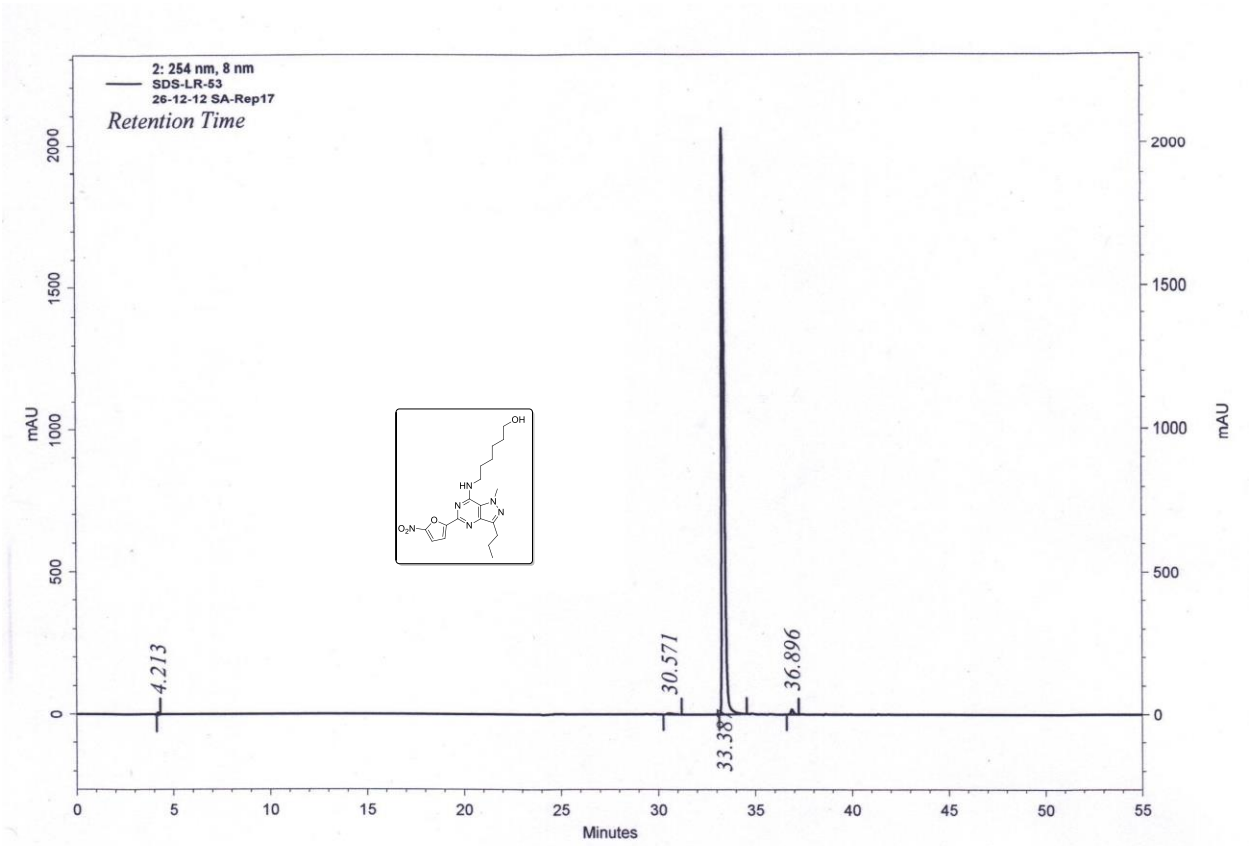
m/z	z	Abund	Formula	Ion
403.20843	1	326763.5	C19 H27 N6 O4	(M+H)+
404.21069	1	77385.1	C19 H27 N6 O4	(M+H)+
405.21287	1	12710.9	C19 H27 N6 O4	(M+H)+
425.18996	1	10795.1	C19 H26 N6 Na O4	(M+Na)+
426.19267	1	2774.4	C19 H26 N6 Na O4	(M+Na)+
441.16296	1	4205.6	C19 H26 K N6 O4	(M+K)+
827.38945	1	18009.8	C38 H52 N12 Na O8	(2M+Na)+
828.39343	1	8280.5	C38 H52 N12 Na O8	(2M+Na)+
829.39711	1	1817.5	C38 H52 N12 Na O8	(2M+Na)+
843.3663	1	1312.6	C38 H52 K N12 O8	(2M+K)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	403.20843	403.20883	0.99	100	100	78.17	78.75
2	404.21069	404.21163	2.33	23.68	23.2	18.51	18.27
3	405.21287	405.21408	2.99	3.89	3.4	3.04	2.68
4	406.21737	406.2165	-2.15	0.35	0.37	0.28	0.29

--- End Of Report ---

HPLC

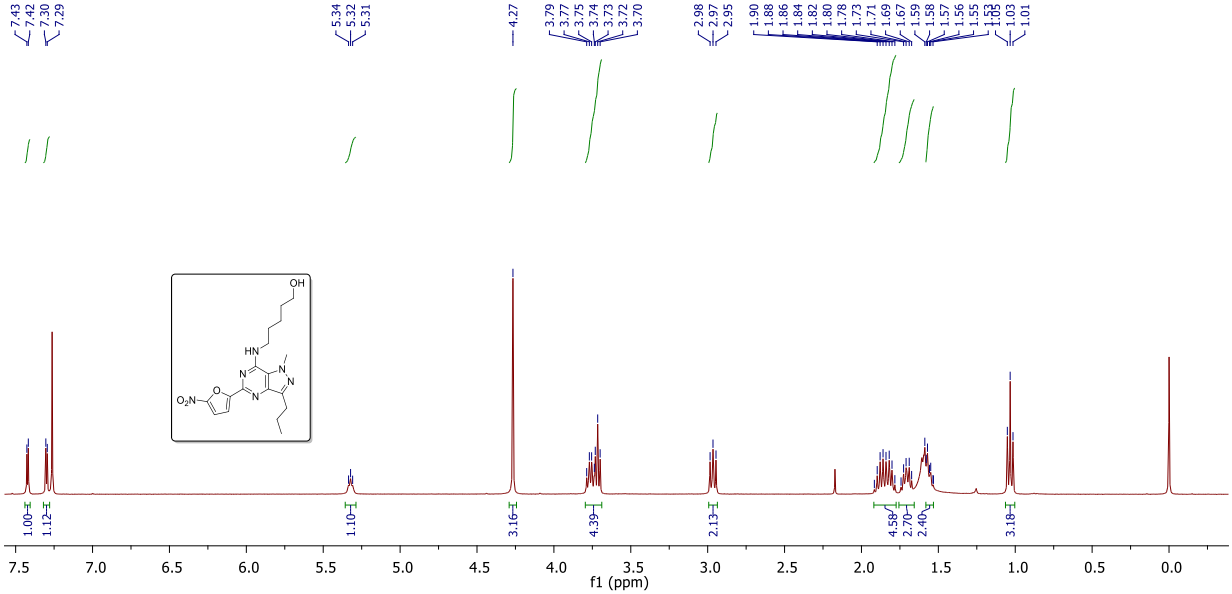


2: 254 nm, 8 nm

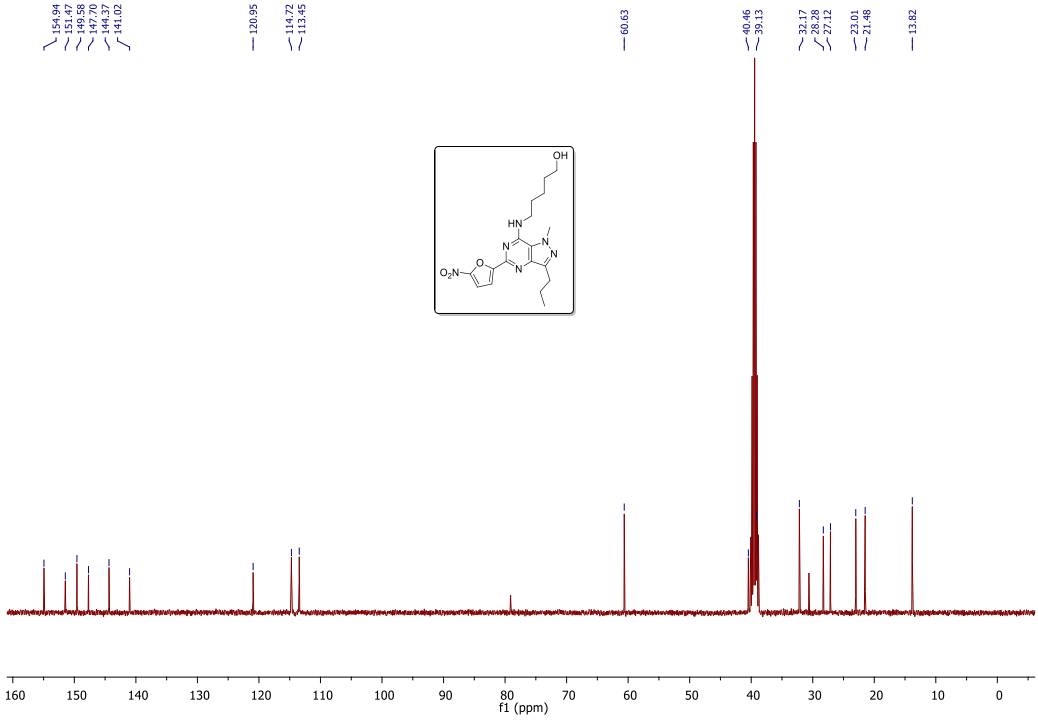
Pk #	Retention Time	Area	Area %	Height	Height %
1	4.213	61261	0.309	9508	0.456
2	30.571	83420	0.421	4194	0.201
3	33.387	19502693	98.432	2053945	98.493
4	36.896	166047	0.838	17730	0.850
Totals		19813421	100.000	2085377	100.000

Compound (25)

^{1}H NMR in $CDCl_3$



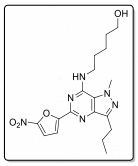
^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report

Data File	GLR-A-47.d	**Sample Name**	GLR-A-47
Sample Type	Sample	**Position**	Vial 4
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-07-2013 PM 12:33:03
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



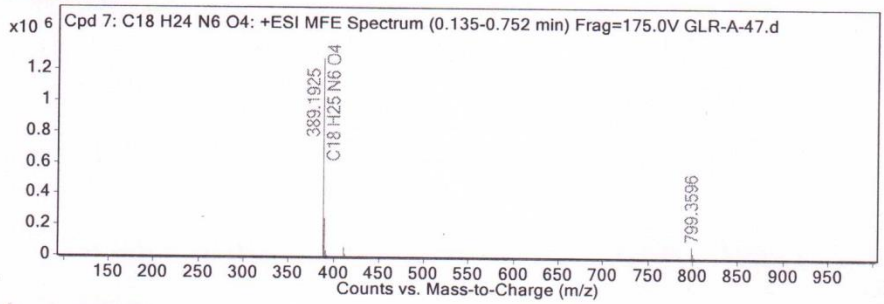
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C18 H24 N6 O4	0.193	388.1853	C18 H24 N6 O4	C18 H24 N6 O4	1.43	C18 H24 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C18 H24 N6 O4	389.1925	0.193	Find by Molecular Feature	388.1853

MFE MS Spectrum



MS Spectrum Peak List

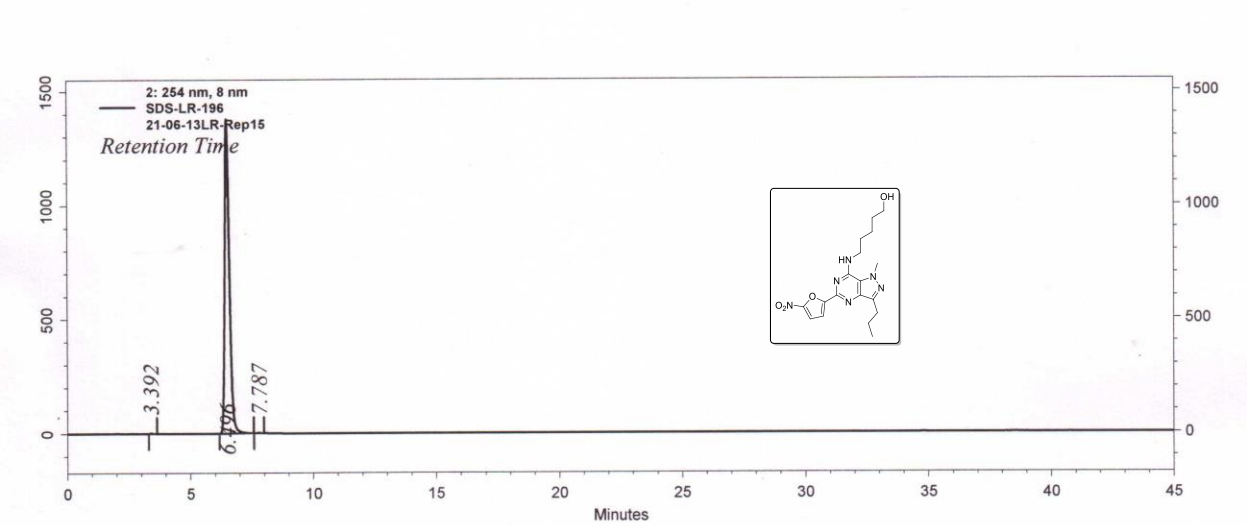
m/z	z	Abund	Formula	Ion
389.1925	1	1272528.63	C18 H25 N6 O4	(M+H)+
390.1959	1	243920.28	C18 H25 N6 O4	(M+H)+
391.1981	1	33209.2	C18 H25 N6 O4	(M+H)+
392.2004	1	3821.87	C18 H25 N6 O4	(M+H)+
411.1743	1	59634.92	C18 H24 N6 Na O4	(M+Na)+
412.1775	1	12861.71	C18 H24 N6 Na O4	(M+Na)+
413.1801	1	2281.33	C18 H24 N6 Na O4	(M+Na)+
799.3596	1	74392.88		(2M+Na)+
800.3621	1	30664.33		(2M+Na)+
801.3647	1	7088.35		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	389.1925	389.1932	1.7	100	100	81.89	79.6
2	390.1959	390.196	0.11	19.17	22.1	15.7	17.59
3	391.1981	391.1984	0.7	2.61	3.15	2.14	2.51
4	392.2004	392.2008	0.99	0.3	0.34	0.25	0.27
5	393.2003	393.2031	7.07	0.03	0.03	0.03	0.02

--- End Of Report ---

HPLC

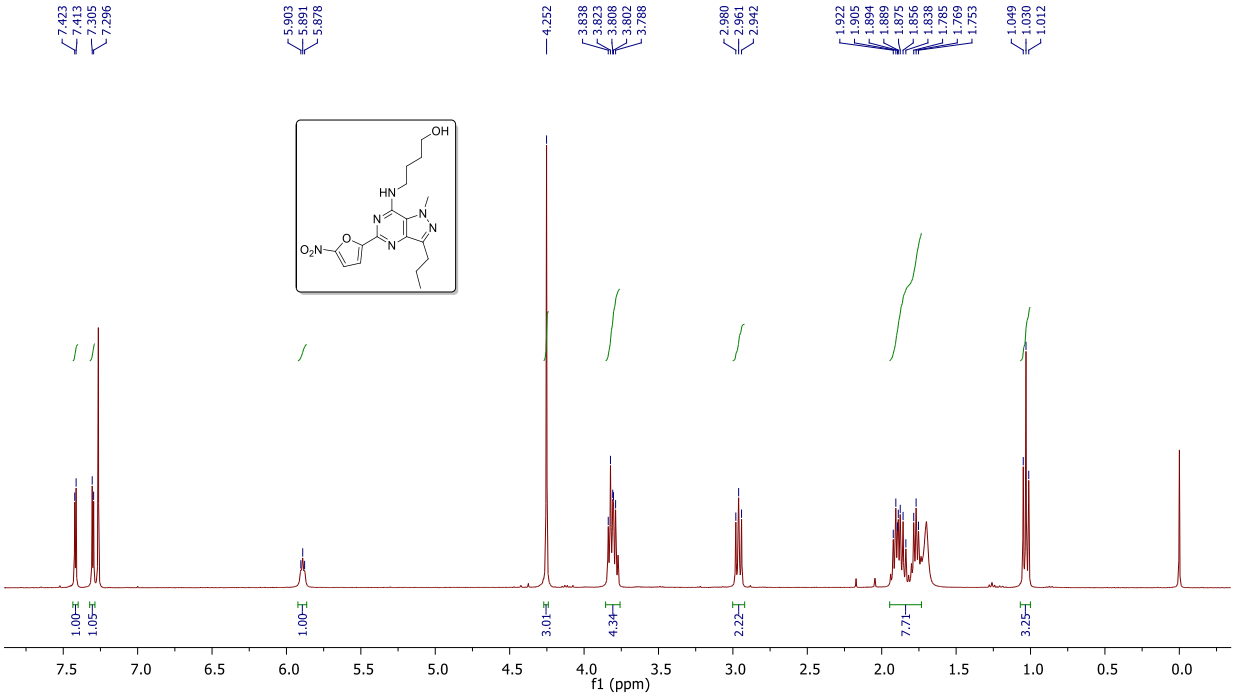


2: 254 nm, 8 nm

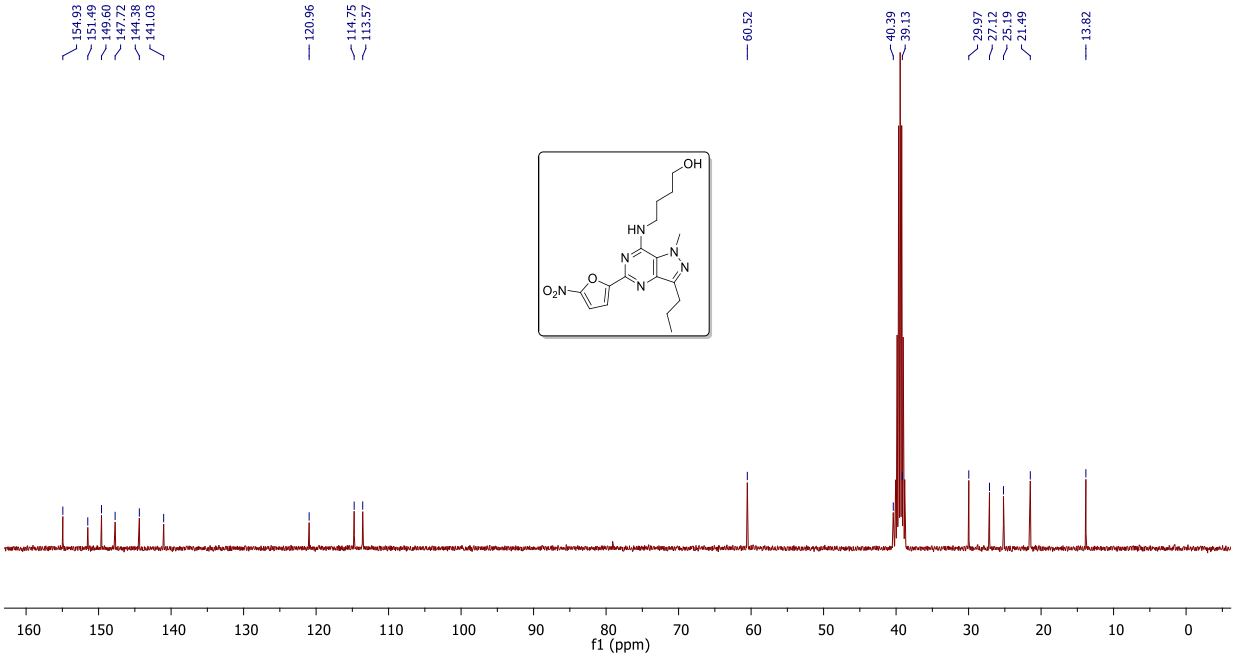
Pk #	Retention Time	Area	Area %	Height	Height %
1	3.392	10279	0.056	1484	0.107
2	6.496	18300925	99.867	1378069	99.799
3	7.787	14146	0.077	1290	0.093
Totals		18325350	100.000	1380843	100.000

Compound (26)

^{1}H NMR in $CDCl_3$

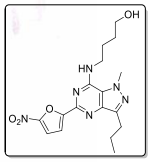


^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report



Data File	GLR-A-51.d	**Sample Name**	GLR-A-51
Sample Type	Sample	**Position**	Vial 5
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-07-2013 PM 12:40:36
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

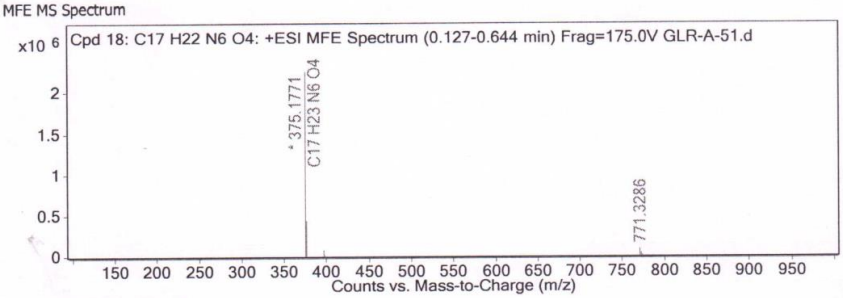
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 18: C17 H22 N6 O4	0.195	374.17	C17 H22 N6 O4	C17 H22 N6 O4	0.67	C17 H22 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 18: C17 H22 N6 O4	375.1771	0.195	Find by Molecular Feature	374.17

MFE MS Spectrum



MS Spectrum Peak List

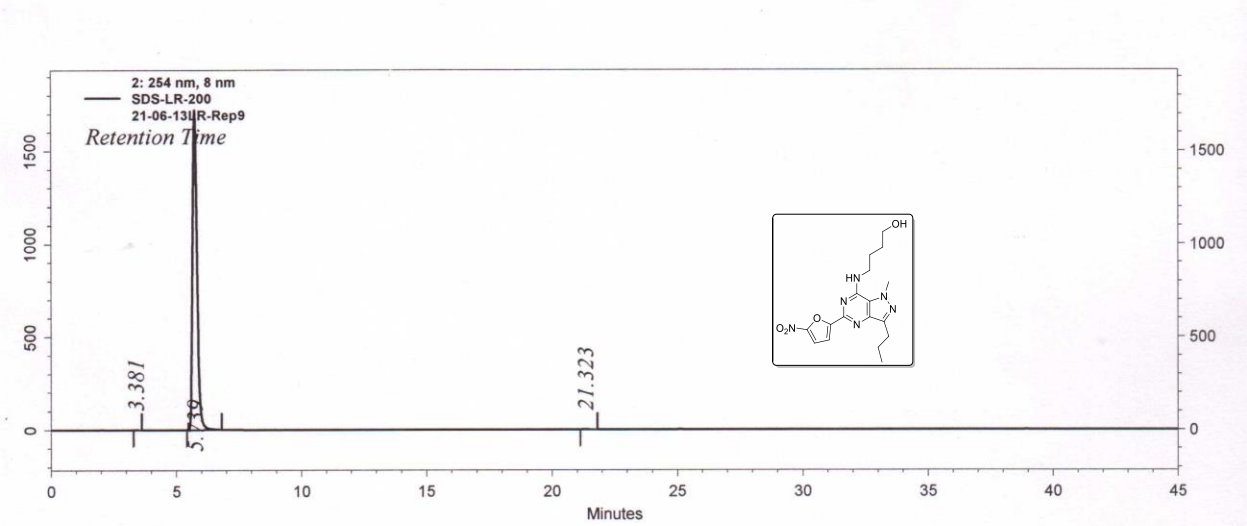
m/z	z	Abund	Formula	Ion
375.1771	1	2258091.5	C17 H23 N6 O4	(M+H)+
376.1806	1	433639.53	C17 H23 N6 O4	(M+H)+
377.1828	1	50726.54	C17 H23 N6 O4	(M+H)+
378.1847	1	4820.64	C17 H23 N6 O4	(M+H)+
397.159	1	72342.15	C17 H22 N6 Na O4	(M+Na)+
398.1619	1	15390.32	C17 H22 N6 Na O4	(M+Na)+
399.164	1	2235.92	C17 H22 N6 Na O4	(M+Na)+
771.3286	1	94778.48		(2M+Na)+
772.3307	1	40370.81		(2M+Na)+
773.3338	1	9694.06		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	375.1771	375.1775	1.01	100	100	82.18	80.48
2	376.1806	376.1803	-1.01	19.2	21	15.78	16.9
3	377.1828	377.1826	-0.39	2.25	2.92	1.85	2.35
4	378.1847	378.185	0.83	0.21	0.31	0.18	0.25
5	379.1847	379.1873	7.07	0.02	0.03	0.02	0.02

--- End Of Report ---

HPLC

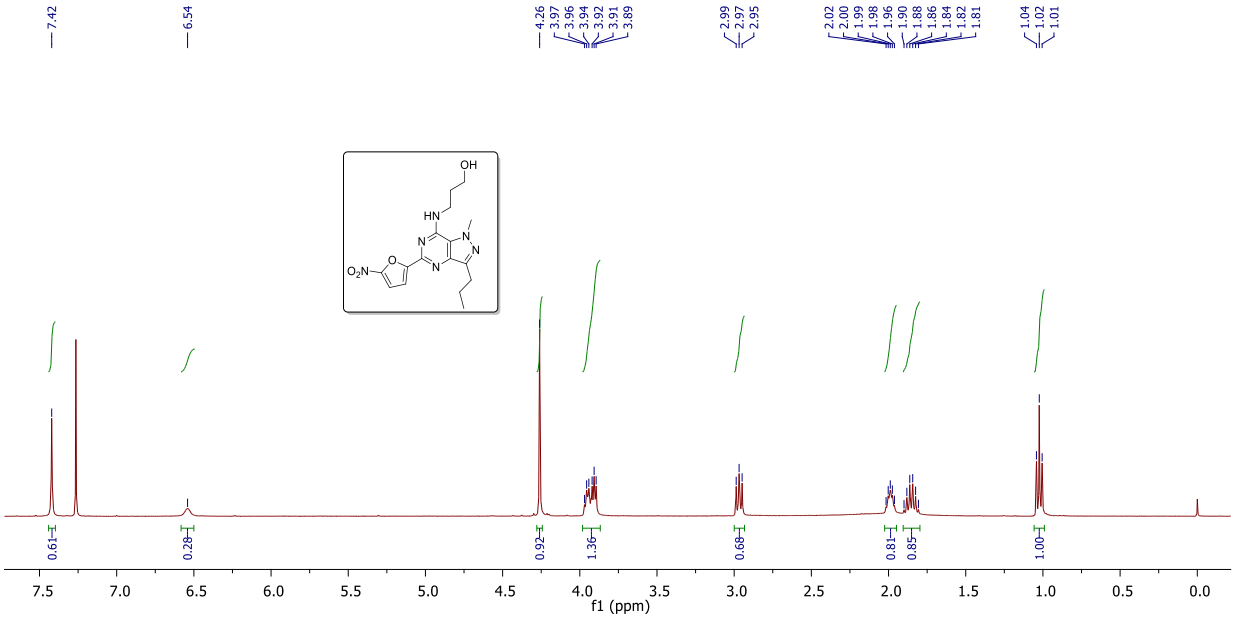


2: 254 nm, 8 nm

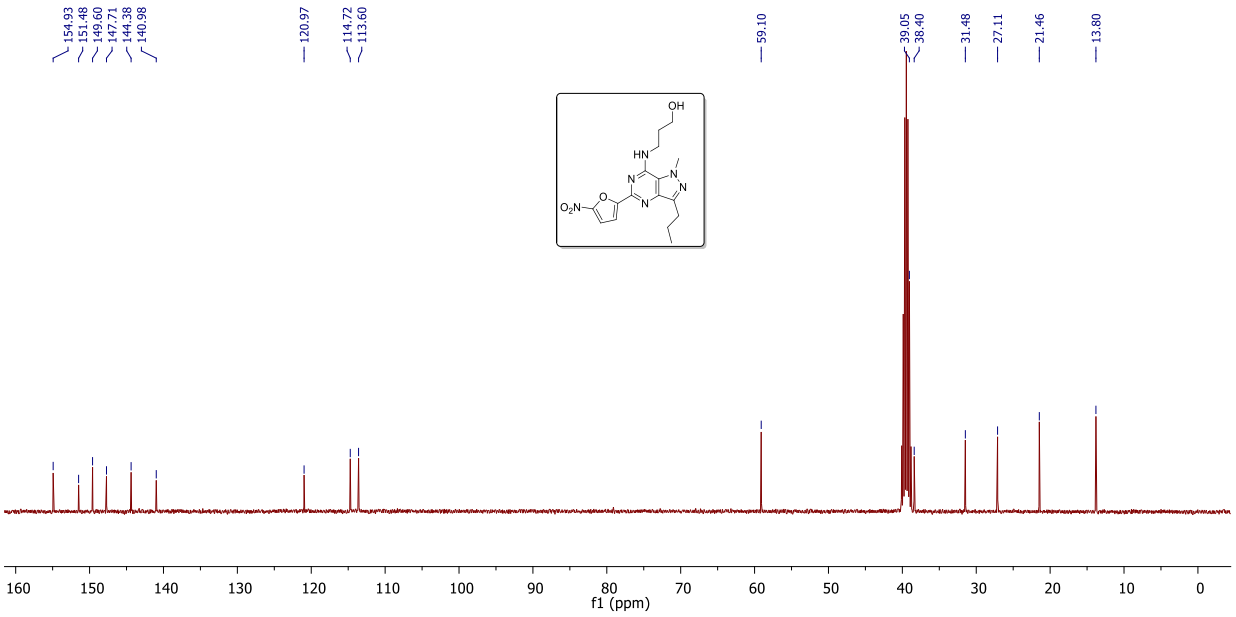
Pk #	Retention Time	Area	Area %	Height	Height %
1	3.381	10594	0.050	1547	0.090
2	5.739	21345161	99.844	1721036	99.815
3	21.323	22860	0.107	1641	0.095
Totals		21378615	100.000	1724224	100.000

Compound (27)

^{1}H NMR in $CDCl_3$

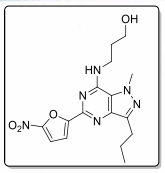


^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report



Data File	GLR-A-50.d	**Sample Name**	GLR-A-50
Sample Type	Sample	**Position**	Vial 6
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-07-2013 PM 12:42:09
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

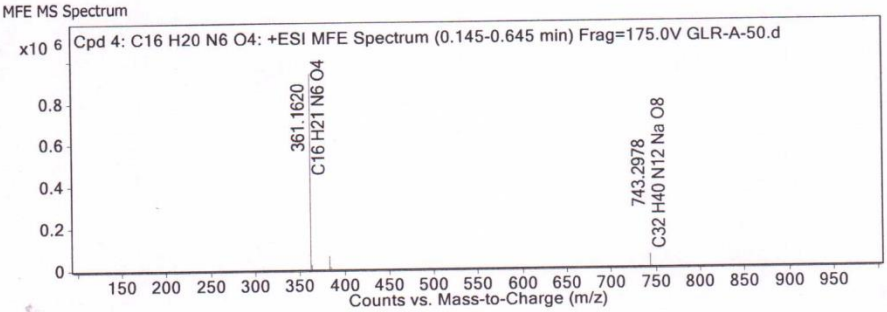
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C16 H20 N6 O4	0.195	360.1547	C16 H20 N6 O4	C16 H20 N6 O4	-0.33	C16 H20 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C16 H20 N6 O4	361.162	0.195	Find by Molecular Feature	360.1547

MFE MS Spectrum



MS Spectrum Peak List

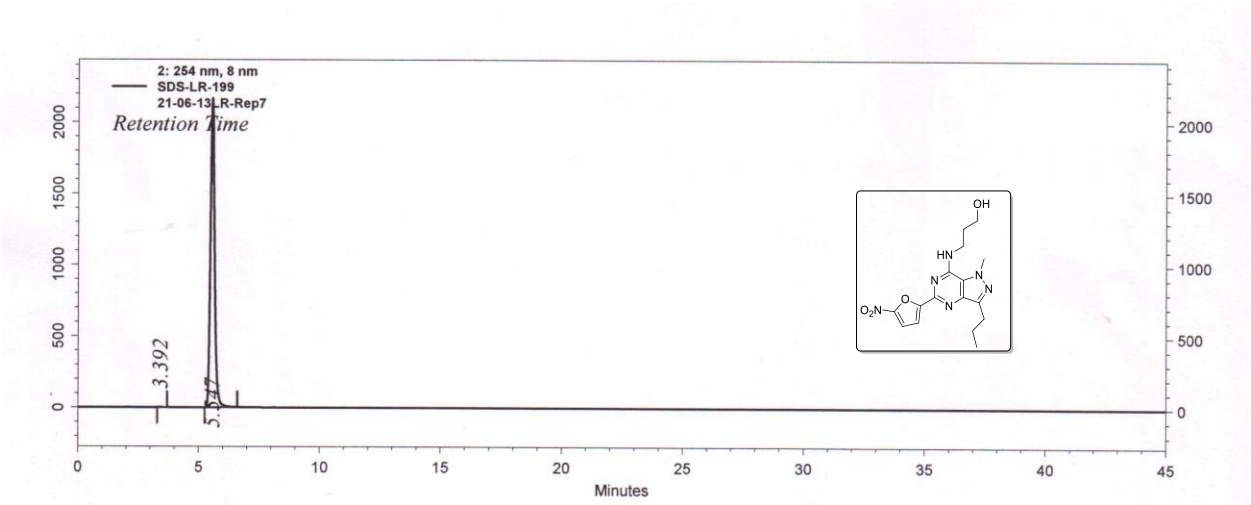
m/z	z	Abund	Formula	Ion
361.162	1	934604.69	C16 H21 N6 O4	(M+H)+
362.1648	1	161417.45	C16 H21 N6 O4	(M+H)+
363.1666	1	21325.7	C16 H21 N6 O4	(M+H)+
364.1688	1	2135.81	C16 H21 N6 O4	(M+H)+
383.1436	1	62944.37	C16 H20 N6 Na O4	(M+Na)+
384.1464	1	12541.51	C16 H20 N6 Na O4	(M+Na)+
385.1486	1	1701.56	C16 H20 N6 Na O4	(M+Na)+
743.2978	1	57376.84	C32 H40 N12 Na O8	(2M+Na)+
744.2997	1	21401.39	C32 H40 N12 Na O8	(2M+Na)+
745.3023	1	5249.12	C32 H40 N12 Na O8	(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	361.162	361.1619	-0.34	100	100	83.45	81.37
2	362.1648	362.1646	-0.56	17.27	19.89	14.41	16.19
3	363.1666	363.1669	0.95	2.28	2.7	1.9	2.2
4	364.1688	364.1692	1.35	0.23	0.28	0.19	0.22
5	365.1623	365.1716	25.38	0.05	0.02	0.04	0.02

--- End Of Report ---

HPLC

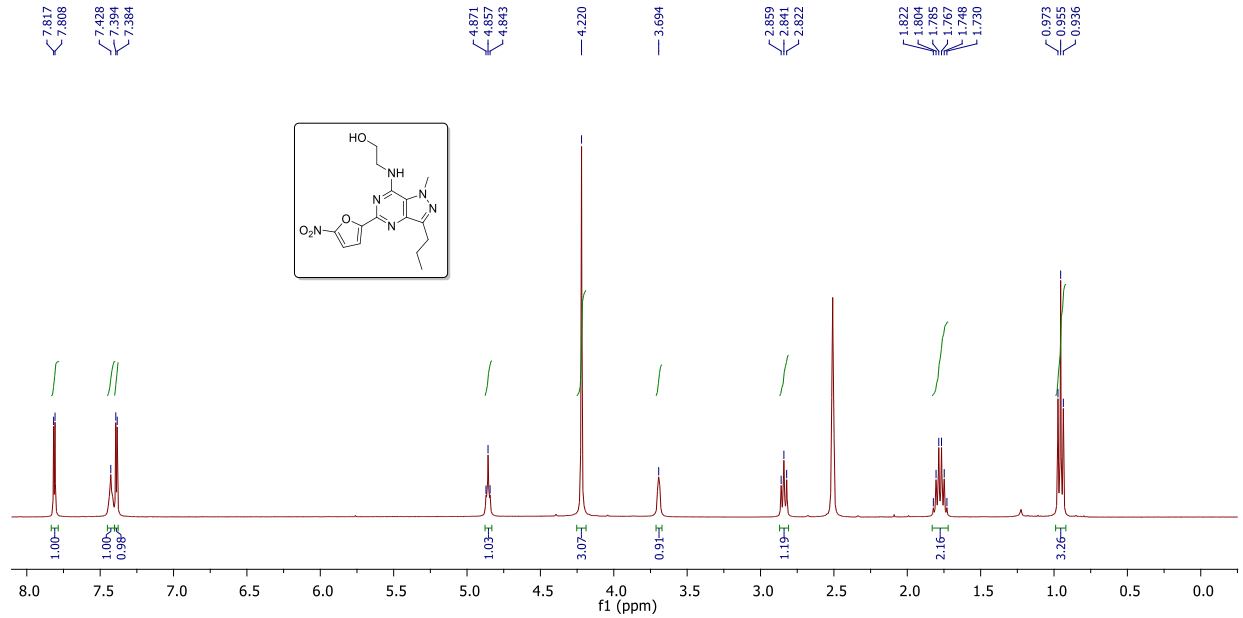


2: 254 nm, 8 nm

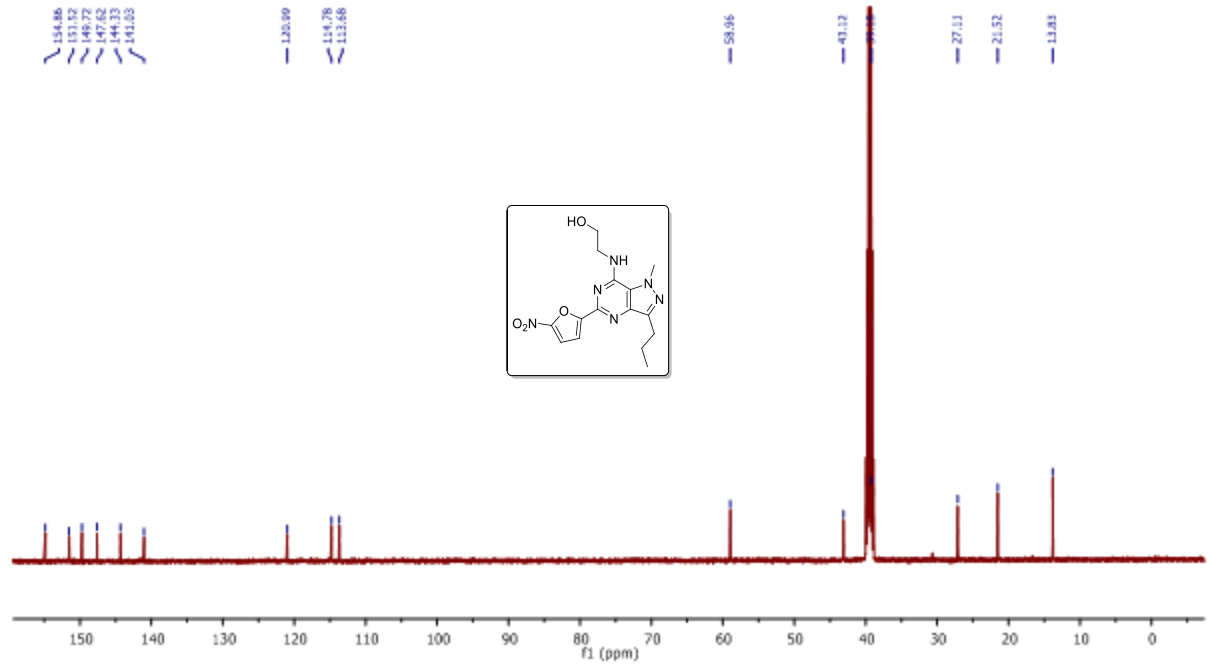
Pk #	Retention Time	Area	Area %	Height	Height %
1	3.392	11129	0.042	1577	0.073
2	5.547	26541690	99.958	2167589	99.927
Totals		26552819	100.000	2169166	100.000

Compound (28)

^{1}H NMR in DMSO-d6

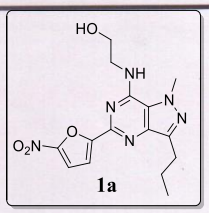


^{13}C NMR in DMSO-d6



HRMS

Qualitative Compound Report



1a

Data File	GLR-1.d	**Sample Name**	GLR-1
Sample Type	Sample	**Position**	Vial 14
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/18/2012 12:58:04 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

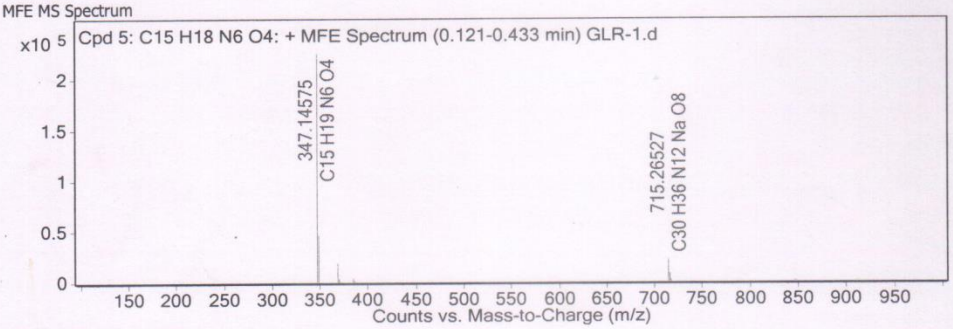
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C15 H18 N6 O4	0.17	346.13848	C15 H18 N6 O4	C15 H18 N6 O4	1.38	C15 H18 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C15 H18 N6 O4	347.14575	0.17	Find by Molecular Feature	346.13848

MFE MS Spectrum



MS Spectrum Peak List

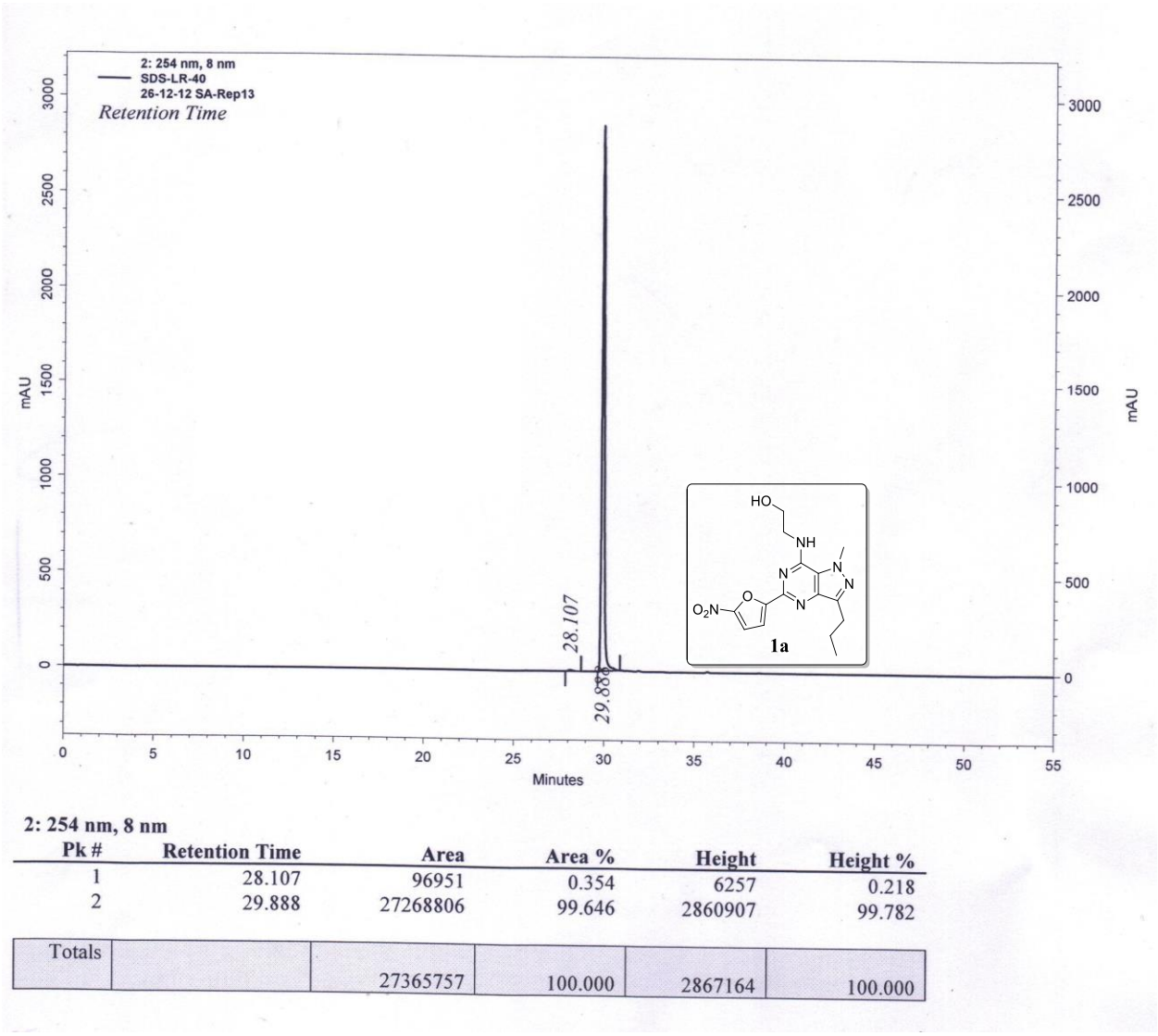
m/z	z	Abund	Formula	Ion
347.14575	1	225247.6	C15 H19 N6 O4	(M+H)+
348.14846	1	46517.4	C15 H19 N6 O4	(M+H)+
349.15045	1	5888.2	C15 H19 N6 O4	(M+H)+
369.12753	1	19064.4	C15 H18 N6 Na O4	(M+Na)+
370.13073	1	3624	C15 H18 N6 Na O4	(M+Na)+
371.13112	1	1591.5	C15 H18 N6 Na O4	(M+Na)+
385.10281	1	3357.7	C15 H18 K N6 O4	(M+K)+
715.26527	1	22254.8	C30 H36 N12 Na O8	(2M+Na)+
716.26916	1	8439.9	C30 H36 N12 Na O8	(2M+Na)+
717.27129	1	1908.5	C30 H36 N12 Na O8	(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	347.14575	347.14623	1.37	100	100	81.13	82.45
2	348.14846	348.14889	1.24	20.65	18.79	16.75	15.49
3	349.15045	349.15116	2.04	2.61	2.49	2.12	2.06

--- End Of Report ---

HPLC

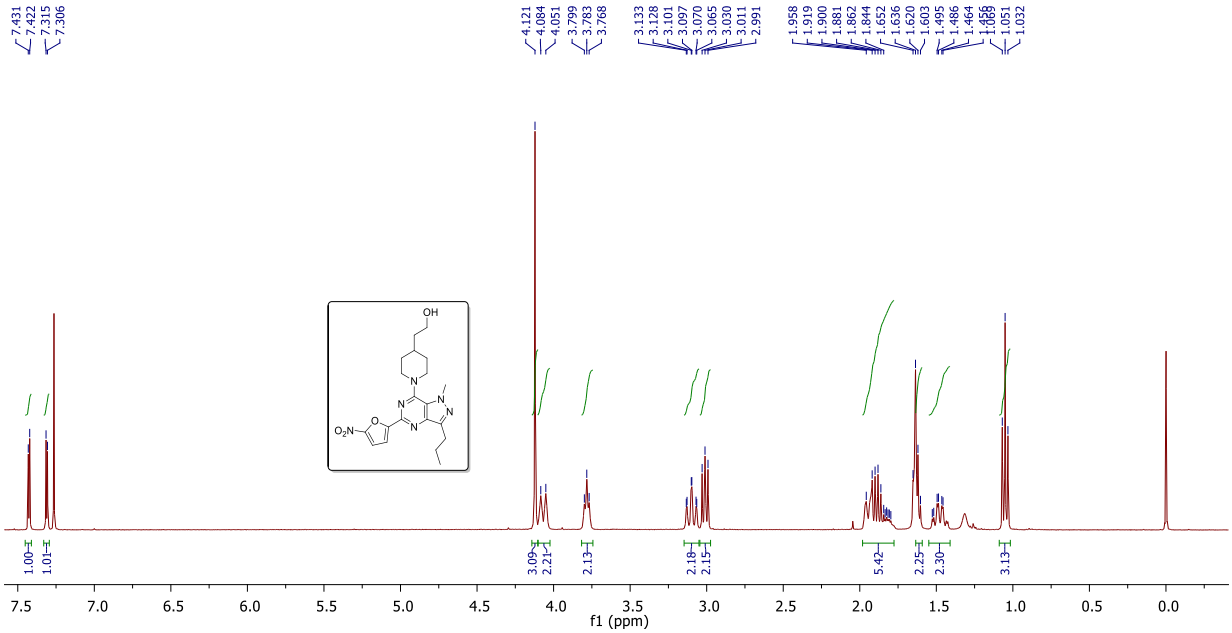


2: 254 nm, 8 nm

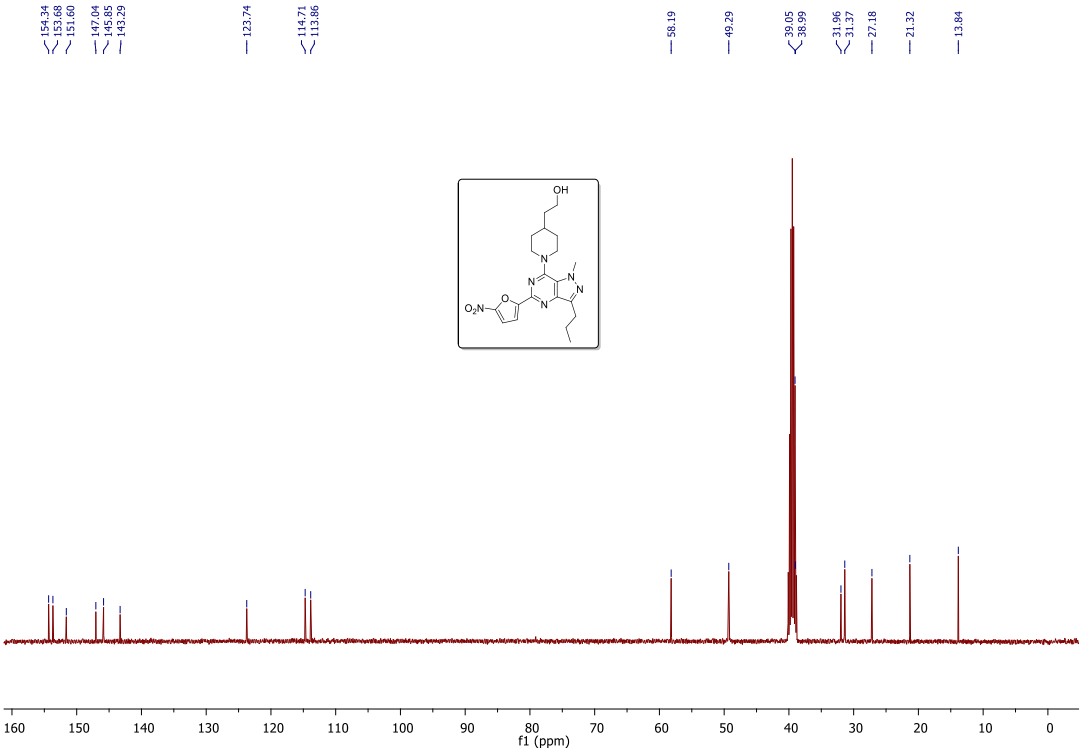
Pk #	Retention Time	Area	Area %	Height	Height %
1	28.107	96951	0.354	6257	0.218
2	29.888	27268806	99.646	2860907	99.782
Totals		27365757	100.000	2867164	100.000

Compound (29)

^{1}H NMR in $CDCl_3$

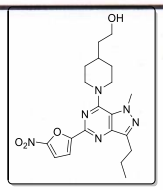


^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report



Data File	GLR-A-46.d	**Sample Name**	GLR-A-46
Sample Type	Sample	**Position**	Vial 7
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-07-2013 PM 12:51:23
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

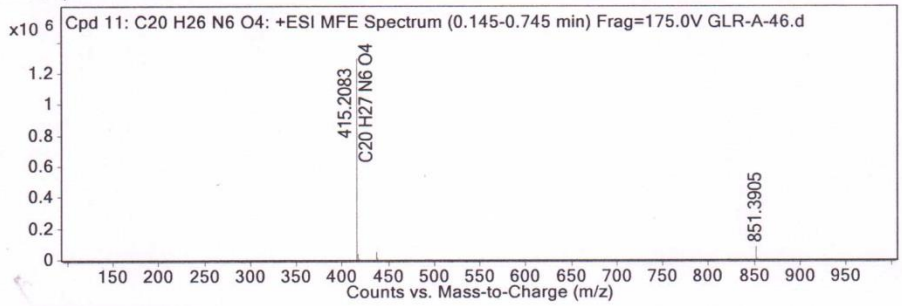
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 11: C20 H26 N6 O4	0.196	414.2011	C20 H26 N6 O4	C20 H26 N6 O4	1.06	C20 H26 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 11: C20 H26 N6 O4	415.2083	0.196	Find by Molecular Feature	414.2011

MFE MS Spectrum



MS Spectrum Peak List

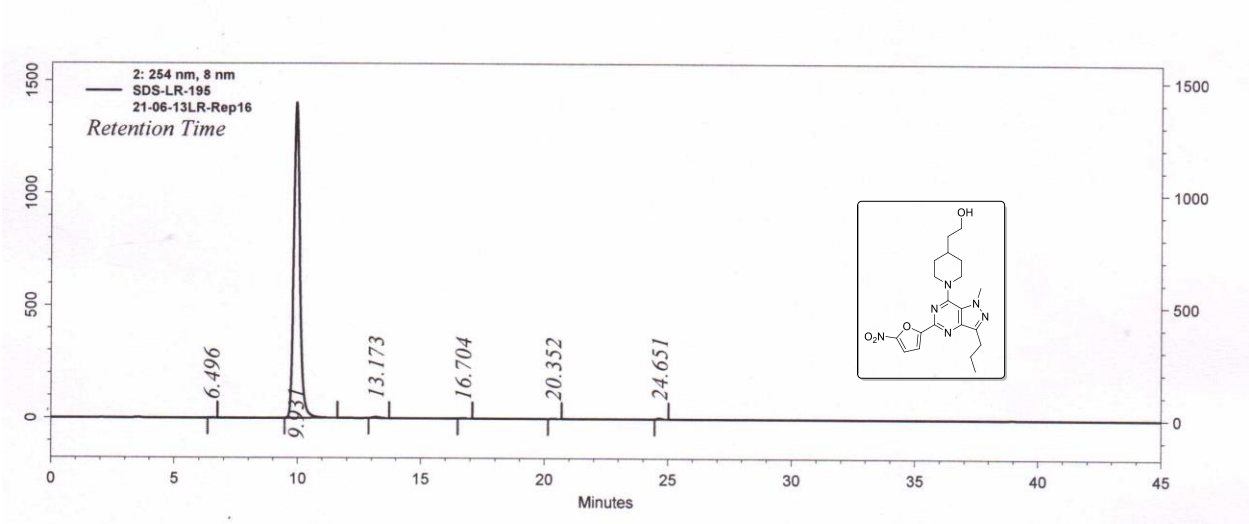
m/z	z	Abund	Formula	Ion
415.2083	1	1292987.38	C20 H27 N6 O4	(M+H)+
416.2117	1	291293.09	C20 H27 N6 O4	(M+H)+
417.2138	1	39021.78	C20 H27 N6 O4	(M+H)+
418.2169	1	4733.37	C20 H27 N6 O4	(M+H)+
437.1901	1	50145.08	C20 H26 N6 Na O4	(M+Na)+
438.1928	1	11900.2	C20 H26 N6 Na O4	(M+Na)+
439.1943	1	2186.7	C20 H26 N6 Na O4	(M+Na)+
851.3905	1	77696.91		(2M+Na)+
852.3931	1	37551.07		(2M+Na)+
853.3957	1	9755.46		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	415.2083	415.2088	1.32	100	100	79.4	77.89
2	416.2117	416.2117	-0.05	22.53	24.29	17.89	18.92
3	417.2138	417.2141	0.76	3.02	3.65	2.4	2.84
4	418.2169	418.2166	-0.69	0.37	0.41	0.29	0.32
5	419.2203	419.219	-3.1	0.03	0.04	0.02	0.03

--- End Of Report ---

HPLC

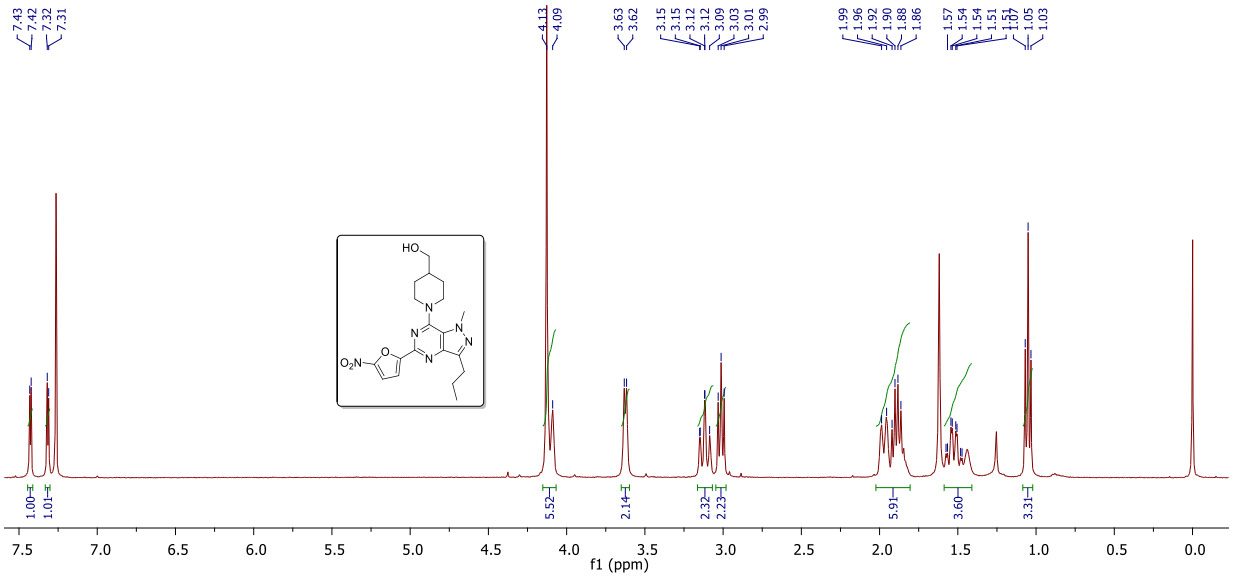


2: 254 nm, 8 nm

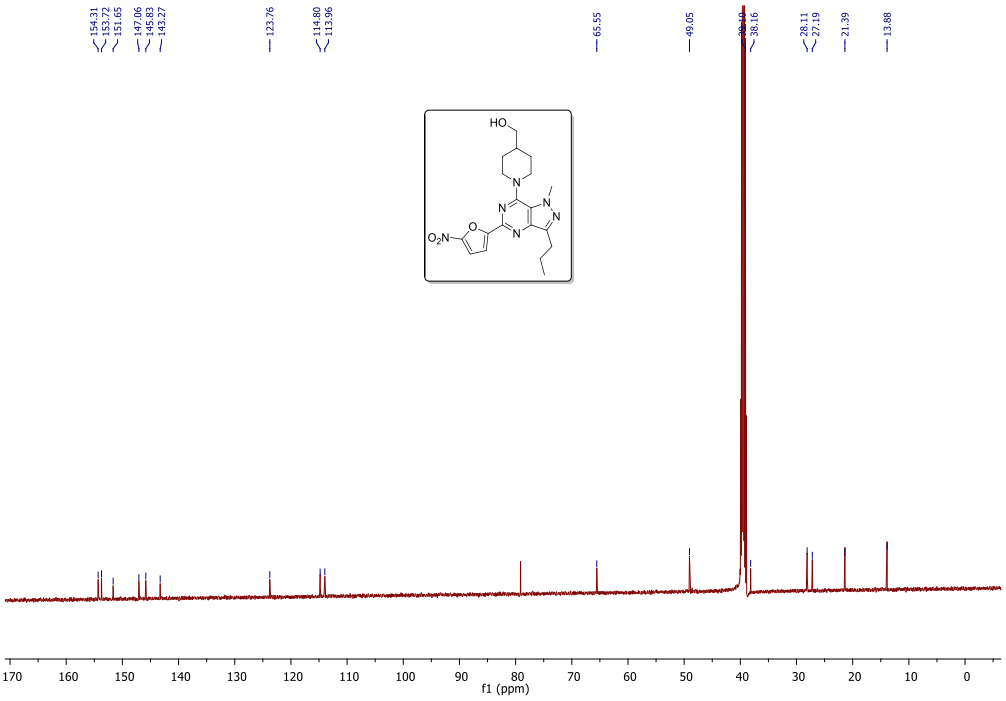
Pk #	Retention Time	Area	Area %	Height	Height %
1	6.496	10741	0.044	967	0.068
2	9.931	24200097	99.287	1403390	99.168
3	13.173	85912	0.352	4511	0.319
4	16.704	11043	0.045	671	0.047
5	20.352	16214	0.067	1096	0.077
6	24.651	49770	0.204	4535	0.320
Totals		24373777	100.000	1415170	100.000

Compound (30)

^{1}H NMR in $CDCl_3$



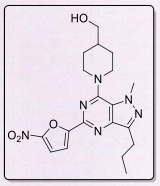
^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report

Data File	GLR-4-36.d	**Sample Name**	GLR-4-36
Sample Type	Sample	**Position**	Vial 7
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/19/2012 12:50:56 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			



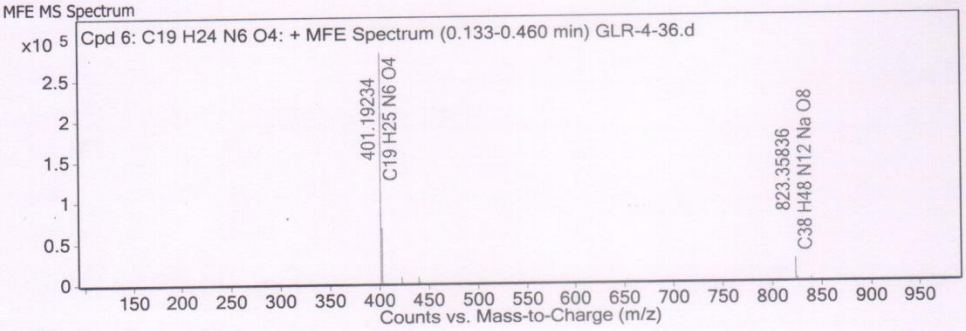
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C19 H24 N6 O4	0.172	400.18506	C19 H24 N6 O4	C19 H24 N6 O4	2.1	C19 H24 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C19 H24 N6 O4	401.19234	0.172	Find by Molecular Feature	400.18506

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
401.19234	1	282970.2	C19 H25 N6 O4	(M+H)+
402.19526	1	67367.8	C19 H25 N6 O4	(M+H)+
403.19781	1	11081.3	C19 H25 N6 O4	(M+H)+
423.17484	1	7723.5	C19 H24 N6 Na O4	(M+Na)+
439.14864	1	7726.5	C19 H24 K N6 O4	(M+K)+
440.15073	1	2042	C19 H24 K N6 O4	(M+K)+
823.35836	1	26678.9	C38 H48 N12 Na O8	(2M+Na)+
824.36126	1	12483.3	C38 H48 N12 Na O8	(2M+Na)+
825.36353	1	3587.6	C38 H48 N12 Na O8	(2M+Na)+
839.33337	1	2868.5	C38 H48 K N12 O8	(2M+K)+

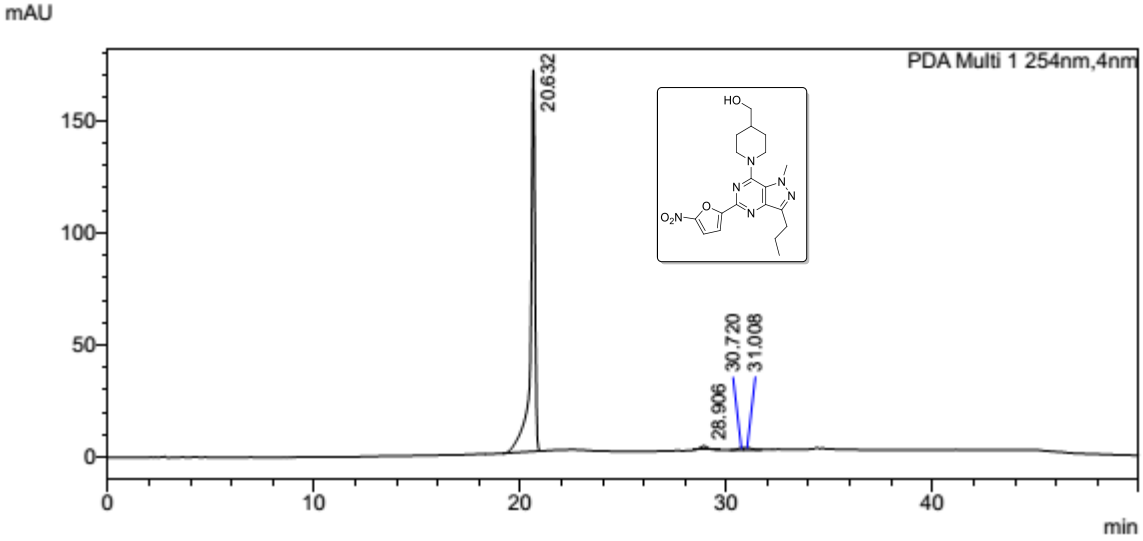
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	401.19234	401.19318	2.1	100	100	77.93	78.77
2	402.19526	402.19598	1.78	23.81	23.18	18.55	18.26
3	403.19781	403.19843	1.54	3.92	3.39	3.05	2.67
4	404.2001	404.20084	1.84	0.59	0.37	0.46	0.29

--- End Of Report ---

HPLC

<Chromatogram>



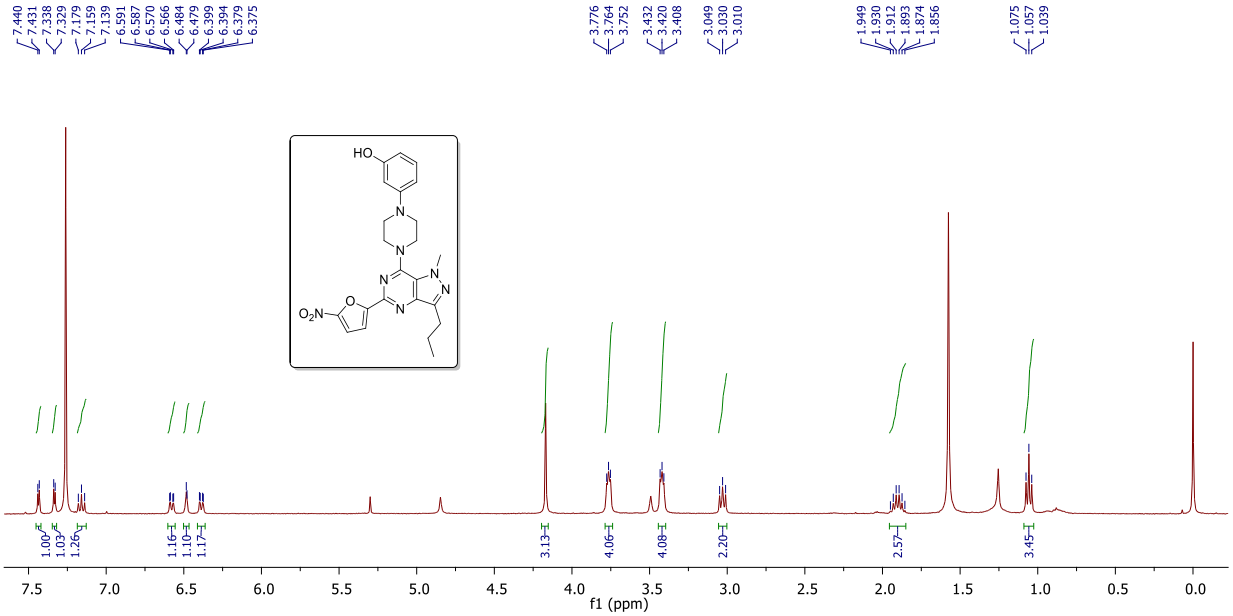
<Peak Table>

PDA Ch1 254nm

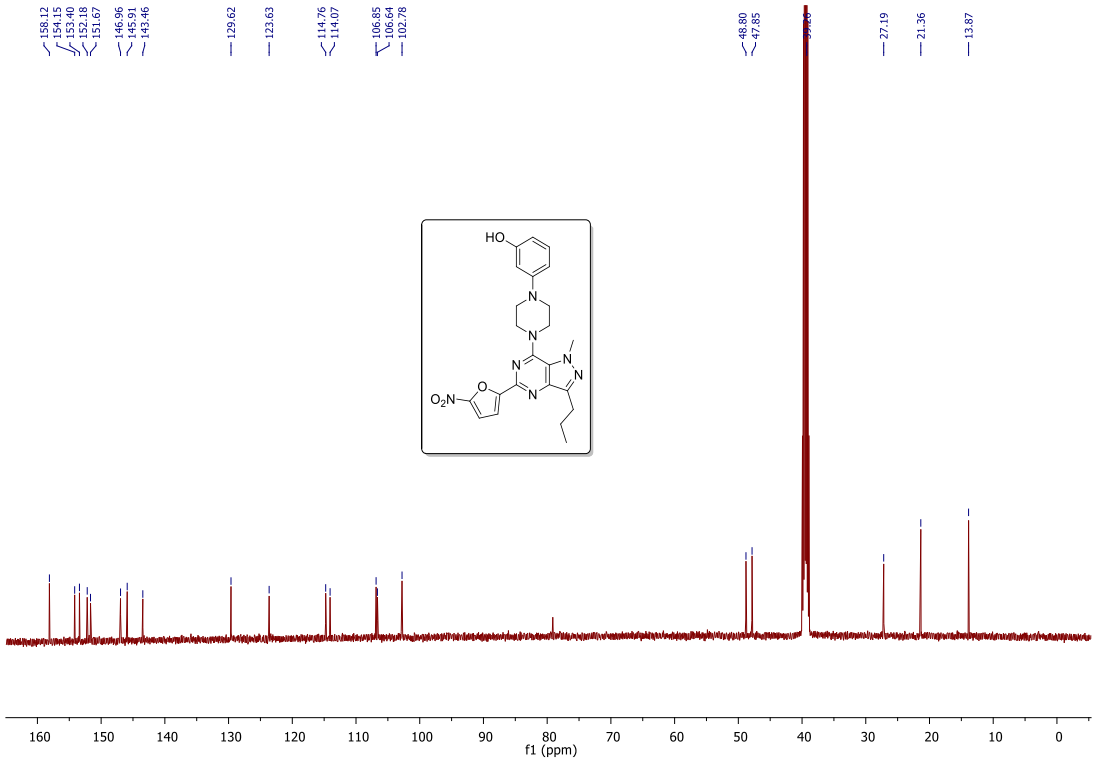
Peak#	Name	Ret. Time	Area	Height	Area%	Height%
1		20.632	2551608	169677	96.403	97.966
2		28.906	56197	1832	2.123	1.058
3		30.720	15467	789	0.584	0.455
4		31.008	23540	902	0.889	0.521
Total			2646813	173199	100.000	100.000

Compound (31)

^{1}H NMR in $CDCl_3$



^{13}C NMR in DMSO-d_6

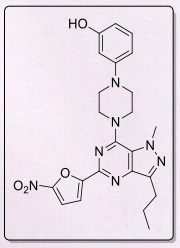


HRMS

Qualitative Compound Report

Data File	GLR-4-38.d	**Sample Name**	GLR-4-38
Sample Type	Sample	**Position**	Vial 14
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/19/2012 1:26:20 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

Sample Group **Info.**

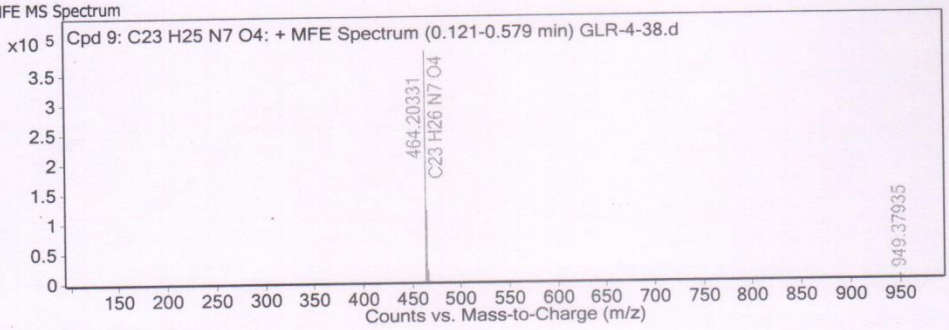


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C23 H25 N7 O4	0.172	463.19602	C23 H25 N7 O4	C23 H25 N7 O4	1.68	C23 H25 N7 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 9: C23 H25 N7 O4	464.20331	0.172	Find by Molecular Feature	463.19602

MFE MS Spectrum



MS Spectrum Peak List

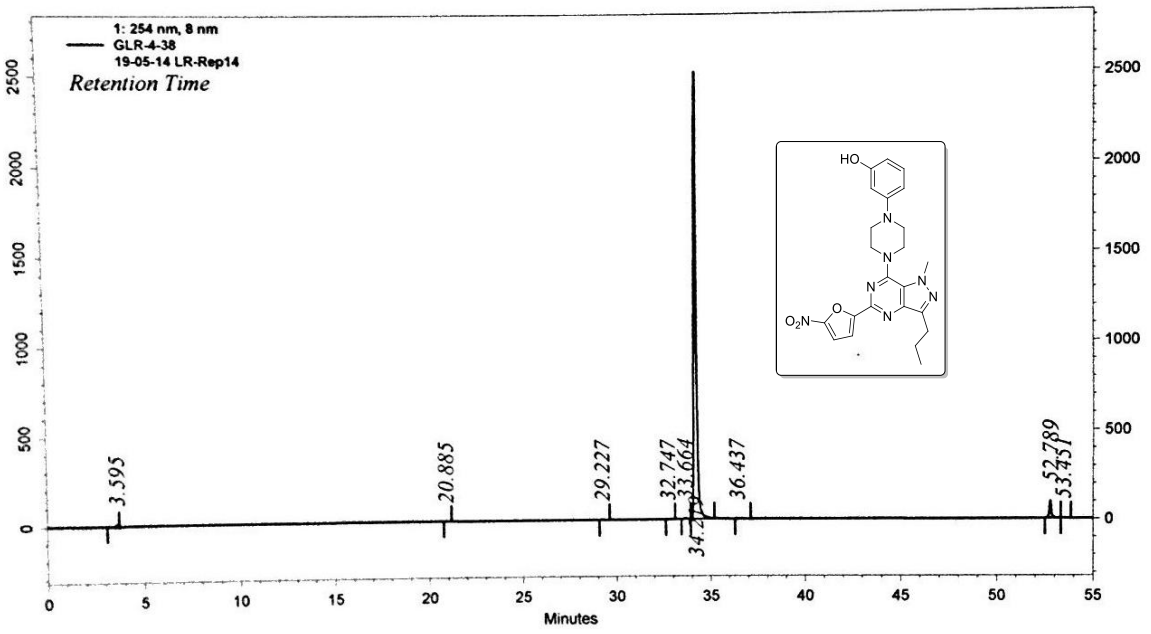
m/z	z	Abund	Formula	Ion
464.20331	1	388142.2	C23 H26 N7 O4	(M+H)+
465.20582	1	120954.3	C23 H26 N7 O4	(M+H)+
466.20898	1	19834	C23 H26 N7 O4	(M+H)+
467.21078	1	2581.2	C23 H26 N7 O4	(M+H)+
949.37935	1	4499.6		(2M+Na)+
950.38136	1	3277.5		(2M+Na)+
951.38441	1	1005.2		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	464.20331	464.20408	1.66	100	100	73.03	75.18
2	465.20582	465.20689	2.3	31.16	27.88	22.76	20.96
3	466.20898	466.20943	0.97	5.11	4.57	3.73	3.44
4	467.21078	467.2119	2.39	0.67	0.55	0.49	0.42

--- End Of Report ---

HPLC

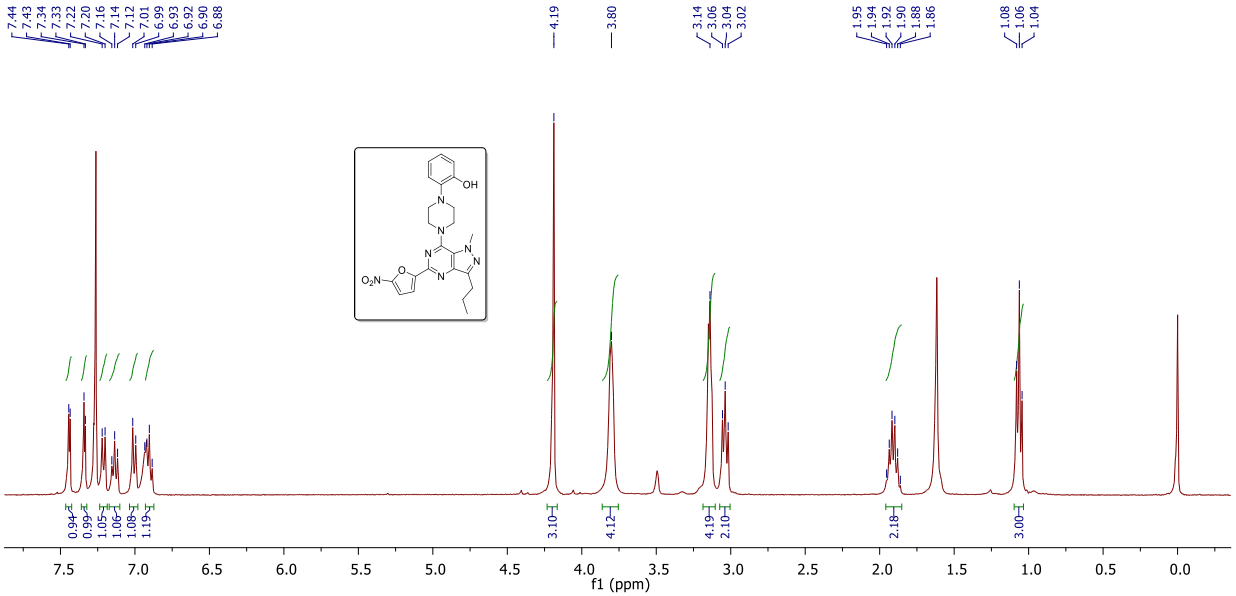


1: 254 nm, 8 nm

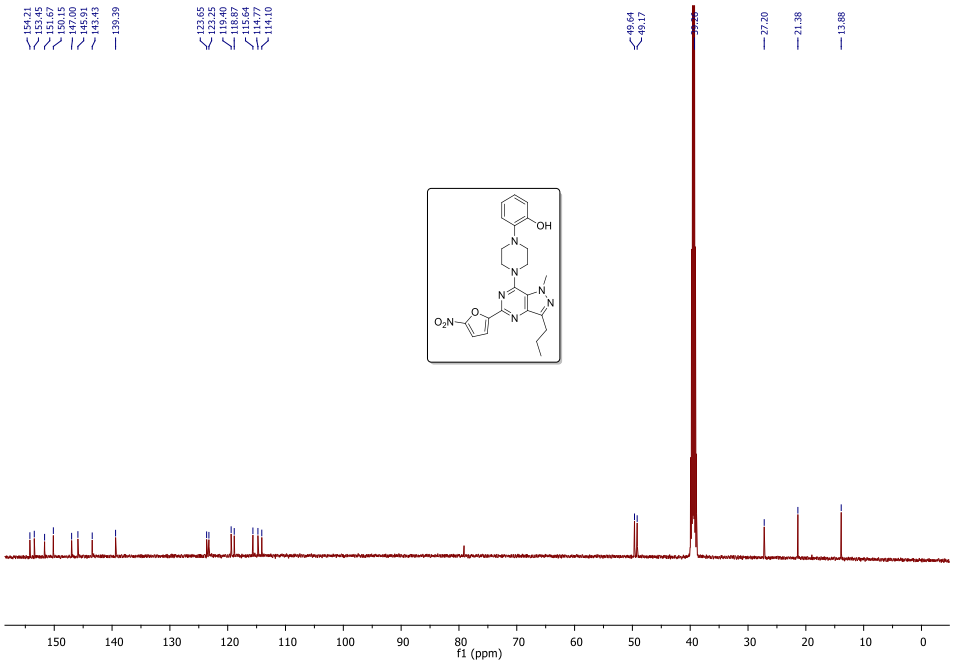
Pk #	Retention Time	Area	Area %	Height	Height %
1	3.595	120378	0.483	15181	0.575
2	20.885	14054	0.056	1582	0.060
3	29.227	33810	0.136	3349	0.127
4	32.747	10754	0.043	980	0.037
5	33.664	69821	0.280	6525	0.247
6	34.219	23947893	96.002	2511024	95.140
7	36.437	36623	0.147	1963	0.074
8	52.789	698526	2.800	97620	3.699
9	53.451	13214	0.053	1065	0.040
Totals		24945073	100.000	2639289	100.000

Compound (32)

^{1}H NMR in $CDCl_3$

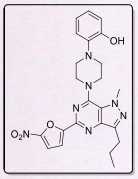


^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report



Data File	GLR-4-39.d	**Sample Name**	GLR-4-39
Sample Type	Sample	**Position**	Vial 9
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/19/2012 1:01:32 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

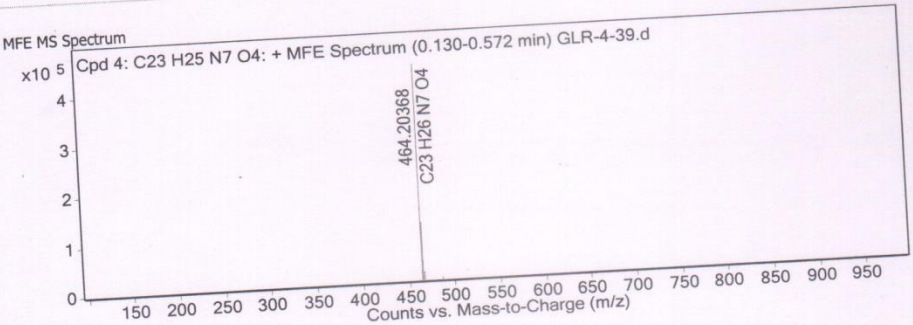
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C23 H25 N7 O4	0.171	463.1964	C23 H25 N7 O4	C23 H25 N7 O4	0.87	C23 H25 N7 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C23 H25 N7 O4	464.20368	0.171	Find by Molecular Feature	463.1964

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
464.20368	1	436361	C23 H26 N7 O4	(M+H)+
465.20611	1	116429.5	C23 H26 N7 O4	(M+H)+
466.20809	1	16902.8	C23 H26 N7 O4	(M+H)+
467.21058	1	2940.3	C23 H26 N7 O4	(M+H)+
486.18616	1	3394.2	C23 H25 N7 Na O4	(M+Na)+
487.18794	1	509.1	C23 H25 N7 Na O4	(M+Na)+

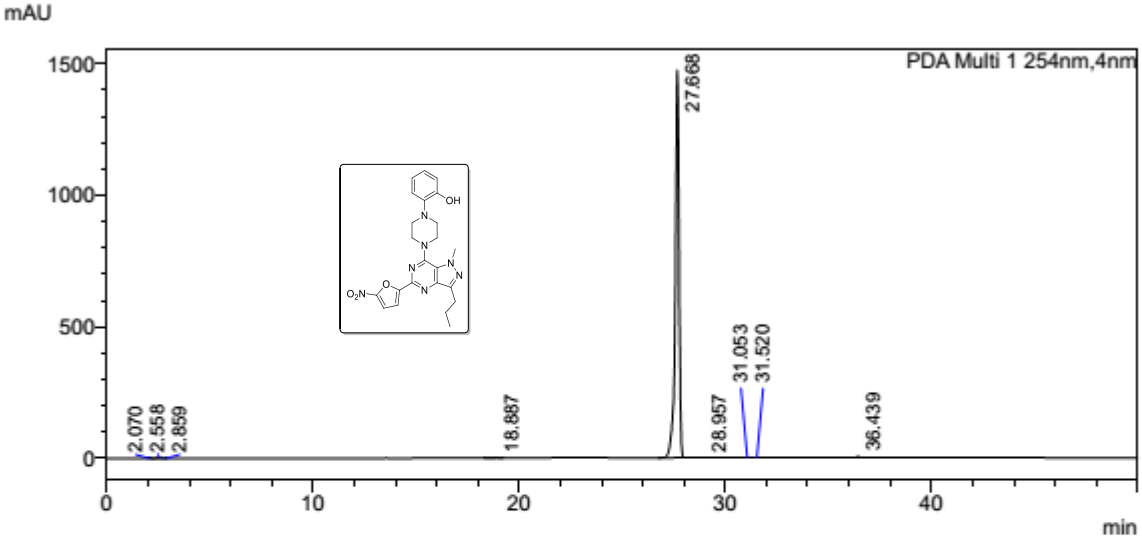
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	464.20368	464.20408	0.85	100	100	76.2	75.18
2	465.20611	465.20689	1.68	26.68	27.88	20.33	20.96
3	466.20809	466.20943	2.89	3.87	4.57	2.95	3.44
4	467.21058	467.2119	2.83	0.67	0.55	0.51	0.42

--- End Of Report ---

HPLC

<Chromatogram>



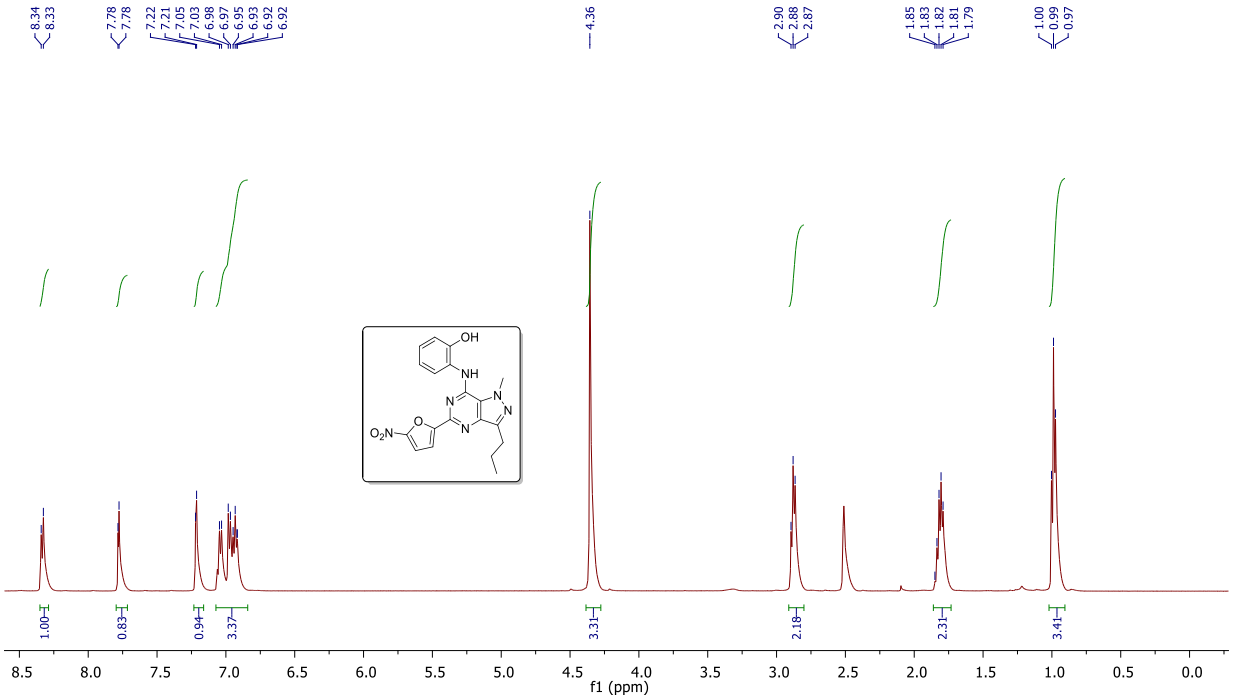
<Peak Table>

PDA Ch1 254nm

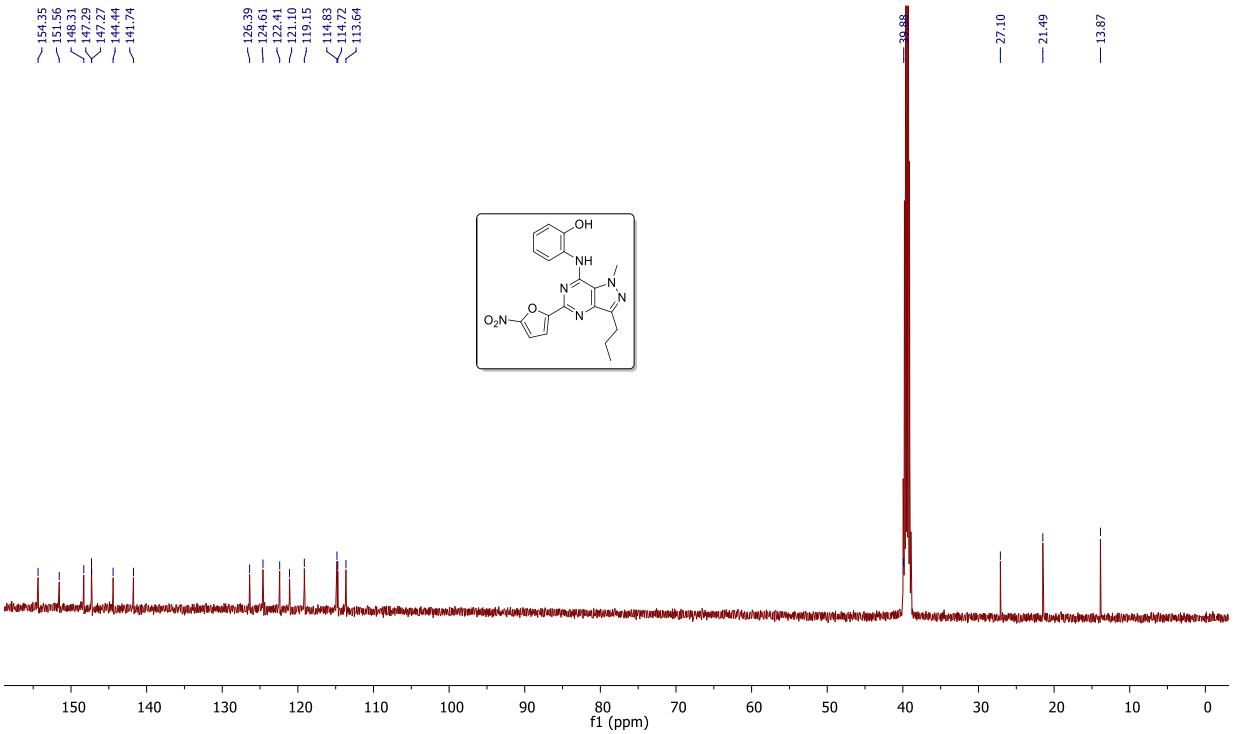
Peak#	Name	Ret. Time	Area	Height	Area%	Height%
1		2.070	3052	423	0.016	0.028
2		2.558	58737	2872	0.308	0.193
3		2.859	3296	954	0.017	0.064
4		18.887	25108	1232	0.132	0.083
5		27.668	18875450	1473646	98.993	99.203
6		28.957	56933	1733	0.299	0.117
7		31.053	4307	275	0.023	0.019
8		31.520	201	37	0.001	0.002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

Compound (33)

^{1}H NMR in DMSO-d$_6$



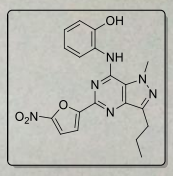
^{13}C NMR in DMSO-d$_6$



HRMS

Qualitative Compound Report

Data File	GCR-4-33.d	**Sample Name**	GCR-4-33
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	29-06-2015 PM 6:33:09
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



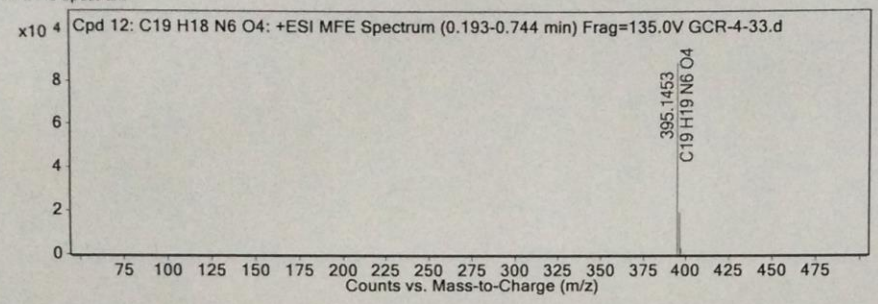
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 12: C19 H18 N6 O4	0.266	394.138	C19 H18 N6 O4	C19 H18 N6 O4	2.54	C19 H18 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 12: C19 H18 N6 O4	395.1453	0.266	Find by Molecular Feature	394.138

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
395.1453	1	88725.32	C19 H19 N6 O4	(M+H)+
396.1479	1	19502.1	C19 H19 N6 O4	(M+H)+
397.1506	1	2852.16	C19 H19 N6 O4	(M+H)+
398.143	1	373.73	C19 H19 N6 O4	(M+H)+

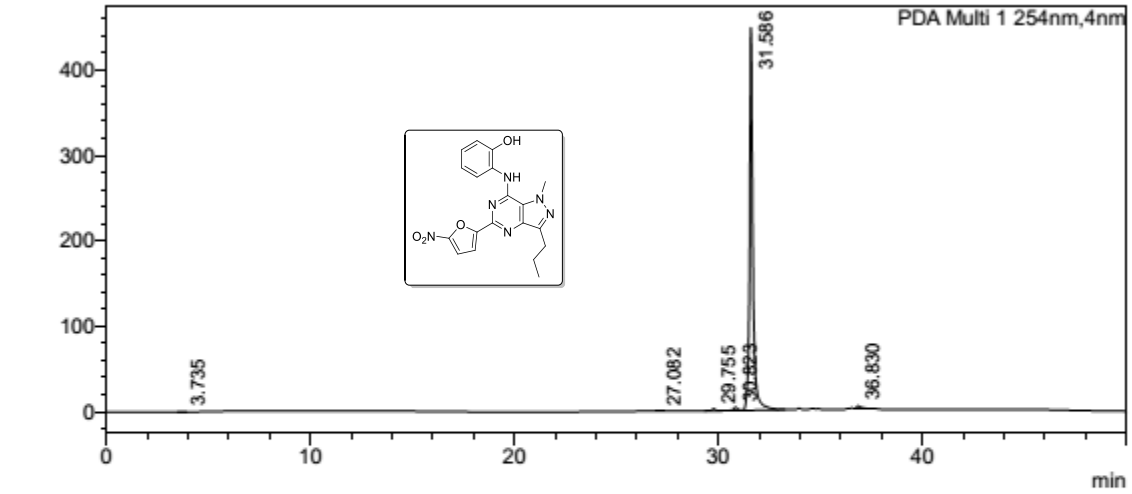
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	395.1453	395.1462	2.36	100	100	79.61	78.83
2	396.1479	396.149	2.87	21.98	23.11	17.5	18.22
3	397.1506	397.1515	2.16	3.21	3.38	2.56	2.66
4	398.143	398.1539	27.25	0.42	0.37	0.34	0.29

--- End Of Report ---

HPLC

<Chromatogram>



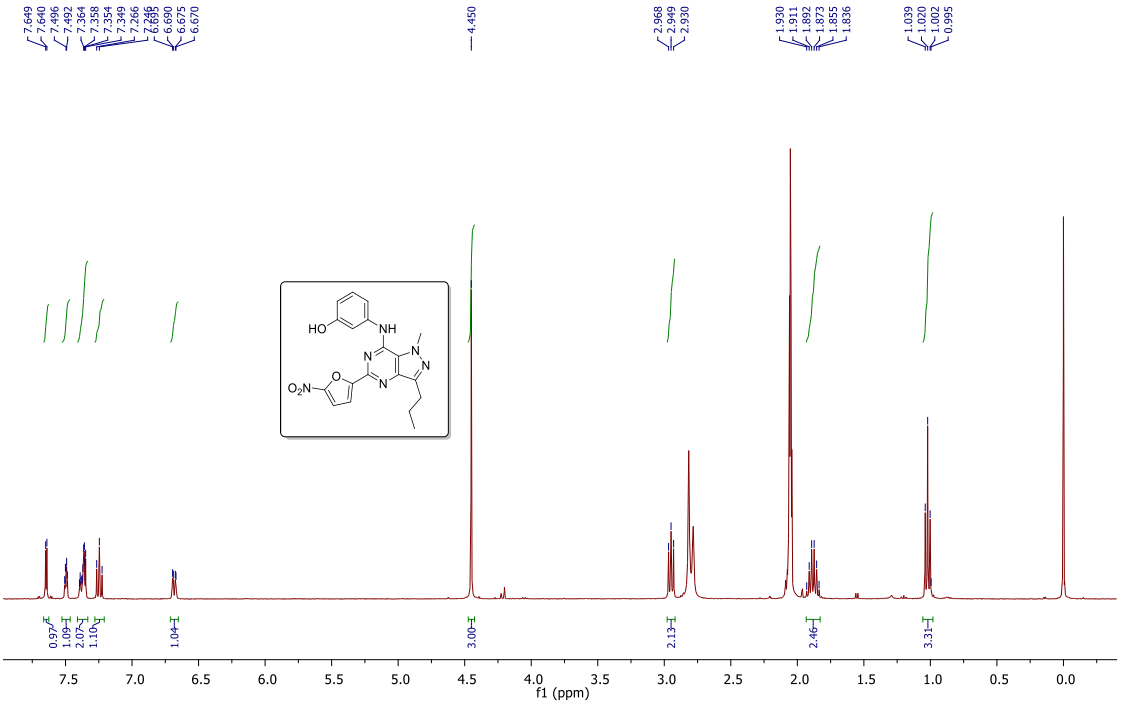
<Peak Table>

PDA Ch1 254nm

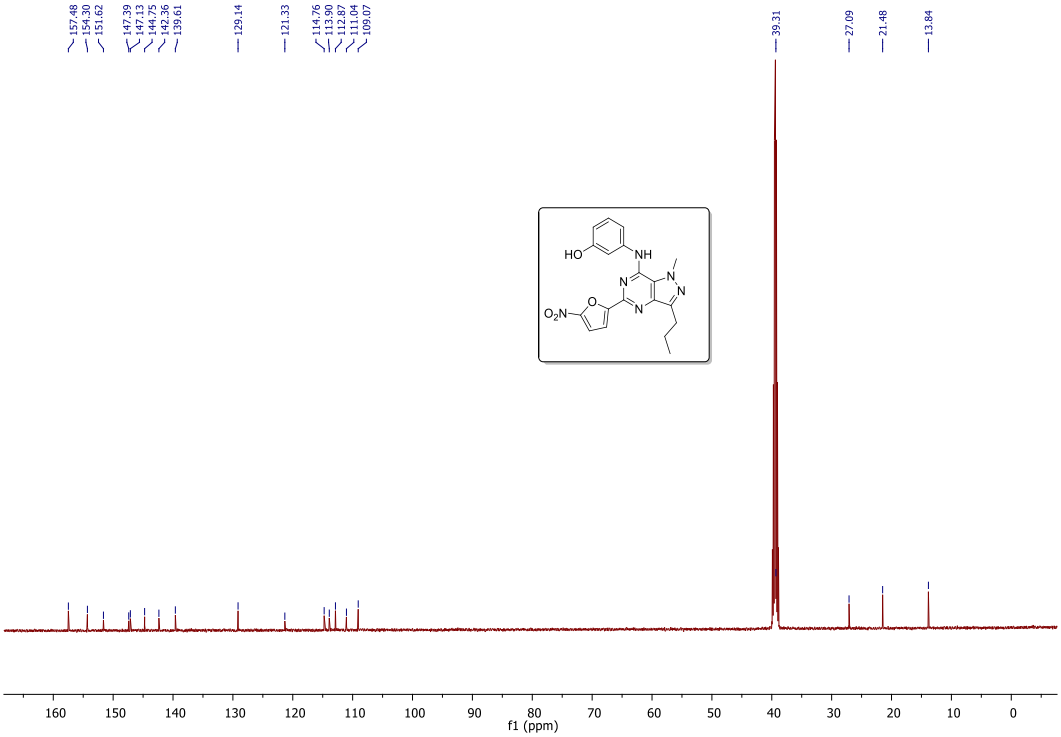
Peak#	Ret. Time	Area	Height	Area%	Height%
1	3.735	3233	275	0.061	0.060
2	27.082	2253	261	0.042	0.057
3	29.755	34028	2442	0.639	0.533
4	30.823	57222	4195	1.075	0.915
5	31.586	5165122	447714	97.060	97.667
6	36.830	59705	3521	1.122	0.768
Total		5321563	458408	100.000	100.000

Compound (34)

^{1}H NMR in Acetone-d$_6$



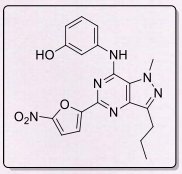
^{13}C NMR in DMSO-d$_6$



HRMS

Qualitative Compound Report

Data File	GLR-4-27.d	**Sample Name**	GLR-4-27
Sample Type	Sample	**Position**	1
Instrument Name	Instrument 1	**User Name**	
Acq Method	29_may__positive.m	**Acquired Time**	6/4/2012 1:15:01 PM
IRM Calibration Status	All Ions Missed	**DA Method**	as.m
Comment			



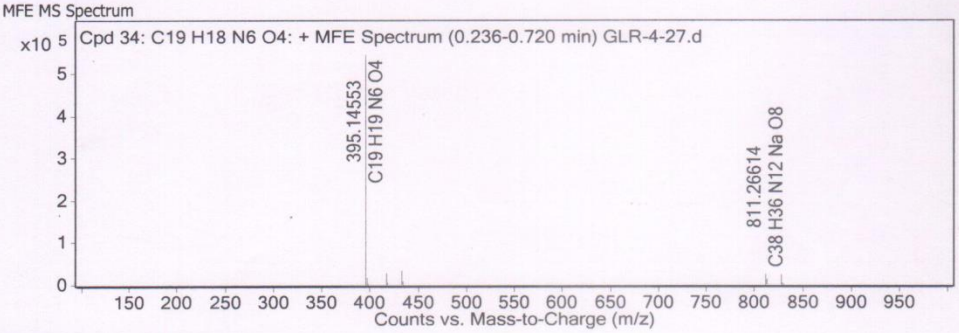
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 34: C19 H18 N6 O4	0.32	394.13826	C19 H18 N6 O4	C19 H18 N6 O4	1.75	C19 H18 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 34: C19 H18 N6 O4	395.14553	0.32	Find by Molecular Feature	394.13826

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
395.14553	1	544598.1	C19 H19 N6 O4	(M+H)+
396.14906	1	117609	C19 H19 N6 O4	(M+H)+
397.15002	1	18189	C19 H19 N6 O4	(M+H)+
417.1278	1	28855.3	C19 H18 N6 Na O4	(M+Na)+
433.10154	1	34032.1	C19 H18 K N6 O4	(M+K)+
434.1044	1	8206	C19 H18 K N6 O4	(M+K)+
811.26614	1	26655.5	C38 H36 N12 Na O8	(2M+Na)+
812.26847	1	13316.7	C38 H36 N12 Na O8	(2M+Na)+
827.23687	1	25617.8	C38 H36 K N12 O8	(2M+K)+
828.2422	1	11309	C38 H36 K N12 O8	(2M+K)+

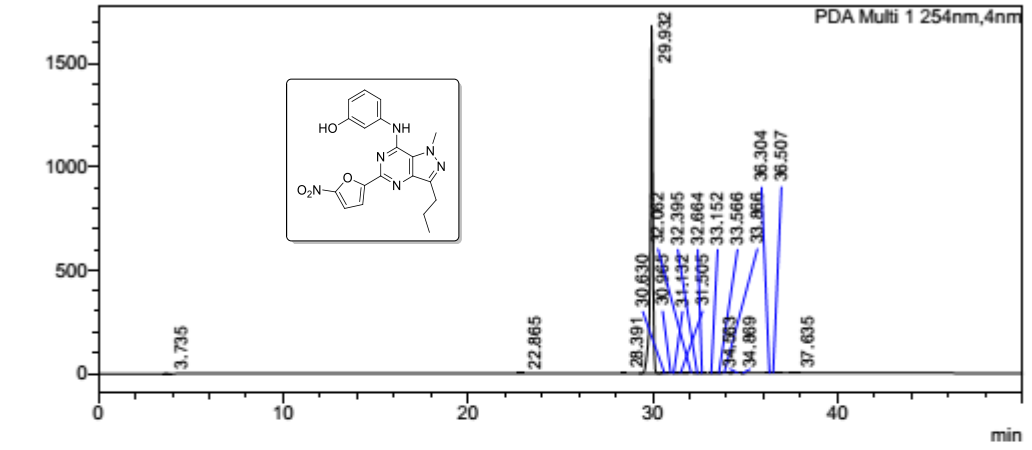
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	395.14553	395.14623	1.76	100	100	79.74	78.83
2	396.14906	396.14902	-0.11	21.6	23.11	17.22	18.22
3	397.15002	397.15146	3.62	3.34	3.38	2.66	2.66
4	398.15323	398.15386	1.6	0.47	0.37	0.37	0.29

--- End Of Report ---

HPLC

<Chromatogram>



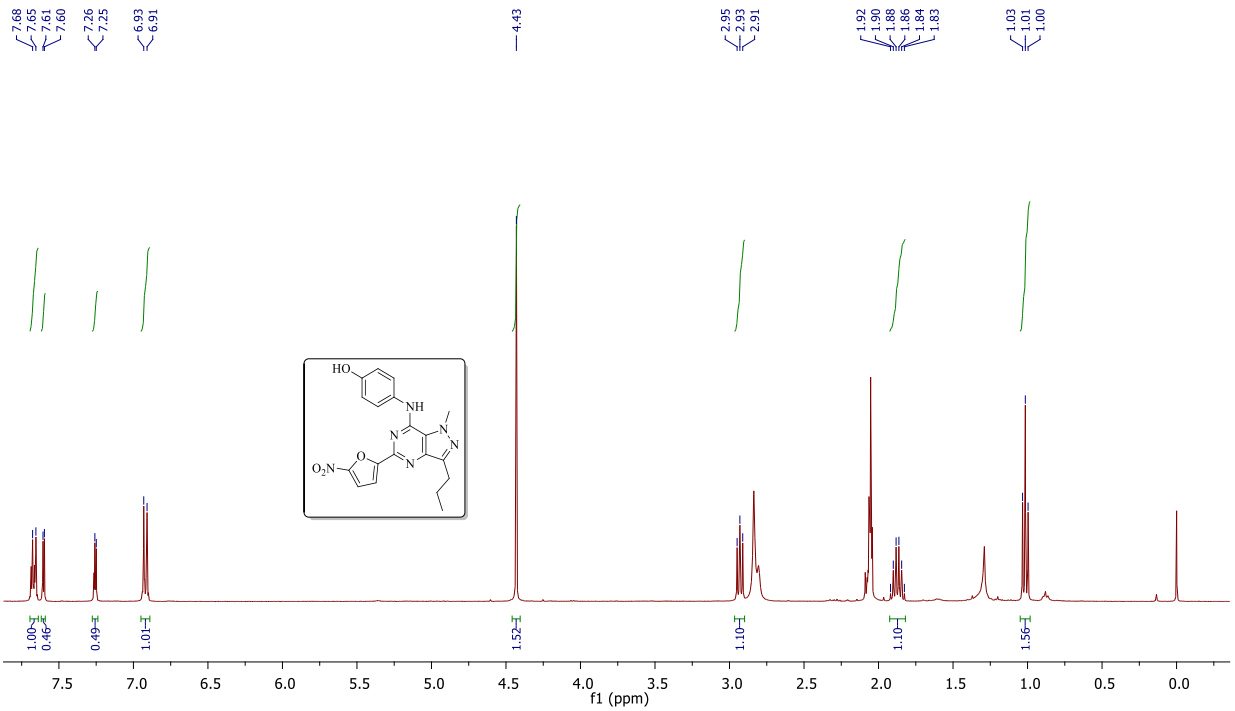
<Peak Table>

PDA Ch1 254nm

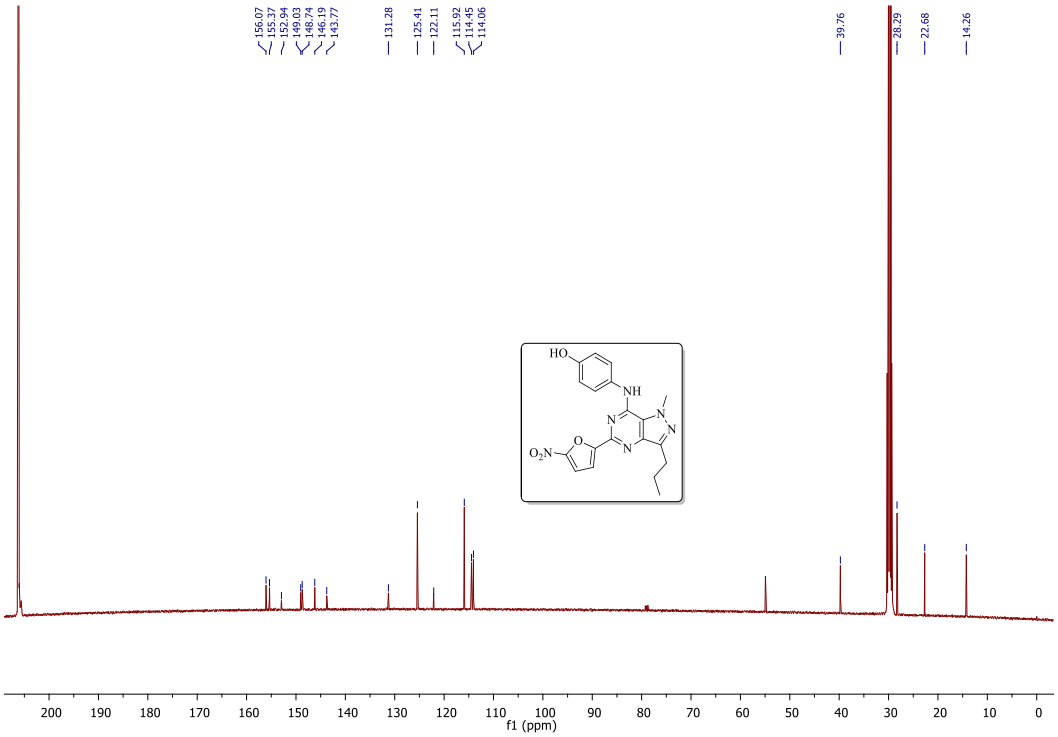
Peak#	Ret. Time	Area	Height	Area%	Height%
1	3.735	3618	307	0.023	0.018
2	22.865	3566	302	0.023	0.018
3	28.391	4146	452	0.026	0.027
4	29.932	15639625	1681682	98.810	99.038
5	30.630	14365	1007	0.091	0.059
6	30.965	14933	1391	0.094	0.082
7	31.132	8188	849	0.052	0.050
8	31.505	14036	1015	0.089	0.060
9	32.062	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)

^{1}H NMR in Acetone- d6



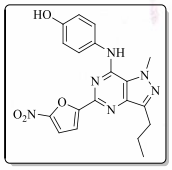
^{13}C NMR in Acetone –d6



HRMS

Qualitative Compound Report

Data File	SDS-LR-59.d	**Sample Name**	SDS-LR-59
Sample Type	Sample	**Position**	Vial 9
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-07-2013 PM 1:00:32
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



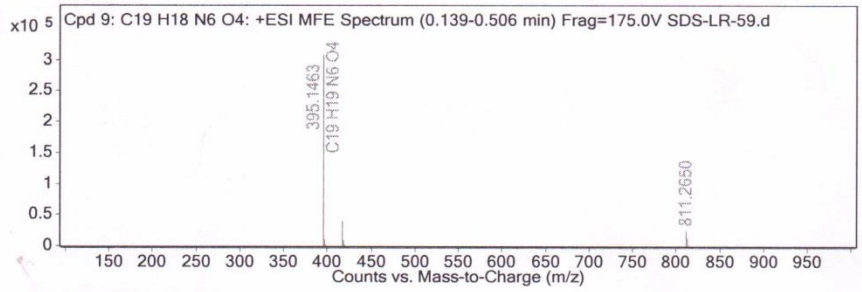
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C19 H18 N6 O4	0.196	394.139	C19 H18 N6 O4	C19 H18 N6 O4	-0.07	C19 H18 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 9: C19 H18 N6 O4	395.1463	0.196	Find by Molecular Feature	394.139

MFE MS Spectrum



MS Spectrum Peak List

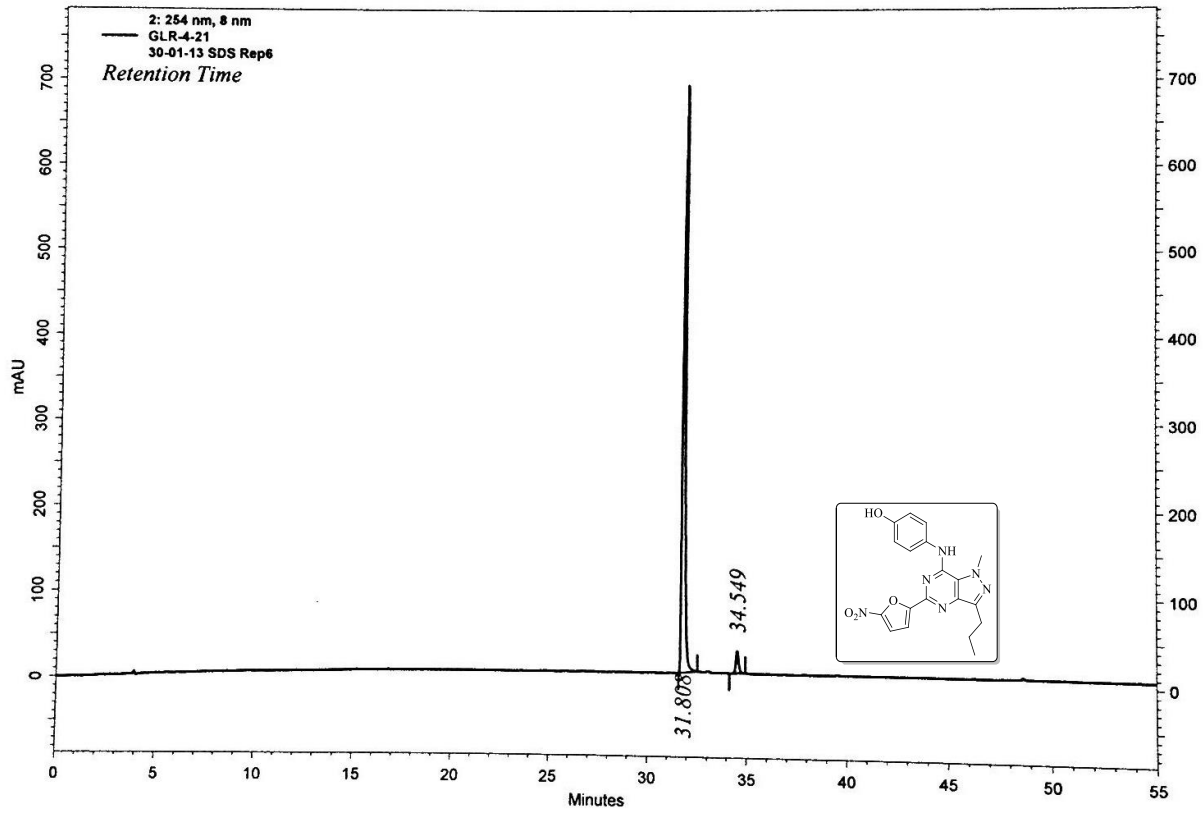
m/z	z	Abund	Formula	Ion
395.1463	1	307886.81	C19 H19 N6 O4	(M+H)+
396.1487	1	69651.94	C19 H19 N6 O4	(M+H)+
397.1511	1	10527.27	C19 H19 N6 O4	(M+H)+
398.1521	1	1216.98	C19 H19 N6 O4	(M+H)+
417.1277	1	39788.2	C19 H18 N6 Na O4	(M+Na)+
418.1314	1	8419.64	C19 H18 N6 Na O4	(M+Na)+
419.1316	1	1643.5	C19 H18 N6 Na O4	(M+Na)+
811.265	1	25112.88		(2M+Na)+
812.2685	1	11525.41		(2M+Na)+
813.2712	1	3134.63		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	395.1463	395.1462	-0.29	100	100	79.09	78.83
2	396.1487	396.149	0.71	22.62	23.11	17.89	18.22
3	397.1511	397.1515	0.78	3.42	3.38	2.7	2.66
4	398.1521	398.1539	4.51	0.4	0.37	0.31	0.29

--- End Of Report ---

HPLC

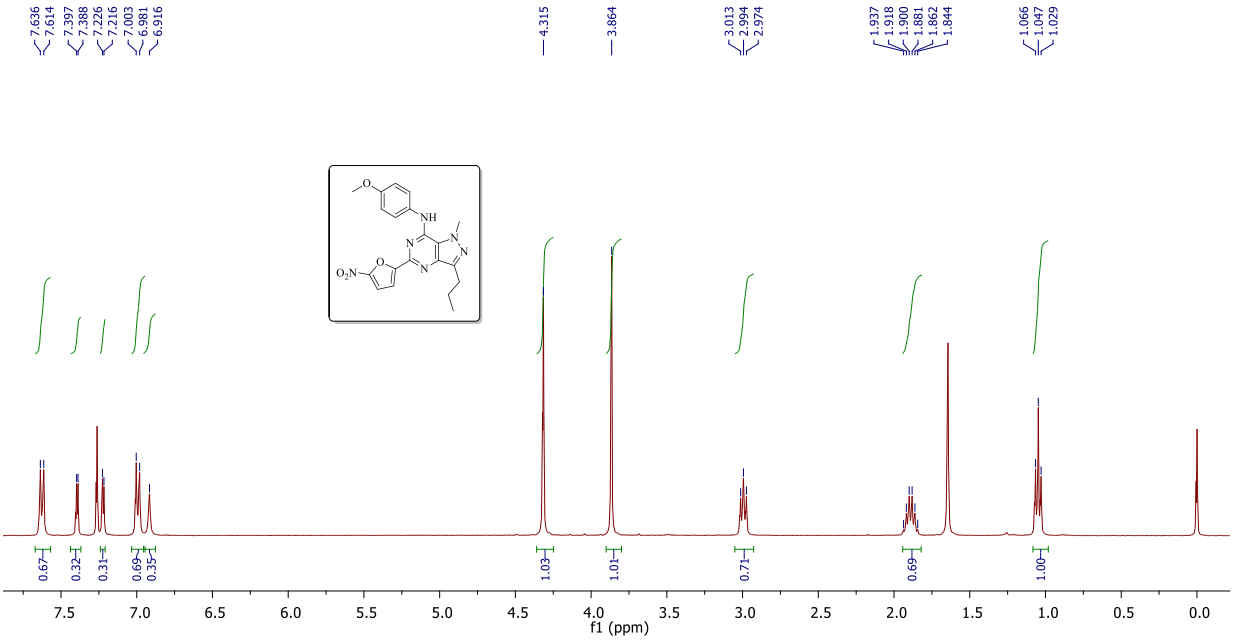


2: 254 nm, 8 nm

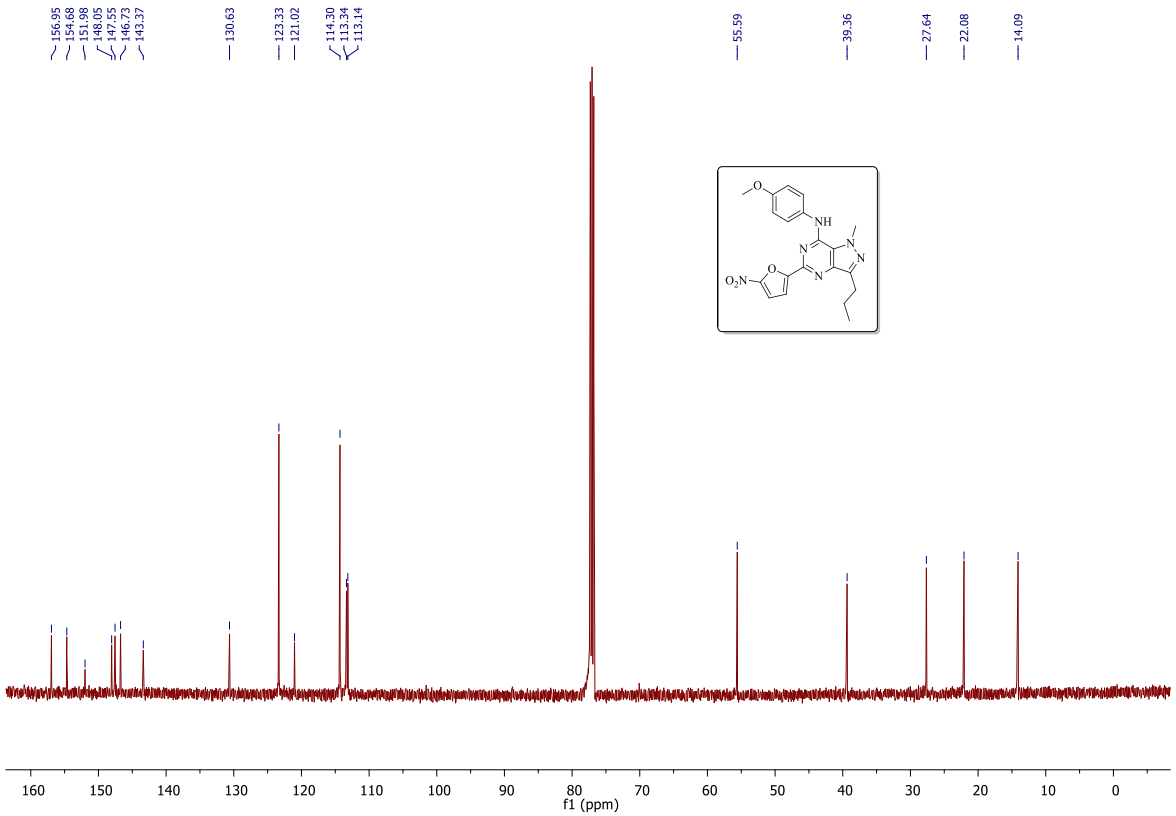
Pk #	Retention Time	Area	Area %	Height	Height %
1	31.808	6510096	96.268	686468	96.419
2	34.549	252349	3.732	25498	3.581
Totals		6762445	100.000	711966	100.000

Compound (36)

^{1}H NMR in $CDCl_3$



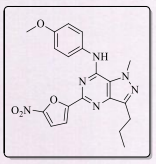
^{13}C NMR in $CDCl_3$



HRMS

Qualitative Compound Report

Data File	GLR-4-32.d	**Sample Name**	GLR-4-32
Sample Type	Sample	**Position**	Vial 4
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/19/2012 12:36:43 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			



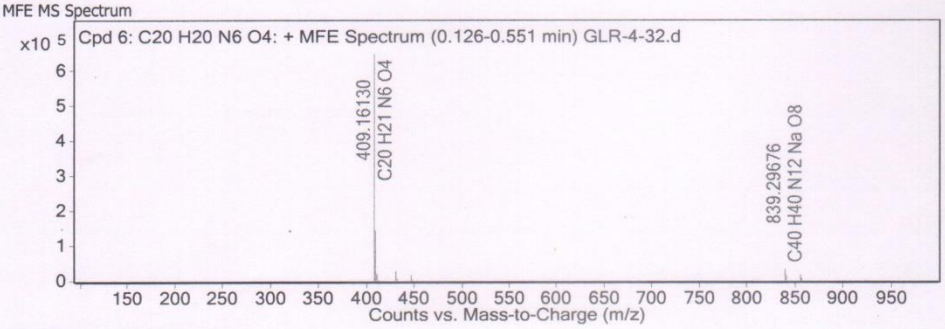
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C20 H20 N6 O4	0.172	408.15402	C20 H20 N6 O4	C20 H20 N6 O4	1.43	C20 H20 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C20 H20 N6 O4	409.1613	0.172	Find by Molecular Feature	408.15402

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
409.1613	1	646423.4	C20 H21 N6 O4	(M+H)+
410.16397	1	143567.2	C20 H21 N6 O4	(M+H)+
411.16613	1	20171.5	C20 H21 N6 O4	(M+H)+
431.14238	1	26980.6	C20 H20 N6 Na O4	(M+Na)+
432.14612	1	6596.8	C20 H20 N6 Na O4	(M+Na)+
447.11766	1	15701.7	C20 H20 K N6 O4	(M+K)+
839.29676	1	33978	C40 H40 N12 Na O8	(2M+Na)+
840.29929	1	15786.4	C40 H40 N12 Na O8	(2M+Na)+
855.27026	1	16701.6	C40 H40 K N12 O8	(2M+K)+
856.27436	1	6608.2	C40 H40 K N12 O8	(2M+K)+

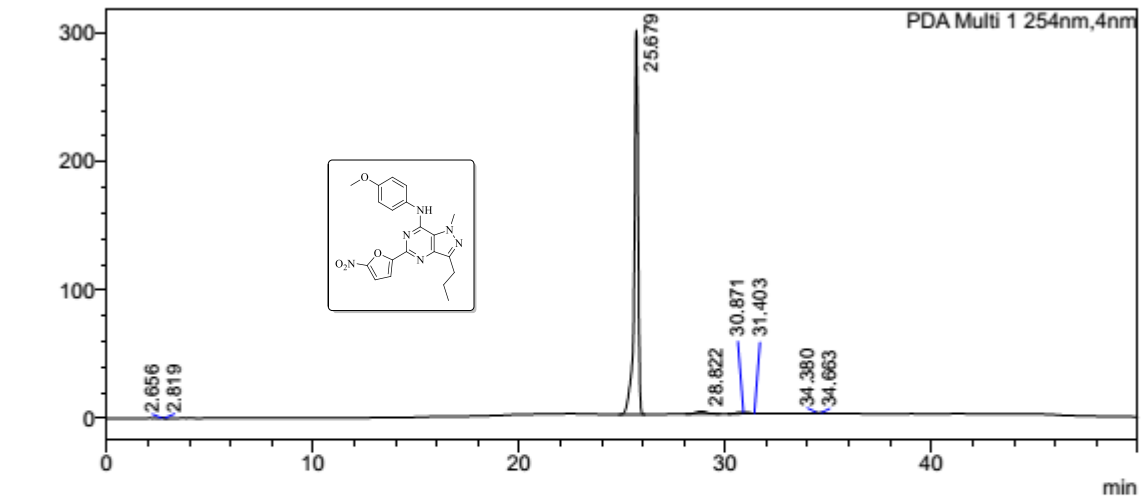
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	409.1613	409.16188	1.42	100	100	79.45	77.97
2	410.16397	410.1647	1.78	22.21	24.22	17.65	18.88
3	411.16613	411.16718	2.56	3.12	3.63	2.48	2.83
4	412.16933	412.16961	0.67	0.53	0.41	0.42	0.32

--- End Of Report ---

HPLC

<Chromatogram>



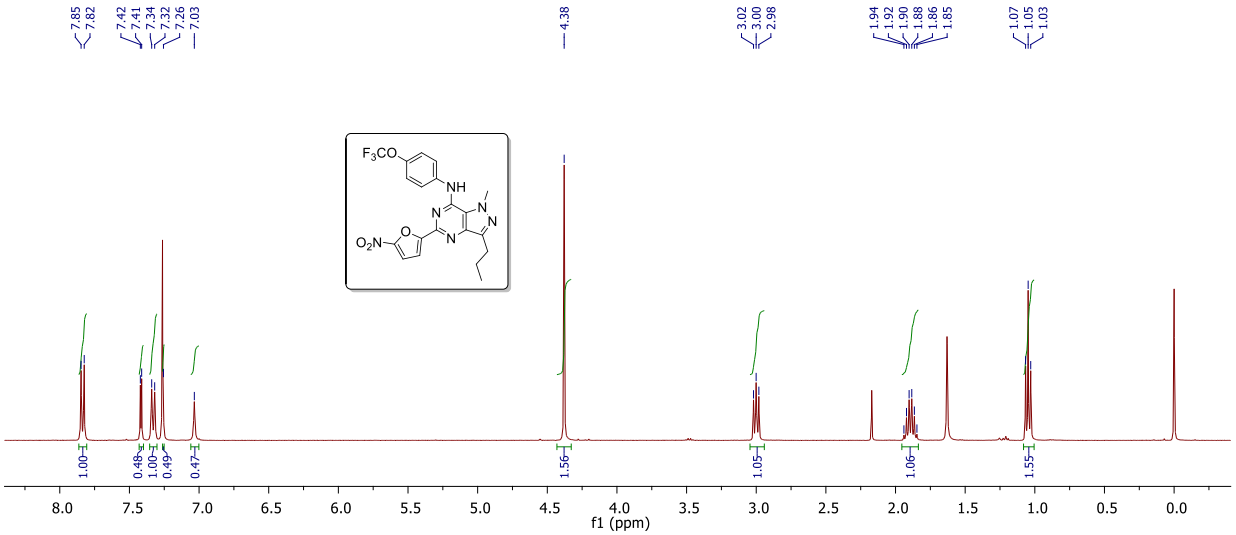
<Peak Table>

PDA Ch1 254nm

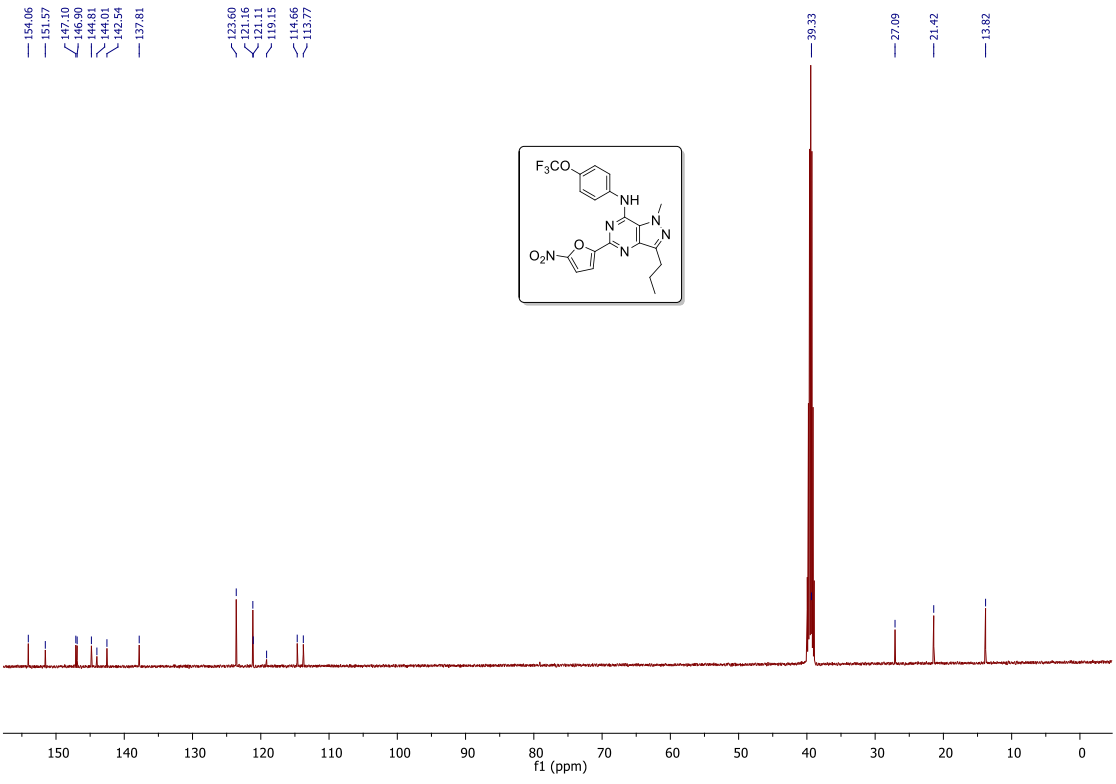
Peak#	Name	Ret. Time	Area	Height	Area%	Height%
1		2.656	1244	193	0.031	0.063
2		2.819	3413	469	0.085	0.154
3		25.679	3867286	299855	96.247	98.190
4		28.822	81184	2126	2.020	0.696
5		30.871	47681	1146	1.187	0.375
6		31.403	3952	397	0.098	0.130
7		34.380	8786	785	0.219	0.257
8		34.663	4528	410	0.113	0.134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

Compound (37)

^{1}H NMR in $CDCl_3$



^{13}C NMR in DMSO-d_6

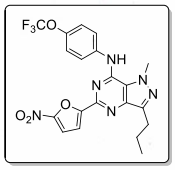


HRMS

Qualitative Compound Report

Data File	GLR-6.d	**Sample Name**	GLR-6
Sample Type	Sample	**Position**	Vial 18
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/18/2012 1:15:54 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

Sample Group **Info.**

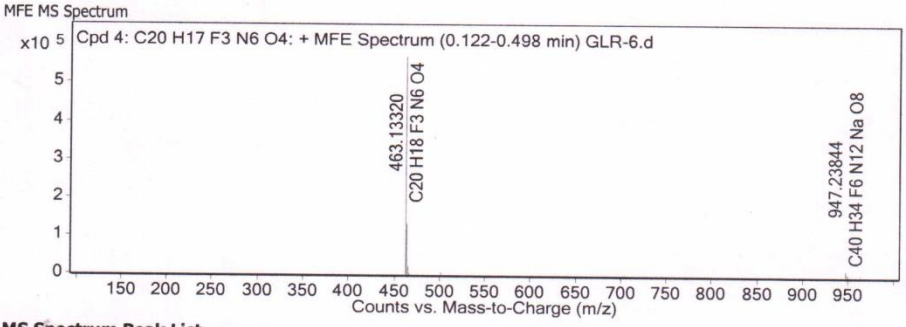


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C20 H17 F3 N6 O4	0.172	462.12592	C20 H17 F3 N6 O4	C20 H17 F3 N6 O4	0.91	C20 H17 F3 N6 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C20 H17 F3 N6 O4	463.1332	0.172	Find by Molecular Feature	462.12592

MFE MS Spectrum



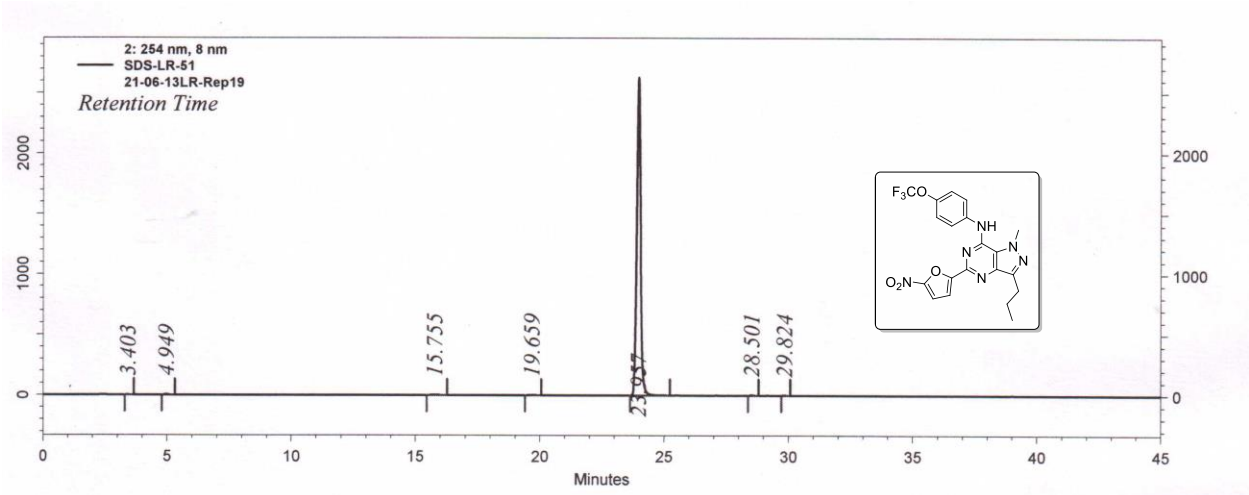
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
463.1332	1	568808.3	C20 H18 F3 N6 O4	(M+H)+
464.13579	1	131893.8	C20 H18 F3 N6 O4	(M+H)+
465.13886	1	20175.6	C20 H18 F3 N6 O4	(M+H)+
466.1372	1	2932.9	C20 H18 F3 N6 O4	(M+H)+
501.08746	1	6053.9	C20 H17 F3 K N6 O4	(M+K)+
502.09058	1	1364.8	C20 H17 F3 K N6 O4	(M+K)+
947.23844	1	14232.7	C40 H34 F6 N12 Na O8	(2M+Na)+
948.24204	1	6514.4	C40 H34 F6 N12 Na O8	(2M+Na)+
949.24633	1	1990.3	C40 H34 F6 N12 Na O8	(2M+Na)+
963.21522	1	1511.5	C40 H34 F6 K N12 O8	(2M+K)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	463.1332	463.13361	0.9	100	100	78.59	77.99
2	464.13579	464.13643	1.36	23.19	24.18	18.22	18.86
3	465.13886	465.1389	0.09	3.55	3.63	2.79	2.83
4	466.1372	466.14133	8.86	0.52	0.41	0.41	0.32

--- End Of Report ---

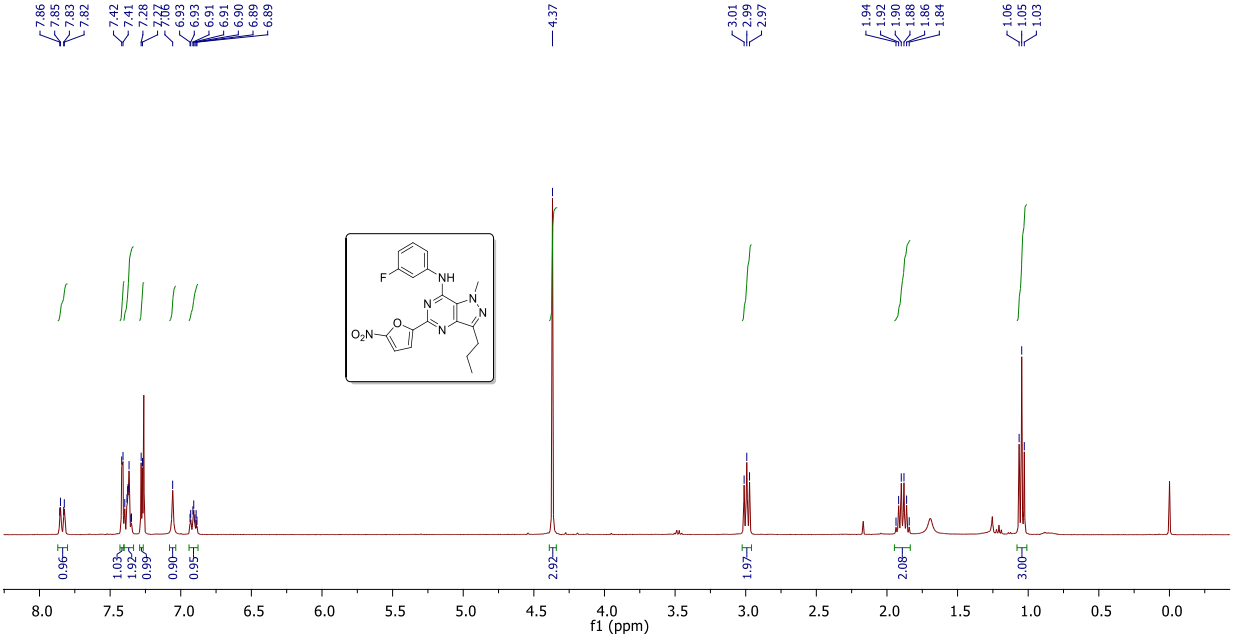


2: 254 nm, 8 nm

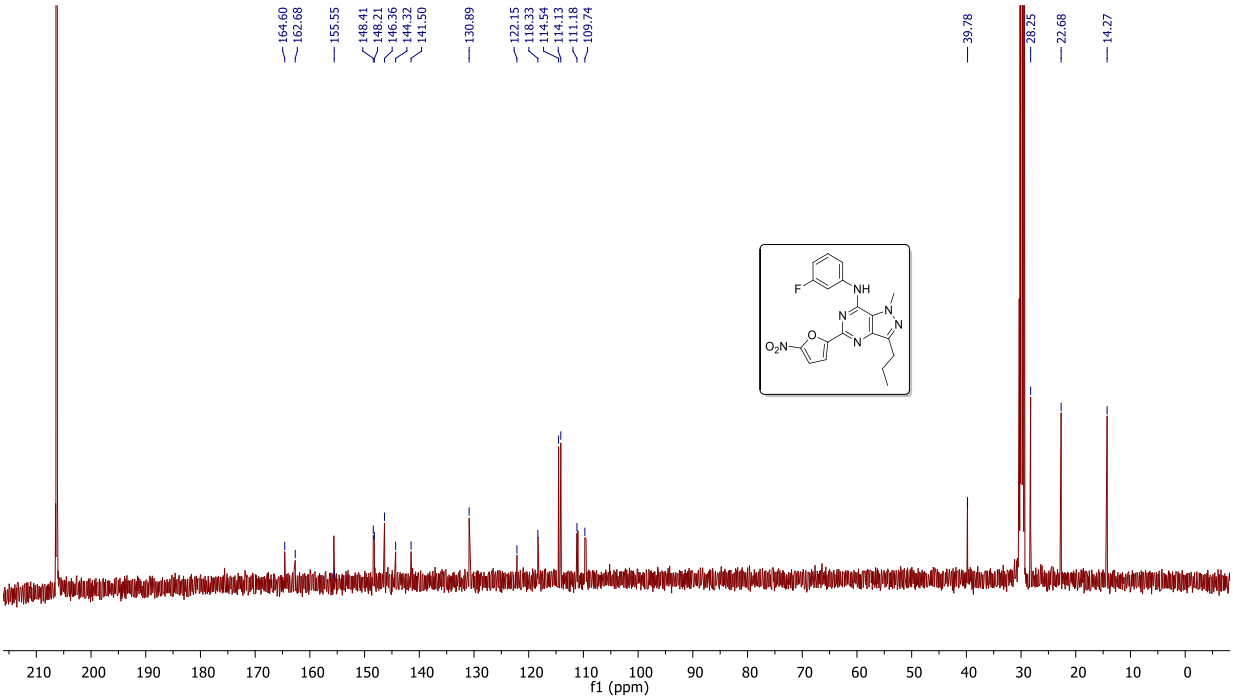
Pk #	Retention Time	Area	Area %	Height	Height %
1	3.403	10275	0.035	1422	0.054
2	4.949	43431	0.148	4175	0.158
3	15.755	41166	0.140	1944	0.074
4	19.659	44427	0.151	2542	0.096
5	23.957	29155654	99.387	2628026	99.422
6	28.501	28367	0.097	3582	0.136
7	29.824	12104	0.041	1610	0.061
Totals		29335424	100.000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

Compound (38)

^{1}H NMR in $CDCl_3$



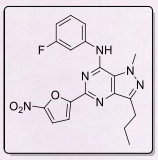
^{13}C NMR in Acetone -d6



HRMS

Qualitative Compound Report

Data File	GLR-4-22.d	**Sample Name**	GLR-4-22
Sample Type	Sample	**Position**	23
Instrument Name	Instrument 1	**User Name**	
Acq Method	29_may__positive.m	**Acquired Time**	6/4/2012 2:56:52 PM
IRM Calibration Status	All Ions Missed	**DA Method**	as.m
Comment			



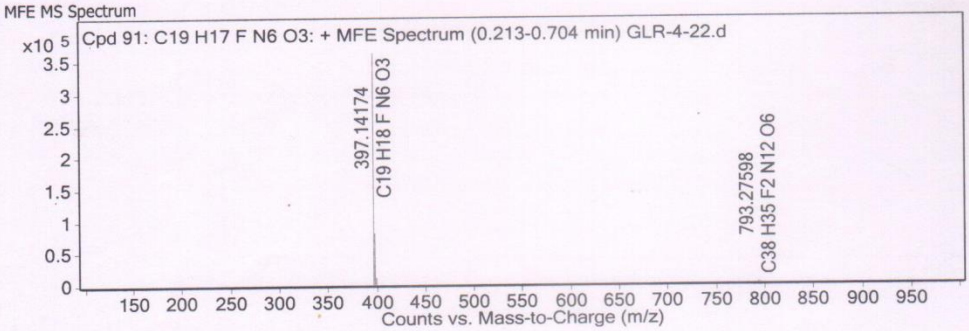
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 91: C19 H17 F N6 O3	0.331	396.13447	C19 H17 F N6 O3	C19 H17 F N6 O3	0.38	C19 H17 F N6 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 91: C19 H17 F N6 O3	397.14174	0.331	Find by Molecular Feature	396.13447

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
397.14174	1	363797.2	C19 H18 F N6 O3	(M+H)+
398.1453	1	79824.5	C19 H18 F N6 O3	(M+H)+
399.14803	1	11748	C19 H18 F N6 O3	(M+H)+
793.27598	1	2116.4	C38 H35 F2 N12 O6	(2M+H)+
794.27897	1	1080.9	C38 H35 F2 N12 O6	(2M+H)+
795.28384	1	800.5	C38 H35 F2 N12 O6	(2M+H)+

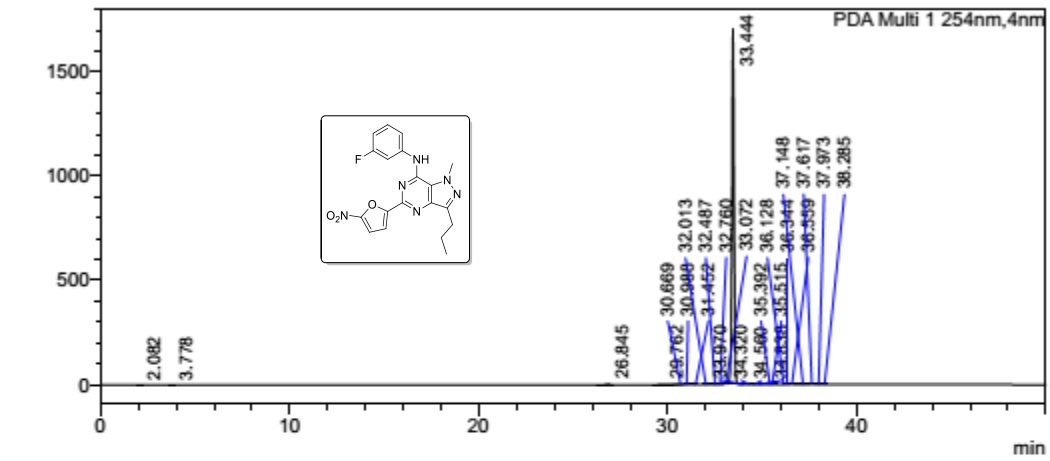
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	397.14174	397.14189	0.4	100	100	79.89	79.22
2	398.1453	398.14468	-1.57	21.94	23.06	17.53	18.27
3	399.14803	399.14718	-2.13	3.23	3.16	2.58	2.5

--- End Of Report ---

HPLC

<Chromatogram>



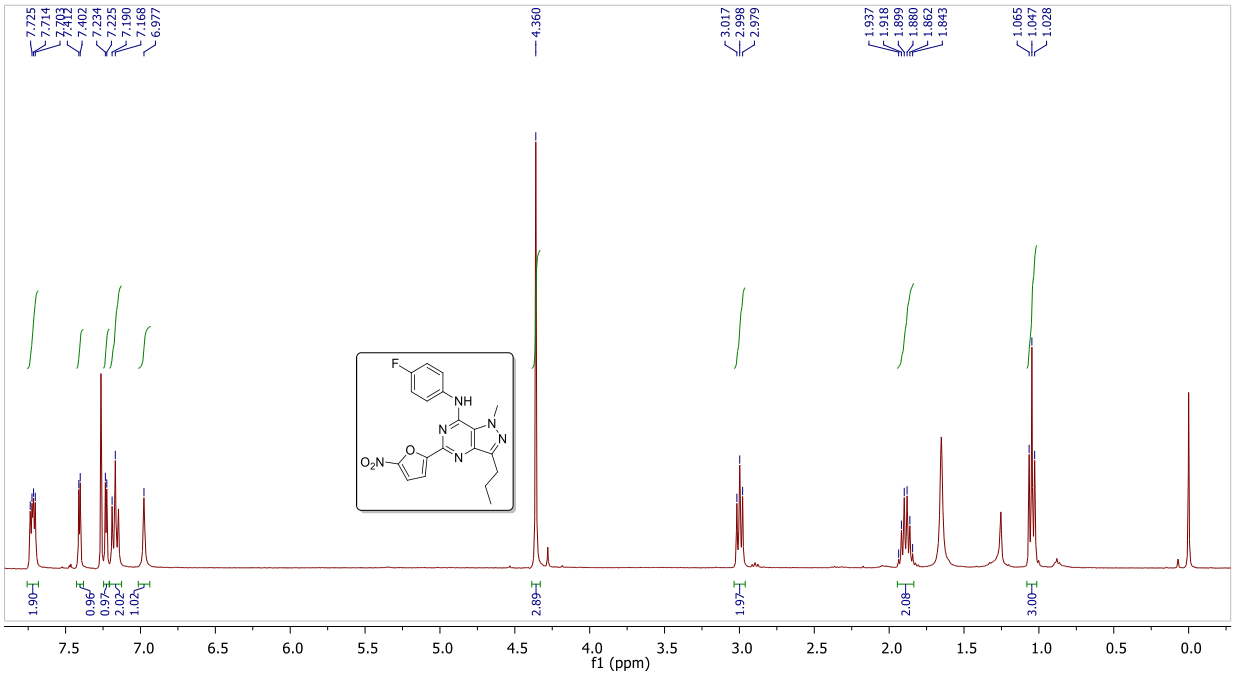
<Peak Table>

PDA Ch1 254nm

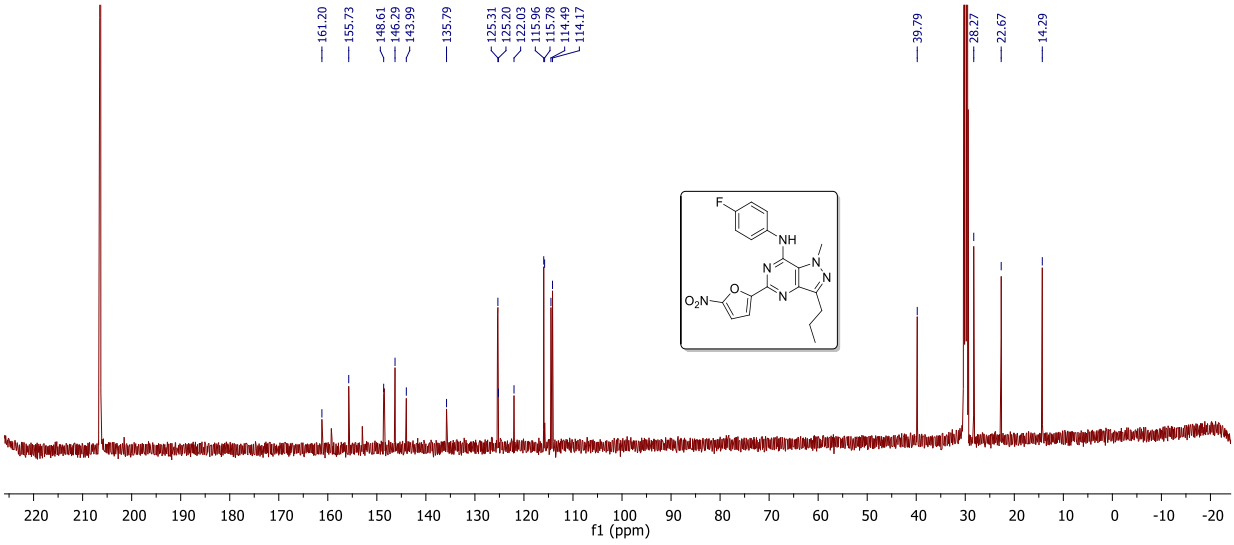
Peak#	Ret. Time	Area	Height	Area%	Height%
1	2.082	3740	436	0.027	0.025
2	3.778	2496	243	0.018	0.014
3	26.845	40589	3569	0.297	0.206
4	29.762	39430	2519	0.288	0.145
5	30.669	13659	971	0.100	0.056
6	30.988	7765	519	0.057	0.030
7	31.452	6511	448	0.048	0.026
8	32.013	3547	297	0.026	0.017
9	32.487	4100	445	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)

^{1}H NMR in $CDCl_3$



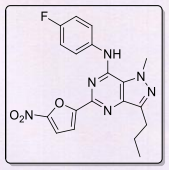
^{13}C NMR in Acetone-d_6



HRMS

Qualitative Compound Report

Data File	GLR-A-20.d	**Sample Name**	GLR-A-20
Sample Type	Sample	**Position**	Vial 10
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-07-2013 PM 1:05:11
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



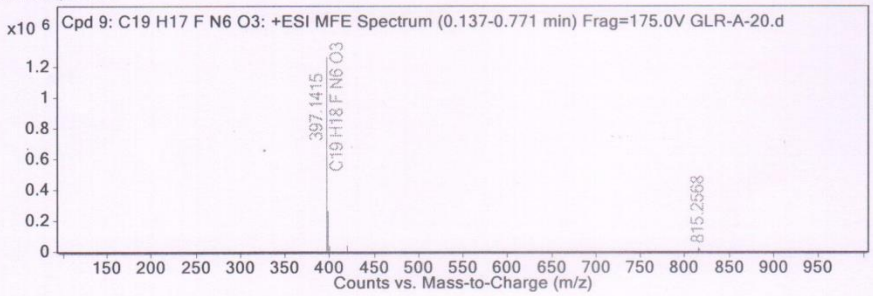
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C19 H17 F N6 O3	0.193	396.1344	C19 H17 F N6 O3	C19 H17 F N6 O3	0.66	C19 H17 F N6 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 9: C19 H17 F N6 O3	397.1415	0.193	Find by Molecular Feature	396.1344

MFE MS Spectrum



MS Spectrum Peak List

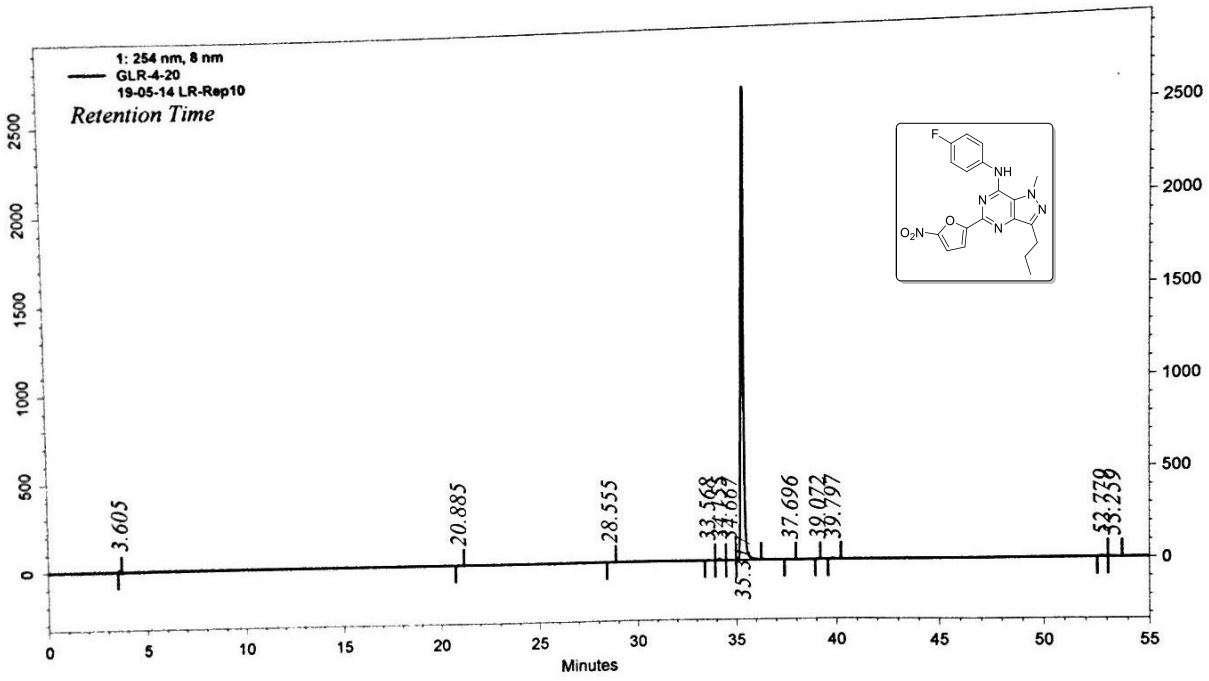
m/z	z	Abund	Formula	Ion
397.1415	1	1264502.5	C19 H18 F N6 O3	(M+H)+
398.1448	1	263032.88	C19 H18 F N6 O3	(M+H)+
399.1468	1	35780.83	C19 H18 F N6 O3	(M+H)+
400.1491	1	3477	C19 H18 F N6 O3	(M+H)+
419.1237	1	33089	C19 H17 F N6 Na O3	(M+Na)+
420.126	1	8806.8	C19 H17 F N6 Na O3	(M+Na)+
421.1289	1	1259.4	C19 H17 F N6 Na O3	(M+Na)+
815.2568	1	23681.71		(2M+Na)+
816.2599	1	11912.44		(2M+Na)+
817.2607	1	3235.56		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	397.1415	397.1419	0.88	100	100	80.71	79.02
2	398.1448	398.1447	-0.41	20.8	23.06	16.79	18.23
3	399.1468	399.1472	0.89	2.83	3.16	2.28	2.5
4	400.1491	400.1496	1.18	0.27	0.32	0.22	0.25

--- End Of Report ---

HPLC

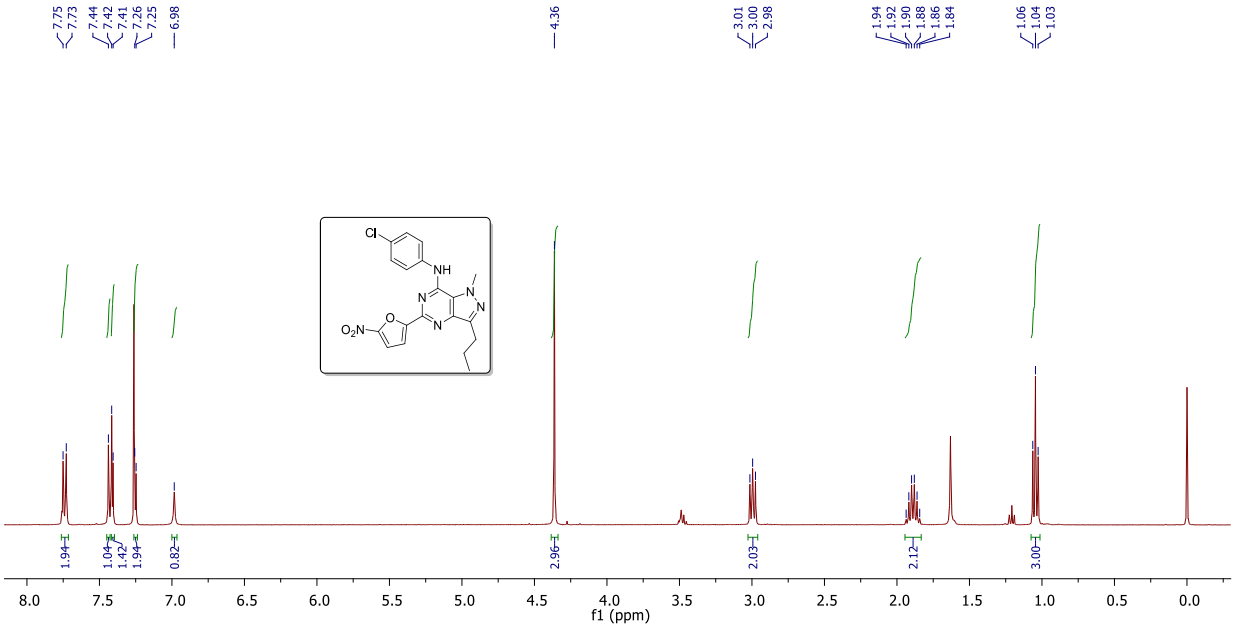


1: 254 nm, 8 nm

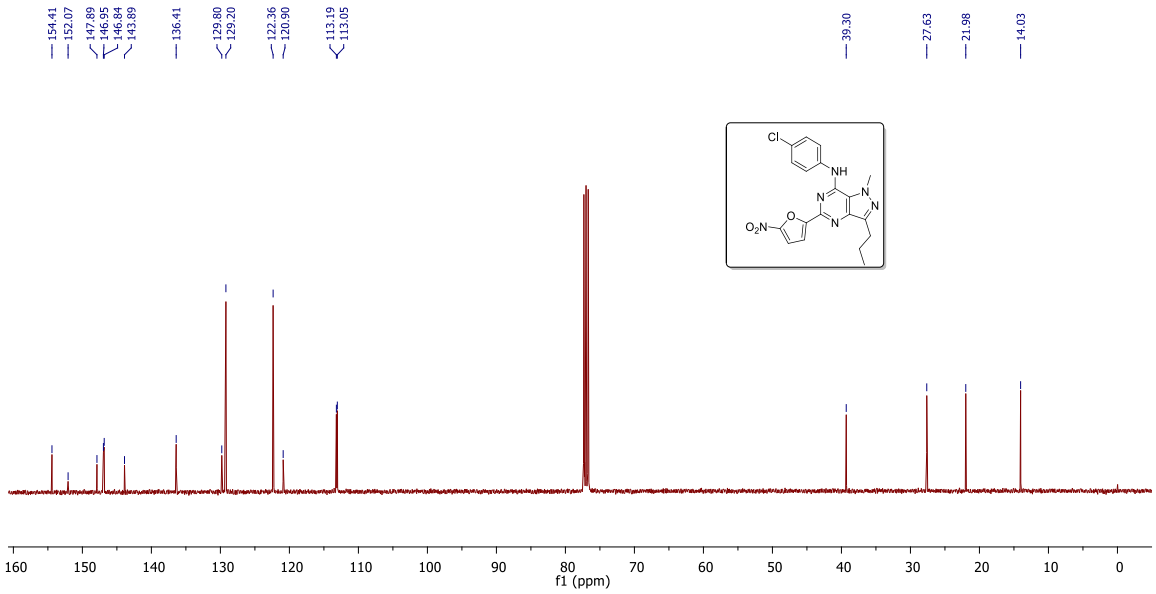
Pk #	Retention Time	Area	Area %	Height	Height %
1	3.605	53859	0.224	12696	0.476
2	20.885	17322	0.072	1864	0.070
3	28.555	11566	0.048	1126	0.042
4	33.568	26433	0.110	2320	0.087
5	34.155	84278	0.350	9090	0.341
6	34.667	30599	0.127	3001	0.112
7	35.317	23700456	98.533	2627329	98.473
8	37.696	20651	0.086	1311	0.049
9	39.072	12697	0.053	1826	0.068
10	39.797	38574	0.160	3617	0.136
11	52.779	35728	0.149	2961	0.111
12	53.259	21219	0.088	918	0.034
Totals		24053382	100.000	2668059	100.000

Compound (40)

^{1}H NMR in $CDCl_3$

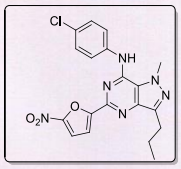


^{13}C NMR in $CDCl_3$



HRMS

Qualitative Compound Report



Data File	GLR-4-41.d	**Sample Name**	GLR-4-41
Sample Type	Sample	**Position**	Vial 11
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/19/2012 1:12:13 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

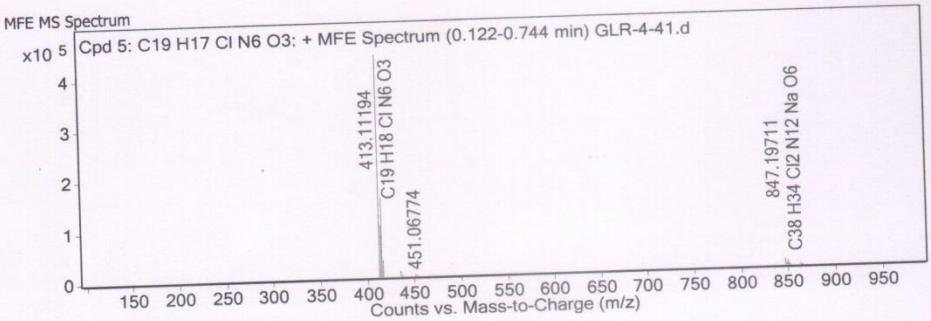
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C19 H17 Cl N6 O3	0.172	412.10463	C19 H17 Cl N6 O3	C19 H17 Cl N6 O3	1.05	C19 H17 Cl N6 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C19 H17 Cl N6 O3	413.11194	0.172	Find by Molecular Feature	412.10463

MFE MS Spectrum



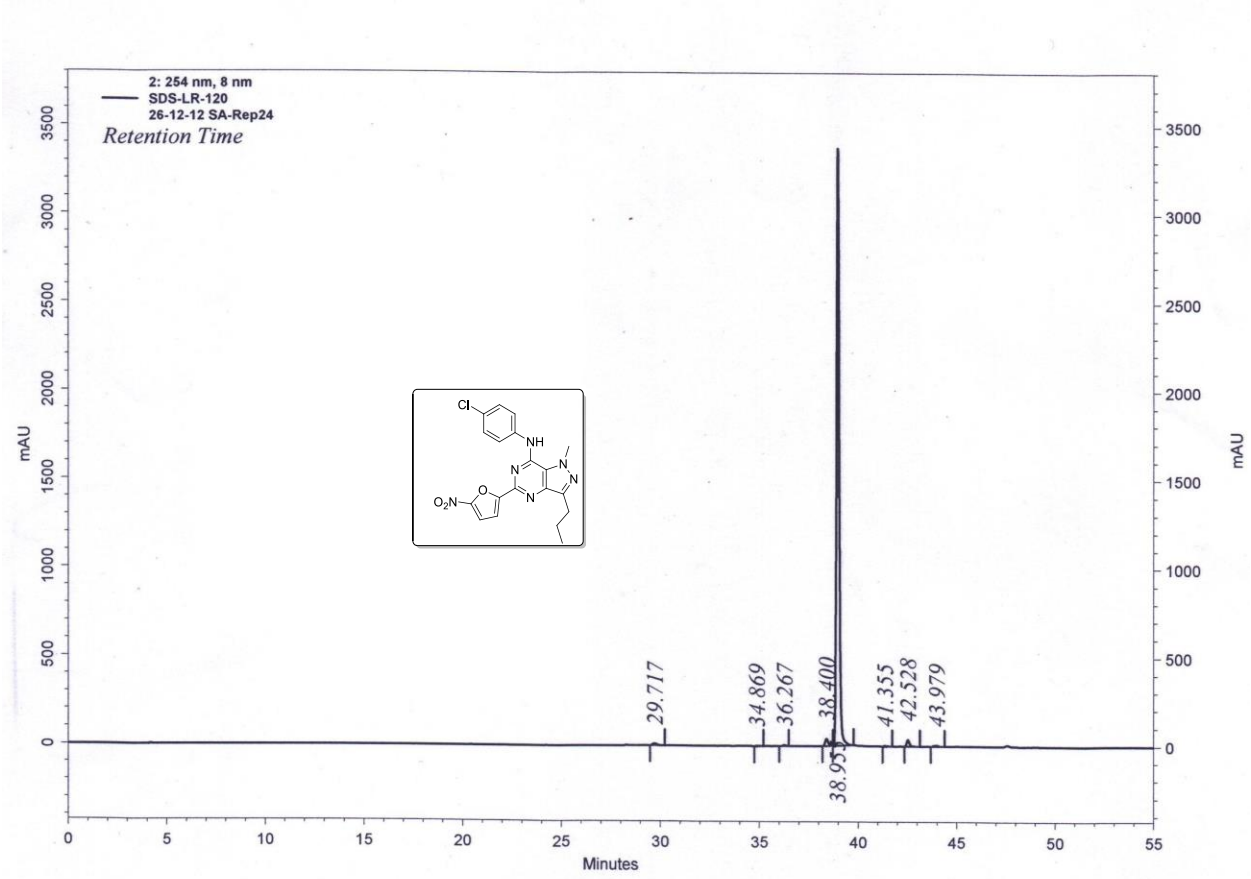
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
413.11194	1	438276.4	C19 H18 Cl N6 O3	(M+H)+
414.11451	1	103107	C19 H18 Cl N6 O3	(M+H)+
415.10911	1	155445.3	C19 H18 Cl N6 O3	(M+H)+
416.112	1	33909.6	C19 H18 Cl N6 O3	(M+H)+
435.0923	1	10911.2	C19 H17 Cl N6 Na O3	(M+Na)+
451.06774	1	4673.1		(M+K)+
847.19711	1	14619.5	C38 H34 Cl2 N12 Na O6	(2M+Na)+
848.20076	1	7708.6	C38 H34 Cl2 N12 Na O6	(2M+Na)+
849.19455	1	11221.8	C38 H34 Cl2 N12 Na O6	(2M+Na)+
850.19643	1	5989.8	C38 H34 Cl2 N12 Na O6	(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	413.11194	413.11234	0.98	100	100	59.69	59.9
2	414.11451	414.11513	1.5	23.53	23.06	14.04	13.81
3	415.10911	415.11013	2.47	35.47	35.16	21.17	21.06
4	416.112	416.11251	1.22	7.74	7.7	4.62	4.61
5	417.11398	417.11487	2.14	0.8	1.04	0.48	0.62

HPLC

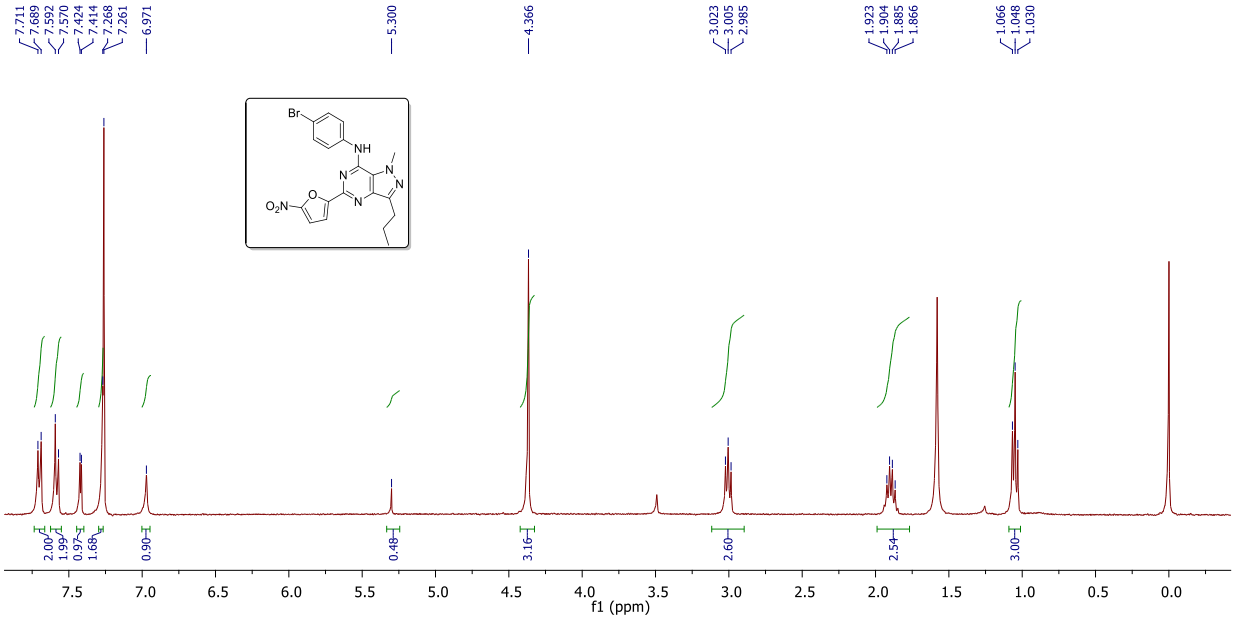


2: 254 nm, 8 nm

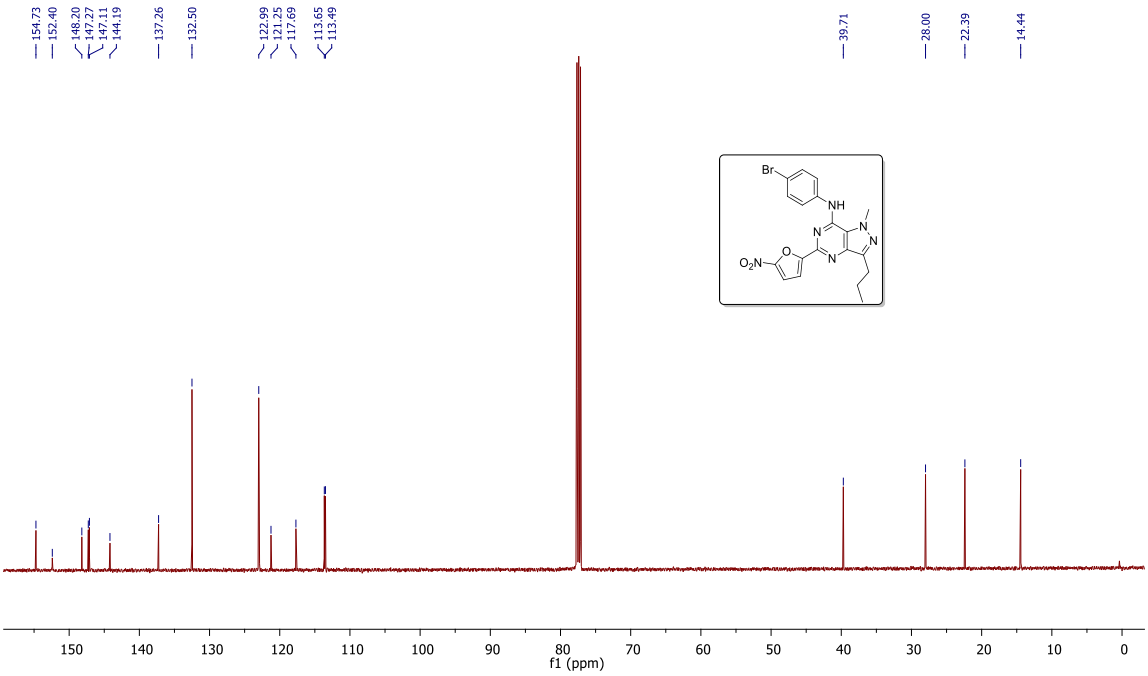
Pk #	Retention Time	Area	Area %	Height	Height %
1	29.717	159938	0.481	10193	0.293
2	34.869	54308	0.163	3676	0.106
3	36.267	58969	0.177	5863	0.168
4	38.400	419656	1.262	40408	1.161
5	38.955	32051096	96.407	3374215	96.911
6	41.355	51231	0.154	4495	0.129
7	42.528	352296	1.060	36584	1.051
8	43.979	98070	0.295	6330	0.182
Totals		33245564	100.000	3481764	100.000

Compound (41)

^{1}H NMR in $CDCl_3$



^{13}C NMR in $CDCl_3$

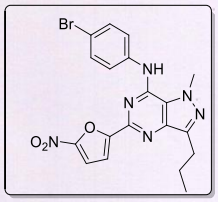


HRMS

Qualitative Compound Report

Data File	GLR-4-40.d	**Sample Name**	GLR-4-40
Sample Type	Sample	**Position**	Vial 10
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/19/2012 1:05:07 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

Sample Group **Info.**

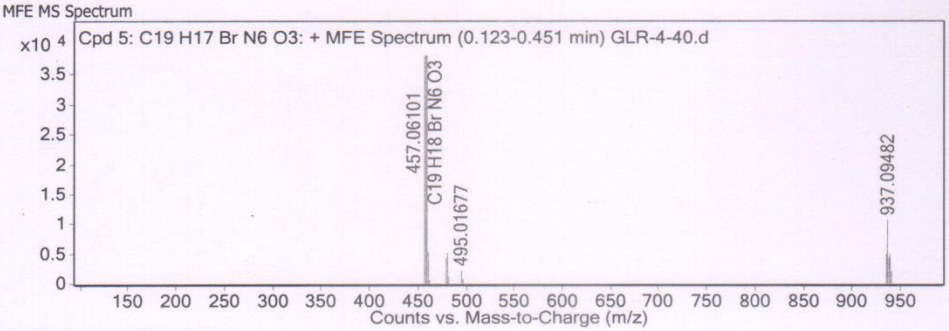


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C19 H17 Br N6 O3	0.173	456.05368	C19 H17 Br N6 O3	C19 H17 Br N6 O3	1.91	C19 H17 Br N6 O3

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



MS Spectrum Peak List

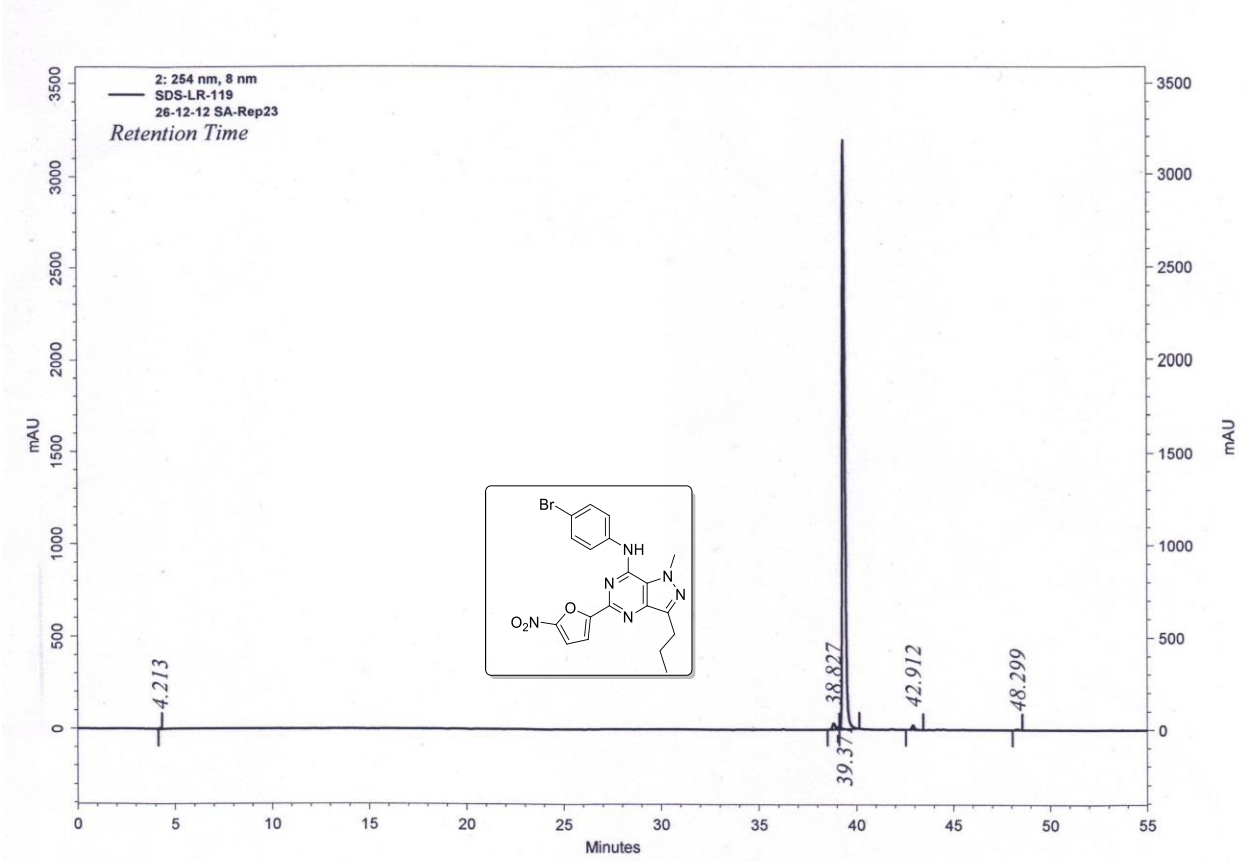
m/z	z	Abund	Formula	Ion
457.06101	1	160124.5	C19 H18 Br N6 O3	(M+H)+
458.06399	1	38239.7	C19 H18 Br N6 O3	(M+H)+
459.05908	1	157646.4	C19 H18 Br N6 O3	(M+H)+
460.06201	1	35501.4	C19 H18 Br N6 O3	(M+H)+
461.06331	1	5224.2	C19 H18 Br N6 O3	(M+H)+
481.03964	1	5088.1	C19 H17 Br N6 Na O3	(M+Na)+
935.09612	1	4998.8		(2M+Na)+
937.09482	1	10595		(2M+Na)+
938.09518	1	4493.5		(2M+Na)+
939.09344	1	4989.1		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	457.06101	457.06183	1.78	100	99.56	40.29	40.05
2	458.06399	458.06461	1.37	23.88	22.96	9.62	9.24
3	459.05908	459.06001	2.04	98.45	100	39.67	40.23
4	460.06201	460.06266	1.43	22.17	22.66	8.93	9.11
5	461.06331	461.06512	3.94	3.26	3.09	1.31	1.24
6	462.06645	462.06753	2.34	0.41	0.31	0.17	0.13

--- End Of Report ---

HPLC

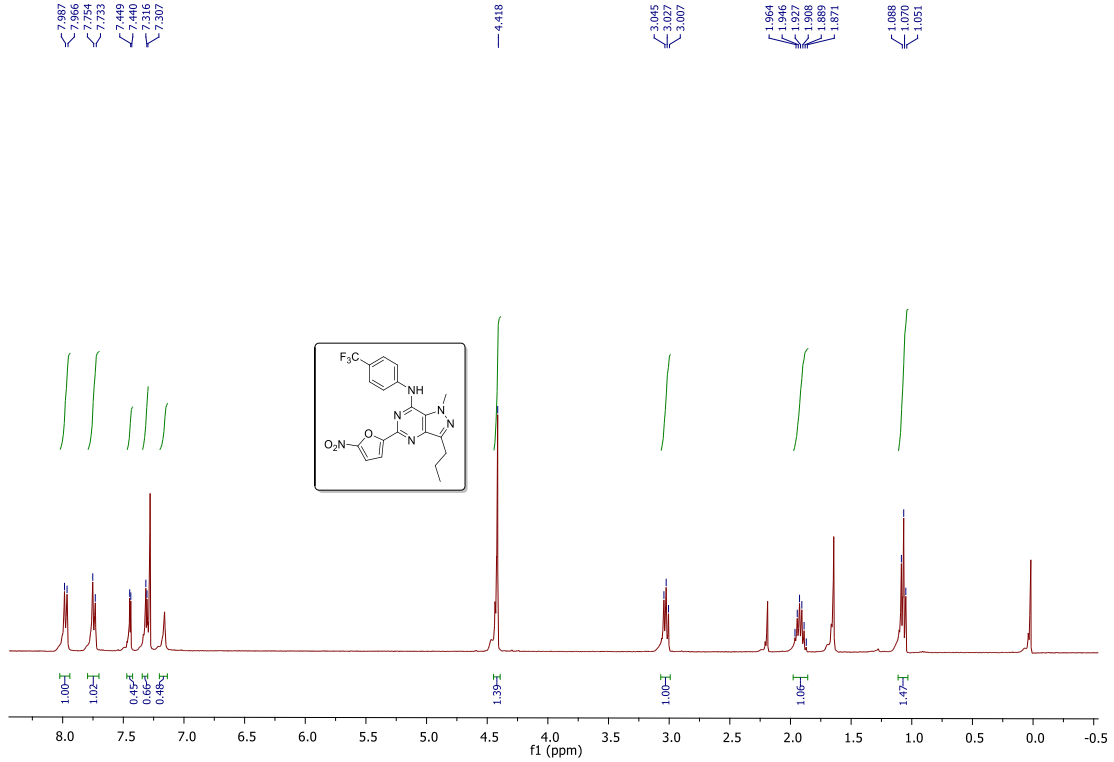


2: 254 nm, 8 nm

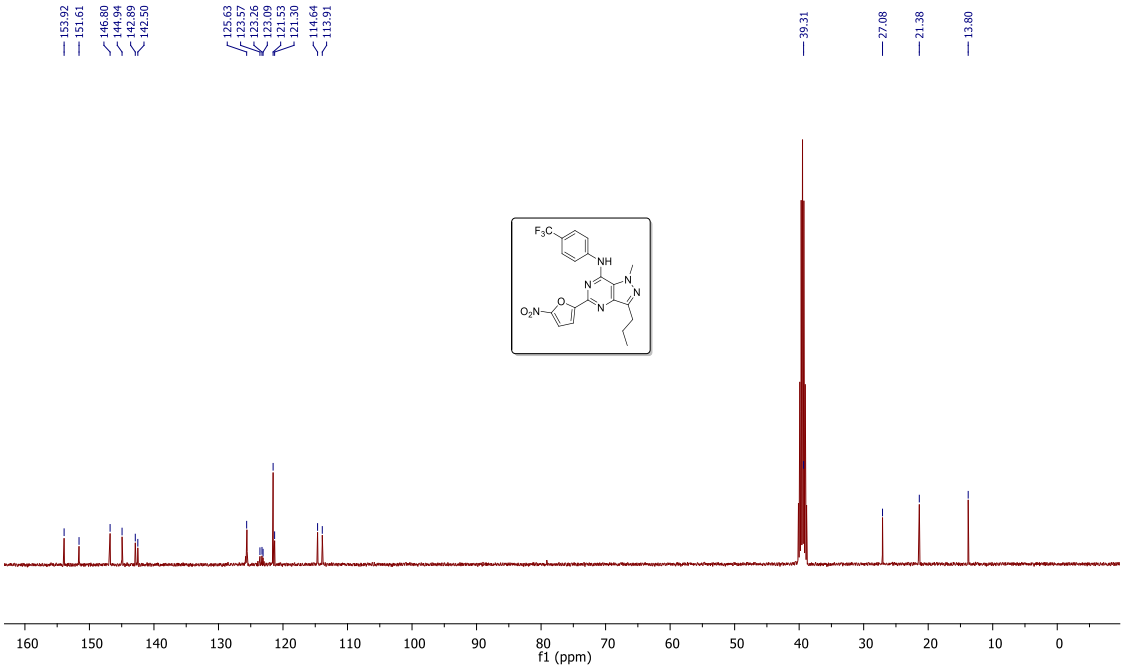
Pk #	Retention Time	Area	Area %	Height	Height %
1	4.213	59426	0.196	9571	0.294
2	38.827	368153	1.216	33966	1.043
3	39.371	29531137	97.536	3184158	97.753
4	42.912	252611	0.834	25108	0.771
5	48.299	65846	0.217	4560	0.140
Totals		30277173	100.000	3257363	100.000

Compound (42)

^{1}H NMR in $CDCl_3$



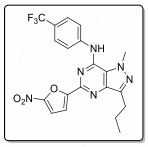
^{13}C NMR in DMSO-d_6



HRMS

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**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/19/2012 12:33:11 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			



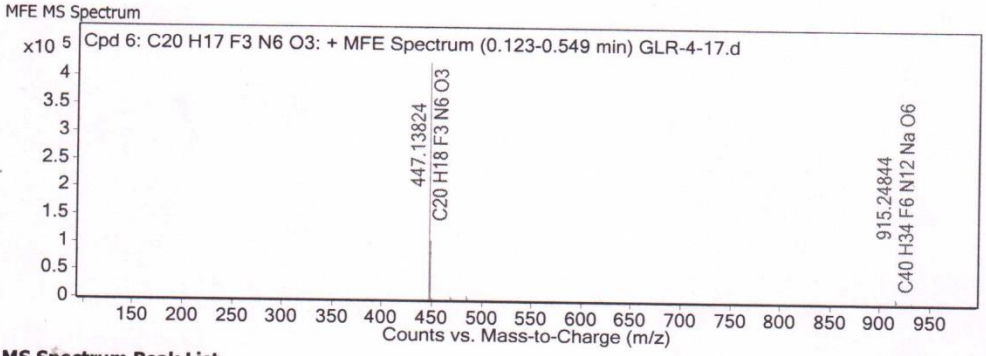
Sample Group **Info.**

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

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C20 H17 F3 N6 O3	447.13824	0.172	Find by Molecular Feature	446.13095

MFE MS Spectrum



MS Spectrum Peak List

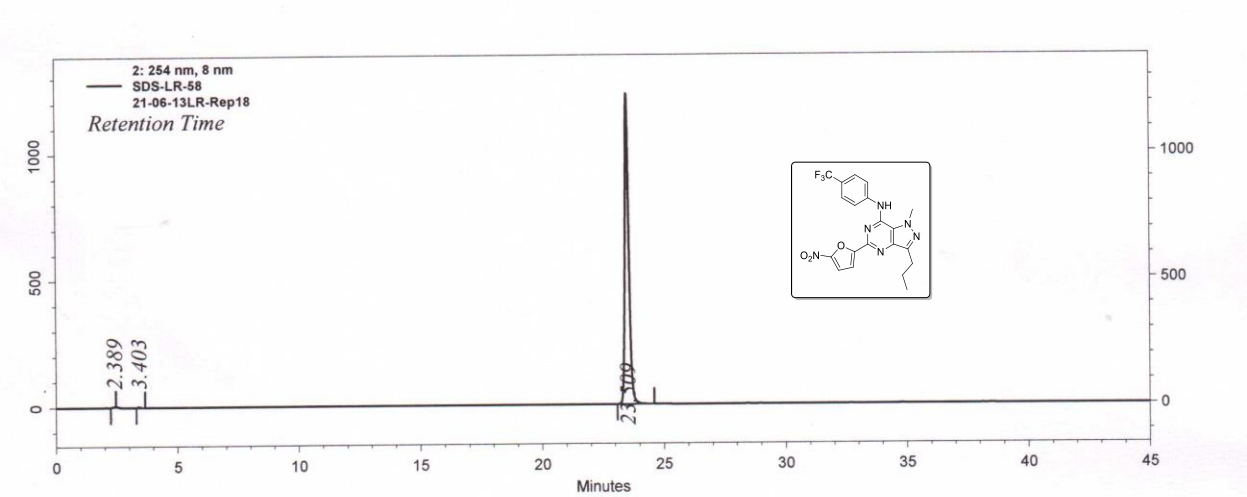
m/z	z	Abund	Formula	Ion
447.13824	1	427502.1	C20 H18 F3 N6 O3	(M+H)+
448.14049	1	106718	C20 H18 F3 N6 O3	(M+H)+
449.14344	1	15102.1	C20 H18 F3 N6 O3	(M+H)+
450.14326	1	1907.9	C20 H18 F3 N6 O3	(M+H)+
469.11917	1	5028.1	C20 H17 F3 N6 Na O3	(M+Na)+
485.09308	1	6205.8	C20 H17 F3 K N6 O3	(M+K)+
486.09766	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

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	447.13824	447.1387	1.03	100	100	77.55	78.18
2	448.14049	448.14151	2.27	24.96	24.14	19.36	18.88
3	449.14344	449.14405	1.34	3.53	3.41	2.74	2.67
4	450.14326	450.1465	7.21	0.45	0.35	0.35	0.28

--- End Of Report ---

HPLC

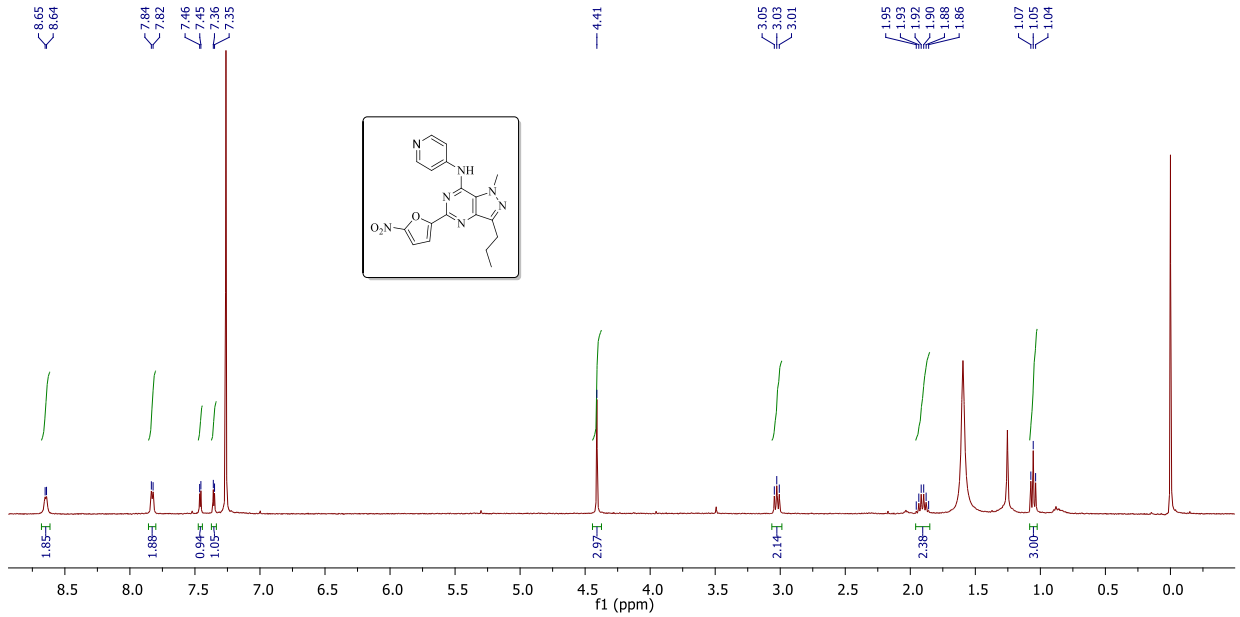


2: 254 nm, 8 nm

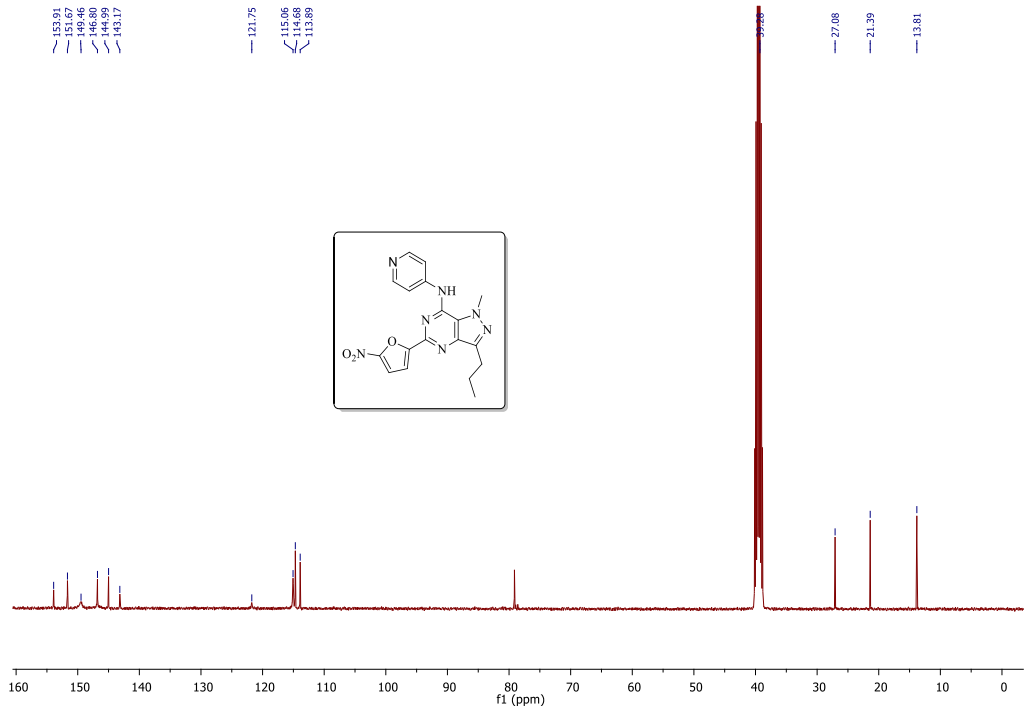
Pk #	Retention Time	Area	Area %	Height	Height %
1	2.389	11776	0.082	1483	0.120
2	3.403	17683	0.124	2485	0.201
3	23.509	14268912	99.794	1230948	99.679
Totals		14298371	100.000	1234916	100.000

Compound (43)

^{1}H NMR in $CDCl_3$



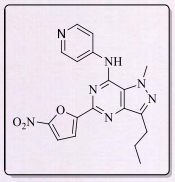
^{13}C NMR in DMSO-d_6



HRMS

Qualitative Compound Report

Data File	GLR-4-35.d	**Sample Name**	GLR-4-35
Sample Type	Sample	**Position**	Vial 6
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/19/2012 12:47:24 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			



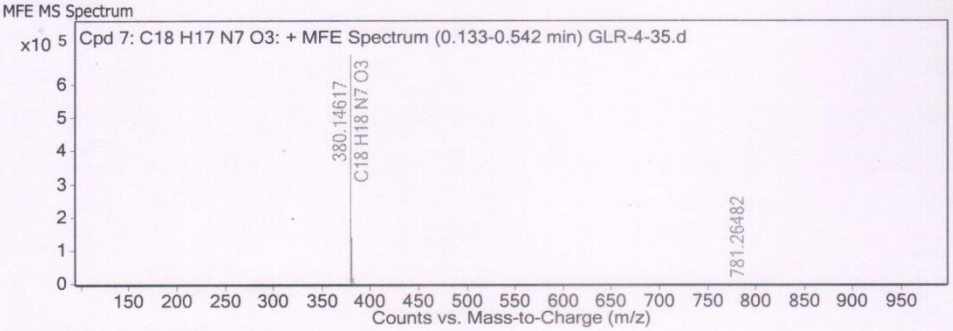
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C18 H17 N7 O3	0.173	379.13889	C18 H17 N7 O3	C18 H17 N7 O3	1.05	C18 H17 N7 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C18 H17 N7 O3	380.14617	0.173	Find by Molecular Feature	379.13889

MFE MS Spectrum



MS Spectrum Peak List

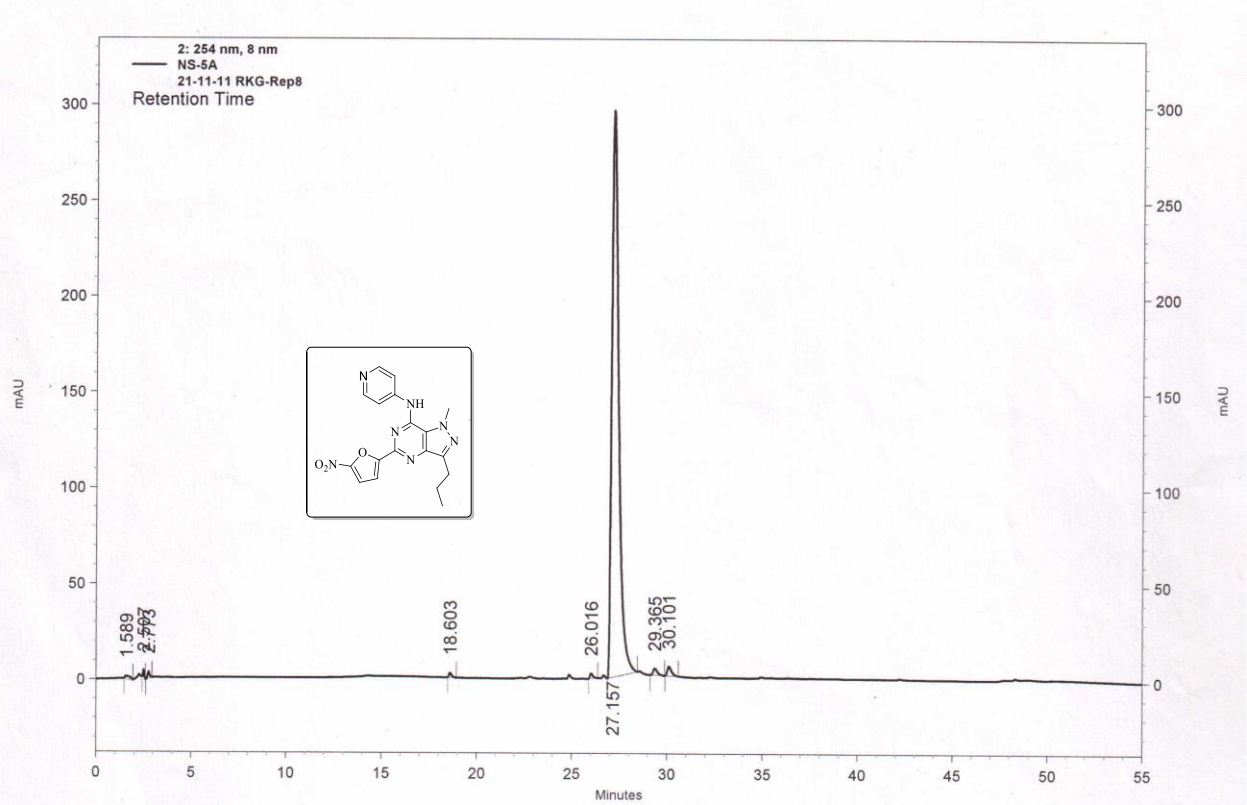
m/z	z	Abund	Formula	Ion
380.14617	1	689556.9	C18 H18 N7 O3	(M+H)+
381.14848	1	137491.3	C18 H18 N7 O3	(M+H)+
382.15117	1	17561.8	C18 H18 N7 O3	(M+H)+
383.15339	1	2329.3	C18 H18 N7 O3	(M+H)+
402.12775	1	1510.2	C18 H17 N7 Na O3	(M+Na)+
418.1014	1	1363.8	C18 H17 K N7 O3	(M+K)+
781.26482	1	1389.7		(2M+Na)+
782.26457	1	910.2		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	380.14617	380.14656	1.04	100	100	81.42	79.59
2	381.14848	381.14923	1.95	19.94	22.35	16.23	17.79
3	382.15117	382.15164	1.23	2.55	3	2.07	2.39
4	383.15339	383.15399	1.57	0.34	0.3	0.28	0.24

--- End Of Report ---

HPLC

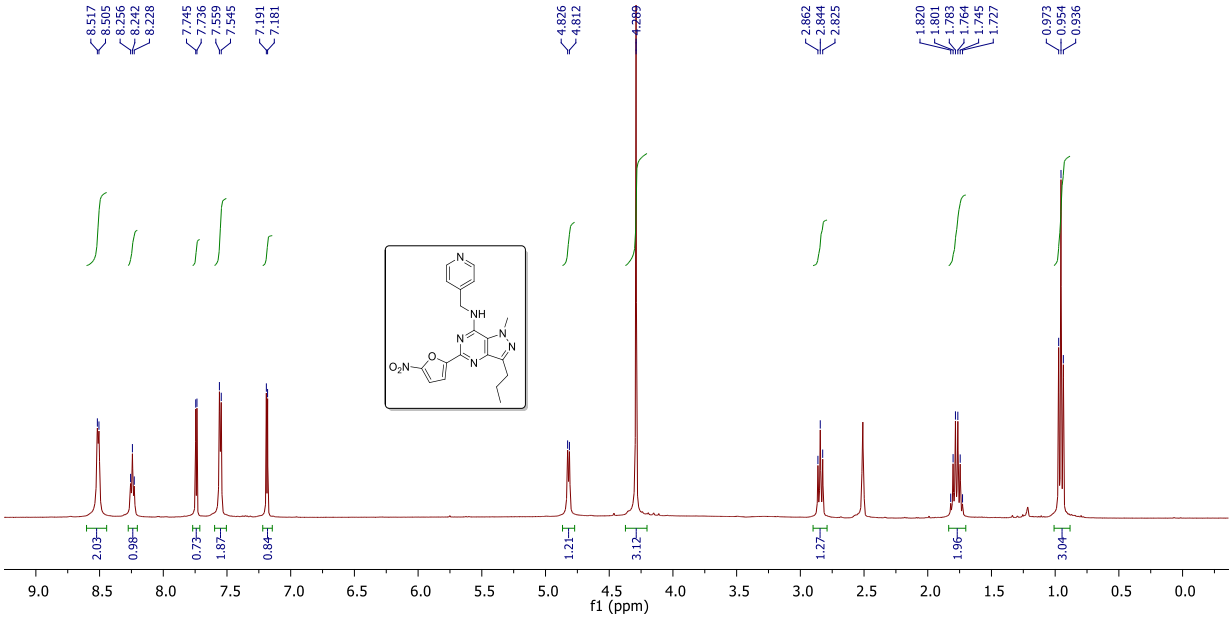


2: 254 nm, 8 nm

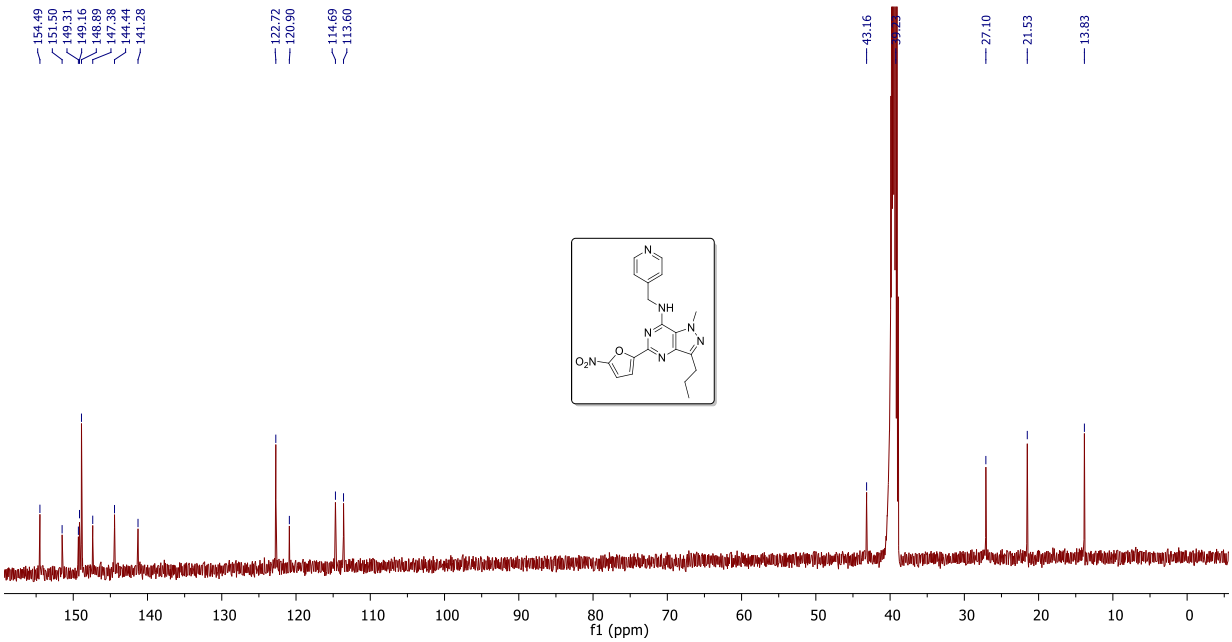
Pk #	Retention Time	Area	Area %	Height	Height %
1	1.589	26311	0.343	1448	0.455
2	2.507	20394	0.266	4462	1.401
3	2.773	27192	0.355	3540	1.112
4	18.603	22055	0.288	2358	0.740
5	26.016	29578	0.386	2679	0.841
6	27.157	7412200	96.721	295666	92.841
7	29.365	51740	0.675	3456	1.085
8	30.101	74020	0.966	4857	1.525
Totals		7663490	100.000	318466	100.000

Compound (44)

^{1}H NMR in DMSO-d$_6$

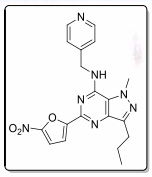


^{13}C NMR in DMSO-d$_6$



HRMS

Qualitative Compound Report



Data File	GLR-A-54.d	**Sample Name**	GLR-A-54
Sample Type	Sample	**Position**	Vial 3
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-07-2013 PM 12:31:29
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

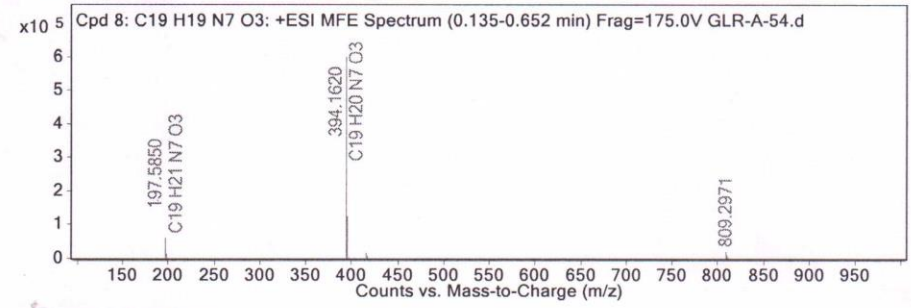
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C19 H19 N7 O3	0.194	393.1547	C19 H19 N7 O3	C19 H19 N7 O3	0.55	C19 H19 N7 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C19 H19 N7 O3	394.162	0.194	Find by Molecular Feature	393.1547

MFE MS Spectrum



MS Spectrum Peak List

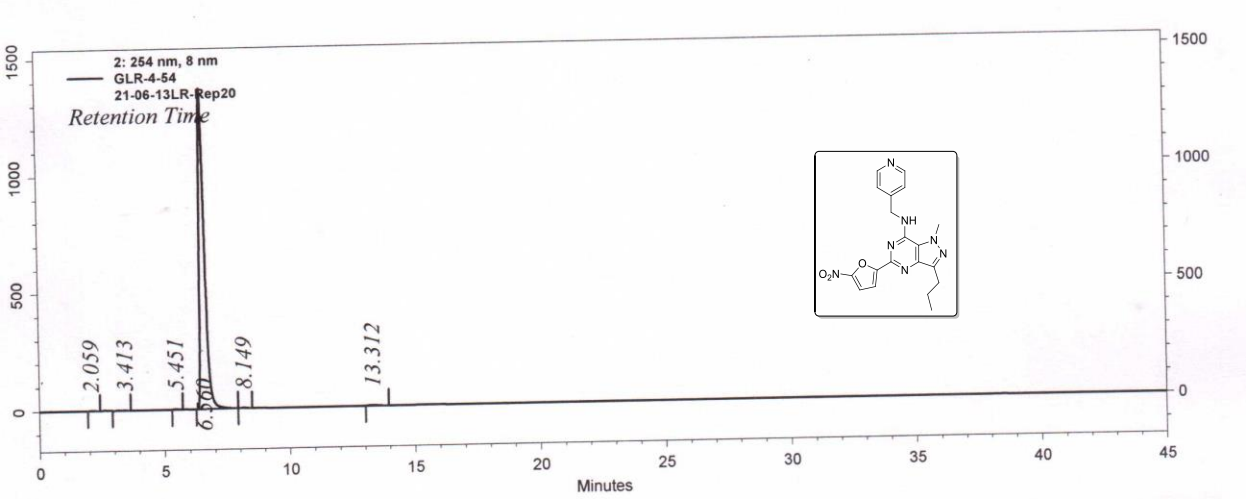
m/z	z	Abund	Formula	Ion
197.585	2	59301.27	C19 H21 N7 O3	(M+2H)+2
198.086	2	12752.76	C19 H21 N7 O3	(M+2H)+2
394.162	1	597924.94	C19 H20 N7 O3	(M+H)+
395.1647	1	126481.34	C19 H20 N7 O3	(M+H)+
396.1671	1	16859.99	C19 H20 N7 O3	(M+H)+
416.1439	1	18440.13	C19 H19 N7 Na O3	(M+Na)+
417.1462	1	5230.56	C19 H19 N7 Na O3	(M+Na)+
809.2971	1	21837.68		(2M+Na)+
810.3	1	10253.06		(2M+Na)+
811.3001	1	2686.42		(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	197.585	197.5847	-1.39	100	100	79.52	78.92
2	198.086	198.0861	0.25	21.51	23.46	17.1	18.52
3	198.5878	198.5873	-2.18	4.25	3.25	3.38	2.57

--- End Of Report ---

HPLC

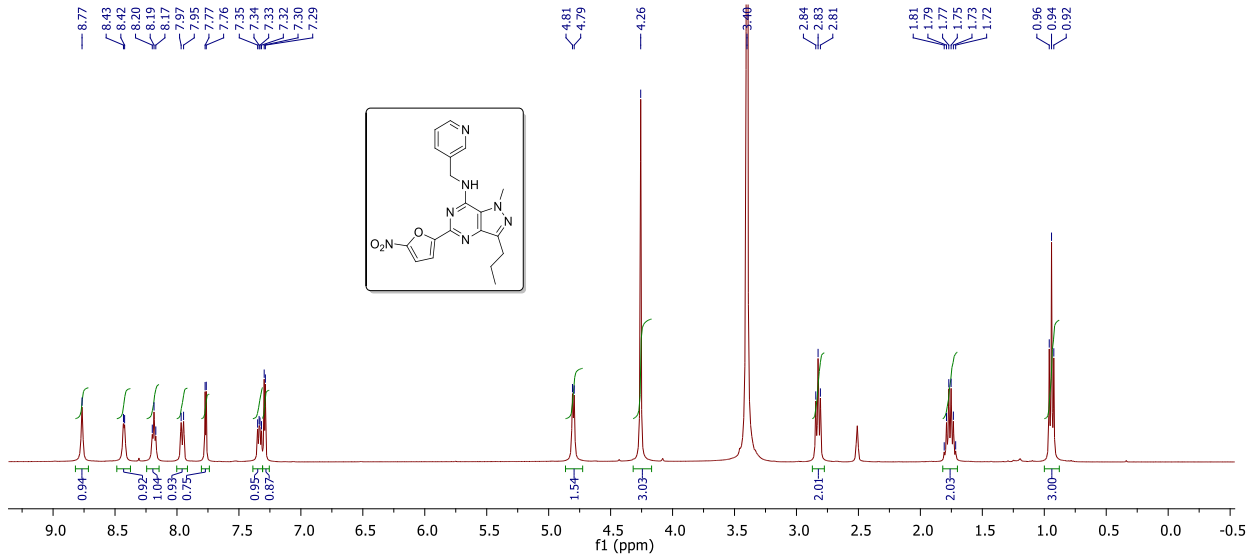


2: 254 nm, 8 nm

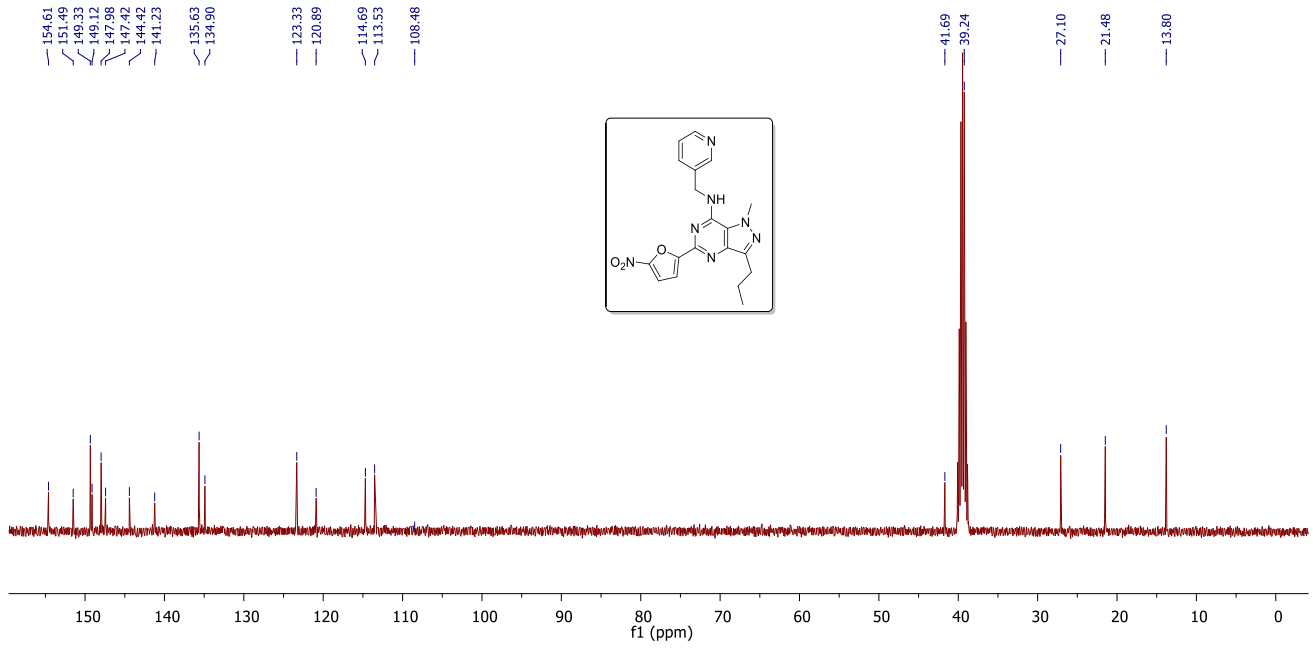
Pk #	Retention Time	Area	Area %	Height	Height %
1	2.059	12756	0.066	1088	0.079
2	3.413	13676	0.070	1318	0.096
3	5.451	19745	0.102	1856	0.135
4	6.560	19313911	99.371	1369377	99.410
5	8.149	23537	0.121	1627	0.118
6	13.312	52458	0.270	2245	0.163
Totals		19436083	100.000	1377511	100.000

Compound (45)

^{1}H NMR in DMSO-d$_6$



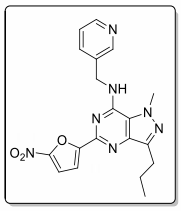
^{13}C NMR in DMSO-d$_6$



HRMS

Qualitative Compound Report

Data File	GLR-A-55.d	**Sample Name**	GLR-A-55
Sample Type	Sample	**Position**	Vial 11
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-07-2013 PM 1:09:45
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



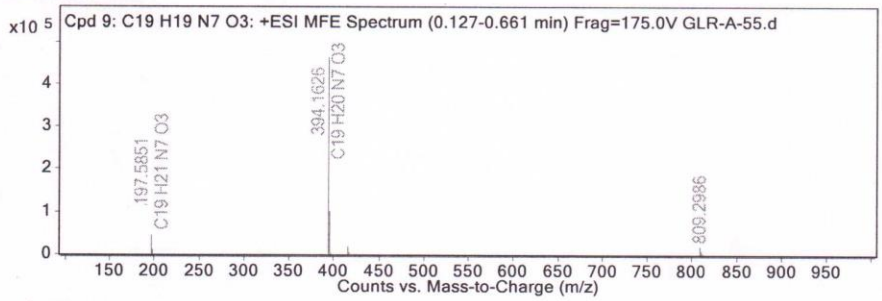
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C19 H19 N7 O3	0.195	393.1552	C19 H19 N7 O3	C19 H19 N7 O3	-0.7	C19 H19 N7 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 9: C19 H19 N7 O3	394.1626	0.195	Find by Molecular Feature	393.1552

MFE MS Spectrum



MS Spectrum Peak List

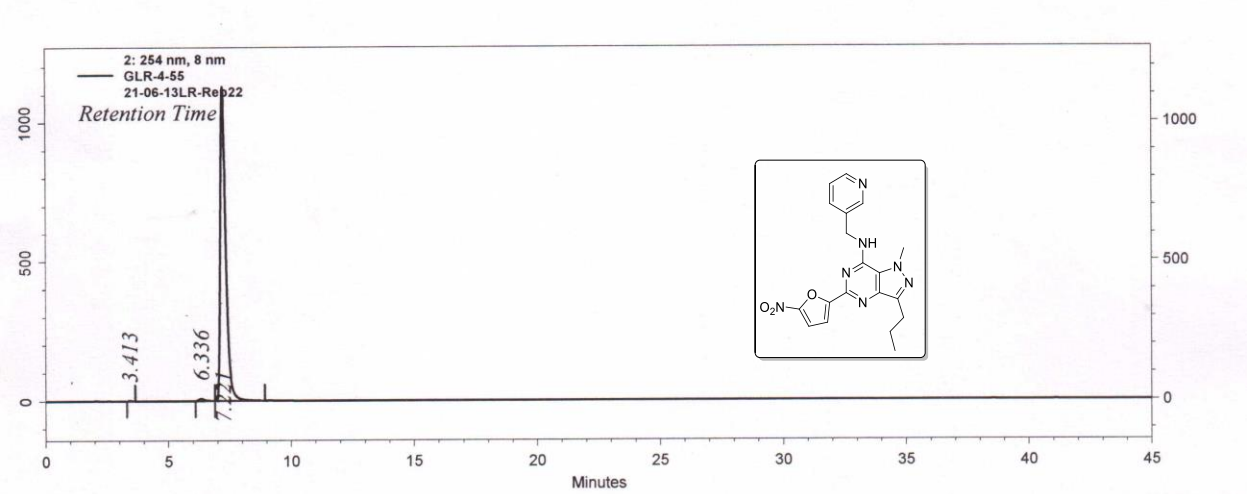
m/z	z	Abund	Formula	Ion
197.5851	2	45138.43	C19 H21 N7 O3	(M+2H)+2
198.086	2	9651.31	C19 H21 N7 O3	(M+2H)+2
394.1626	1	461941.72	C19 H20 N7 O3	(M+H)+
395.1648	1	101419.98	C19 H20 N7 O3	(M+H)+
396.1672	1	14377.99	C19 H20 N7 O3	(M+H)+
416.1435	1	19339.75	C19 H19 N7 Na O3	(M+Na)+
417.1465	1	4140.78	C19 H19 N7 Na O3	(M+Na)+
809.2986	1	17577.36		(2M+Na)+
810.3006	1	8031.12		(2M+Na)+
811.3009	1	1677.14		(2M+Na)+

Predicted Isotope Match Table

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 ---

HPLC

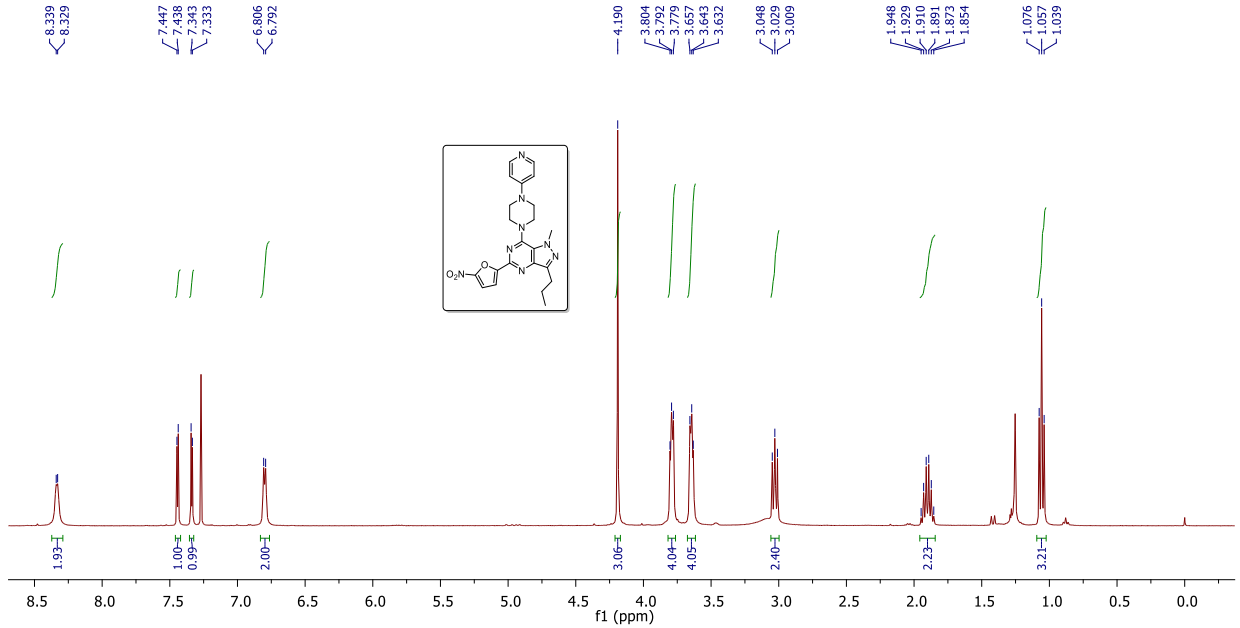


2: 254 nm, 8 nm

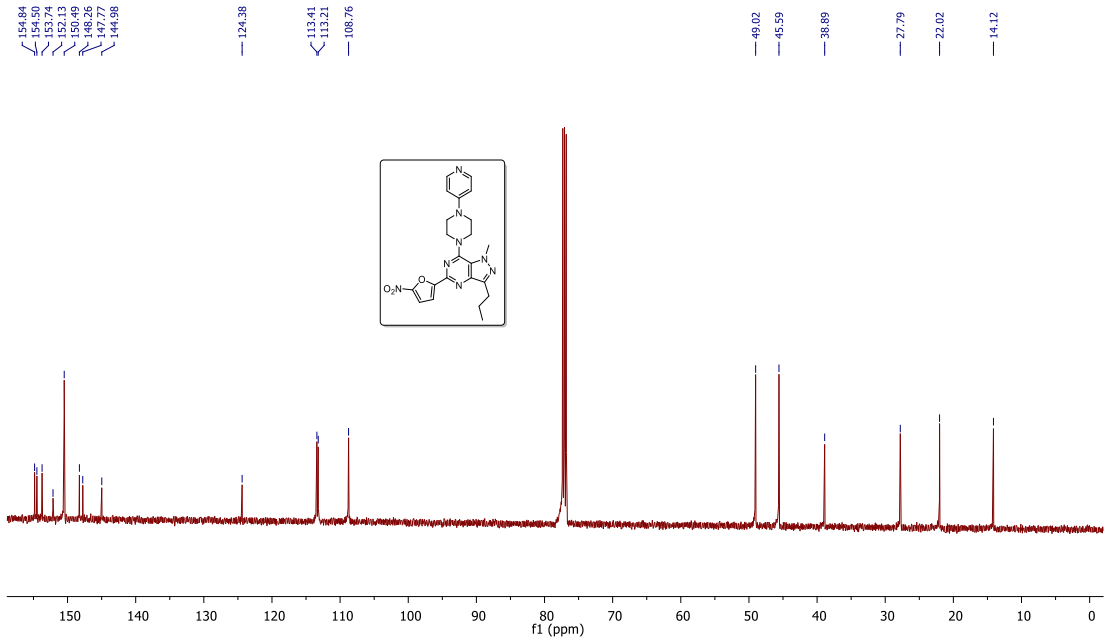
Pk #	Retention Time	Area	Area %	Height	Height %
1	3.413	12013	0.069	1712	0.150
2	6.336	124836	0.718	7744	0.680
3	7.221	17260308	99.213	1129344	99.170
Totals		17397157	100.000	1138800	100.000

Compound (46)

^{1}H NMR in $CDCl_3$



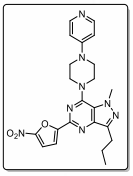
^{13}C NMR in $CDCl_3$



HRMS

Qualitative Compound Report

Data File	GLR-A-53.d	**Sample Name**	GLR-A-53
Sample Type	Sample	**Position**	Vial 8
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-07-2013 PM 12:55:56
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



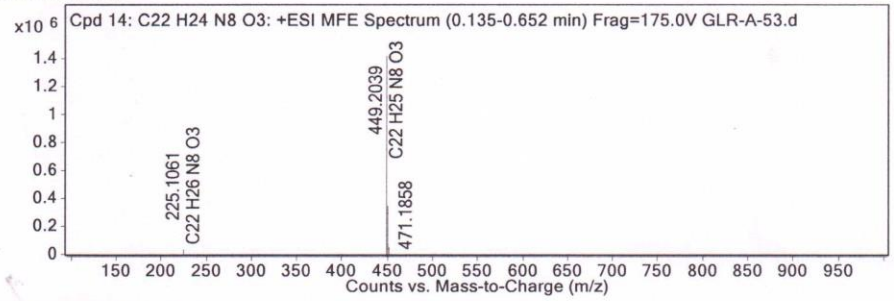
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 14: C22 H24 N8 O3	0.196	448.1968	C22 H24 N8 O3	C22 H24 N8 O3	0.8	C22 H24 N8 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 14: C22 H24 N8 O3	449.2039	0.196	Find by Molecular Feature	448.1968

MFE MS Spectrum



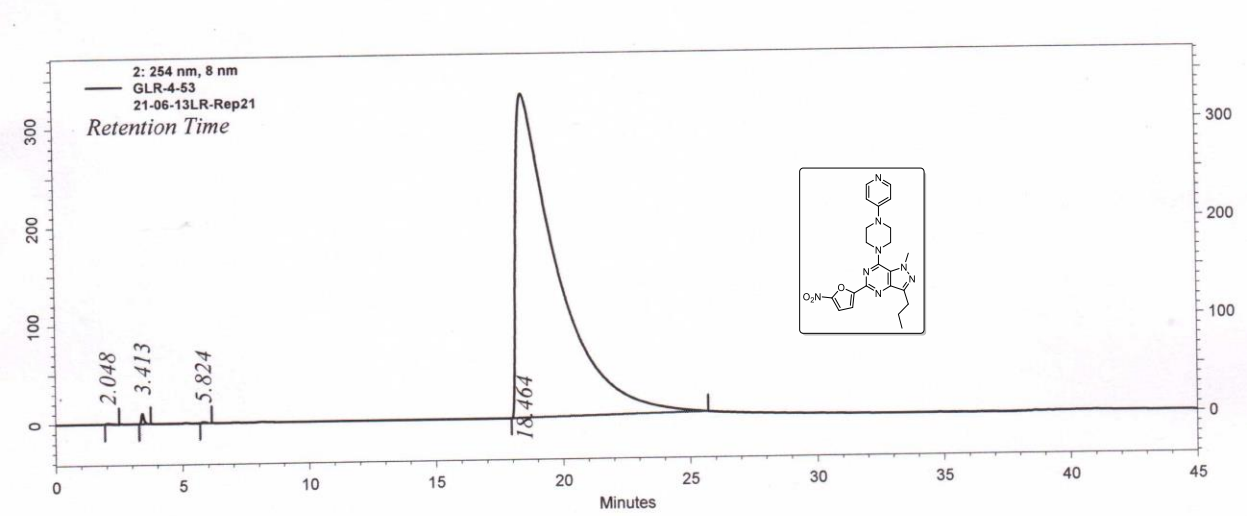
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
225.1061	2	34854.21	C22 H26 N8 O3	(M+2H)+2
225.6072	2	7801.15	C22 H26 N8 O3	(M+2H)+2
226.1092	2	2365.38	C22 H26 N8 O3	(M+2H)+2
449.2039	1	1414743.25	C22 H25 N8 O3	(M+H)+
450.2073	1	346527.56	C22 H25 N8 O3	(M+H)+
451.2093	1	49575.61	C22 H25 N8 O3	(M+H)+
452.212	1	5524.13	C22 H25 N8 O3	(M+H)+
453.2119	1	839.33	C22 H25 N8 O3	(M+H)+
471.1858	1	2462.44		(M+Na)+
472.1885	1	1203.29		(M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	225.1061	225.1058	-0.96	100	100	76.87	75.9
2	225.6072	225.6072	-0.02	22.38	27.13	17.21	20.59
3	226.1092	226.1085	-3.08	6.79	4.16	5.22	3.16
4	226.6073	226.6097	10.61	0.92	0.46	0.71	0.35

HPLC



2: 254 nm, 8 nm

Pk #	Retention Time	Area	Area %	Height	Height %
1	2.048	15484	0.042	863	0.252
2	3.413	75574	0.204	10325	3.017
3	5.824	10940	0.030	966	0.282
4	18.464	36973719	99.725	330017	96.448
Totals		37075717	100.000	342171	100.000

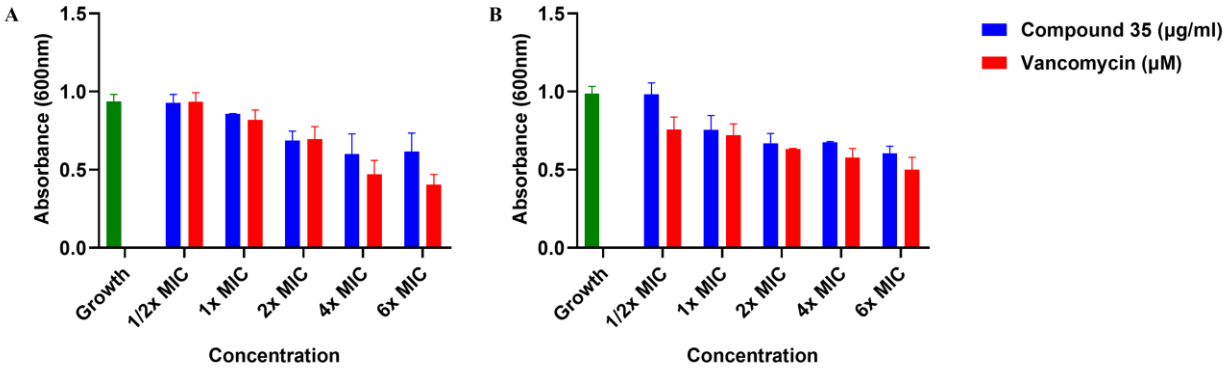


Figure S1. The graph represents the preformed biofilm disruption at different concentrations of the compound **35 (**1/2x, 1x, 2x, 4x and 6x MIC) while vancomycin is used as drug control at respective concentrations. The untreated cells or growth control in (A) *S. aureus* and (B) MRSA show the biofilm 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.

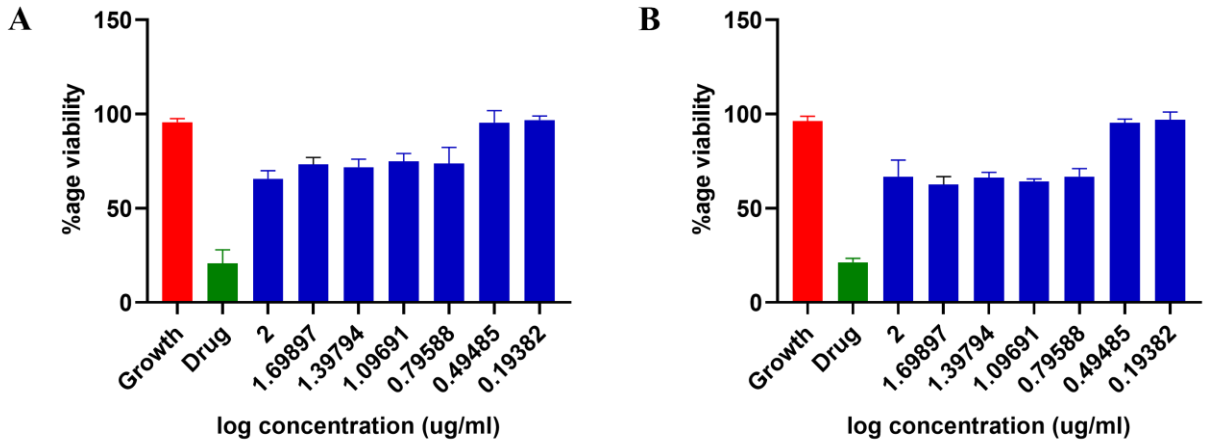


Figure S2. The compound **35** (blue bars) shows >50% growth of macrophage cells RAW264.7 at all concentrations ranging from 100µg/ml to 1.5µg/ml when exposed for A) 48 h and B) 72 h. The untreated cells (red) act as growth control. Drug control (green), Doxorubicin was used at a concentration of 10µM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

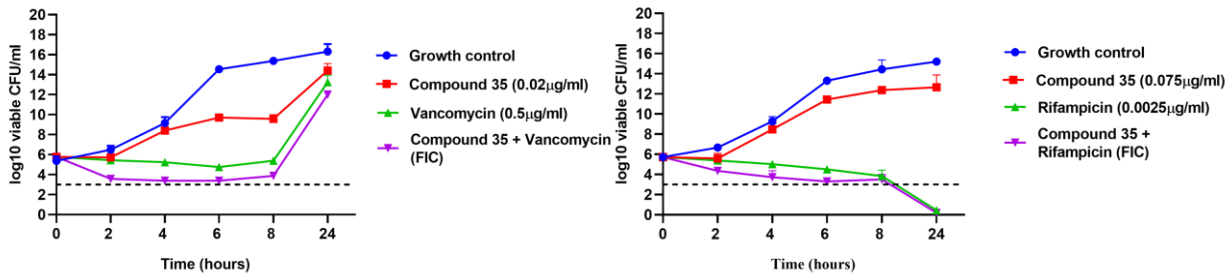


Figure S3. Killing efficacy of synergistic combinations of (A) compound **35** with vancomycin in *S. aureus and (B)* compound **35** with rifampicin in MRSA strains. Sub-inhibitory concentrations of vancomycin (0.5μg/ml), and compound 35 (0.02μg/ml) in *S. aureus* and rifampicin (0.0025μg/ml) and compound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

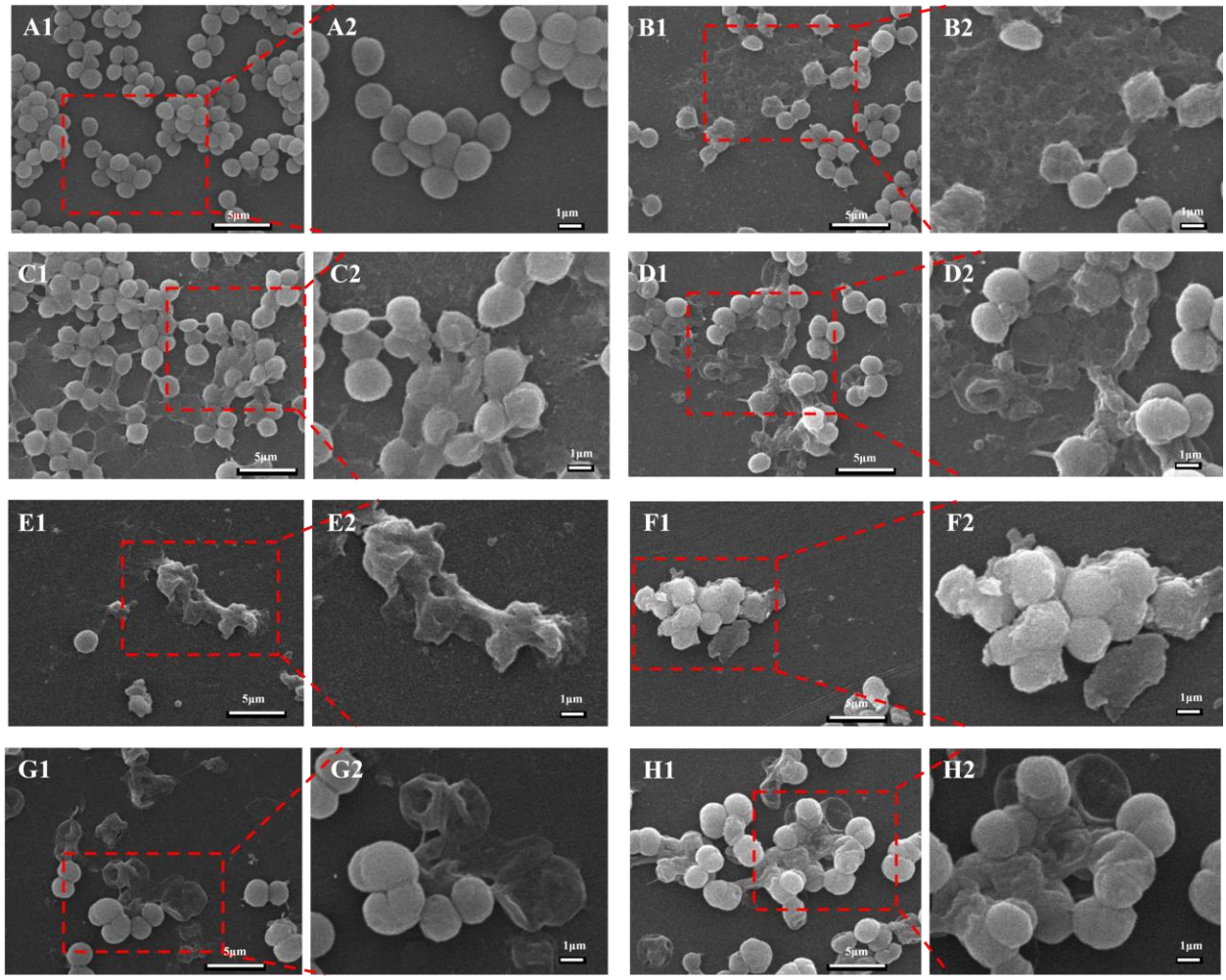


Figure S4. Scanning electron micrographs of MRSA at 2 hours of incubation with compound **35**, including images at 5µm and 1µm scales, with the 1µm scale image providing a magnified view of a portion of the 5µm scale image. Panels A1 and A2 depict the morphology of untreated cells, which appear in clusters. 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.

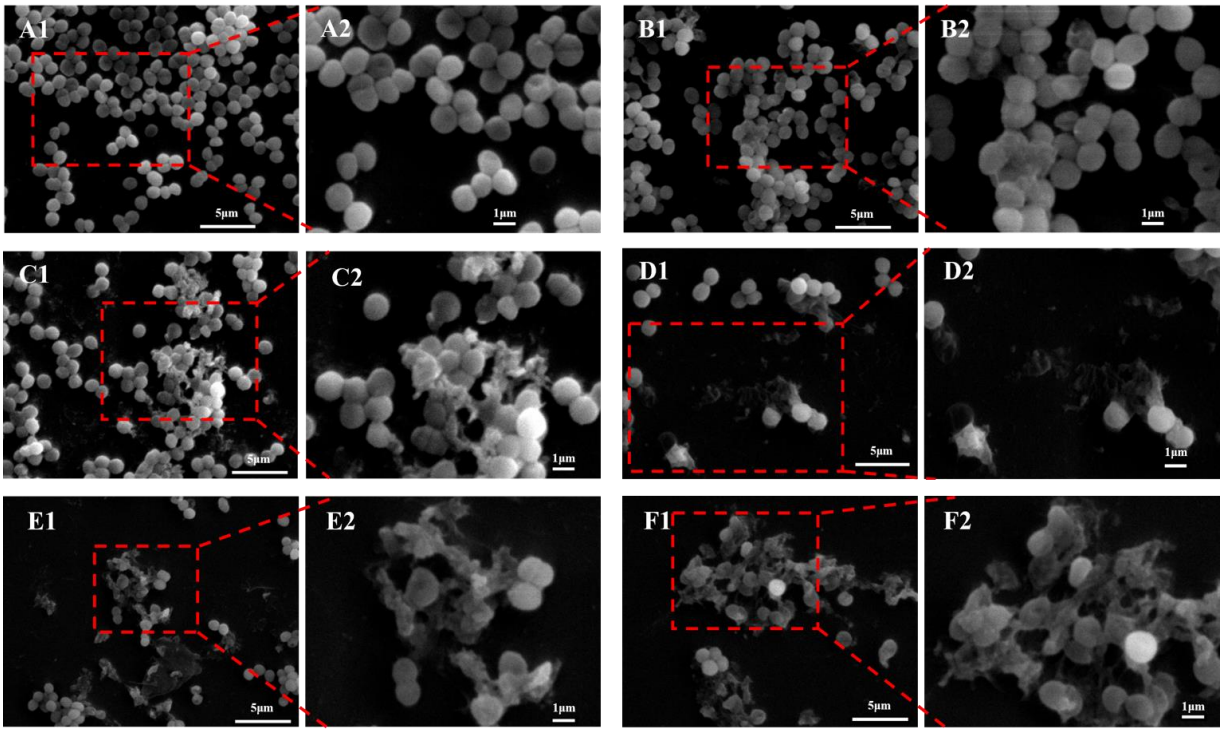


Figure S5. Scanning electron micrographs of MRSA at 6 hours of incubation with compound **35**, including images at 5µm and 1µm scales, with the 1µm scale image providing a magnified view of a portion of the 5µm scale image. Panels A1 and A2 depict the morphology of untreated cells, which appear in clusters. 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).

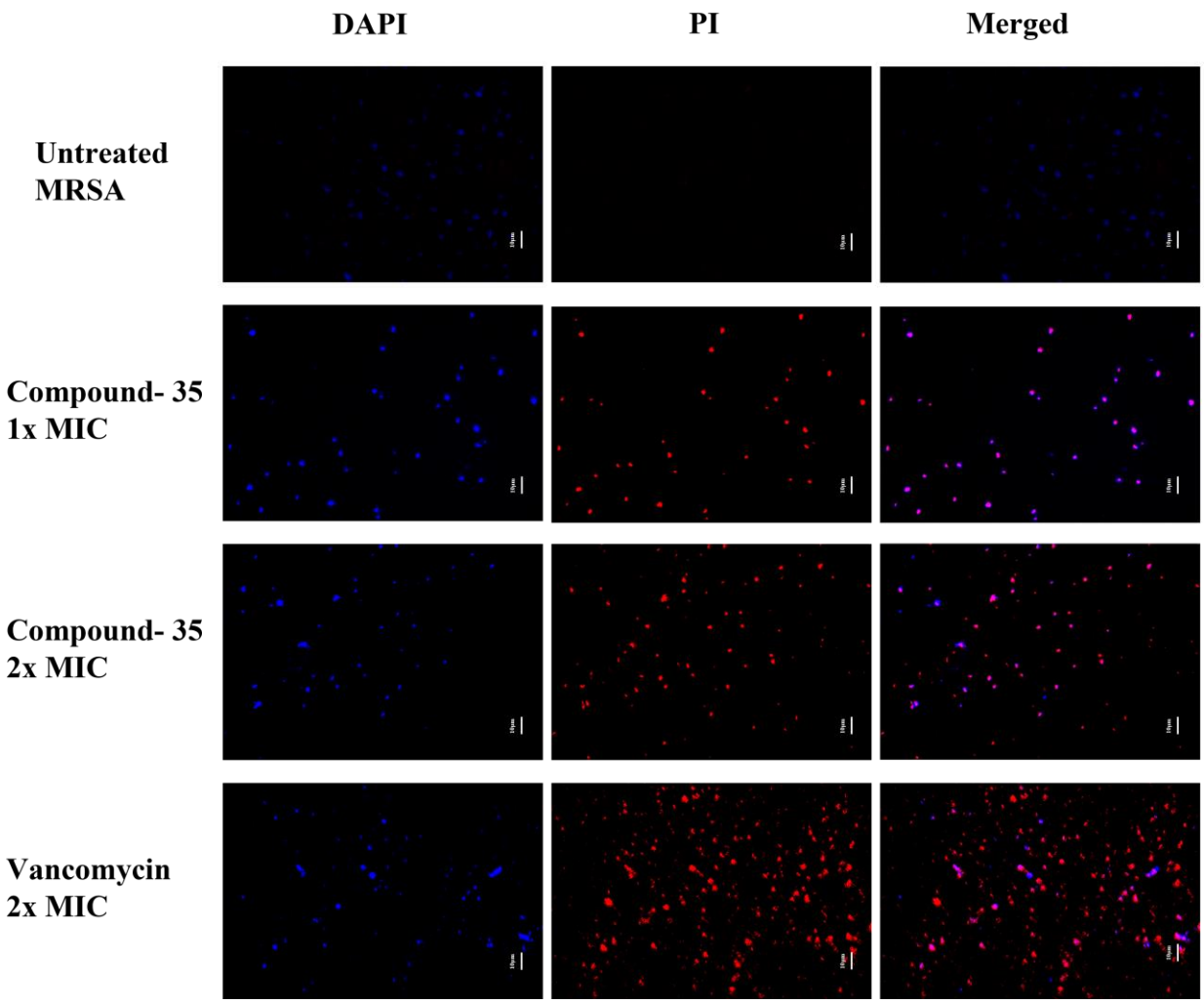


Figure S6. Fluorescence micrographs of MRSA stained with DAPI and PI after treatment with compound **35** at 1X and 2X MIC. Vancomycin, at 2X MIC, served as a positive control. In the blank control (untreated bacteria), DAPI staining was present without PI staining, signifying intact bacterial membranes. 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.