Electronic Supplementary Material (ESI) for MedChemComm.

Novel alkyne-azide cycloaddition analogues of dehydrozingerone as potential anti-prostate cancer inhibitors via PI3K/Akt/NF-kB pathway.

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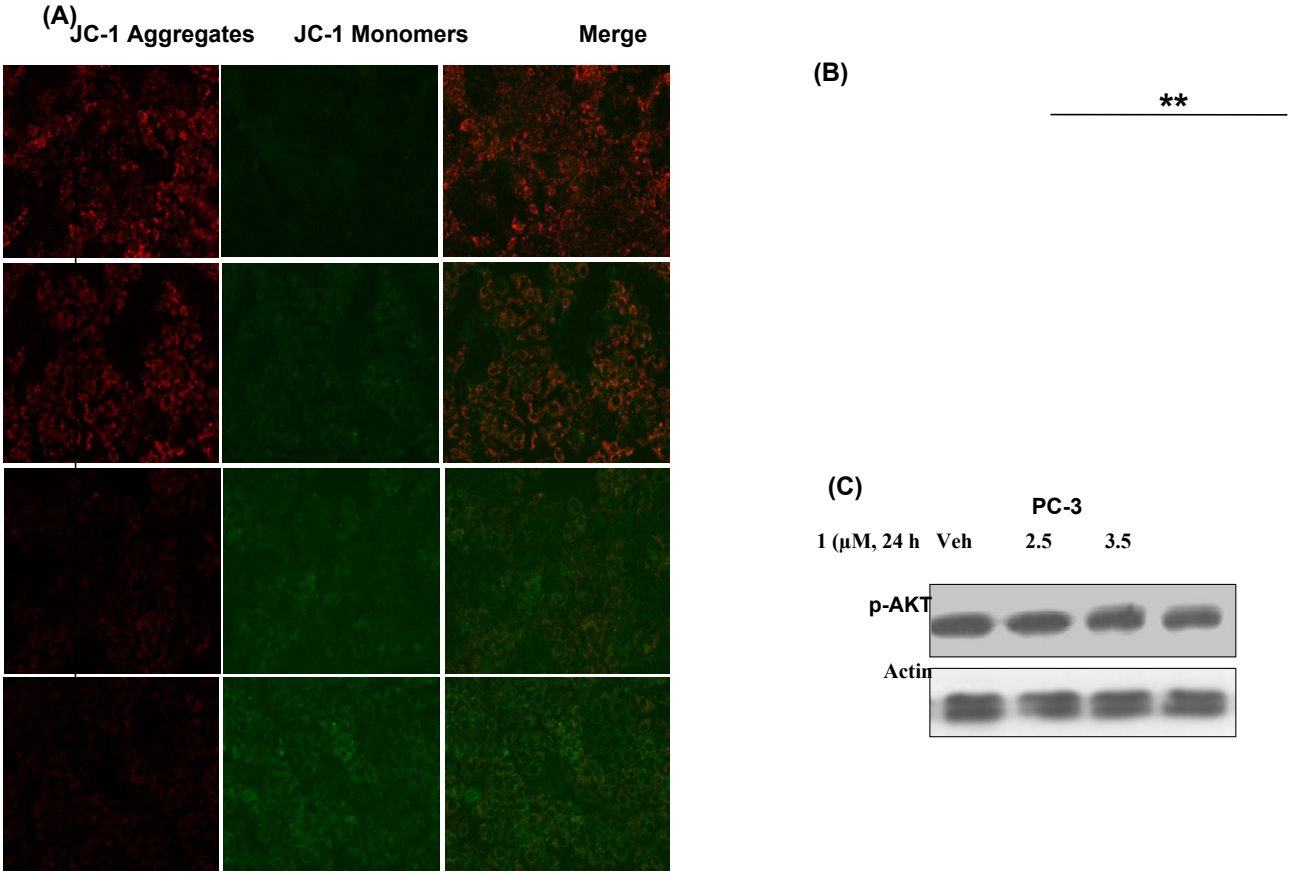
¶ *Contributed equally*



Supplementary Figure. 1). Apoptotic effect of compound 7. (A) PC-3 cells, after the indicated treatment for 24 h, were stained with JC-1 dye to check the mitochondrial membrane potential loss. (B) Caspase glow assay was carried out to check the caspase 3/7 activity in PC-3 cells, after the cells were treated for the set time point. (C)PC-3 cells were treated with indicated concentrations of compound 7 and analysed for phospho-AKT (p-AKT) through western blotting. Data from three independent experiments were subjected to statistical analysis. SD ± $^{**}P<0.01$.

HPLC and HRESIMS of 1:

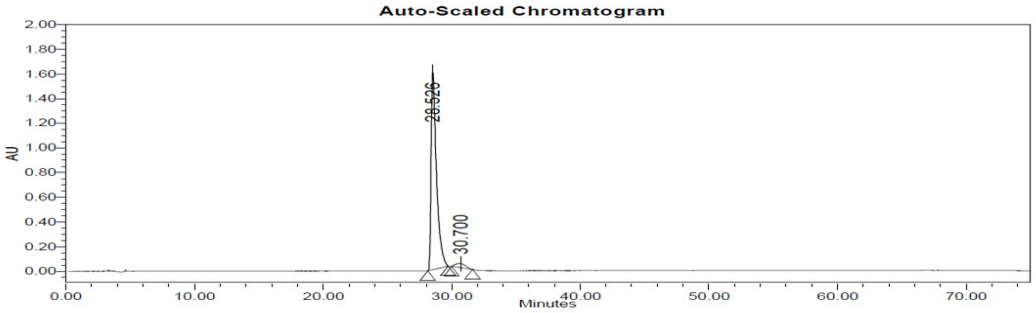
NPC DIVISION IIIM JAMMU

Reported by User: System

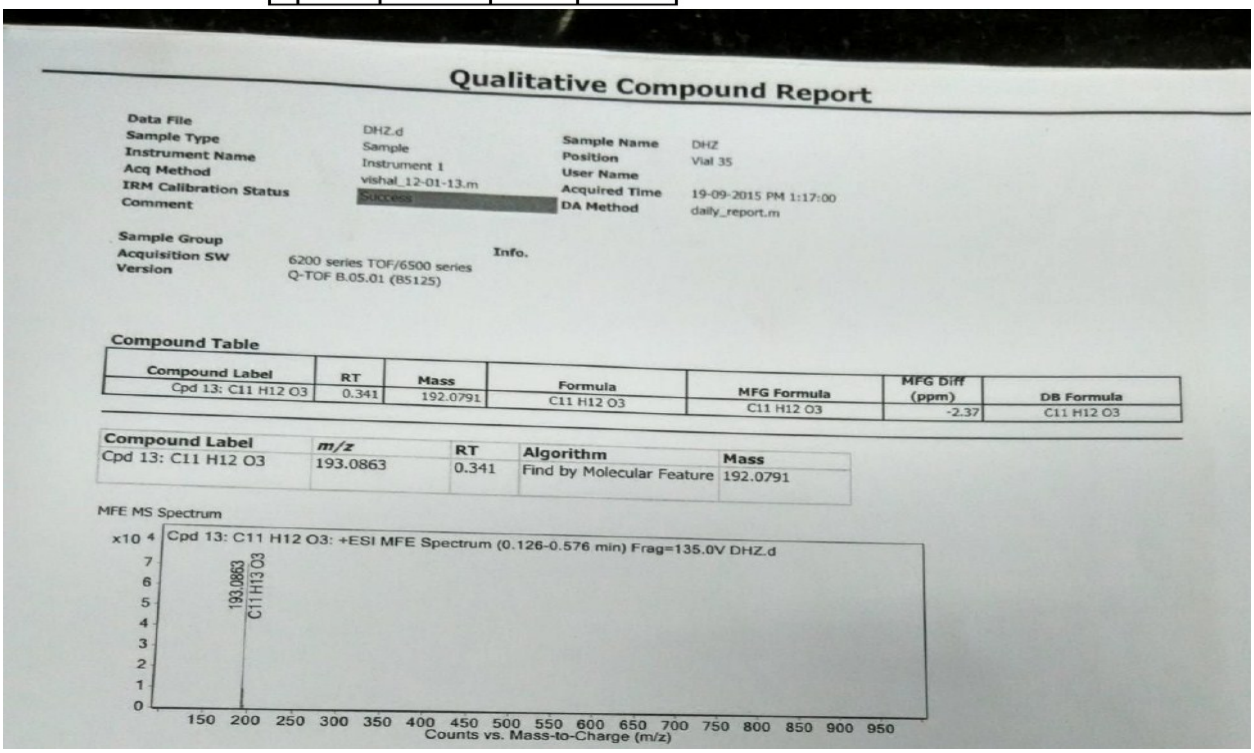
Project Name: NP

SAMPLE INFORMATION

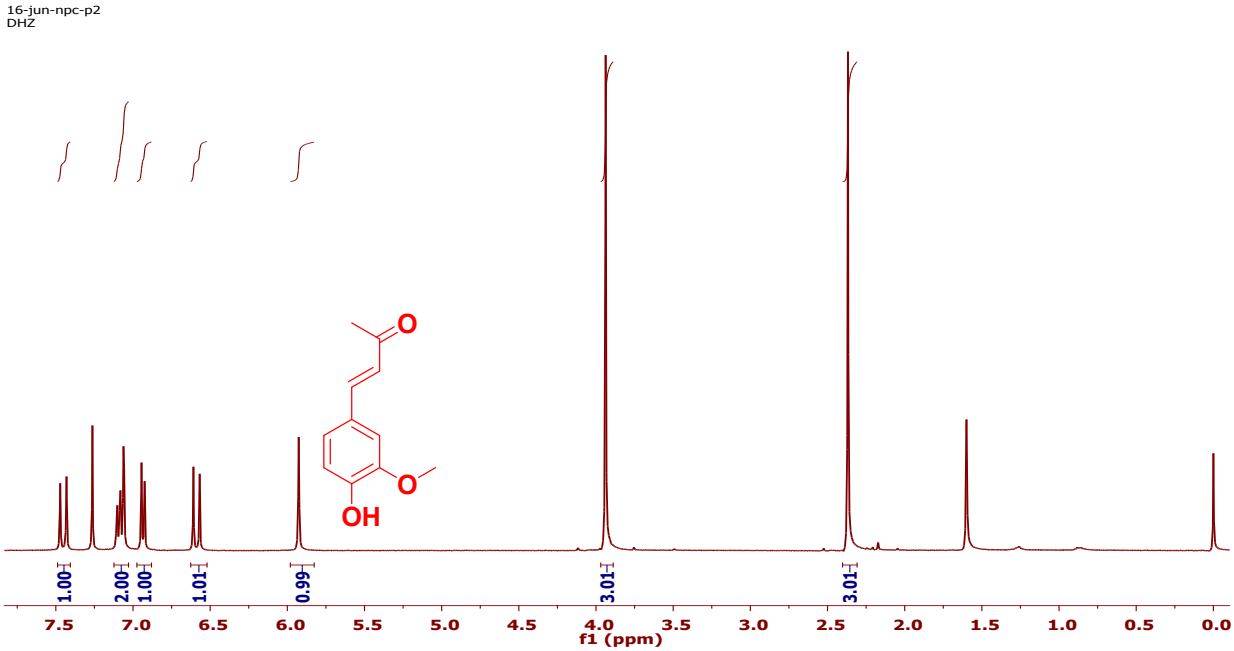
Sample Name:	Sample-15	Acquired By:	System
		Date Acquired:	9/29/2015 10:04:30 AM
Sample Type:	Unknown	Acq. Method Set:	Belerica 1
Vial:	14	Date Processed:	10/7/2015 10:50:06 AM
Injection #:	1	Processing Method:	Purity profile
Injection Volume:	10.00 ul	Channel Name:	W2996 335.0nm-1.2
Run Time:	75.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 335.0 nm at 1.2
Sample Set Name:	Echinacea	Flow rate: 0.6 ml/min	
column_name	RP-18,5um	Sample conc:	
		Mobile phase: ACN:1.5%AcOH in Water(Gradient)	

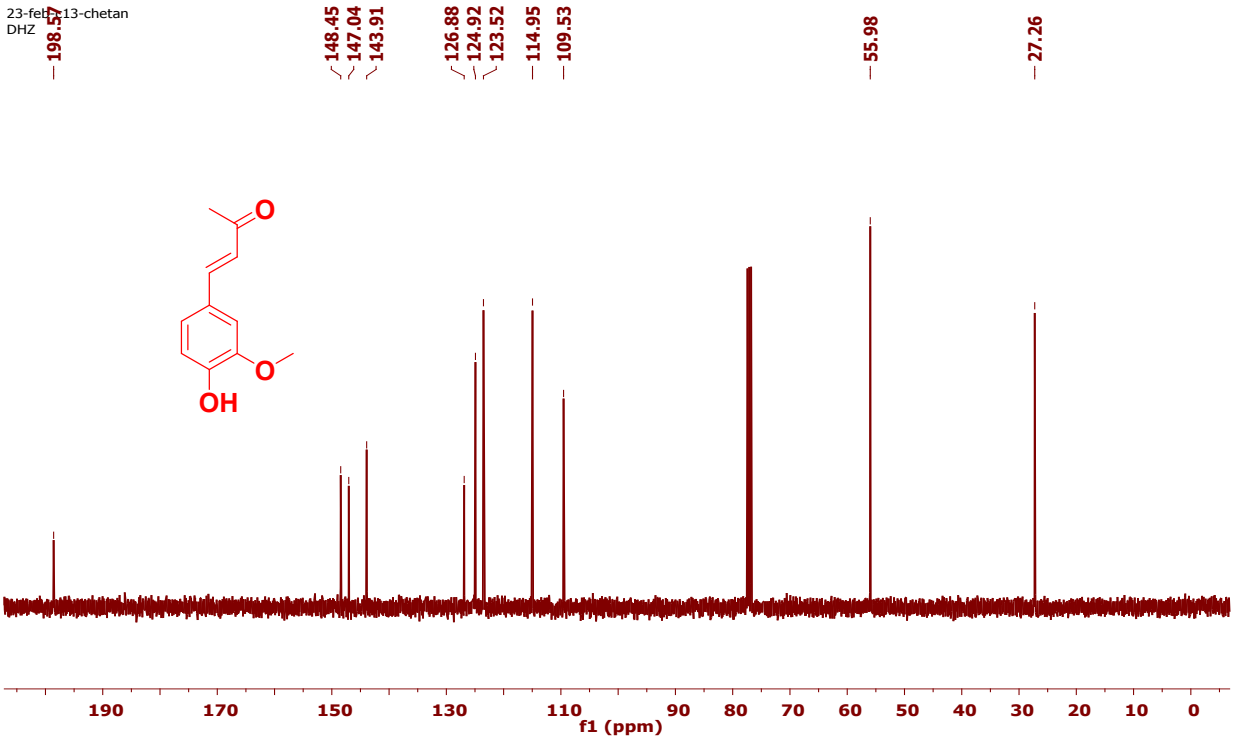


	RT	Area (µV*sec)	% Area	Height (µV)
1	28.526	47165894	96.36	1600274
2	30.700	1781087	3.64	32352

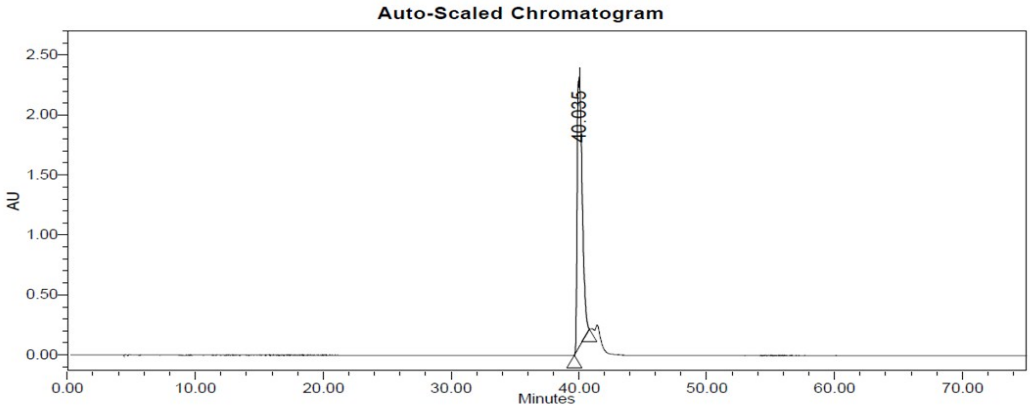


^{1}H and ^{13}C NMR of 1:





HPLC and HRESIMS of 2:



	RT	Area (µV*sec)	% Area	Height (µV)
1	40.035	62392418	100.00	2237236

Qualitative Compound Report

Data File	PRO-Br.d	**Sample Name**	PRO-Br
Sample Type	Sample	**Position**	Vial 31
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 3:10:24
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

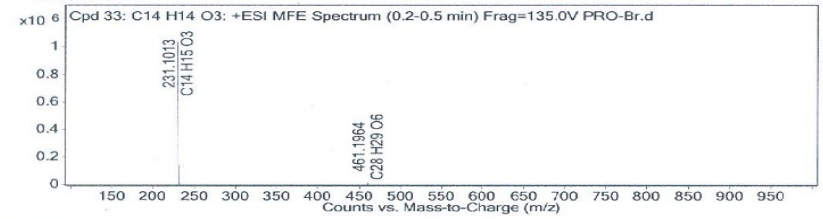
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 33: C14 H14 O3	0.3	230.094	C14 H14 O3	C14 H14 O3	1.17	C14 H14 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 33: C14 H14 O3	231.1013	0.3	Find by Molecular Feature	230.094

MFE MS Spectrum



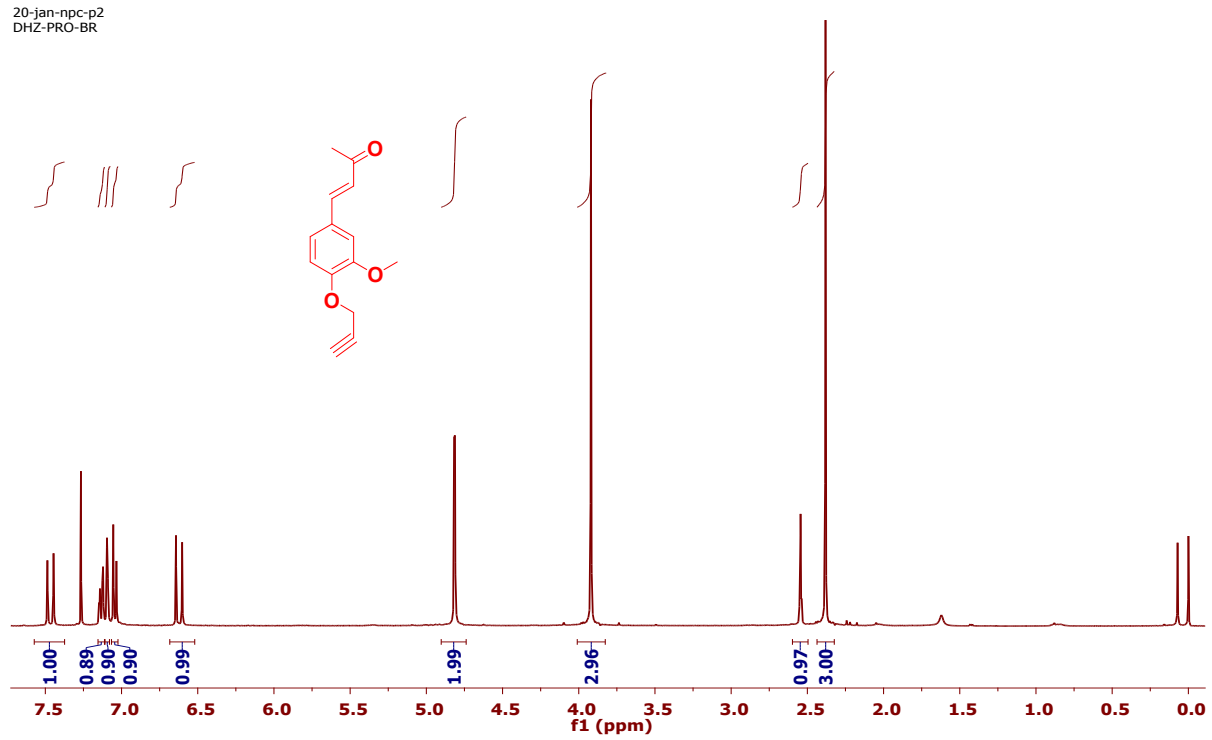
MS Spectrum Peak List

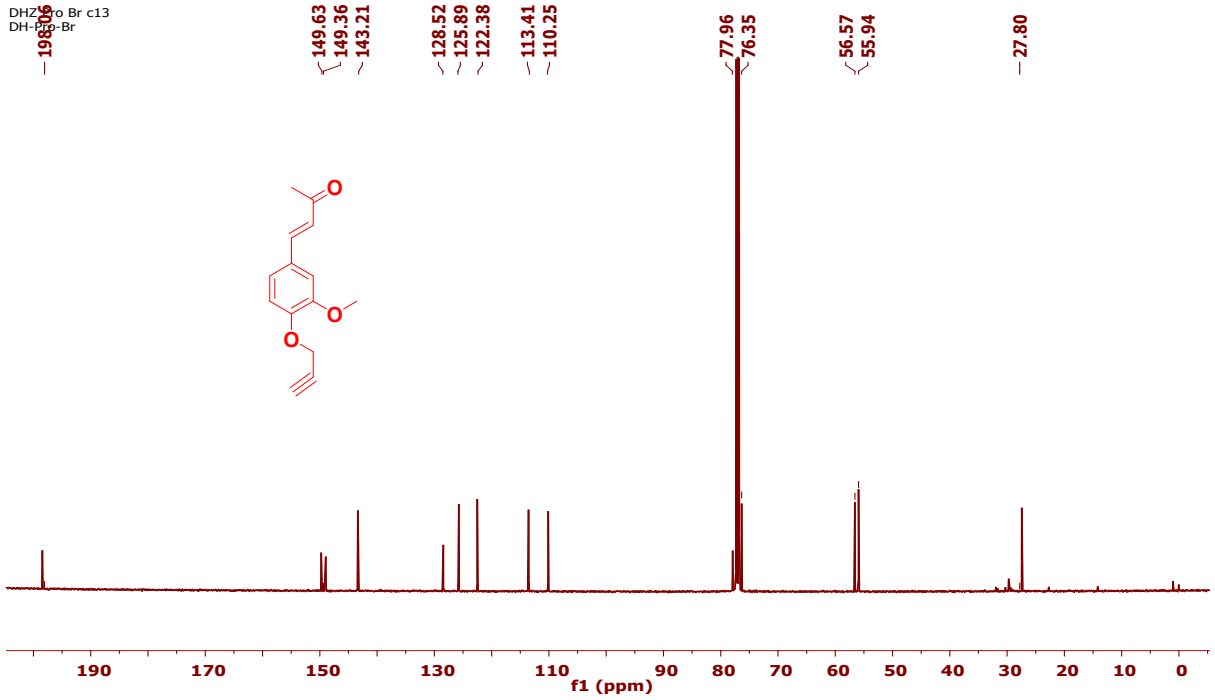
m/z	z	Abund	Formula	Ion
231.1013	1	1036604.69	C14 H15 O3	(M+H)+
232.1048	1	140231.11	C14 H15 O3	(M+H)+
233.1087	1	17586.13	C14 H15 O3	(M+H)+
461.1964	1	9484.1	C28 H29 O6	(2M+H)+
462.2004	1	3055.12	C28 H29 O6	(2M+H)+

Predicted Isotope Match Table

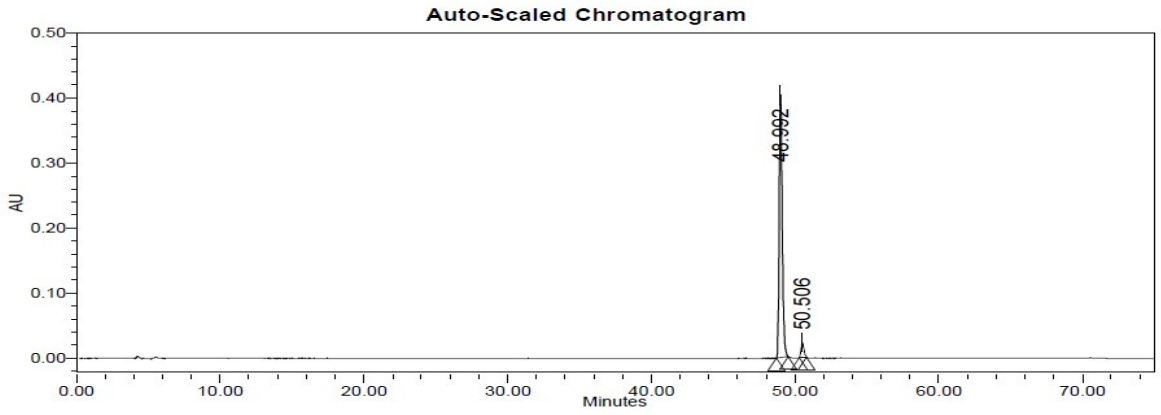
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	231.1013	231.1016	1.38	100	100	86.66	85.25
2	232.1048	232.105	0.55	13.53	15.43	11.72	13.15
3	233.1087	233.1075	-5.33	1.7	1.72	1.47	1.47
4	234.1134	234.1101	-14.03	0.16	0.14	0.14	0.12

^{1}H and ^{13}C NMR of 2:





HPLC and HRESIMS of 3



	RT	Area (μV*sec)	% Area	Height (μV)
1	48.992	5814422	94.78	404589
2	50.506	320109	5.22	23075

Qualitative Compound Report

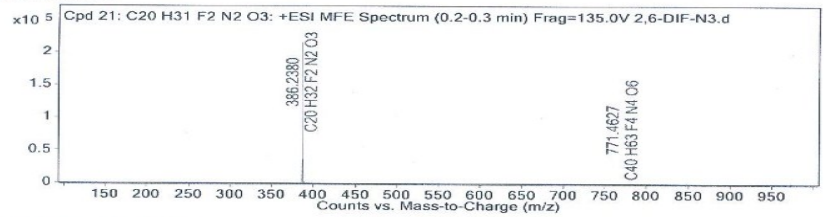
Data File	2,6-DIF-N3.d	**Sample Name**	2,6-DIF-N3
Sample Type	Sample	**Position**	Vial 30
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 3:06:05
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			
Sample Group		**Info.**	
Acquisition 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 21: C20 H31 F2 N2 O3	0.3	385.2307	C20 H31 F2 N2 O3	C20 H31 F2 N2 O3	-1.18	C20 H31 F2 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 21: C20 H31 F2 N2 O3	386.238	0.3	Find by Molecular Feature	385.2307

MFE MS Spectrum



MS Spectrum Peak List

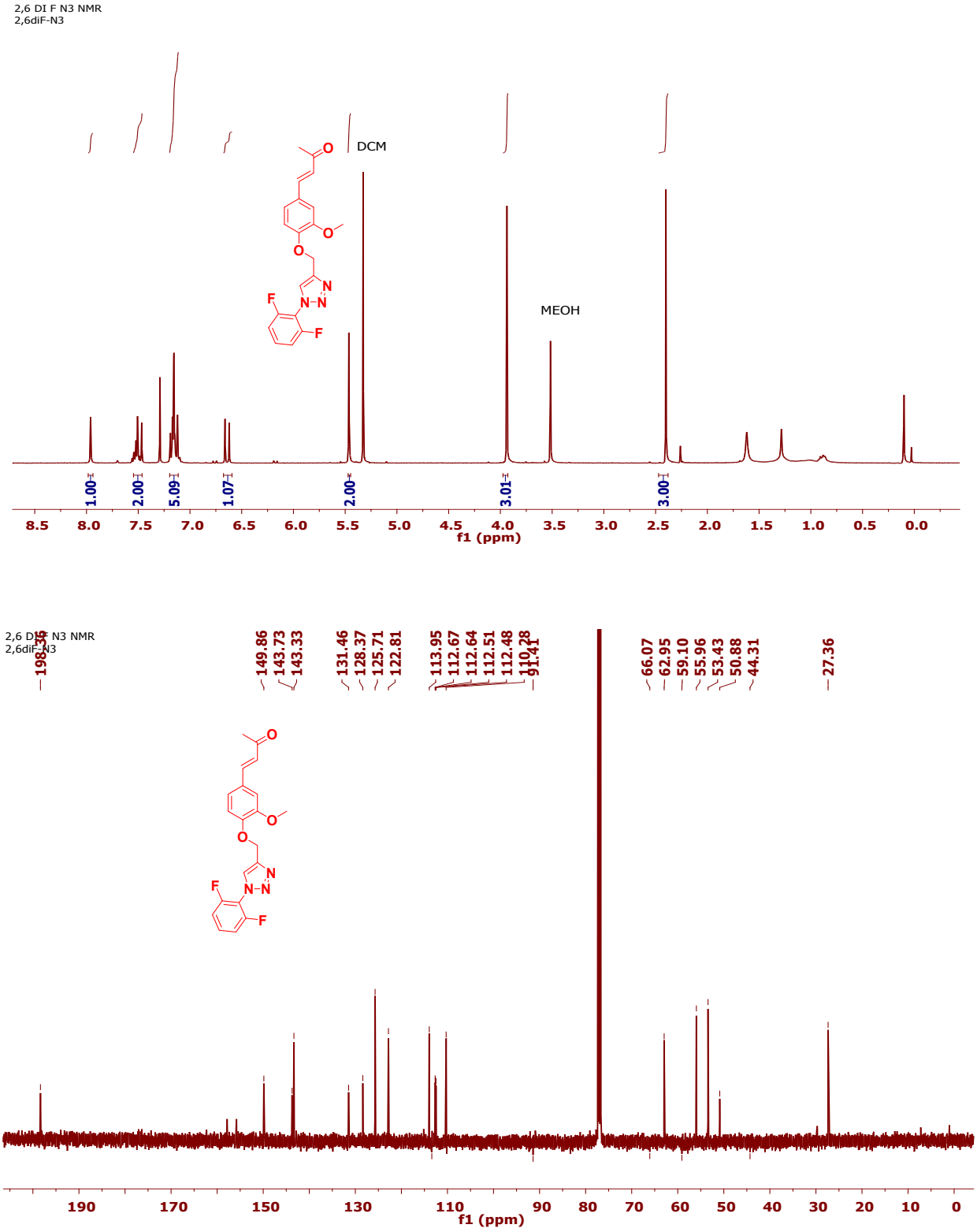
m/z	z	Abund	Formula	Ion
386.238	1	215126.67	C20 H32 F2 N2 O3	(M+H)+
387.2405	1	36599.47	C20 H32 F2 N2 O3	(M+H)+
388.2509	1	2904.31	C20 H32 F2 N2 O3	(M+H)+
389.2524	1	577.94	C20 H32 F2 N2 O3	(M+H)+
771.4627	1	294.13	C40 H63 F4 N4 O6	(2M+H)+

Predicted Isotope Match Table

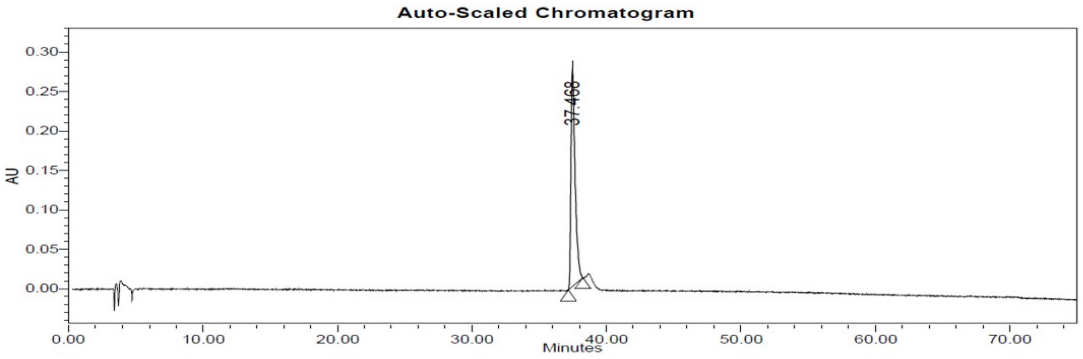
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	386.238	386.2376	-1.21	100	100	84.29	79.2
2	387.2405	387.2408	0.7	17.01	22.84	14.34	18.09
3	388.2509	388.2435	-19.07	1.35	3.11	1.14	2.46
4	389.2524	389.2462	-16.02	0.27	0.31	0.23	0.25

--- End Of Report ---

^{1}H and ^{13}C NMR of 3:



HPLC and HRESIMS of 4



	RT	Area (μV*sec)	% Area	Height (μV)
1	37.468	5894953	100.00	275920

Qualitative Compound Report

Data File	2-N3.d	**Sample Name**	2-N3
Sample Type	Sample	**Position**	Vial 24
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 2:35:46
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

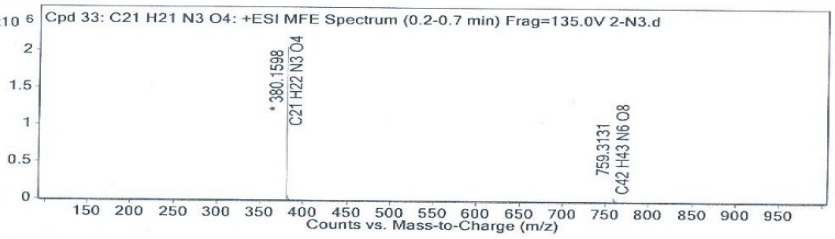
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 33: C21 H21 N3 O4	0.3	379.1528	C21 H21 N3 O4	C21 H21 N3 O4	1.16	C21 H21 N3 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 33: C21 H21 N3 O4	380.1598	0.3	Find by Molecular Feature	379.1528

MFE MS Spectrum



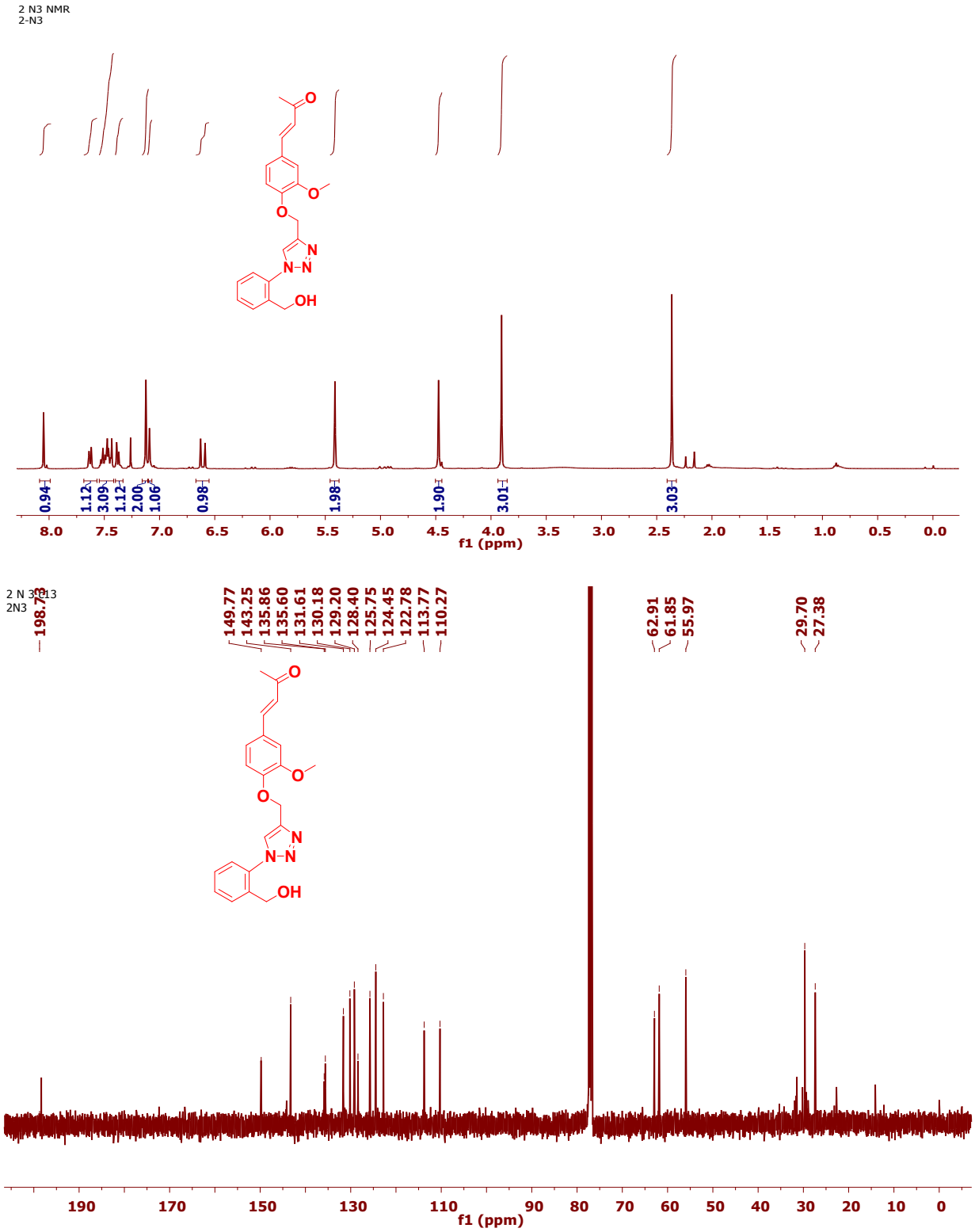
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
380.1598	1	2058134.38	C21 H22 N3 O4	(M+H)+
381.164	1	461431.16	C21 H22 N3 O4	(M+H)+
382.1664	1	60787.25	C21 H22 N3 O4	(M+H)+
759.3131	1	50214.82	C42 H43 N6 O8	(2M+H)+
760.3165	1	24011.39	C42 H43 N6 O8	(2M+H)+

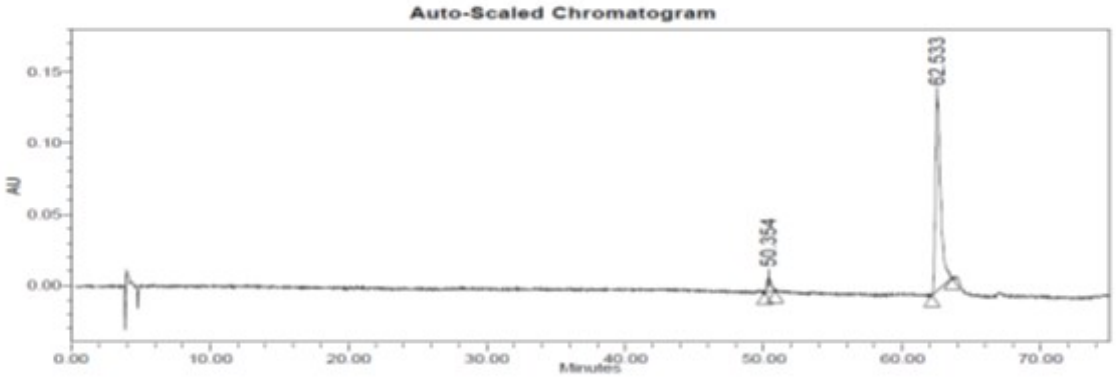
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	380.1598	380.1605	1.71	100	100	79.56	77.97
2	381.164	381.1636	-1.12	22.42	24.21	17.84	18.88
3	382.1664	382.1662	-0.33	2.95	3.63	2.35	2.83
4	383.1694	383.1688	-1.42	0.32	0.41	0.26	0.32

^{1}H and ^{13}C NMR of 4:



HPLC and HRESIMS of 5



	RT	Area (µV*sec)	% Area	Height (µV)
1	50.354	206653	5.39	9735
2	62.533	3625498	94.61	136099

Qualitative Compound Report

Data File	AZOBENZENE.d	**Sample Name**	AZOBENZENE
Sample Type	Sample	**Position**	Vial 27
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 2:53:07
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

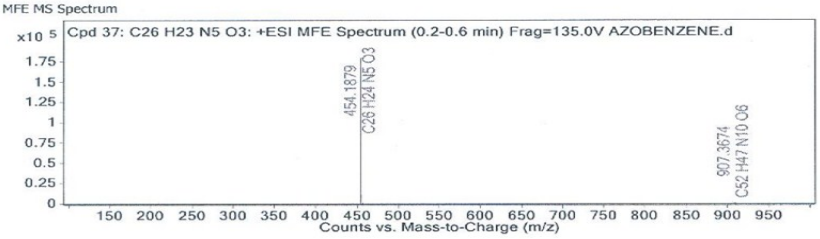
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 37: C26 H23 N5 O3	0.3	453.1806	C26 H23 N5 O3	C26 H23 N5 O3	-1.11	C26 H23 N5 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 37: C26 H23 N5 O3	454.1879	0.3	Find by Molecular Feature	453.1806

MFE MS Spectrum



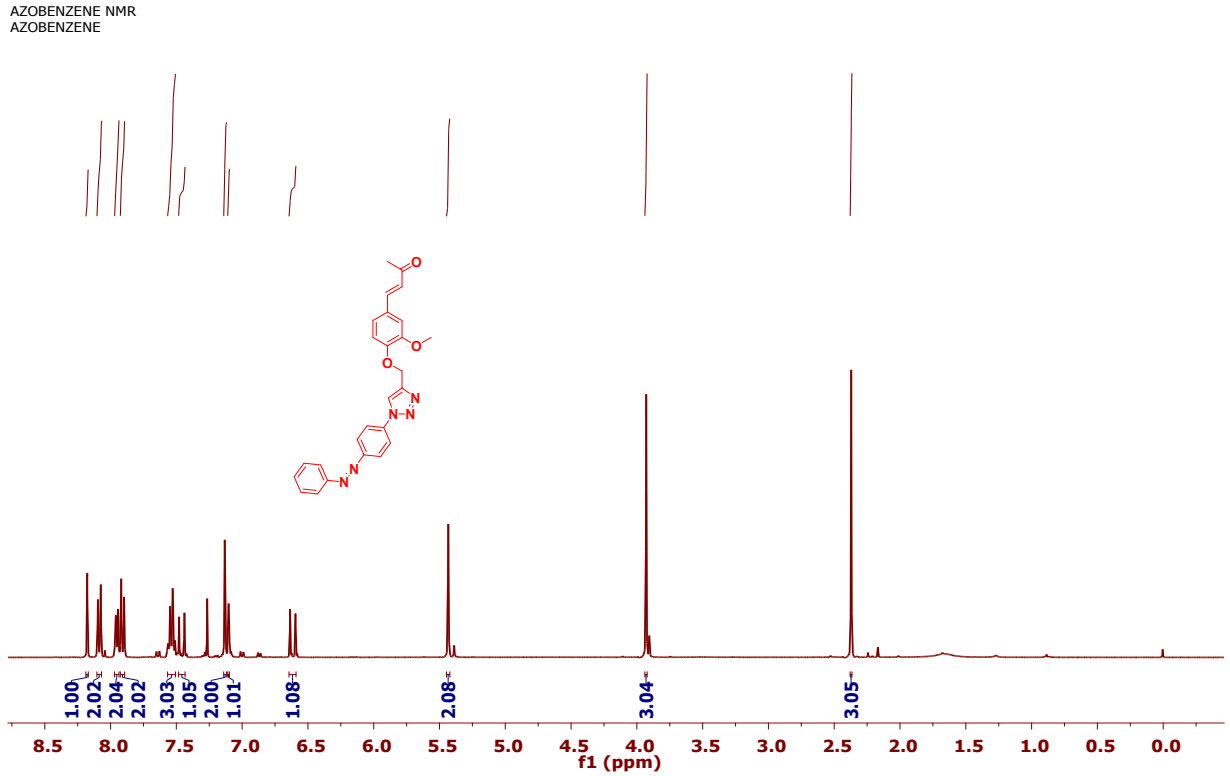
MS Spectrum Peak List

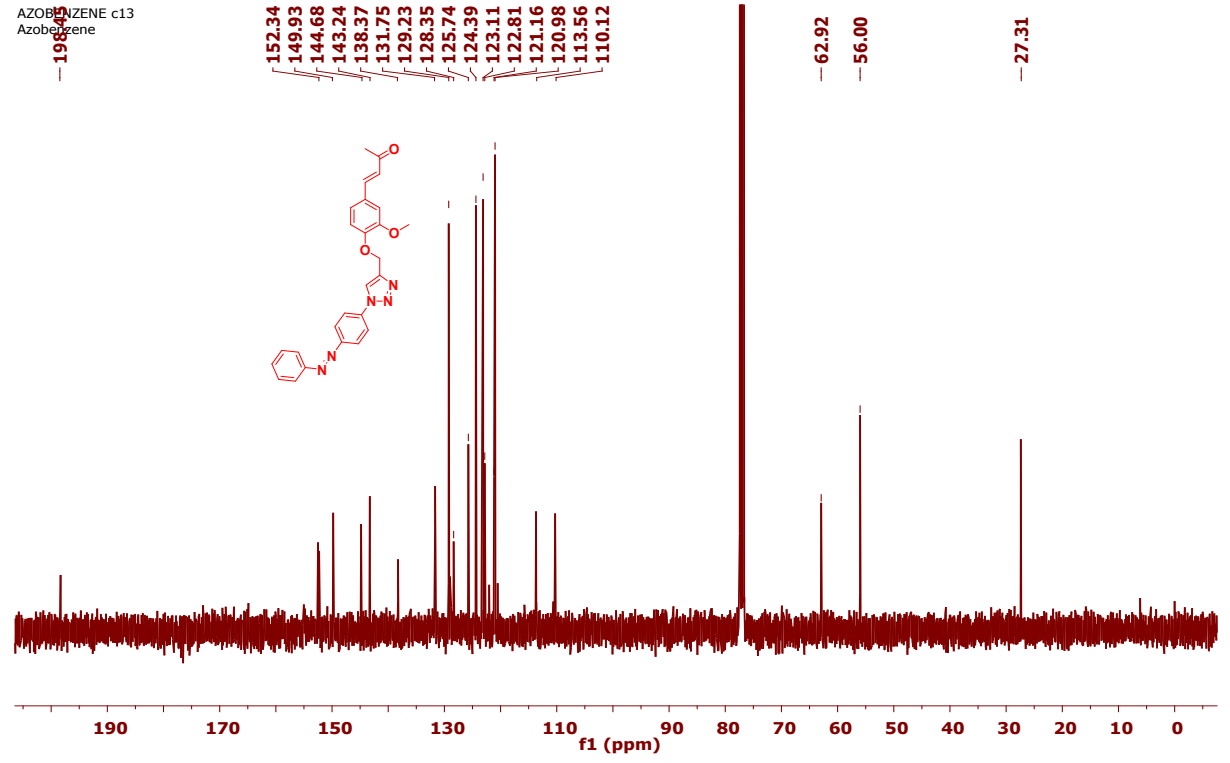
m/z	z	Abund	Formula	Ion
454.1879	1	178845.95	C26 H24 N5 O3	(M+H)+
455.1908	1	51649.05	C26 H24 N5 O3	(M+H)+
456.1941	1	9802.76	C26 H24 N5 O3	(M+H)+
907.3674	1	2202.82	C52 H47 N10 O6	(2M+H)+
908.3706	1	1390.57	C52 H47 N10 O6	(2M+H)+

Predicted Isotope Match Table

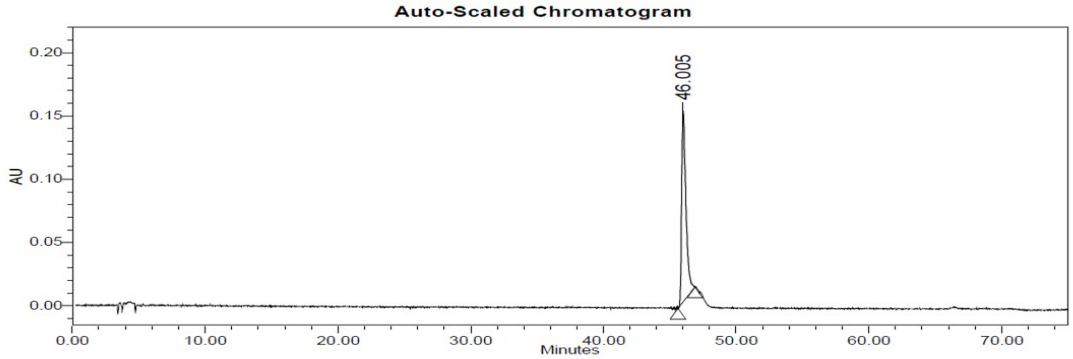
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	454.1879	454.1874	-1.09	100	100	74.07	73.53
2	455.1908	455.1904	-0.86	28.88	30.34	21.39	22.31
3	456.1941	456.1931	-2.1	5.48	5.06	4.06	3.72
4	457.1989	457.1958	-6.68	0.65	0.61	0.48	0.45

^{1}H and ^{13}C NMR of 5:





HPLC AND HRESIMS of 6:



	RT	Area (μV*sec)	% Area	Height (μV)
1	46.005	3414763	100.00	151068

Qualitative Compound Report

Data File	4-OMe-N3.d	**Sample Name**	4-OMe-N3
Sample Type	Sample	**Position**	Vial 19
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 2:09:43
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

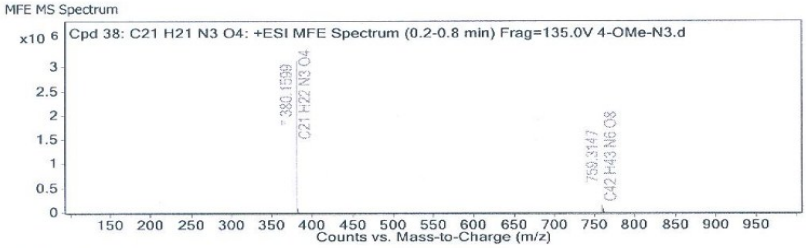
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 38: C21 H21 N3 O4	0.3	379.1529	C21 H21 N3 O4	C21 H21 N3 O4	0.81	C21 H21 N3 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 38: C21 H21 N3 O4	380.1599	0.3	Find by Molecular Feature	379.1529

MFE MS Spectrum



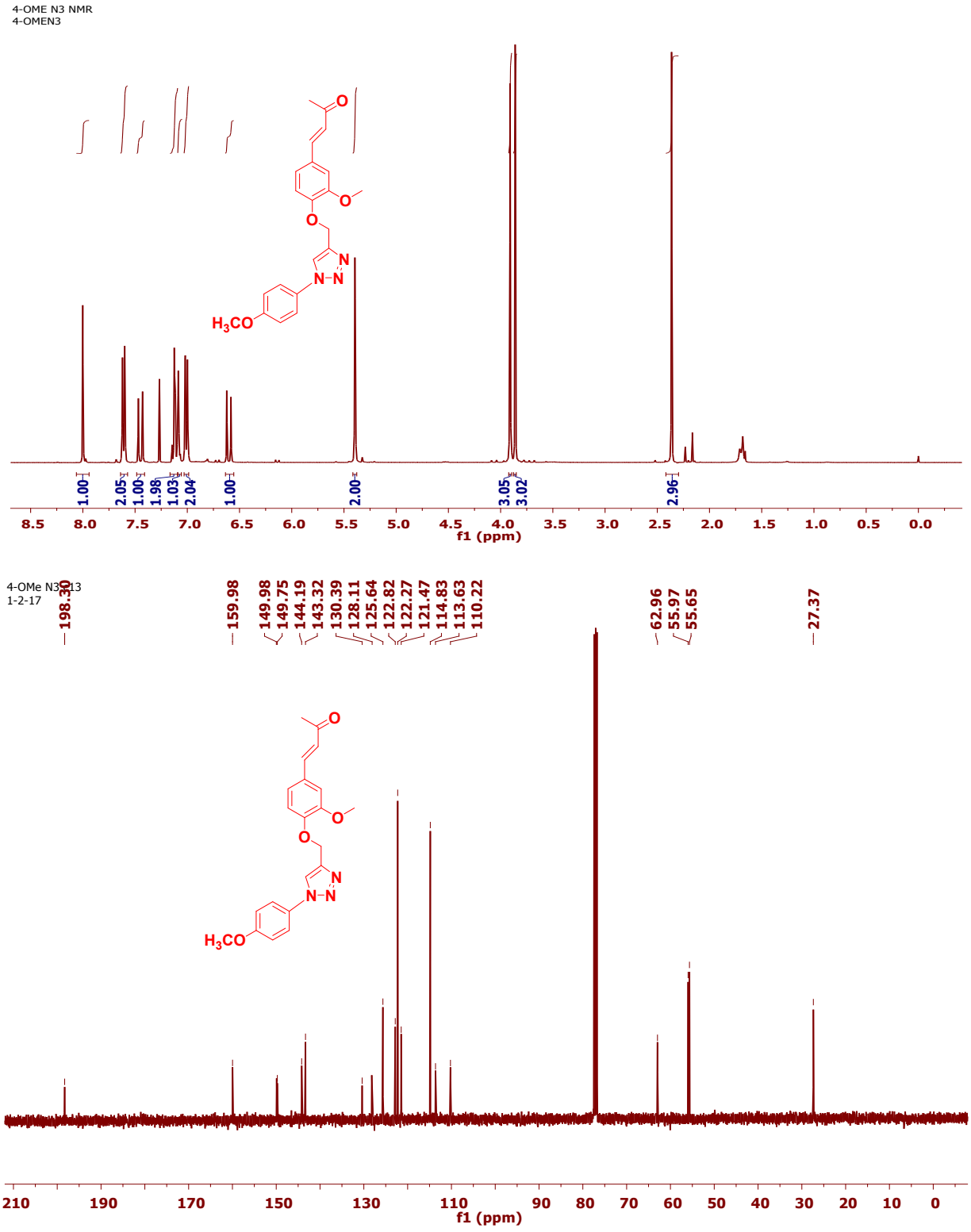
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
380.1599	1	3128396.25	C21 H22 N3 O4	(M+H)+
381.1645	1	686203	C21 H22 N3 O4	(M+H)+
382.1669	1	93718.7	C21 H22 N3 O4	(M+H)+
759.3147	1	145659.97	C42 H43 N6 O8	(2M+H)+
760.3178	1	67842.76	C42 H43 N6 O8	(2M+H)+

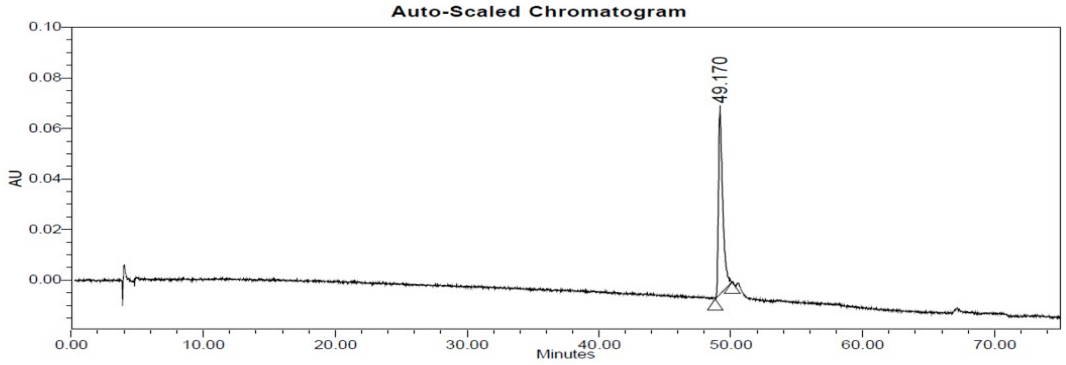
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	380.1599	380.1605	1.57	100	100	79.86	77.97
2	381.1645	381.1636	-2.33	21.93	24.21	17.52	18.88
3	382.1669	382.1662	-1.66	3	3.63	2.39	2.83
4	383.1693	383.1688	-1.36	0.28	0.41	0.23	0.32

^{1}H and ^{13}C NMR of 6:



HPLC AND HRESIMS of 7:



	RT	Area (µV*sec)	% Area	Height (µV)
1	49.170	1648682	100.00	71347

Qualitative Compound Report

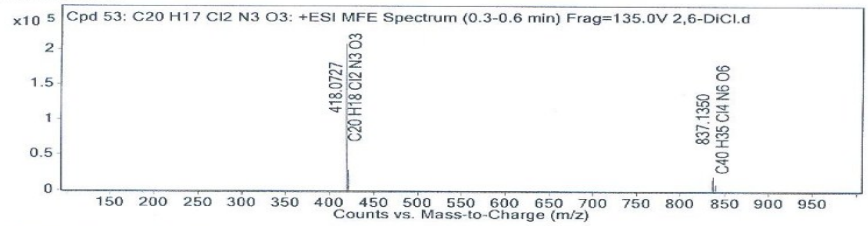
Data File	2,6-DiCl.d	**Sample Name**	2,6-DiCl
Sample Type	Sample	**Position**	Vial 26
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 2:44:22
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			
Sample Group		**Info.**	
Acquisition 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 53: C20 H17 Cl2 N3 O3	0.4	417.0654	C20 H17 Cl2 N3 O3	C20 H17 Cl2 N3 O3	-1.76	C20 H17 Cl2 N3 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 53: C20 H17 Cl2 N3 O3	418.0727	0.4	Find by Molecular Feature	417.0654

MFE MS Spectrum



MS Spectrum Peak List

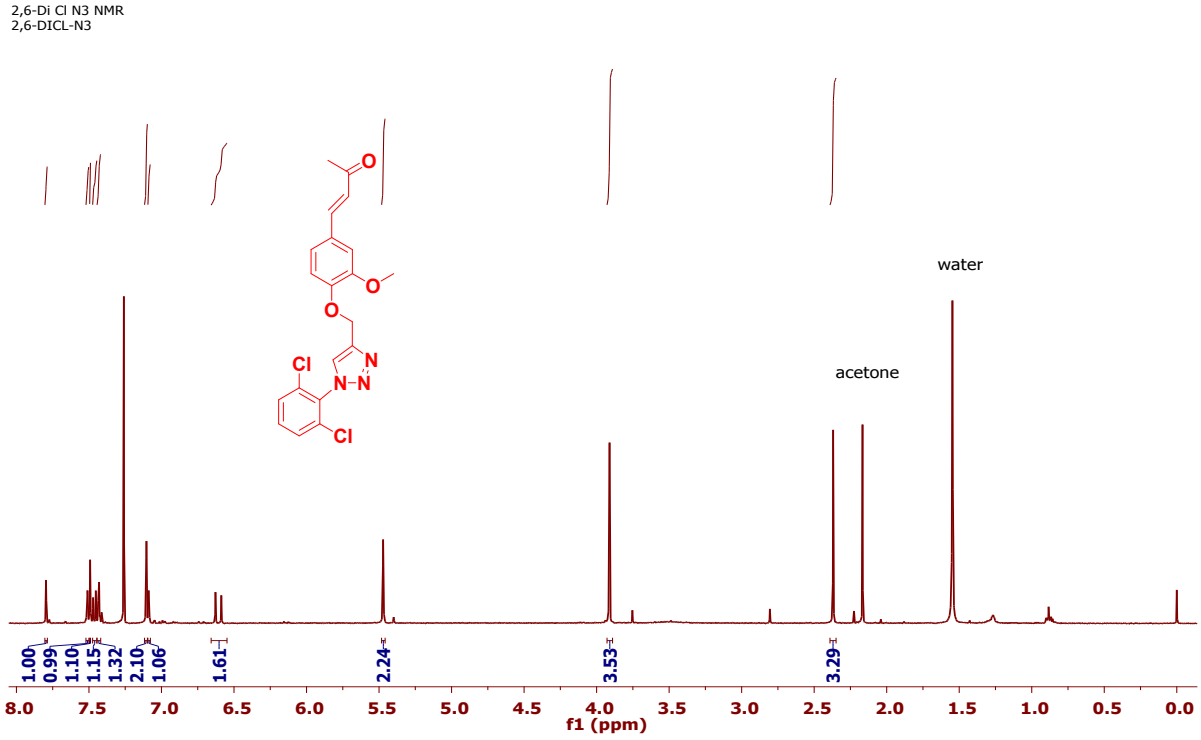
m/z	z	Abund	Formula	Ion
418.0727	1	208120.92	C20 H18 Cl2 N3 O3	(M+H)+
419.076	1	45114.04	C20 H18 Cl2 N3 O3	(M+H)+
420.0701	1	124211.38	C20 H18 Cl2 N3 O3	(M+H)+
421.0731	1	29334.54	C20 H18 Cl2 N3 O3	(M+H)+
422.068	1	22162.6	C20 H18 Cl2 N3 O3	(M+H)+

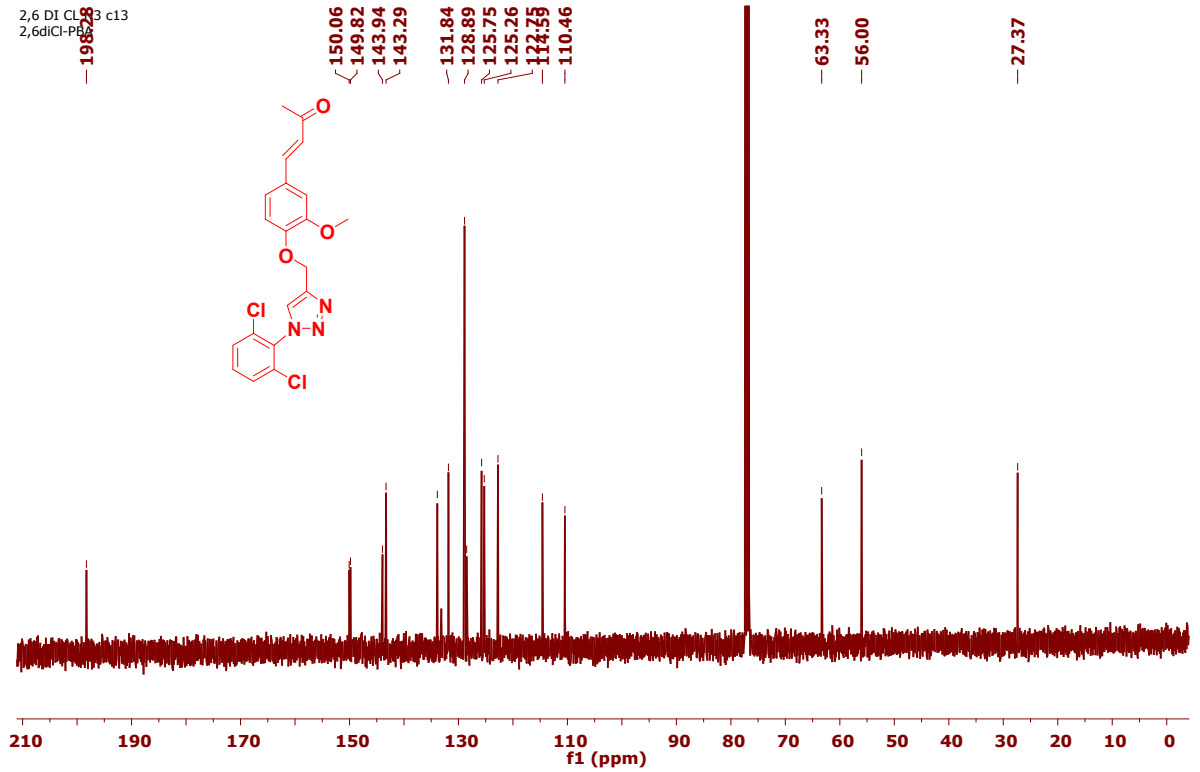
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	418.0727	418.072	-1.77	100	100	48.52	45.97
2	419.076	419.0751	-2.28	21.68	23.05	10.52	10.59
3	420.0701	420.0694	-1.59	59.68	67.15	28.96	30.87
4	421.0731	421.0723	-1.93	14.09	15.07	6.84	6.93
5	422.068	422.0675	-1.11	10.65	12.28	5.17	5.65

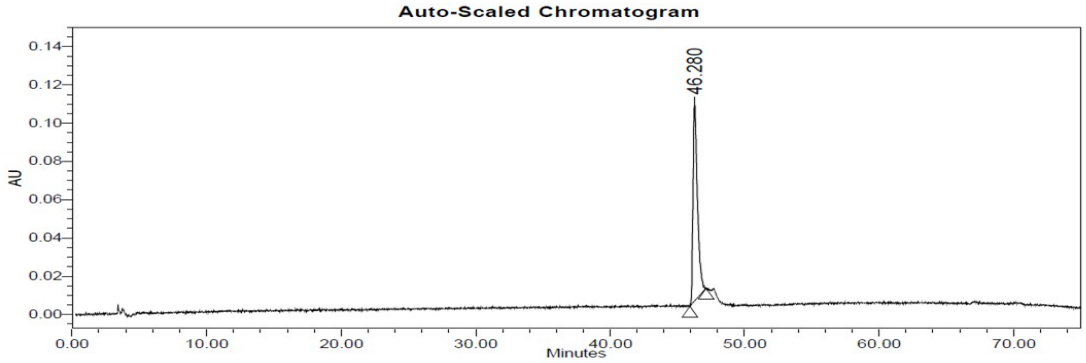
--- End Of Report ---

^{1}H and ^{13}C NMR of 7:





HPLC AND HRESIMS of 8-



	RT	Area (μV*sec)	% Area	Height (μV)
1	46.280	2356079	100.00	102622

Qualitative Compound Report

Data File	O-ANISIDINE.d	**Sample Name**	O-ANISIDINE
Sample Type	Sample	**Position**	Vial 20
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 2:14:04
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

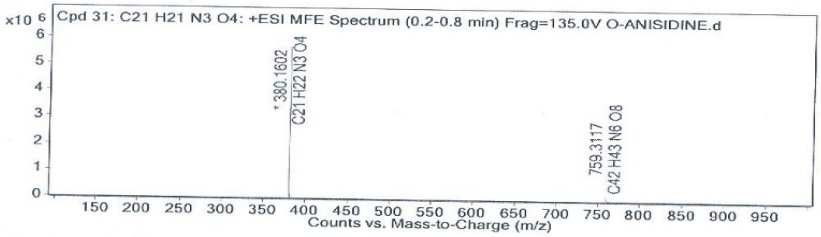
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 31: C21 H21 N3 O4	0.3	379.1528	C21 H21 N3 O4	C21 H21 N3 O4	1.18	C21 H21 N3 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 31: C21 H21 N3 O4	380.1602	0.3	Find by Molecular Feature	379.1528

MFE MS Spectrum



MS Spectrum Peak List

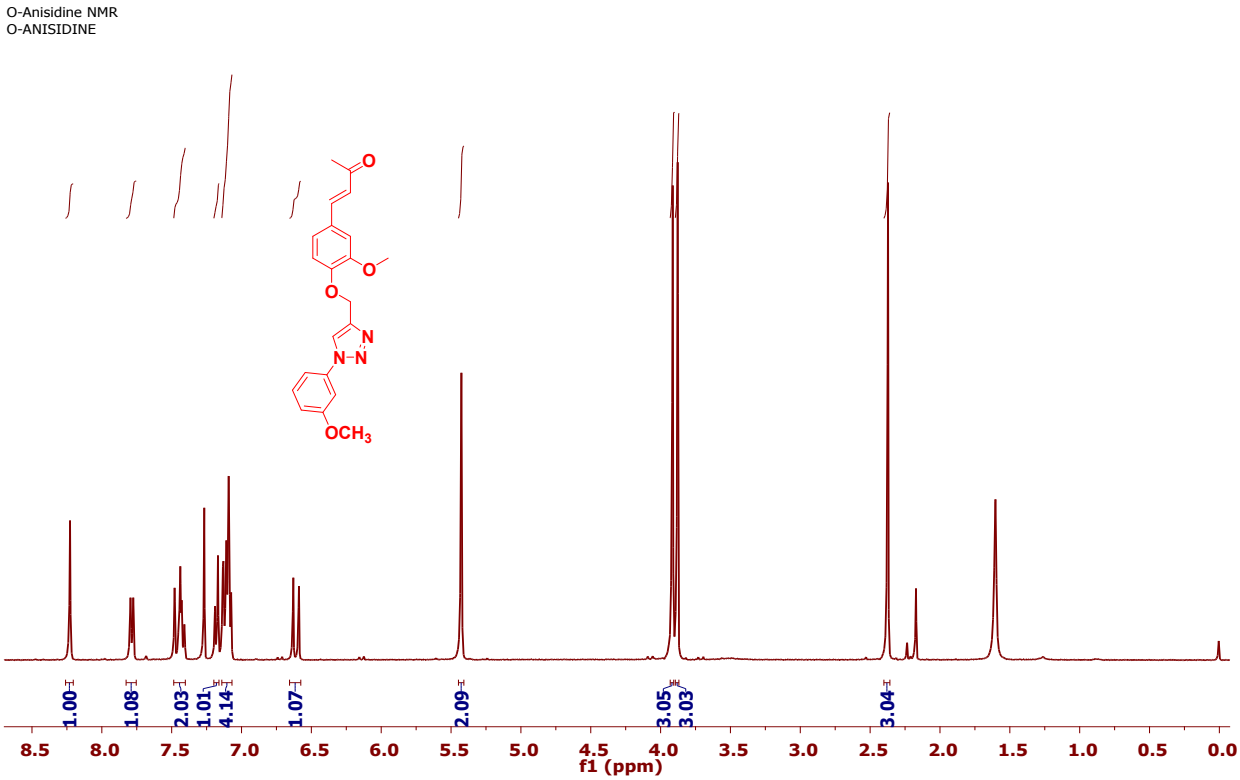
m/z	z	Abund	Formula	Ion
380.1602	1	5667660.5	C21 H22 N3 O4	(M+H)+
381.1624	1	1246876.25	C21 H22 N3 O4	(M+H)+
382.1655	1	167291.45	C21 H22 N3 O4	(M+H)+
759.3117	1	166346.47	C42 H43 N6 O8	(2M+H)+
760.3145	1	80817.66	C42 H43 N6 O8	(2M+H)+

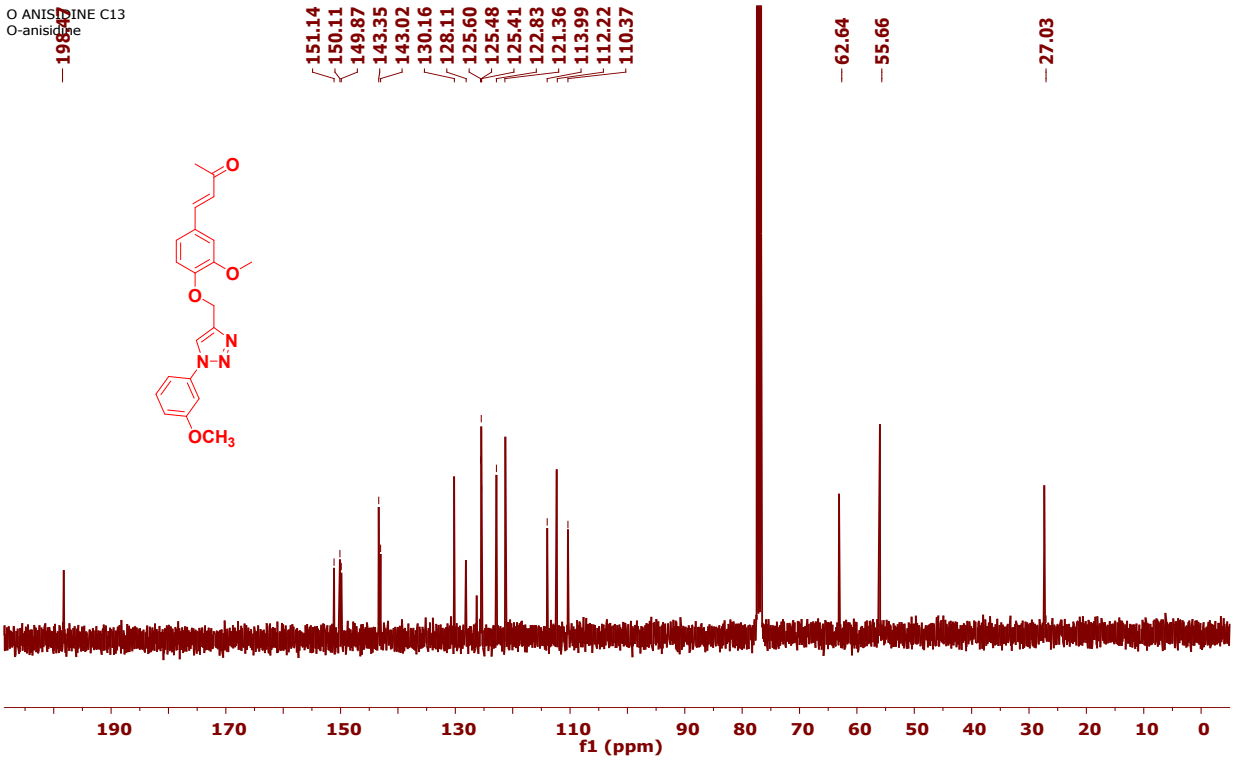
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	380.1602	380.1605	0.7	100	100	79.77	77.95
2	381.1624	381.1636	3.16	22	24.21	17.55	18.88
3	382.1655	382.1662	1.98	2.95	3.63	2.35	2.83
4	383.1674	383.1688	3.81	0.36	0.41	0.29	0.32
5	384.1692	384.1714	5.66	0.04	0.04	0.03	0.03

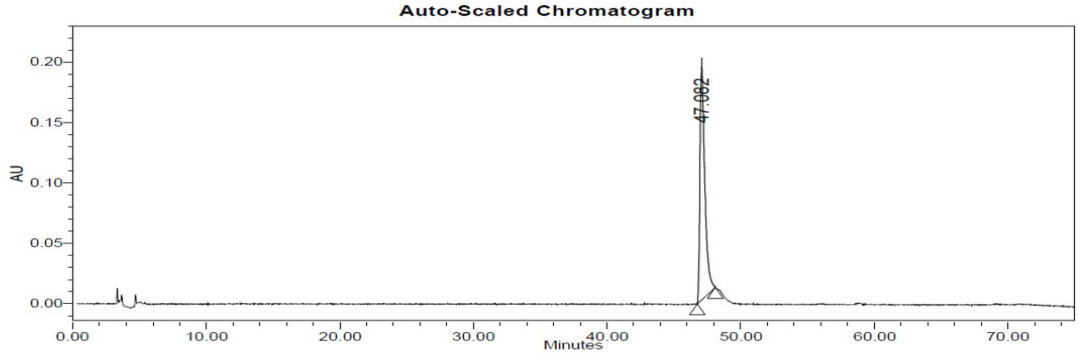
--- End Of Report ---

^{1}H and ^{13}C NMR of 8:





HPLC AND HRESIMS of 9:



	RT	Area (μV*sec)	% Area	Height (μV)
1	47.082	4811458	100.00	193723

Qualitative Compound Report

Data File	m-anisidine.d	**Sample Name**	m-anisidine
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-03-2017 PM 12:46:55
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

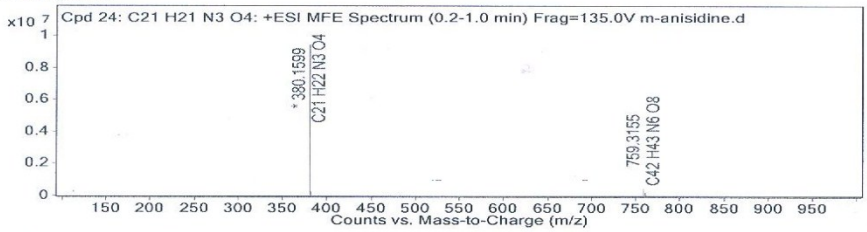
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 24: C21 H21 N3 O4	0.3	379.1527	C21 H21 N3 O4	C21 H21 N3 O4	1.27	C21 H21 N3 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 24: C21 H21 N3 O4	380.1599	0.3	Find by Molecular Feature	379.1527

MFE MS Spectrum



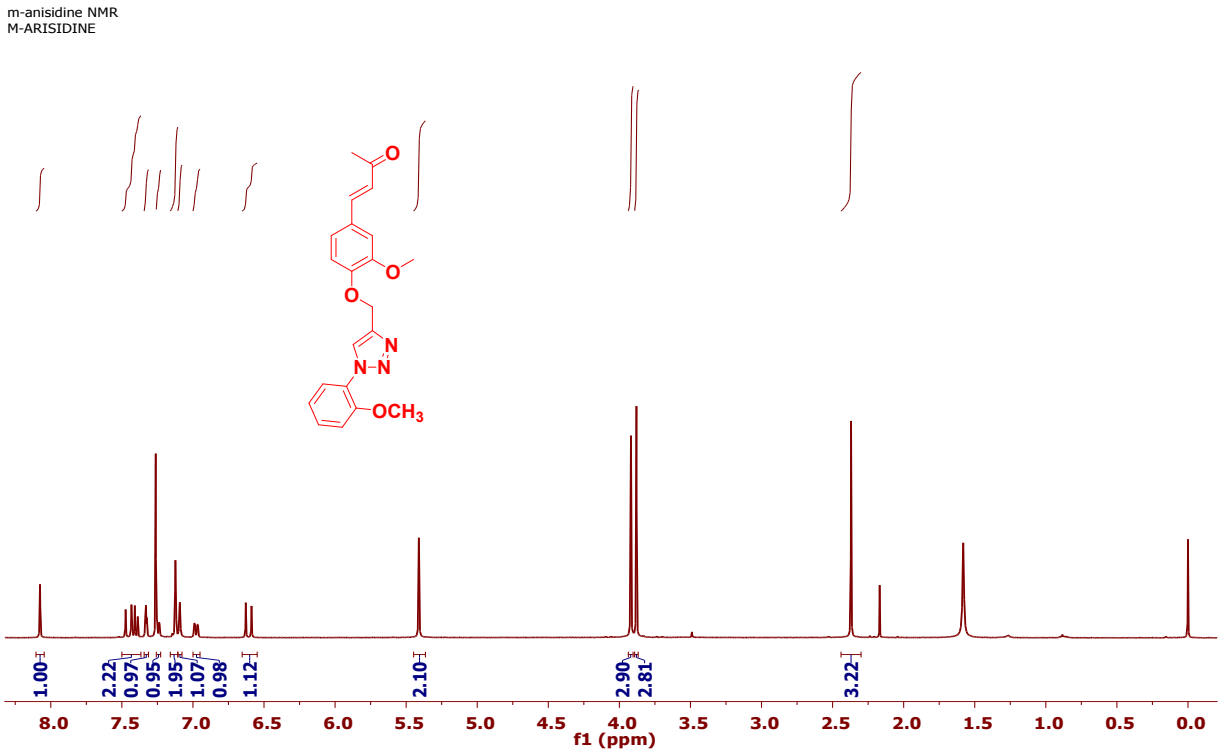
MS Spectrum Peak List

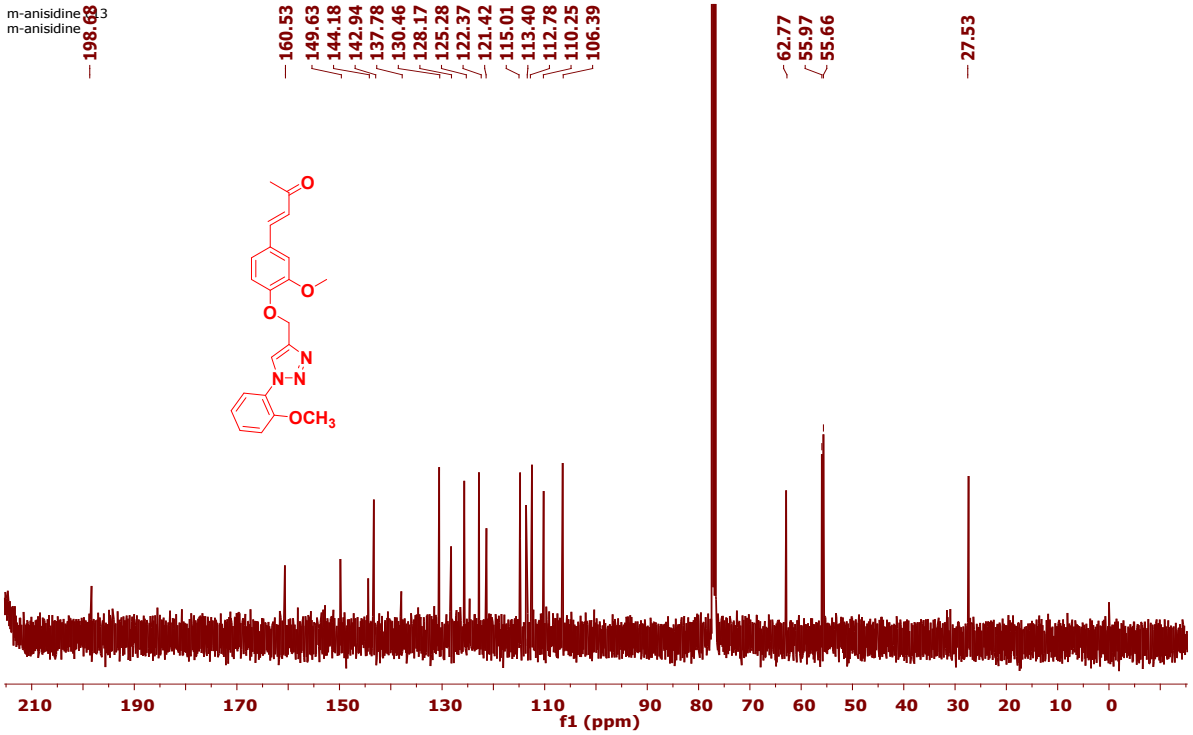
m/z	z	Abund	Formula	Ion
380.1599	1	9418078	C21 H22 N3 O4	(M+H)+
381.1635	1	2033427.38	C21 H22 N3 O4	(M+H)+
382.1663	1	262618.13	C21 H22 N3 O4	(M+H)+
759.3155	1	435239.63	C42 H43 N6 O8	(2M+H)+
760.3182	1	201223.38	C42 H43 N6 O8	(2M+H)+

Predicted Isotope Match Table

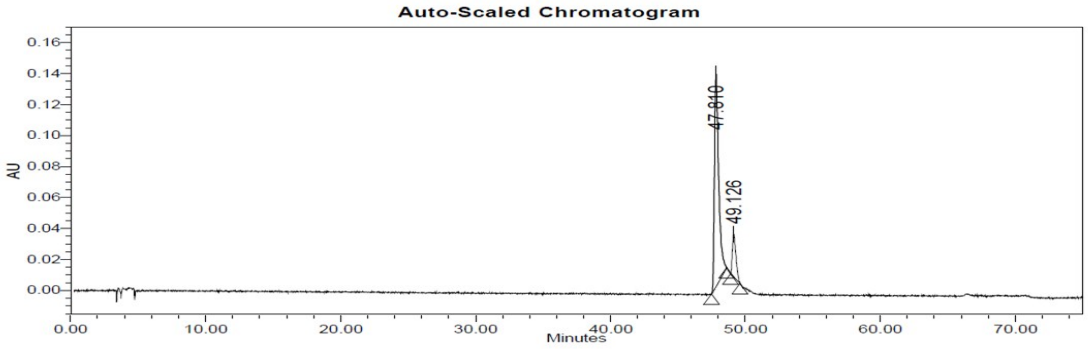
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	380.1599	380.1605	1.53	100	100	80.21	77.95
2	381.1635	381.1636	0.22	21.59	24.21	17.32	18.88
3	382.1663	382.1662	-0.07	2.79	3.63	2.24	2.83
4	383.1684	383.1688	0.97	0.26	0.41	0.21	0.32
5	384.1706	384.1714	1.93	0.03	0.04	0.03	0.03

^{1}H and ^{13}C NMR of 9:





HPLC AND HRESIMS of 10



	RT	Area (µV*sec)	% Area	Height (µV)
1	47.810	2994221	85.24	137808
2	49.126	518514	14.76	27725

Qualitative Compound Report

Data File	4-ABN.d	**Sample Name**	4-ABN
Sample Type	Sample	**Position**	Vial 25
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 2:40:03
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

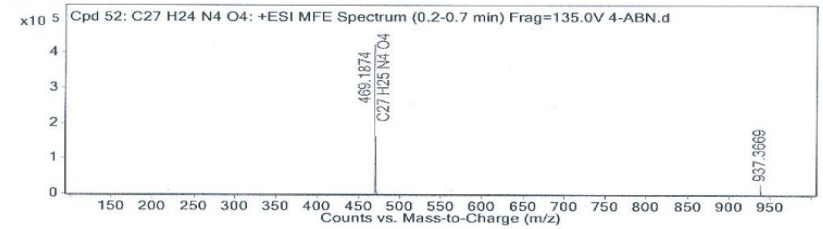
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 52: C27 H24 N4 O4	0.3	468.1804	C27 H24 N4 O4	C27 H24 N4 O4	-1.36	C27 H24 N4 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 52: C27 H24 N4 O4	469.1874	0.3	Find by Molecular Feature	468.1804

MFE MS Spectrum



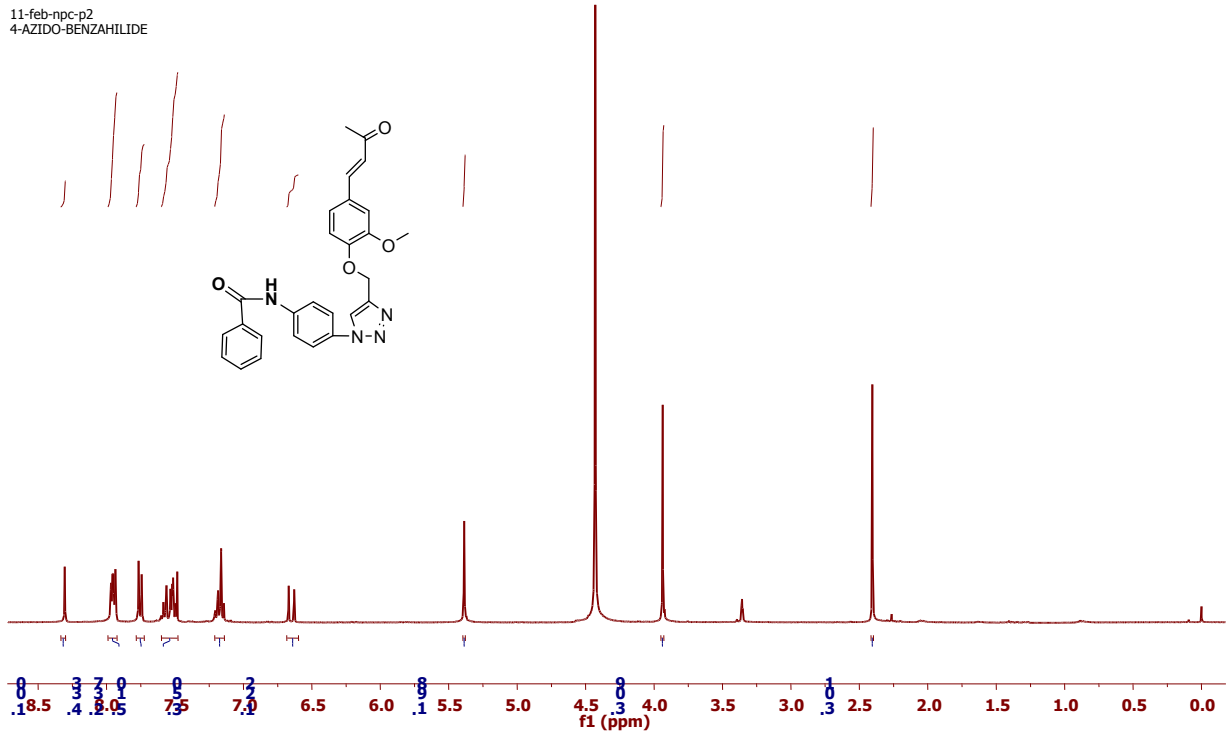
MS Spectrum Peak List

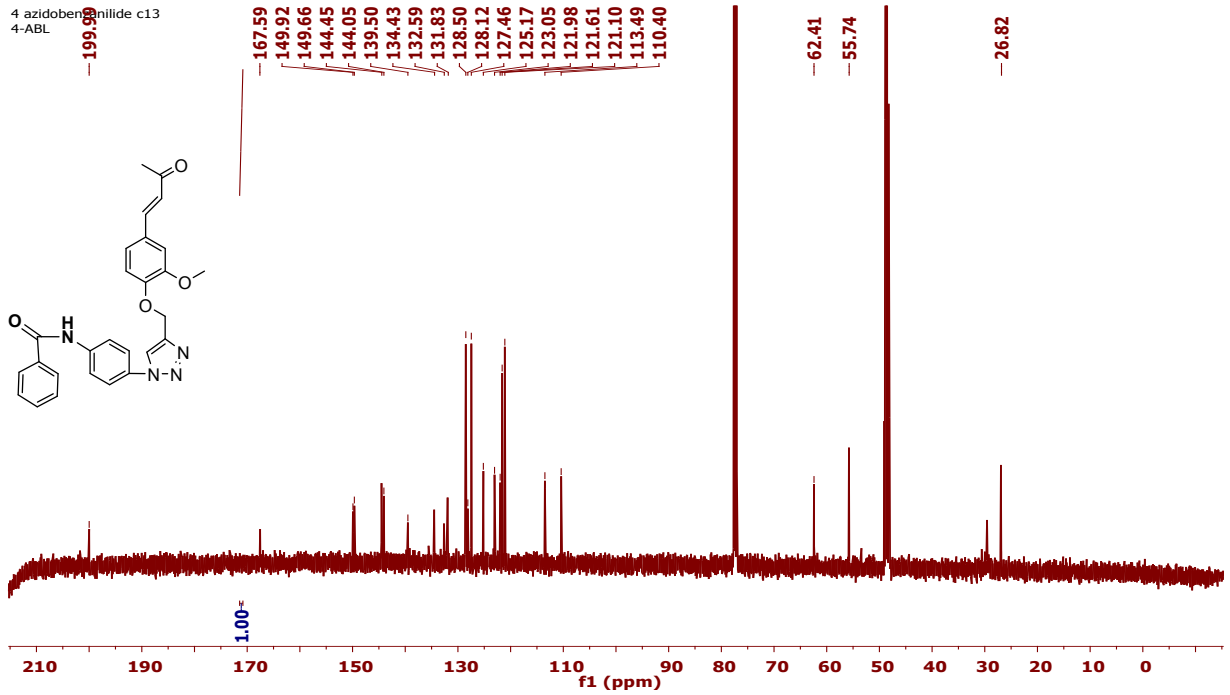
m/z	z	Abund	Formula	Ion
469.1874	1	423718.28	C27 H25 N4 O4	(M+H)+
470.191	1	162967.69	C27 H25 N4 O4	(M+H)+
471.1945	1	34089.97	C27 H25 N4 O4	(M+H)+
937.3669	1	29577.66		(2M+H)+
938.3707	1	25261.61		(2M+H)+

Predicted Isotope Match Table

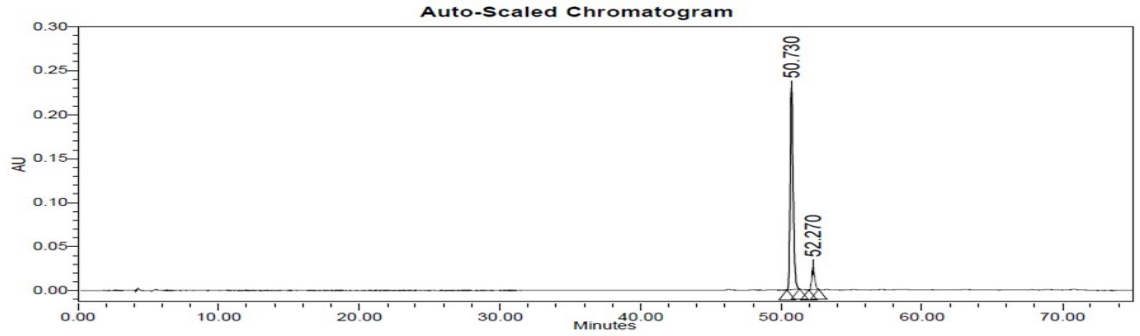
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	469.1874	469.187	-0.88	100	100	67.41	72.79
2	470.191	470.1901	-1.93	38.46	31.1	25.93	22.64
3	471.1945	471.1929	-3.38	8.05	5.5	5.42	4
4	472.199	472.1956	-7.26	1.45	0.71	0.98	0.52
5	473.1988	473.1982	-1.36	0.34	0.07	0.23	0.05
6	474.2112	474.2008	-21.9	0.04	0.01	0.03	0

^{1}H and ^{13}C NMR of 10:





HPLC and HRESIMS of 11



	RT	Area (μV*sec)	% Area	Height (μV)
1	50.730	3373764	90.06	229498
2	52.270	372346	9.94	25703

Qualitative Compound Report

Data File	4-NO2-N3.d	**Sample Name**	4-NO2-N3
Sample Type	Sample	**Position**	Vial 17
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 2:01:04
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

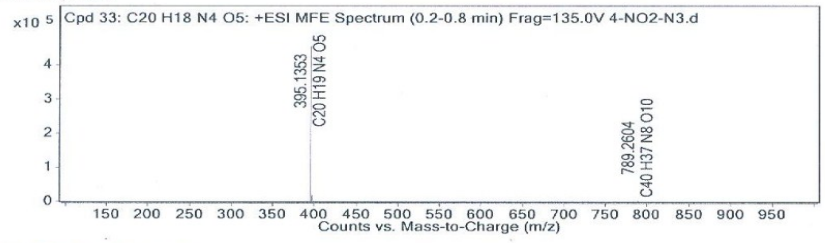
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 33: C20 H18 N4 O5	0.3	394.1279	C20 H18 N4 O5	C20 H18 N4 O5	-0.5	C20 H18 N4 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 33: C20 H18 N4 O5	395.1353	0.3	Find by Molecular Feature	394.1279

MFE MS Spectrum



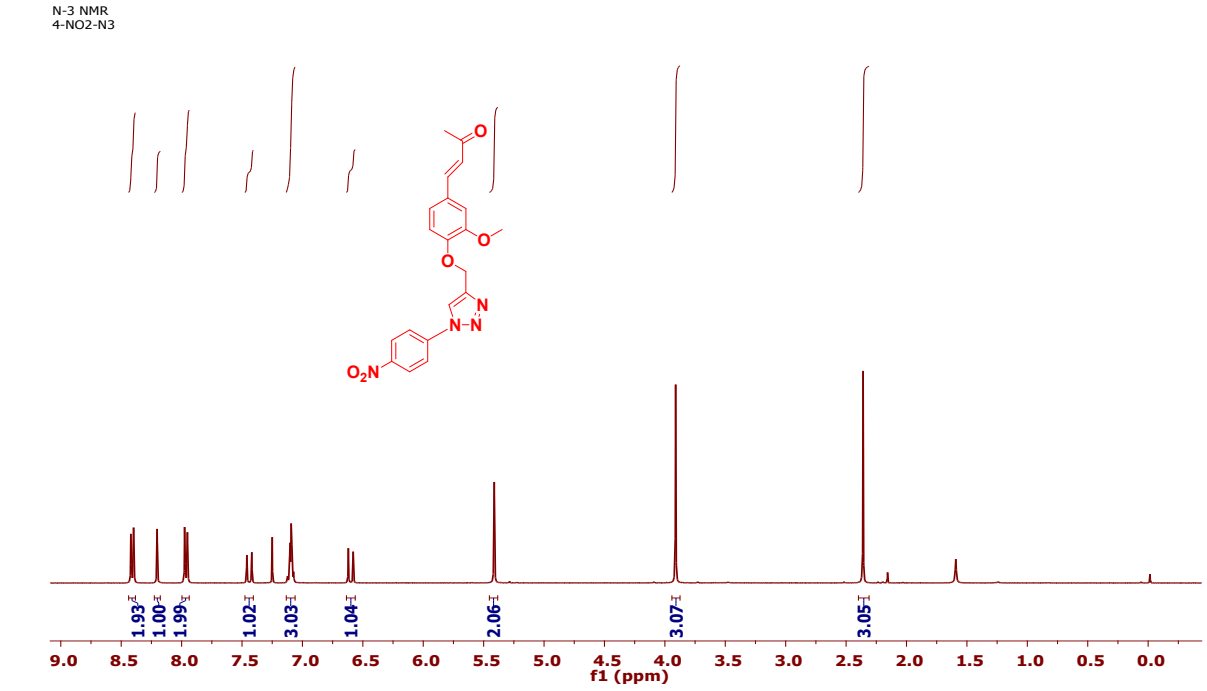
MS Spectrum Peak List

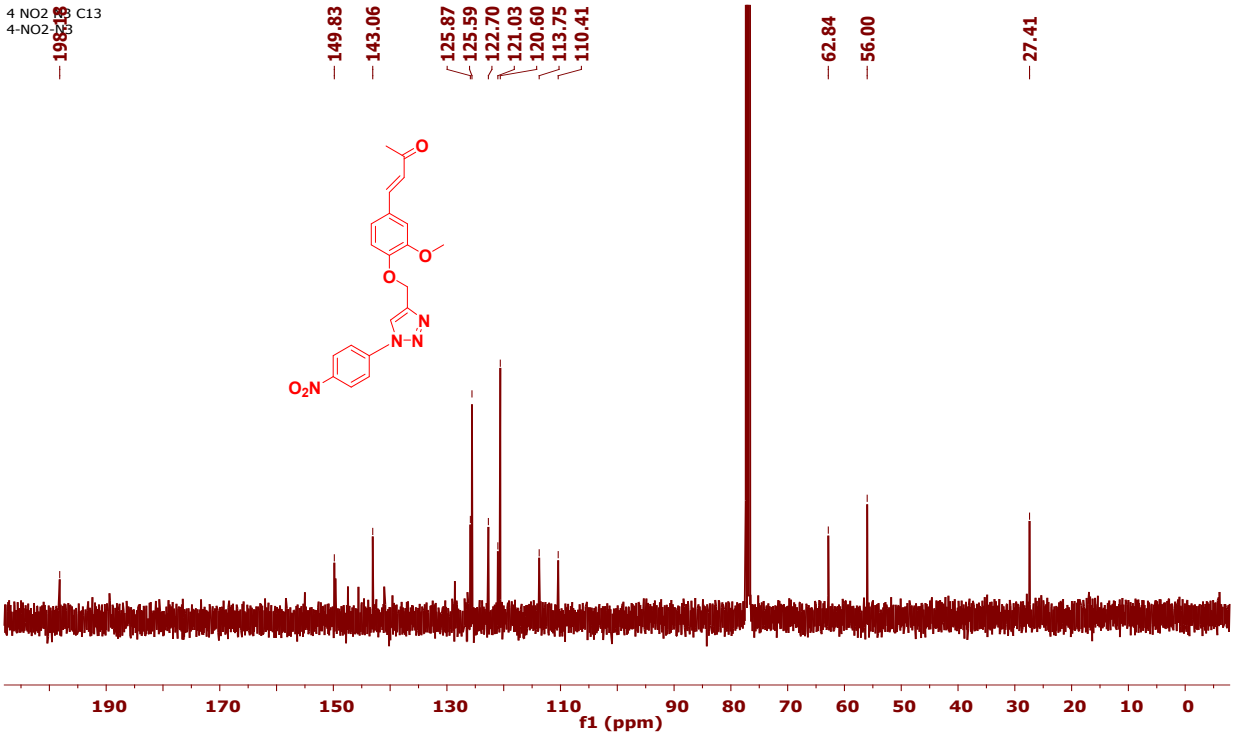
m/z	z	Abund	Formula	Ion
395.1353	1	453710.78	C20 H19 N4 O5	(M+H)+
396.138	1	110469.45	C20 H19 N4 O5	(M+H)+
397.1403	1	16790.17	C20 H19 N4 O5	(M+H)+
398.143	1	2259.07	C20 H19 N4 O5	(M+H)+
789.2604	1	1785.77	C40 H37 N8 O10	(2M+H)+

Predicted Isotope Match Table

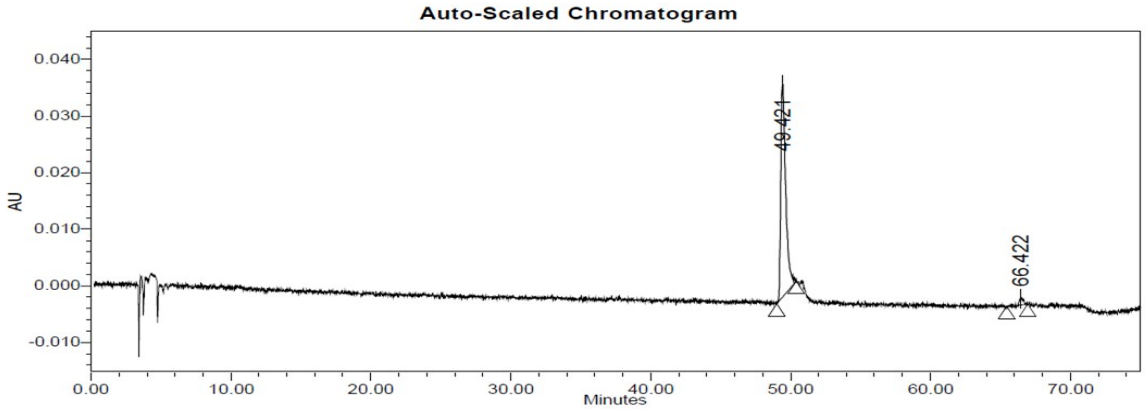
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	395.1353	395.135	-0.68	100	100	77.79	78.37
2	396.138	396.138	0.07	24.35	23.5	18.94	18.42
3	397.1403	397.1405	0.51	3.7	3.67	2.88	2.88
4	398.143	398.143	-0.08	0.5	0.43	0.39	0.34

^{1}H and ^{13}C NMR of 11:





HPLC AND HRESIMS of 12



	RT	Area (μV*sec)	% Area	Height (μV)
1	49.421	899113	96.70	37602
2	66.422	30662	3.30	1072

Qualitative Compound Report

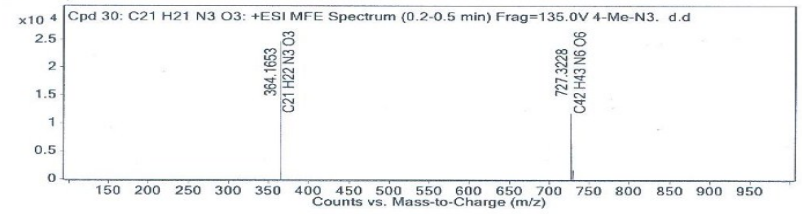
Data File	4-Me-N3. d.d	**Sample Name**	4-Me-N3
Sample Type	Sample	**Position**	Vial 29
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 4:42:18
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			
Sample Group		**Info.**	
Acquisition 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 30: C21 H21 N3 O3	0.3	363.1582	C21 H21 N3 O3	C21 H21 N3 O3	0.29	C21 H21 N3 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 30: C21 H21 N3 O3	364.1653	0.3	Find by Molecular Feature	363.1582

MFE MS Spectrum



MS Spectrum Peak List

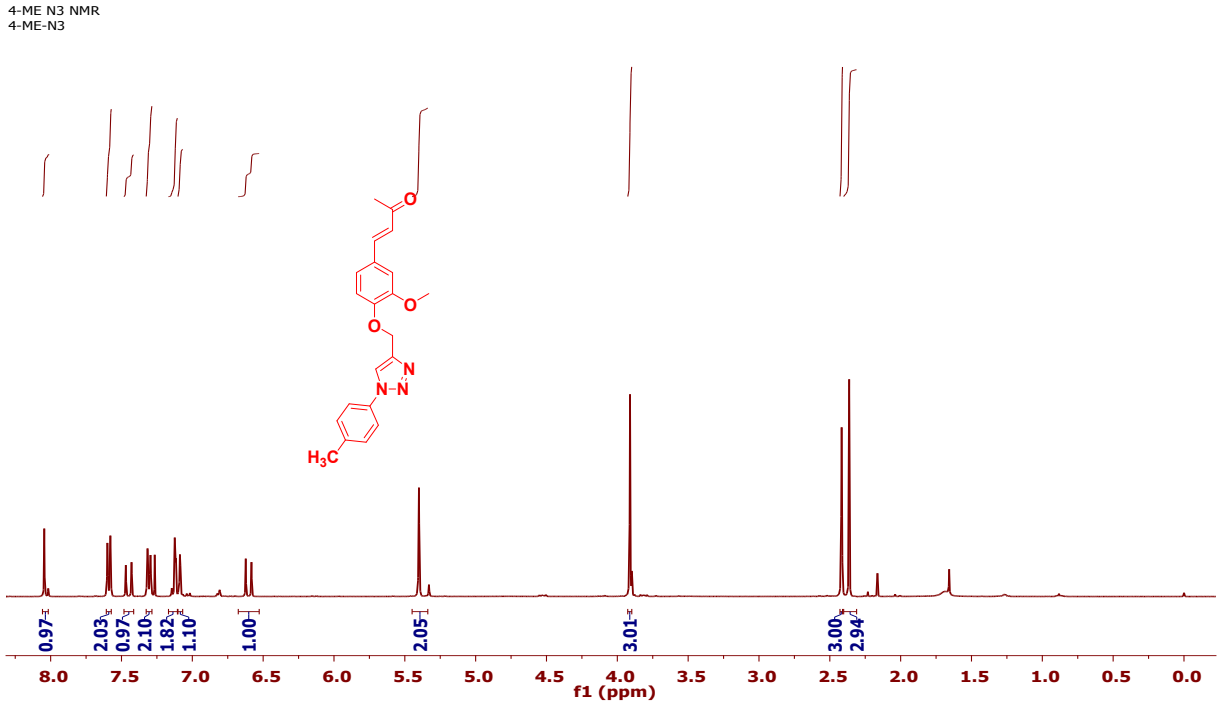
m/z	z	Abund	Formula	Ion
364.1653	1	24685.71	C21 H22 N3 O3	(M+H)+
365.1684	1	4761.32	C21 H22 N3 O3	(M+H)+
727.3228	1	11785.11	C42 H43 N6 O6	(2M+H)+
728.3263	1	6549.75	C42 H43 N6 O6	(2M+H)+
729.3291	1	1627.17	C42 H43 N6 O6	(2M+H)+

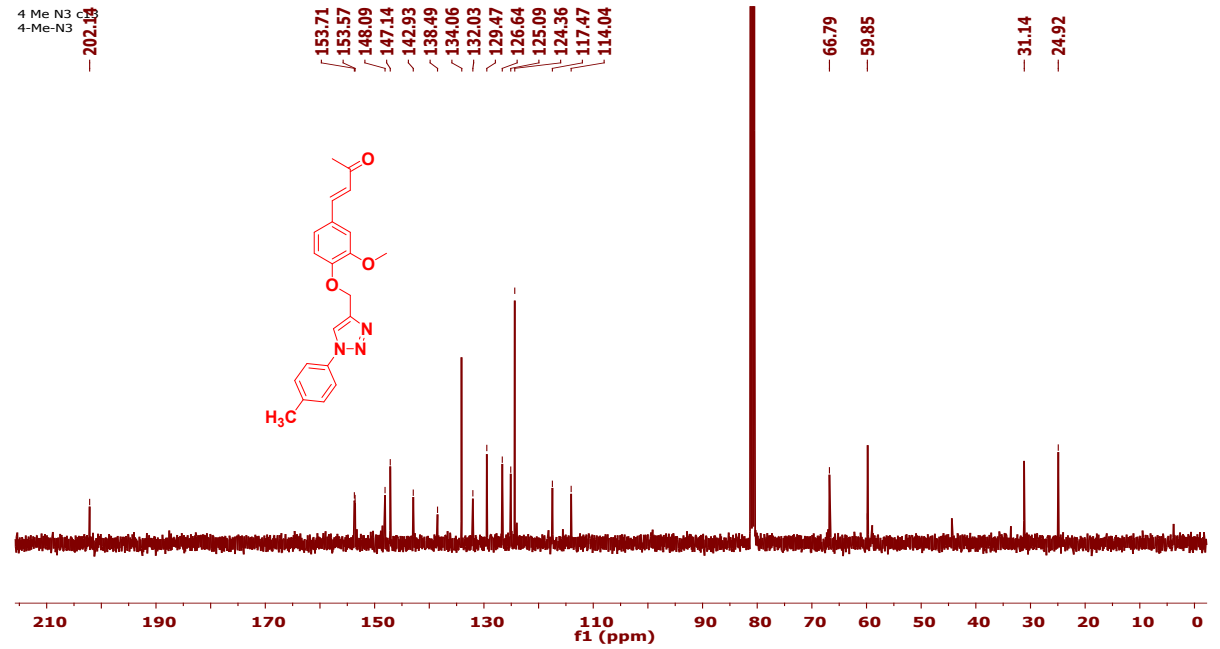
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	364.1653	364.1656	0.7	100	100	80.15	78.38
2	365.1684	365.1687	0.86	19.29	24.18	15.46	18.95
3	366.1748	366.1714	-9.24	5.47	3.41	4.39	2.68

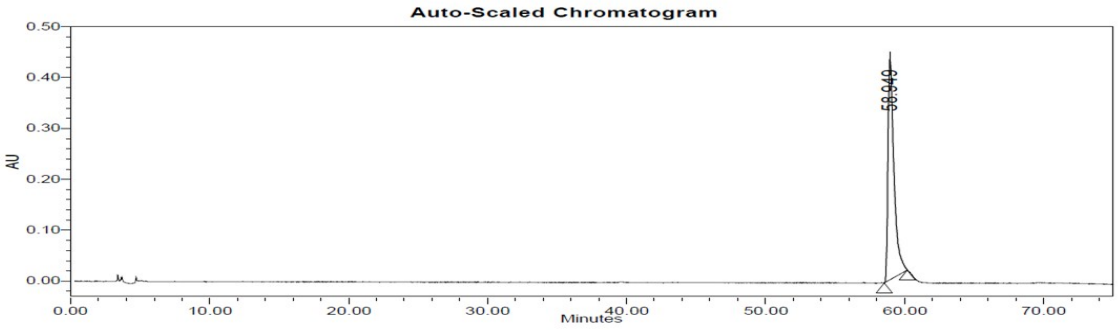
End Of Report

^{1}H and ^{13}C NMR of 12:





HPLC AND HRESIMS of 13



	RT	Area (µV*sec)	% Area	Height (µV)
1	58.949	13004162	100.00	433743

Qualitative Compound Report

Data File	DiCF3.d	**Sample Name**	DiCF3
Sample Type	Sample	**Position**	Vial 22
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 2:27:05
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

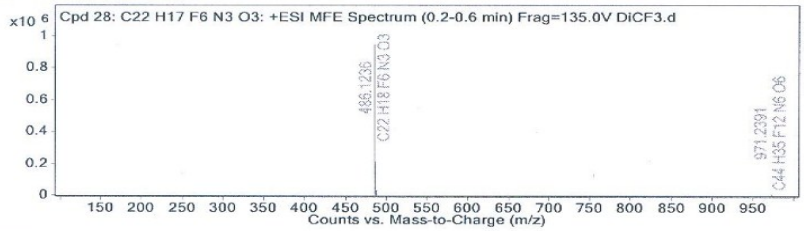
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 28: C22 H17 F6 N3 O3	0.3	485.1164	C22 H17 F6 N3 O3	C22 H17 F6 N3 O3	2.06	C22 H17 F6 N3 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 28: C22 H17 F6 N3 O3	486.1236	0.3	Find by Molecular Feature	485.1164

MFE MS Spectrum



MS Spectrum Peak List

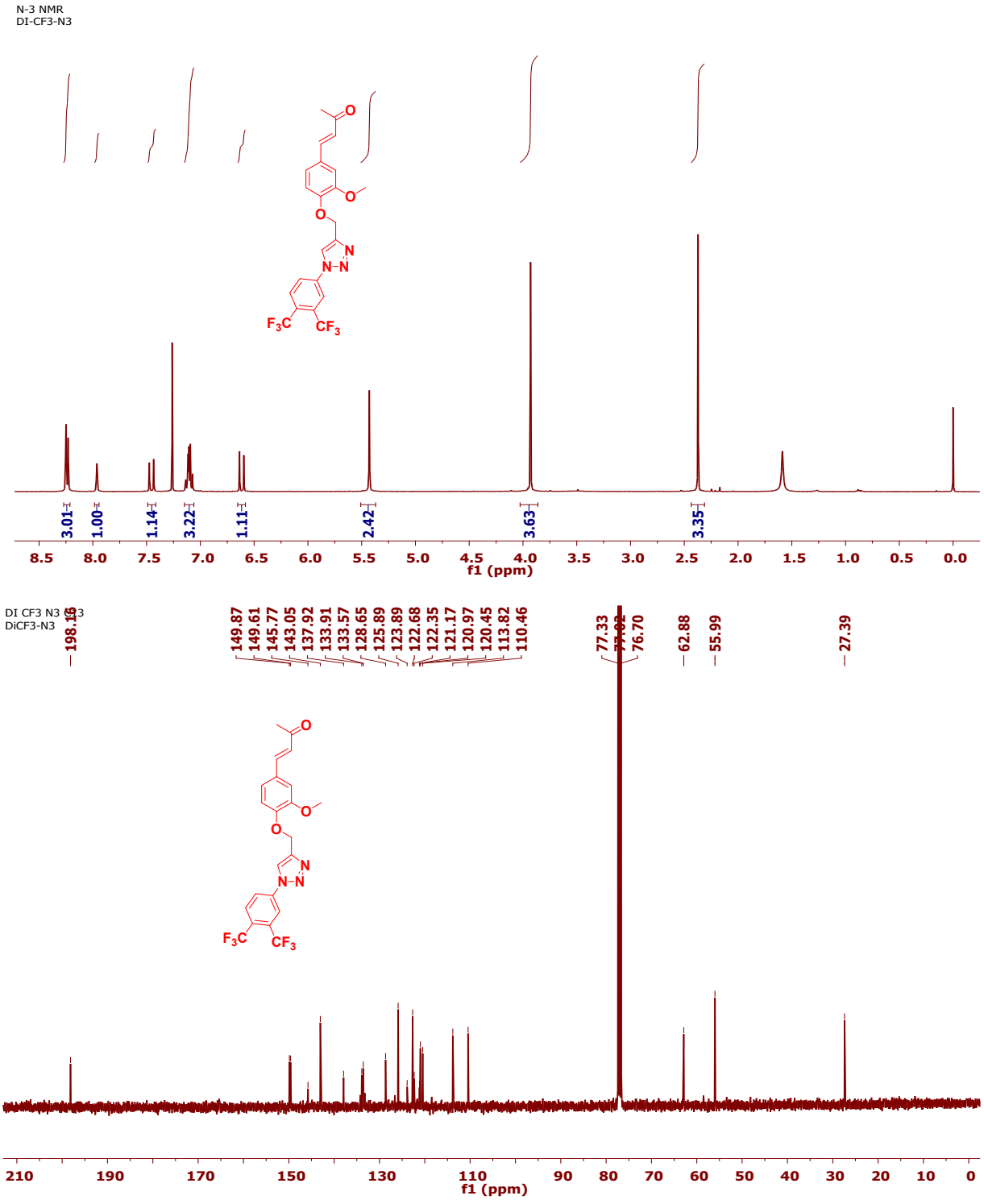
m/z	z	Abund	Formula	Ion
486.1236	1	946160.19	C22 H18 F6 N3 O3	(M+H)+
487.127	1	214418.77	C22 H18 F6 N3 O3	(M+H)+
488.1298	1	32304.5	C22 H18 F6 N3 O3	(M+H)+
971.2391	1	9787.14	C44 H35 F12 N6 O6	(2M+H)+
972.2433	1	5623.22	C44 H35 F12 N6 O6	(2M+H)+

Predicted Isotope Match Table

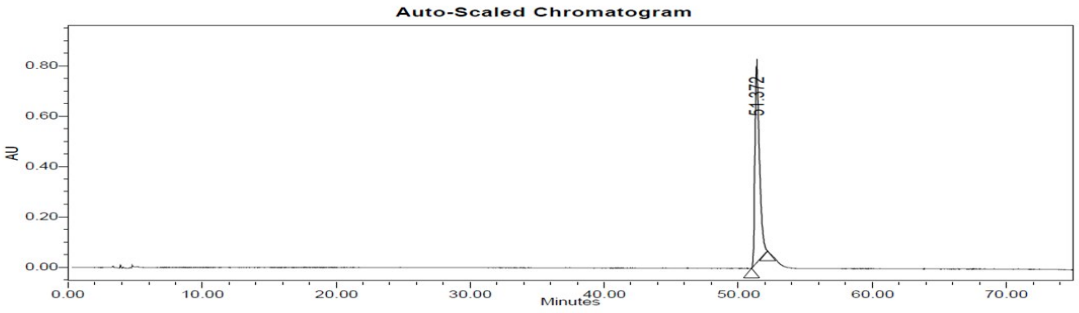
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	486.1236	486.1247	2.18	100	100	79.05	77.34
2	487.127	487.1278	1.58	22.66	25.21	17.91	19.5
3	488.1298	488.1306	1.61	3.41	3.66	2.7	2.83
4	489.1318	489.1332	2.79	0.36	0.39	0.29	0.3
5	490.1355	490.1358	0.54	0.06	0.03	0.05	0.03
6	491.1367	491.1384	3.36	0.01	0	0.01	0

--- End Of Report ---

^{1}H and ^{13}C NMR of 13:



HPLC AND HRESIMS of 14



	RT	Area (µV*sec)	% Area	Height (µV)
1	51.372	18650988	100.00	781377

Qualitative Compound Report

Data File	Et-4-N3.d	**Sample Name**	Et-4-N3
Sample Type	Sample	**Position**	Vial 21
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 2:21:24
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

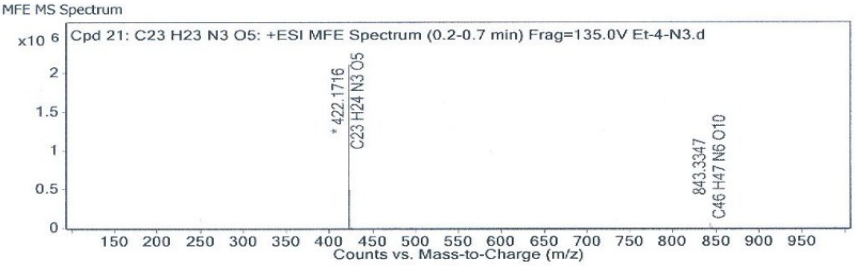
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 21: C23 H23 N3 O5	0.3	421.1645	C23 H23 N3 O5	C23 H23 N3 O5	-1.64	C23 H23 N3 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 21: C23 H23 N3 O5	422.1716	0.3	Find by Molecular Feature	421.1645

MFE MS Spectrum



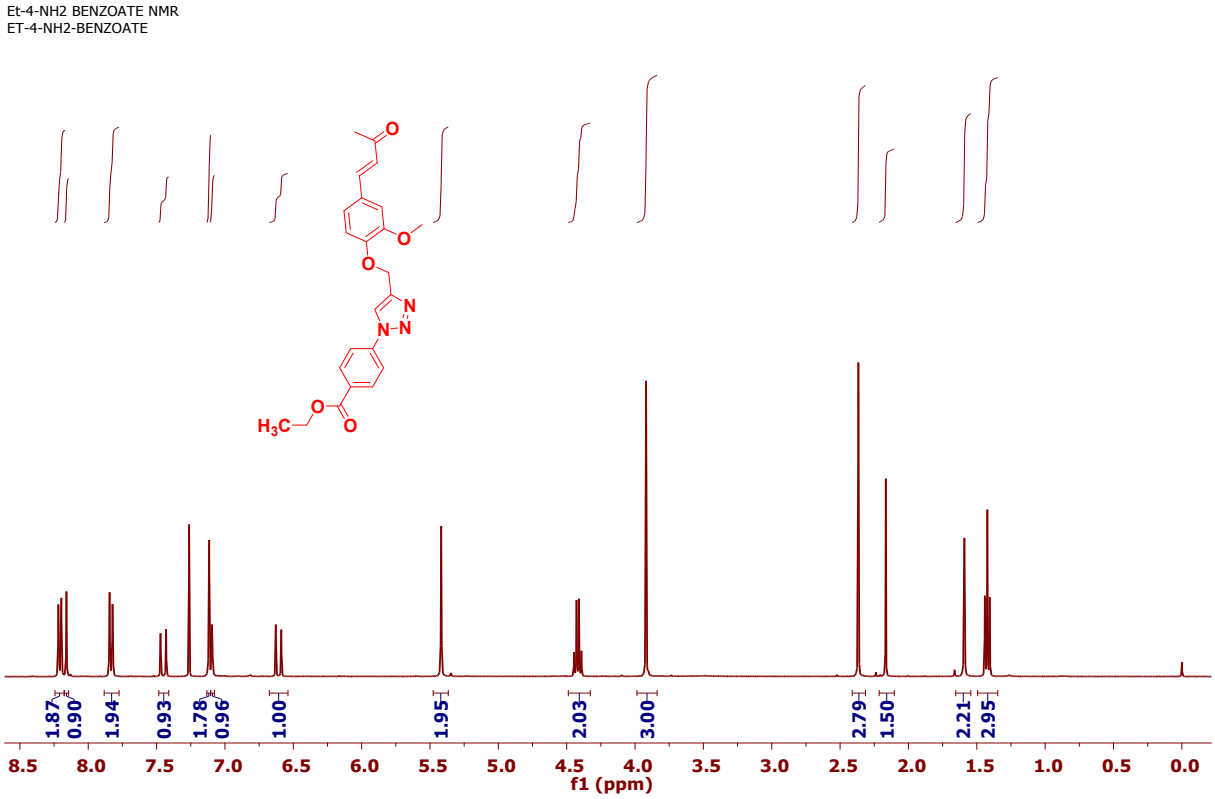
MS Spectrum Peak List

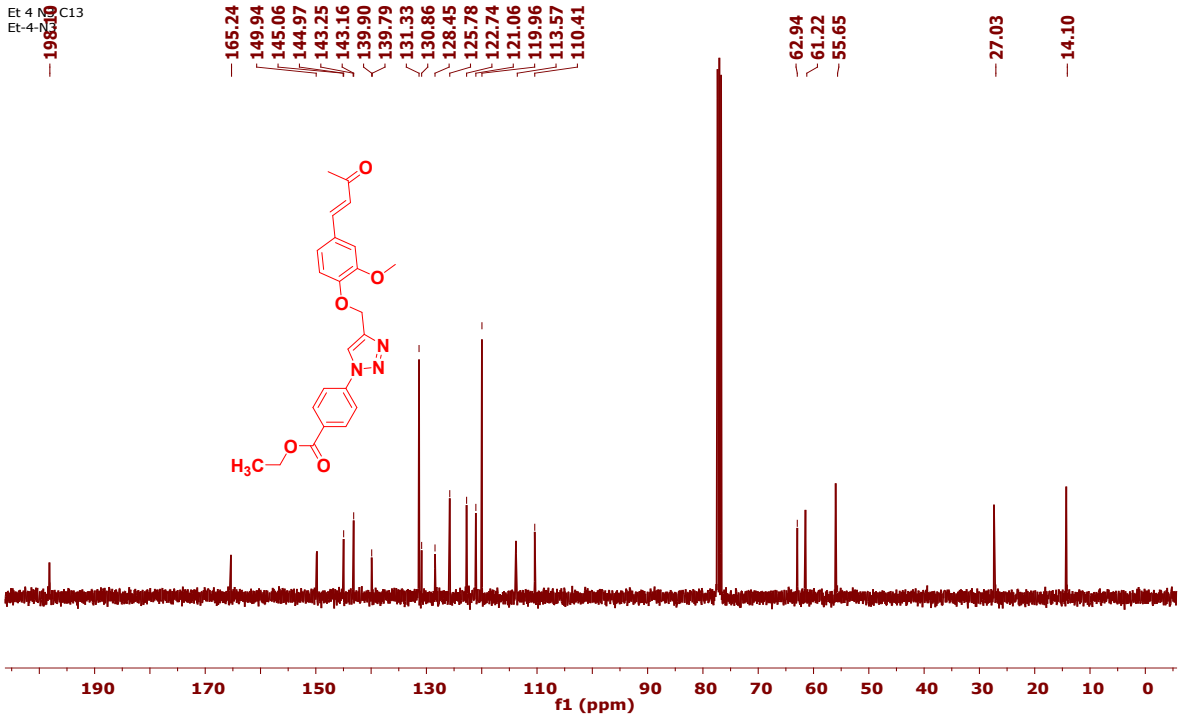
m/z	z	Abund	Formula	Ion
422.1716	1	2107891	C23 H24 N3 O5	(M+H)+
423.1754	1	492218.19	C23 H24 N3 O5	(M+H)+
424.1775	1	77694.05	C23 H24 N3 O5	(M+H)+
843.3347	1	58736.14	C46 H47 N6 O10	(2M+H)+
844.3382	1	31014.43	C46 H47 N6 O10	(2M+H)+

Predicted Isotope Match Table

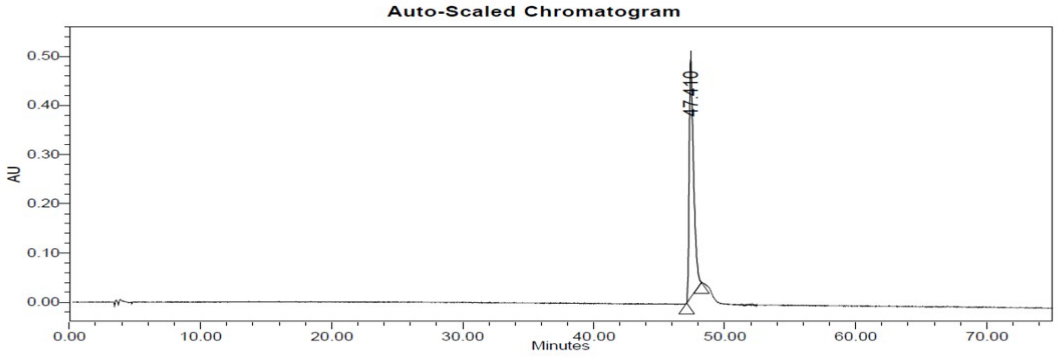
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	422.1716	422.171	-1.32	100	100	78.42	76.09
2	423.1754	423.1742	-2.96	23.35	26.44	18.31	20.12
3	424.1775	424.1768	-1.67	3.69	4.39	2.89	3.34
4	425.1804	425.1794	-2.21	0.43	0.54	0.34	0.41
5	426.1827	426.182	-1.78	0.05	0.05	0.04	0.04

^{1}H and ^{13}C NMR of 14:





HPLC AND HRESIMS of 15



	RT	Area (µV*sec)	% Area	Height (µV)
1	47.410	11173027	100.00	485713

Qualitative Compound Report

Data File	2-CL-N3.d	**Sample Name**	2-CL-N3
Sample Type	Sample	**Position**	Vial 18
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 2:05:24
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

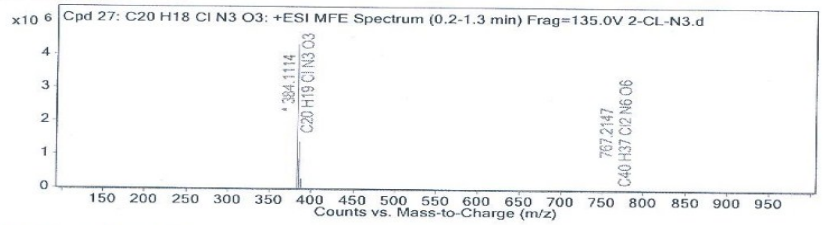
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 27: C20 H18 Cl N3 O3	0.3	383.1041	C20 H18 Cl N3 O3	C20 H18 Cl N3 O3	-1.07	C20 H18 Cl N3 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 27: C20 H18 Cl N3 O3	384.1114	0.3	Find by Molecular Feature	383.1041

MFE MS Spectrum



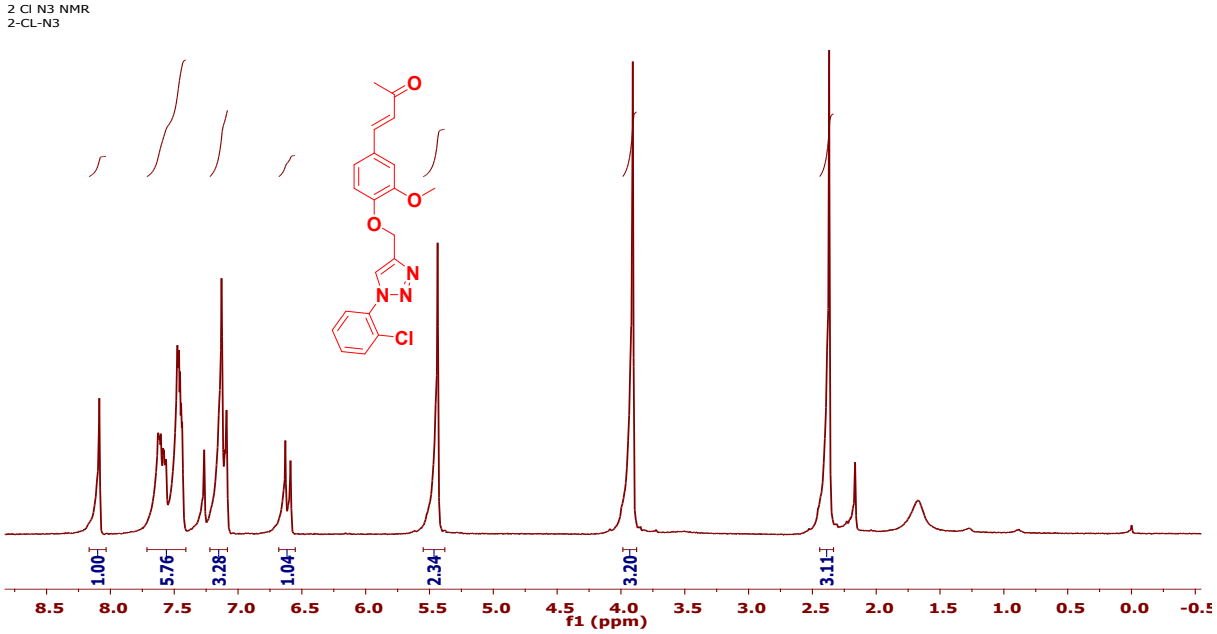
MS Spectrum Peak List

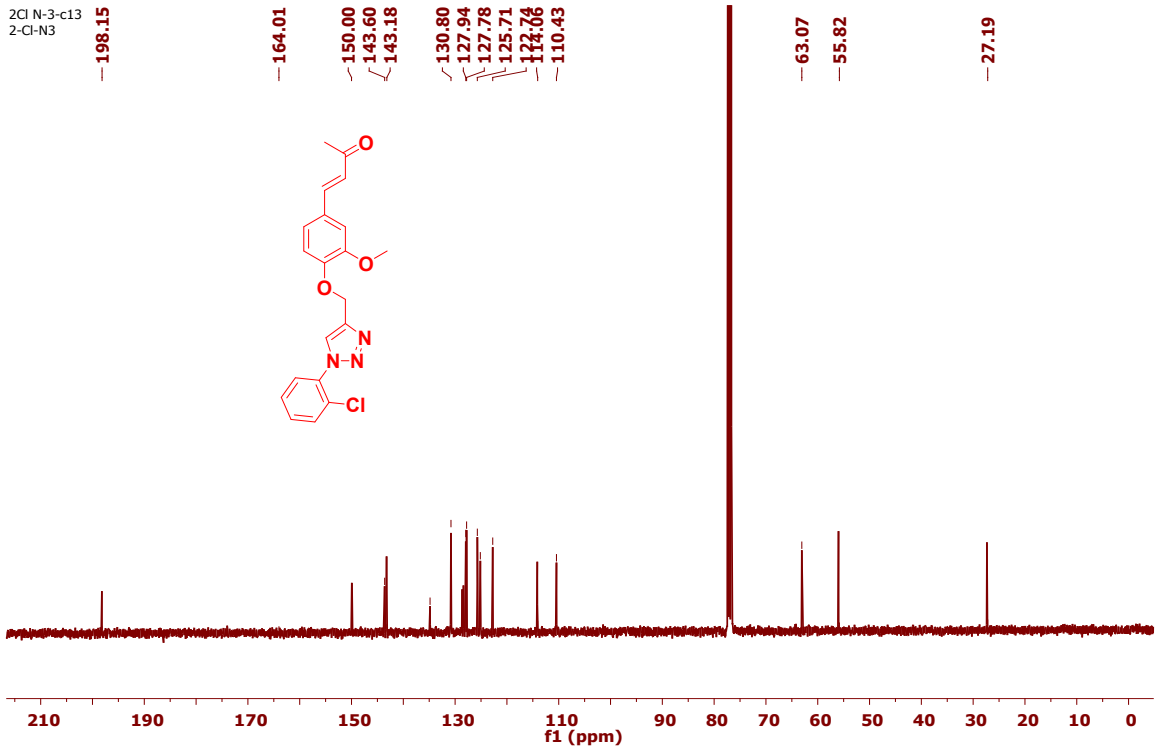
m/z	z	Abund	Formula	Ion
384.1114	1	4310781.5	C20 H19 Cl N3 O3	(M+H)+
385.1145	1	876818.56	C20 H19 Cl N3 O3	(M+H)+
386.109	1	1399216.13	C20 H19 Cl N3 O3	(M+H)+
387.1121	1	286429.41	C20 H19 Cl N3 O3	(M+H)+
388.1145	1	34656.31	C20 H19 Cl N3 O3	(M+H)+

Predicted Isotope Match Table

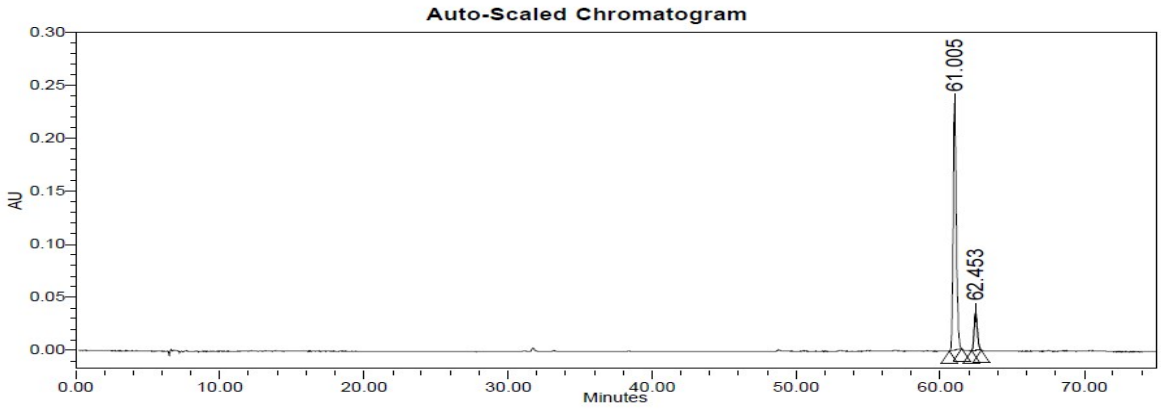
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	384.1114	384.1109	-1.18	100	100	62.37	59.86
2	385.1145	385.114	-1.22	20.34	23.06	12.69	13.8
3	386.109	386.1088	-0.46	32.46	35.15	20.24	21.04
4	387.1121	387.1114	-1.78	6.64	7.7	4.14	4.61
5	388.1145	388.114	-1.46	0.8	1.04	0.5	0.62
6	389.1165	389.1165	-0.06	0.08	0.1	0.05	0.06
7	390.1158	390.119	8.39	0.02	0.01	0.01	0

^{1}H and ^{13}C NMR of 15:





HPLC AND HRESIMS of 16



	RT	Area (μV*sec)	% Area	Height (μV)
1	61.005	3533336	86.64	233206
2	62.453	544676	13.36	35509

Qualitative Compound Report

Data File	BiPhenyl.d	**Sample Name**	BiPhenyl
Sample Type	Sample	**Position**	Vial 32
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 3:19:08
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

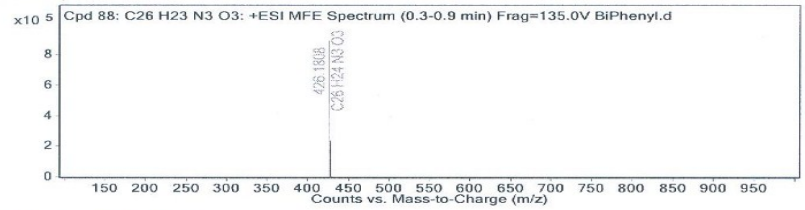
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 88: C26 H23 N3 O3	0.4	425.1736	C26 H23 N3 O3	C26 H23 N3 O3	0.72	C26 H23 N3 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 88: C26 H23 N3 O3	426.1808	0.4	Find by Molecular Feature	425.1736

MFE MS Spectrum



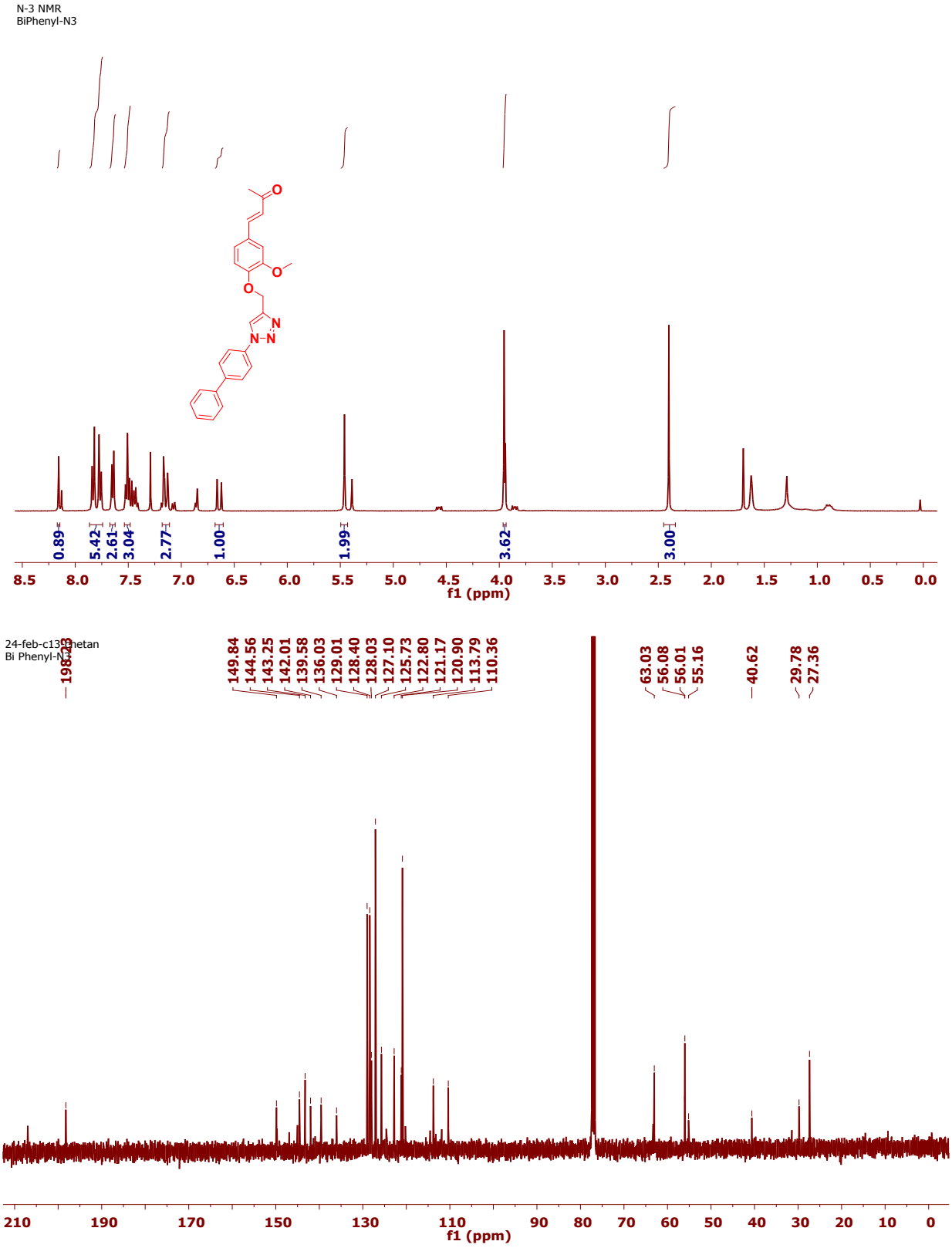
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
426.1808	1	891663.13	C26 H24 N3 O3	(M+H)+
427.1843	1	236538.78	C26 H24 N3 O3	(M+H)+
428.1876	1	30722	C26 H24 N3 O3	(M+H)+
429.1901	1	3786.38	C26 H24 N3 O3	(M+H)+

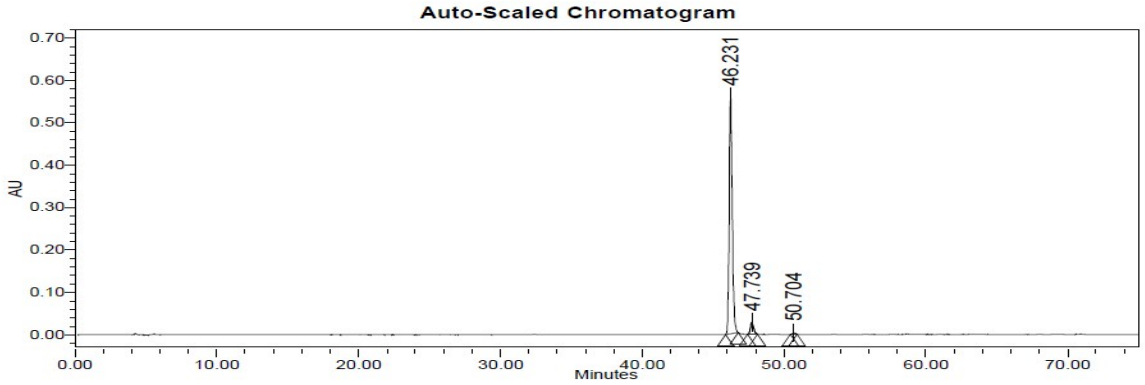
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	426.1808	426.1812	0.91	100	100	76.69	74.06
2	427.1843	427.1844	0.25	26.53	29.61	20.34	21.93
3	428.1876	428.1873	-0.92	3.45	4.85	2.64	3.59
4	429.1901	429.19	-0.35	0.42	0.57	0.33	0.42

^{1}H and ^{13}C NMR of 16



HPLC AND HRESIMS of 17



	RT	Area (μV*sec)	% Area	Height (μV)
1	46.231	8483846	94.64	559419
2	47.739	435132	4.85	27874
3	50.704	45153	0.50	3156

Qualitative Compound Report

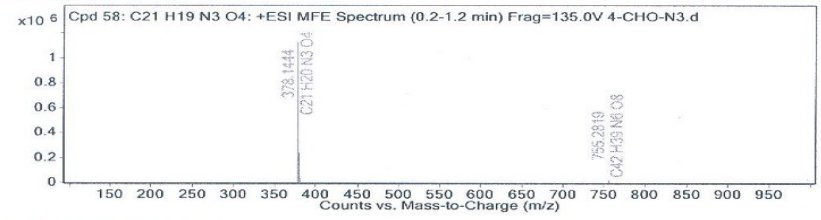
Data File	4-CHO-N3.d	**Sample Name**	4-CHO-N3
Sample Type	Sample	**Position**	Vial 33
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 3:23:29
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			
Sample Group		**Info.**	
Acquisition 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 58: C21 H19 N3 O4	0.3	377.1373	C21 H19 N3 O4	C21 H19 N3 O4	0.65	C21 H19 N3 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 58: C21 H19 N3 O4	378.1444	0.3	Find by Molecular Feature	377.1373

MFE MS Spectrum



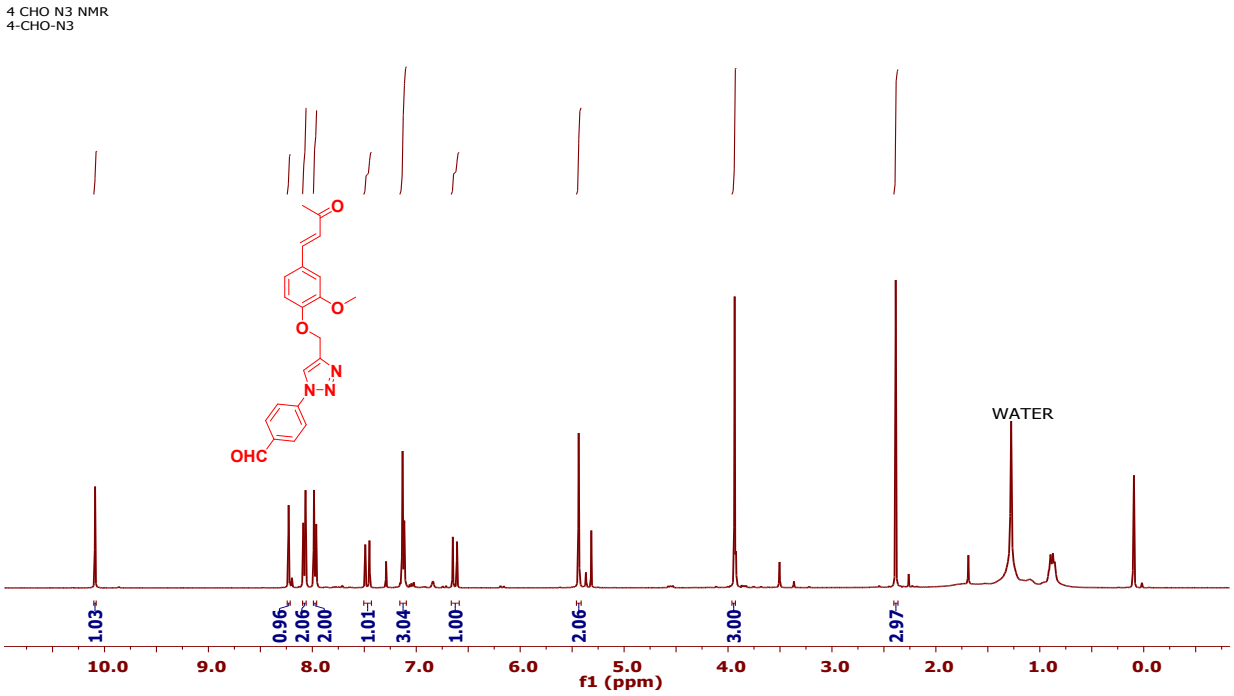
MS Spectrum Peak List

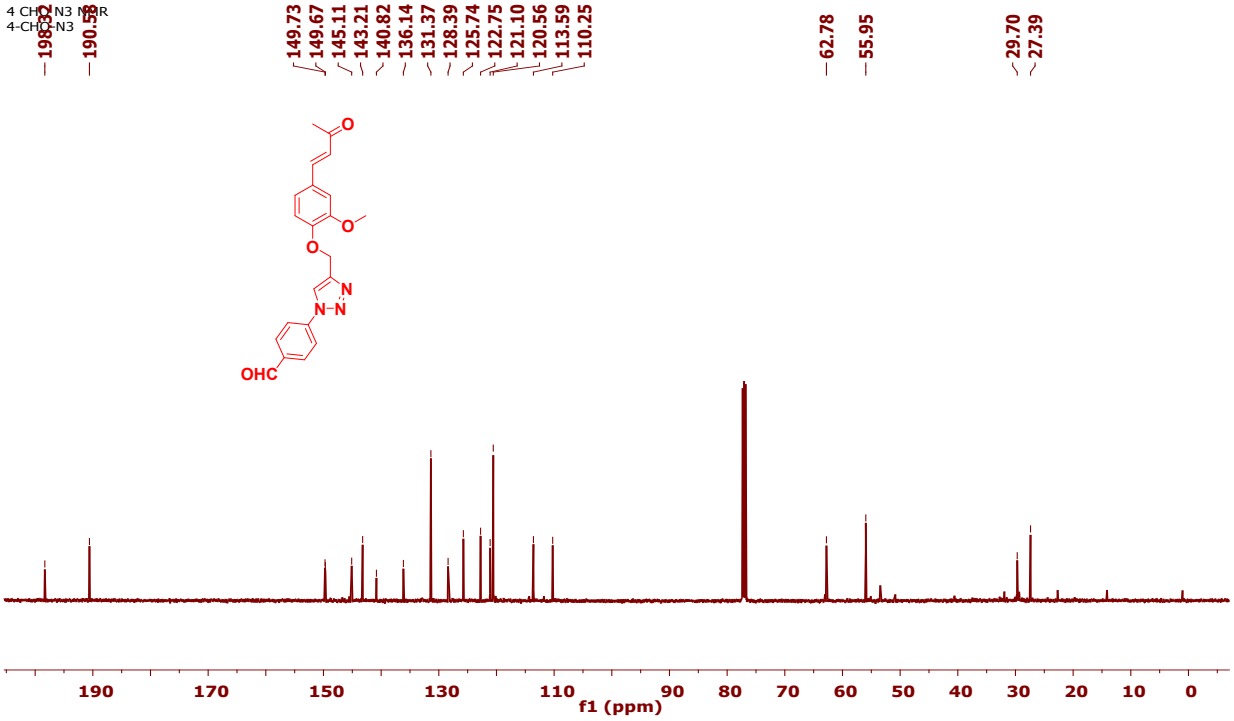
m/z	z	Abund	Formula	Ion
378.1444	1	1125335.38	C21 H20 N3 O4	(M+H)+
379.1481	1	244306.41	C21 H20 N3 O4	(M+H)+
380.1522	1	39587.66	C21 H20 N3 O4	(M+H)+
755.2819	1	16195.12	C42 H39 N6 O8	(2M+H)+
756.2848	1	7187.93	C42 H39 N6 O8	(2M+H)+

Predicted Isotope Match Table

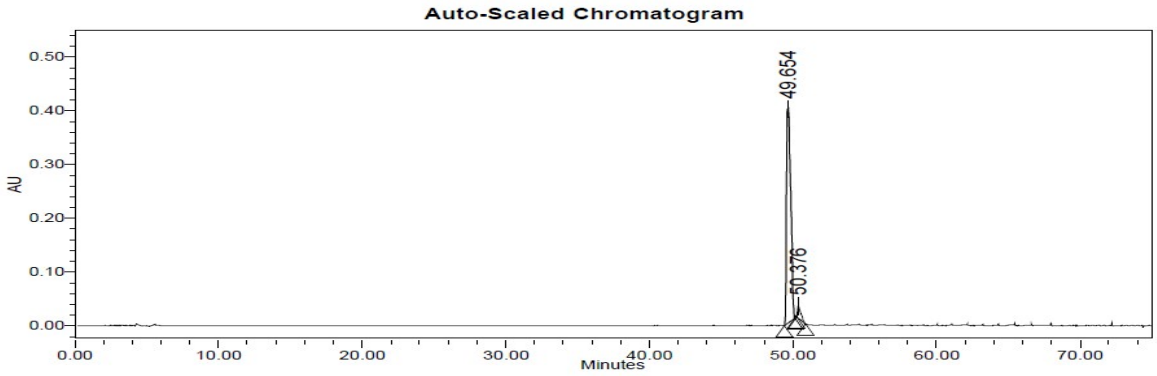
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	378.1444	378.1448	1.08	100	100	79.57	77.99
2	379.1481	379.1479	-0.33	21.71	24.19	17.27	18.87
3	380.1522	380.1506	-4.22	3.52	3.62	2.8	2.83
4	381.1568	381.1532	-9.52	0.46	0.41	0.36	0.32

^{1}H and C^{13}NMR of 17:





HPLC AND HRESIMS of 18



	RT	Area (μV*sec)	% Area	Height (μV)
1	49.654	8370568	95.70	400375
2	50.376	376084	4.30	22312

Qualitative Compound Report

Data File	Aniline.d	**Sample Name**	Aniline
Sample Type	Sample	**Position**	Vial 35
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 3:35:06
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

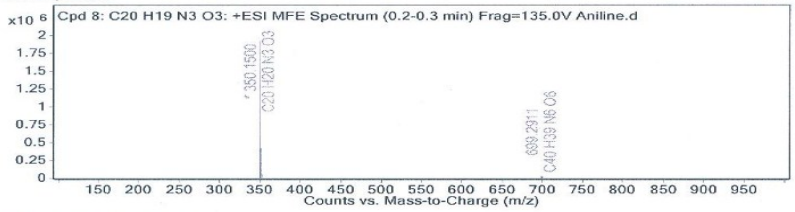
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C20 H19 N3 O3	0.3	349.1426	C20 H19 N3 O3	C20 H19 N3 O3	0.1	C20 H19 N3 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C20 H19 N3 O3	350.15	0.3	Find by Molecular Feature	349.1426

MFE MS Spectrum



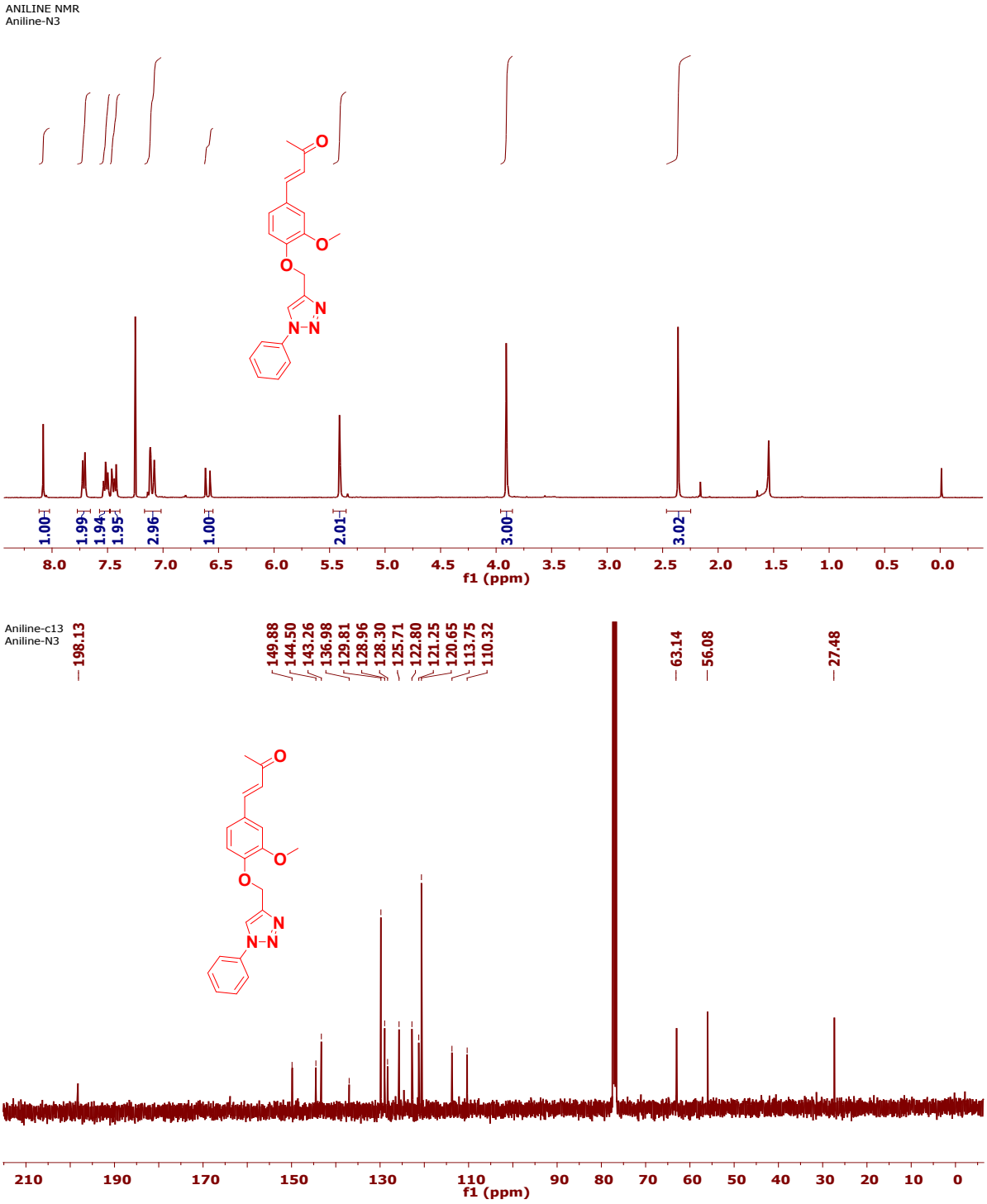
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
350.15	1	1924937.5	C20 H20 N3 O3	(M+H)+
351.1526	1	420266.5	C20 H20 N3 O3	(M+H)+
352.1554	1	63142.94	C20 H20 N3 O3	(M+H)+
699.2911	1	37086.18	C40 H39 N6 O6	(2M+H)+
700.2941	1	17492.96	C40 H39 N6 O6	(2M+H)+

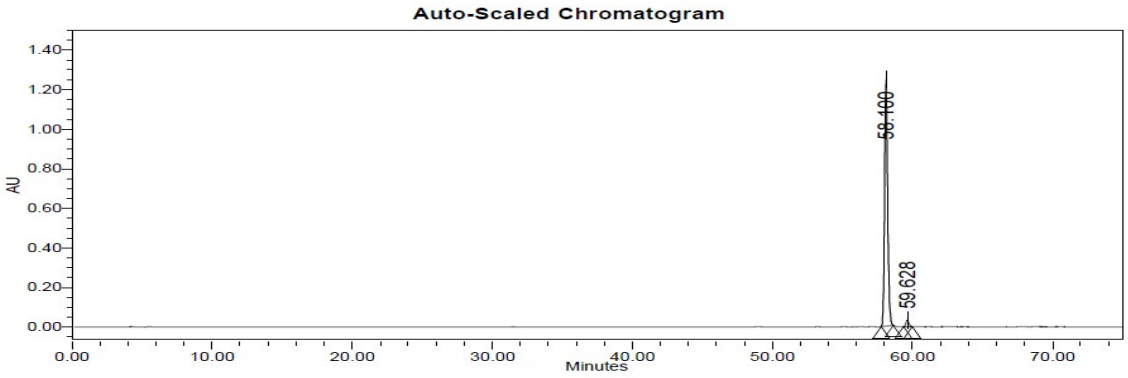
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	350.15	350.1499	-0.14	100	100	79.73	79.02
2	351.1526	351.153	1.03	21.83	23.07	17.41	18.23
3	352.1554	352.1557	0.93	3.28	3.16	2.62	2.5
4	353.1576	353.1583	1.93	0.31	0.32	0.24	0.25

^{1}H and ^{13}C NMR of 18:



HPLC AND HRESIMS of 19



	RT	Area (µV*sec)	% Area	Height (µV)
1	58.100	19175550	97.53	1247757
2	59.628	486537	2.47	32357

Qualitative Compound Report

Data File	3-Br-5F-N3.d	**Sample Name**	3-Br-5F-N3
Sample Type	Sample	**Position**	Vial 36
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	02-03-2017 PM 3:36:27
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

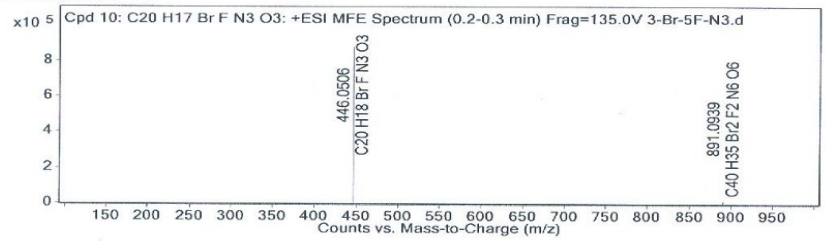
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 10: C20 H17 Br F N3 O3	0.3	445.0433	C20 H17 Br F N3 O3	C20 H17 Br F N3 O3	0.92	C20 H17 Br F N3 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 10: C20 H17 Br F N3 O3	446.0506	0.3	Find by Molecular Feature	445.0433

MFE MS Spectrum



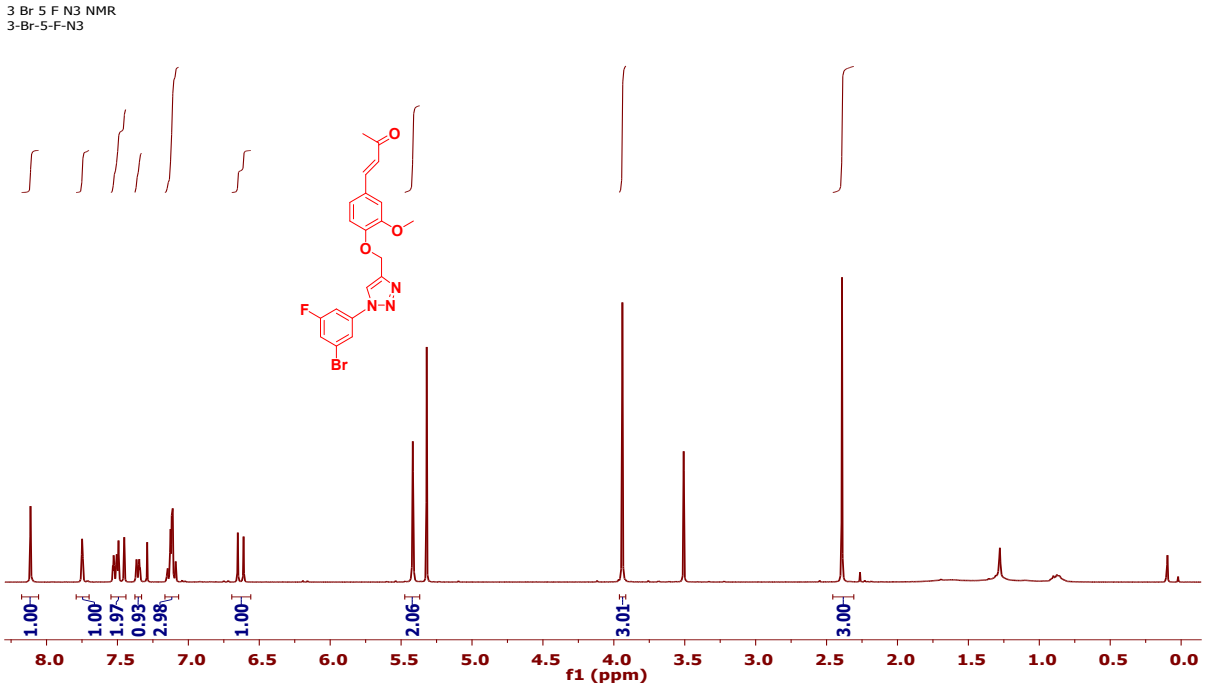
MS Spectrum Peak List

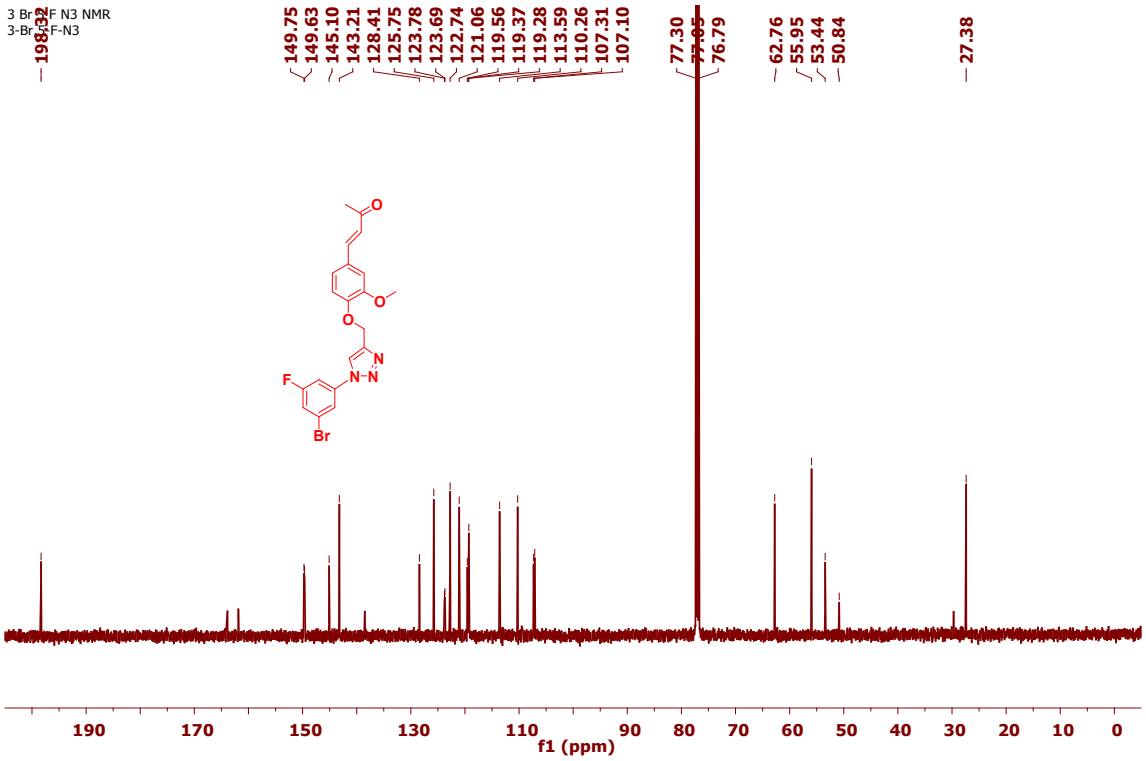
m/z	z	Abund	Formula	Ion
446.0506	1	878484.63	C20 H18 Br F N3 O3	(M+H)+
891.0939	1	16904.63	C40 H35 Br2 F2 N6 O6	(2M+H)+

Predicted Isotope Match Table

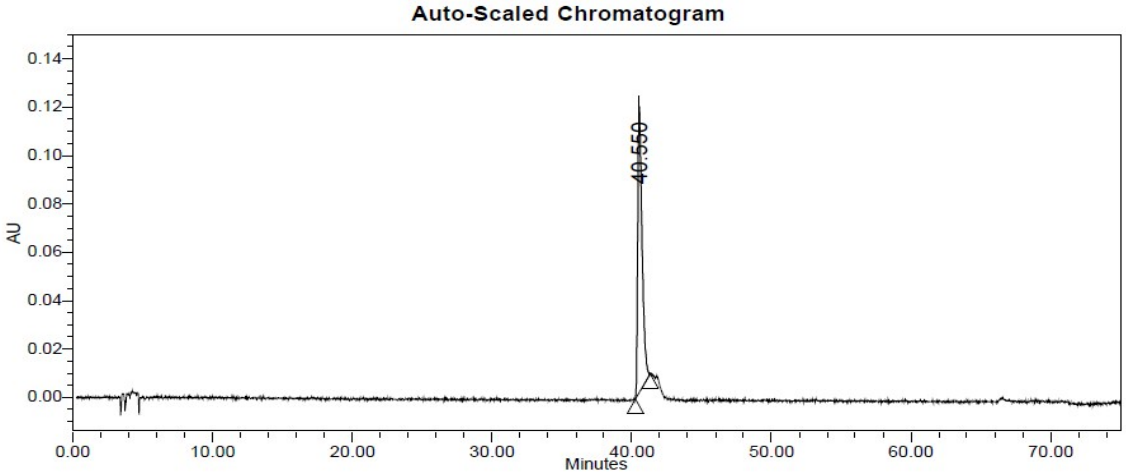
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	446.0506	446.051	0.91	100	100	100	100

^{1}H and ^{13}C NMR of 19:





HPLC AND HRESIMS OF and 20:



	RT	Area (µV*sec)	% Area	Height (µV)
1	40.550	2514012	100.00	118268

Qualitative Compound Report

Data File	2-NH2OH.d	**Sample Name**	2-NH2OH
Sample Type	Sample	**Position**	Vial 3
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	09-03-2017 PM 12:51:13
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

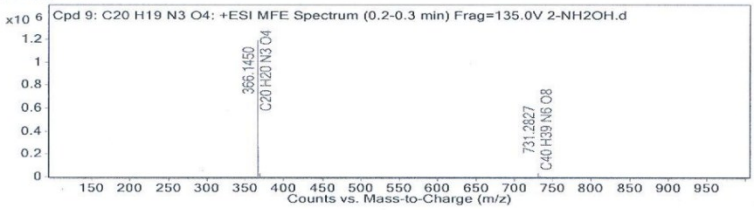
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C20 H19 N3 O4	0.3	365.1378	C20 H19 N3 O4	C20 H19 N3 O4	-0.76	C20 H19 N3 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 9: C20 H19 N3 O4	366.145	0.3	Find by Molecular Feature	365.1378

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
366.145	1	1192157	C20 H20 N3 O4	(M+H)+
367.1487	1	260299.53	C20 H20 N3 O4	(M+H)+
368.1509	1	34069.24	C20 H20 N3 O4	(M+H)+
731.2827	1	31077.24	C40 H39 N6 O8	(2M+H)+
732.2861	1	16645.95	C40 H39 N6 O8	(2M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	366.145	366.1448	-0.44	100	100	80.2	79.06
2	367.1487	367.1479	-2.17	21.83	23.11	17.51	18.27
3	368.1509	368.1505	-1.09	2.86	3.37	2.29	2.67

^{1}H and C^{13} NMR of 20: