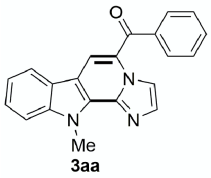
Qualitative Compound Report

Data File	VNS-137.d	**Sample Name**	VNS-137
Sample Type	Sample	**Position**	P1-F6
Instrument Name	Instrument 1	**User Name**	
Acq Method	isocratic.m	**Acquired Time**	5/6/2017 9:18:36 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



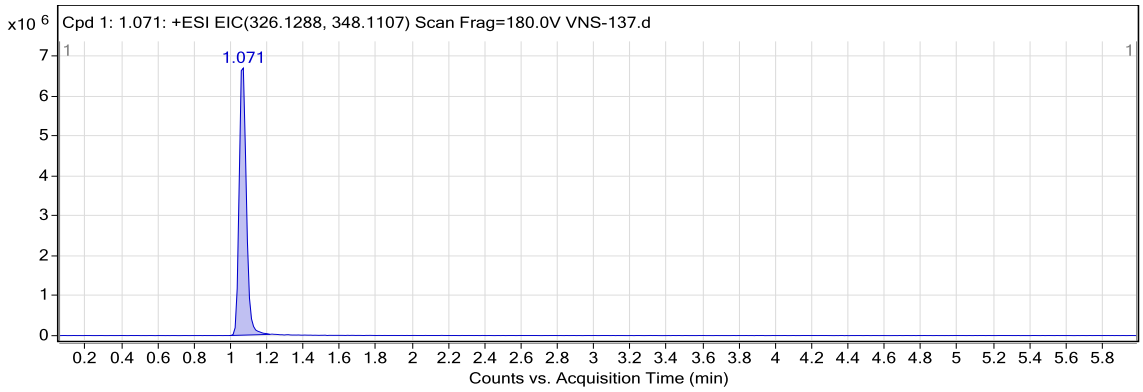
3aa

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

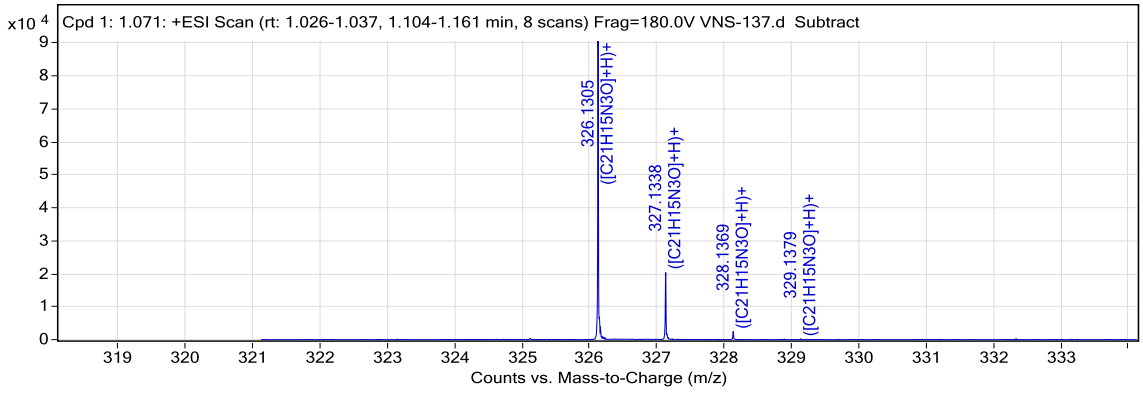
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 1.071	1.071	325.1233	93207	C21 H15 N3 O	325.1215	5.46

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 1.071	326.1305	1.071	Find By Formula	325.1233



MS Zoomed Spectrum



MS Spectrum Peak List

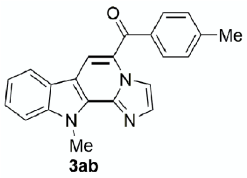
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
326.1305	326.1288	-5.3	1	93207.3	C21H15N3O	(M+H)+
327.1338	327.1319	-6.01	1	20552.85	C21H15N3O	(M+H)+

328.1369	328.1348	-6.47	1	2525.31	C21H15N3O	(M+H)+
329.1379	329.1376	-0.75	1	256.97	C21H15N3O	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-284.d	**Sample Name**	VNS-284
Sample Type	Sample	**Position**	P1-E3
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	11/3/2017 6:23:55 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



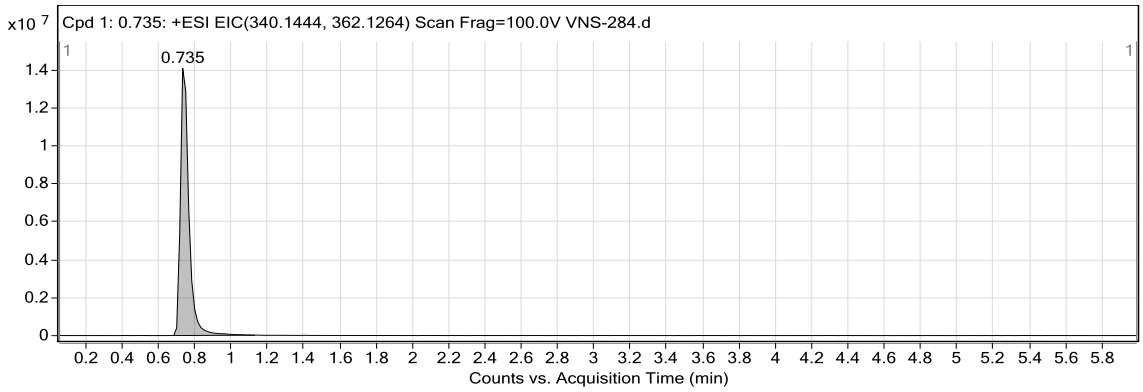
3ab

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

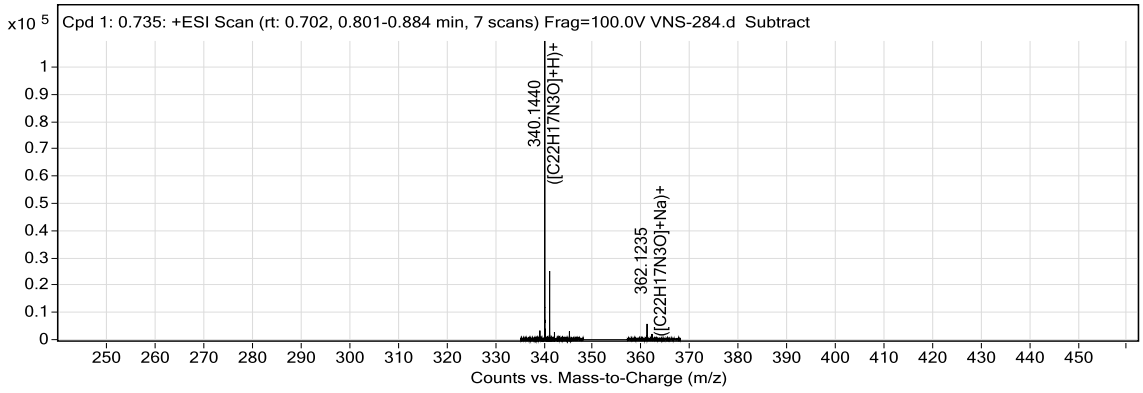
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.735	0.735	339.1366	109581	C22 H17 N3 O	339.1372	-1.52

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.735	340.144	0.735	Find By Formula	339.1366



MS Zoomed Spectrum



MS Spectrum Peak List

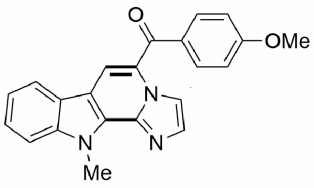
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
340.144	340.1444	1.35	1	109580.52	C22H17N3O	(M+H)+
341.147	341.1475	1.6	1	26168.45	C22H17N3O	(M+H)+

342.1485	342.1505	5.87	1	2782.65	C22H17N3O	(M+H)+
343.1496	343.1534	10.93	1	255.73	C22H17N3O	(M+H)+
362.1235	362.1264	7.96	1	162.39	C22H17N3O	(M+Na)+
363.1288	363.1295	1.95	1	49.84	C22H17N3O	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-286.d	**Sample Name**	VNS-286
Sample Type	Sample	**Position**	P1-E1
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	11/3/2017 5:55:22 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



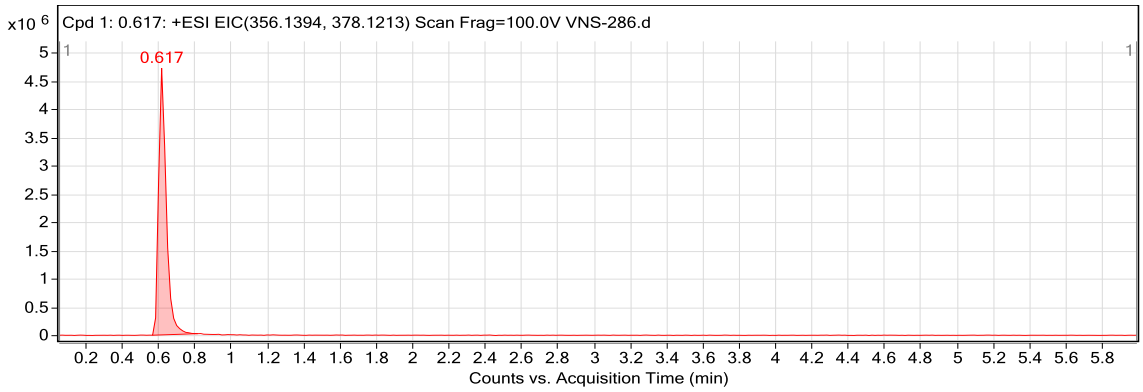
3ac

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

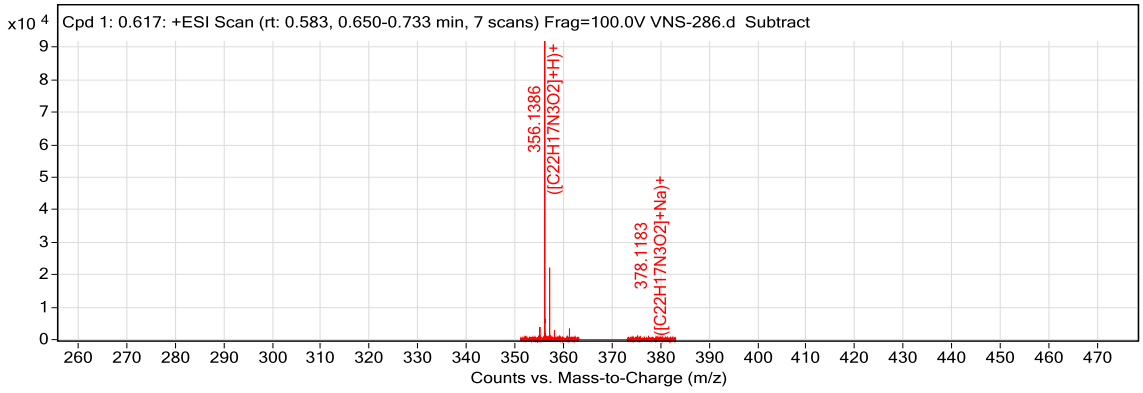
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.617	0.617	355.1313	94081	C22 H17 N3 O2	355.1321	-2.14

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.617	356.1386	0.617	Find By Formula	355.1313



MS Zoomed Spectrum



MS Spectrum Peak List

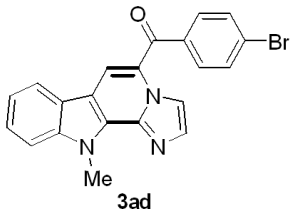
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
356.1386	356.1394	2.13	1	94080.96	C22H17N3O2	(M+H)+
357.1417	357.1425	2.01	1	22150.59	C22H17N3O2	(M+H)+

358.1445	358.1453	2.41	1	2834.64	C22H17N3O2	(M+H)+
378.1183	378.1213	7.8	1	320.97	C22H17N3O2	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-285.d	**Sample Name**	VNS-285
Sample Type	Sample	**Position**	P1-E2
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	11/3/2017 6:09:37 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



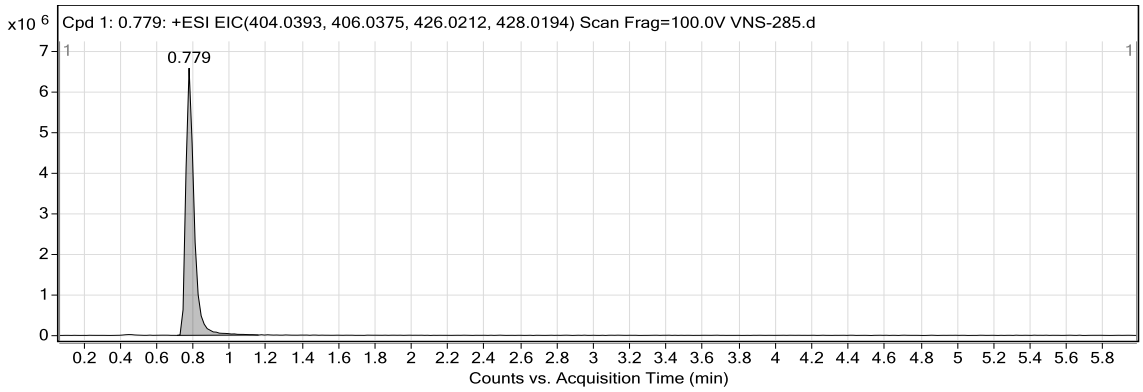
3ad

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

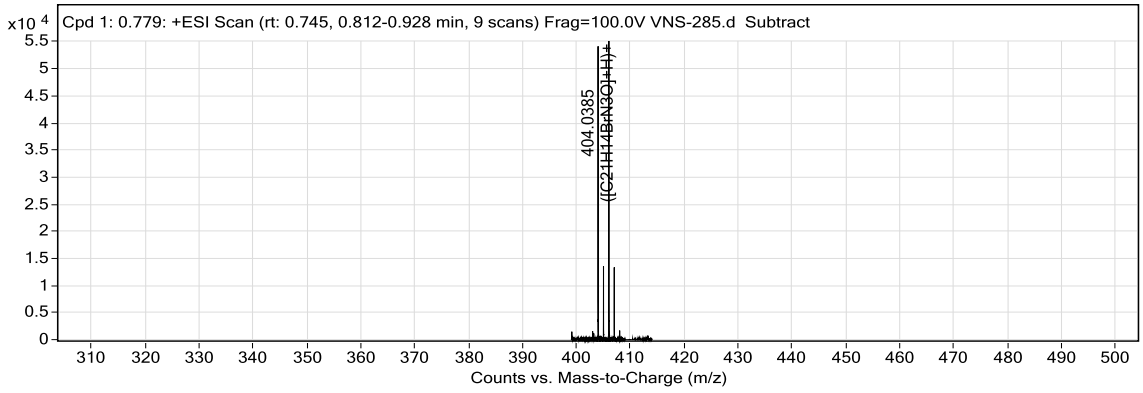
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.779	0.779	403.0311	55979	C21 H14 Br N3 O	403.032	-2.17

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.779	404.0385	0.779	Find By Formula	403.0311



MS Zoomed Spectrum



MS Spectrum Peak List

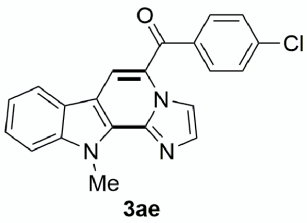
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
404.0385	404.0393	2.02	1	55979.33	C21H14BrN3O	(M+H)+
405.0417	405.0424	1.72	1	13586.75	C21H14BrN3O	(M+H)+

406.0365	406.0375	2.38	1	55145.09	C21H14BrN3O	(M+H)+
407.0396	407.0404	1.93	1	13339.66	C21H14BrN3O	(M+H)+
408.0417	408.0433	4.01	1	1707.46	C21H14BrN3O	(M+H)+
409.0362	409.0461	24.36	1	57.35	C21H14BrN3O	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-283.d	**Sample Name**	VNS-283
Sample Type	Sample	**Position**	P1-E4
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	11/3/2017 6:38:09 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



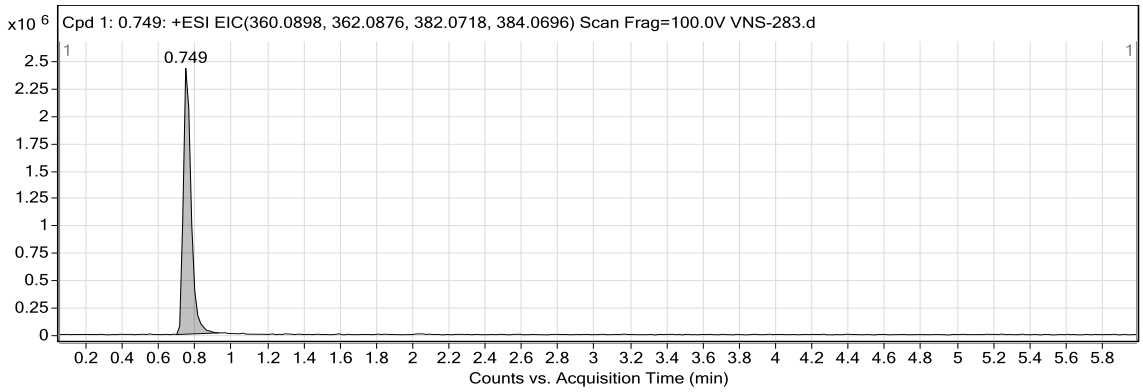
3ae

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

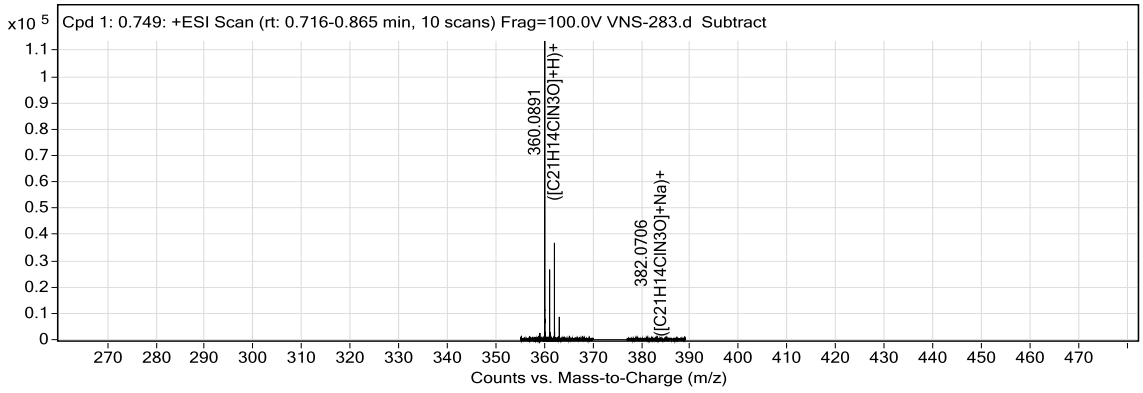
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.749	0.749	359.0818	114003	C21 H14 Cl N3 O	359.0825	-2.16

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.749	360.0891	0.749	Find By Formula	359.0818



MS Zoomed Spectrum



MS Spectrum Peak List

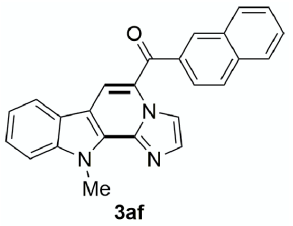
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
360.0891	360.0898	1.87	1	114003.01	C21H14ClN3O	(M+H)+
361.0923	361.0929	1.66	1	27275.65	C21H14ClN3O	(M+H)+

362.0864	362.0876	3.42	1	36830.79	C21H14ClN3O	(M+H)+
363.0895	363.0902	1.99	1	8648.16	C21H14ClN3O	(M+H)+
364.0937	364.093	-1.94	1	856.3	C21H14ClN3O	(M+H)+
365.1025	365.0958	-18.34	1	70.32	C21H14ClN3O	(M+H)+
382.0706	382.0718	3.04	1	164.5	C21H14ClN3O	(M+Na)+
383.06	383.0748	38.86	1	56.62	C21H14ClN3O	(M+Na)+
384.0555	384.0696	36.75	1	31.99	C21H14ClN3O	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-276.d	**Sample Name**	VNS-276
Sample Type	Sample	**Position**	P1-E5
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	11/3/2017 6:52:19 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



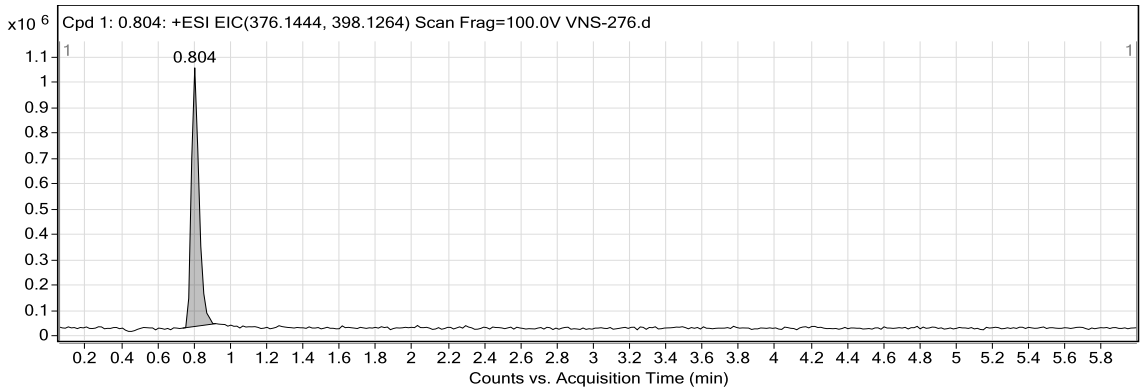
3af

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

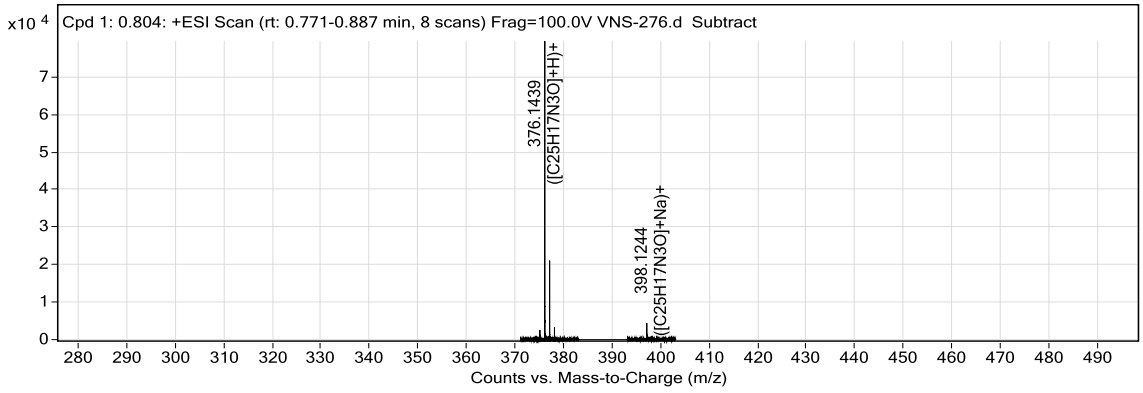
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.804	0.804	375.1367	79705	C25 H17 N3 O	375.1372	-1.34

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.804	376.1439	0.804	Find By Formula	375.1367



MS Zoomed Spectrum



MS Spectrum Peak List

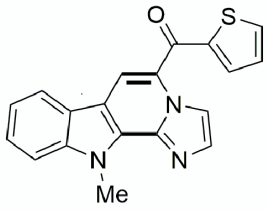
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
376.1439	376.1444	1.31	1	79704.78	C25H17N3O	(M+H)+
377.147	377.1476	1.4	1	21254.08	C25H17N3O	(M+H)+

378.1501	378.1506	1.31	1	3311.29	C25H17N3O	(M+H)+
398.1244	398.1264	4.92	1	246.99	C25H17N3O	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-273.d	**Sample Name**	VNS-273
Sample Type	Sample	**Position**	P1-E6
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	11/3/2017 7:06:29 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



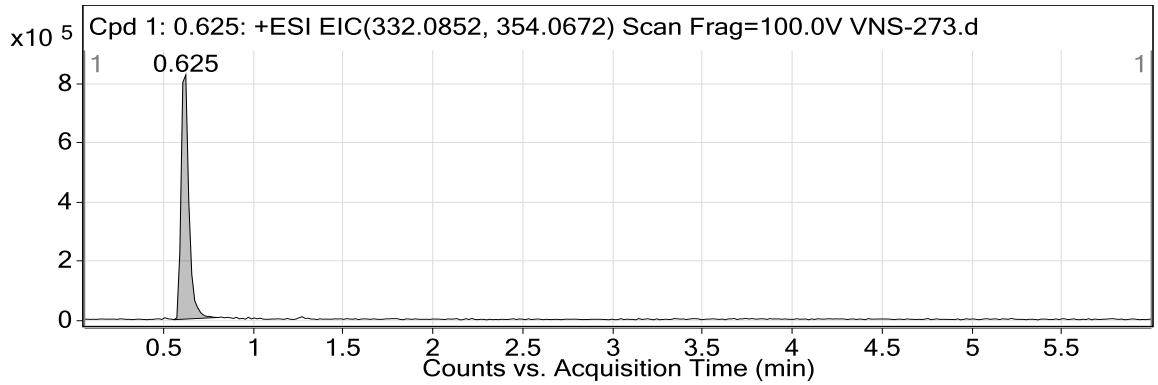
3ag

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

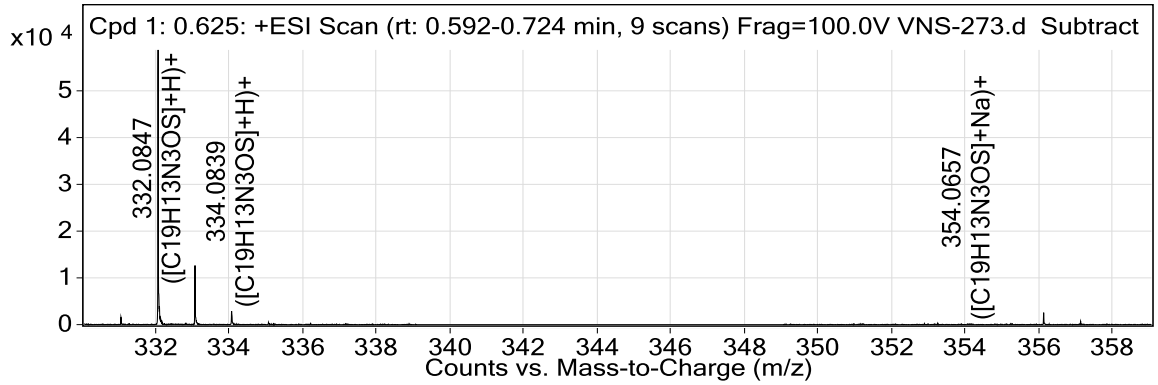
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.625	0.625	331.0774	59370	C19 H13 N3 O S	331.0779	-1.6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.625	332.0847	0.625	Find By Formula	331.0774



MS Zoomed Spectrum



MS Spectrum Peak List

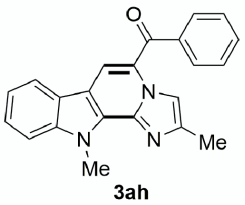
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
332.0847	332.0852	1.57	1	59370.24	C19H13N3OS	(M+H)+
333.0876	333.0881	1.48	1	12627.26	C19H13N3OS	(M+H)+

334.0839	334.0847	2.38	1	2871.35	C19H13N3OS	(M+H)+
354.0657	354.0672	4.06	1	164.33	C19H13N3OS	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-313.d	**Sample Name**	VNS-313
Sample Type	Sample	**Position**	P2-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	10/17/2017 5:15:30 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



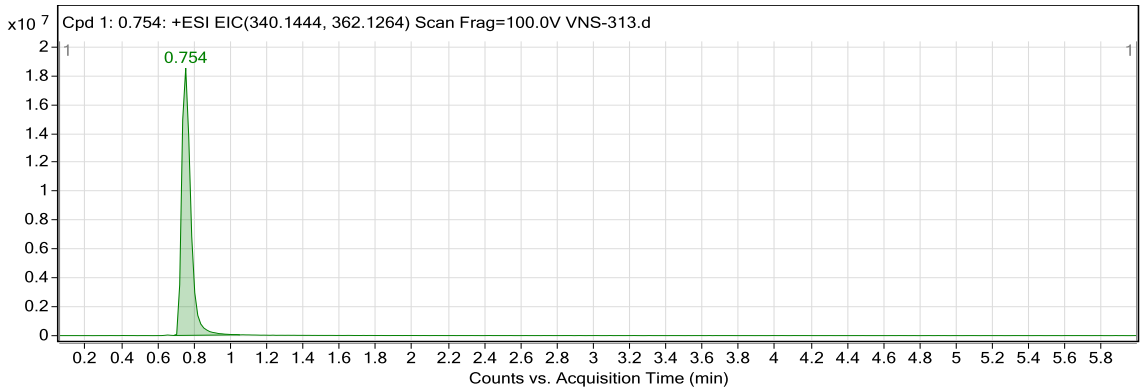
3ah

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

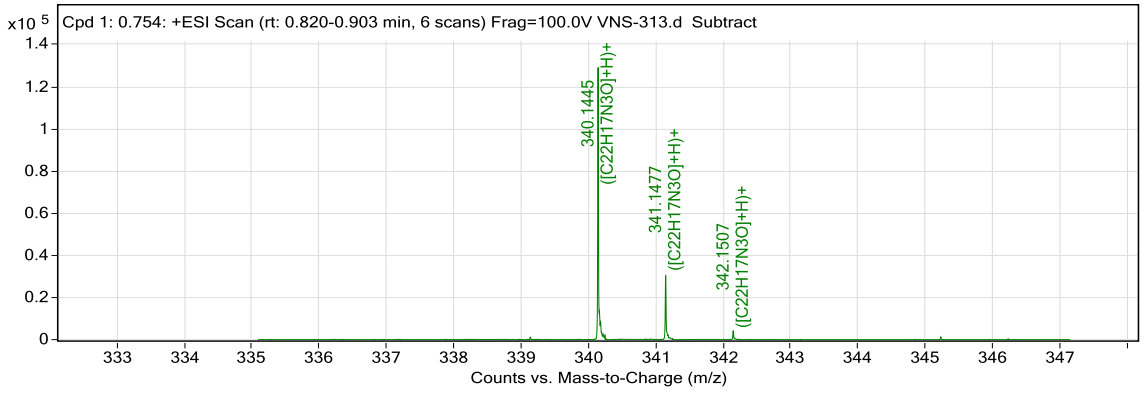
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.754	0.754	339.1372	129251	C22 H17 N3 O	339.1372	0.15

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.754	340.1445	0.754	Find By Formula	339.1372



MS Zoomed Spectrum



MS Spectrum Peak List

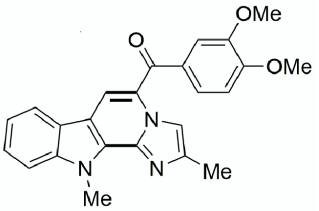
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
340.1445	340.1444	-0.06	1	129250.7	C22H17N3O	(M+H)+
341.1477	341.1475	-0.45	1	31428.92	C22H17N3O	(M+H)+

342.1507	342.1505	-0.61	1	4270.49	C22H17N3O	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-150d.d	**Sample Name**	VNS-150
Sample Type	Sample	**Position**	P1-F4
Instrument Name	Instrument 1	**User Name**	
Acq Method	isocratic.m	**Acquired Time**	5/6/2017 8:51:21 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



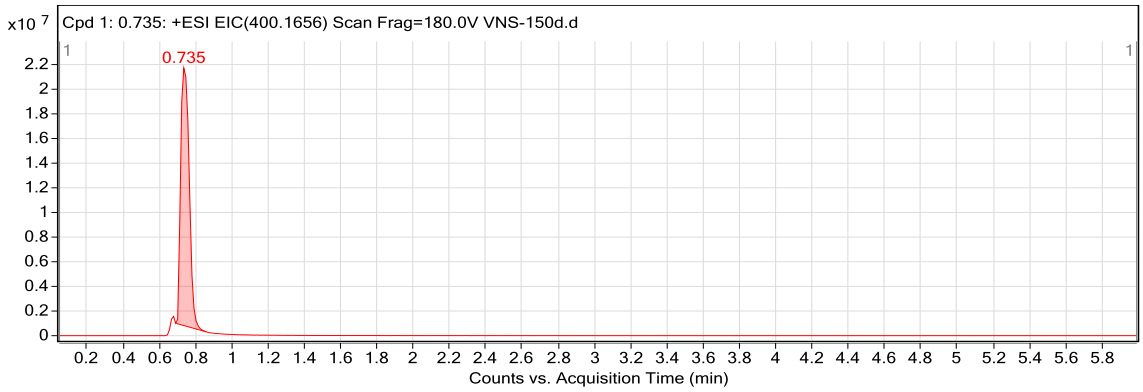
3ai

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

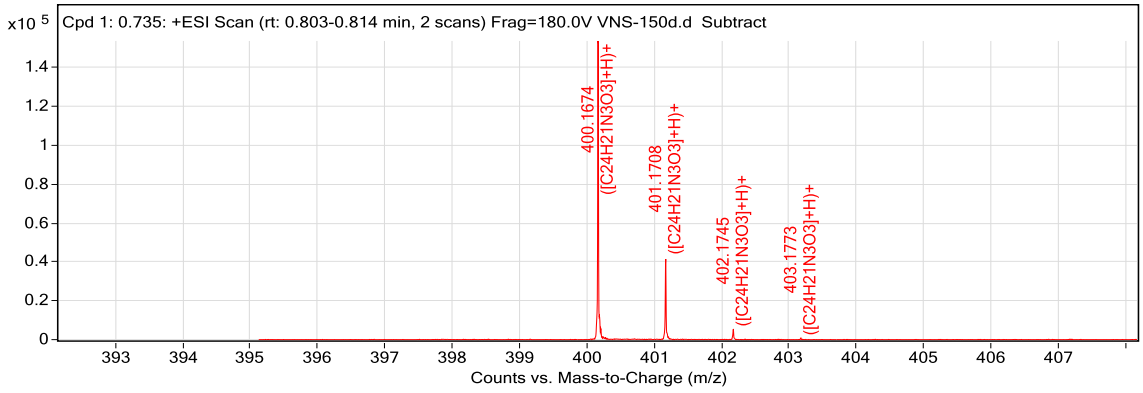
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.735	0.735	399.1602	159833	C24 H21 N3 O3	399.1583	4.86

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.735	400.1674	0.735	Find By Formula	399.1602



MS Zoomed Spectrum



MS Spectrum Peak List

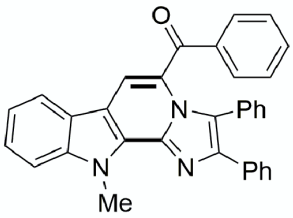
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
400.1674	400.1656	-4.64	1	159833.07	C24H21N3O3	(M+H)+
401.1708	401.1687	-5.25	1	42485.81	C24H21N3O3	(M+H)+

402.1745	402.1715	-7.28	1	5453.59	C24H21N3O3	(M+H)+
403.1773	403.1742	-7.69	1	898.2	C24H21N3O3	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-147.d	**Sample Name**	VNS-147
Sample Type	Sample	**Position**	P2-C5
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min_reg.m	**Acquired Time**	11/14/2017 12:34:23 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



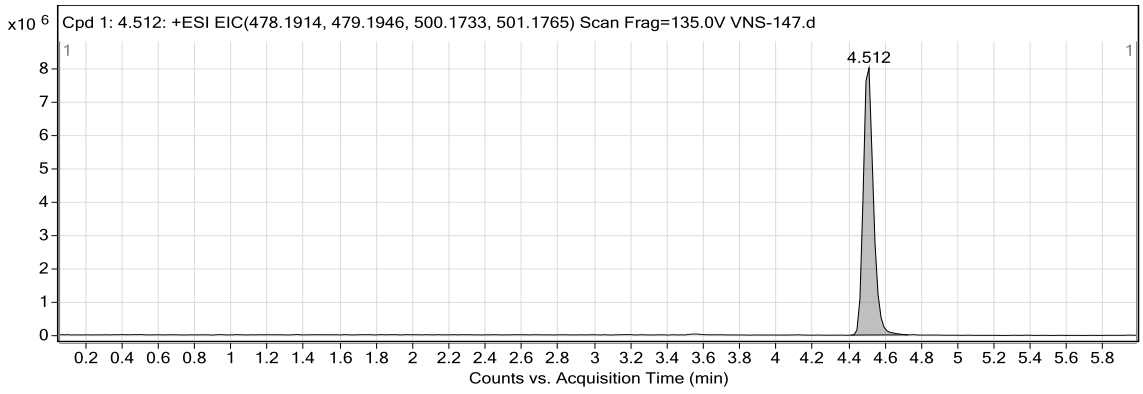
3aj

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

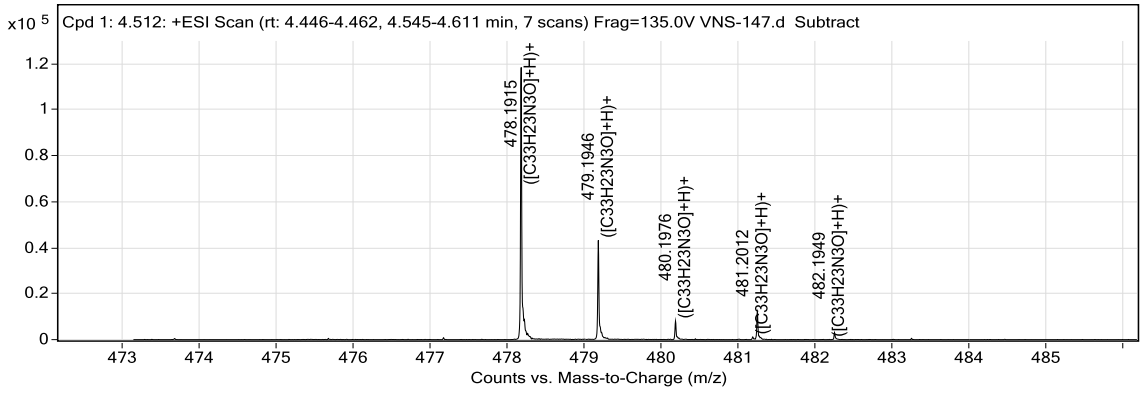
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 4.512	4.512	477.1842	120047	C33 H23 N3 O	477.1841	0.13

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 4.512	478.1915	4.512	Find By Formula	477.1842



MS Zoomed Spectrum



MS Spectrum Peak List

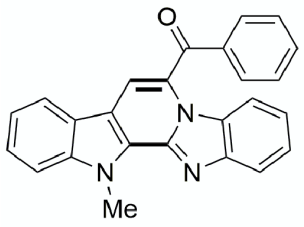
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
478.1915	478.1914	-0.19	1	120047.36	C33H23N3O	(M+H)+
479.1946	479.1946	-0.07	1	43183.11	C33H23N3O	(M+H)+

480.1976	480.1977	0.26	1	8081.5	C33H23N3O	(M+H)+
481.2012	481.2008	-0.91	1	1164.46	C33H23N3O	(M+H)+
482.1949	482.2038	18.37	1	109.8	C33H23N3O	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-159.d	**Sample Name**	VNS-159
Sample Type	Sample	**Position**	P2-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min.m	**Acquired Time**	9/7/2017 5:17:35 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



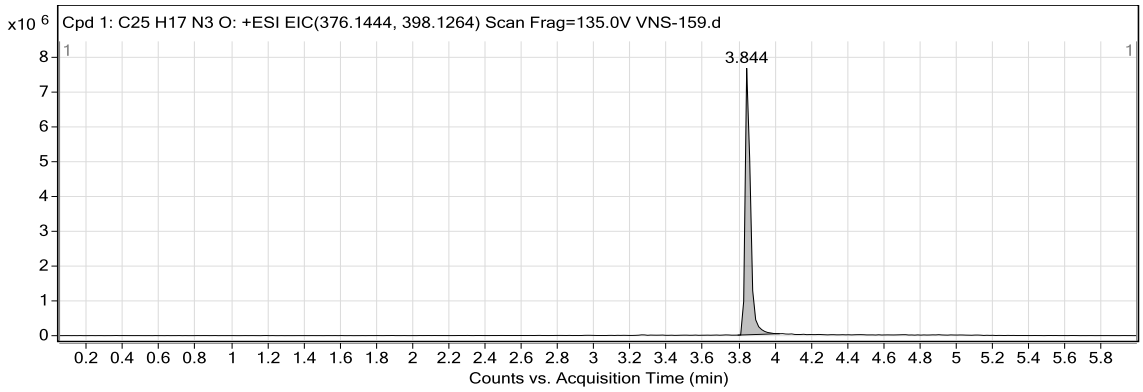
3ak

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

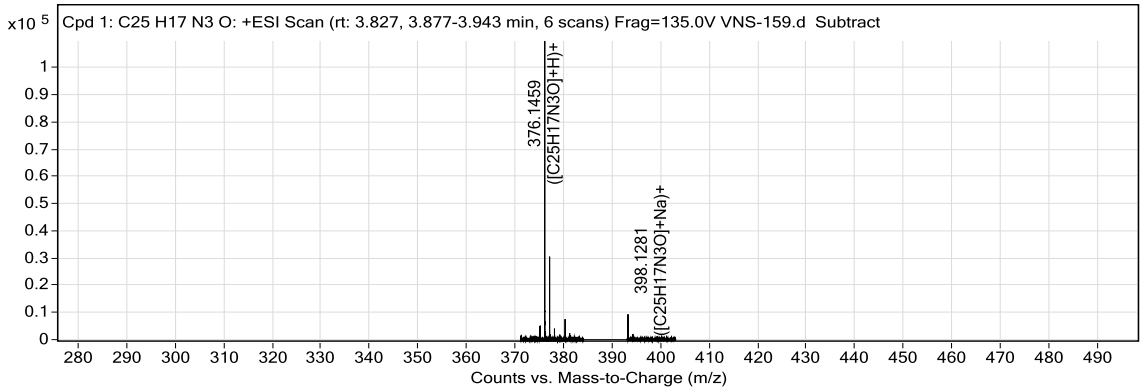
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C25 H17 N3 O	3.844	375.1386	112006	C25 H17 N3 O	375.1372	3.92

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C25 H17 N3 O	376.1459	3.844	Find By Formula	375.1386



MS Zoomed Spectrum



MS Spectrum Peak List

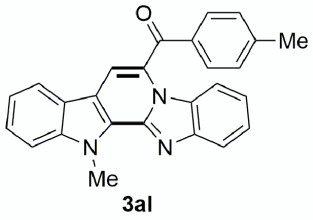
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
376.1459	376.1444	-3.87	1	112006.33	C25H17N3O	(M+H)+
377.1491	377.1476	-3.94	1	30676.33	C25H17N3O	(M+H)+

378.1521	378.1506	-4.01	1	4147.81	C25H17N3O	(M+H)+
379.1561	379.1535	-6.82	1	535.4	C25H17N3O	(M+H)+
398.1281	398.1264	-4.24	1	350.01	C25H17N3O	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-144.d	**Sample Name**	VNS-144
Sample Type	Sample	**Position**	P2-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min.m	**Acquired Time**	9/7/2017 5:03:24 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



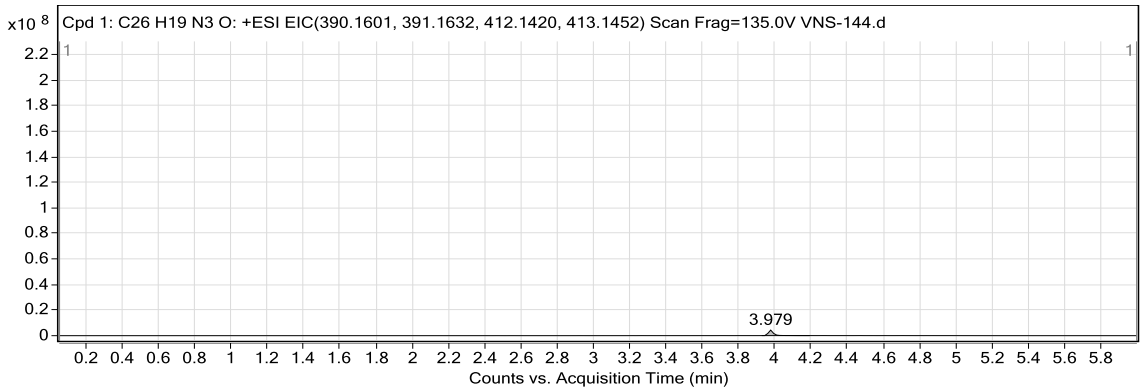
3al

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

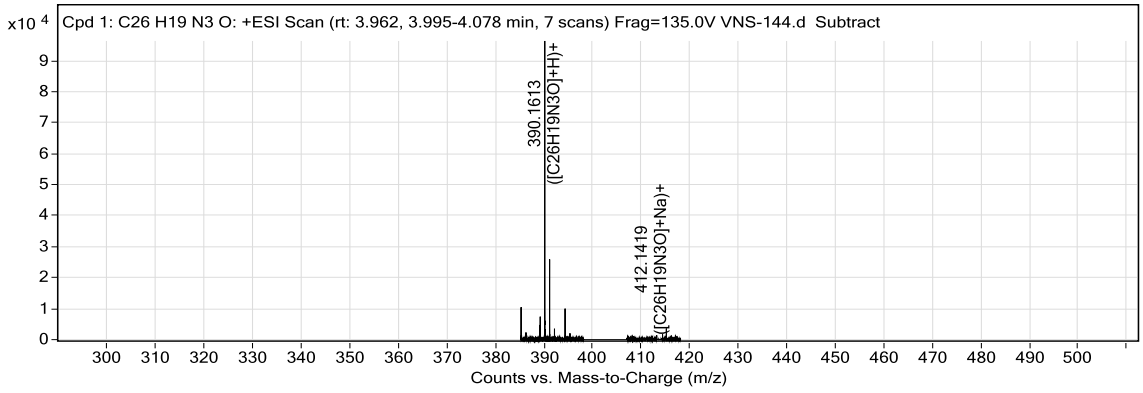
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C26 H19 N3 O	3.979	389.154	96943	C26 H19 N3 O	389.1528	2.98

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C26 H19 N3 O	390.1613	3.979	Find By Formula	389.154



MS Zoomed Spectrum



MS Spectrum Peak List

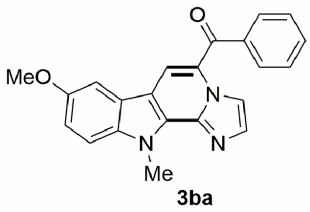
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
390.1613	390.1601	-2.98	1	96942.93	C26H19N3O	(M+H)+
391.1644	391.1632	-3.05	1	26699.53	C26H19N3O	(M+H)+

392.1674	392.1663	-2.97	1	3525.64	C26H19N3O	(M+H)+
393.1694	393.1692	-0.39	1	341.87	C26H19N3O	(M+H)+
412.1419	412.142	0.43	1	692.93	C26H19N3O	(M+Na)+
413.1458	413.1452	-1.42	1	276.24	C26H19N3O	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-179.d	**Sample Name**	VNS-179
Sample Type	Sample	**Position**	P2-B8
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min.m	**Acquired Time**	9/7/2017 6:28:05 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



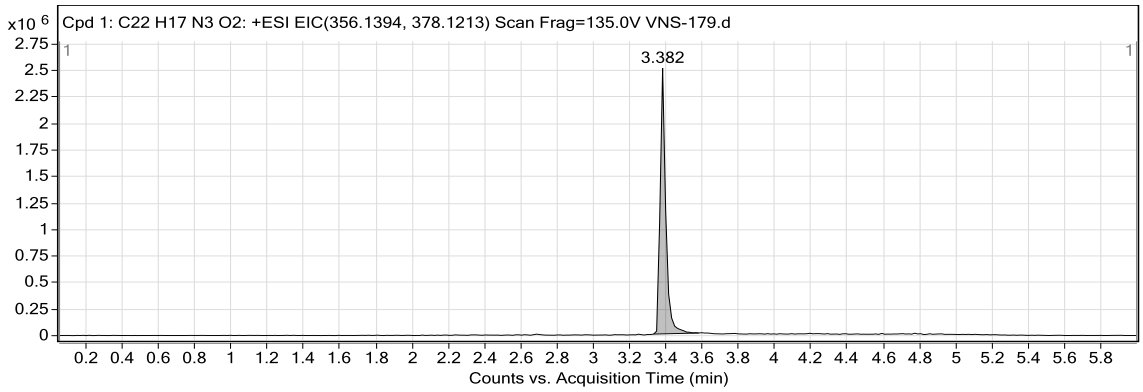
3ba

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

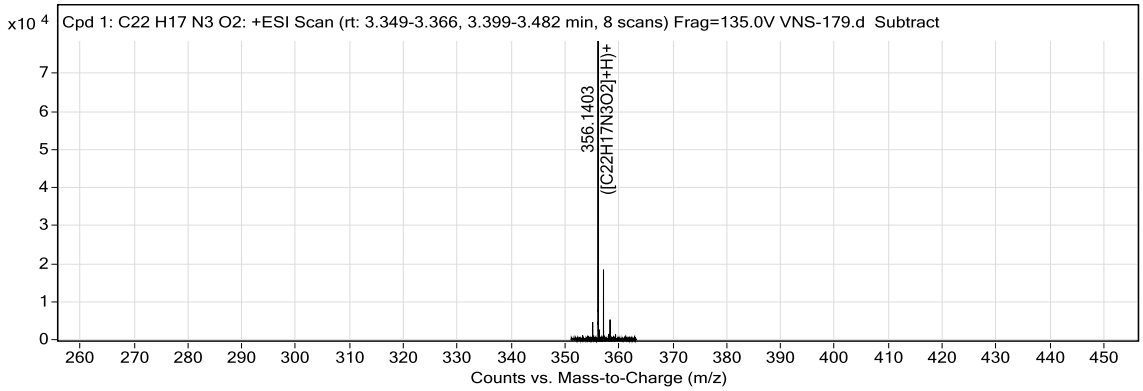
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C22 H17 N3 O2	3.382	355.1331	78694	C22 H17 N3 O2	355.1321	2.85

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H17 N3 O2	356.1403	3.382	Find By Formula	355.1331



MS Zoomed Spectrum



MS Spectrum Peak List

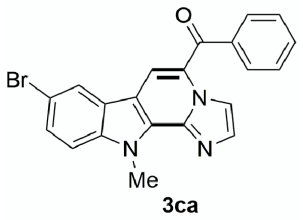
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
356.1403	356.1394	-2.72	1	78693.92	C22H17N3O2	(M+H)+
357.1436	357.1425	-3.19	1	18875.11	C22H17N3O2	(M+H)+

358.147	358.1453	-4.62	1	1536.82	C22H17N3O2	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS 275 (1).d	**Sample Name**	VNS 275-1
Sample Type	Sample	**Position**	P1-C6
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min_reg.m	**Acquired Time**	12/5/2017 5:00:38 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



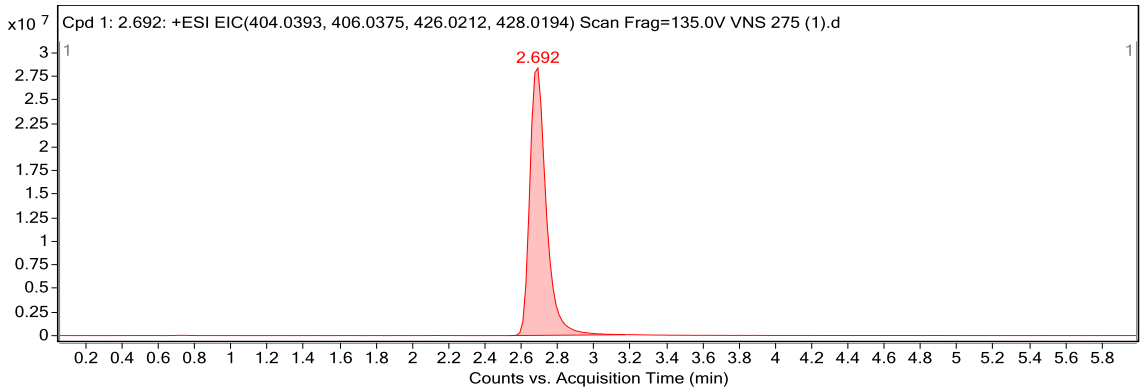
3ca

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

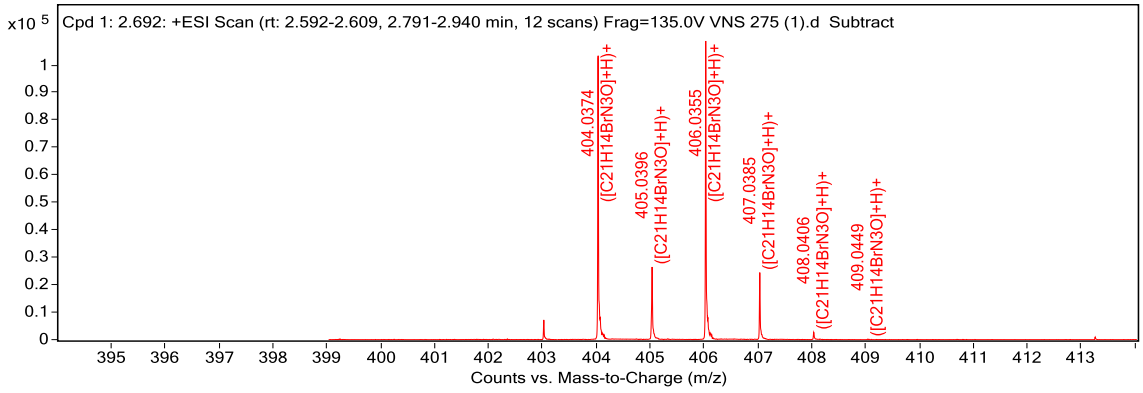
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 2.692	2.692	403.03	108940	C21 H14 Br N3 O	403.032	-5.12

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 2.692	406.0355	2.692	Find By Formula	403.03



MS Zoomed Spectrum



MS Spectrum Peak List

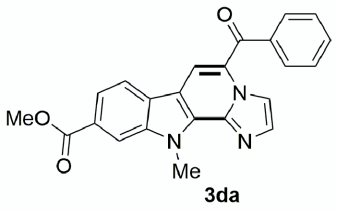
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
404.0374	404.0393	4.74	1	106761.1	C21H14BrN3O	(M+H)+
405.0396	405.0424	6.95	1	26466.05	C21H14BrN3O	(M+H)+

406.0355	406.0375	5.02	1	108939.78	C21H14BrN3O	(M+H)+
407.0385	407.0404	4.71	1	24431.22	C21H14BrN3O	(M+H)+
408.0406	408.0433	6.65	1	2702.13	C21H14BrN3O	(M+H)+
409.0449	409.0461	3.1	1	218.44	C21H14BrN3O	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-316.d	**Sample Name**	VNS-316
Sample Type	Sample	**Position**	P2-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	10/17/2017 6:54:42 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



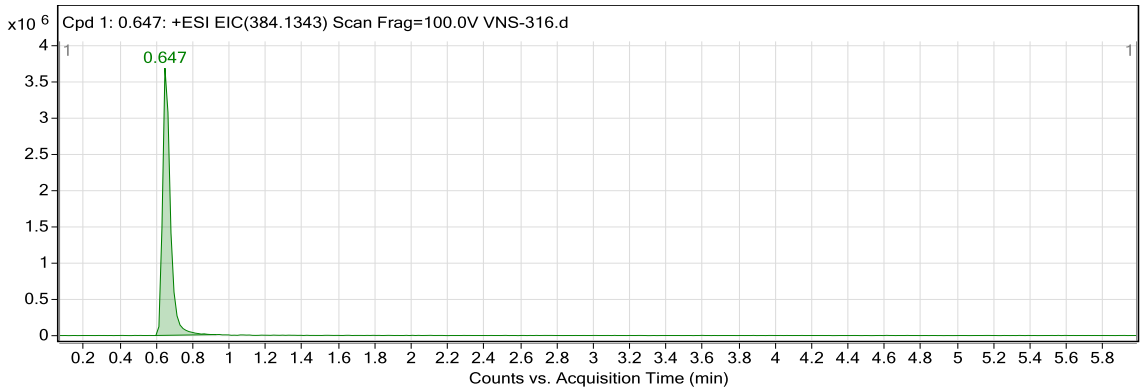
3da

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

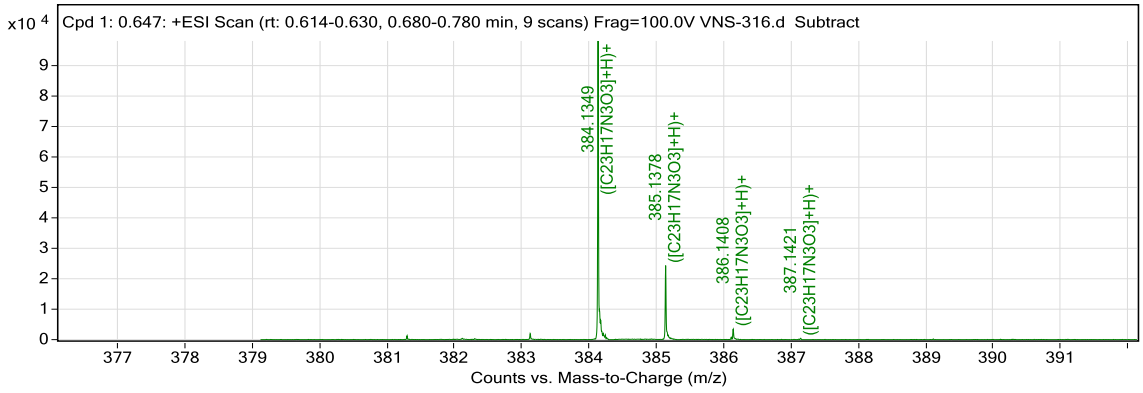
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.647	0.647	383.1276	97902	C23 H17 N3 O3	383.127	1.54

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.647	384.1349	0.647	Find By Formula	383.1276



MS Zoomed Spectrum



MS Spectrum Peak List

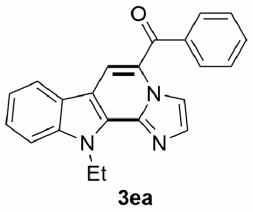
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
384.1349	384.1343	-1.65	1	97902.03	C23H17N3O3	(M+H)+
385.1378	385.1374	-1.1	1	24281.51	C23H17N3O3	(M+H)+

386.1408	386.1402	-1.72	1	3546.58	C23H17N3O3	(M+H)+
387.1421	387.1428	2.06	1	461.66	C23H17N3O3	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-325.d	**Sample Name**	VNS-325
Sample Type	Sample	**Position**	P2-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min_reg.m	**Acquired Time**	11/14/2017 12:06:03 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



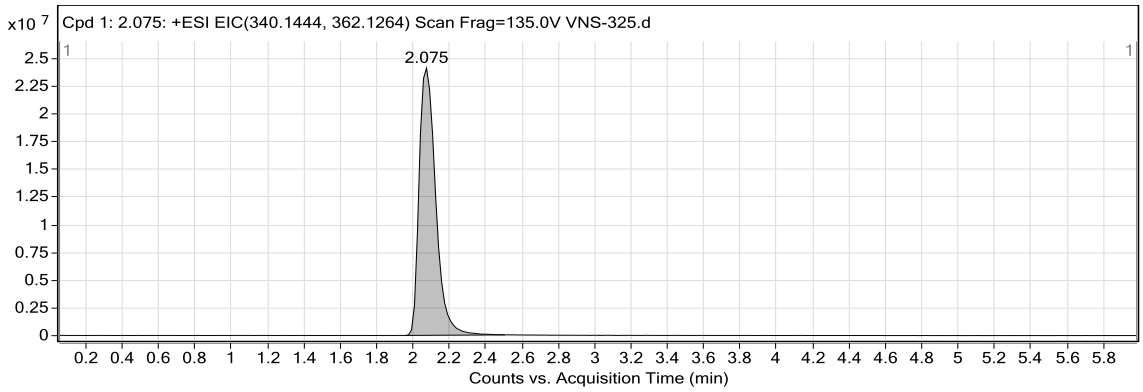
3ea

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

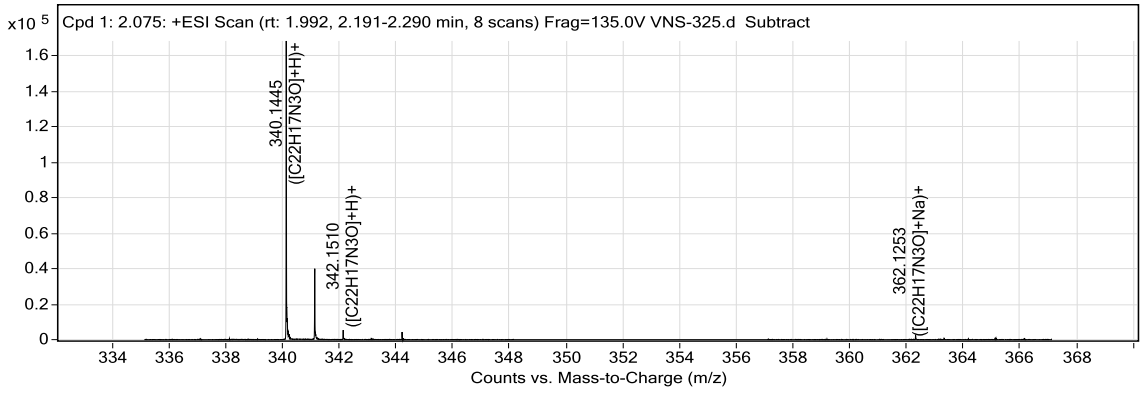
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 2.075	2.075	339.1373	169526	C22 H17 N3 O	339.1372	0.34

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 2.075	340.1445	2.075	Find By Formula	339.1373



MS Zoomed Spectrum



MS Spectrum Peak List

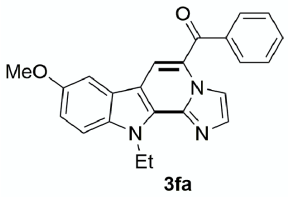
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
340.1445	340.1444	-0.31	1	169525.58	C22H17N3O	(M+H)+
341.1476	341.1475	-0.28	1	40299.86	C22H17N3O	(M+H)+

342.151	342.1505	-1.33	1	5382.74	C22H17N3O	(M+H)+
343.1551	343.1534	-5.03	1	599.81	C22H17N3O	(M+H)+
362.1253	362.1264	2.9	1	242.28	C22H17N3O	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-301.d	**Sample Name**	VNS-301
Sample Type	Sample	**Position**	P2-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	10/17/2017 7:08:50 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



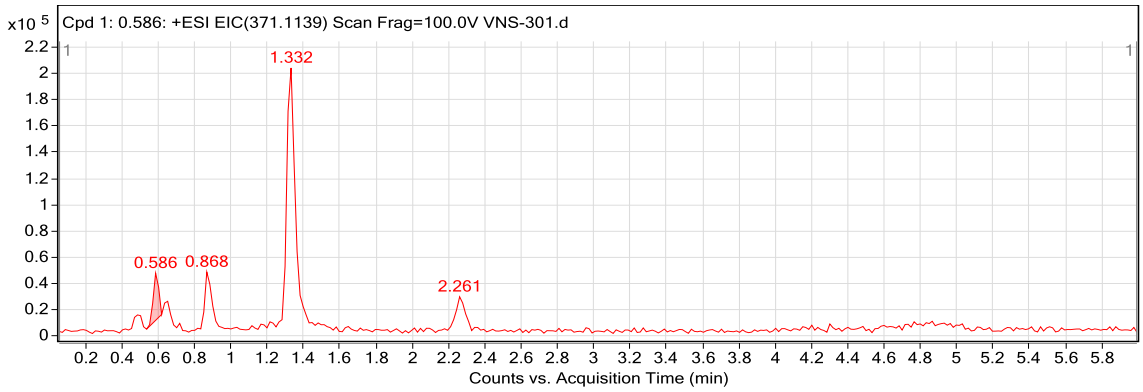
3fa

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

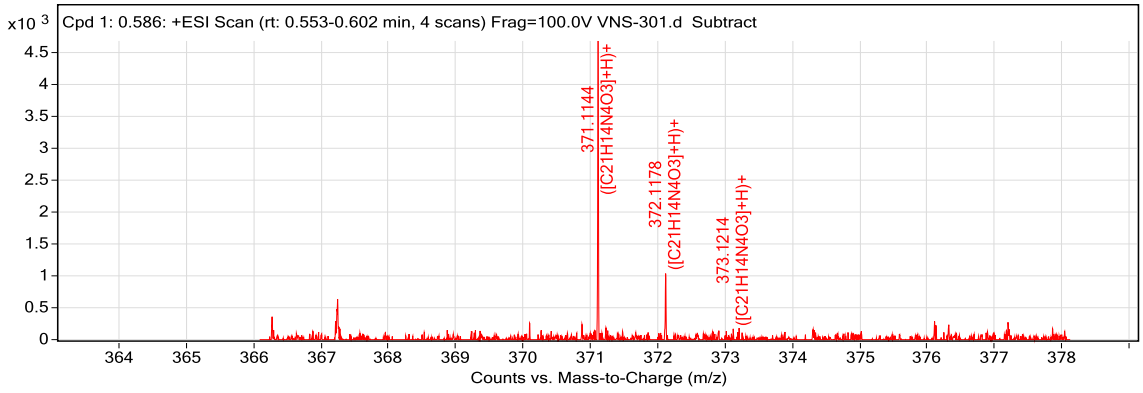
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.586	0.586	370.1073	4687	C21 H14 N4 O3	370.1066	1.81

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.586	371.1144	0.586	Find By Formula	370.1073



MS Zoomed Spectrum



MS Spectrum Peak List

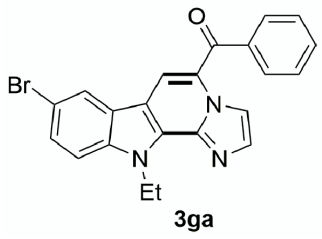
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
371.1144	371.1139	-1.51	1	4687.17	C21H14N4O3	(M+H)+
372.1178	372.1169	-2.63	1	1050.41	C21H14N4O3	(M+H)+

373.1214	373.1195	-4.87	1	173.01	C21H14N4O3	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-164.d	**Sample Name**	VNS-164
Sample Type	Sample	**Position**	P2-B3
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min.m	**Acquired Time**	9/7/2017 5:31:41 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



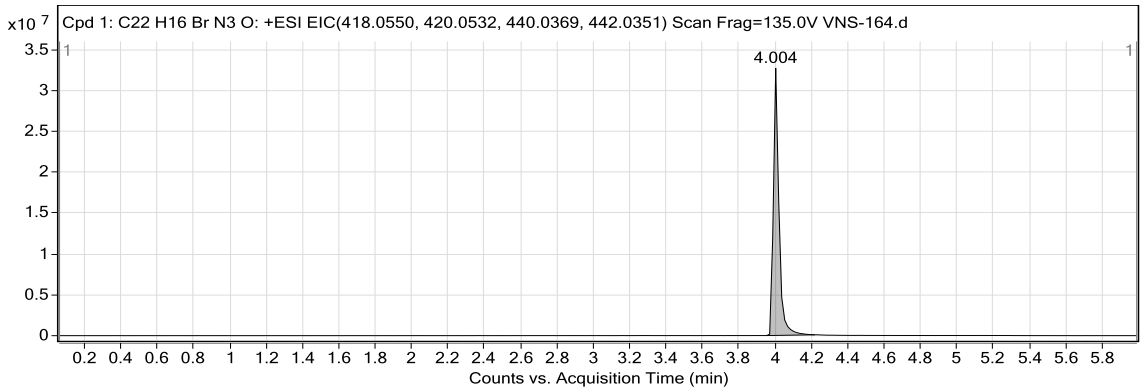
3ga

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

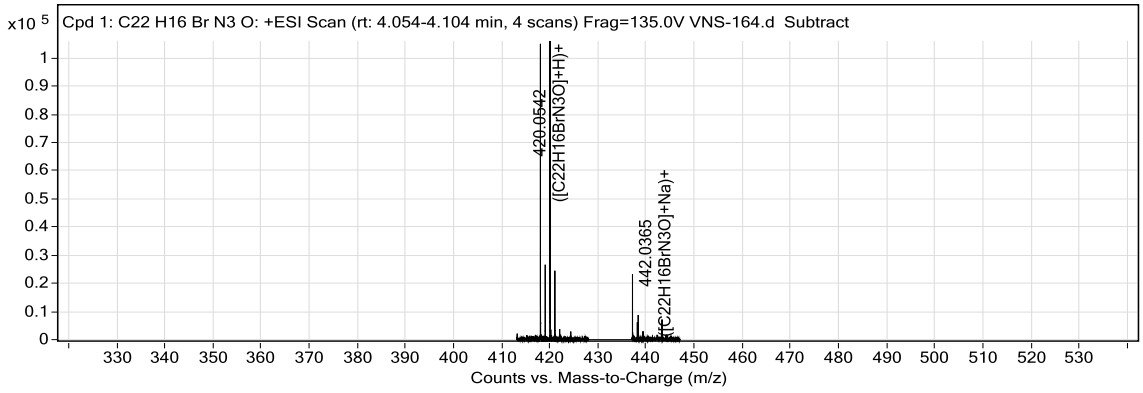
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C22 H16 Br N3 O	4.004	417.0488	106103	C22 H16 Br N3 O	417.0477	2.78

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H16 Br N3 O	420.0542	4.004	Find By Formula	417.0488



MS Zoomed Spectrum



MS Spectrum Peak List

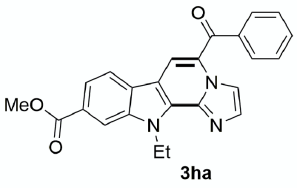
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
418.0562	418.055	-3.08	1	105236.59	C22H16BrN3O	(M+H)+
419.0592	419.0581	-2.73	1	26670.97	C22H16BrN3O	(M+H)+

420.0542	420.0532	-2.37	1	106103.23	C22H16BrN3O	(M+H)+
421.0574	421.0561	-3.12	1	24522.99	C22H16BrN3O	(M+H)+
422.0601	422.059	-2.46	1	3761.58	C22H16BrN3O	(M+H)+
423.0656	423.0619	-8.83	1	357.85	C22H16BrN3O	(M+H)+
442.0365	442.0351	-3.22	1	71.77	C22H16BrN3O	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-176.d	**Sample Name**	VNS-176
Sample Type	Sample	**Position**	P2-B7
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min.m	**Acquired Time**	9/7/2017 6:56:19 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



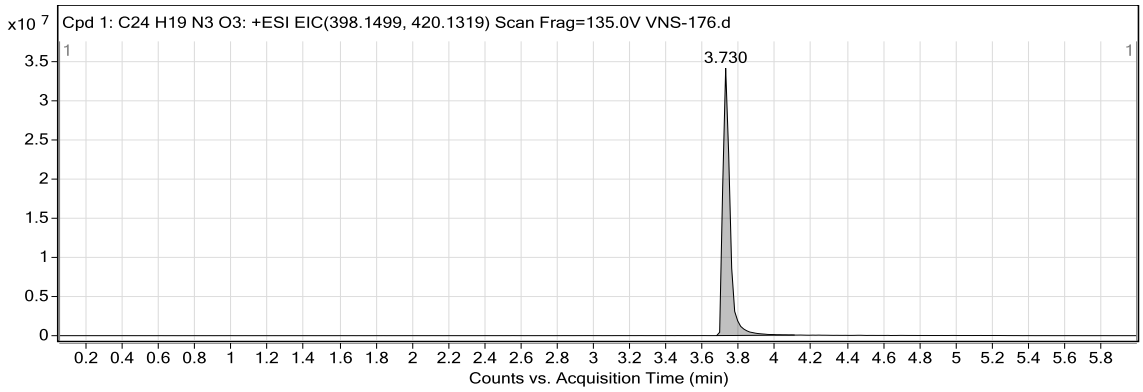
3ha

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

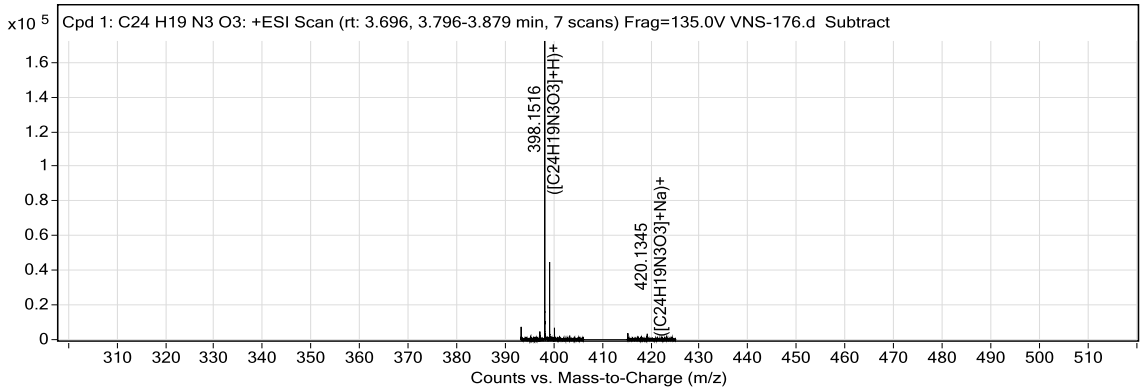
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C24 H19 N3 O3	3.73	397.1443	172894	C24 H19 N3 O3	397.1426	4.2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C24 H19 N3 O3	398.1516	3.73	Find By Formula	397.1443



MS Zoomed Spectrum



MS Spectrum Peak List

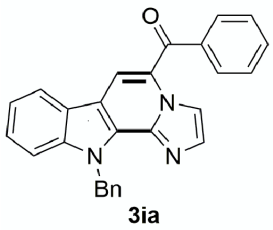
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
398.1516	398.1499	-4.24	1	172894.21	C24H19N3O3	(M+H)+
399.1547	399.153	-4.17	1	44813.51	C24H19N3O3	(M+H)+

400.1571	400.1559	-3.06	1	6828.53	C24H19N3O3	(M+H)+
401.1604	401.1586	-4.61	1	842.34	C24H19N3O3	(M+H)+
420.1345	420.1319	-6.23	1	185.31	C24H19N3O3	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-172.d	**Sample Name**	VNS-172
Sample Type	Sample	**Position**	P2-B5
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min.m	**Acquired Time**	9/7/2017 5:59:53 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



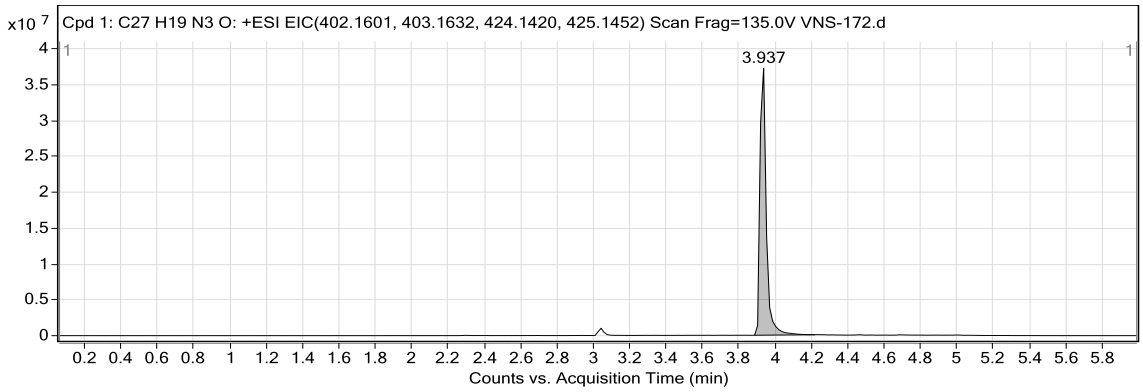
3ia

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

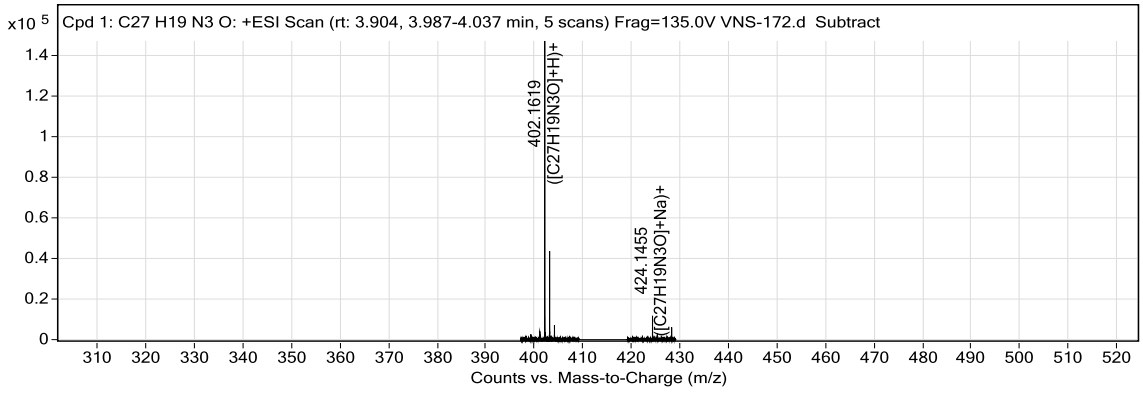
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C27 H19 N3 O	3.937	401.1547	149071	C27 H19 N3 O	401.1528	4.63

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C27 H19 N3 O	402.1619	3.937	Find By Formula	401.1547



MS Zoomed Spectrum



MS Spectrum Peak List

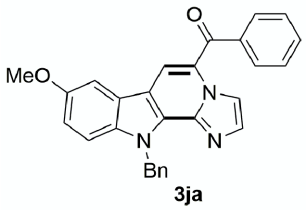
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
402.1619	402.1601	-4.58	1	149071.1	C27H19N3O	(M+H)+
403.1652	403.1632	-4.92	1	43604.49	C27H19N3O	(M+H)+

404.1676	404.1663	-3.27	1	7210.09	C27H19N3O	(M+H)+
424.1455	424.142	-8.28	1	342.69	C27H19N3O	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-177.d	**Sample Name**	VNS-177
Sample Type	Sample	**Position**	P1-F3
Instrument Name	Instrument 1	**User Name**	
Acq Method	isocratic.m	**Acquired Time**	5/6/2017 8:37:39 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



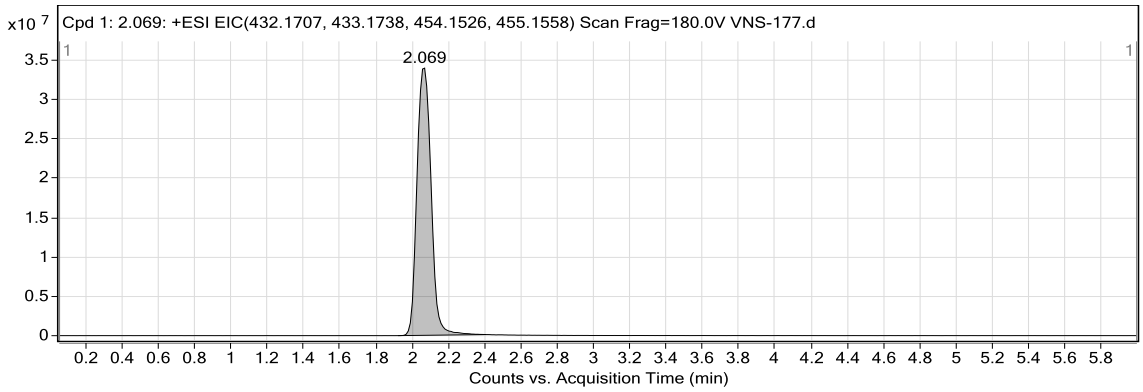
3ja

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

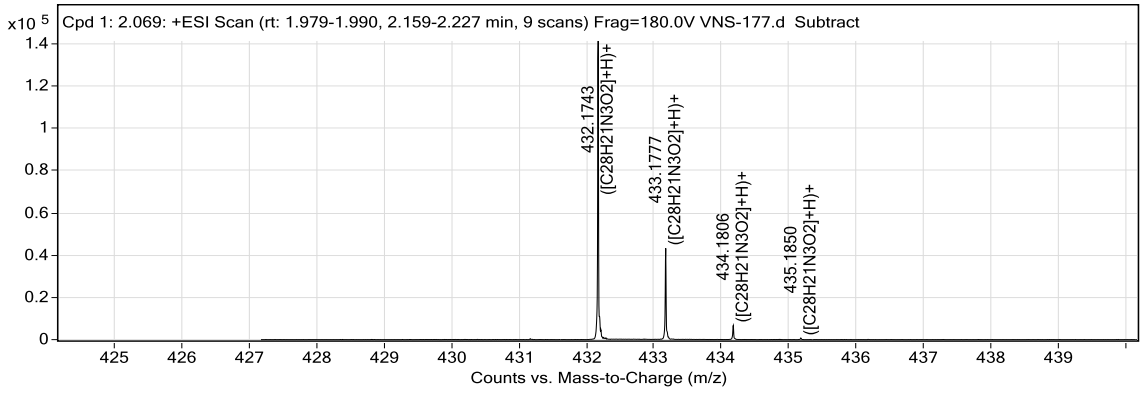
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 2.069	2.069	431.1671	144566	C28 H21 N3 O2	431.1634	8.56

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 2.069	432.1743	2.069	Find By Formula	431.1671



MS Zoomed Spectrum



MS Spectrum Peak List

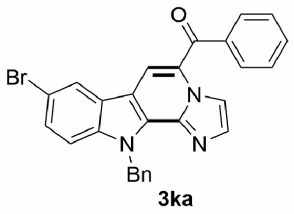
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
432.1743	432.1707	-8.4	1	144565.89	C28H21N3O2	(M+H)+
433.1777	433.1738	-8.88	1	43416.58	C28H21N3O2	(M+H)+

434.1806	434.1768	-8.83	1	6902.43	C28H21N3O2	(M+H)+
435.185	435.1797	-12.3	1	801.01	C28H21N3O2	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-315.d	**Sample Name**	VNS-315
Sample Type	Sample	**Position**	P2-A5
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	10/17/2017 6:12:12 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



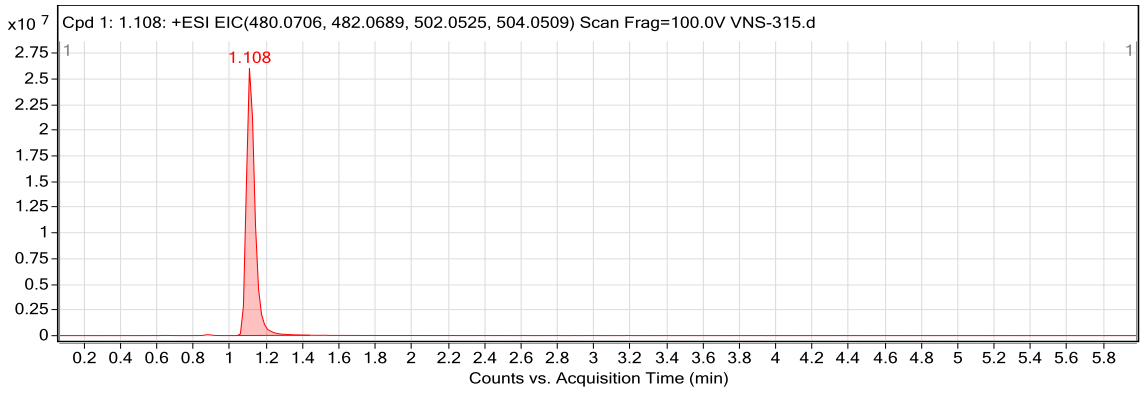
3ka

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

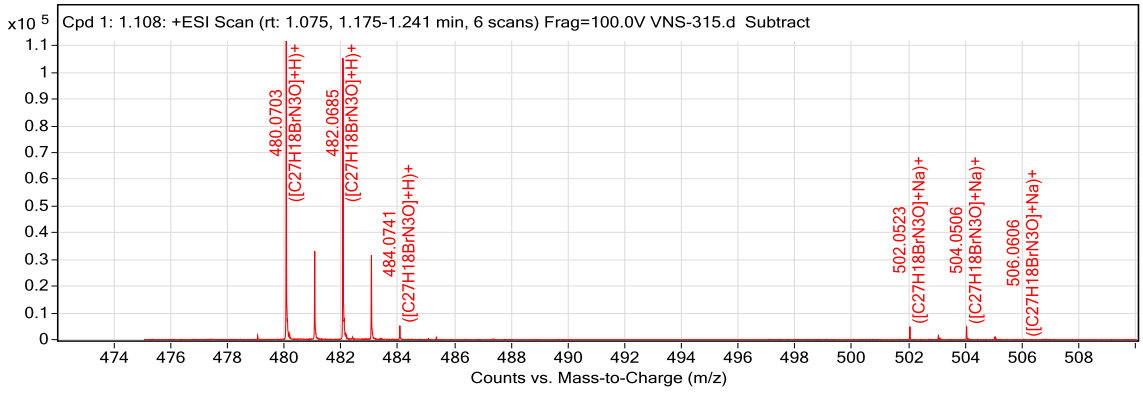
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 1.108	1.108	479.063	112171	C27 H18 Br N3 O	479.0633	-0.76

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 1.108	480.0703	1.108	Find By Formula	479.063



MS Zoomed Spectrum



MS Spectrum Peak List

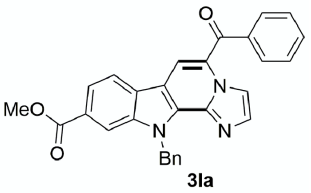
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
480.0703	480.0706	0.65	1	112171.29	C27H18BrN3O	(M+H)+
481.0733	481.0738	0.97	1	33136.67	C27H18BrN3O	(M+H)+

482.0685	482.0689	0.81	1	108131.98	C27H18BrN3O	(M+H)+
483.0715	483.0718	0.7	1	32090.18	C27H18BrN3O	(M+H)+
484.0741	484.0748	1.4	1	5375.45	C27H18BrN3O	(M+H)+
485.0777	485.0778	0.16	1	455.97	C27H18BrN3O	(M+H)+
502.0523	502.0525	0.48	1	4954.27	C27H18BrN3O	(M+Na)+
503.0558	503.0557	-0.13	1	1458.76	C27H18BrN3O	(M+Na)+
504.0506	504.0509	0.62	1	4851.39	C27H18BrN3O	(M+Na)+
505.0523	505.0538	2.87	1	1140.21	C27H18BrN3O	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-294.d	**Sample Name**	VNS-294
Sample Type	Sample	**Position**	P1-E7
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	11/3/2017 7:20:39 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



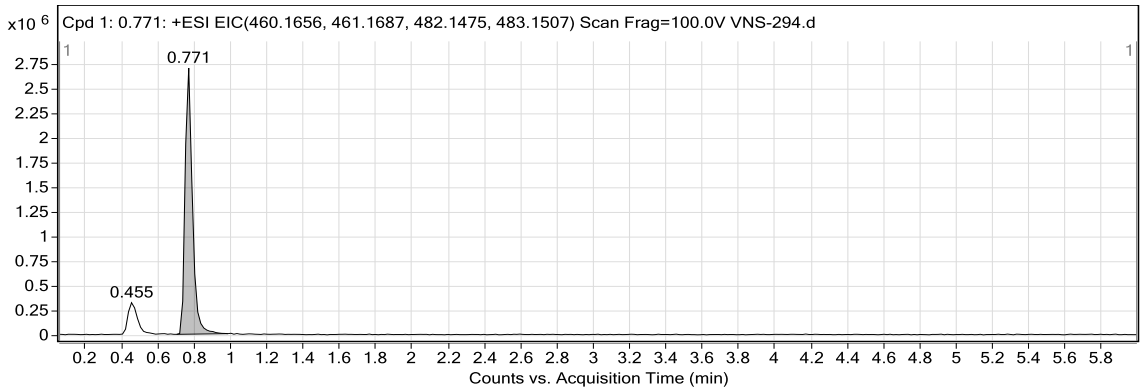
3la

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

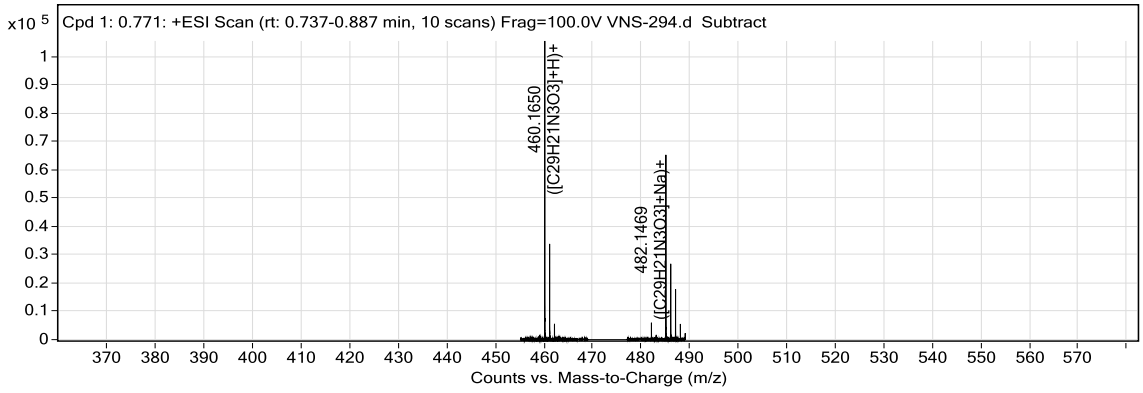
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.771	0.771	459.1577	106683	C29 H21 N3 O3	459.1583	-1.25

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.771	460.165	0.771	Find By Formula	459.1577



MS Zoomed Spectrum



MS Spectrum Peak List

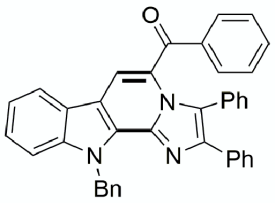
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
460.165	460.1656	1.16	1	106682.93	C29H21N3O3	(M+H)+
461.168	461.1687	1.57	1	34006.96	C29H21N3O3	(M+H)+

462.1715	462.1717	0.31	1	5490.15	C29H21N3O3	(M+H)+
463.1749	463.1745	-0.84	1	783.56	C29H21N3O3	(M+H)+
464.165	464.1772	26.29	1	85.73	C29H21N3O3	(M+H)+
482.1469	482.1475	1.28	1	6057.23	C29H21N3O3	(M+Na)+
483.15	483.1507	1.45	1	1718.46	C29H21N3O3	(M+Na)+
484.1504	484.1536	6.6	1	295.43	C29H21N3O3	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-173.d	**Sample Name**	VNS-173
Sample Type	Sample	**Position**	P2-B6
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min.m	**Acquired Time**	9/7/2017 6:13:58 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



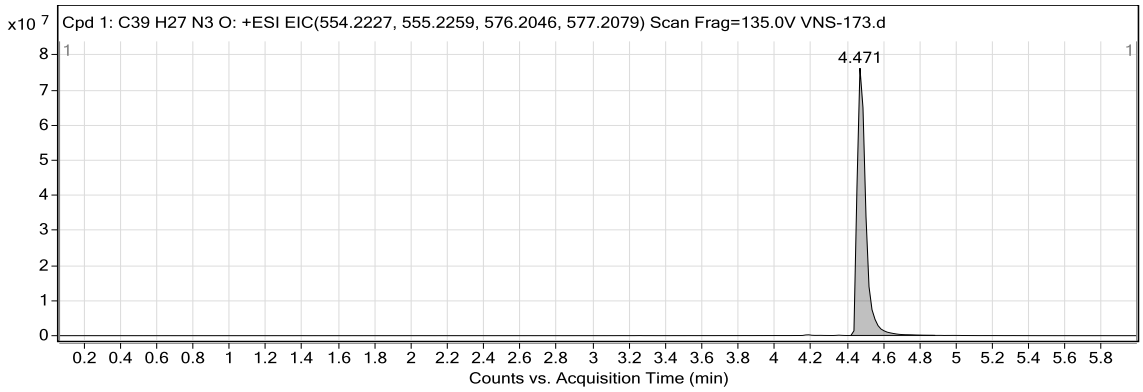
3ij

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

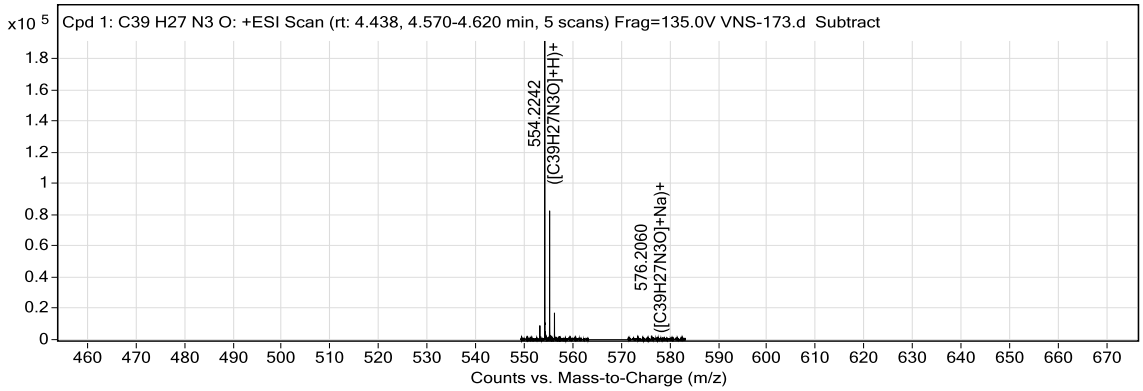
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C39 H27 N3 O	4.471	553.2169	193359	C39 H27 N3 O	553.2154	2.65

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C39 H27 N3 O	554.2242	4.471	Find By Formula	553.2169



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
554.2242	554.2227	-2.7	1	193358.99	C39H27N3O	(M+H)+
555.2273	555.2259	-2.58	1	82863.7	C39H27N3O	(M+H)+

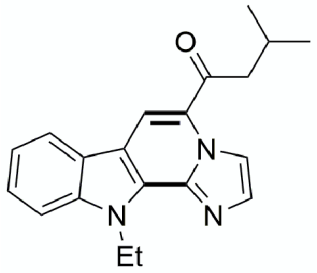
556.2304	556.2291	-2.34	1	17580.66	C39H27N3O	(M+H)+
557.2337	557.2322	-2.67	1	2232.21	C39H27N3O	(M+H)+
558.2353	558.2353	-0.06	1	250.5	C39H27N3O	(M+H)+
576.206	576.2046	-2.31	1	2500.07	C39H27N3O	(M+Na)+
577.2101	577.2079	-3.82	1	995.07	C39H27N3O	(M+Na)+
578.2099	578.211	1.92	1	240.23	C39H27N3O	(M+Na)+

--- End Of Report ---

HRMS Facility, BITS Pilani, Pilani Campus
Compound Report

Data File	VNS-407.d	**Sample Name**	VNS-407
Sample Type	Sample	**Position**	P2-B8
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min_reg.m	**Acquired Time**	3/22/2018 5:30:12 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

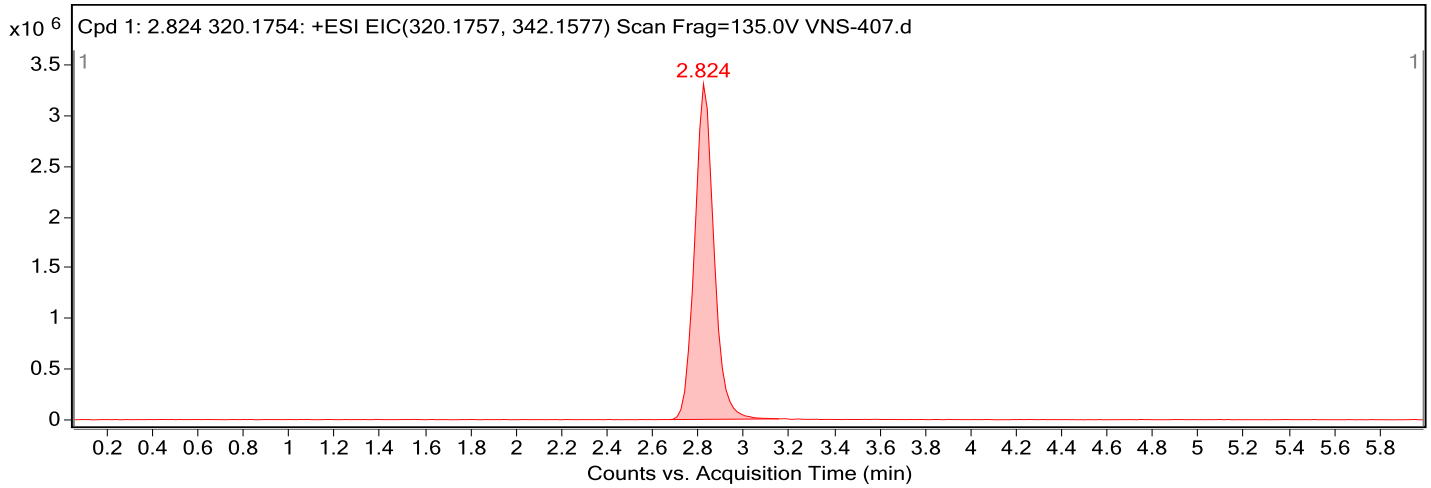


3em

Compound Table

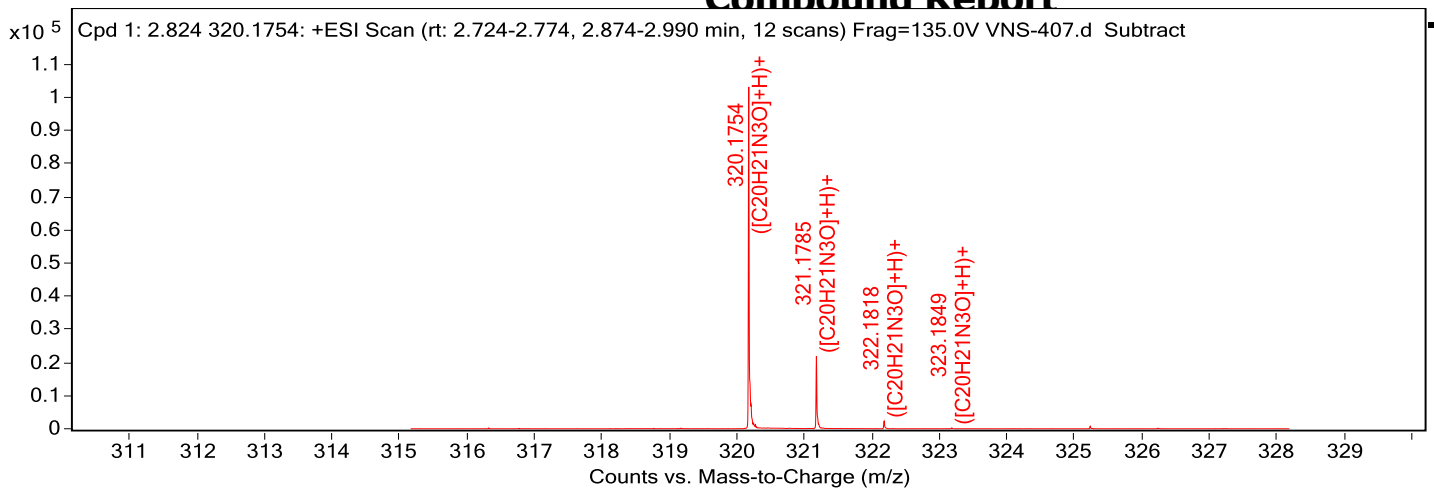
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 2.824 320.1754	2.824	319.1681	103878	C20 H21 N3 O	319.1685	-1.04

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 2.824 320.1754	320.1754	2.824	Find By Formula	319.1681



MS Zoomed Spectrum

HRMS Facility, BITS Pilani, Pilani Campus
Compound Report



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
320.1754	320.1757	1.09	1	103877.73	C20H21N3O	(M+H)+
321.1785	321.1788	0.95	1	21875.81	C20H21N3O	(M+H)+
322.1818	322.1818	-0.17	1	2339.64	C20H21N3O	(M+H)+
323.1849	323.1846	-1.05	1	276.28	C20H21N3O	(M+H)+

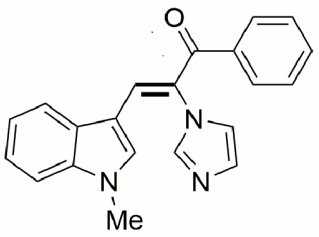
Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

---End Of Report---

Qualitative Compound Report

Data File	VNS-139.d	**Sample Name**	VNS-139
Sample Type	Sample	**Position**	P2-C6
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min_reg.m	**Acquired Time**	11/14/2017 12:48:33 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



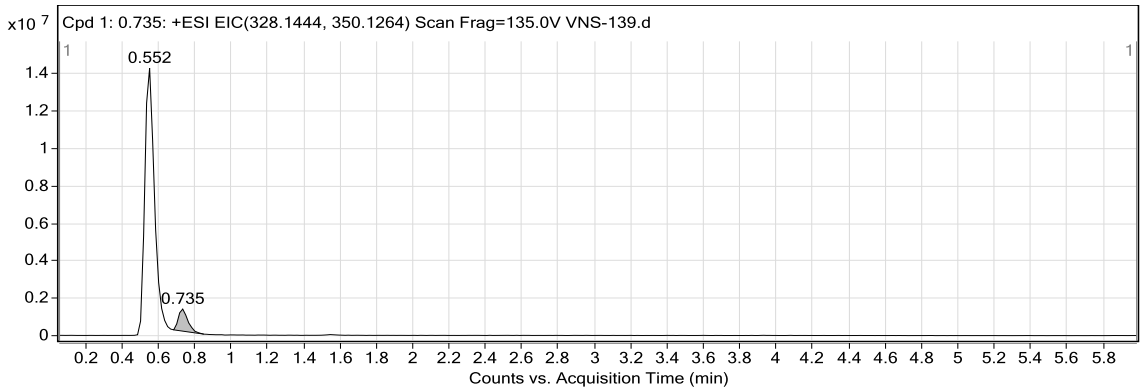
4aa

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

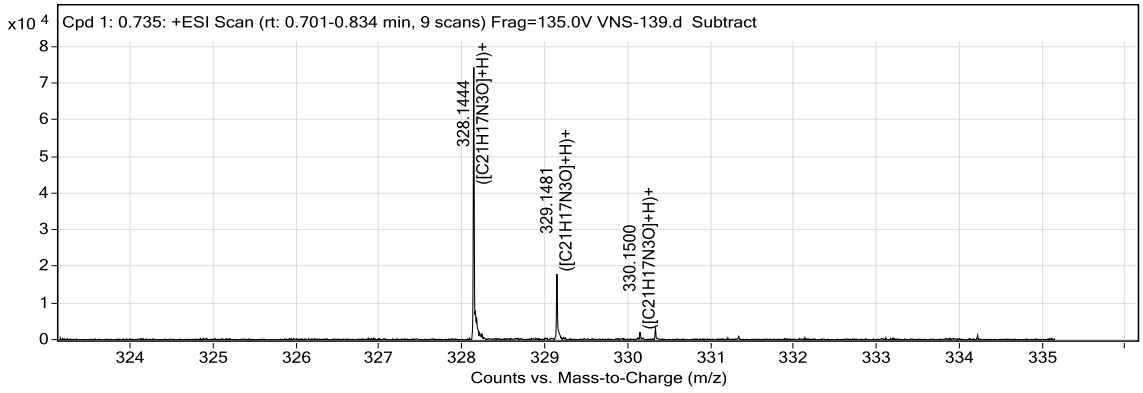
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.735	0.735	327.1372	75762	C21 H17 N3 O	327.1372	0.15

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.735	328.1444	0.735	Find By Formula	327.1372



MS Zoomed Spectrum



MS Spectrum Peak List

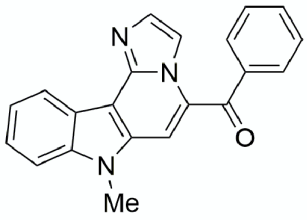
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
328.1444	328.1444	0.16	1	75761.53	C21H17N3O	(M+H)+
329.1481	329.1475	-1.67	1	17875.14	C21H17N3O	(M+H)+

330.15	330.1505	1.38	1	2055.91	C21H17N3O	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-189.d	**Sample Name**	VNS-189
Sample Type	Sample	**Position**	P2-B10
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min.m	**Acquired Time**	9/7/2017 6:42:12 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



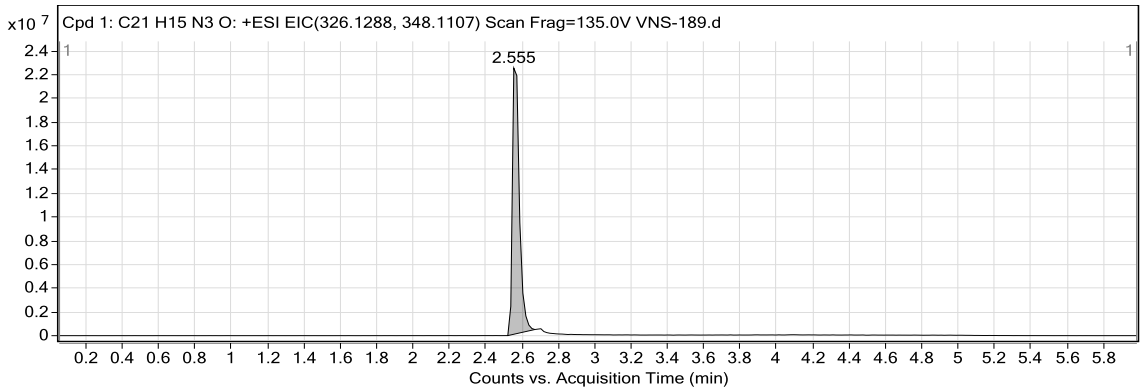
6aa

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

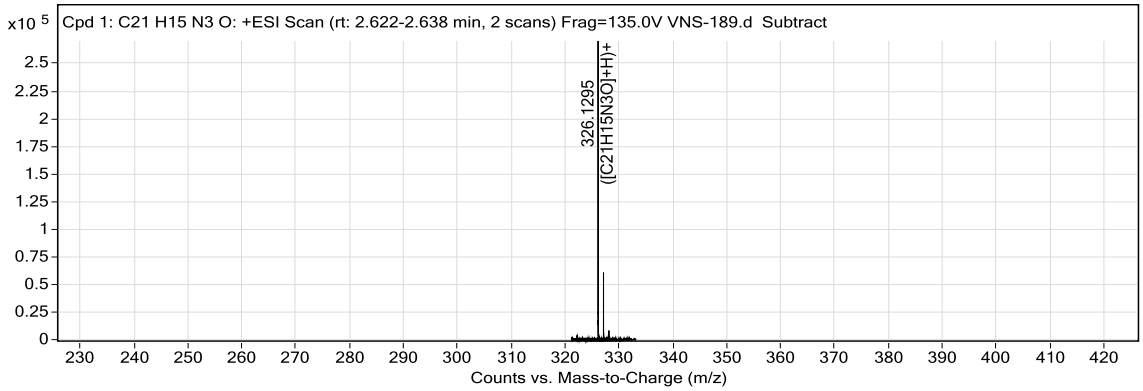
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C21 H15 N3 O	2.555	325.1223	272182	C21 H15 N3 O	325.1215	2.35

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H15 N3 O	326.1295	2.555	Find By Formula	325.1223



MS Zoomed Spectrum



MS Spectrum Peak List

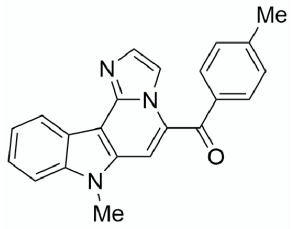
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
326.1295	326.1288	-2.17	1	272181.91	C21H15N3O	(M+H)+
327.1329	327.1319	-3.11	1	60794.95	C21H15N3O	(M+H)+

328.1356	328.1348	-2.42	1	8300.87	C21H15N3O	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-303.d	**Sample Name**	VNS-303
Sample Type	Sample	**Position**	P2-A6
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	10/17/2017 6:26:26 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



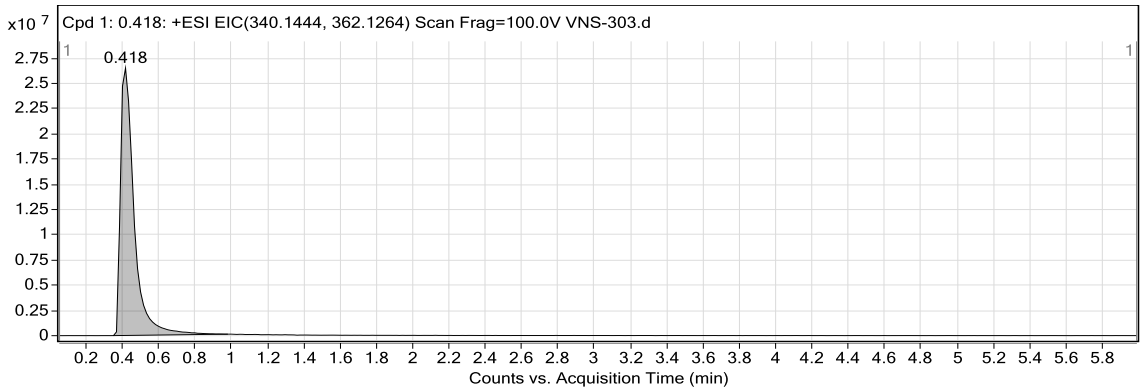
6ab

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

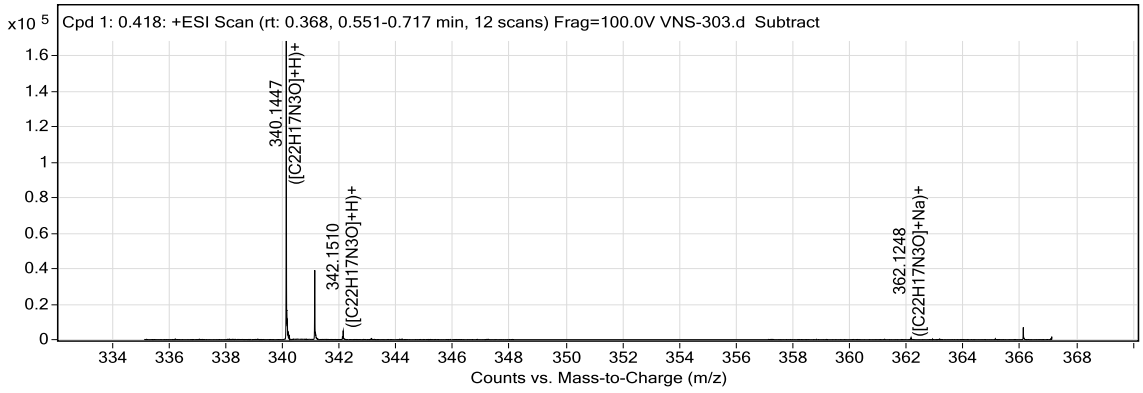
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.418	0.418	339.1374	168408	C22 H17 N3 O	339.1372	0.74

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.418	340.1447	0.418	Find By Formula	339.1374



MS Zoomed Spectrum



MS Spectrum Peak List

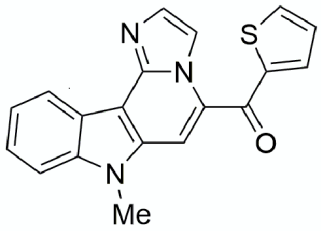
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
340.1447	340.1444	-0.7	1	168407.69	C22H17N3O	(M+H)+
341.1478	341.1475	-0.89	1	40224.33	C22H17N3O	(M+H)+

342.151	342.1505	-1.36	1	5102.59	C22H17N3O	(M+H)+
343.1529	343.1534	1.38	1	549.72	C22H17N3O	(M+H)+
362.1248	362.1264	4.3	1	151.28	C22H17N3O	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-304.d	**Sample Name**	VNS-304
Sample Type	Sample	**Position**	P2-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	10/17/2017 6:40:34 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



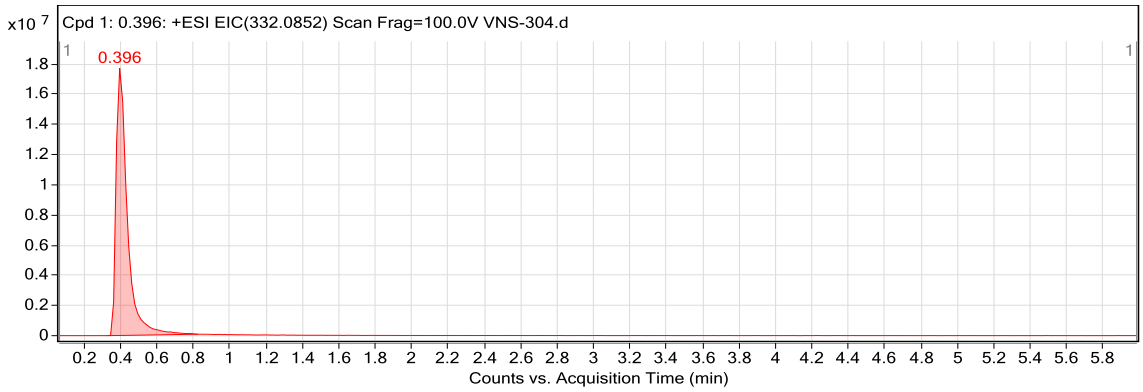
6ag

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

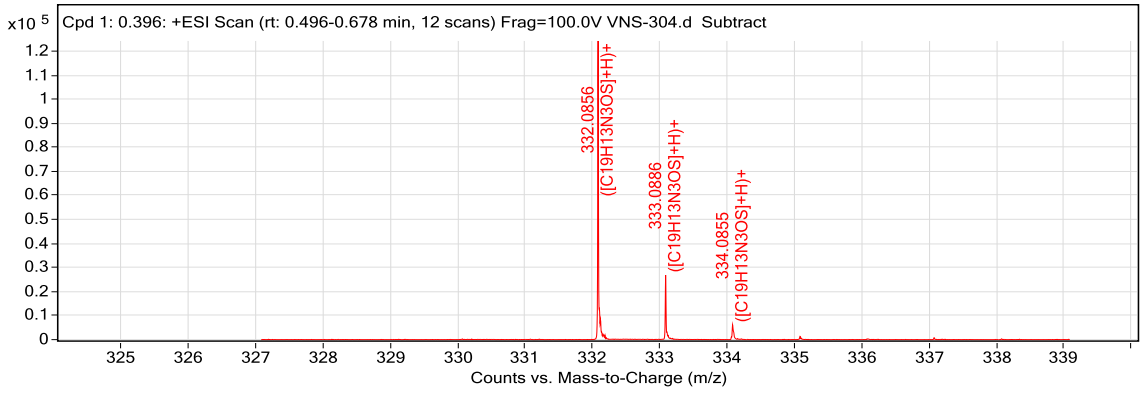
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.396	0.396	331.0783	125134	C19 H13 N3 O S	331.0779	1.15

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.396	332.0856	0.396	Find By Formula	331.0783



MS Zoomed Spectrum



MS Spectrum Peak List

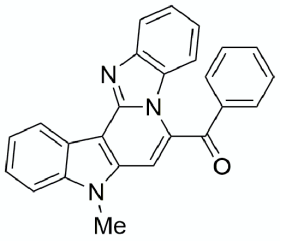
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
332.0856	332.0852	-1.03	1	125134.48	C19H13N3OS	(M+H)+
333.0886	333.0881	-1.37	1	26902.98	C19H13N3OS	(M+H)+

334.0855	334.0847	-2.44	1	6151.82	C19H13N3OS	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-310.d	**Sample Name**	VNS-310
Sample Type	Sample	**Position**	P1-F5
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min_reg.m	**Acquired Time**	10/16/2017 1:35:39 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



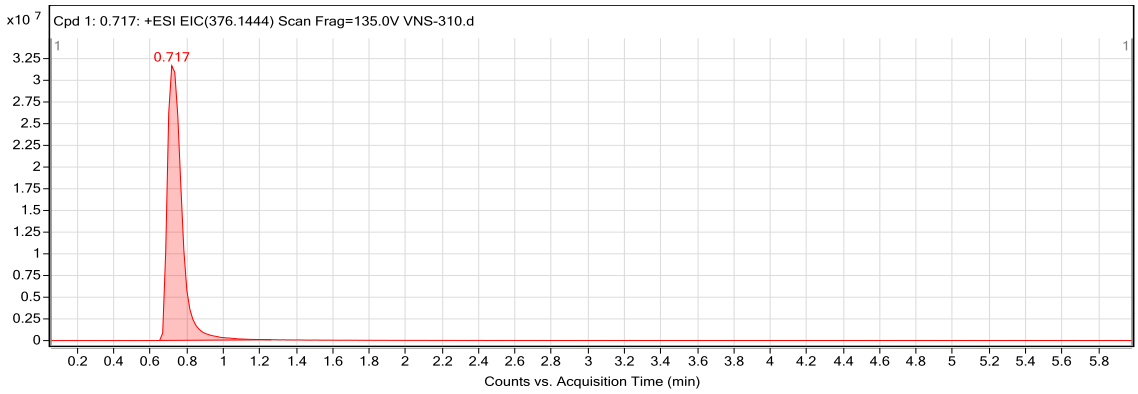
6ak

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

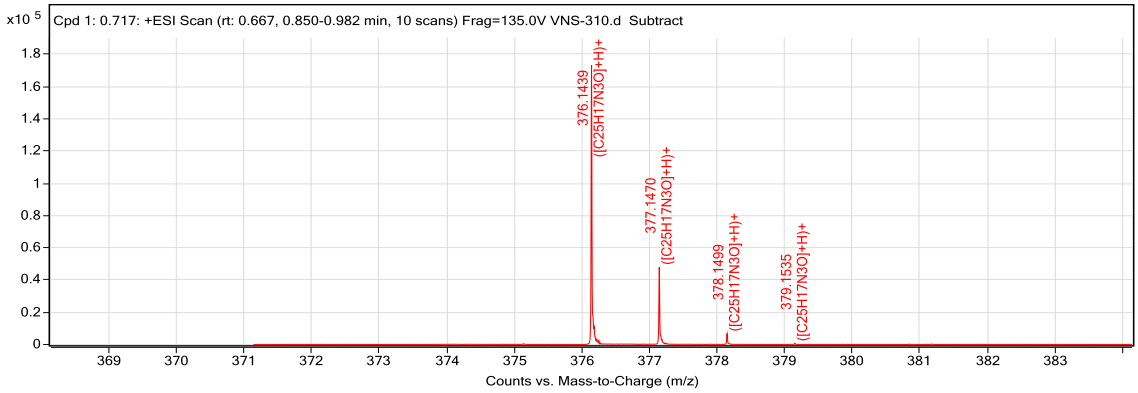
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.717	0.717	375.1366	173538	C25 H17 N3 O	375.1372	-1.51

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.717	376.1439	0.717	Find By Formula	375.1366



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
376.1439	376.1444	1.5	1	173537.87	C25H17N3O	(M+H)+
377.147	377.1476	1.49	1	48067.19	C25H17N3O	(M+H)+

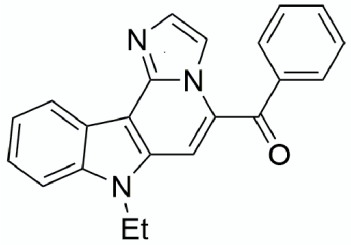
378.1499	378.1506	1.88	1	6761.76	C25H17N3O	(M+H)+
379.1535	379.1535	0.1	1	696.02	C25H17N3O	(M+H)+

--- End Of Report ---

HRMS Facility, BITS Pilani, Pilani Campus
Compound Report

Data File	VNS-408.d	**Sample Name**	VNS-408
Sample Type	Sample	**Position**	P2-F3
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_meoh_grad_6min_reg.m	**Acquired Time**	4/2/2018 11:55:13 AM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

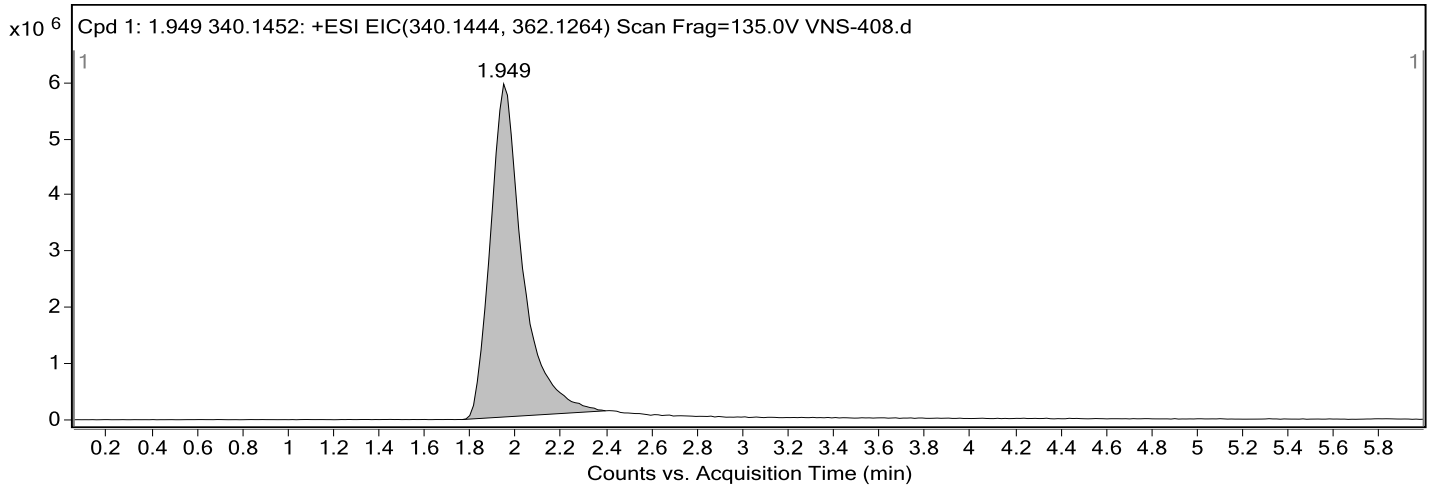


6ba

Compound Table

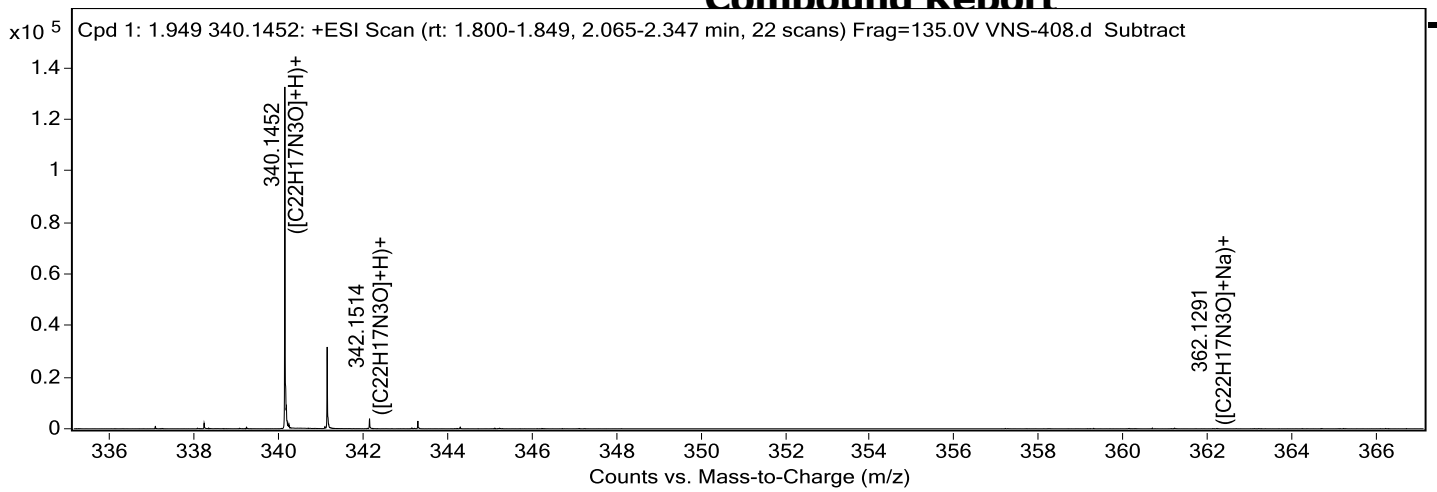
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 1.949 340.1452	1.949	339.1379	134267	C22 H17 N3 O	339.1372	2.24

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 1.949 340.1452	340.1452	1.949	Find By Formula	339.1379



MS Zoomed Spectrum

HRMS Facility, BITS Pilani, Pilani Campus
Compound Report



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
340.1452	340.1444	-2.11	1	134267.2	C22H17N3O	(M+H)+
341.1484	341.1475	-2.63	1	31758.67	C22H17N3O	(M+H)+
342.1514	342.1505	-2.67	1	3903.94	C22H17N3O	(M+H)+
343.1541	343.1534	-2.26	1	359.02	C22H17N3O	(M+H)+
362.1291	362.1264	-7.49	1	89.77	C22H17N3O	(M+Na)+

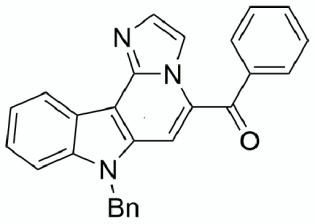
Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

---End Of Report---

Qualitative Compound Report

Data File	VNS-298.d	**Sample Name**	VNS-298
Sample Type	Sample	**Position**	P2-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	10/17/2017 5:29:38 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



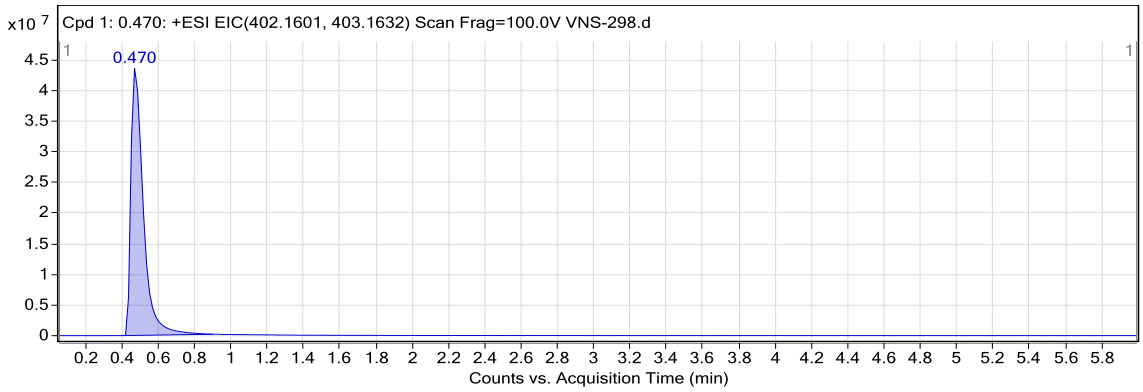
6ca

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

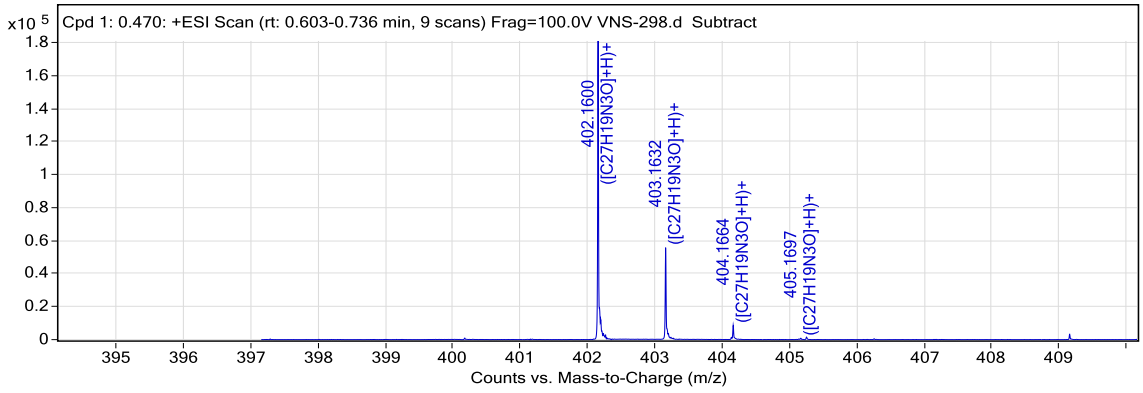
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.470	0.47	401.1528	182387	C27 H19 N3 O	401.1528	-0.15

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.470	402.16	0.47	Find By Formula	401.1528



MS Zoomed Spectrum



MS Spectrum Peak List

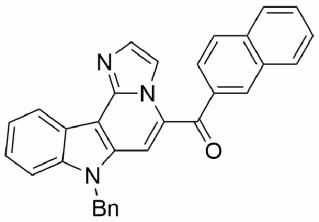
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
402.16	402.1601	0.2	1	182386.78	C27H19N3O	(M+H)+
403.1632	403.1632	0.03	1	55884.43	C27H19N3O	(M+H)+

404.1664	404.1663	-0.17	1	8579.77	C27H19N3O	(M+H)+
405.1697	405.1693	-1.02	1	866.82	C27H19N3O	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-307.d	**Sample Name**	VNS-307
Sample Type	Sample	**Position**	P2-A4
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	10/17/2017 5:57:59 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



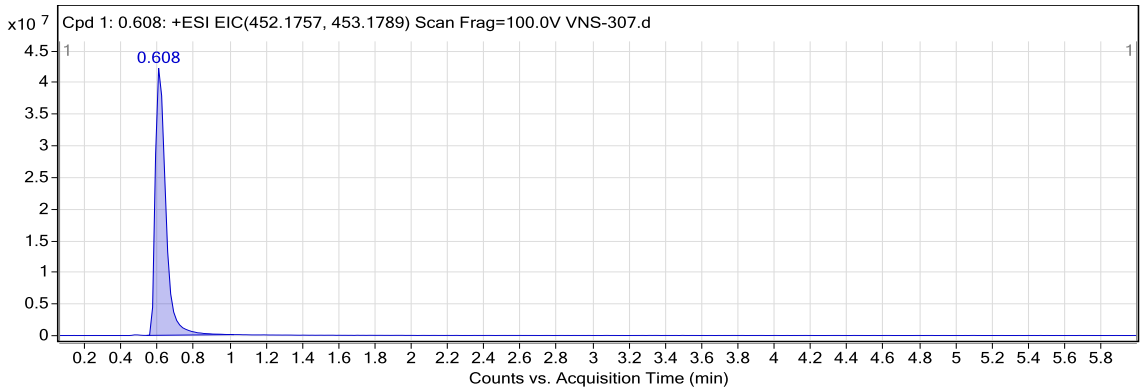
6cf

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

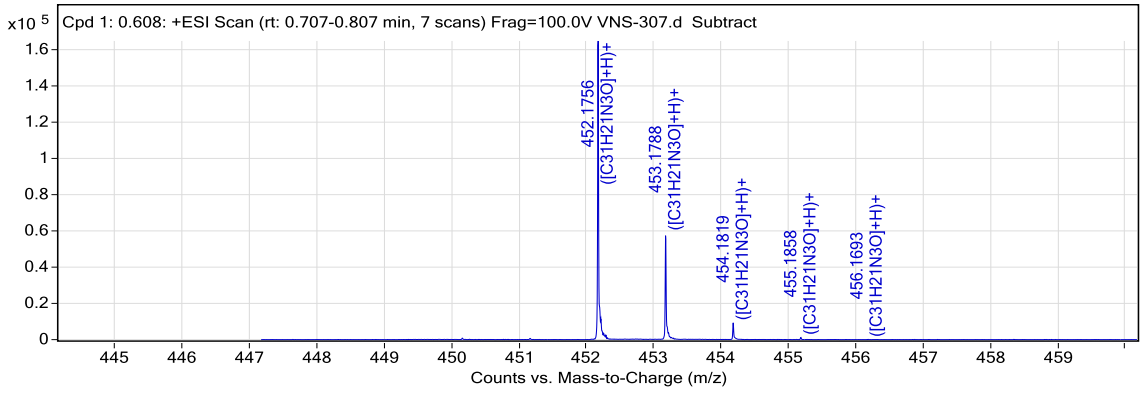
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.608	0.608	451.1683	169777	C31 H21 N3 O	451.1685	-0.37

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.608	452.1756	0.608	Find By Formula	451.1683



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
452.1756	452.1757	0.38	1	169776.58	C31H21N3O	(M+H)+
453.1788	453.1789	0.36	1	58692.47	C31H21N3O	(M+H)+

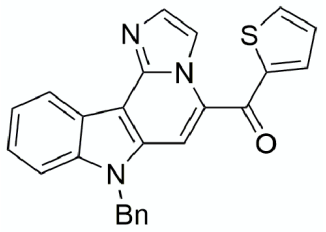
454.1819	454.182	0.21	1	9269.29	C31H21N3O	(M+H)+
455.1858	455.185	-1.71	1	1237.33	C31H21N3O	(M+H)+
456.1693	456.188	40.96	1	98.14	C31H21N3O	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-306.d	**Sample Name**	VNS-306
Sample Type	Sample	**Position**	P2-A10
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACNisocratic.m	**Acquired Time**	10/17/2017 7:23:03 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



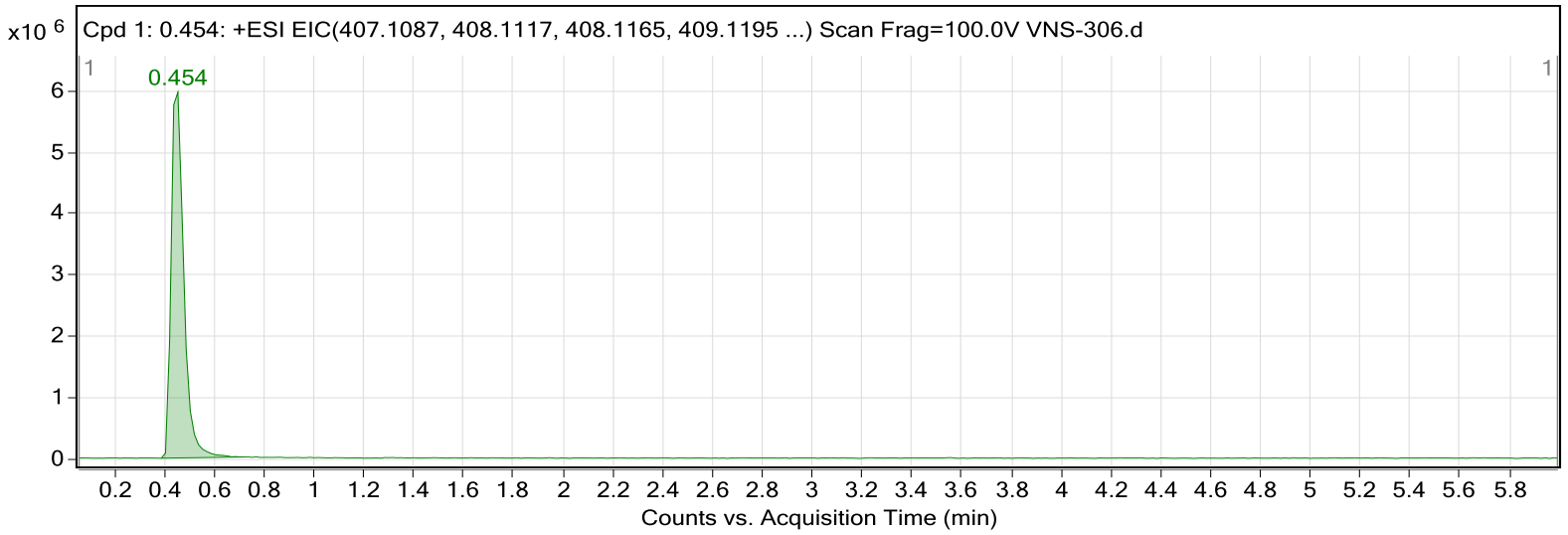
6cg

Compound Table

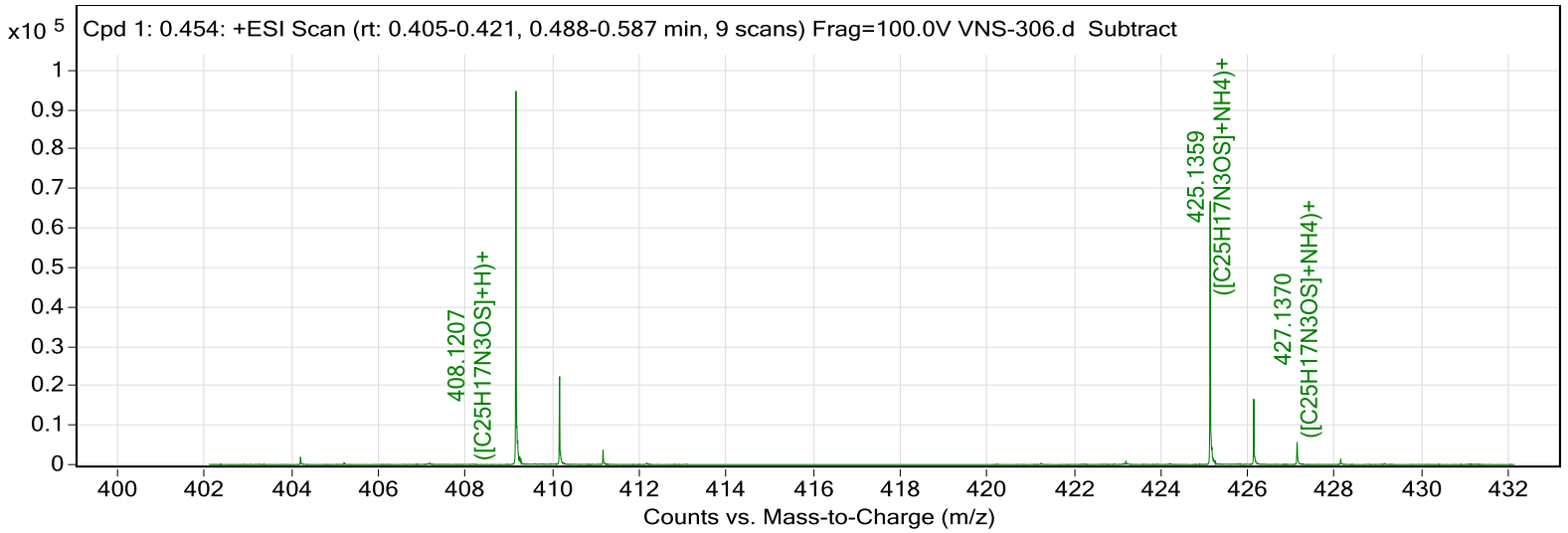
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.454	0.454	407.1022	68525	C25 H17 N3 O S	407.1092	-17.26

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.454	425.1359	0.454	Find By Formula	407.1022

Qualitative Compound Report



MS Zoomed Spectrum



MS Spectrum Peak List

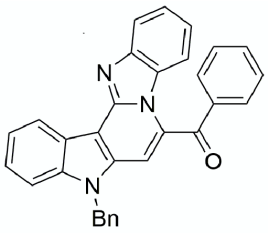
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
407.1024	407.1087	15.55	1	94.98	C25H17N3OS	M+

408.1207	408.1165	-10.24	1	100.96	C25H17N3OS	(M+H)+
425.1359	425.1431	16.84	1	68524.92	C25H17N3OS	(M+NH4)+
426.1394	426.146	15.51	1	16654.03	C25H17N3OS	(M+NH4)+
427.137	427.1438	15.99	1	5746.11	C25H17N3OS	(M+NH4)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-300.d	**Sample Name**	VNS-300
Sample Type	Sample	**Position**	P1-F4
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min_reg.m	**Acquired Time**	10/16/2017 1:21:26
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



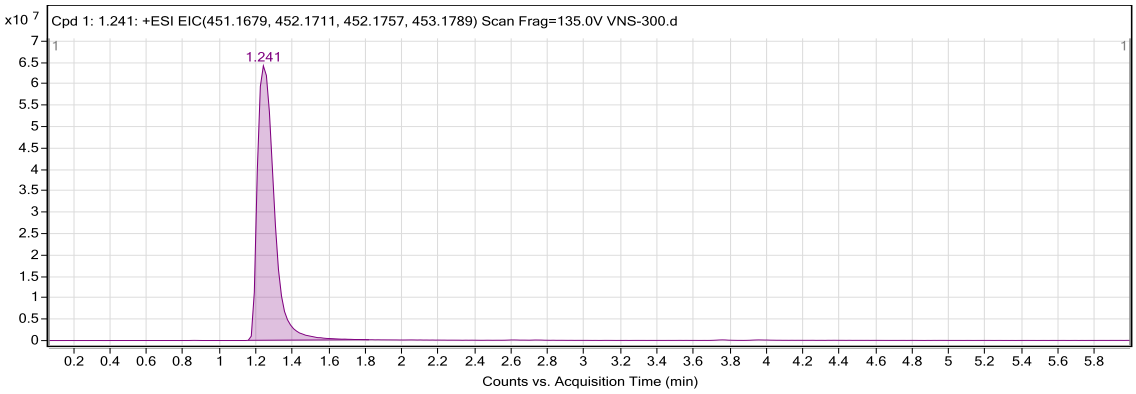
6ck

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

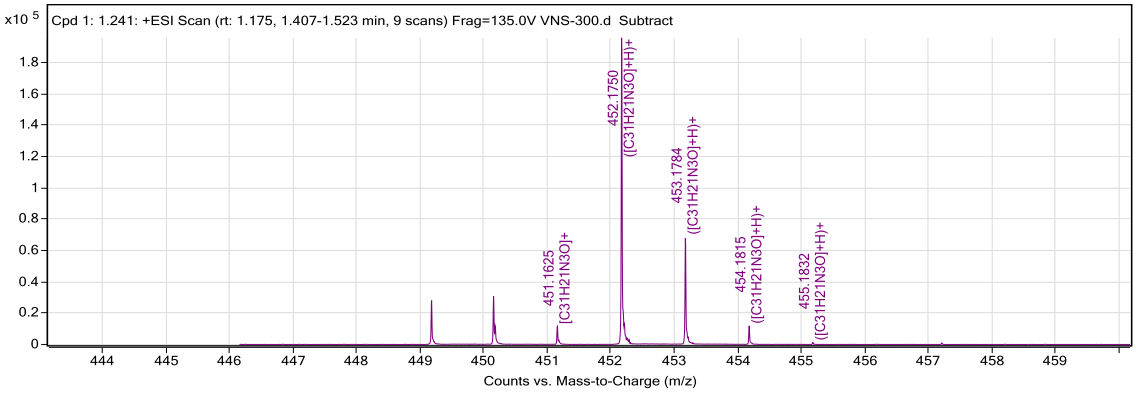
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 1.241	1.241	451.1676	199667	C31 H21 N3 O	451.1685	-1.99

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 1.241	452.175	1.241	Find By Formula	451.1676



MS Zoomed Spectrum



MS Spectrum Peak List

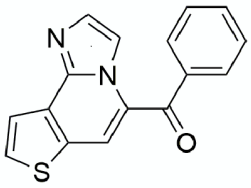
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
451.1625	451.1679	12.05	1	11670.51	C31H21N3O	M+
452.175	452.1757	1.72	1	199666.93	C31H21N3O	(M+H)+

453.1784	453.1789	1.14	1	68832.83	C31H21N3O	(M+H)+
454.1815	454.182	1.16	1	11934.04	C31H21N3O	(M+H)+
455.1832	455.185	4.02	1	1256.98	C31H21N3O	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-192.d	**Sample Name**	VNS-192
Sample Type	Sample	**Position**	P2-F10
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min_reg.m	**Acquired Time**	10/12/2017 7:09:13 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



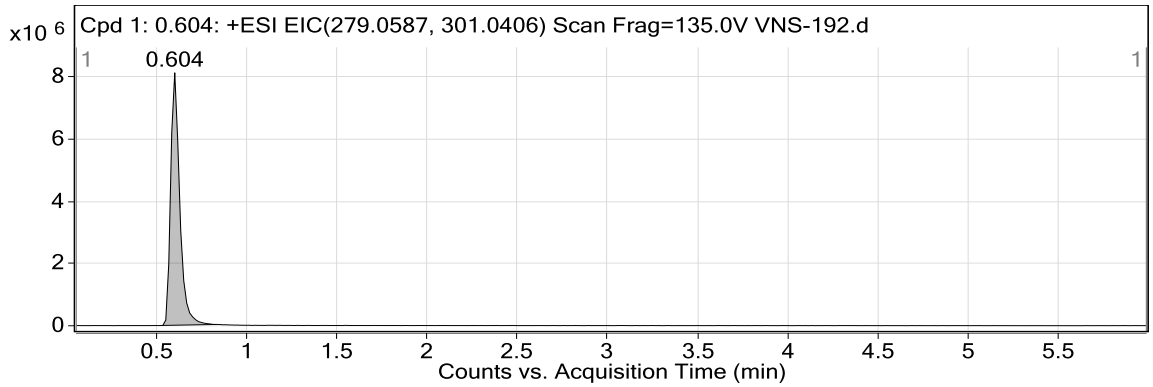
8aa

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

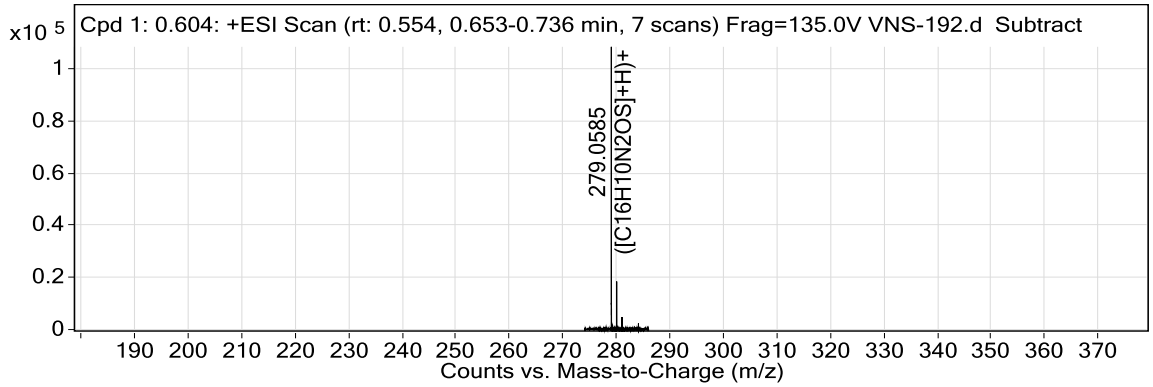
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.604	0.604	278.0511	108781	C16 H10 N2 O S	278.0514	-0.91

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.604	279.0585	0.604	Find By Formula	278.0511



MS Zoomed Spectrum



MS Spectrum Peak List

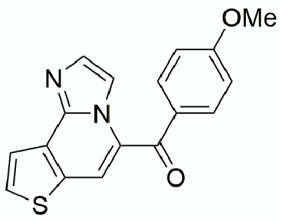
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
279.0585	279.0587	0.72	1	108781.22	C16H10N2OS	(M+H)+
280.0615	280.0616	0.33	1	18784.48	C16H10N2OS	(M+H)+

281.0554	281.0574	7.32	1	4883.85	C16H10N2OS	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	VNS-317.d	**Sample Name**	VNS-317
Sample Type	Sample	**Position**	P2-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min_reg.m	**Acquired Time**	11/27/2017 12:14:04 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



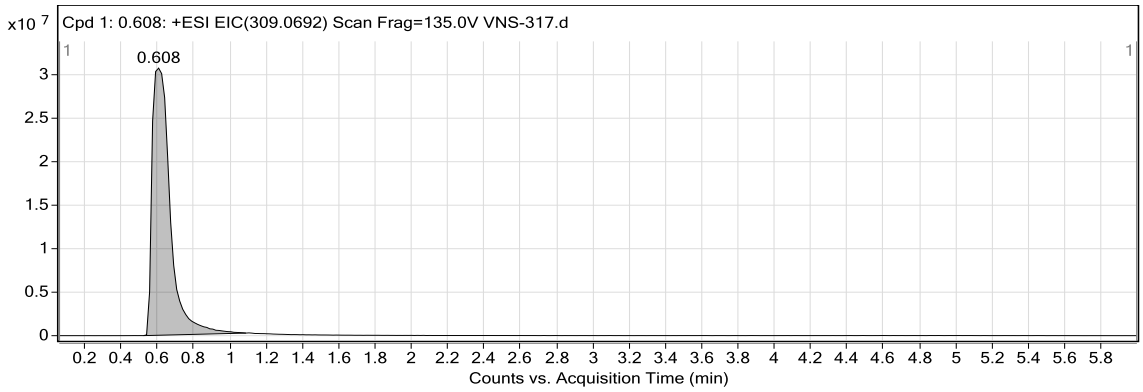
8ac

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

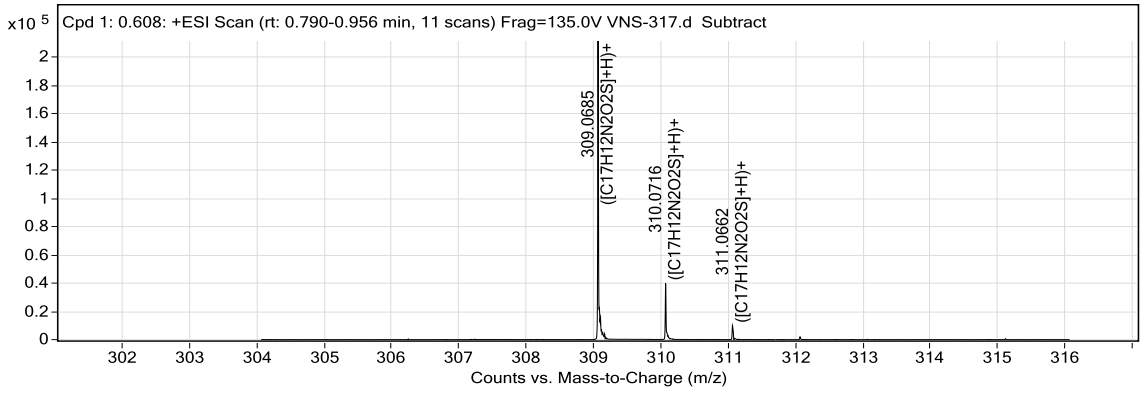
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.608	0.608	308.0612	213340	C17 H12 N2 O2 S	308.0619	-2.49

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.608	309.0685	0.608	Find By Formula	308.0612



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
309.0685	309.0692	2.37	1	213340.44	C17H12N2O2S	(M+H)+
310.0716	310.0722	1.87	1	40240.71	C17H12N2O2S	(M+H)+

311.0662	311.0684	7.08	1	10086.35	C17H12N2O2S	(M+H)+

--- End Of Report ---

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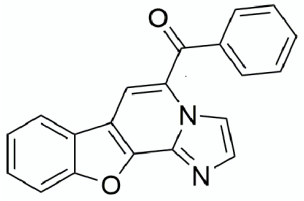
Compound Report

Data File	VNS-405.d	**Sample Name**	VNS-405
Sample Type	Sample	**Position**	P2-B6
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_acn_grad_6min_reg.m	**Acquired Time**	3/22/2018 5:01:57 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)



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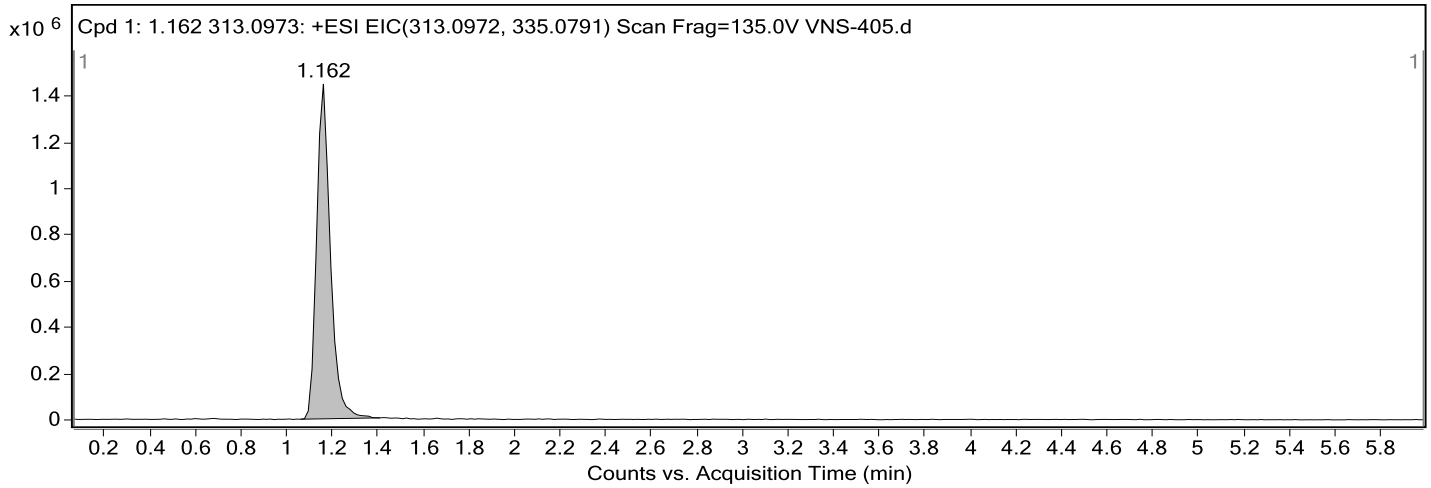
Compound Table

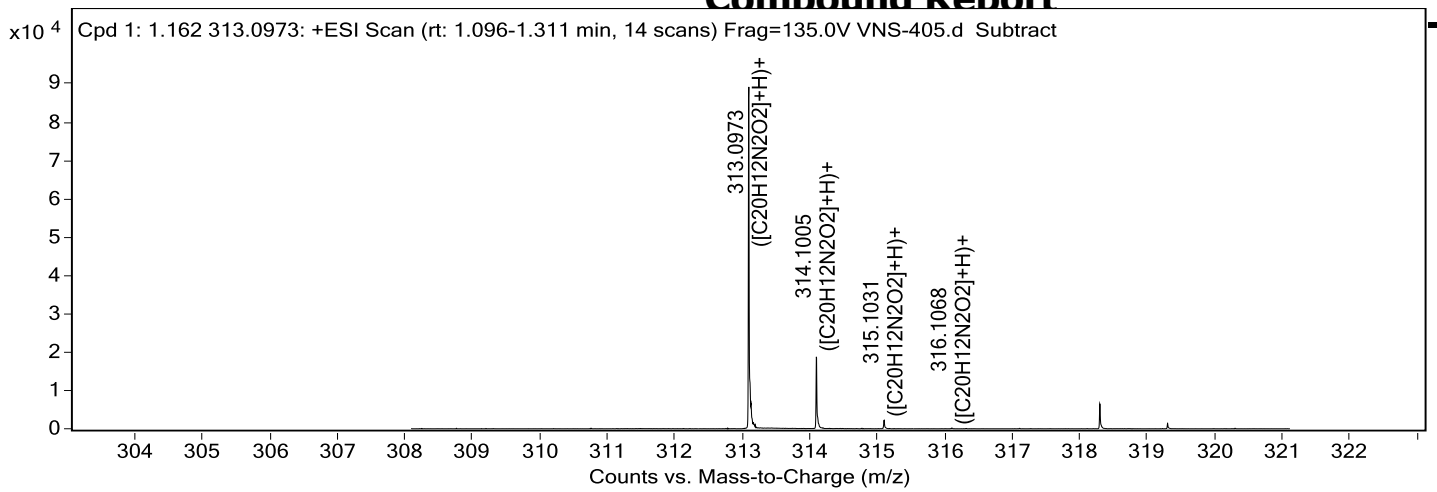
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 1.162 313.0973	1.162	312.09	91565	C20 H12 N2 O2	312.0899	0.34

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 1.162 313.0973	313.0973	1.162	Find By Formula	312.09



MS Zoomed Spectrum

HRMS Facility, BITS Pilani, Pilani Campus
Compound Report



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
313.0973	313.0972	-0.31	1	91565.14	C20H12N2O2	(M+H)+
314.1005	314.1003	-0.56	1	19327.24	C20H12N2O2	(M+H)+
315.1031	315.1032	0.34	1	2291.82	C20H12N2O2	(M+H)+
316.1068	316.1059	-2.84	1	216.83	C20H12N2O2	(M+H)+

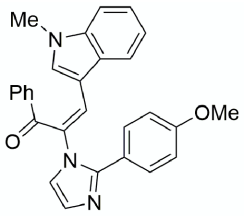
Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

Note: Please acknowledge the work done by HRMS Facility at BITS Pilani, Pilani Campus funded by DST-FIST in your publication.

---End Of Report---

Qualitative Compound Report

Data File	VNS-287.d	**Sample Name**	VNS-287
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	water_meoh_grad_6min_reg.m	**Acquired Time**	1/23/2018 5:52:24 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			



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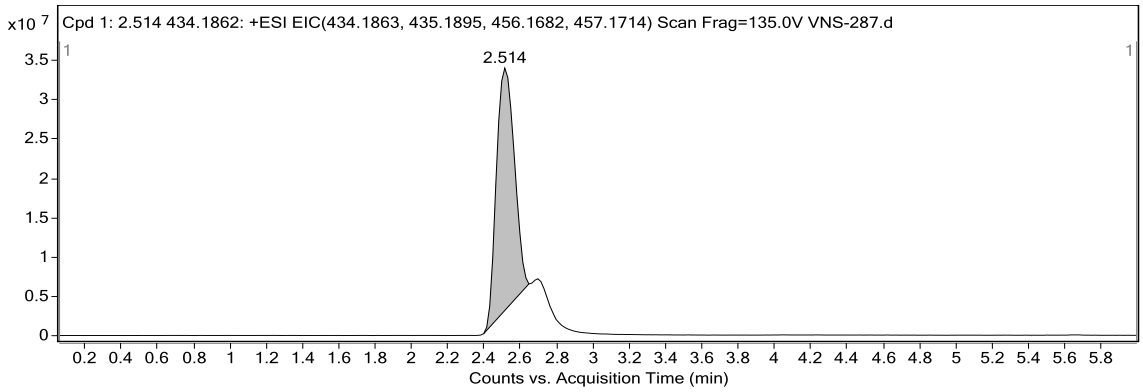
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

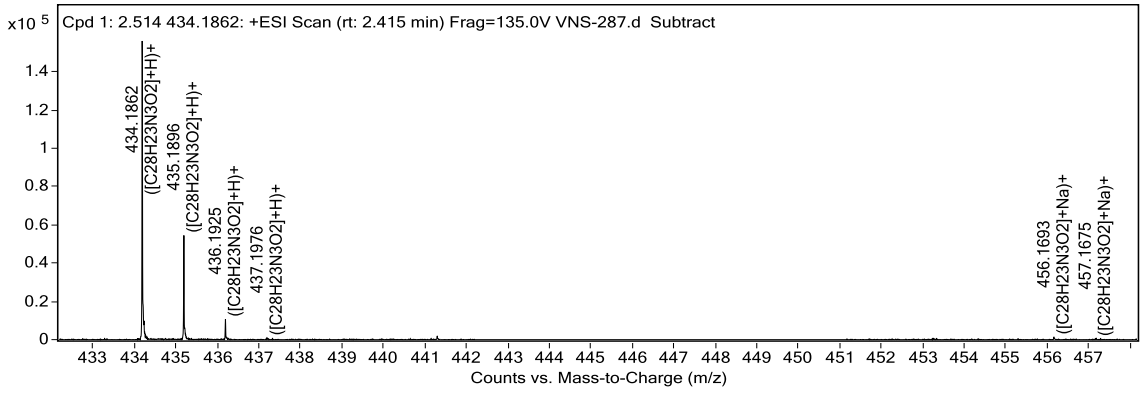
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 2.514 434.1862	2.514	433.179	159144	C28 H23 N3 O2	433.179	0

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 2.514 434.1862	434.1862	2.514	Find By Formula	433.179



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
434.1862	434.1863	0.13	1	159143.82	C28H23N3O2	(M+H)+
435.1896	435.1895	-0.33	1	54569.84	C28H23N3O2	(M+H)+

436.1925	436.1925	0.02	1	10673.36	C28H23N3O2	(M+H)+
437.1976	437.1953	-5.17	1	924.88	C28H23N3O2	(M+H)+
456.1693	456.1682	-2.35	1	1394.65	C28H23N3O2	(M+Na)+
457.1675	457.1714	8.62	1	525.93	C28H23N3O2	(M+Na)+
458.1717	458.1744	5.8	1	87.78	C28H23N3O2	(M+Na)+

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