# **Supplementary File**

### **Fragment Patron OIC1C and OIC1MS**

$$H_2N \longrightarrow N \longrightarrow NH_2$$

m/z: 1032.72 (100.0%), 1033.72 (74.8%), 1034.72 (27.5%), 1035.73 (6.7%), 1036.73 (1.4%)

m/z: [ M-748 ]

Fragment patron OIC1C and OIC1MS

### Fragment Patron OIC2C and OIC2MS

m/z: 1296.81 (100.0%), 1297.82 (95.4%), 1298.82 (45.9%), 1299.82 (15.8%), 1300.83 (3.2%), 1297.81 (2.2%), 1298.81 (2.1%)

m/z: 570.28 (100.0%), 571.28 (45.1%), 572.29 (9.3%), 573.29 (1.3%)

m/z: 372.16 (100.0%), 373.17 (29.4%), 374.17 (4.2%)

[M-100]

### **Qualitative Analysis Report of OIC1C**

# **Qualitative Analysis Report**

 Data Filename
 OT292\_ID\_1\_CHCL3.d
 Sample Name
 OIC1C

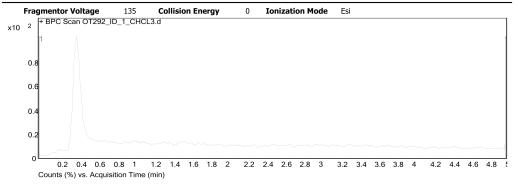
 Sample Type
 Sample
 Position
 P1-F4

 Instrument Name
 Instrument 1
 User Name

 Acq Method
 ESI\_POS\_SCAN\_100AC N-ID.m
 IRM Calibration Status Success
 Success

 DA Method
 ESI-NEG\_FLAV\_MGV.m
 Comment

### **User Chromatograms**



#### **User Spectra**

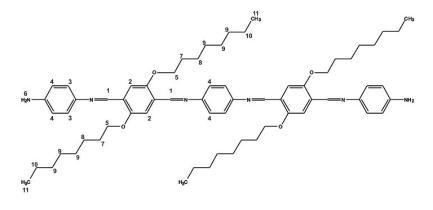
Fragmentor Voltage	Collision Energy	Ionization Mode				
135	0	Esi				
0 2 + Scan (0.304-0.599 mi	in, 60 scans) OT292_ID_1_CF	HCL3.d				
1	286					
0.8		571				
0.6						
0.4						
0.2						
108 213	345	615 660				
0 100 200 Counts (%) vs. Mass-to	300 400	500 600 700	800	900	1000	1100

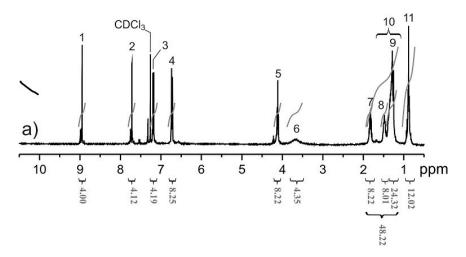
Peak List

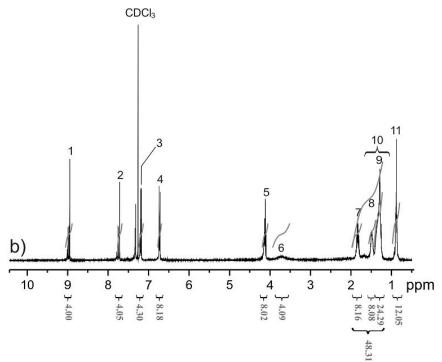
m/z	z	Abund.
102		22194
108		28342
109		26047
135	2	21836
213		24040
286		272724
481		26897
571		218979
572	1	25956
572	1	62412

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# OIC1MS-1H-NMR







### **Qualitative Analysis Report of OIC1MS**

# **Qualitative Analysis Report**

 Data Filename
 OT290\_ID\_CHCL3\_1.d
 Sample Name
 OIC1MS

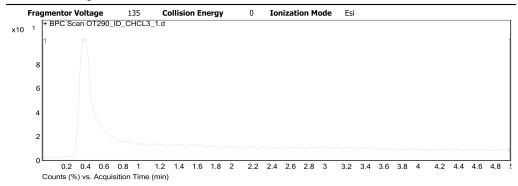
 Sample Type
 Sample
 Position
 P1-F2

 Instrument Name
 Instrument 1
 User Name

 Acq Method
 ESI\_POS\_SCAN\_100AC N-ID.m
 IRM Calibration Status
 Success

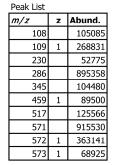
 DA Method
 ESI\_NEG\_FLAV\_MGV.m
 Comment

#### **User Chromatograms**



#### **User Spectra**

ge Collis	sion Energy	Ioniz	ation Mode				
	0		Esi				
0.814 min, 104 scans	s) OT290_ID_CI	HCL3_1.d					
286		5	71				
	345	517					
220	400	500	600 700	800	900	1000	1100
•	0.814 min, 104 scan 286	0 0.814 min, 104 scans) OT290_ID_Cl 286 286	0 0.814 min, 104 scans) OT290_ID_CHCL3_1.d 286 5 286 5	0 Esi 0.814 min, 104 scans) OT290_ID_CHCL3_1.d  286 571  286 571	0 Esi 0.814 min, 104 scans) OT290_ID_CHCL3_1.d  286 571  286 571	0 Esi  0.814 min, 104 scans) OT290_ID_CHCL3_1.d  286 571  286 571	0 Esi  0.814 min, 104 scans) OT290_ID_CHCL3_1.d  286 571  286 571



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### **Qualitative Analysis Report of OIC2C**

# **Qualitative Analysis Report**

 Data Filename
 OT294\_ID\_CHCL3\_1.d
 Sample Name
 0IC2C

Sample TypeSamplePositionP1-F6

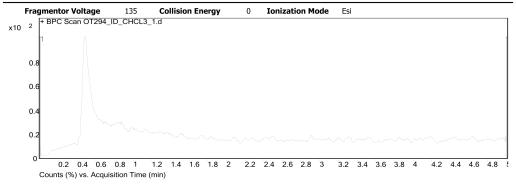
Instrument Name Instrument 1 User Name

Acq Method ESI\_POS\_SCAN\_100AC IRM Calibration Status

N-ID.m

**DA Method** ESI-NEG\_FLAV\_MGV.m **Comment** 

### **User Chromatograms**



#### **User Spectra**

Fragmentor Volt	age	Collision Ene	ergy I	onization Mo	de				
135		0		Esi					
x10 <sup>2</sup> + Scan (0.389	-0.679 min, 5	9 scans) OT294	_ID_CHCL3_1.d						
1	197								
0.8									
0.6									
0.4 102	225			571					
0.2		275 374			74	7			
0 136	200	300 4	481 00 500	609	700	800	900	1000	1100
Counts (%) vs			00 500	300	700	800	900	1000	1100

#### Peak List

m/z	z	Abund.
102		35402
197	1	93105
225	1	35414
247		16949
275	1	22885
374		24116
569		28743
571		19448
571	1	34728
747		18376

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### **Qualitative Analysis Report of OIC2MS**

# **Qualitative Analysis Report**

 Data Filename
 OT293\_ID\_1\_CHCL3.d
 Sample Name
 OIC2MS

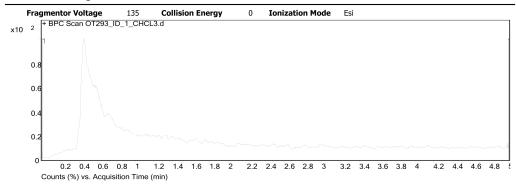
 Sample Type
 Sample
 Position
 P1-F5

 Instrument Name
 Instrument 1
 User Name

 Acq Method
 ESI\_POS\_SCAN\_100AC N-ID.m
 IRM Calibration Status Comment
 Success

 DA Method
 ESI-NEG\_FLAV\_MGV.m
 Comment

#### **User Chromatograms**



#### **User Spectra**

Fragmentor Voltage	Collision Energy	Ionization Mode				
135	0	Esi				
10 <sup>2</sup> + Scan (0.339-0.799 min	, 93 scans) OT293_ID_1_CI	HCL3.d				
1						
0.8						
0.6						
0.4						
0.2 149 225	301 <sub>374</sub>	571 659 659	747			
0 100 200	300 400	500 600 7	00 800	900	1000	1100

r dart Eloc						
m/z	z	Abund.				
149		29365				
196		51949				
197	2	152117				
225	2	39366				
247	1	36498				

Peak List

197	2	152117
225	2	39366
247	1	36498
287		29097
301	1	43953
315	1	25483
374		40382
571		27394

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# OIC2MS-1H-NMR

