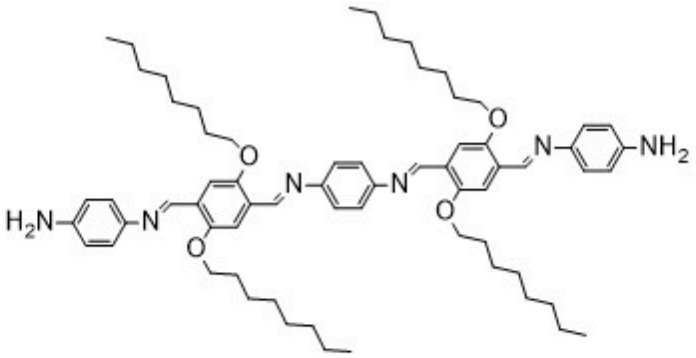
Supplementary File

Fragment Patron OIC1C and OIC1MS



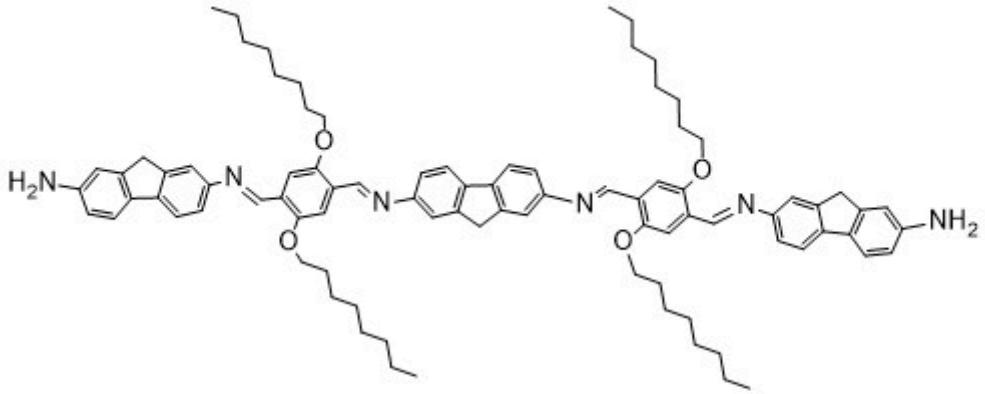
m/z: 1032.72 (100.0%), 1033.72 (74.8%), 1034.72 (27.5%), 1035.73 (6.7%), 1036.73 (1.4%)

m/z: 284.13 (100.0%), 285.13 (22.4%), 286.14 (2.3%)

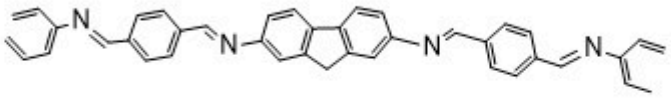
m/z: [M-748]

Fragment patron OIC1C and OIC1MS

Fragment Patron OIC2C and OIC2MS

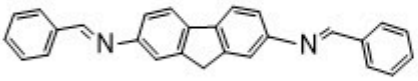


m/z: 1296.81 (100.0%), 1297.82 (95.4%), 1298.82 (45.9%), 1299.82 (15.8%), 1300.83 (3.2%), 1297.81 (2.2%), 1298.81 (2.1%)



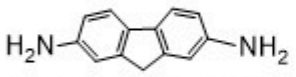
m/z: 570.28 (100.0%), 571.28 (45.1%), 572.29 (9.3%), 573.29 (1.3%)

[M-726]



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

[M-923]



m/z: 196.10 (100.0%), 197.10 (14.8%)

[M-100]

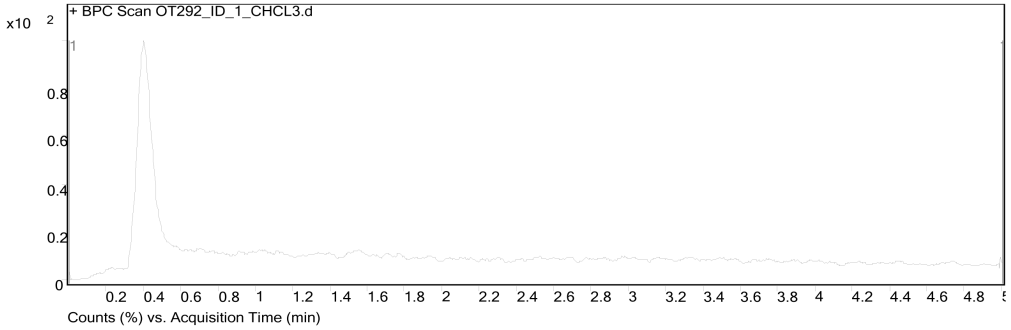
Qualitative Analysis Report of OIC1C

Qualitative Analysis Report

Data Filename	OT292_ID_1_CHCL3.d	**Sample Name**	0IC1C
Sample Type	Sample	**Position**	P1-F4
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI_POS_SCAN_100ACN-ID.m	**IRM Calibration Status**	Success
DA Method	ESI-NEG_FLAV_MGV.m	**Comment**	

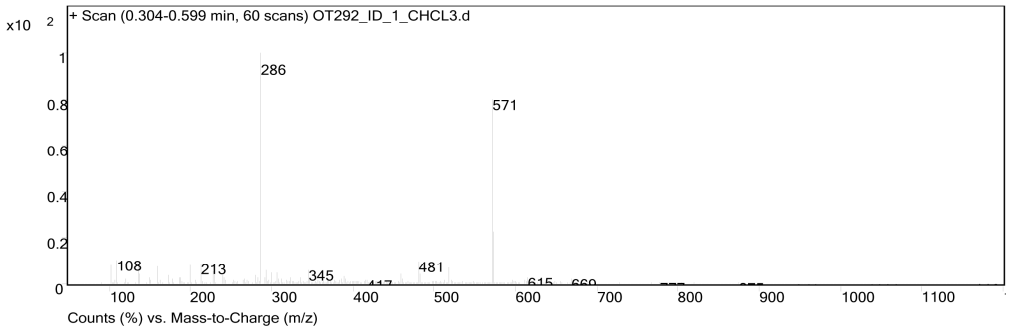
User Chromatograms

Fragmentor Voltage 135 **Collision Energy** 0 **Ionization Mode** Esi



User Spectra

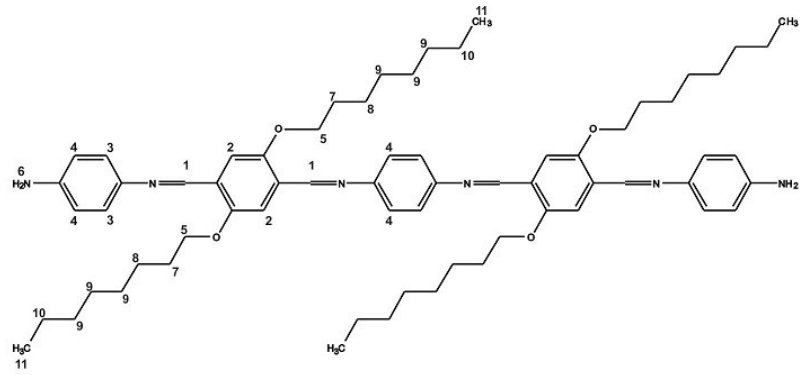
Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	Esi

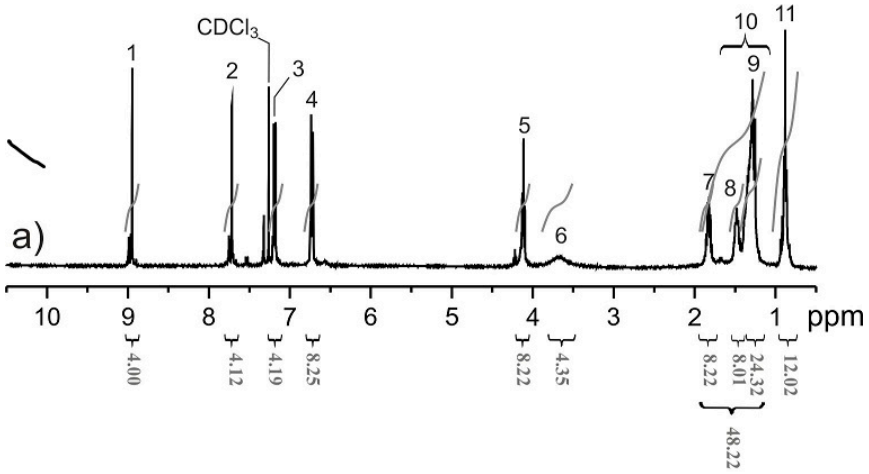


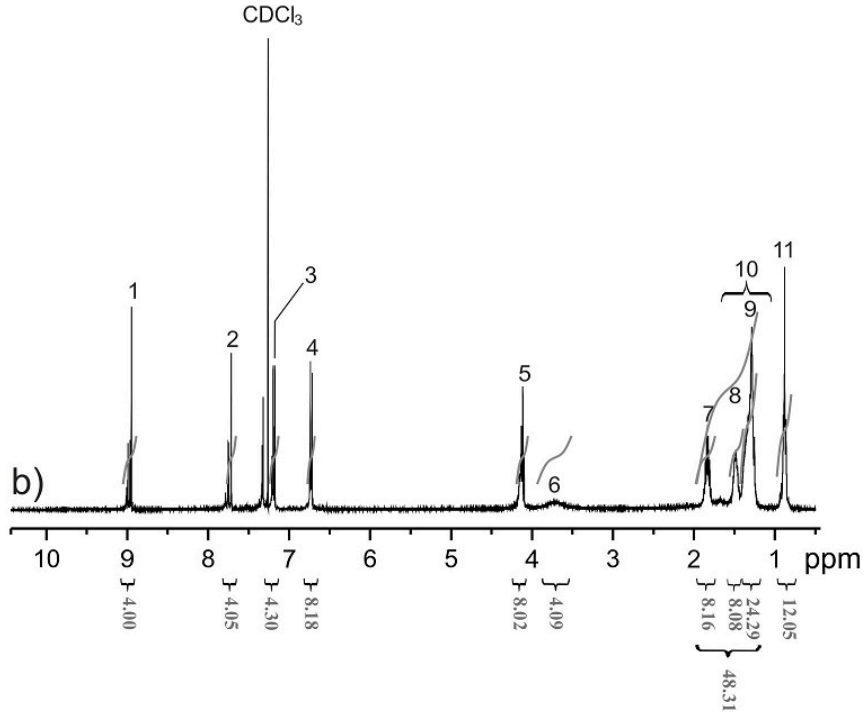
Peak List

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

OIC1MS-1H-NMR







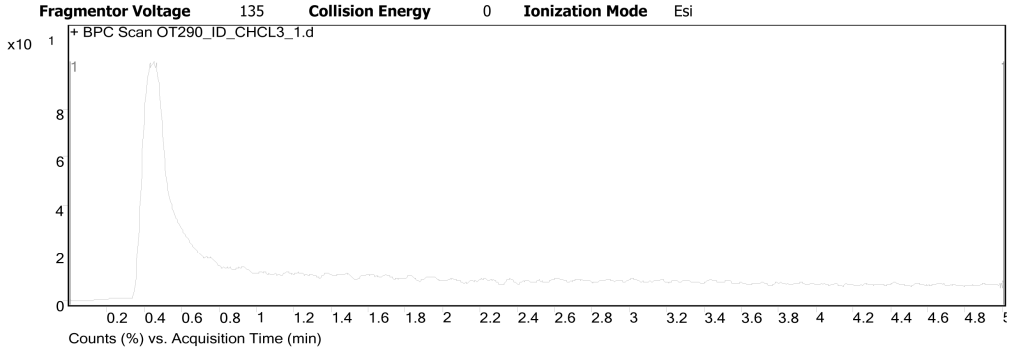
Qualitative Analysis Report of OIC1MS

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_100ACN-ID.m	**IRM Calibration Status**	Success
DA Method	ESI-NEG_FLAV_MGV.m	**Comment**	

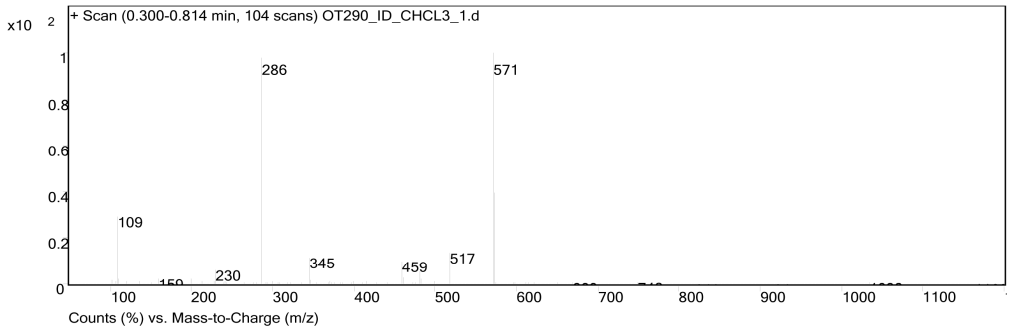
User Chromatograms

Fragmentor Voltage 135 **Collision Energy** 0 **Ionization Mode** Esi



User Spectra

Fragmentor Voltage 135 **Collision Energy** 0 **Ionization Mode** Esi



Peak List

m/z	z	Abund.
108		105085
109	1	268831
230		52775
286		895358
345		104480
459	1	89500
517		125566
571		915530
572	1	363141
573	1	68925

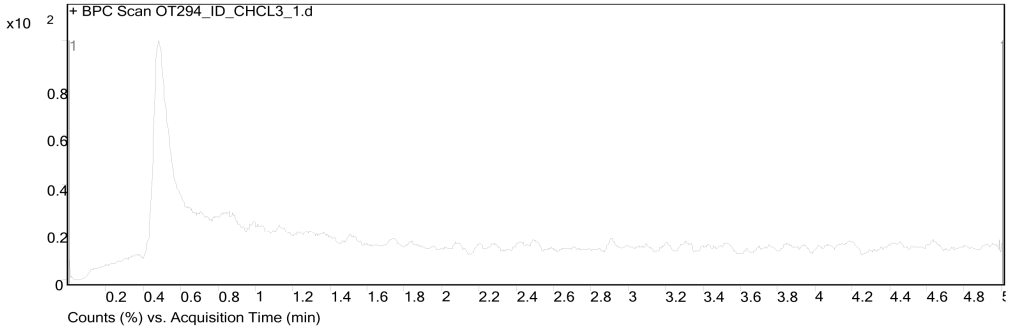
Qualitative Analysis Report of OIC2C

Qualitative Analysis Report

Data Filename	OT294_ID_CHCL3_1.d	**Sample Name**	0IC2C
Sample Type	Sample	**Position**	P1-F6
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI_POS_SCAN_100ACN-ID.m	**IRM Calibration Status**	Success
DA Method	ESI-NEG_FLAV_MGV.m	**Comment**	

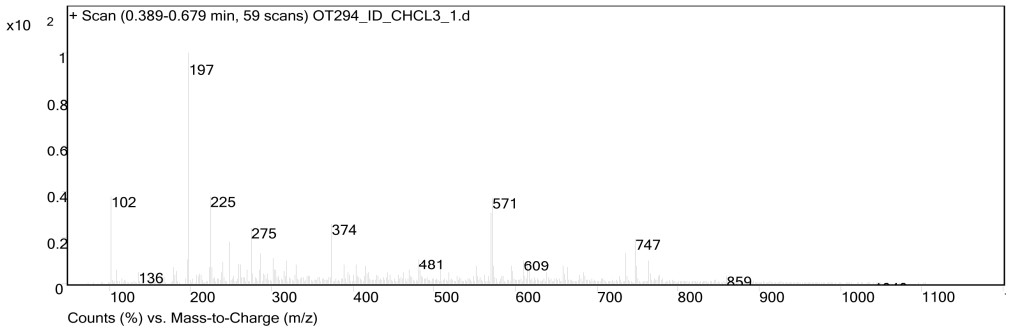
User Chromatograms

Fragmentor Voltage 135 **Collision Energy** 0 **Ionization Mode** Esi



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	Esi



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

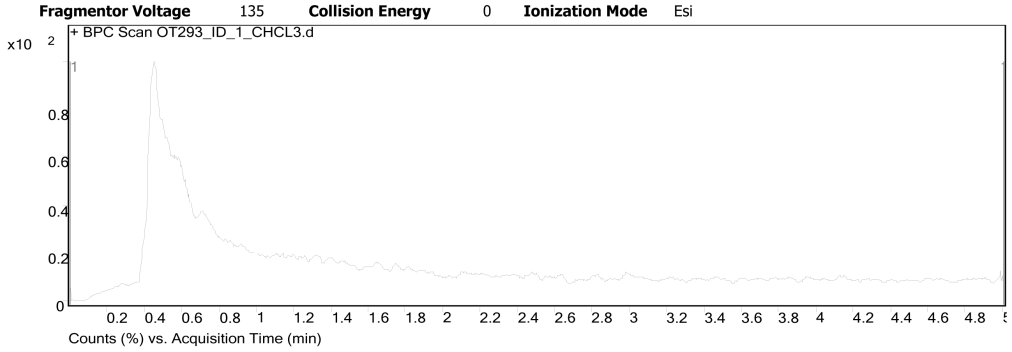
Qualitative Analysis Report of OIC2MS

Qualitative Analysis Report

Data Filename	OT293_ID_1_CHCL3.d	**Sample Name**	0IC2MS
Sample Type	Sample	**Position**	P1-F5
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI_POS_SCAN_100ACN-ID.m	**IRM Calibration Status**	Success
DA Method	ESI-NEG_FLAV_MGV.m	**Comment**	

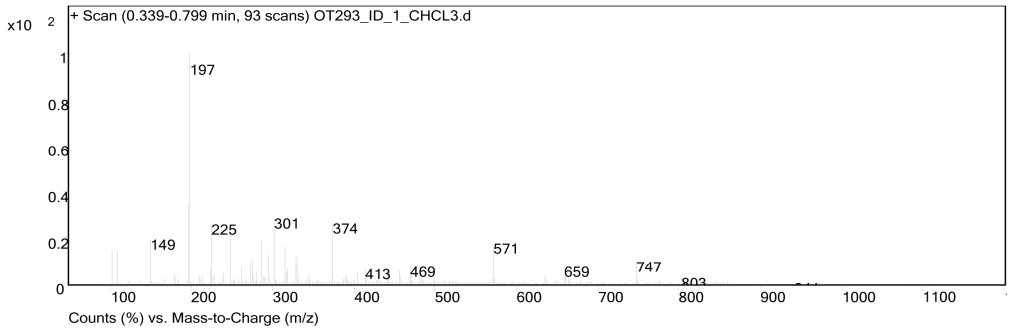
User Chromatograms

Fragmentor Voltage 135 **Collision Energy** 0 **Ionization Mode** Esi



User Spectra

Fragmentor Voltage 135 **Collision Energy** 0 **Ionization Mode** Esi



Peak List

m/z	z	Abund.
149		29365
196		51949
197	2	152117
225	2	39366
247	1	36498
287		29097
301	1	43953
315	1	25483
374		40382
571		27394

OIC2MS-1H-NMR