

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
 Data File : VN074554.D
 Acq On : 17 Sep 2022 14:27
 Operator : JC\MD
 Sample : N4648-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 N48854-1040

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
 Title : SW846 8260

Signal : TIC: VN074554.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	48	53	60	rBV2	193102	362833	21.07%	3.110%
2	2.687	130	136	141	rBV3	53310	132324	7.69%	1.134%
3	3.187	219	221	231	rVB6	32459	69648	4.05%	0.597%
4	4.234	390	399	407	rBV2	18067	50307	2.92%	0.431%
5	4.710	468	480	496	rBV2	143790	494055	28.70%	4.235%
6	5.010	517	531	544	rBV3	69428	227817	13.23%	1.953%
7	7.622	967	975	985	rVB4	11751	30883	1.79%	0.265%
8	7.951	1021	1031	1036	rBV	239672	563117	32.71%	4.827%
9	8.016	1036	1042	1052	rVB	369703	830425	48.23%	7.119%
10	8.375	1092	1103	1116	rBV	266853	642163	37.30%	5.505%
11	8.904	1184	1193	1205	rBV	583829	1224958	71.15%	10.501%
12	10.274	1421	1426	1430	rVB5	11590	21272	1.24%	0.182%
13	10.380	1436	1444	1452	rBV	950786	1721709	100.00%	14.760%
14	10.445	1452	1455	1460	rVB3	17206	28009	1.63%	0.240%
15	11.686	1655	1666	1677	rBV	937064	1632033	94.79%	13.991%
16	11.786	1678	1683	1690	rVB3	16609	33048	1.92%	0.283%
17	11.892	1695	1701	1710	rVB3	29176	61031	3.54%	0.523%
18	12.221	1751	1757	1765	rBV5	23199	47848	2.78%	0.410%
19	12.298	1765	1770	1775	rBV5	12782	20963	1.22%	0.180%
20	12.674	1826	1834	1844	rBV	750319	1274109	74.00%	10.923%
21	12.998	1884	1889	1893	rVB7	11138	18797	1.09%	0.161%
22	13.310	1937	1942	1946	rVB4	14550	23358	1.36%	0.200%
23	13.615	1987	1994	2002	rVV	942704	1545935	89.79%	13.253%
24	13.674	2002	2004	2011	rVB6	13223	21683	1.26%	0.186%
25	14.368	2117	2122	2126	rBV5	12792	22665	1.32%	0.194%
26	14.509	2140	2146	2150	rVB6	12681	25288	1.47%	0.217%
27	14.804	2190	2196	2201	rVV5	28804	56694	3.29%	0.486%
28	14.857	2201	2205	2211	rVV8	10330	19913	1.16%	0.171%
29	15.133	2247	2252	2257	rBV6	16726	33473	1.94%	0.287%
30	15.204	2259	2264	2272	rVV9	29669	68922	4.00%	0.591%
31	15.280	2272	2277	2281	rVB6	10094	19302	1.12%	0.165%
32	15.439	2297	2304	2310	rBV	151660	289515	16.82%	2.482%
33	16.268	2436	2445	2449	rBV8	10315	28016	1.63%	0.240%
34	16.739	2518	2525	2531	rBV8	11664	22825	1.33%	0.196%

Sum of corrected areas: 11664938

Instrument :

MSVOA_N

ClientSampleId :

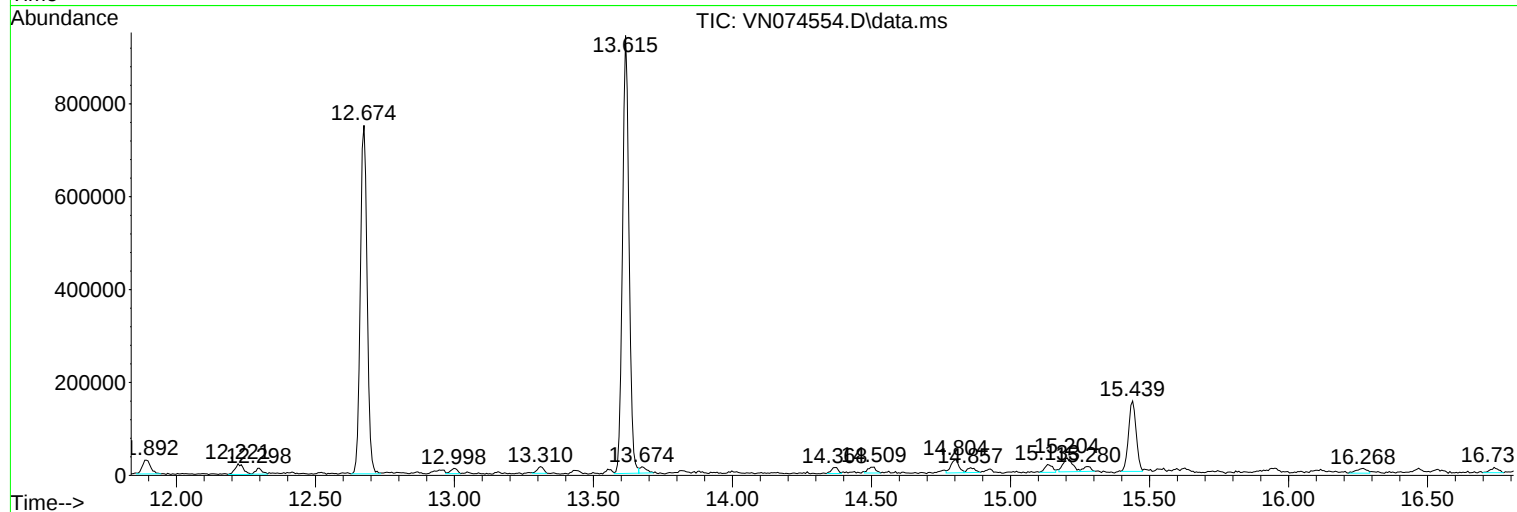
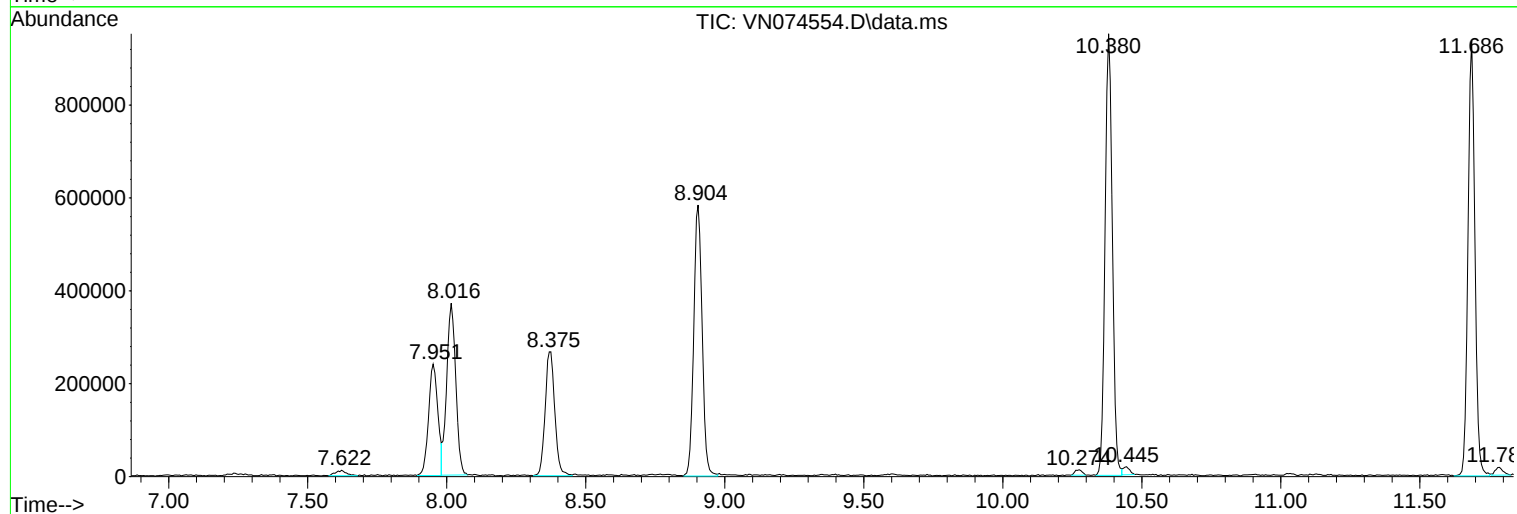
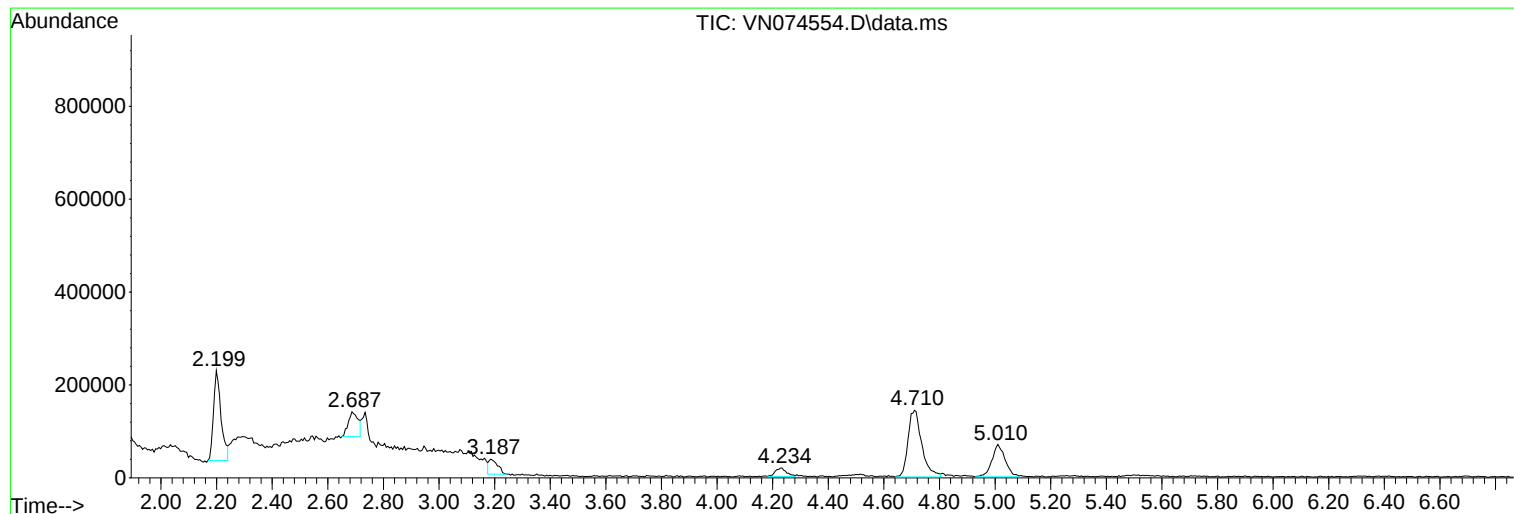
N48854-1040

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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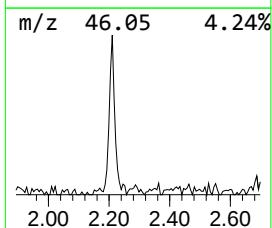
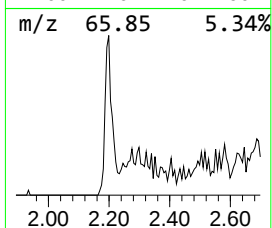
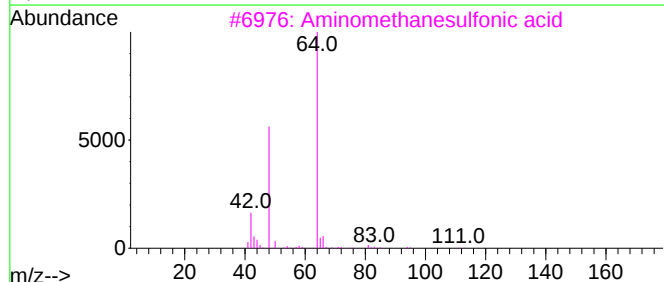
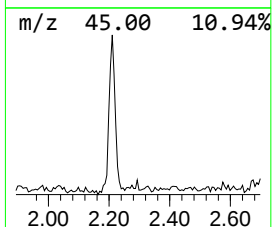
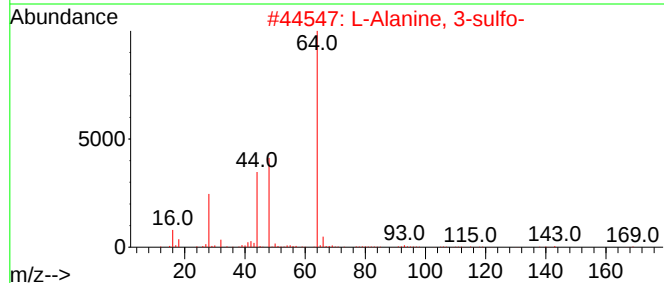
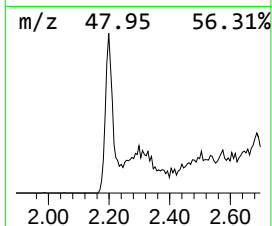
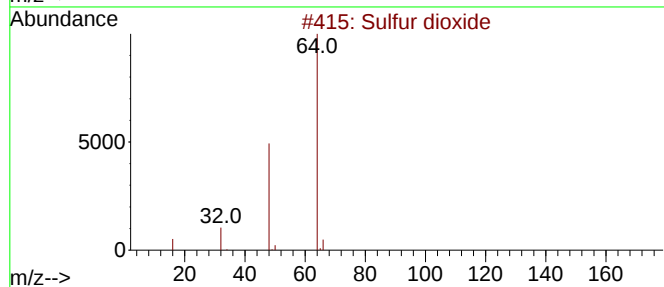
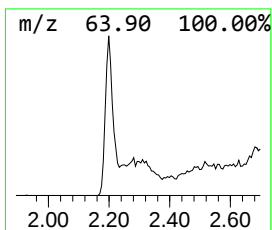
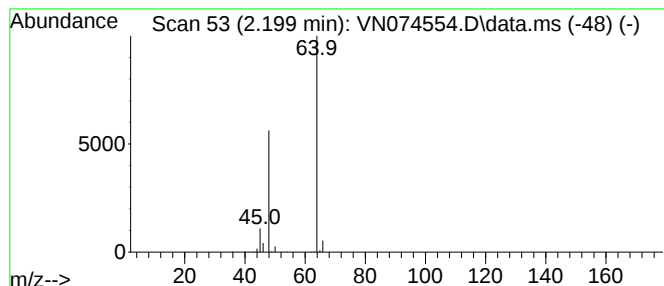
Instrument :
MSVOA_N
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.199	21.85 ug/l	362833	Pentafluorobenzene	8.016	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	5
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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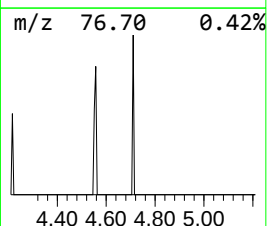
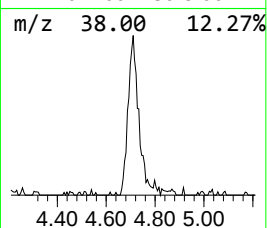
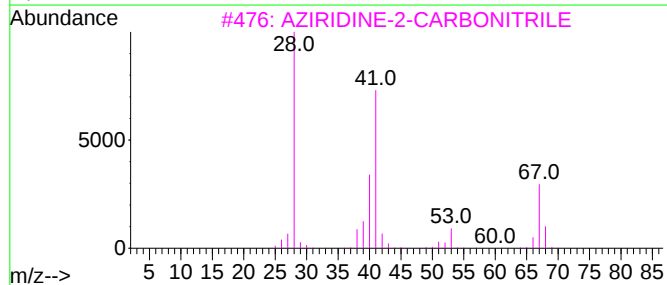
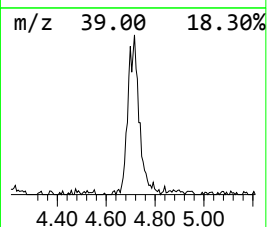
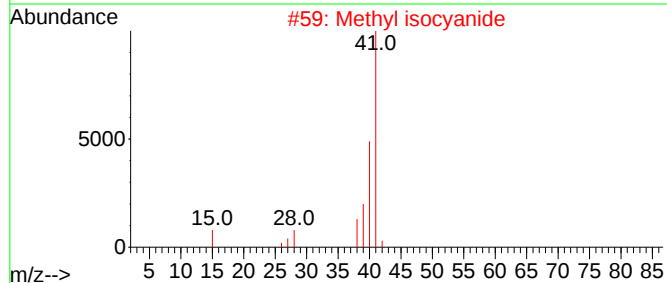
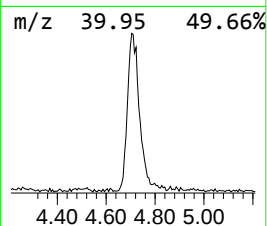
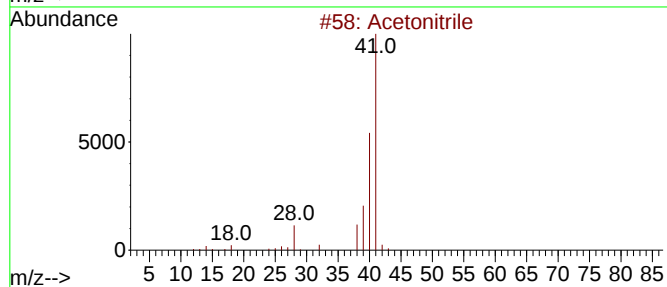
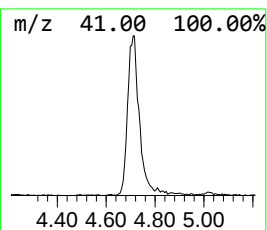
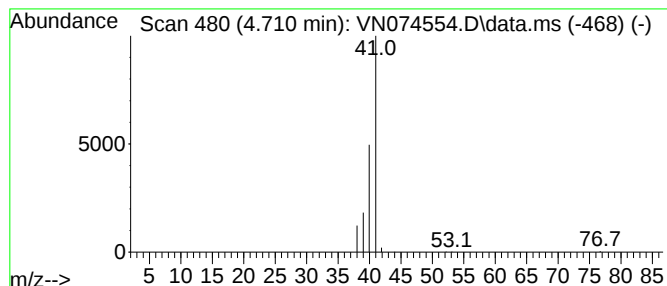
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Peak Number 3 Acetonitrile Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.710	29.75 ug/l	494055	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetonitrile	41	C2H3N	000075-05-8	50
2			Methyl isocyanide	41	C2H3N	000593-75-9	50
3			AZIRIDINE-2-CARBONITRILE	68	C3H4N2	033898-53-2	2
4			2-Aziranecarbonitrile, 1-formyl	96	C4H4N2O	1000196-87-5	2
5			Ethyl isocyanide	55	C3H5N	000624-79-3	1



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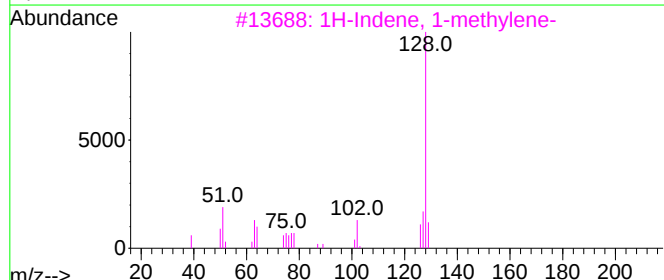
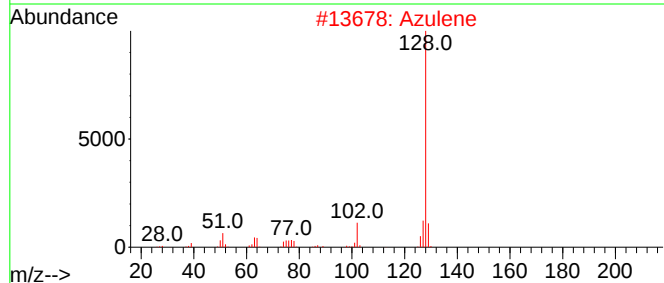
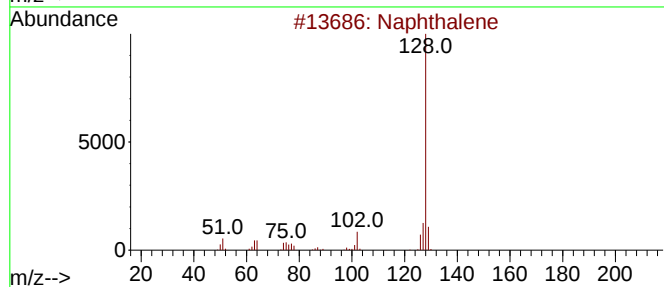
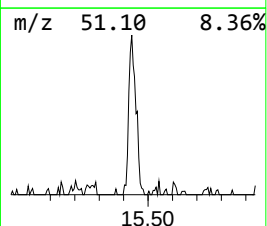
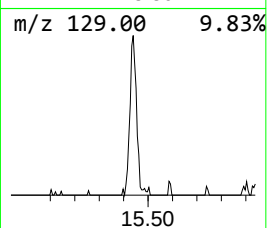
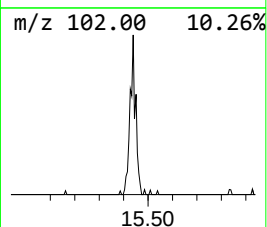
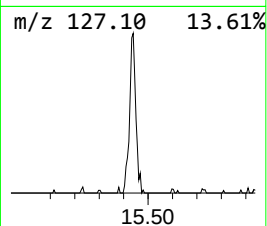
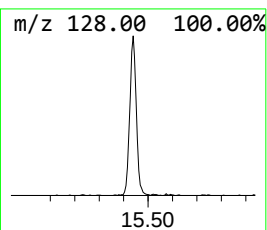
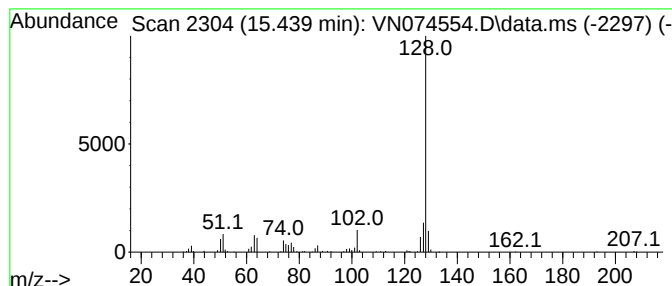
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.439	9.36 ug/l	289515	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	94
2			Azulene	128	C10H8	000275-51-4	91
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	83
4			N-Methyl-9-aza-tricyclo[6.2.2.0(...	185	C12H11NO	013131-19-6	78
5			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	64



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	21.9	ug/l	362833	1	8.016	830425	50.0
unknown2.687	2.687	8.0	ug/l	132324	1	8.016	830425	50.0
Acetonitrile	4.710	29.8	ug/l	494055	1	8.016	830425	50.0
Azulene	15.439	9.4	ug/l	289515	4	13.615	1545940	50.0