

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
 Data File : VN074567.D
 Acq On : 17 Sep 2022 19:43
 Operator : JC\MD
 Sample : N4663-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 HW-9

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: VN074567.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	rBV	243850	471468	24.54%	3.407%
2	2.687	131	136	142	rBV5	58876	163459	8.51%	1.181%
3	4.504	438	445	449	rBV5	8500	21703	1.13%	0.157%
4	7.234	908	909	918	rVB3	12739	21017	1.09%	0.152%
5	7.951	1020	1031	1036	rBV	246090	588141	30.61%	4.250%
6	8.016	1036	1042	1051	rVB	391204	868116	45.18%	6.273%
7	8.369	1092	1102	1113	rBV	284736	655625	34.12%	4.738%
8	8.904	1184	1193	1204	rBV	617761	1299181	67.61%	9.388%
9	10.380	1435	1444	1453	rBV	987333	1808094	94.10%	13.066%
10	10.722	1498	1502	1511	rVB6	9751	21138	1.10%	0.153%
11	11.686	1658	1666	1675	rVB	1041348	1784620	92.87%	12.896%
12	12.674	1827	1834	1841	rBV	840812	1446302	75.27%	10.452%
13	12.839	1860	1862	1868	rVB6	18326	26302	1.37%	0.190%
14	13.504	1958	1975	1987	rBV7	147217	691219	35.97%	4.995%
15	13.615	1987	1994	2008	rVB	1098405	1921549	100.00%	13.886%
16	13.786	2018	2023	2027	rBV7	23658	48054	2.50%	0.347%
17	13.939	2044	2049	2056	rBV6	48761	85647	4.46%	0.619%
18	14.010	2056	2061	2062	rBV5	16846	24628	1.28%	0.178%
19	14.092	2071	2075	2076	rBV4	18728	23444	1.22%	0.169%
20	14.227	2092	2098	2099	rBV3	29554	47271	2.46%	0.342%
21	14.268	2100	2105	2109	rVB4	54878	95841	4.99%	0.693%
22	14.327	2109	2115	2120	rVB9	26442	54008	2.81%	0.390%
23	14.410	2123	2129	2131	rBV3	40890	69451	3.61%	0.502%
24	14.451	2131	2136	2137	rVV5	39295	64254	3.34%	0.464%
25	14.480	2137	2141	2150	rVB2	94337	168722	8.78%	1.219%
26	14.562	2151	2155	2159	rBV6	10475	20802	1.08%	0.150%
27	14.610	2159	2163	2171	rVB10	23288	47556	2.47%	0.344%
28	14.686	2171	2176	2178	rBV6	19118	30814	1.60%	0.223%
29	14.757	2184	2188	2194	rBV7	16032	31184	1.62%	0.225%
30	14.810	2194	2197	2200	rVV5	14487	19718	1.03%	0.142%
31	14.868	2200	2207	2212	rVV4	91079	182841	9.52%	1.321%
32	14.927	2214	2217	2222	rVB6	17690	28485	1.48%	0.206%
33	15.068	2235	2241	2243	rBV7	25127	45572	2.37%	0.329%
34	15.127	2248	2251	2255	rVV5	36165	62456	3.25%	0.451%
35	15.174	2255	2259	2263	rVV5	41528	73724	3.84%	0.533%
36	15.239	2265	2270	2277	rVB4	68046	157996	8.22%	1.142%

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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

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37	15.398	2292	2297	2301	rVB7	17983	33094	1.72%	0.239%
38	15.492	2306	2313	2319	rBV6	32744	77807	4.05%	0.562%
39	15.574	2321	2327	2328	rBV4	21951	32991	1.72%	0.238%
40	15.727	2350	2353	2360	rVB9	10292	21993	1.14%	0.159%
41	15.815	2360	2368	2375	rBV9	24671	65218	3.39%	0.471%
42	15.904	2379	2383	2387	rBV5	17653	28273	1.47%	0.204%
43	16.033	2399	2405	2409	rBV4	20215	38492	2.00%	0.278%
44	16.092	2409	2415	2421	rBV3	65487	134066	6.98%	0.969%
45	16.262	2435	2444	2454	rBV5	59392	156129	8.13%	1.128%
46	16.739	2518	2525	2532	rBV8	33163	79612	4.14%	0.575%

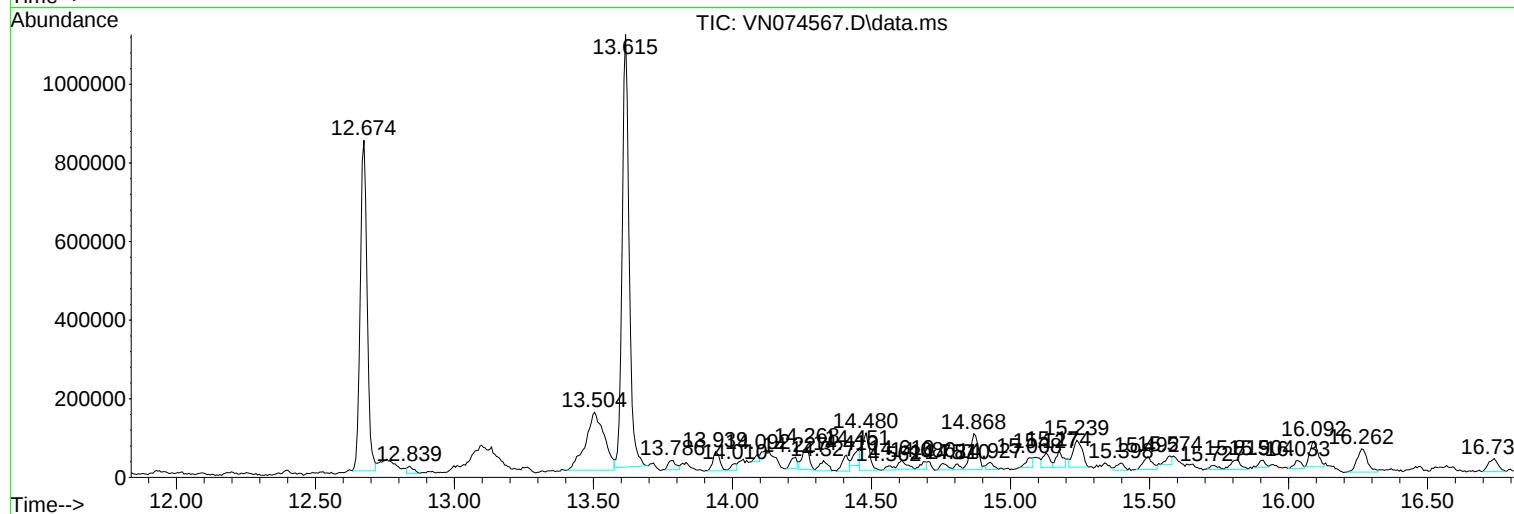
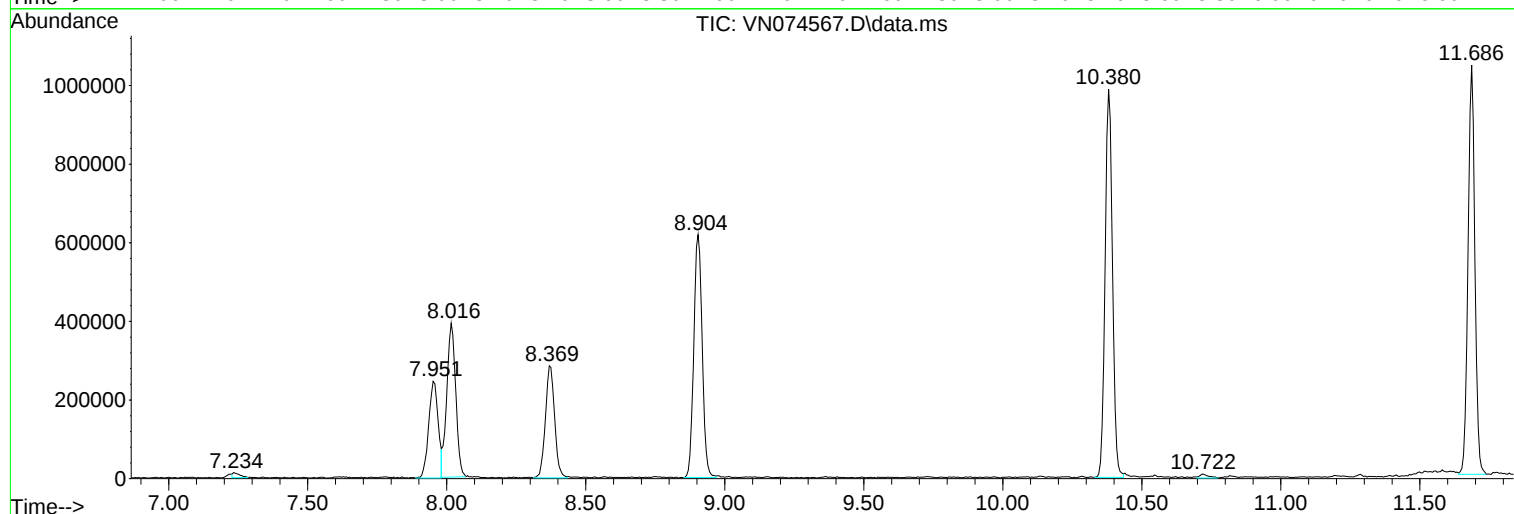
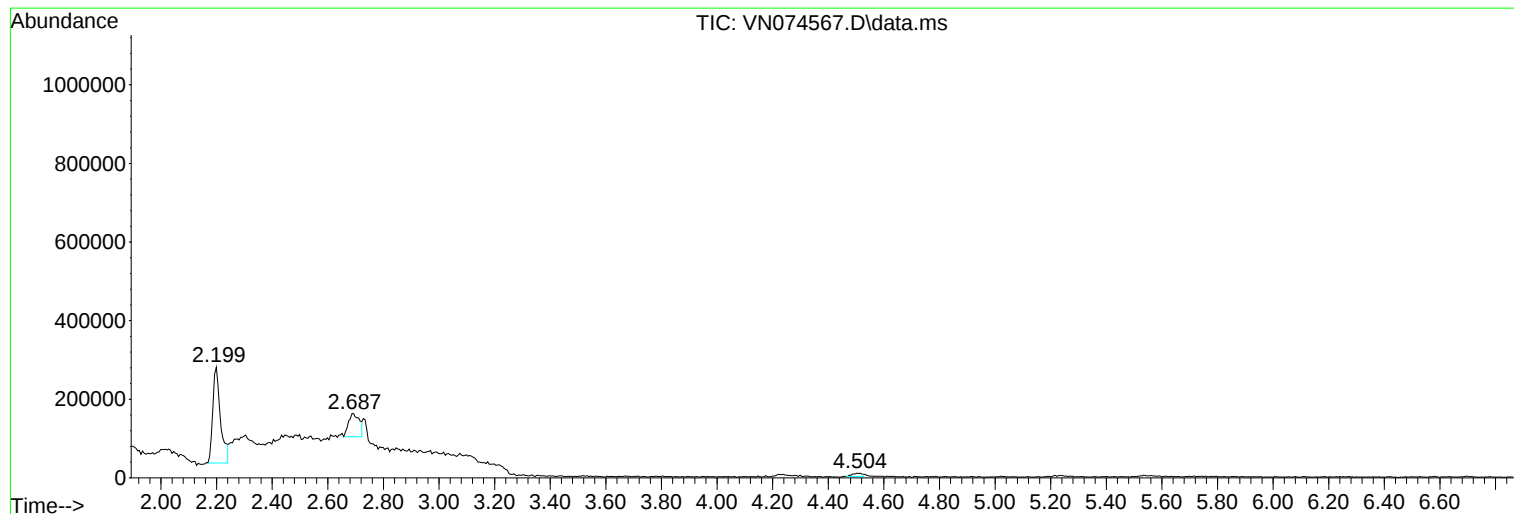
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



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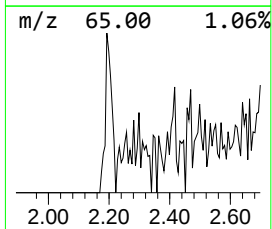
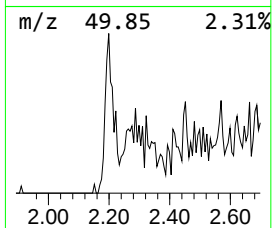
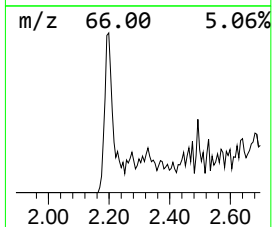
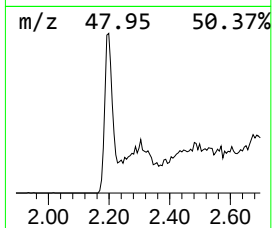
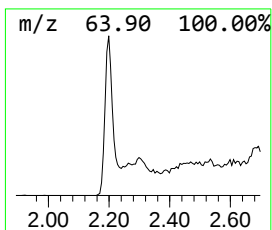
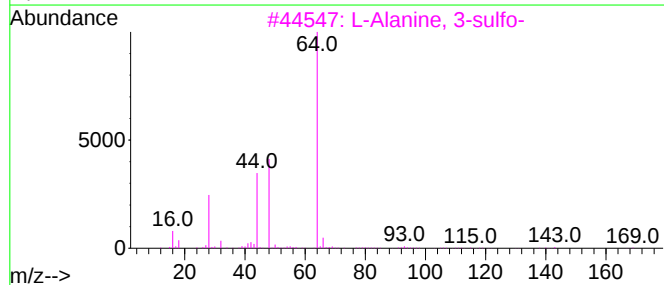
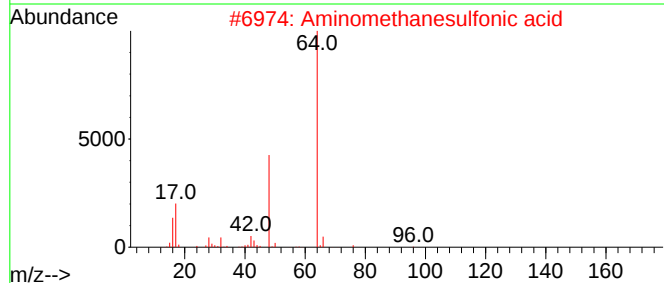
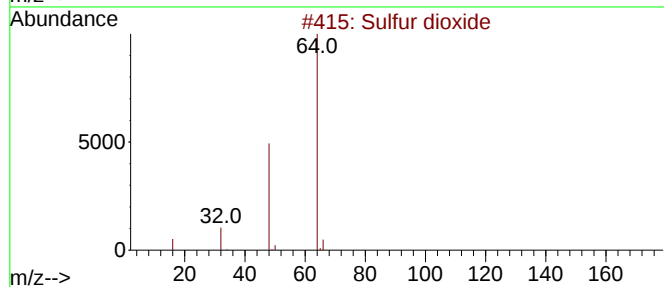
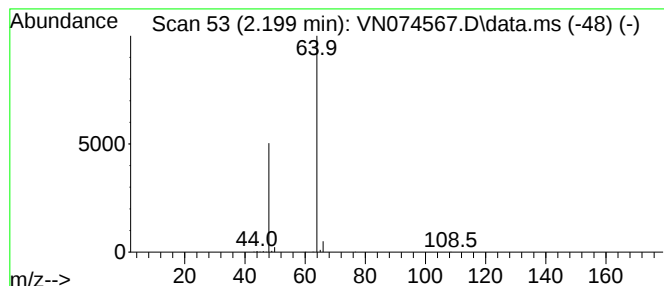
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	27.15 ug/l	471468	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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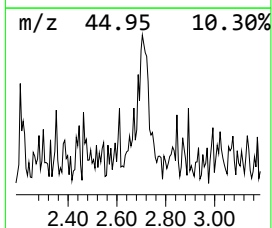
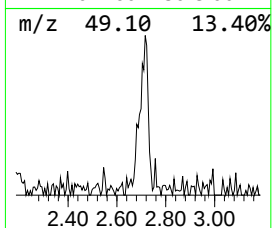
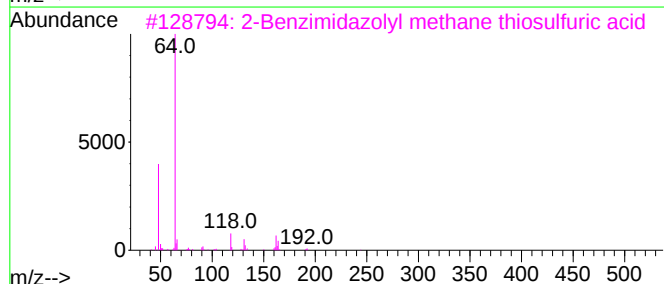
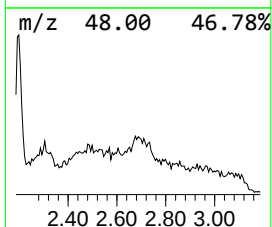
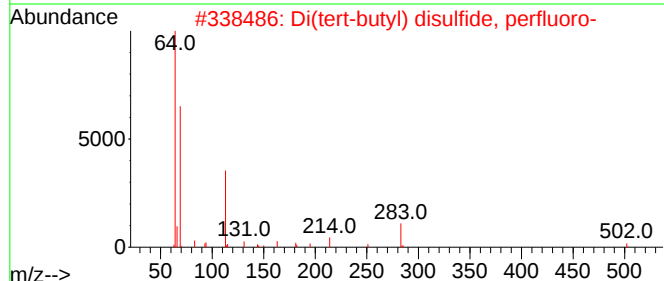
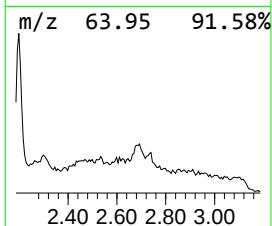
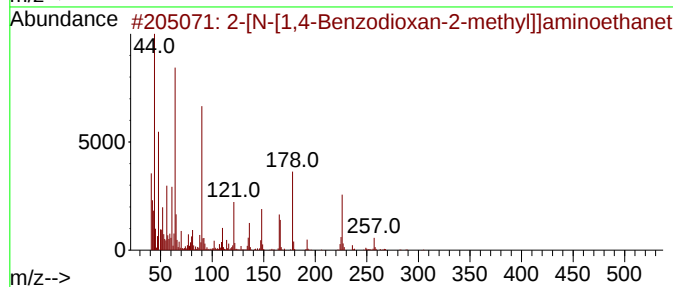
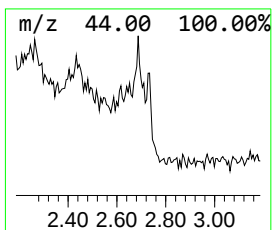
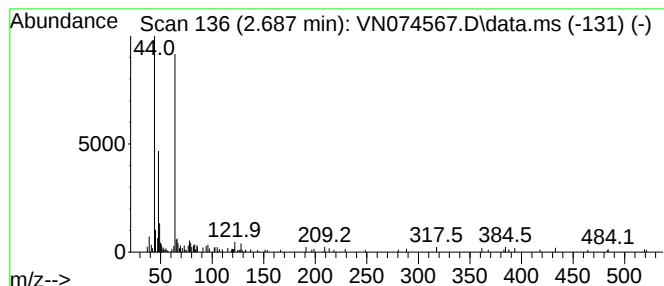
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-[N-[1,4-Benzodioxan-2-met... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.687	9.41 ug/l	163459	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2		[N-[1,4-Benzodioxan-2-methyl]]...	305	C11H15NO5S2	060311-26-4	64
2			Di(tert-butyl) disulfide, perflu...	502	C8F18S2	034880-30-3	64
3			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	59
4			2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	50
5			Sulfur dioxide	64	O2S	007446-09-5	45



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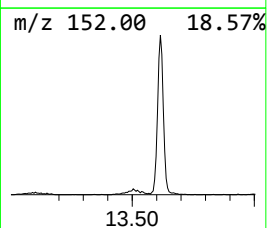
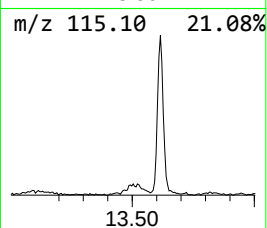
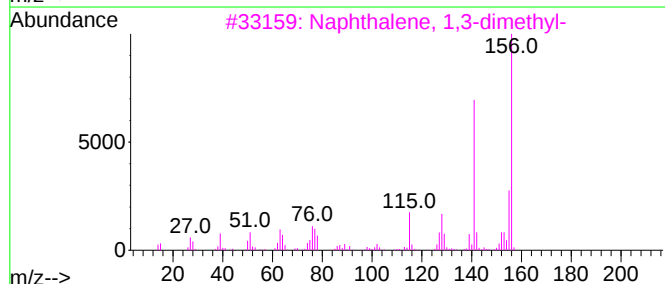
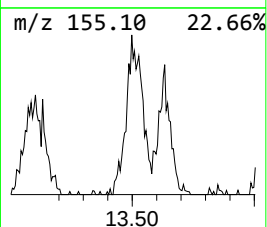
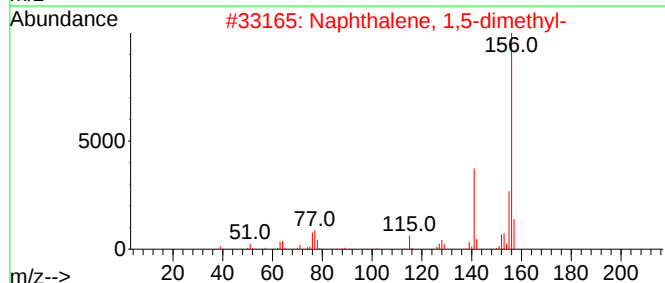
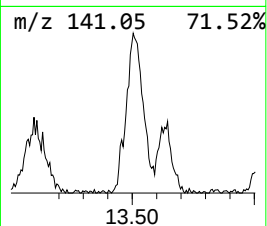
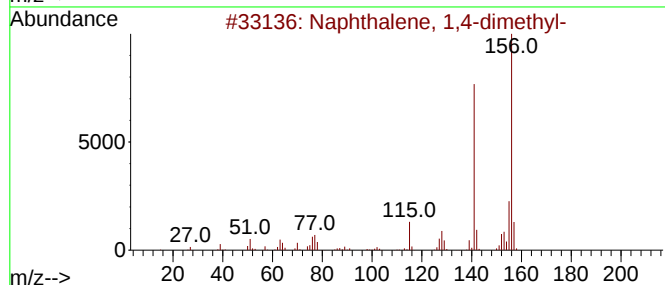
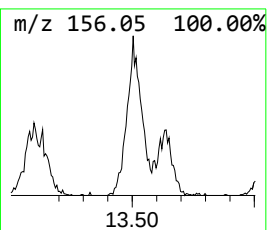
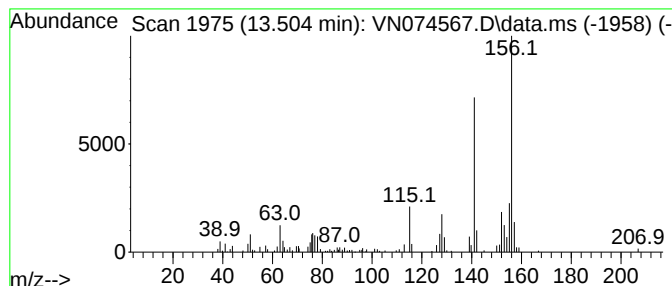
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Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 1,4-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.504	17.99 ug/l	691219	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
2			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	95
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	95
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	94



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	27.1	ug/l	471468	1	8.016	868116	50.0
2-[N-[1,4-Benzo...	2.687	9.4	ug/l	163459	1	8.016	868116	50.0
Naphthalene, 1,...	13.504	18.0	ug/l	691219	4	13.616	1921550	50.0