

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100322\
 Data File : VX031848.D
 Acq On : 03 Oct 2022 20:58
 Operator : JC/MD
 Sample : N4860-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-05

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_X\Method\82X100322W.M
 Title : SW846 8260

Signal : TIC: VX031848.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	25	30	41	rBV2	7520	23181	3.57%	0.589%
2	5.385	693	705	720	rBV	79726	235537	36.28%	5.983%
3	5.556	722	733	745	rVB2	80238	228513	35.19%	5.804%
4	5.952	789	798	814	rBV	78627	211798	32.62%	5.380%
5	6.763	920	931	944	rBV	111553	265345	40.87%	6.740%
6	8.647	1234	1240	1251	rBV	416165	649295	100.00%	16.492%
7	10.055	1465	1471	1479	rBV	293551	383317	59.04%	9.736%
8	11.079	1634	1639	1654	rBV	340762	439883	67.75%	11.173%
9	11.890	1769	1772	1778	rVB	5214	6744	1.04%	0.171%
10	12.024	1788	1794	1804	rBV	429542	532440	82.00%	13.524%
11	12.177	1815	1819	1824	rVB	10165	12212	1.88%	0.310%
12	12.250	1825	1831	1837	rVV	33240	43004	6.62%	1.092%
13	12.311	1837	1841	1849	rVB3	10080	14895	2.29%	0.378%
14	12.646	1891	1896	1901	rBV	40450	51760	7.97%	1.315%
15	12.719	1901	1908	1912	rBV3	7309	13060	2.01%	0.332%
16	12.841	1920	1928	1934	rVB	17214	26334	4.06%	0.669%
17	13.030	1955	1959	1966	rVB3	16201	23750	3.66%	0.603%
18	13.134	1969	1976	1980	rVV	21419	28473	4.39%	0.723%
19	13.195	1980	1986	1991	rVB2	14214	18169	2.80%	0.461%
20	13.347	2006	2011	2015	rBV2	8765	11829	1.82%	0.300%
21	13.396	2015	2019	2021	rVV3	5579	7500	1.16%	0.191%
22	13.427	2022	2024	2034	rVB7	4706	6932	1.07%	0.176%
23	13.622	2052	2056	2057	rVV2	18556	22144	3.41%	0.562%
24	13.664	2060	2063	2068	rVB	38395	49279	7.59%	1.252%
25	13.750	2073	2077	2081	rBV	8731	11297	1.74%	0.287%
26	13.798	2081	2085	2090	rVB5	4925	8343	1.28%	0.212%
27	13.853	2090	2094	2099	rVB	45243	55844	8.60%	1.418%
28	13.926	2099	2106	2110	rBV	72658	92184	14.20%	2.341%
29	13.975	2110	2114	2117	rBV2	7841	10858	1.67%	0.276%
30	14.103	2132	2135	2139	rVB4	6901	7005	1.08%	0.178%
31	14.213	2149	2153	2155	rBV4	7676	11294	1.74%	0.287%
32	14.323	2167	2171	2175	rBV	15230	19257	2.97%	0.489%
33	14.378	2175	2180	2184	rVB	19641	27743	4.27%	0.705%
34	14.420	2184	2187	2193	rVB5	4801	7396	1.14%	0.188%
35	14.481	2193	2197	2201	rBV4	17007	26107	4.02%	0.663%
36	14.524	2201	2204	2210	rVB4	4656	6897	1.06%	0.175%

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37	14.615	2210	2219	2220	rBV4	13356	28662	4.41%	0.728%
38	14.634	2220	2222	2226	rVV2	13550	18517	2.85%	0.470%
39	14.676	2226	2229	2233	rVB2	18419	22524	3.47%	0.572%
40	14.725	2233	2237	2242	rBV2	9770	13851	2.13%	0.352%
41	14.792	2243	2248	2250	rBV2	13907	19837	3.06%	0.504%
42	14.823	2250	2253	2255	rVV2	10619	13942	2.15%	0.354%
43	14.847	2255	2257	2261	rVB3	14475	16763	2.58%	0.426%
44	14.914	2261	2268	2274	rBV6	12273	27029	4.16%	0.687%
45	15.048	2284	2290	2294	rBV6	4986	8876	1.37%	0.225%
46	15.182	2306	2312	2319	rVB6	13659	28514	4.39%	0.724%
47	15.255	2319	2324	2331	rVB5	10239	17820	2.74%	0.453%
48	15.377	2339	2344	2346	rBV5	6820	10232	1.58%	0.260%
49	15.609	2378	2382	2387	rVB4	6374	11440	1.76%	0.291%
50	15.658	2387	2390	2396	rVB7	5393	10113	1.56%	0.257%
51	15.725	2396	2401	2409	rBV6	4962	14113	2.17%	0.358%
52	15.810	2409	2415	2418	rBV2	9675	17049	2.63%	0.433%
53	15.847	2418	2421	2435	rVB9	8136	19664	3.03%	0.499%
54	15.987	2439	2444	2448	rBV2	14722	25768	3.97%	0.655%
55	16.322	2492	2499	2505	rVB7	4404	12649	1.95%	0.321%
56	16.530	2527	2533	2541	rBV10	3954	9990	1.54%	0.254%

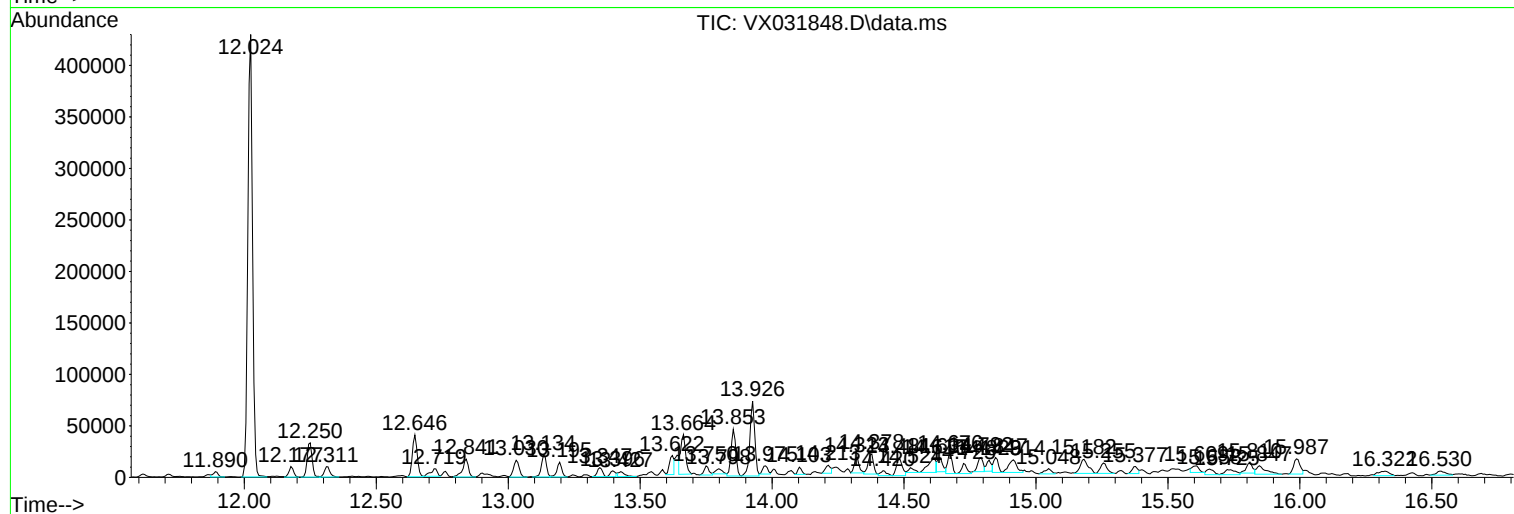
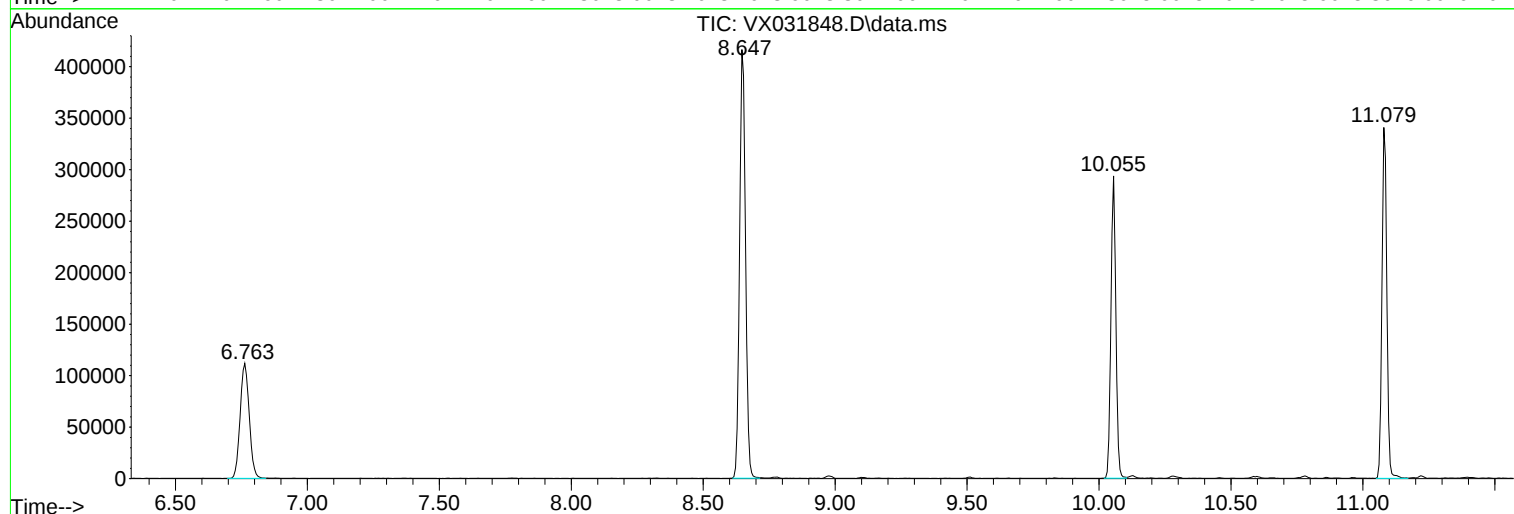
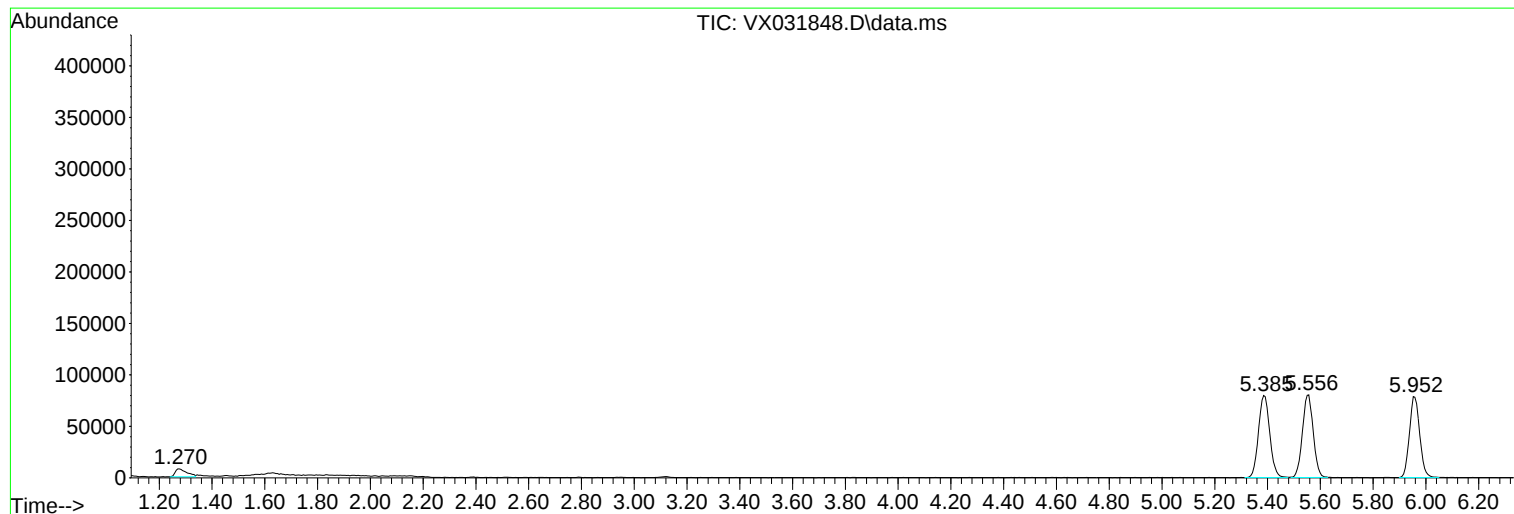
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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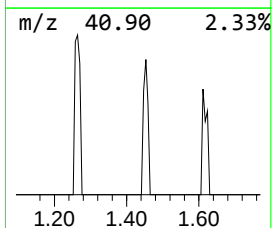
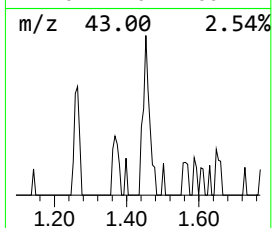
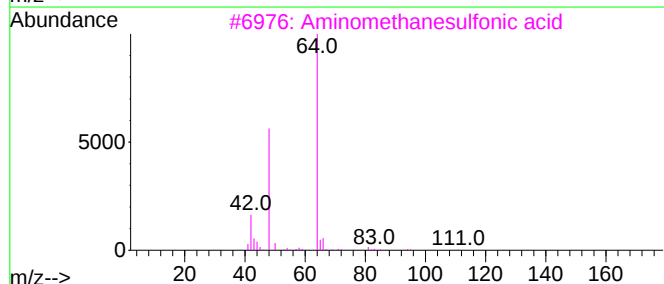
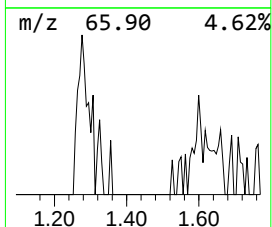
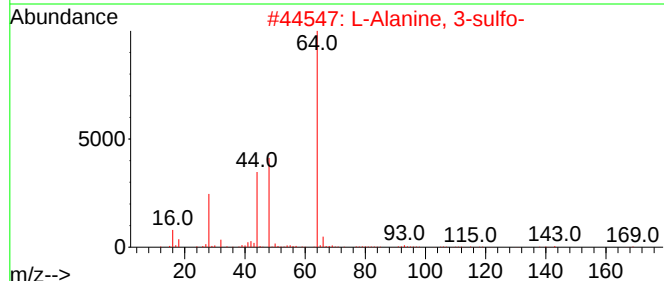
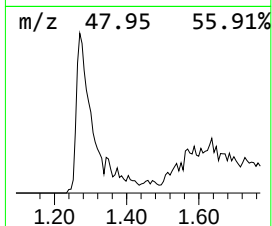
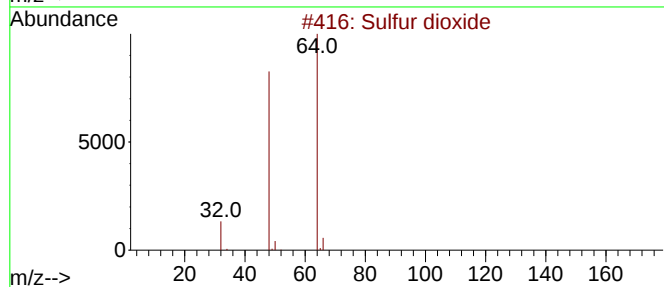
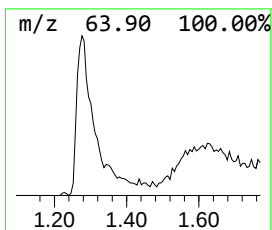
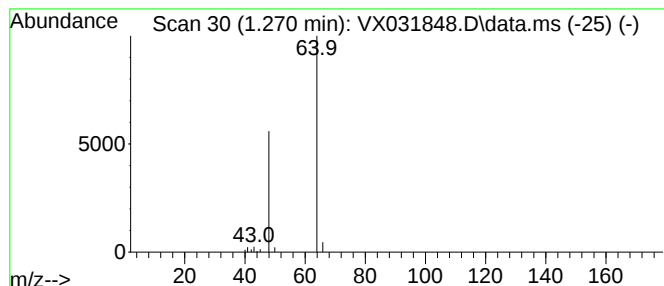
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100322W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	5.07 ug/l	23181	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	4



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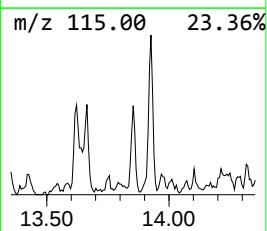
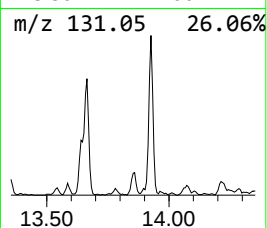
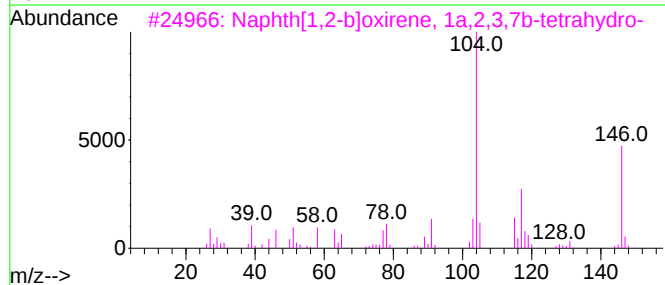
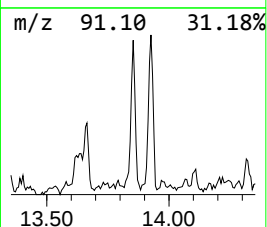
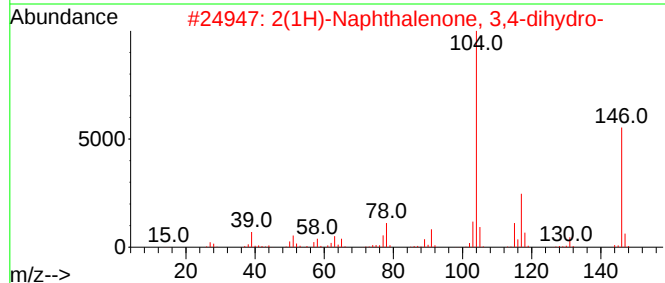
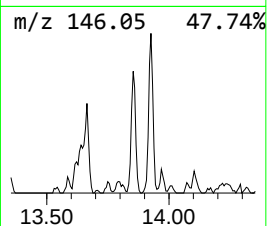
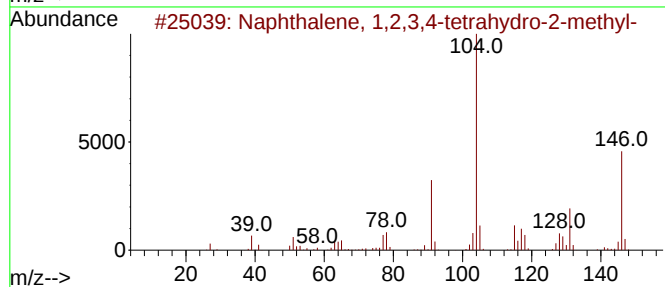
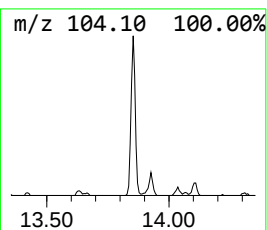
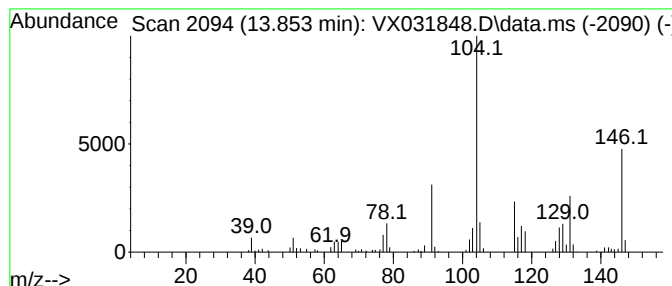
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.853	5.24 ug/l	55844	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	93
2			2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	64
3			Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	62
4			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	50
5			2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	38



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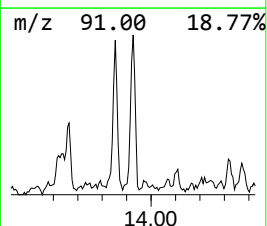
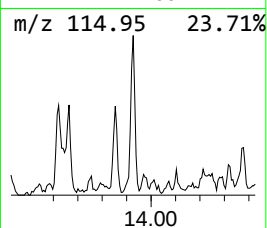
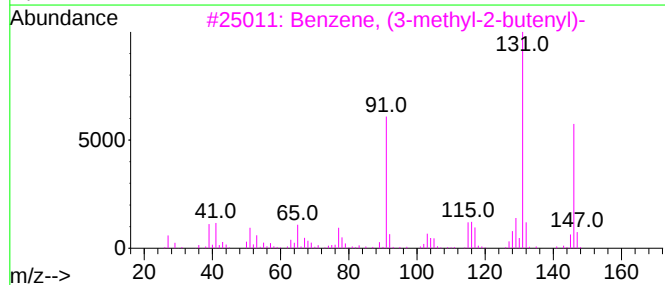
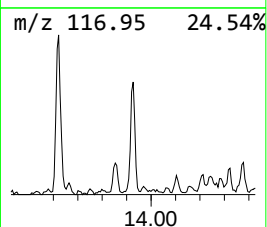
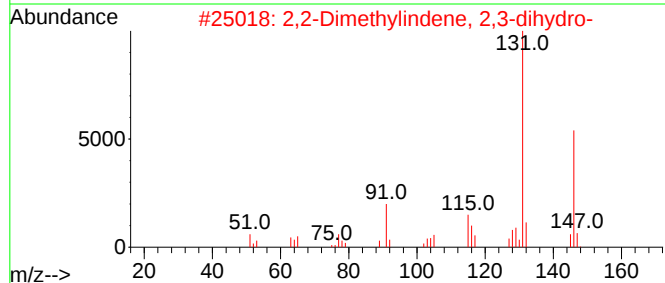
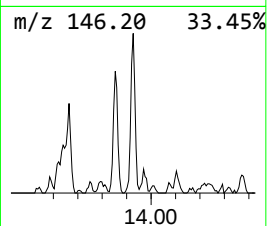
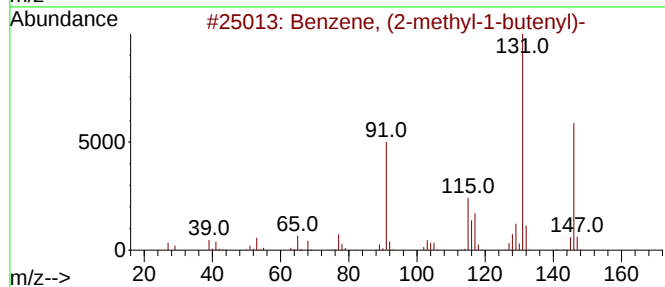
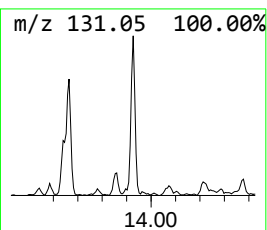
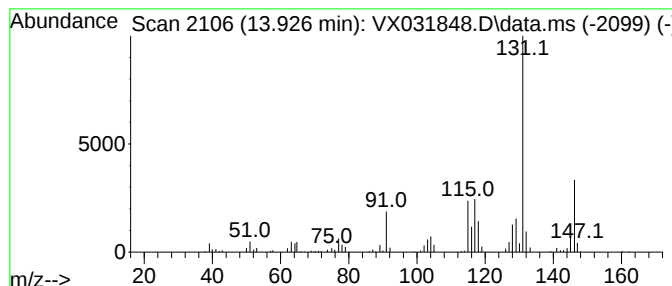
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Peak Number 3 Benzene, (2-methyl-1-butenyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.926	8.66 ug/l	92184	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	93
2			2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	91
3			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	90
4			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	87
5			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	81



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.270	5.1	ug/l	23181	1	5.556	228513	50.0
Naphthalene, 1,...	13.853	5.2	ug/l	55844	4	12.024	532440	50.0
Benzene, (2-met...	13.926	8.7	ug/l	92184	4	12.024	532440	50.0