

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092922\
 Data File : VX031774.D
 Acq On : 29 Sep 2022 15:32
 Operator : JC/MD
 Sample : N4860-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 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\82X092622W.M
 Title : SW846 8260

Signal : TIC: VX031774.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	23	30	40	rBV	8724	25905	5.04%	0.793%
2	5.385	692	705	721	rBV2	65698	192541	37.46%	5.891%
3	5.556	721	733	748	rVB	67258	190742	37.11%	5.836%
4	5.958	788	799	815	rBV	68941	186004	36.18%	5.691%
5	6.763	921	931	942	rBV	95265	224809	43.73%	6.879%
6	8.647	1232	1240	1256	rBV	324525	514054	100.00%	15.729%
7	10.055	1465	1471	1479	rBV	243888	321194	62.48%	9.828%
8	11.079	1634	1639	1645	rBV	275441	354347	68.93%	10.842%
9	11.890	1769	1772	1777	rVB2	4451	5495	1.07%	0.168%
10	12.024	1788	1794	1805	rBV	345338	439195	85.44%	13.438%
11	12.177	1814	1819	1824	rVB	8610	10318	2.01%	0.316%
12	12.250	1826	1831	1835	rVV	28801	34699	6.75%	1.062%
13	12.317	1837	1842	1850	rVB	9009	12897	2.51%	0.395%
14	12.646	1891	1896	1902	rBV	35427	43328	8.43%	1.326%
15	12.719	1906	1908	1912	rVV2	5753	7419	1.44%	0.227%
16	12.762	1912	1915	1919	rVB	4543	5361	1.04%	0.164%
17	12.841	1919	1928	1934	rBV	15253	22167	4.31%	0.678%
18	12.902	1934	1938	1941	rBV3	3141	5335	1.04%	0.163%
19	13.030	1954	1959	1965	rVB2	13903	18907	3.68%	0.579%
20	13.134	1970	1976	1980	rVV	18734	24209	4.71%	0.741%
21	13.195	1980	1986	1991	rVB	12116	15160	2.95%	0.464%
22	13.347	2007	2011	2015	rVB2	8671	10185	1.98%	0.312%
23	13.396	2015	2019	2021	rBV2	4895	6672	1.30%	0.204%
24	13.426	2021	2024	2029	rVB6	3719	5566	1.08%	0.170%
25	13.585	2046	2050	2052	rBV3	5084	5559	1.08%	0.170%
26	13.615	2052	2055	2057	rVV	15574	20761	4.04%	0.635%
27	13.664	2060	2063	2071	rVV	33015	44353	8.63%	1.357%
28	13.750	2074	2077	2080	rVV	6892	8970	1.74%	0.274%
29	13.798	2081	2085	2090	rVV3	4861	9667	1.88%	0.296%
30	13.853	2090	2094	2099	rVB	38728	47936	9.33%	1.467%
31	13.926	2099	2106	2110	rBV	59779	78098	15.19%	2.390%
32	13.975	2110	2114	2117	rVV4	7163	10944	2.13%	0.335%
33	14.103	2132	2135	2142	rVB5	6023	7500	1.46%	0.229%
34	14.213	2148	2153	2156	rBV4	6698	11473	2.23%	0.351%
35	14.323	2167	2171	2174	rBV	12018	14894	2.90%	0.456%
36	14.371	2175	2179	2184	rVB2	16780	24688	4.80%	0.755%

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37	14.420	2184	2187	2192	rVB4	4110	5629	1.10%	0.172%
38	14.481	2192	2197	2202	rBV2	12901	22339	4.35%	0.684%
39	14.530	2202	2205	2210	rVB5	4026	5793	1.13%	0.177%
40	14.609	2210	2218	2221	rBV4	11885	28313	5.51%	0.866%
41	14.634	2221	2222	2225	rVV3	12871	12135	2.36%	0.371%
42	14.676	2225	2229	2233	rVB2	14449	18901	3.68%	0.578%
43	14.725	2233	2237	2242	rBV3	7788	10434	2.03%	0.319%
44	14.792	2242	2248	2250	rVV2	12309	19377	3.77%	0.593%
45	14.823	2250	2253	2254	rVV2	10291	11545	2.25%	0.353%
46	14.847	2254	2257	2261	rVV4	12876	17600	3.42%	0.539%
47	14.908	2261	2267	2276	rVV7	10090	27030	5.26%	0.827%
48	15.048	2283	2290	2293	rBV6	3931	6823	1.33%	0.209%
49	15.182	2306	2312	2319	rVB5	12009	24393	4.75%	0.746%
50	15.255	2319	2324	2331	rVB5	9280	15049	2.93%	0.460%
51	15.377	2339	2344	2347	rBV4	6234	10548	2.05%	0.323%
52	15.597	2376	2380	2382	rBV5	3238	5273	1.03%	0.161%
53	15.658	2386	2390	2396	rVB8	4090	9445	1.84%	0.289%
54	15.743	2396	2404	2409	rBV7	4526	12993	2.53%	0.398%
55	15.810	2409	2415	2418	rBV4	8681	14777	2.87%	0.452%
56	15.987	2440	2444	2449	rBV3	12288	22002	4.28%	0.673%
57	16.530	2528	2533	2538	rBV6	3247	6493	1.26%	0.199%

Sum of corrected areas: 3268244

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Instrument :
MSVOA_X
ClientSampleId :
MW-05

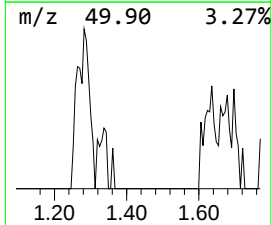
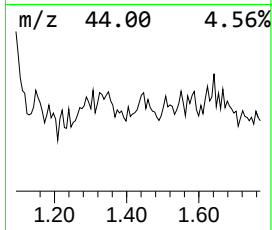
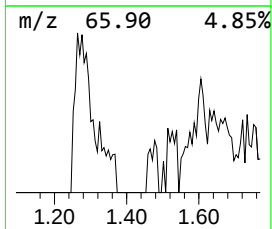
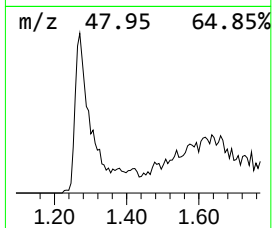
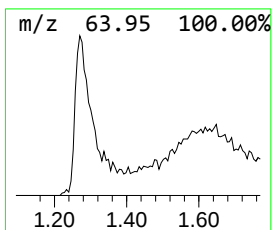
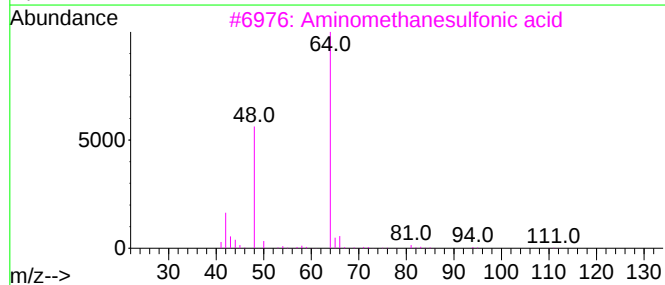
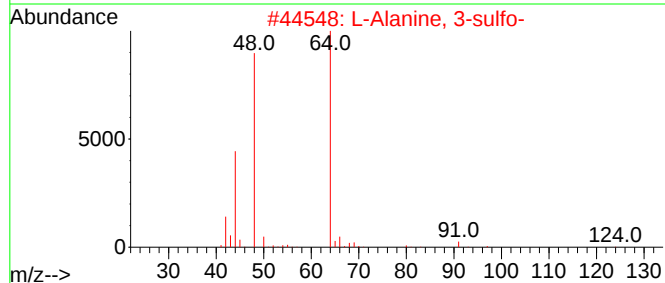
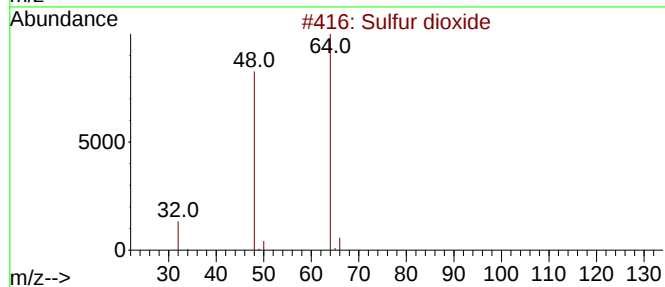
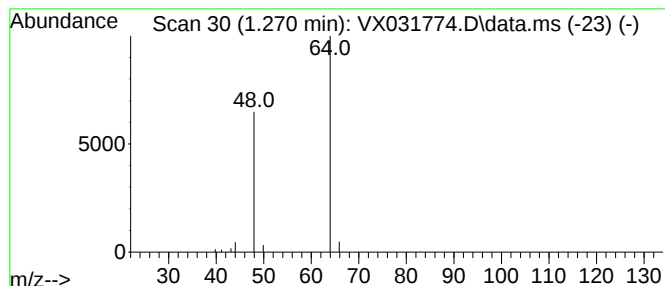
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092622W.M
Quant Title : SW846 8260

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.
1.270	6.79 ug/l	25905	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	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	4



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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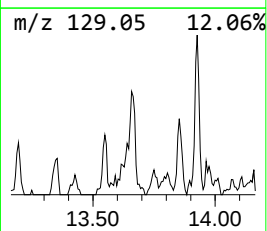
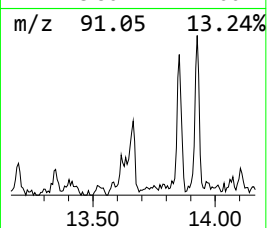
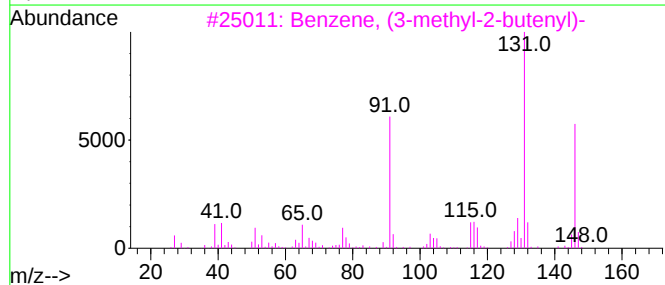
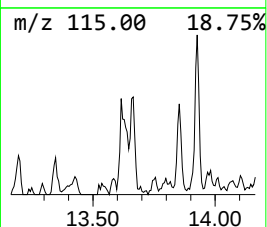
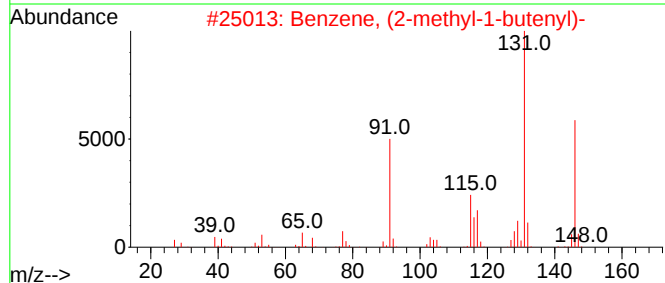
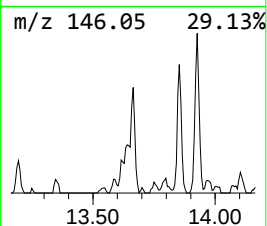
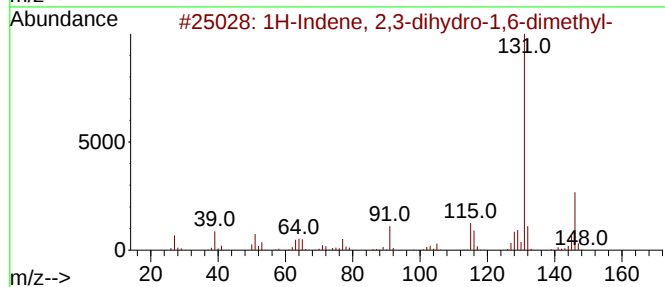
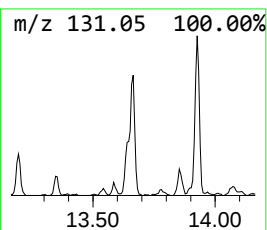
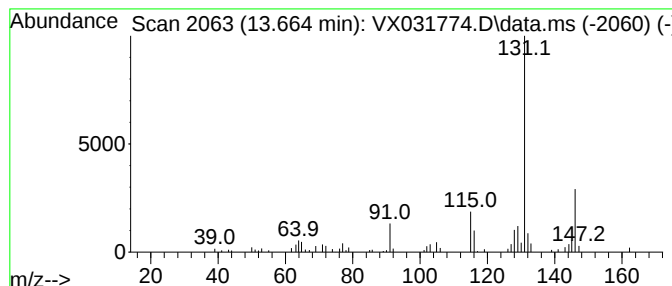
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092622W.M
Quant Title : SW846 8260

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

Peak Number 2 1H-Indene, 2,3-dihydro-1,6-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.664	5.05 ug/l	44353	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	94
2			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	93
3			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	93
4			1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	91
5			Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	90



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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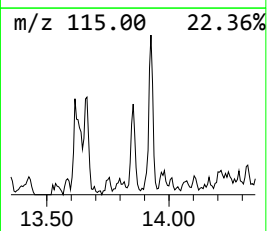
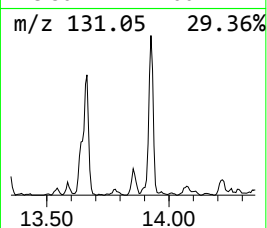
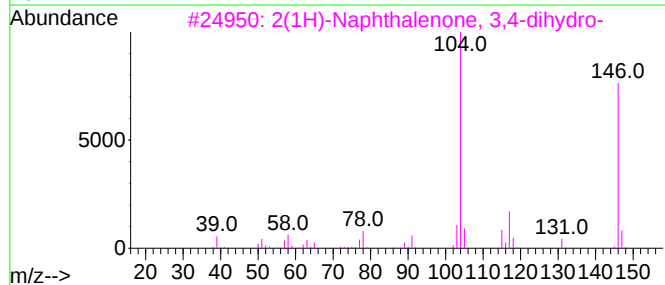
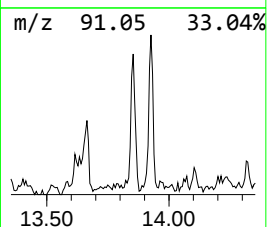
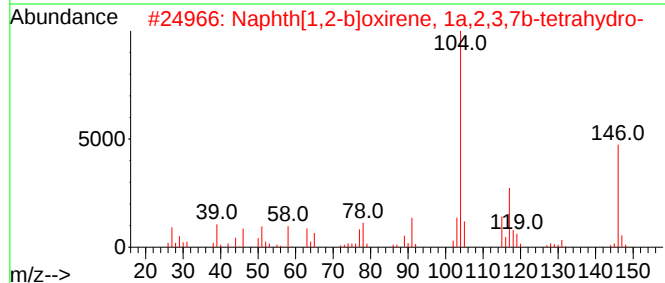
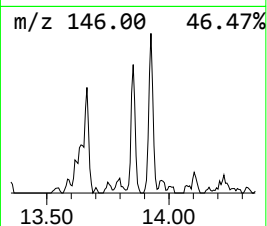
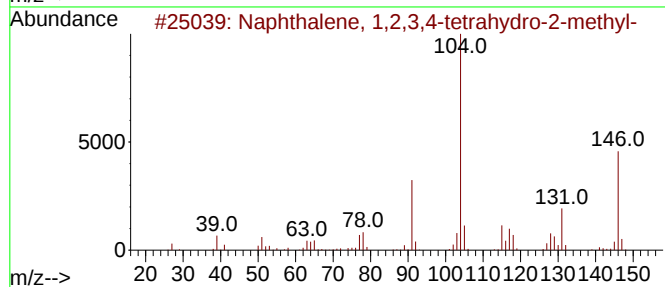
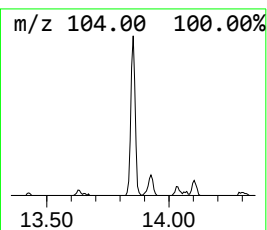
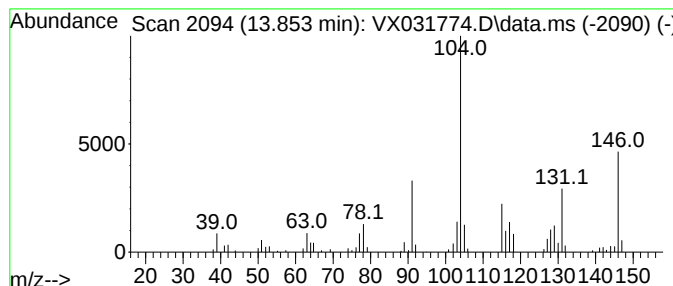
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092622W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.853	5.46 ug/l	47936	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	90
2			Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	62
3			2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	58
4			2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	50
5			Acetic acid, 2-phenylethyl ester	164	C10H12O2	000103-45-7	27



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ClientSampleId :
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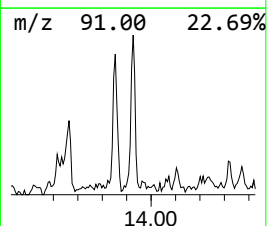
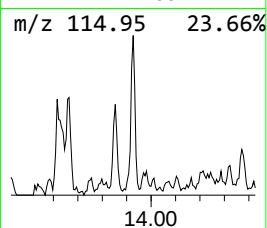
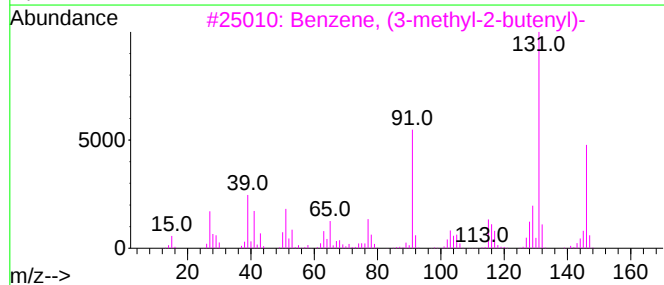
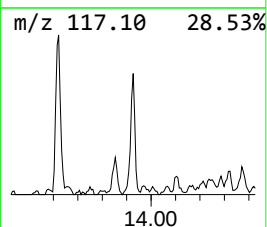
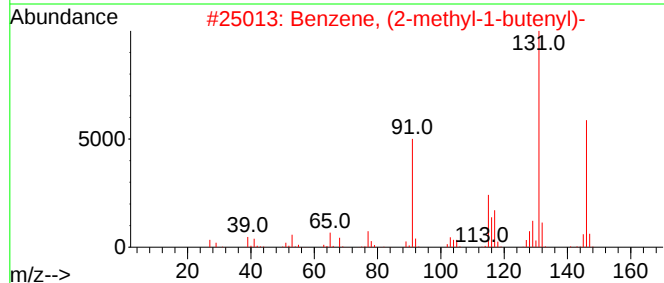
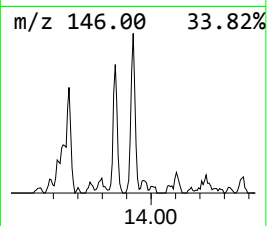
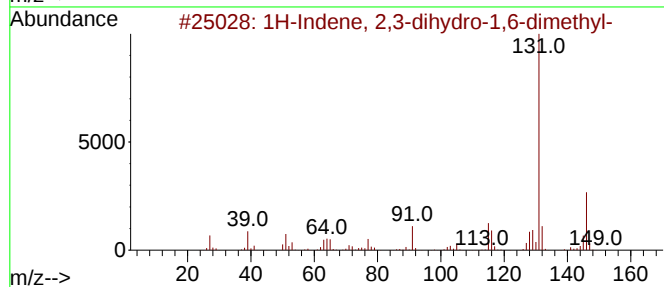
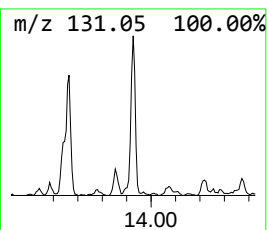
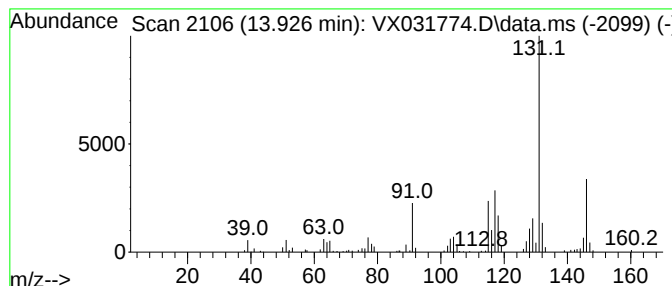
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092622W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, (2-methyl-1-butenyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.926	8.89 ug/l	78098	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	93		
2	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	93		
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	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	81		



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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	1.270	6.8	ug/l	25905	1	5.556	190742	50.0
1H-Indene, 2,3-...	13.664	5.0	ug/l	44353	4	12.024	439195	50.0
Naphthalene, 1,...	13.853	5.5	ug/l	47936	4	12.024	439195	50.0
Benzene, (2-met...	13.926	8.9	ug/l	78098	4	12.024	439195	50.0