

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
 Data File : VX029247.D
 Acq On : 06 Jun 2022 18:41
 Operator : JC/MD
 Sample : N3160-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-3

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\82X053122W.M
 Title : SW846 8260

Signal : TIC: VX029247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	15	rVB	53503	45971	2.46%	0.262%
2	1.270	25	30	41	rBV5	9883	28481	1.53%	0.162%
3	1.355	41	44	50	rVB2	16221	20898	1.12%	0.119%
4	2.337	200	205	209	rBV3	11481	20401	1.09%	0.116%
5	2.386	209	213	222	rVB	11069	19325	1.04%	0.110%
6	2.782	268	278	293	rVB	53145	122073	6.54%	0.695%
7	3.099	323	330	338	rBV2	9774	22336	1.20%	0.127%
8	4.050	478	486	498	rVB3	7149	21222	1.14%	0.121%
9	4.215	501	513	526	rBV	91179	270382	14.48%	1.538%
10	4.458	540	553	563	rVB3	6275	23596	1.26%	0.134%
11	5.117	647	661	663	rBV6	15631	44867	2.40%	0.255%
12	5.391	694	706	720	rBV2	214124	612650	32.82%	3.486%
13	5.556	720	733	740	rVV	322573	955389	51.18%	5.436%
14	5.623	740	744	760	rVB	119174	327449	17.54%	1.863%
15	5.958	789	799	811	rBV	215125	569516	30.51%	3.240%
16	6.251	827	847	860	rBV	481009	1477454	79.14%	8.406%
17	6.763	921	931	947	rBV	549706	1285389	68.85%	7.313%
18	6.970	957	965	975	rBV4	10968	28245	1.51%	0.161%
19	7.373	1023	1031	1041	rVB4	16634	39339	2.11%	0.224%
20	7.501	1044	1052	1057	rBV2	25995	55445	2.97%	0.315%
21	7.561	1057	1062	1066	rVV2	35917	79850	4.28%	0.454%
22	7.604	1066	1069	1076	rVB2	29224	57703	3.09%	0.328%
23	7.775	1090	1097	1105	rVB3	24800	52087	2.79%	0.296%
24	7.988	1124	1132	1141	rVB	397631	763389	40.89%	4.343%
25	8.110	1143	1152	1160	rBV	413066	804213	43.08%	4.575%
26	8.311	1180	1185	1192	rVB7	10150	21276	1.14%	0.121%
27	8.391	1192	1198	1202	rBV3	15248	27712	1.48%	0.158%
28	8.653	1225	1241	1249	rBV	1107407	1866899	100.00%	10.621%
29	8.976	1291	1294	1299	rVB2	15781	24400	1.31%	0.139%
30	9.104	1307	1315	1320	rVB5	10249	22238	1.19%	0.127%
31	9.165	1320	1325	1328	rBV	18173	27493	1.47%	0.156%
32	9.518	1376	1383	1389	rBV5	11115	26896	1.44%	0.153%
33	10.055	1466	1471	1478	rBV	1208779	1601672	85.79%	9.112%
34	10.274	1503	1507	1510	rBV4	14772	23843	1.28%	0.136%
35	10.585	1550	1558	1566	rBV8	13549	35231	1.89%	0.200%
36	11.085	1634	1640	1645	rBV	971086	1250672	66.99%	7.115%

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Integrator: RTE

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37	11.219	1658	1662	1667	rVB3	19099	28405	1.52%	0.162%
38	11.402	1686	1692	1702	rBV10	7115	22587	1.21%	0.129%
39	11.866	1760	1768	1770	rBV	48806	68834	3.69%	0.392%
40	11.890	1770	1772	1776	rVB	40502	47118	2.52%	0.268%
41	12.024	1789	1794	1804	rBV	1328191	1608785	86.17%	9.153%
42	12.317	1837	1842	1851	rVB2	54905	100575	5.39%	0.572%
43	12.408	1851	1857	1862	rBV	33601	43848	2.35%	0.249%
44	12.475	1863	1868	1872	rVV	36268	47142	2.53%	0.268%
45	12.603	1882	1889	1894	rBV5	14928	31359	1.68%	0.178%
46	12.725	1906	1909	1913	rVB4	23025	31606	1.69%	0.180%
47	12.835	1920	1927	1934	rVB3	42516	88531	4.74%	0.504%
48	12.902	1934	1938	1939	rBV2	47941	54962	2.94%	0.313%
49	12.926	1939	1942	1947	rVB2	62115	84528	4.53%	0.481%
50	13.030	1955	1959	1966	rVB2	35161	55199	2.96%	0.314%
51	13.115	1966	1973	1974	rBV2	35262	52548	2.81%	0.299%
52	13.140	1974	1977	1982	rVB	68718	89207	4.78%	0.508%
53	13.195	1982	1986	1991	rBV	28988	35629	1.91%	0.203%
54	13.250	1991	1995	1998	rBV3	14727	24299	1.30%	0.138%
55	13.292	1998	2002	2008	rVB5	28398	48588	2.60%	0.276%
56	13.512	2034	2038	2041	rBV3	27076	44482	2.38%	0.253%
57	13.579	2046	2049	2053	rVV2	77451	109136	5.85%	0.621%
58	13.621	2053	2056	2061	rVV2	55681	114665	6.14%	0.652%
59	13.670	2061	2064	2068	rVV3	43263	70621	3.78%	0.402%
60	13.756	2072	2078	2081	rBV	49570	68149	3.65%	0.388%
61	13.798	2081	2085	2090	rVB4	36814	55379	2.97%	0.315%
62	13.853	2090	2094	2099	rVB2	68853	96285	5.16%	0.548%
63	13.926	2099	2106	2111	rBV3	85945	163191	8.74%	0.928%
64	13.975	2111	2114	2118	rBV3	28325	37903	2.03%	0.216%
65	14.073	2126	2130	2133	rBV2	29366	40372	2.16%	0.230%
66	14.213	2149	2153	2163	rVB4	79467	142668	7.64%	0.812%
67	14.322	2163	2171	2176	rBV	77349	113824	6.10%	0.648%
68	14.377	2176	2180	2184	rVB2	62760	82861	4.44%	0.471%
69	14.420	2184	2187	2193	rVB2	39574	53197	2.85%	0.303%
70	14.481	2193	2197	2203	rBV2	79901	150726	8.07%	0.858%
71	14.579	2210	2213	2216	rBV3	18346	25158	1.35%	0.143%
72	14.615	2216	2219	2225	rVV3	54873	92971	4.98%	0.529%
73	14.676	2225	2229	2233	rVB2	69187	89192	4.78%	0.507%
74	14.725	2233	2237	2243	rBV3	24227	38565	2.07%	0.219%
75	14.792	2243	2248	2251	rVV2	51266	85656	4.59%	0.487%
76	14.847	2255	2257	2261	rVV2	47951	55920	3.00%	0.318%

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ClientSampleId :
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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

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77	14.920	2267	2269	2273	rVB4	19029	22540	1.21%	0.128%
78	15.048	2282	2290	2293	rBV4	18136	40496	2.17%	0.230%
79	15.182	2307	2312	2320	rVB2	59060	109763	5.88%	0.624%
80	15.255	2320	2324	2330	rVB4	28718	50398	2.70%	0.287%
81	15.377	2339	2344	2346	rBV6	18632	29354	1.57%	0.167%
82	15.408	2346	2349	2353	rVV	32054	41871	2.24%	0.238%
83	15.481	2357	2361	2365	rVV2	29011	48316	2.59%	0.275%
84	15.530	2365	2369	2374	rVV5	19372	37773	2.02%	0.215%
85	15.615	2378	2383	2386	rVV3	45815	76136	4.08%	0.433%
86	15.652	2386	2389	2397	rVB5	27838	48108	2.58%	0.274%
87	15.731	2397	2402	2408	rBV3	15415	35449	1.90%	0.202%
88	15.810	2411	2415	2417	rVV3	16716	24394	1.31%	0.139%
89	15.847	2417	2421	2430	rVB3	23066	41509	2.22%	0.236%

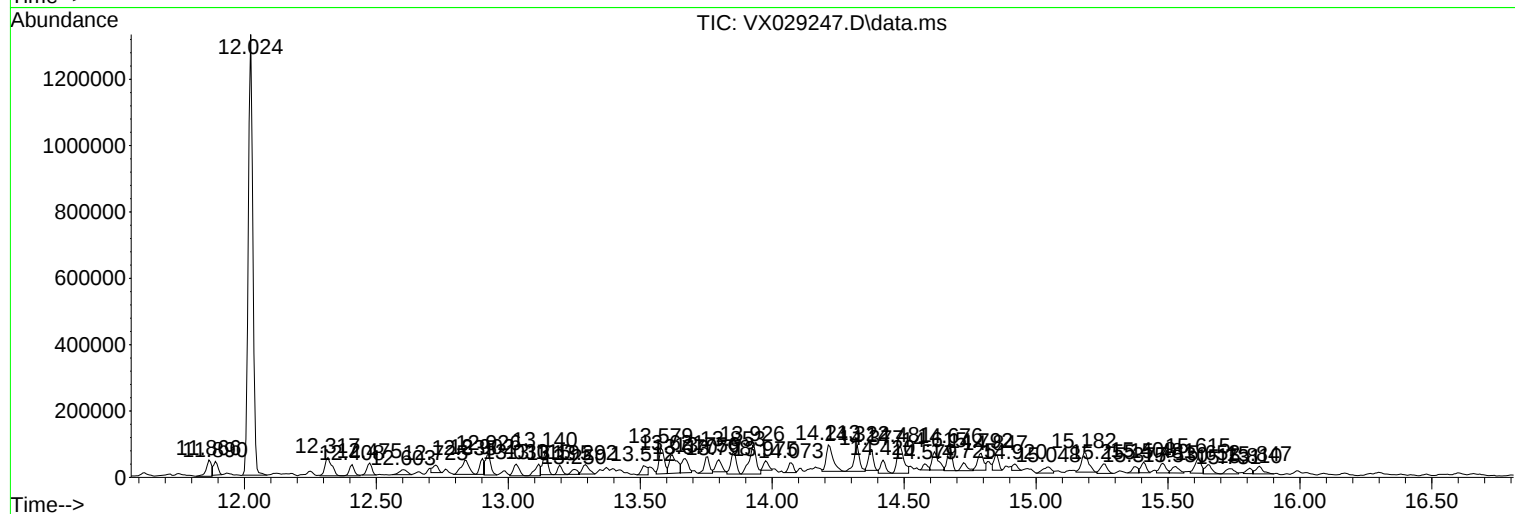
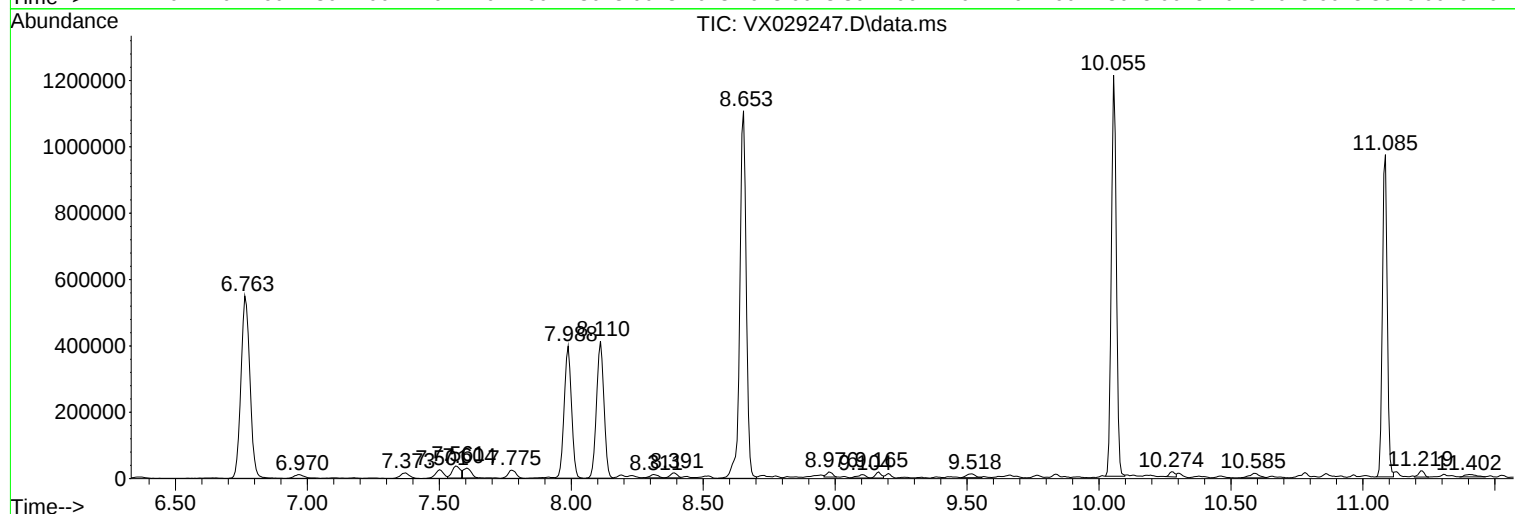
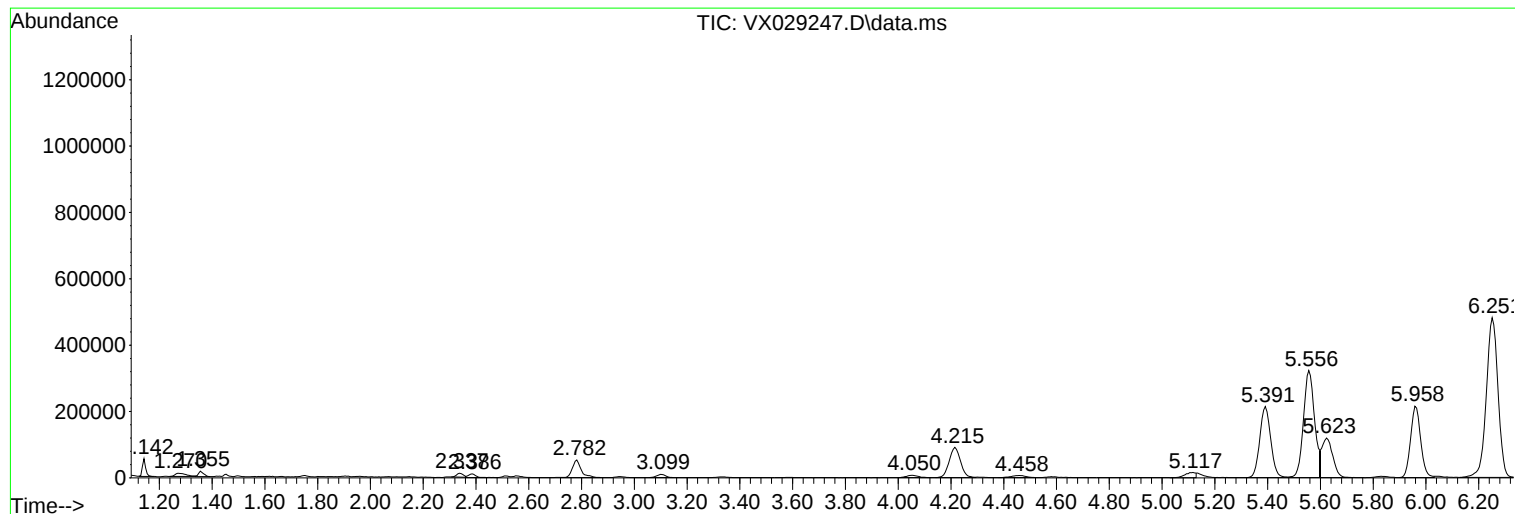
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Instrument :
MSVOA_X
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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



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Instrument :
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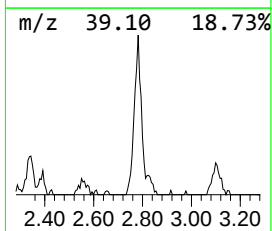
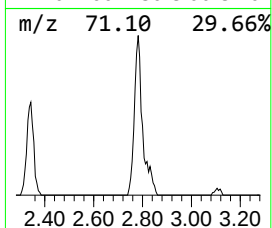
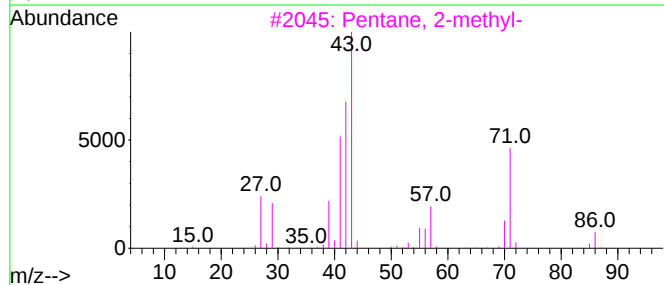
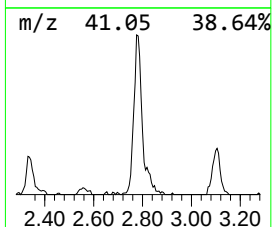
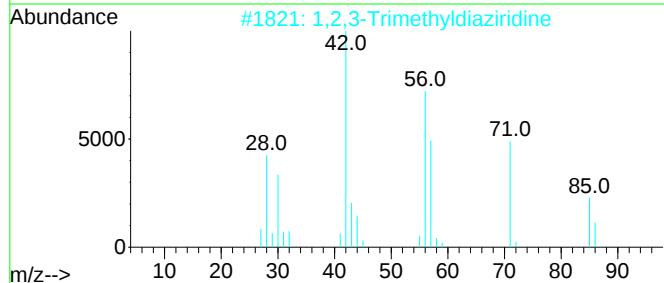
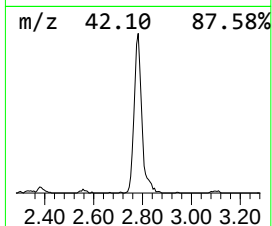
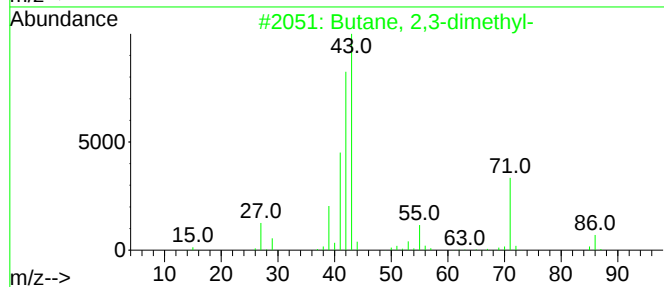
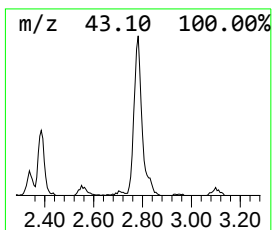
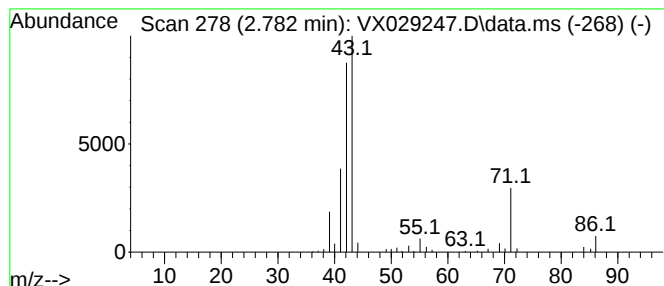
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	6.39 ug/l	122073	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2			1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	59
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	43
4			Tetrahydrofuran	72	C4H8O	000109-99-9	36
5			Pyrrolidine	71	C4H9N	000123-75-1	9



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ALS Vial : 21 Sample Multiplier: 1

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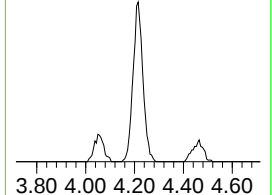
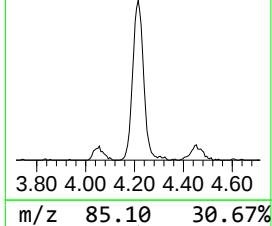
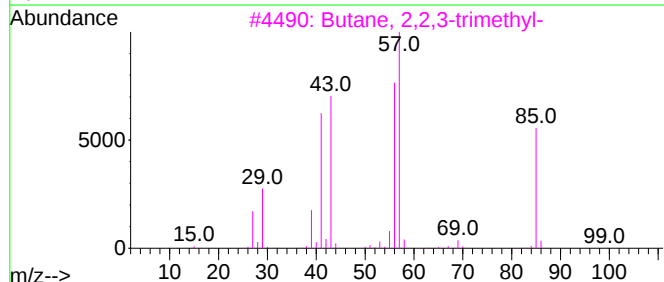
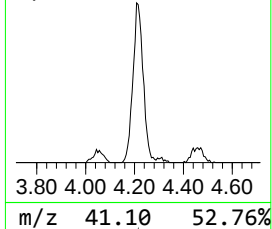
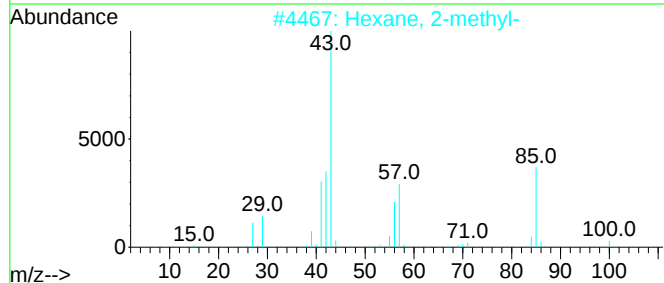
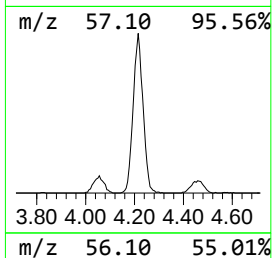
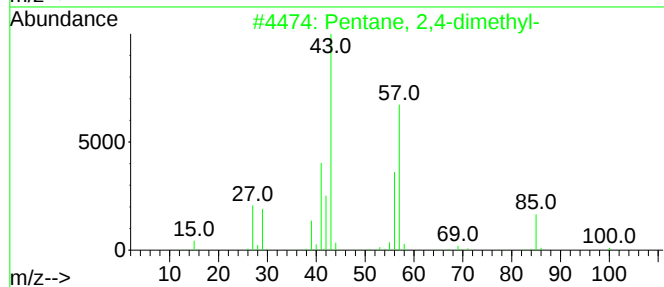
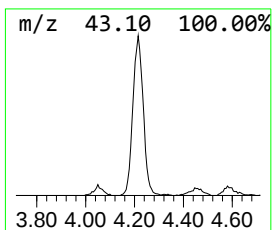
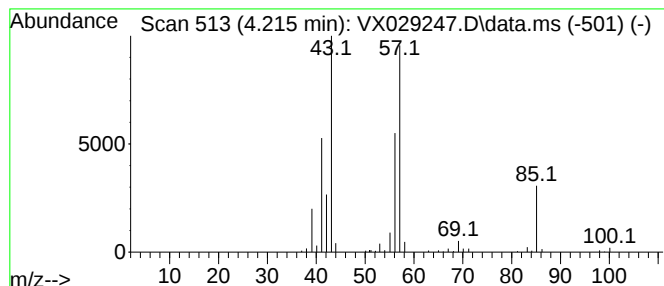
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.215	14.15 ug/l	270382	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2			Hexane, 2-methyl-	100	C7H16	000591-76-4	72
3			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
4			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	53
5			Heptane, 3-methyl-	114	C8H18	000589-81-1	50



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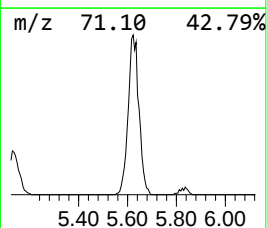
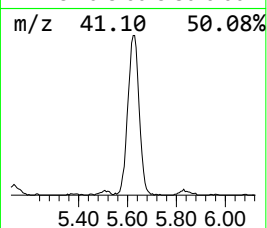
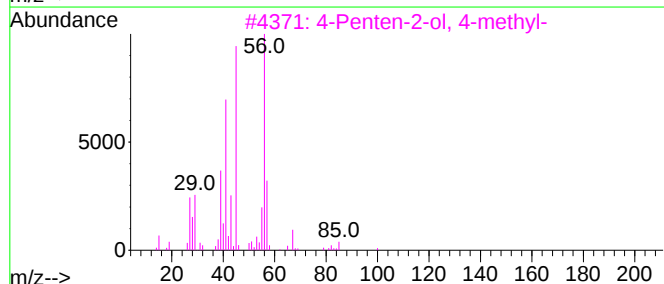
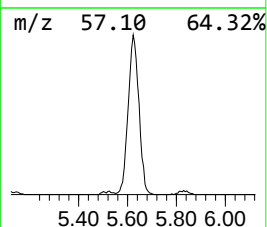
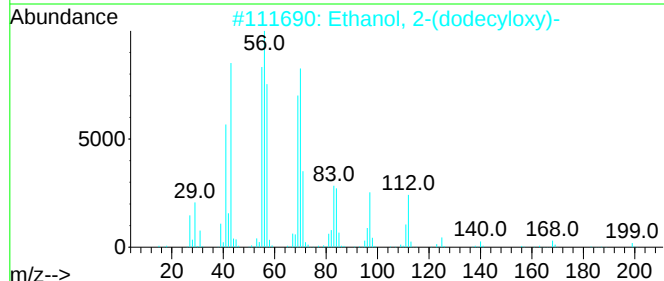
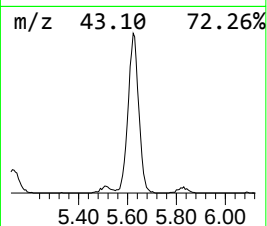
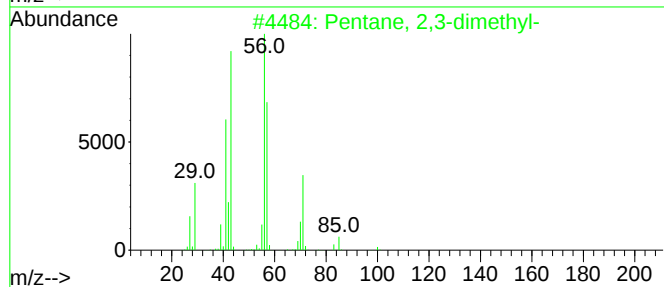
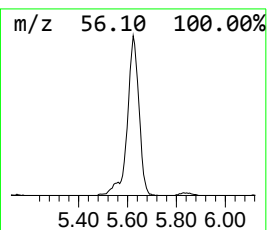
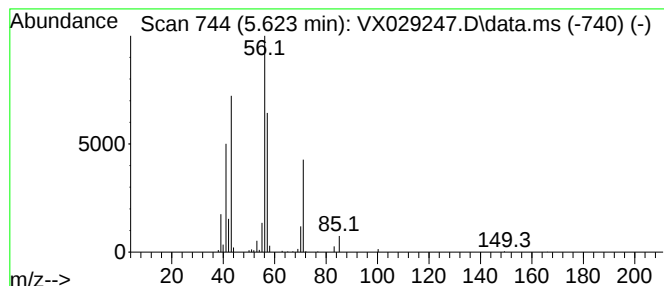
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.623	17.14 ug/l	327449	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	56
3			4-Penten-2-ol, 4-methyl-	100	C6H12O	002004-67-3	38
4			1-Octene, 2-methyl-	126	C9H18	004588-18-5	33
5			Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	33



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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

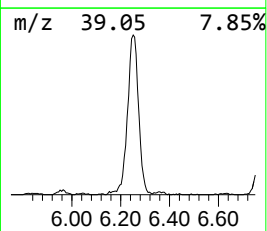
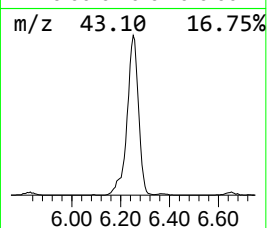
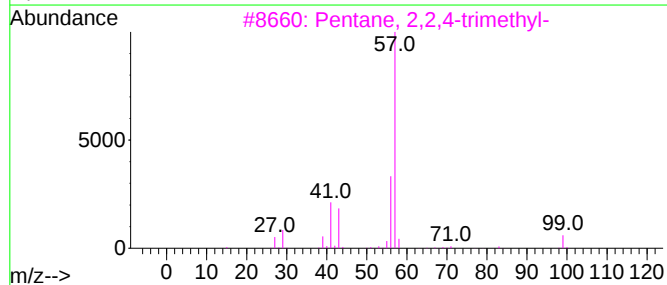
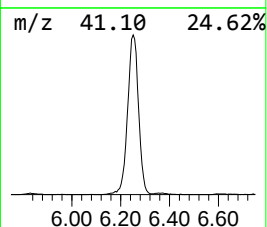
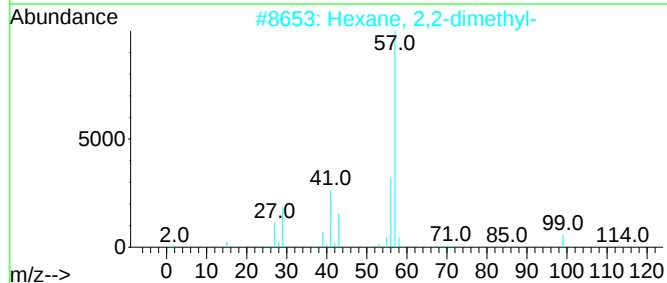
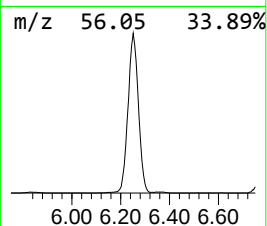
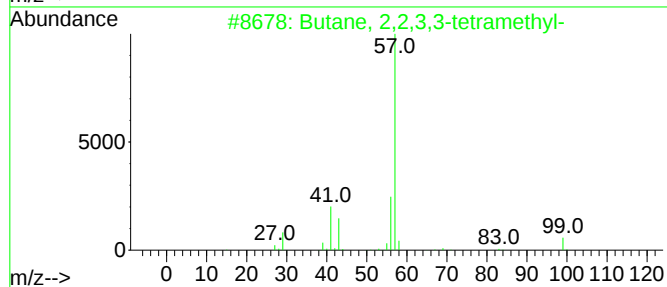
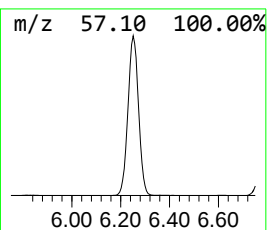
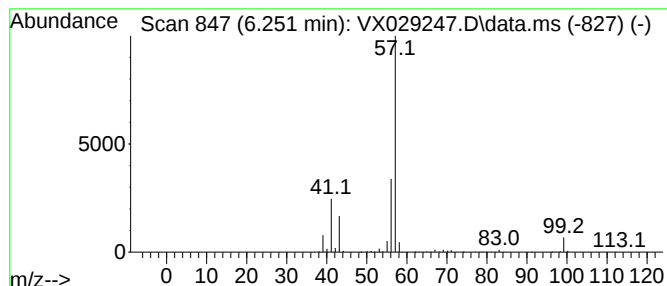
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Quant Title : SW846 8260

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

Peak Number 4 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	57.47 ug/l	1477450	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	59
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029247.D
Acq On : 06 Jun 2022 18:41
Operator : JC/MD
Sample : N3160-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

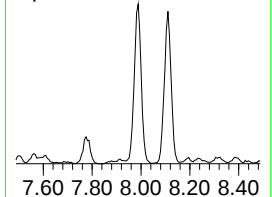
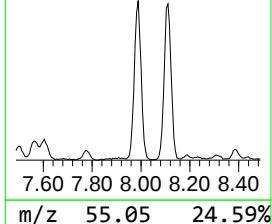
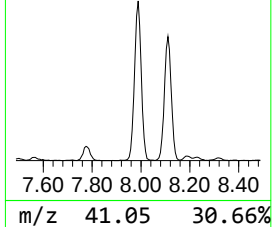
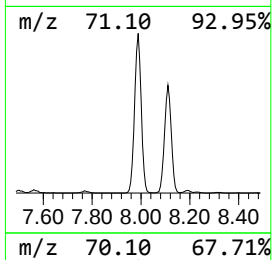
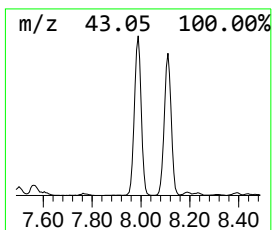
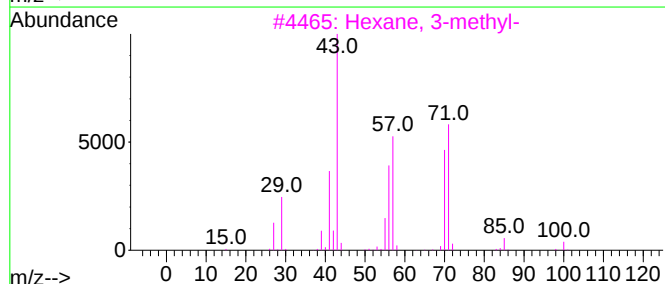
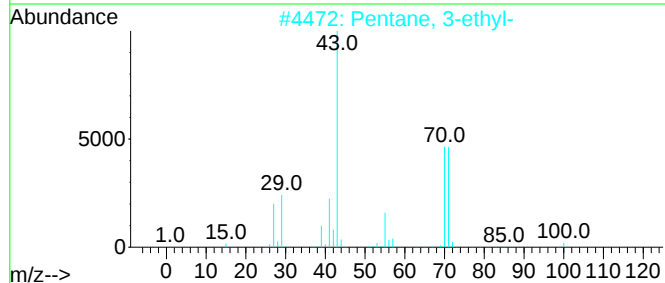
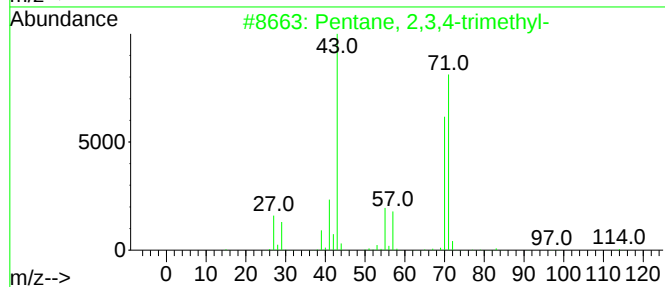
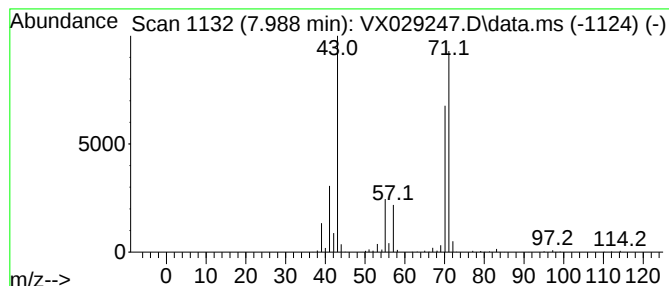
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.988	29.69 ug/l	763389	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	78
4			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	78
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029247.D
Acq On : 06 Jun 2022 18:41
Operator : JC/MD
Sample : N3160-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

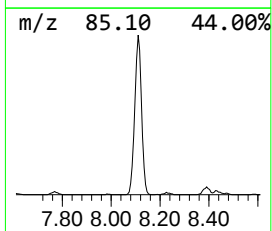
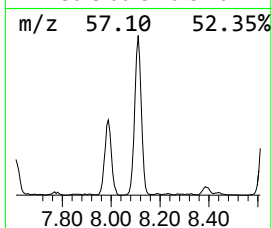
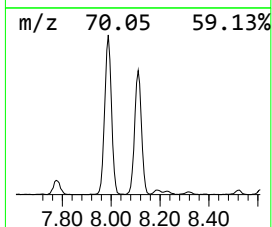
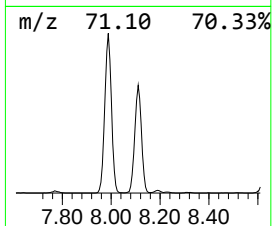
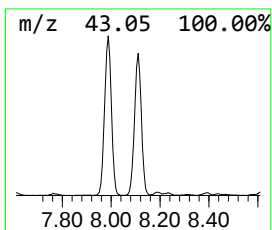
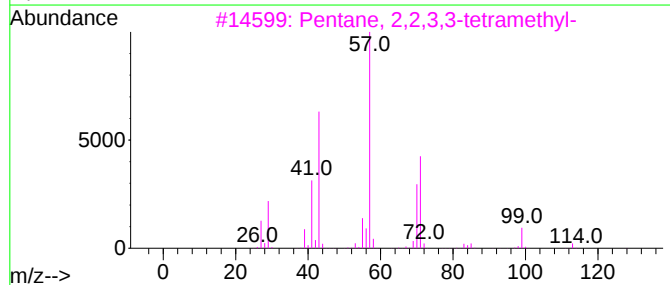
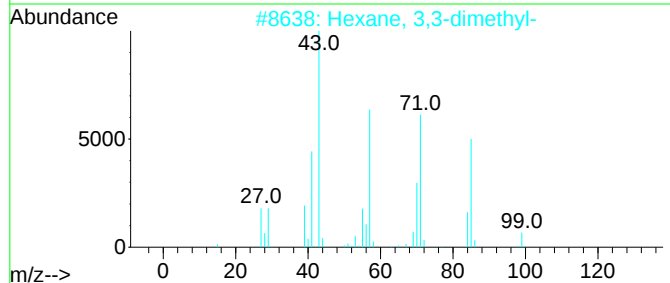
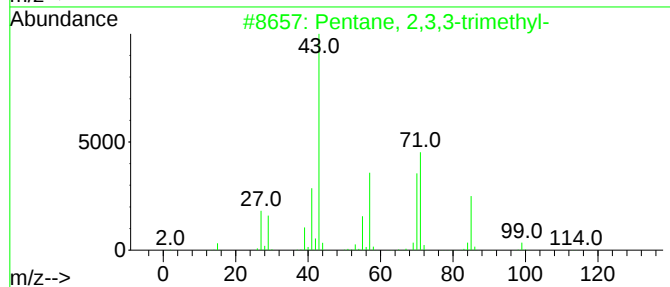
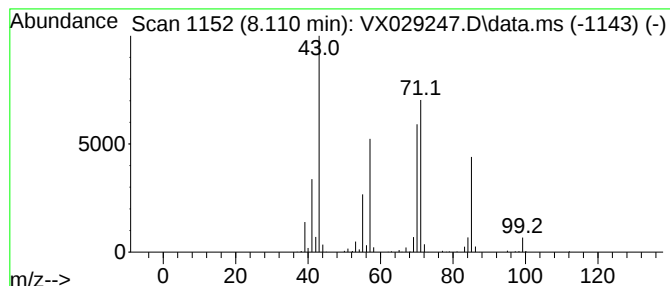
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	31.28 ug/l	804213	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	72
3			Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	53
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029247.D
Acq On : 06 Jun 2022 18:41
Operator : JC/MD
Sample : N3160-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

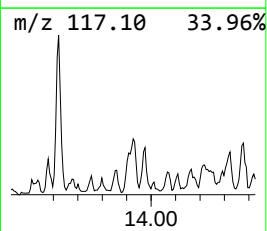
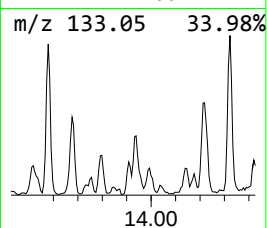
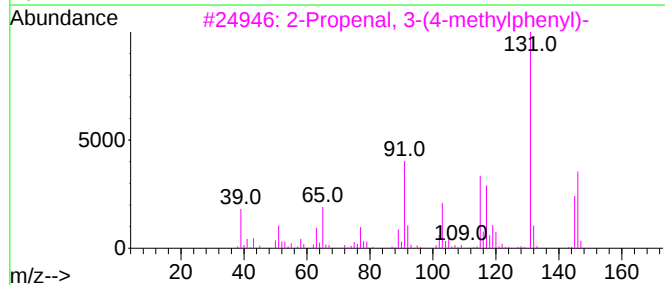
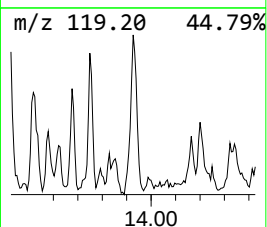
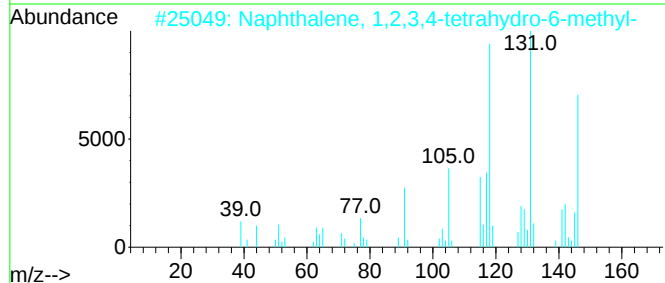
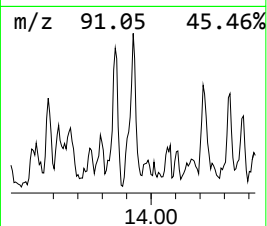
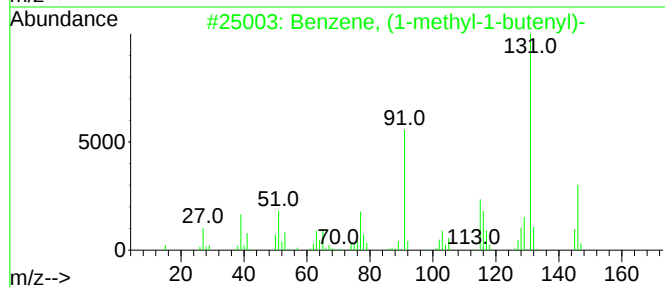
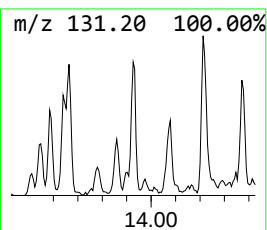
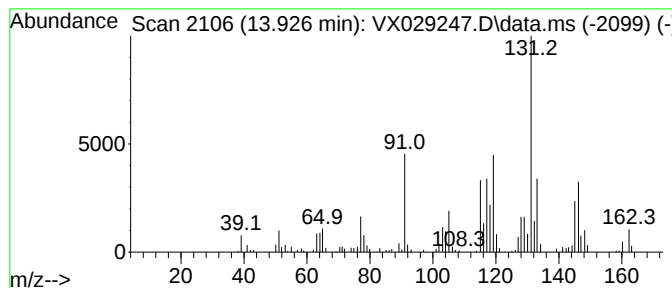
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, (1-methyl-1-butenyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.926	5.07 ug/l	163191	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	86
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	70
3			2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	58
4			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	55
5			Benzene, (1,1-dimethyl-2-propenyl)-	146	C11H14	018321-36-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060622\
Data File : VX029247.D
Acq On : 06 Jun 2022 18:41
Operator : JC/MD
Sample : N3160-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053122W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2,3-dim...	2.782	6.4	ug/l	122073	1	5.556	955389	50.0
Pentane, 2,4-di...	4.215	14.2	ug/l	270382	1	5.556	955389	50.0
Pentane, 2,3-di...	5.623	17.1	ug/l	327449	1	5.556	955389	50.0
Butane, 2,2,3,3...	6.251	57.5	ug/l	1477450	2	6.763	1285390	50.0
Pentane, 2,3,4-...	7.988	29.7	ug/l	763389	2	6.763	1285390	50.0
Pentane, 2,3,3-...	8.110	31.3	ug/l	804213	2	6.763	1285390	50.0
Benzene, (1-met...	13.926	5.1	ug/l	163191	4	12.024	1608790	50.0