

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
 Data File : VX029583.D
 Acq On : 18 Jun 2022 20:29
 Operator : JC/MD
 Sample : N3290-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-11A

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\82X061822W.M
 Title : SW846 8260

Signal : TIC: VX029583.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	23	29	43	rBV	49164	124619	8.66%	0.931%
2	1.752	105	109	116	rVB	12239	16660	1.16%	0.124%
3	2.337	195	205	222	rVB	109305	228268	15.86%	1.705%
4	2.782	267	278	289	rBV	383665	821971	57.10%	6.139%
5	2.971	299	309	321	rBV2	15902	40681	2.83%	0.304%
6	3.117	324	333	345	rVB	14189	34086	2.37%	0.255%
7	4.050	478	486	496	rBV3	6816	21053	1.46%	0.157%
8	4.215	496	513	523	rBV2	81136	250674	17.41%	1.872%
9	4.452	538	552	565	rBV6	12683	52969	3.68%	0.396%
10	5.129	651	663	682	rVB5	16666	68969	4.79%	0.515%
11	5.391	692	706	722	rBV2	151844	452038	31.40%	3.376%
12	5.556	722	733	739	rVV	289426	851154	59.13%	6.357%
13	5.623	739	744	759	rVB	199775	591551	41.10%	4.418%
14	5.849	769	781	790	rBV3	14702	44886	3.12%	0.335%
15	5.958	790	799	809	rBV	162261	431265	29.96%	3.221%
16	6.251	828	847	858	rBV2	148928	487283	33.85%	3.639%
17	6.361	858	865	876	rVB4	17942	51696	3.59%	0.386%
18	6.763	922	931	943	rBV	439499	1035814	71.96%	7.736%
19	7.171	994	998	1006	rVB2	15191	33419	2.32%	0.250%
20	7.367	1022	1030	1043	rVB2	29262	73084	5.08%	0.546%
21	7.501	1043	1052	1057	rBV2	15220	33949	2.36%	0.254%
22	7.562	1057	1062	1065	rVV3	14066	29860	2.07%	0.223%
23	7.604	1066	1069	1077	rVB	18369	35825	2.49%	0.268%
24	7.775	1090	1097	1106	rVB2	26292	54785	3.81%	0.409%
25	7.897	1106	1117	1122	rBV6	5183	18390	1.28%	0.137%
26	7.988	1122	1132	1143	rVB	130070	283804	19.72%	2.120%
27	8.110	1143	1152	1162	rBV	266662	541436	37.61%	4.044%
28	8.318	1178	1186	1193	rBV6	16858	41161	2.86%	0.307%
29	8.391	1193	1198	1200	rVV3	9142	15851	1.10%	0.118%
30	8.427	1200	1204	1210	rVB	20908	36755	2.55%	0.275%
31	8.513	1211	1218	1225	rVB4	23110	49207	3.42%	0.368%
32	8.653	1225	1241	1251	rBV	877432	1439445	100.00%	10.751%
33	8.842	1265	1272	1277	rVV5	12975	31132	2.16%	0.233%
34	8.927	1281	1286	1290	rVV	16619	29207	2.03%	0.218%
35	8.976	1290	1294	1299	rVV2	23995	39028	2.71%	0.291%
36	9.104	1307	1315	1320	rVV3	25881	50932	3.54%	0.380%

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37	9.165	1320	1325	1335	rVV	103092	171999	11.95%	1.285%
38	9.452	1364	1372	1377	rBV5	24118	58585	4.07%	0.438%
39	9.506	1377	1381	1387	rVB3	15529	28719	2.00%	0.214%
40	9.659	1401	1406	1417	rVB	13859	26193	1.82%	0.196%

41	9.769	1417	1424	1432	rBV2	21374	39142	2.72%	0.292%
42	10.019	1460	1465	1466	rBV2	21353	29025	2.02%	0.217%
43	10.055	1466	1471	1476	rVB	877369	1137533	79.03%	8.496%
44	10.104	1476	1479	1482	rBV2	17093	21988	1.53%	0.164%
45	10.195	1491	1494	1498	rBV	15851	21631	1.50%	0.162%

46	10.256	1498	1504	1505	rVV5	8298	18172	1.26%	0.136%
47	10.305	1505	1512	1517	rVB	38560	72612	5.04%	0.542%
48	10.586	1550	1558	1564	rBV6	11760	25161	1.75%	0.188%
49	10.646	1564	1568	1578	rVB2	17534	24265	1.69%	0.181%
50	10.793	1582	1592	1598	rBV8	28578	73498	5.11%	0.549%

51	10.848	1598	1601	1606	rVB4	10584	15964	1.11%	0.119%
52	10.970	1614	1621	1625	rBV3	19433	33385	2.32%	0.249%
53	11.018	1625	1629	1631	rVV	16786	22638	1.57%	0.169%
54	11.049	1631	1634	1635	rVV	18245	21011	1.46%	0.157%
55	11.085	1635	1640	1644	rVV	667228	881564	61.24%	6.584%

56	11.122	1644	1646	1649	rVV4	16573	22931	1.59%	0.171%
57	11.177	1649	1655	1659	rVB	18752	31650	2.20%	0.236%
58	11.268	1666	1670	1673	rBV3	12644	19927	1.38%	0.149%
59	11.305	1673	1676	1680	rVB2	22311	28816	2.00%	0.215%
60	11.390	1686	1690	1695	rBV5	10137	19968	1.39%	0.149%

61	11.451	1695	1700	1709	rVB3	10420	23546	1.64%	0.176%
62	11.616	1718	1727	1731	rBV4	9913	17923	1.25%	0.134%
63	11.701	1736	1741	1746	rBV5	10577	21521	1.50%	0.161%
64	11.750	1746	1749	1754	rVV	13846	17755	1.23%	0.133%
65	11.890	1769	1772	1779	rVB	38216	54053	3.76%	0.404%

66	12.024	1788	1794	1801	rBV	881478	1076800	74.81%	8.042%
67	12.091	1801	1805	1807	rBV3	11343	16939	1.18%	0.127%
68	12.177	1816	1819	1824	rVB	20302	25590	1.78%	0.191%
69	12.250	1824	1831	1838	rBV	325086	404874	28.13%	3.024%
70	12.311	1838	1841	1852	rVB7	8777	22422	1.56%	0.167%

71	12.616	1884	1891	1894	rVB2	15707	21774	1.51%	0.163%
72	12.719	1902	1908	1912	rVV3	19060	33402	2.32%	0.249%
73	12.762	1912	1915	1920	rVB	15435	20560	1.43%	0.154%
74	12.841	1920	1928	1934	rBV2	29759	43286	3.01%	0.323%
75	13.030	1952	1959	1969	rBV3	39891	66797	4.64%	0.499%

76	13.195	1978	1986	1991	rVB2	31471	49753	3.46%	0.372%
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Title : SW846 8260

77	13.292	1998	2002	2007	rBV2	12088	17381	1.21%	0.130%
78	13.426	2016	2024	2029	rVB3	12802	19737	1.37%	0.147%
79	13.622	2052	2056	2063	rVV3	18775	30151	2.09%	0.225%
80	13.780	2074	2082	2091	rBV2	25935	55584	3.86%	0.415%
81	14.323	2166	2171	2175	rBV2	10592	14804	1.03%	0.111%
82	14.603	2210	2217	2220	rBV3	8170	14515	1.01%	0.108%
83	14.640	2220	2223	2233	rVB3	9758	15221	1.06%	0.114%
84	14.780	2241	2246	2251	rBV4	9392	15210	1.06%	0.114%

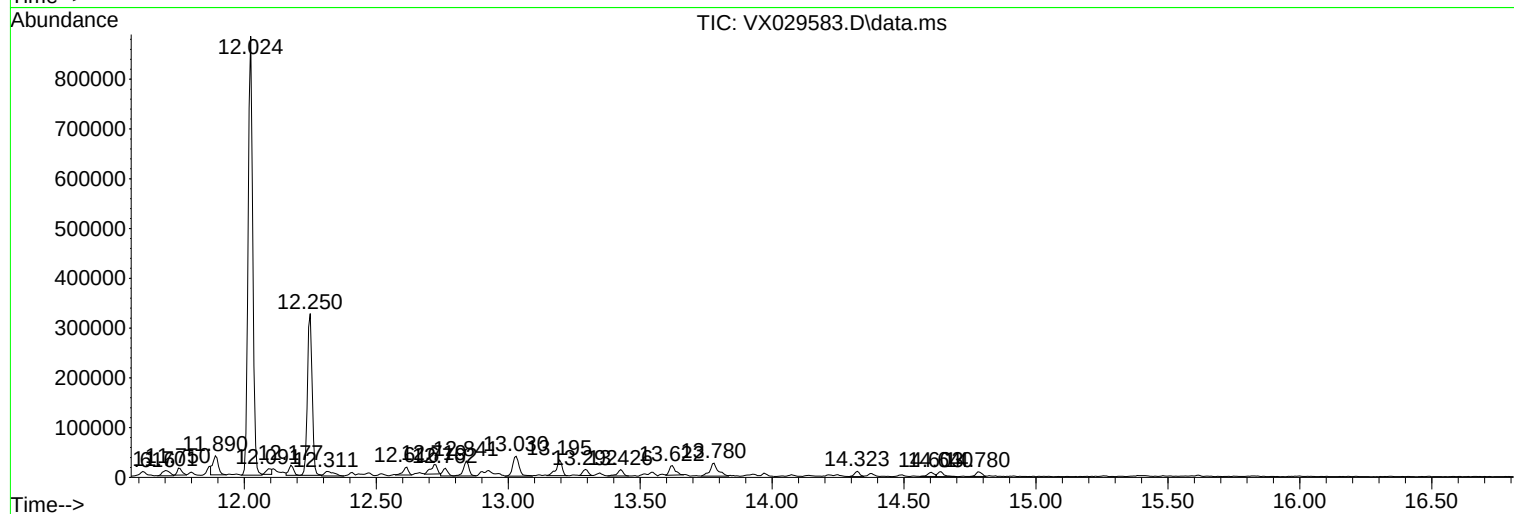
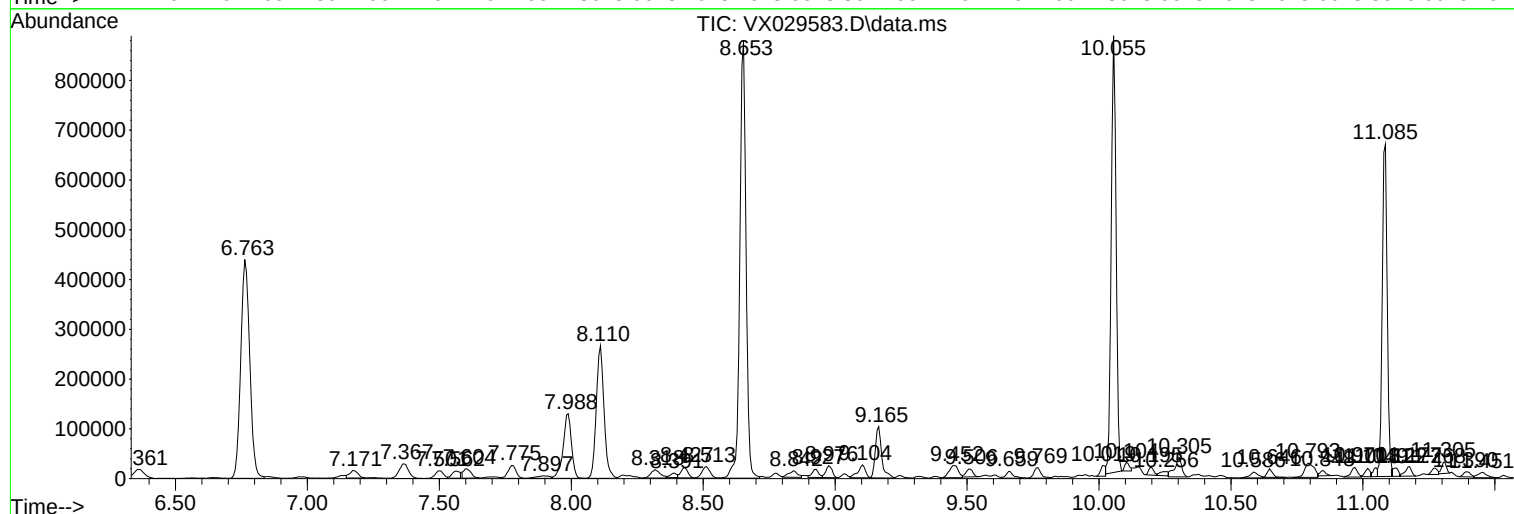
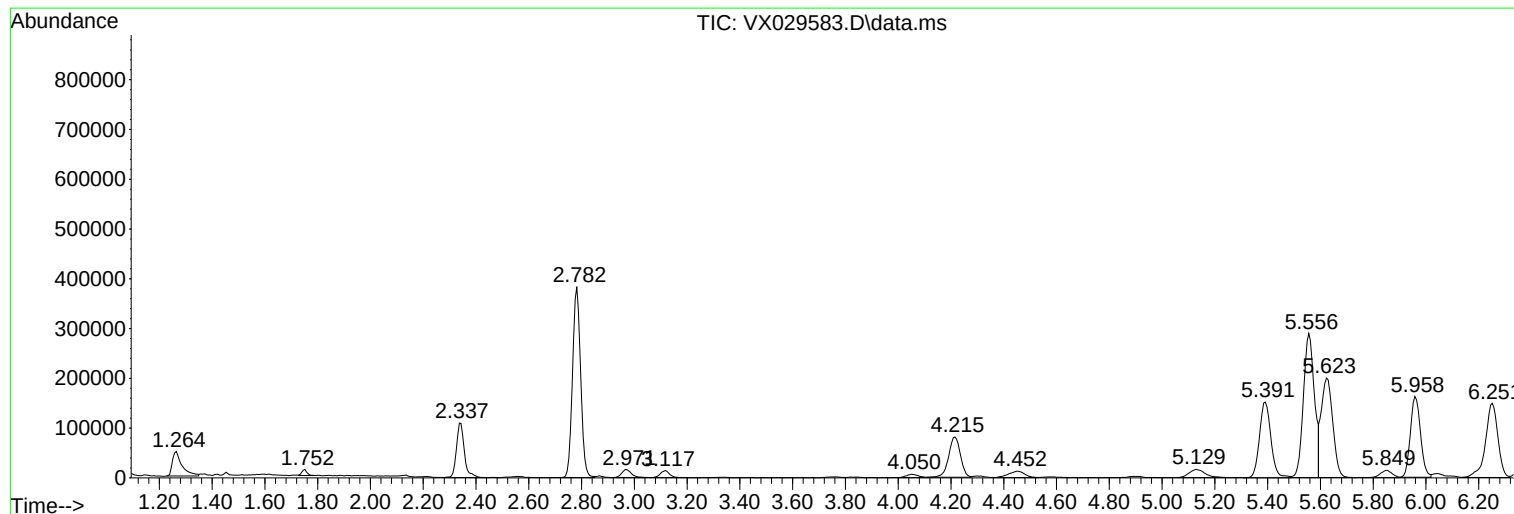
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Instrument :
MSVOA_X
ClientSampleId :
MW-11A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
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MW-11A

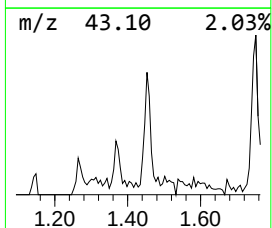
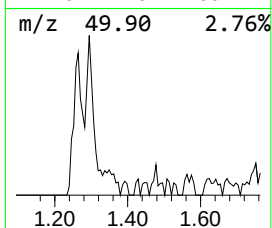
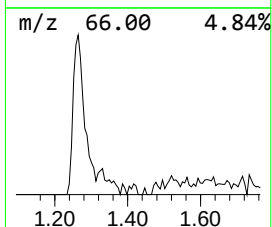
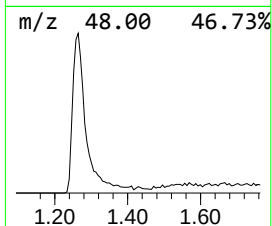
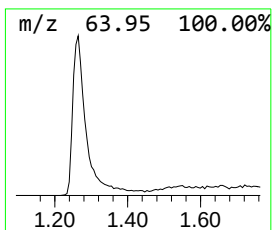
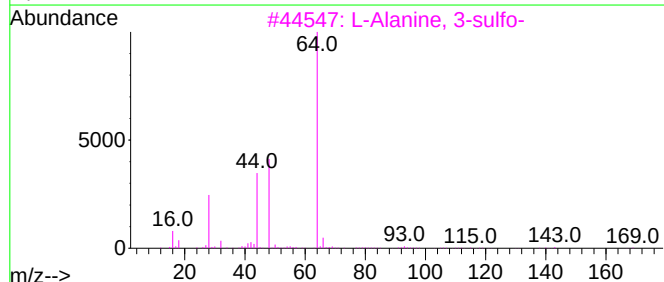
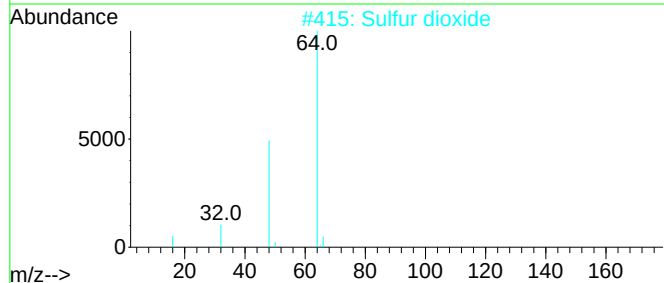
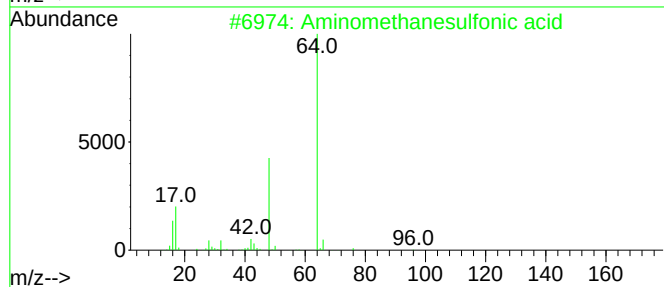
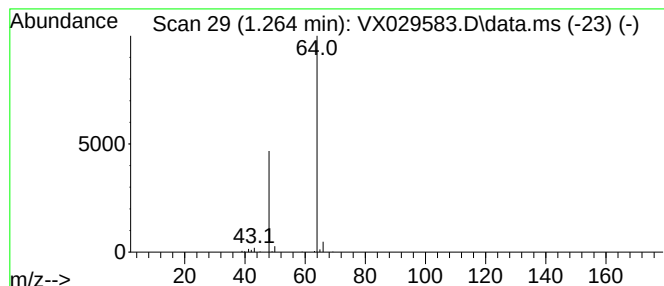
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	7.32 ug/l	124619	Pentafluorobenzene	5.556

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



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ALS Vial : 31 Sample Multiplier: 1

Instrument :
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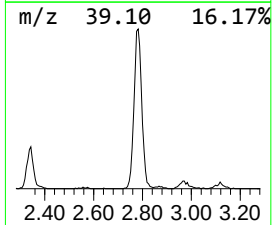
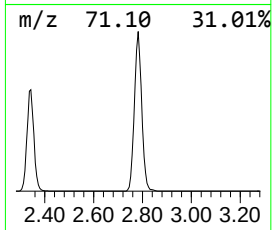
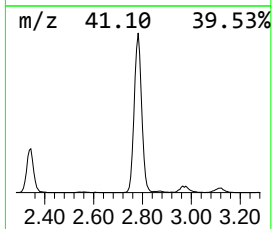
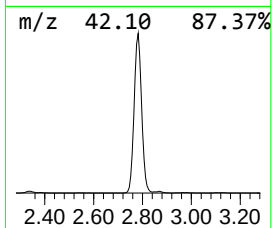
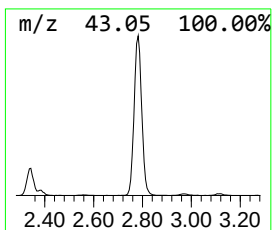
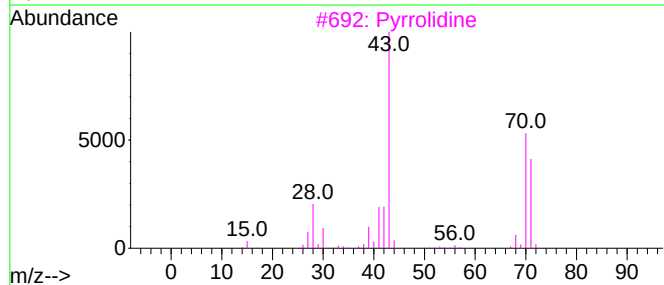
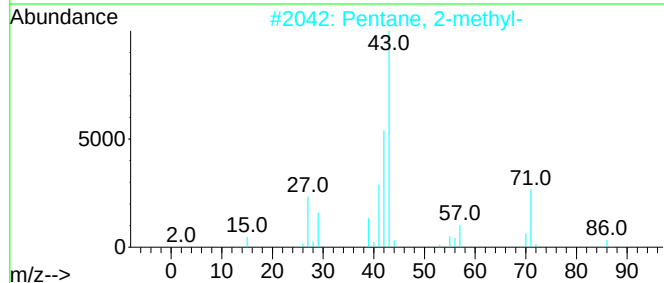
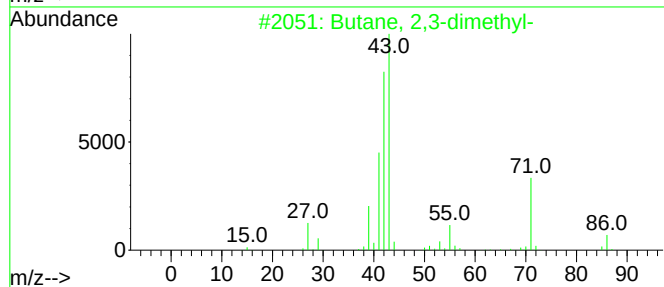
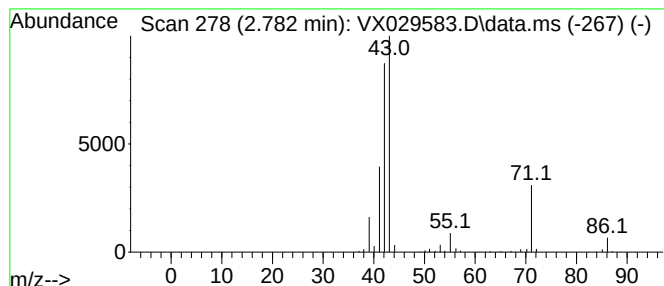
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	48.29 ug/l	821971	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3			Pyrrolidine	71	C4H9N	000123-75-1	22
4			Propanoic acid, 2-methyl-, 2-pro...	128	C7H12O2	015727-77-2	12
5			Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	12



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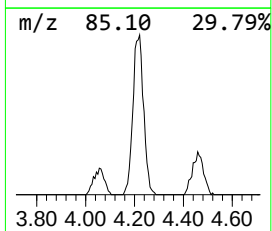
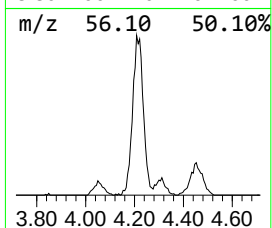
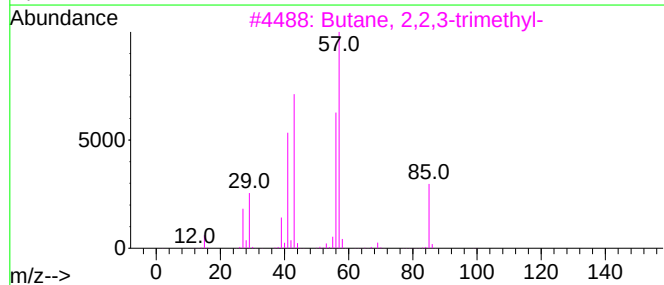
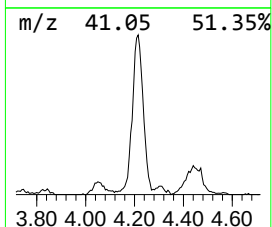
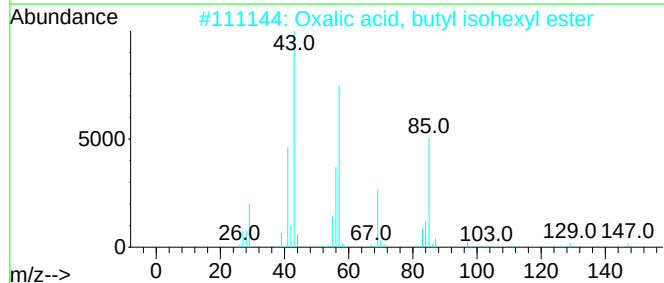
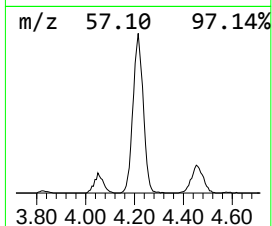
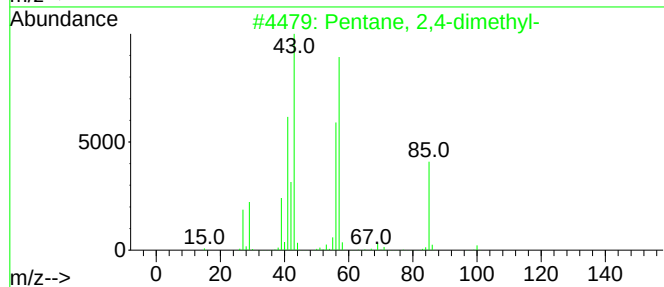
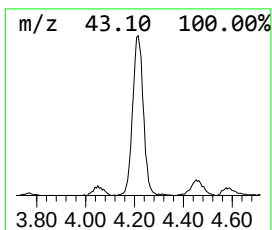
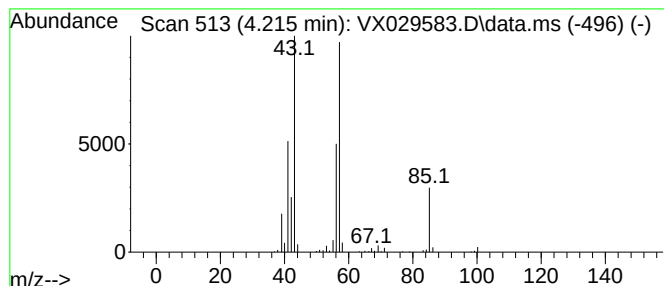
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.215	14.73 ug/l	250674	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	94
2			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	64
3			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
4			Hexane, 1-(hexyloxy)-5-methyl-	200	C13H28O	074421-19-5	56
5			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	53



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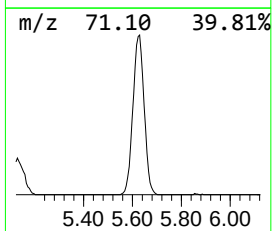
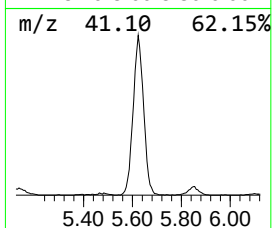
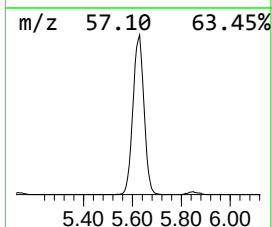
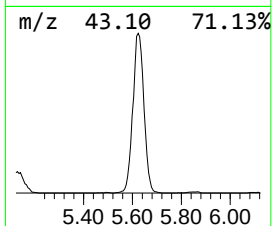
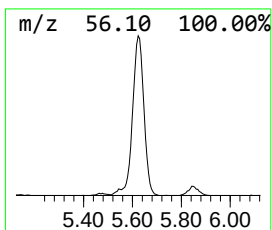
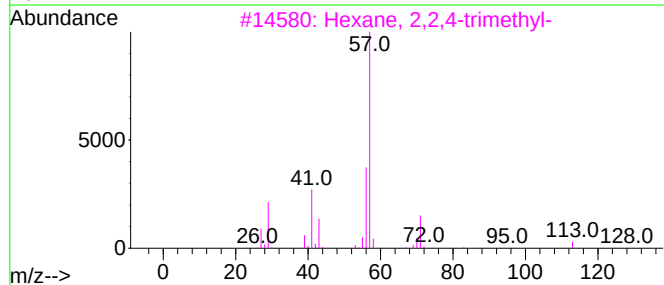
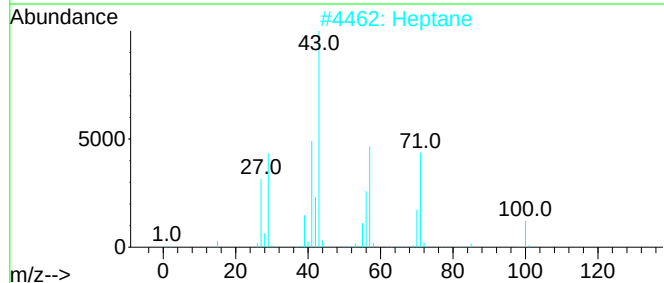
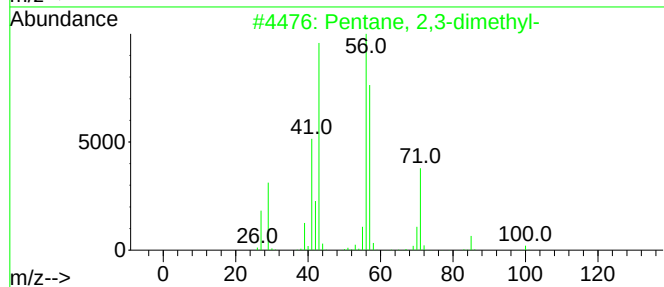
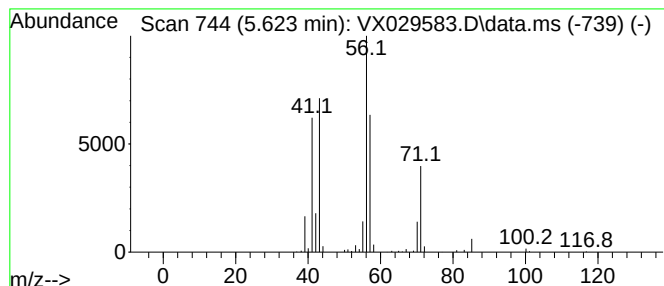
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.623	34.75 ug/l	591551	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Heptane	100	C7H16	000142-82-5	47
3			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45
4			Hexyl octyl ether	214	C14H30O	017071-54-4	43
5			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029583.D
Acq On : 18 Jun 2022 20:29
Operator : JC/MD
Sample : N3290-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11A

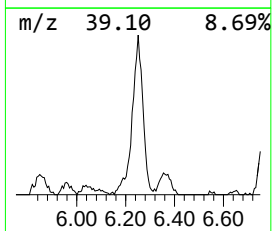
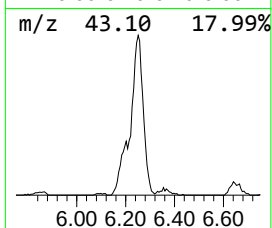
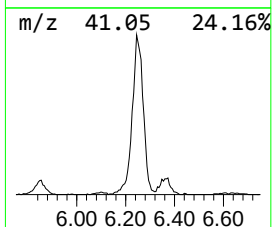
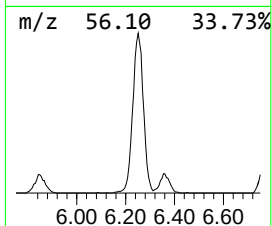
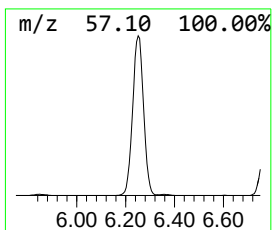
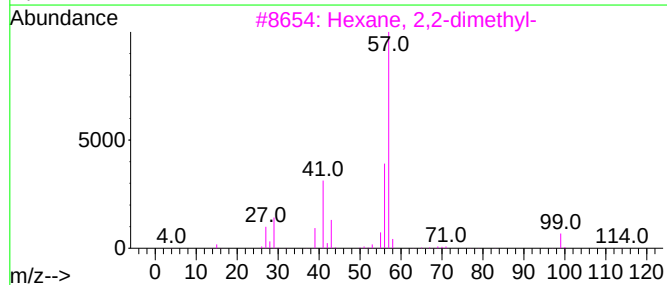
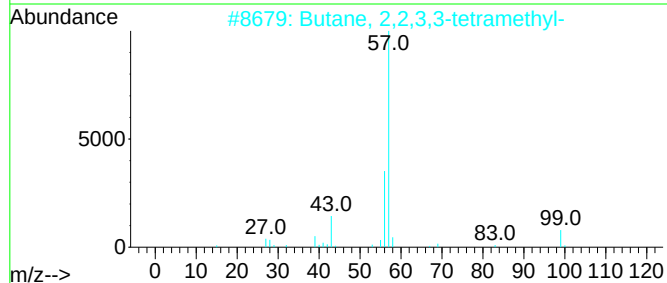
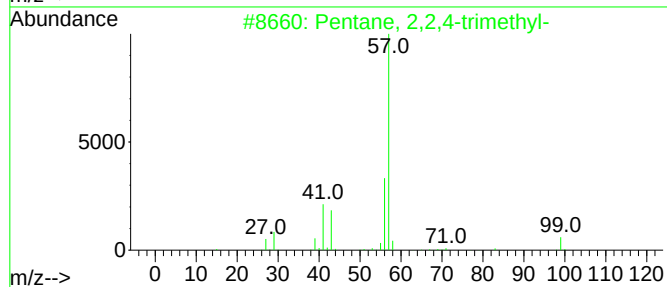
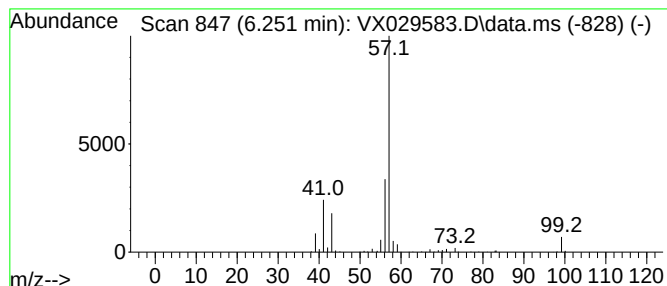
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	23.52 ug/l	487283	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	53
5			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029583.D
Acq On : 18 Jun 2022 20:29
Operator : JC/MD
Sample : N3290-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11A

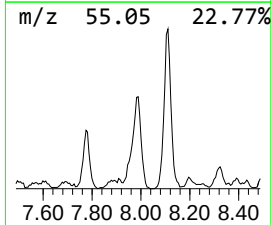
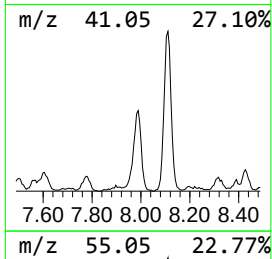
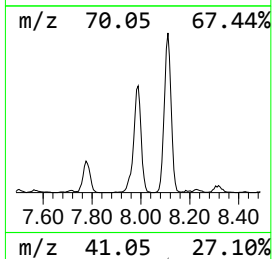
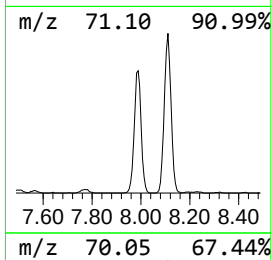
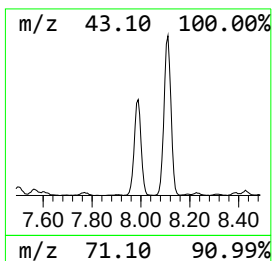
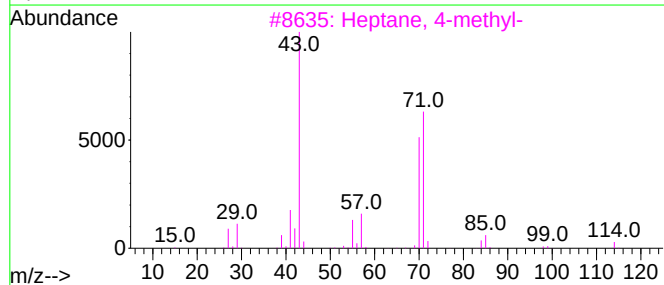
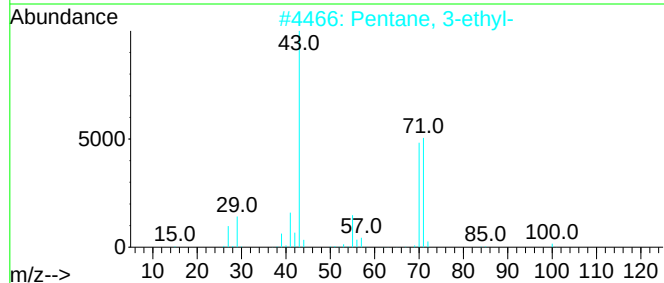
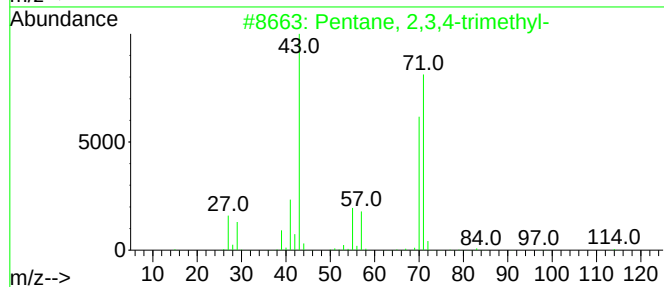
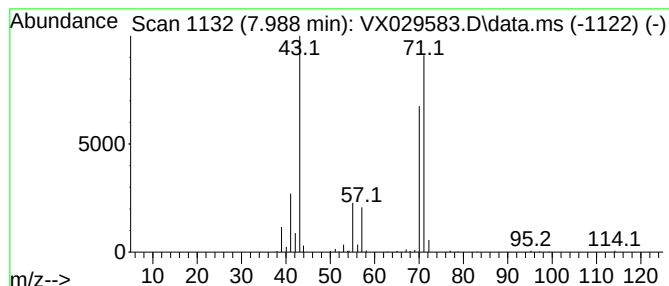
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3,4-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.988	13.70 ug/l	283804	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			Heptane, 4-methyl-	114	C8H18	000589-53-7	74
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	74
5			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029583.D
Acq On : 18 Jun 2022 20:29
Operator : JC/MD
Sample : N3290-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11A

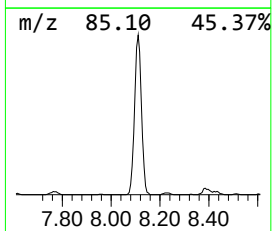
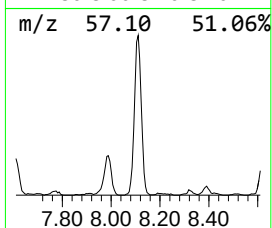
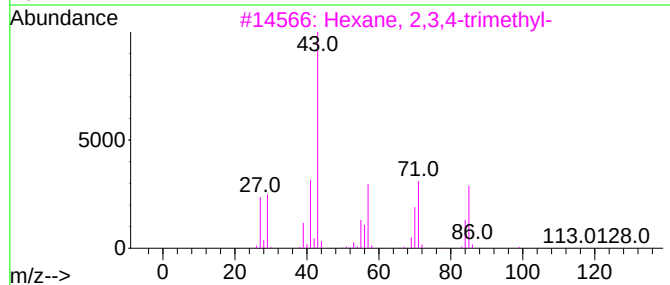
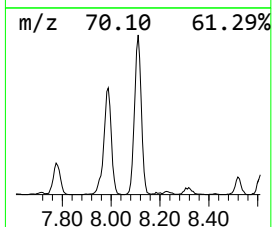
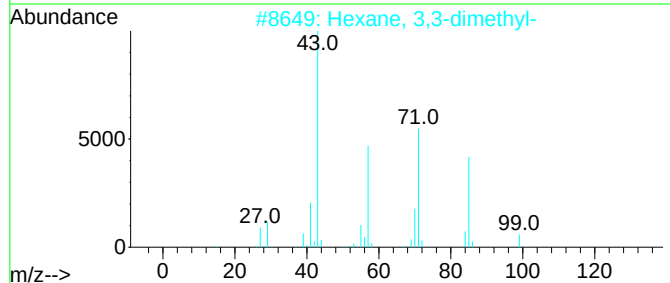
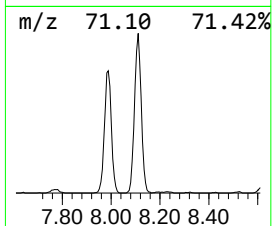
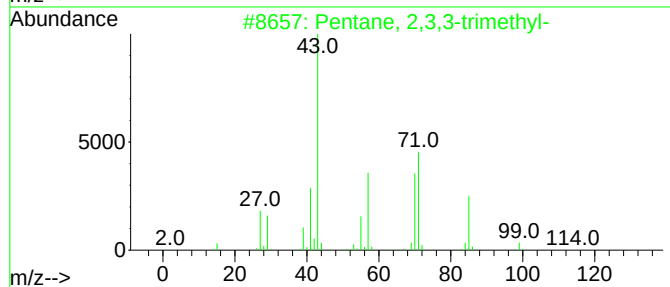
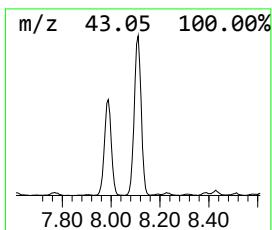
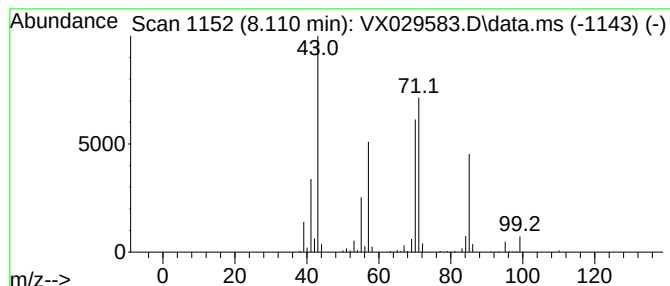
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	26.14 ug/l	541436	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			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	53
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029583.D
Acq On : 18 Jun 2022 20:29
Operator : JC/MD
Sample : N3290-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11A

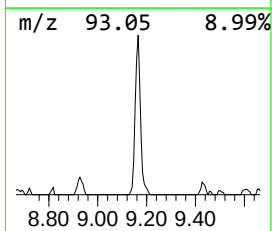
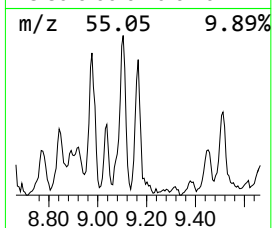
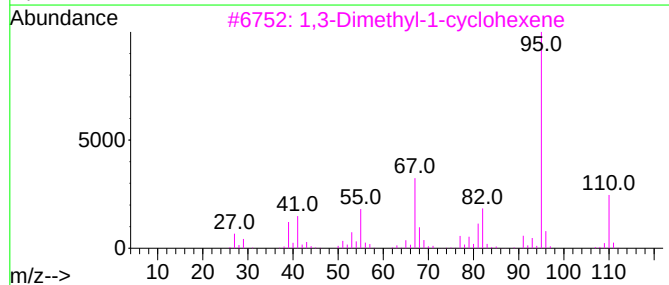
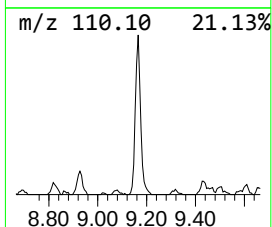
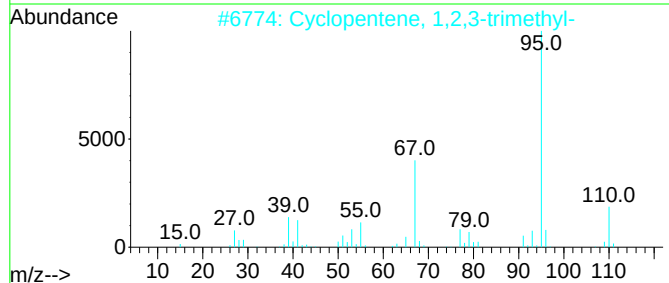
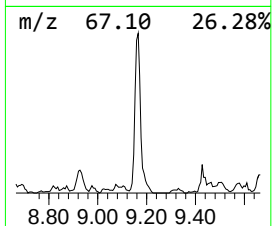
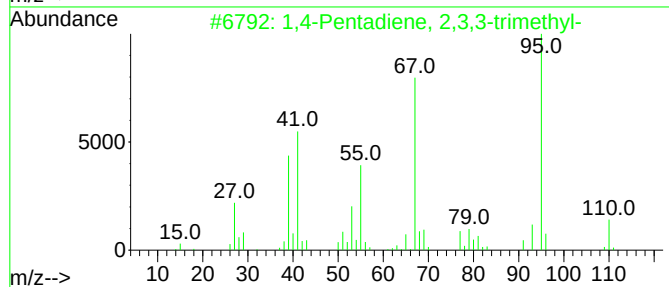
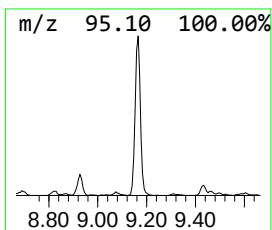
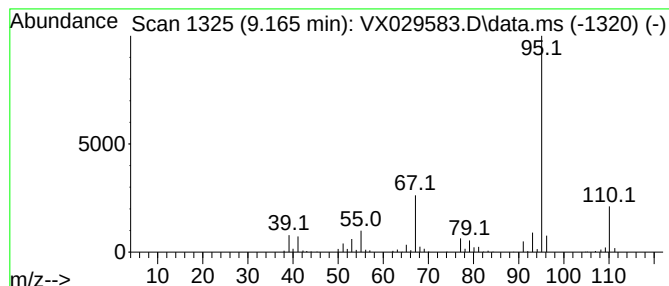
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Quant Title : SW846 8260

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

Peak Number 8 1,4-Pentadiene, 2,3,3-trime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.165	7.56 ug/l	171999	Chlorobenzene-d5	10.055

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	91
2		Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	91
3		1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	91
4		Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	90
5		5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029583.D
Acq On : 18 Jun 2022 20:29
Operator : JC/MD
Sample : N3290-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11A

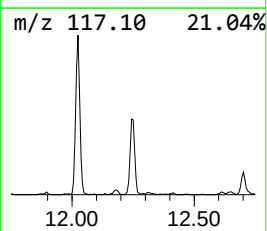
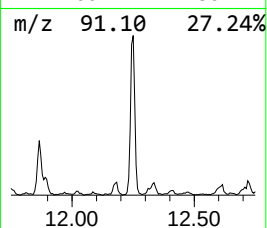
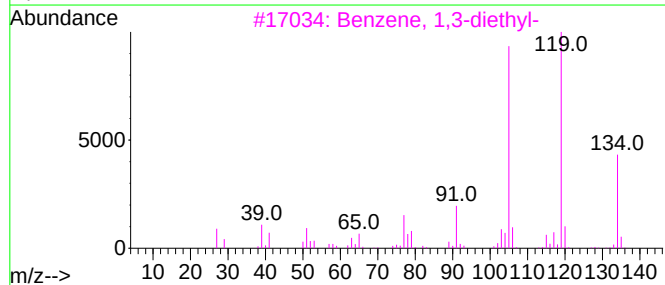
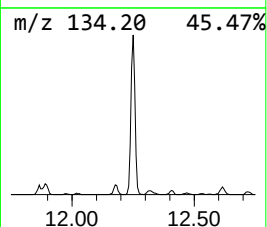
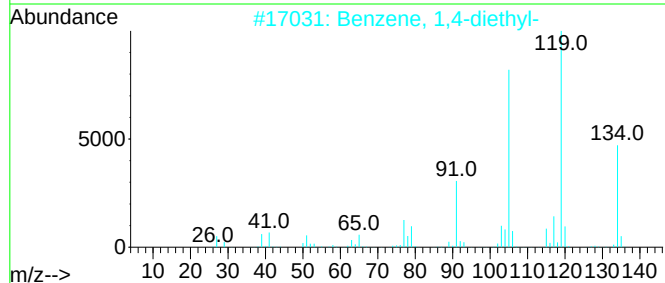
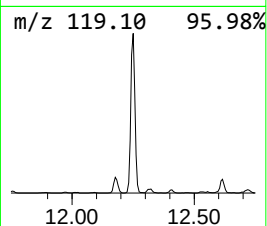
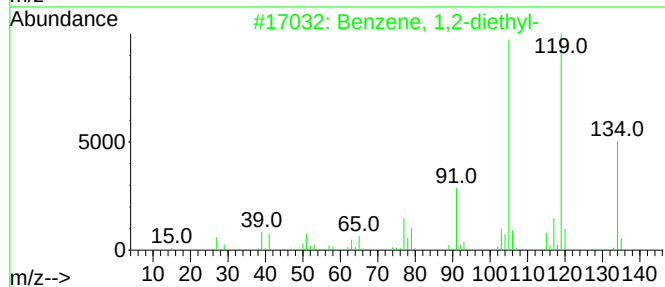
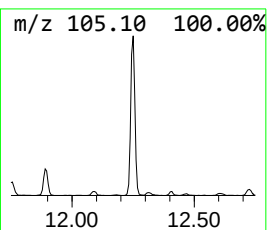
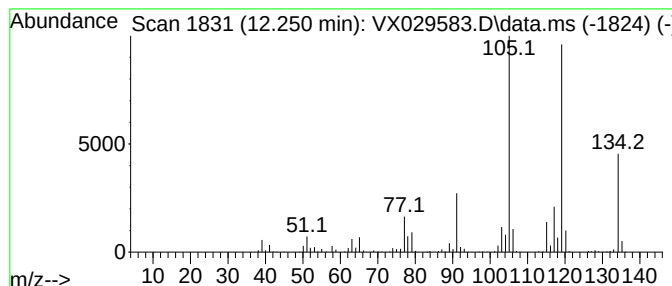
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2-diethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	18.80 ug/l	404874	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	97
2			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	97
3			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	93
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	83
5			2,6-Dimethyl-1,3,5,7-octatetraen...	134	C10H14	000460-01-5	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029583.D
Acq On : 18 Jun 2022 20:29
Operator : JC/MD
Sample : N3290-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.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
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Butane, 2,3-dim...	2.782	48.3	ug/l	821971	1	5.556	851154	50.0
Pentane, 2,4-di...	4.215	14.7	ug/l	250674	1	5.556	851154	50.0
Pentane, 2,3-di...	5.623	34.8	ug/l	591551	1	5.556	851154	50.0
Pentane, 2,2,4-...	6.251	23.5	ug/l	487283	2	6.763	1035810	50.0
Pentane, 2,3,4-...	7.988	13.7	ug/l	283804	2	6.763	1035810	50.0
Pentane, 2,3,3-...	8.110	26.1	ug/l	541436	2	6.763	1035810	50.0
1,4-Pentadiene,...	9.165	7.6	ug/l	171999	3	10.055	1137530	50.0
Benzene, 1,2-di...	12.250	18.8	ug/l	404874	4	12.024	1076800	50.0