

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
 Data File : VX022229.D
 Acq On : 27 May 2021 13:56
 Operator : JC/MD
 Sample : M2535-02 20X
 Misc : 5.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GHOST-2D

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\82X051921W.M

Title : SW846 8260

Signal : TIC: VX022229.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.563	73	78	81	rBV6	3465	6834	1.39%	0.195%
2	1.593	81	83	91	rVB7	4275	5352	1.09%	0.153%
3	1.740	104	107	112	rVB3	4097	5498	1.12%	0.157%
4	2.831	282	286	294	rVB2	4313	8796	1.79%	0.252%
5	3.105	325	331	339	rVB2	3432	7605	1.55%	0.218%
6	3.447	381	387	396	rBV3	3849	8229	1.68%	0.235%
7	4.215	506	513	519	rBV4	2424	5643	1.15%	0.161%
8	4.312	522	529	538	rVB3	4537	11664	2.38%	0.334%
9	5.397	696	707	715	rBV	49894	140052	28.57%	4.006%
10	5.562	724	734	753	rVB2	77846	236229	48.19%	6.757%
11	5.824	768	777	778	rBV2	5892	8748	1.78%	0.250%
12	5.964	790	800	811	rBV2	60054	160381	32.72%	4.588%
13	6.166	826	833	839	rBV5	2663	8160	1.66%	0.233%
14	6.257	839	848	858	rVV	19288	56396	11.51%	1.613%
15	6.361	858	865	875	rVB4	3363	8368	1.71%	0.239%
16	6.617	899	907	916	rVB6	3692	9325	1.90%	0.267%
17	6.769	922	932	942	rBV	137172	330080	67.34%	9.442%
18	7.385	1022	1033	1041	rBV5	16906	43298	8.83%	1.238%
19	7.501	1046	1052	1057	rBV3	3379	7336	1.50%	0.210%
20	7.562	1057	1062	1067	rBV3	3577	7402	1.51%	0.212%
21	7.665	1074	1079	1084	rVB3	3337	5946	1.21%	0.170%
22	7.988	1121	1132	1141	rVB2	20874	42486	8.67%	1.215%
23	8.110	1144	1152	1161	rVV2	28039	61452	12.54%	1.758%
24	8.190	1161	1165	1171	rVV2	5694	10218	2.08%	0.292%
25	8.281	1175	1180	1184	rVV4	4045	7941	1.62%	0.227%
26	8.440	1201	1206	1210	rBV3	3944	5778	1.18%	0.165%
27	8.653	1228	1241	1249	rBV	303552	490154	100.00%	14.020%
28	8.921	1279	1285	1291	rBV6	2917	5595	1.14%	0.160%
29	8.976	1291	1294	1301	rVB3	4411	7273	1.48%	0.208%
30	9.104	1308	1315	1320	rBV4	3790	6676	1.36%	0.191%
31	9.519	1376	1383	1387	rBV5	3405	7778	1.59%	0.222%
32	9.561	1387	1390	1395	rVB	4385	6091	1.24%	0.174%
33	9.616	1395	1399	1404	rBV4	3549	5688	1.16%	0.163%
34	9.909	1443	1447	1452	rVB4	3634	5551	1.13%	0.159%
35	10.055	1466	1471	1477	rVV	280650	377244	76.96%	10.791%
36	10.195	1490	1494	1501	rVB2	8032	12239	2.50%	0.350%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

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Start Thrs: 0.2

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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 Title : SW846 8260

37	10.305	1501	1512	1517	rVV	136022	190330	38.83%	5.444%
38	10.360	1519	1521	1532	rVB6	2674	5049	1.03%	0.144%
39	10.585	1552	1558	1563	rBV5	2780	4924	1.00%	0.141%
40	10.646	1563	1568	1576	rVB	8933	12545	2.56%	0.359%
41	10.963	1614	1620	1624	rBV	6902	9633	1.97%	0.276%
42	11.085	1634	1640	1645	rBV	217017	271251	55.34%	7.759%
43	11.122	1645	1646	1651	rVB3	7610	6821	1.39%	0.195%
44	11.305	1669	1676	1682	rVB	19006	25044	5.11%	0.716%
45	11.384	1682	1689	1696	rVV	73423	100907	20.59%	2.886%
46	11.457	1696	1701	1714	rVB	42250	58810	12.00%	1.682%
47	11.616	1722	1727	1732	rBV	30755	38139	7.78%	1.091%
48	11.756	1745	1750	1758	rVB	129782	159527	32.55%	4.563%
49	11.939	1776	1780	1783	rVB	5665	6651	1.36%	0.190%
50	12.024	1789	1794	1800	rBV	265050	317312	64.74%	9.076%
51	12.091	1800	1805	1809	rVV	30487	39964	8.15%	1.143%
52	12.250	1825	1831	1833	rBV	19927	27360	5.58%	0.783%
53	12.323	1838	1843	1849	rVB3	14136	23142	4.72%	0.662%
54	12.469	1863	1867	1872	rVB3	4044	6189	1.26%	0.177%
55	12.536	1872	1878	1880	rBV	6047	8483	1.73%	0.243%
56	12.616	1887	1891	1895	rBV	8570	10251	2.09%	0.293%
57	12.701	1901	1905	1915	rVB5	3716	6886	1.40%	0.197%
58	12.927	1935	1942	1945	rBV2	3631	4969	1.01%	0.142%
59	12.963	1945	1948	1954	rVB	4802	6223	1.27%	0.178%
60	13.292	1999	2002	2007	rVB2	5967	7778	1.59%	0.222%
61	13.780	2077	2082	2087	rBV2	5611	6961	1.42%	0.199%
62	14.640	2217	2223	2228	rVB	5635	7384	1.51%	0.211%

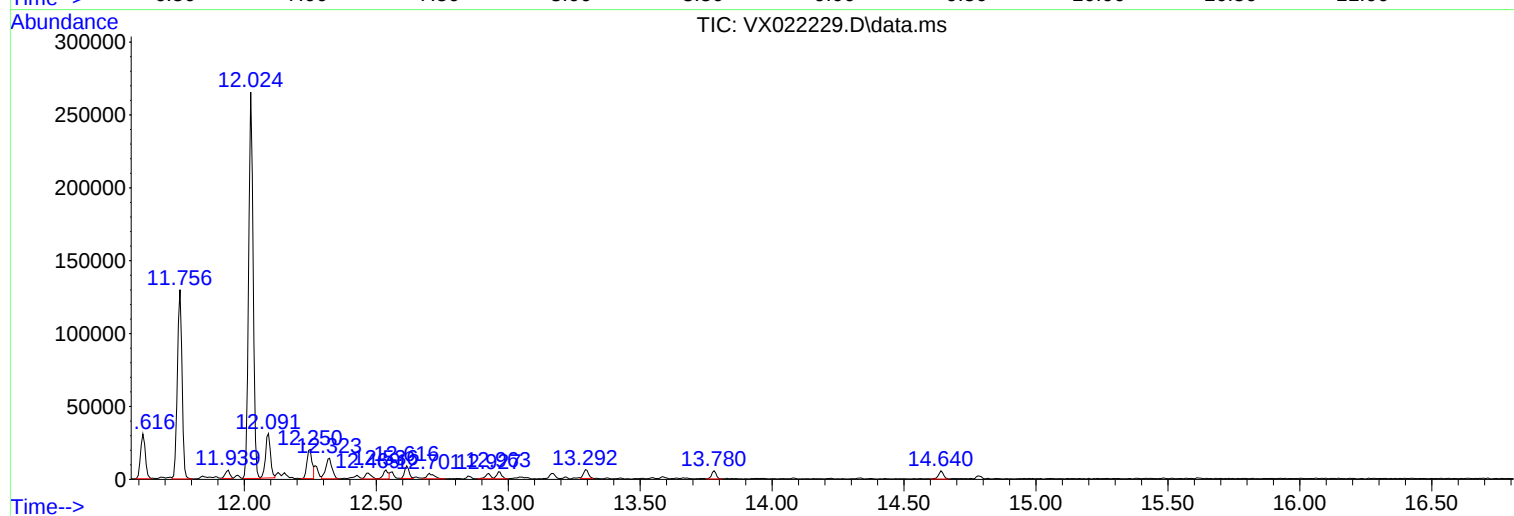
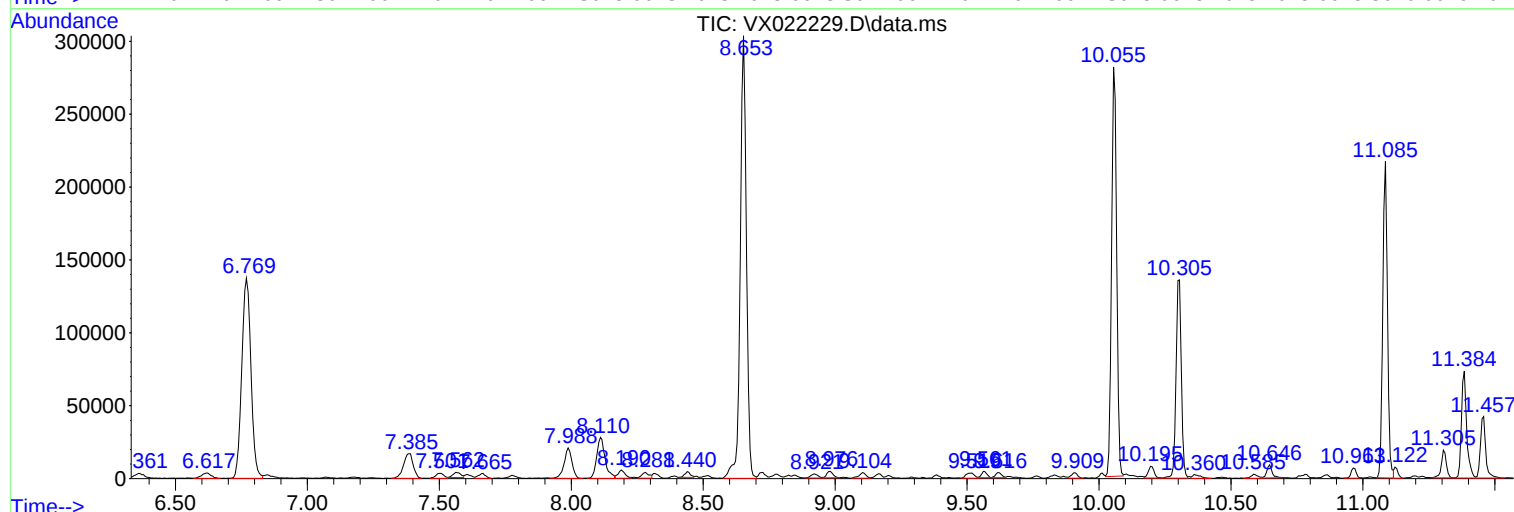
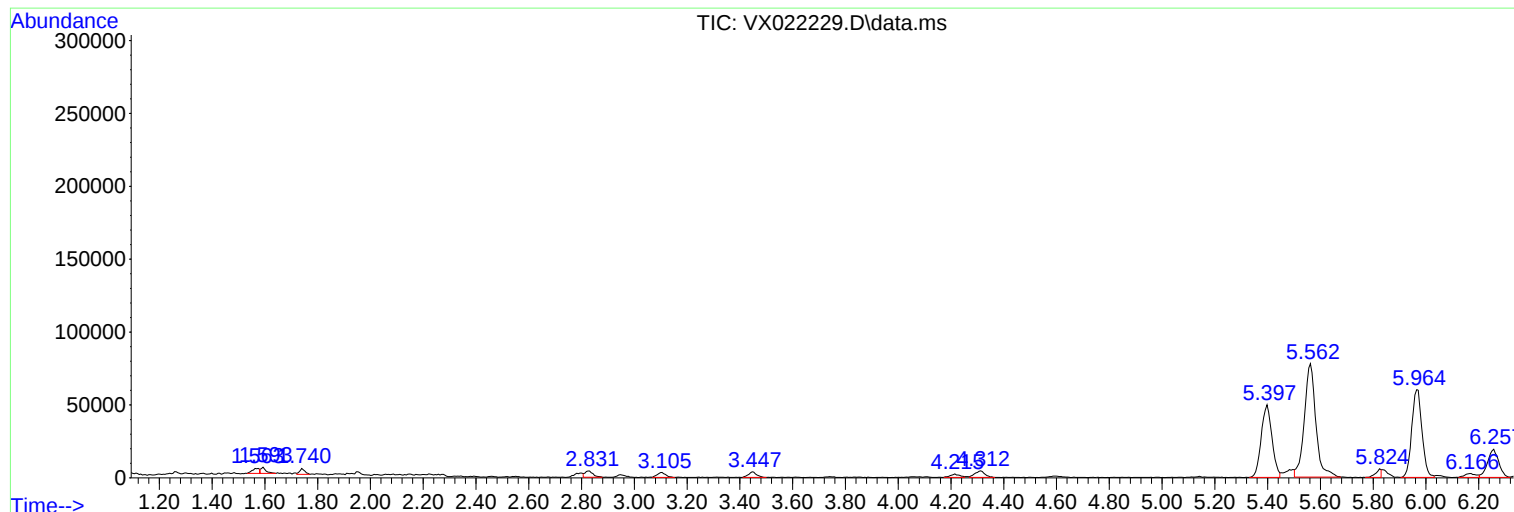
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Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

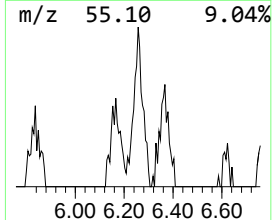
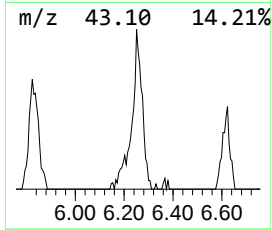
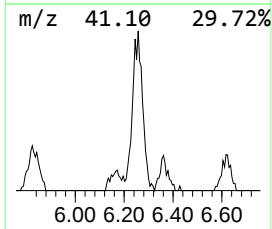
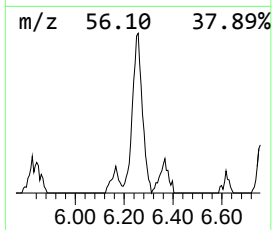
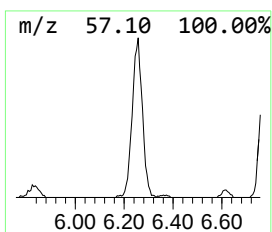
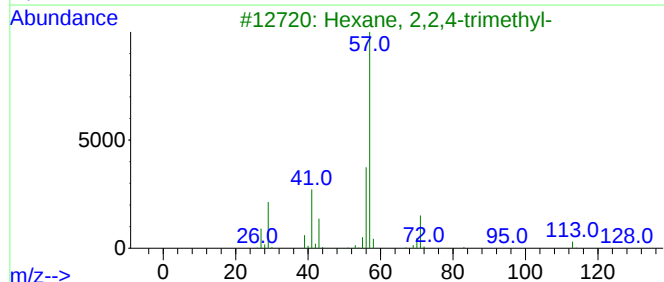
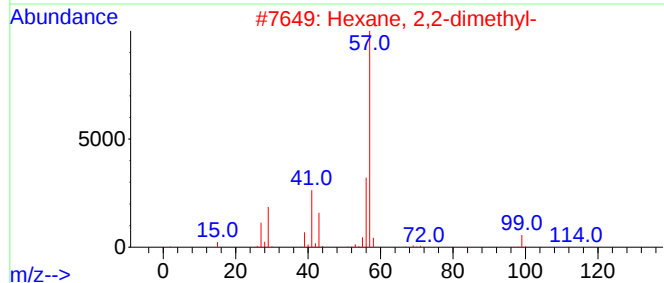
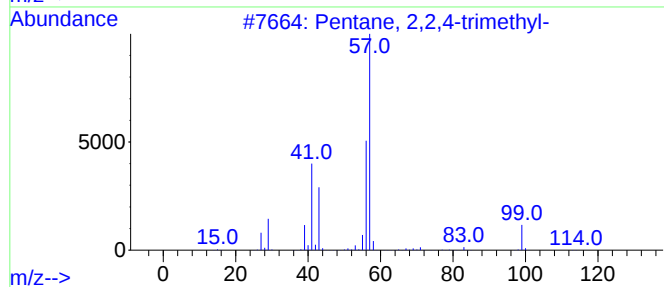
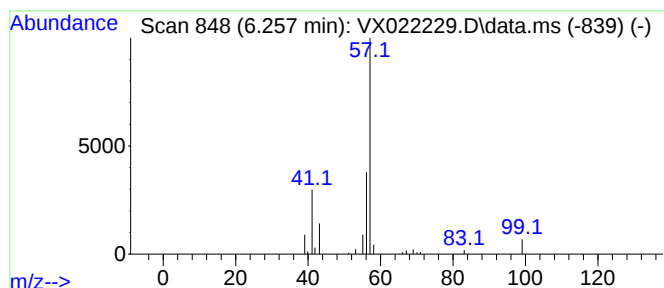
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Pentane, 2,2,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.257	8.54 ug/l	56396	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	56



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

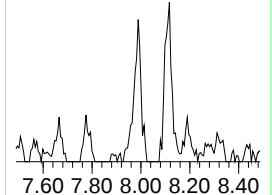
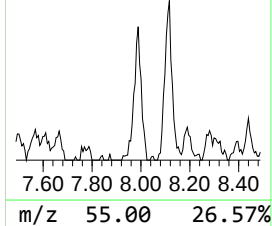
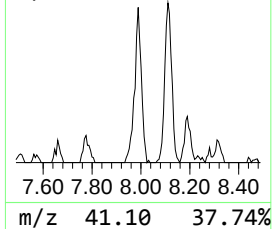
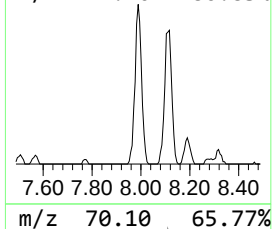
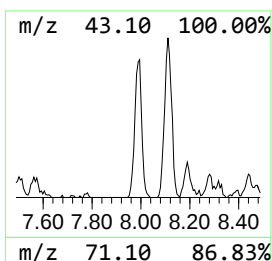
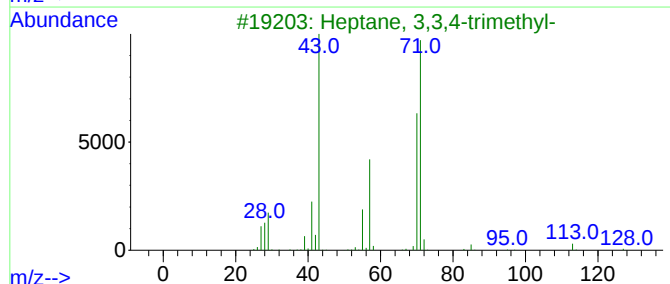
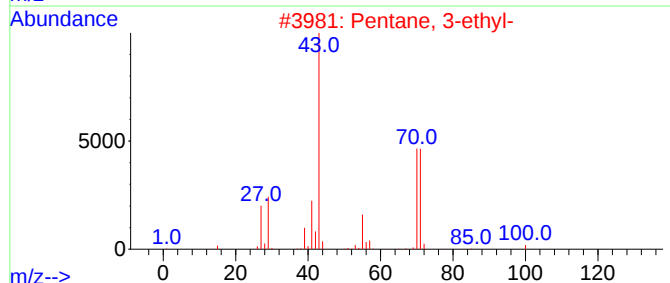
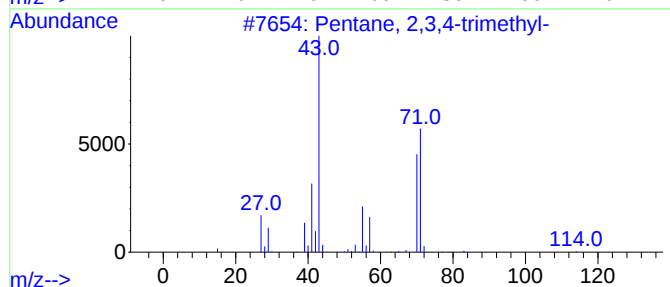
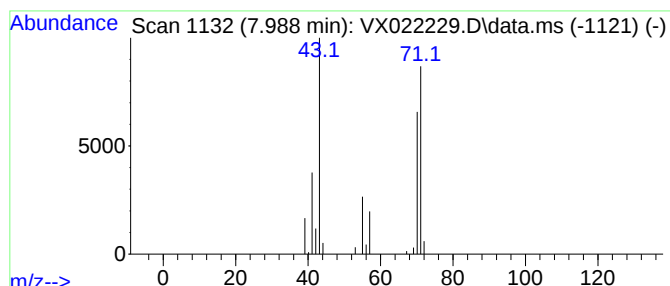
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.988	6.44 ug/l	42486	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	83
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	64
4			2,2'-Bifuran, octahydro-	142	C8H14O2	001592-33-2	56
5			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	53



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Misc : 5.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

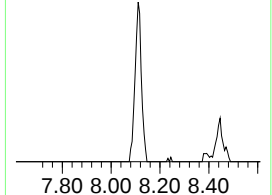
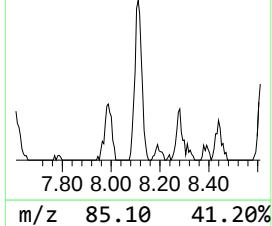
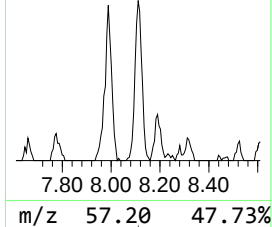
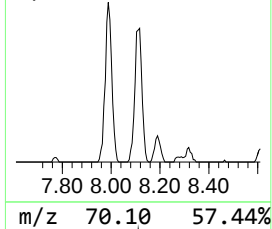
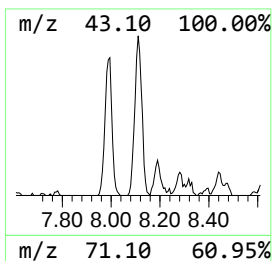
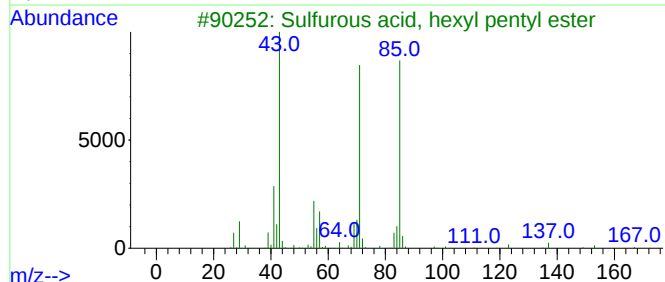
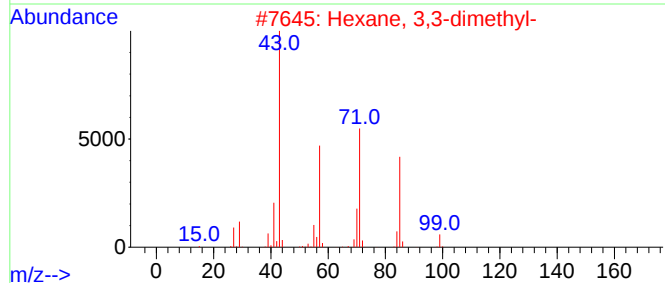
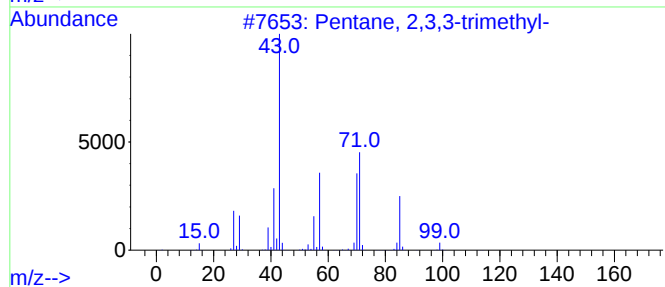
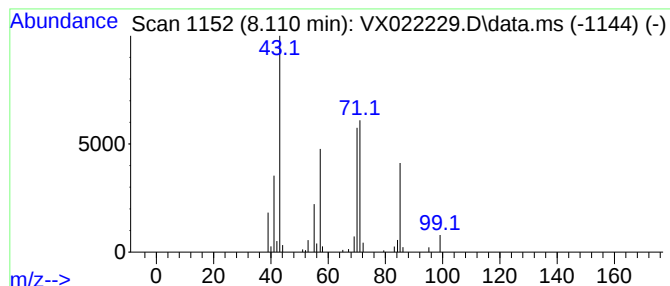
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	9.31 ug/l	61452	1,4-Difluorobenzene	6.769

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	64
3			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	59
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

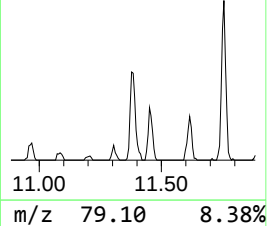
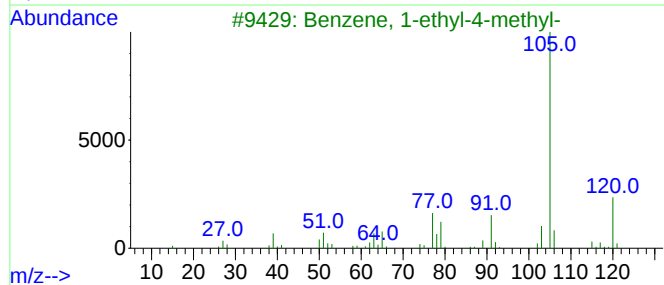
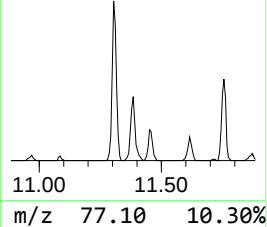
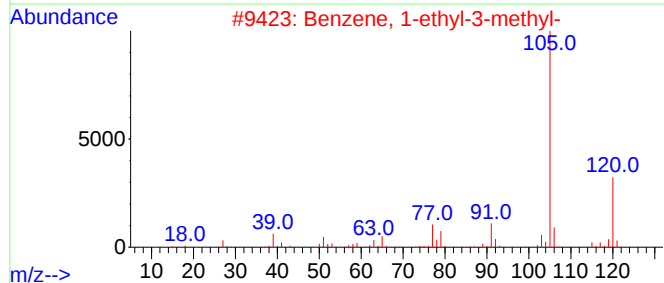
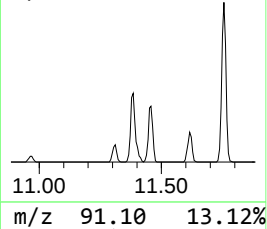
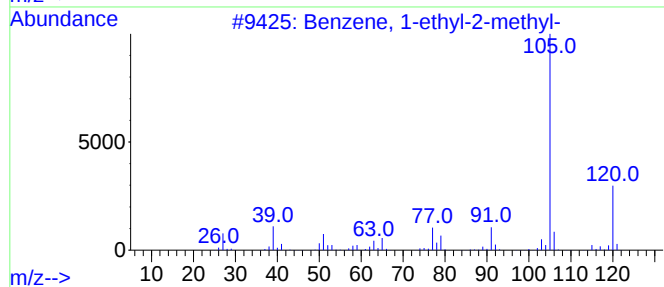
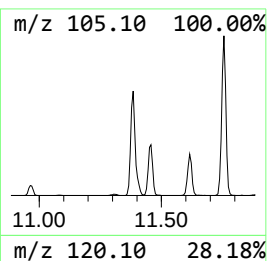
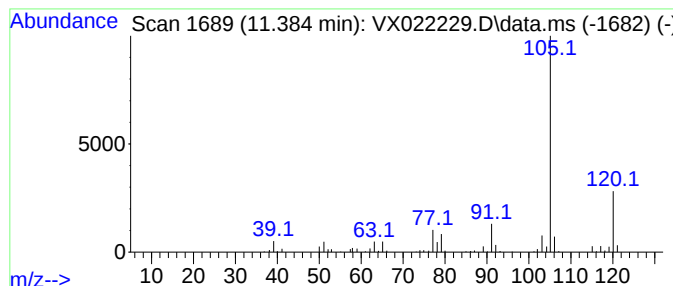
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	15.90 ug/l	100907	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022229.D
Acq On : 27 May 2021 13:56
Operator : JC/MD
Sample : M2535-02 20X
Misc : 5.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

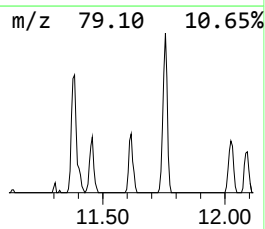
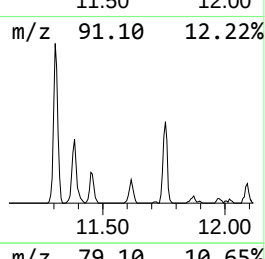
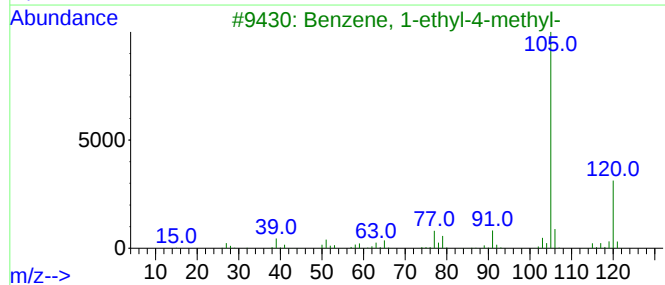
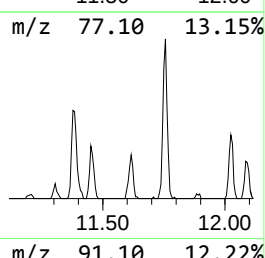
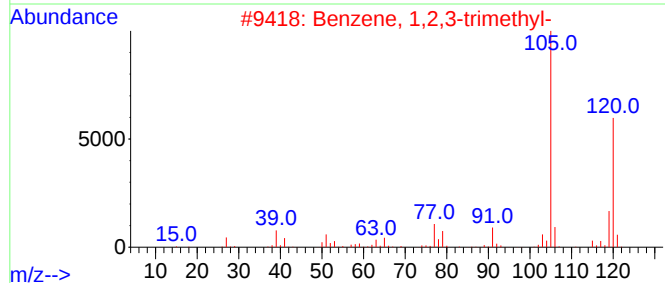
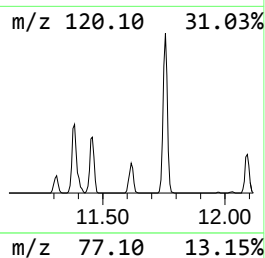
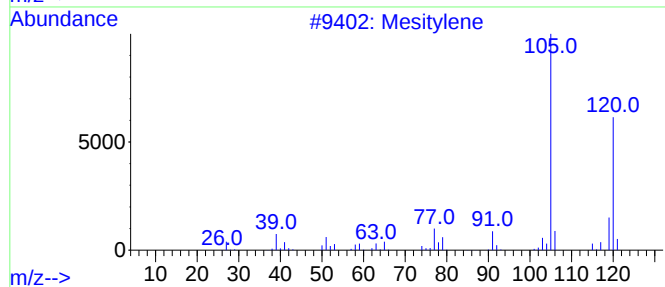
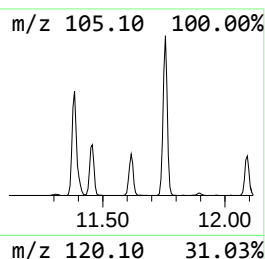
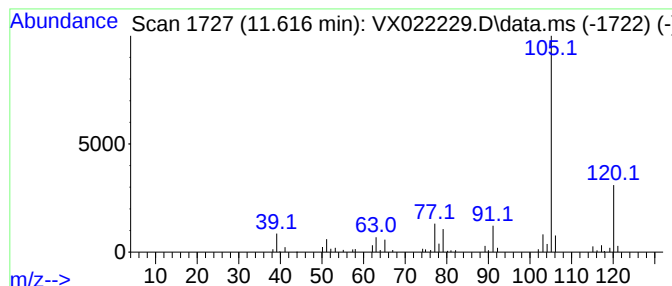
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Mesitylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	6.01 ug/l	38139	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	91
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022229.D
Acq On : 27 May 2021 13:56
Operator : JC/MD
Sample : M2535-02 20X
Misc : 5.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

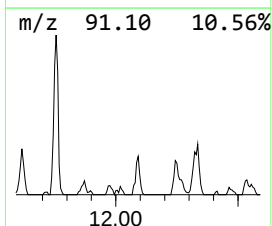
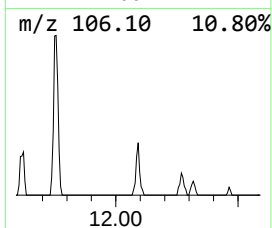
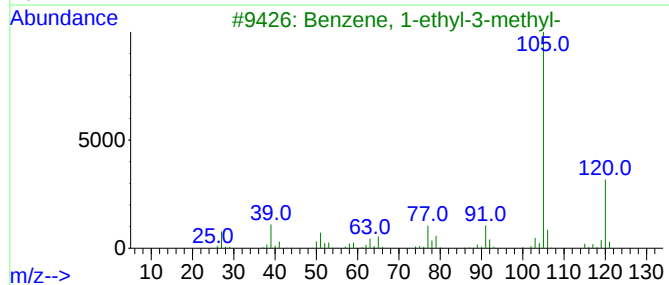
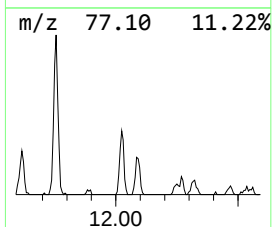
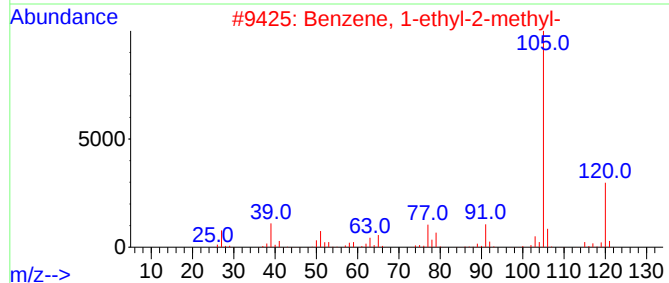
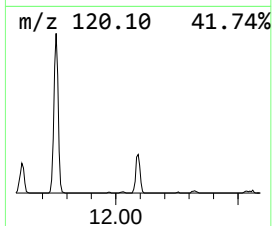
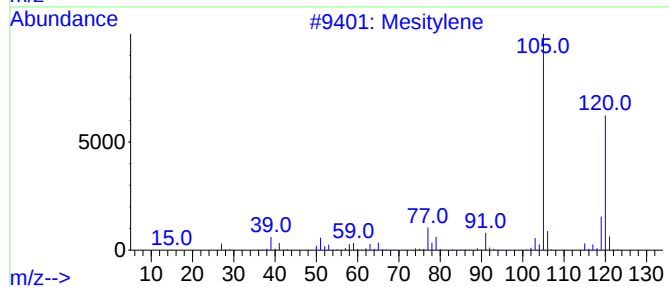
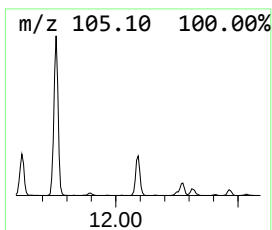
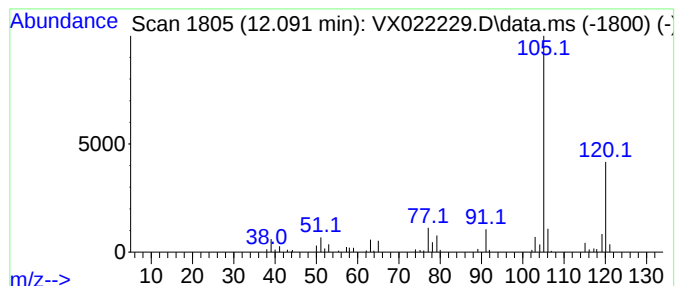
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	6.30 ug/l	39964	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	91
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022229.D
Acq On : 27 May 2021 13:56
Operator : JC/MD
Sample : M2535-02 20X
Misc : 5.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,2,4-...	6.257	8.5	ug/l	56396	2	6.769	330080	50.0
Pentane, 2,3,4-...	7.988	6.4	ug/l	42486	2	6.769	330080	50.0
Pentane, 2,3,3-...	8.110	9.3	ug/l	61452	2	6.769	330080	50.0
Benzene, 1-ethy...	11.384	15.9	ug/l	100907	4	12.024	317312	50.0
Mesitylene	11.616	6.0	ug/l	38139	4	12.024	317312	50.0
Benzene, 1-ethy...	12.091	6.3	ug/l	39964	4	12.024	317312	50.0