

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052521\
 Data File : VX022173.D
 Acq On : 25 May 2021 13:49
 Operator : JC/MD
 Sample : M2504-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-2

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: VX022173.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.337	200	205	211	rBV2	9446	17760	2.33%	0.435%
2	2.782	270	278	287	rBV	31314	66791	8.76%	1.637%
3	5.397	696	707	722	rBV3	52134	148859	19.53%	3.648%
4	5.562	722	734	743	rBV	79634	238826	31.33%	5.853%
5	5.970	789	801	812	rBV	62452	162192	21.28%	3.975%
6	6.257	835	848	859	rBV	255554	762225	100.00%	18.681%
7	6.769	921	932	943	rBV	141922	340787	44.71%	8.352%
8	7.604	1061	1069	1080	rVB	10188	22901	3.00%	0.561%
9	7.781	1091	1098	1104	rBV3	5380	10531	1.38%	0.258%
10	7.988	1123	1132	1144	rVB	162257	325279	42.67%	7.972%
11	8.110	1144	1152	1161	rBV	133616	257086	33.73%	6.301%
12	8.427	1200	1204	1211	rVB	6597	11996	1.57%	0.294%
13	8.653	1229	1241	1251	rBV	300633	482779	63.34%	11.832%
14	9.244	1333	1338	1347	rVV	57791	94648	12.42%	2.320%
15	9.458	1363	1373	1379	rBV3	8630	16796	2.20%	0.412%
16	9.951	1447	1454	1459	rBV	7750	12202	1.60%	0.299%
17	10.055	1466	1471	1478	rVB	275132	379331	49.77%	9.297%
18	11.085	1635	1640	1646	rBV	221865	270258	35.46%	6.624%
19	12.024	1789	1794	1801	rVB	263027	319482	41.91%	7.830%
20	12.250	1827	1831	1838	rBV	21832	27144	3.56%	0.665%
21	12.701	1900	1905	1912	rBV4	6583	10674	1.40%	0.262%
22	13.030	1954	1959	1965	rVB2	5569	8192	1.07%	0.201%
23	13.122	1969	1974	1980	rBV3	12720	23805	3.12%	0.583%
24	13.237	1990	1993	1998	rVB2	10098	12303	1.61%	0.302%
25	13.304	1998	2004	2008	rBV	7727	9250	1.21%	0.227%
26	13.542	2040	2043	2049	rVV3	11509	15928	2.09%	0.390%
27	13.646	2053	2060	2061	rVV2	8777	14788	1.94%	0.362%
28	13.664	2061	2063	2071	rVB	15103	17411	2.28%	0.427%

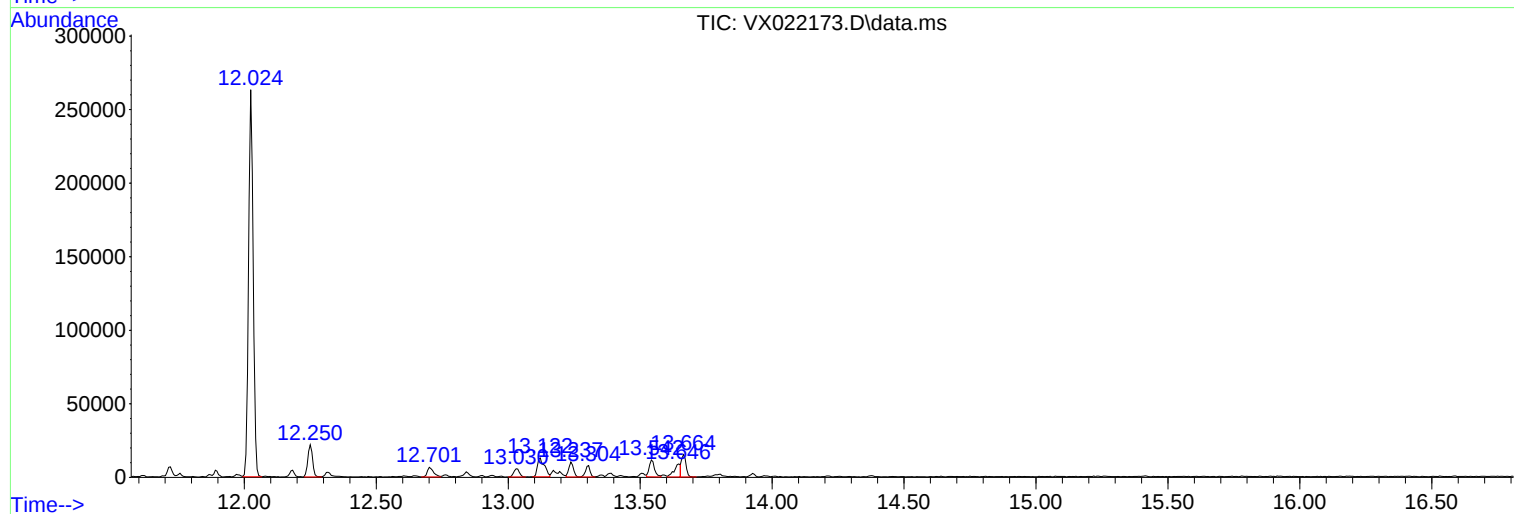
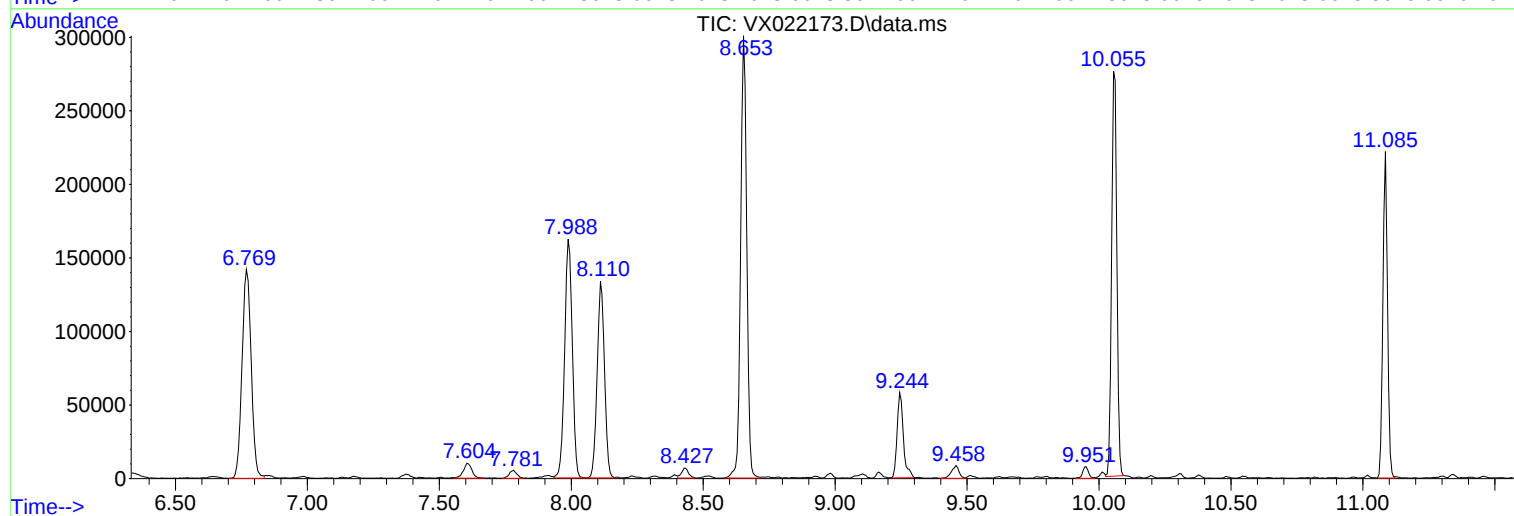
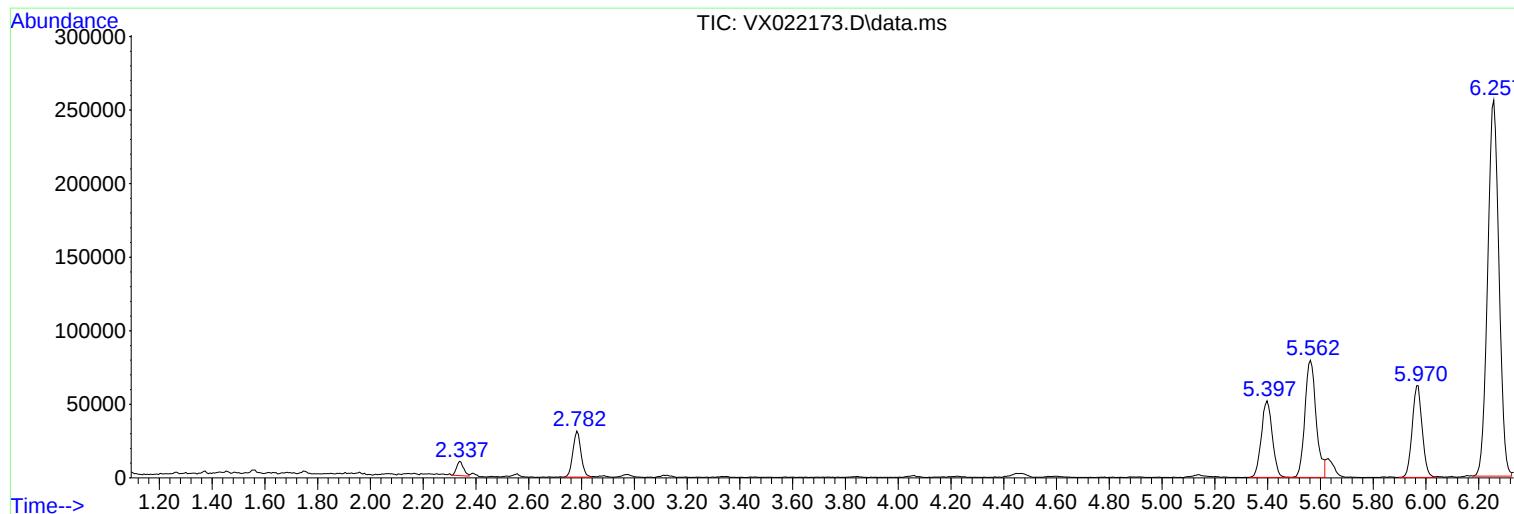
Sum of corrected areas: 4080224

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052521\
Data File : VX022173.D
Acq On : 25 May 2021 13:49
Operator : JC/MD
Sample : M2504-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052521\
Data File : VX022173.D
Acq On : 25 May 2021 13:49
Operator : JC/MD
Sample : M2504-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

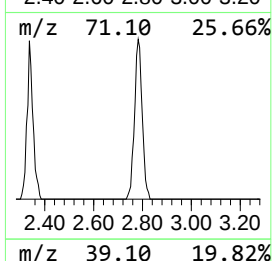
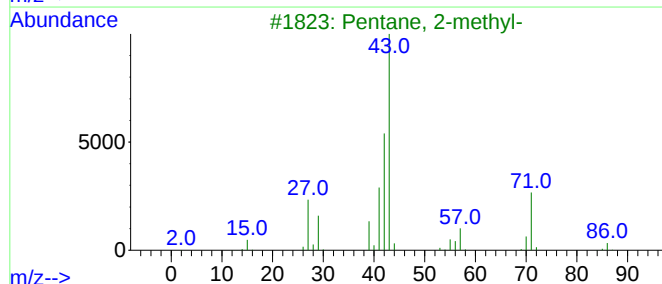
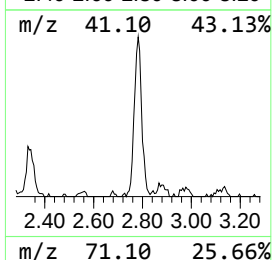
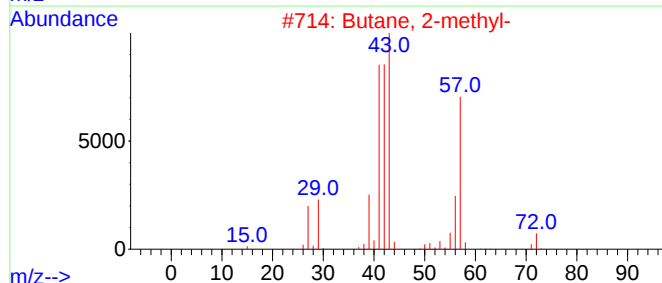
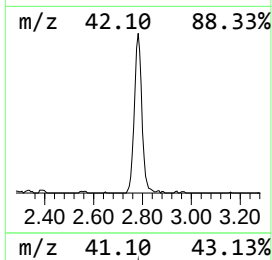
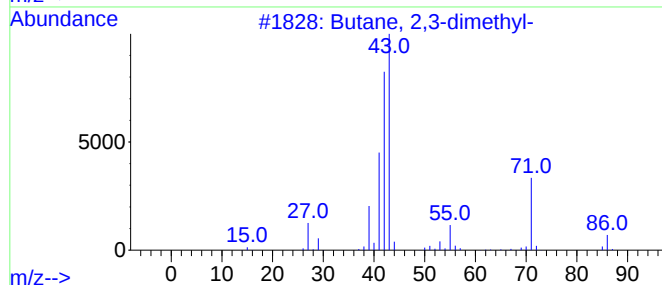
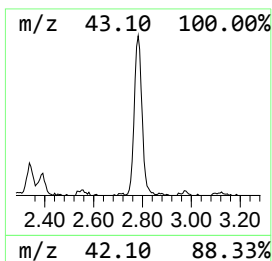
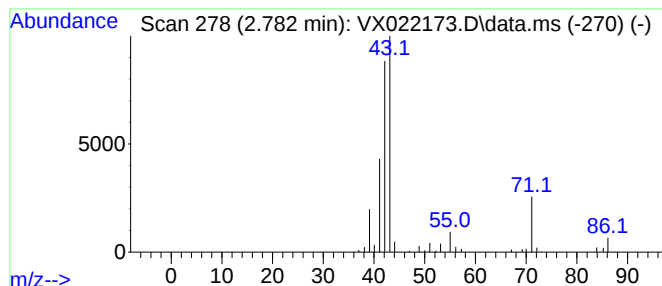
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	13.98 ug/l	66791	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2			Butane, 2-methyl-	72	C5H12	000078-78-4	38
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	38
4			Tetrahydrofuran	72	C4H8O	000109-99-9	36
5			Pentane	72	C5H12	000109-66-0	36



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052521\
Data File : VX022173.D
Acq On : 25 May 2021 13:49
Operator : JC/MD
Sample : M2504-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

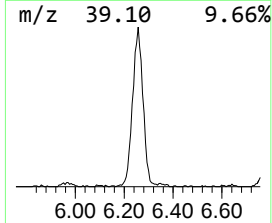
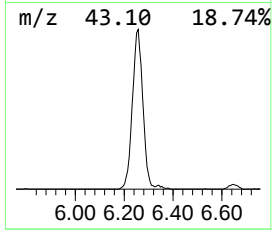
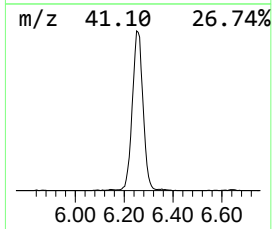
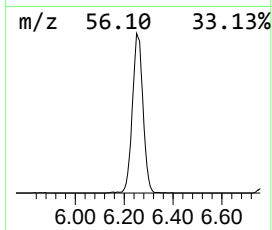
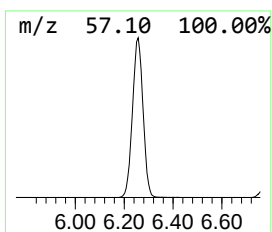
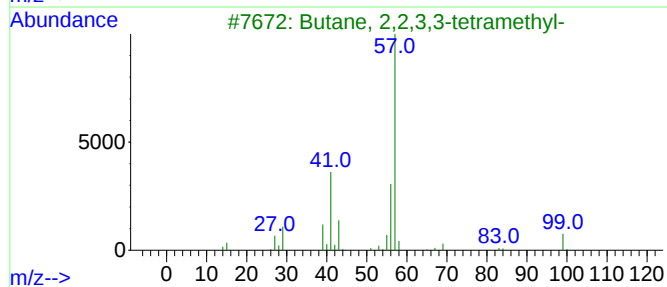
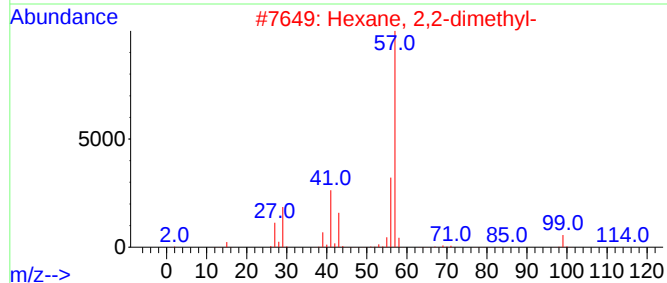
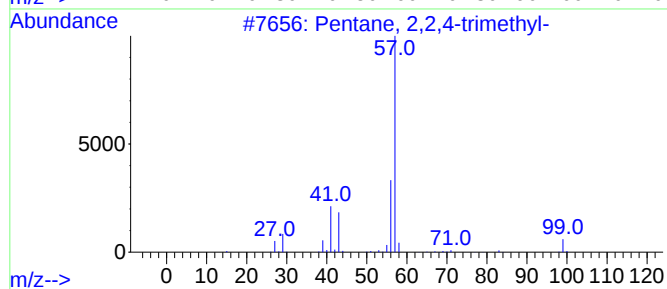
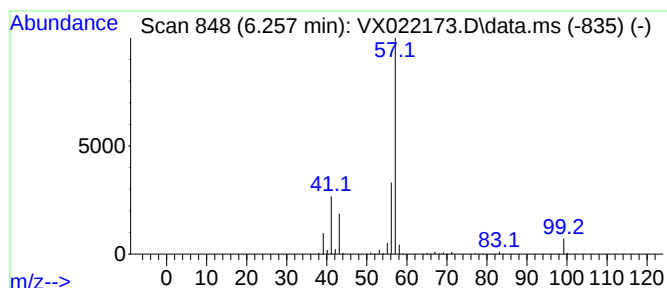
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.257	111.83 ug/l	762225	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	78
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052521\
Data File : VX022173.D
Acq On : 25 May 2021 13:49
Operator : JC/MD
Sample : M2504-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

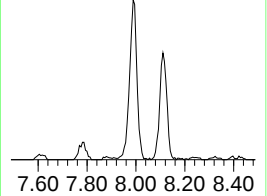
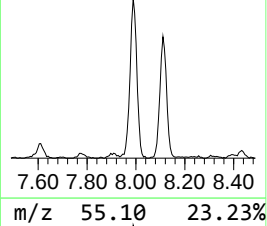
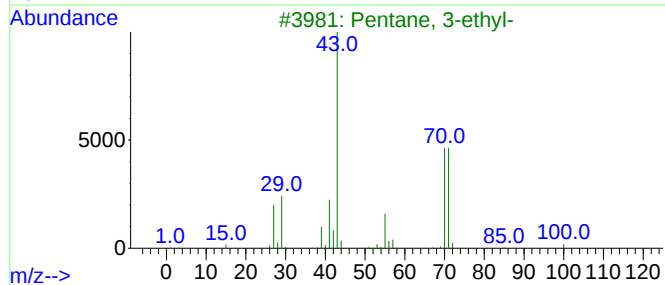
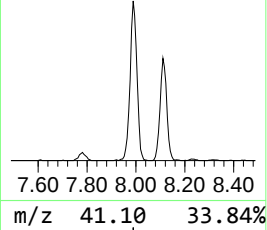
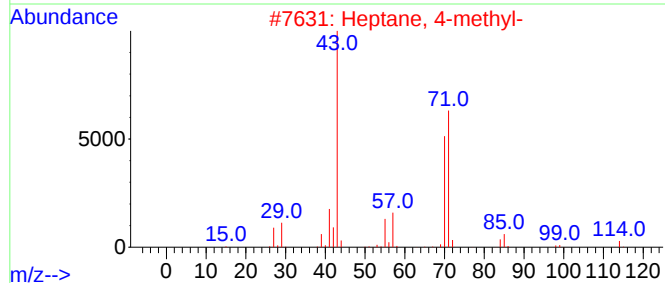
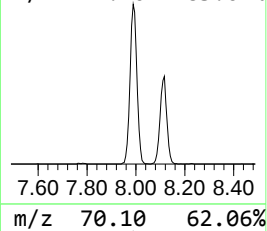
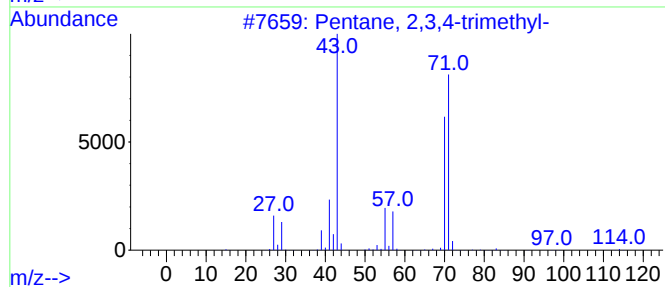
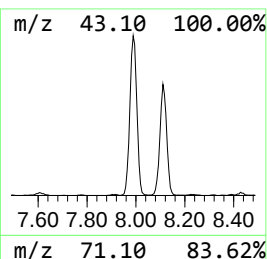
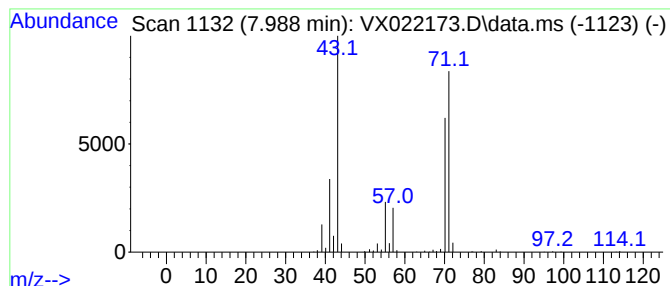
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.988	47.72 ug/l	325279	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	91
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	78
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052521\
Data File : VX022173.D
Acq On : 25 May 2021 13:49
Operator : JC/MD
Sample : M2504-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

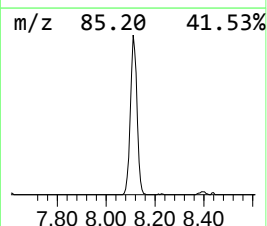
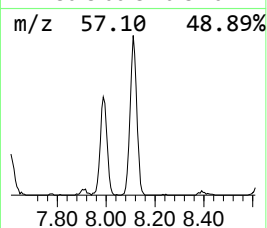
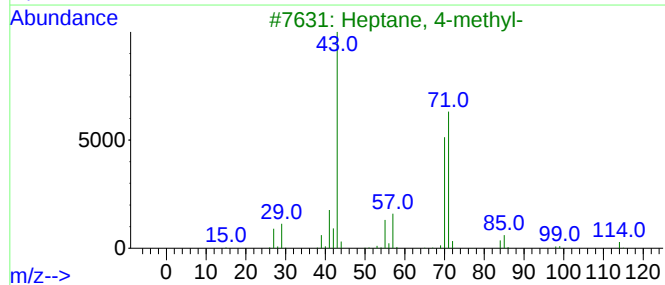
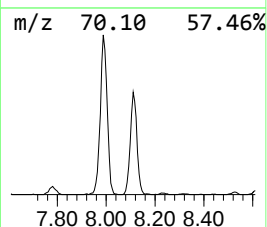
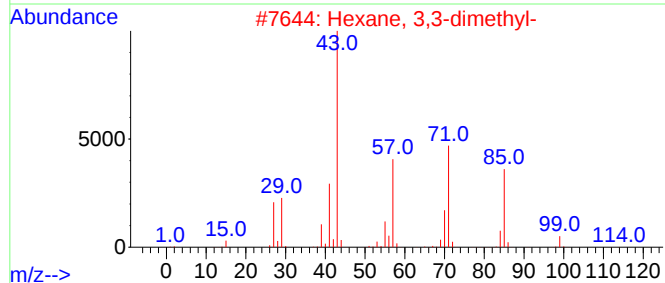
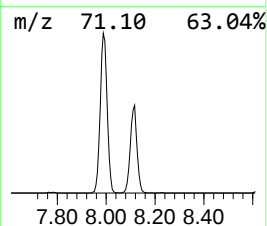
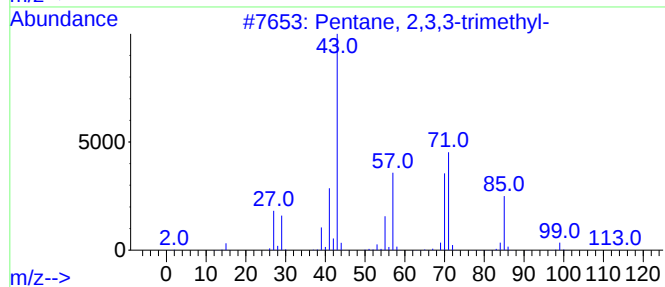
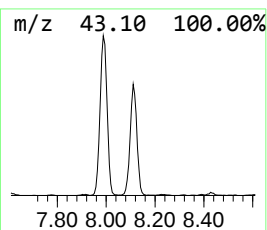
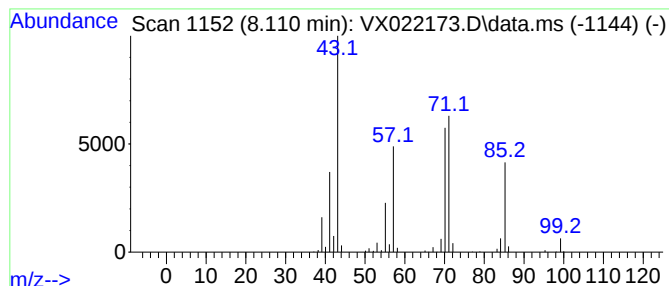
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	37.72 ug/l	257086	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			Heptane, 4-methyl-	114	C8H18	000589-53-7	53
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	53
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052521\
Data File : VX022173.D
Acq On : 25 May 2021 13:49
Operator : JC/MD
Sample : M2504-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

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
Butane, 2,3-dim...	2.782	14.0	ug/l	66791	1	5.556	238826	50.0
Pentane, 2,2,4-...	6.257	111.8	ug/l	762225	2	6.769	340787	50.0
Pentane, 2,3,4-...	7.988	47.7	ug/l	325279	2	6.769	340787	50.0
Pentane, 2,3,3-...	8.110	37.7	ug/l	257086	2	6.769	340787	50.0