

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
 Data File : VX026638.D
 Acq On : 27 Jan 2022 20:30
 Operator : JC/MD
 Sample : N1297-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-14DB

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\82X011122W.M
 Title : SW846 8260

Signal : TIC: VX026638.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	52	rVB	11190	11372	1.69%	0.205%
2	1.752	104	109	120	rVB	195548	265496	39.37%	4.776%
3	2.343	199	206	221	rVB	21969	46696	6.92%	0.840%
4	2.788	270	279	284	rBV	64591	143725	21.31%	2.586%
5	3.105	320	331	344	rBV	99074	225451	33.43%	4.056%
6	4.062	480	488	498	rVB2	2633	7878	1.17%	0.142%
7	4.221	503	514	522	rVV2	12583	37789	5.60%	0.680%
8	4.312	522	529	538	rVB2	5128	14480	2.15%	0.260%
9	5.111	649	660	661	rBV3	4048	7849	1.16%	0.141%
10	5.391	693	706	717	rBV2	75277	220096	32.64%	3.960%
11	5.556	722	733	741	rVV	134470	396965	58.87%	7.141%
12	5.623	741	744	758	rVB2	31900	84343	12.51%	1.517%
13	5.849	770	781	790	rBV6	5078	16614	2.46%	0.299%
14	5.958	790	799	809	rVV	86054	228903	33.95%	4.118%
15	6.044	809	813	823	rVV	9394	23816	3.53%	0.428%
16	6.166	823	833	841	rVV4	16471	56268	8.34%	1.012%
17	6.257	841	848	859	rVV4	32642	98355	14.59%	1.769%
18	6.361	859	865	874	rVB4	4558	12837	1.90%	0.231%
19	6.763	922	931	942	rBV	210154	497912	73.84%	8.957%
20	7.367	1021	1030	1041	rBV5	6267	15702	2.33%	0.282%
21	7.775	1090	1097	1103	rBV4	4254	8539	1.27%	0.154%
22	7.982	1122	1131	1140	rVB	13416	31584	4.68%	0.568%
23	8.110	1144	1152	1162	rBV2	23841	55929	8.29%	1.006%
24	8.513	1212	1218	1224	rVB4	5529	10793	1.60%	0.194%
25	8.604	1227	1233	1235	rBV3	6196	10737	1.59%	0.193%
26	8.653	1235	1241	1251	rVB	426516	674319	100.00%	12.131%
27	8.842	1265	1272	1279	rVB3	5513	11087	1.64%	0.199%
28	8.976	1290	1294	1299	rVB2	4571	6851	1.02%	0.123%
29	9.098	1307	1314	1320	rBV3	4990	9402	1.39%	0.169%
30	9.165	1320	1325	1334	rVB	9536	15032	2.23%	0.270%
31	10.055	1465	1471	1477	rVB	431354	564364	83.69%	10.153%
32	10.963	1613	1620	1625	rBV	76465	96692	14.34%	1.739%
33	11.079	1634	1639	1646	rBV	311661	407184	60.38%	7.325%
34	11.616	1722	1727	1732	rVB	11272	14026	2.08%	0.252%
35	11.866	1763	1768	1770	rBV2	9623	11920	1.77%	0.214%
36	11.890	1770	1772	1778	rVB	12449	13907	2.06%	0.250%

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Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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37	12.024	1788	1794	1800	rBV	394099	474545	70.37%	8.537%
38	12.244	1823	1830	1837	rVB2	60750	81966	12.16%	1.475%
39	12.311	1837	1841	1843	rVV2	7729	10328	1.53%	0.186%
40	12.335	1843	1845	1849	rVV	10415	10711	1.59%	0.193%
41	12.408	1852	1857	1862	rVB2	11974	15439	2.29%	0.278%
42	12.530	1872	1877	1883	rBV	7854	9427	1.40%	0.170%
43	12.616	1886	1891	1894	rBV	25409	30975	4.59%	0.557%
44	12.701	1900	1905	1912	rBV	102876	127324	18.88%	2.291%
45	12.920	1935	1941	1945	rBV2	7098	9713	1.44%	0.175%
46	13.170	1979	1982	1992	rVB	22502	29278	4.34%	0.527%
47	13.292	1997	2002	2008	rVB2	102407	132219	19.61%	2.379%
48	13.426	2019	2024	2031	rVB	9516	12596	1.87%	0.227%
49	13.542	2040	2043	2047	rVV	15336	21545	3.20%	0.388%
50	13.585	2047	2050	2056	rVV2	11280	21374	3.17%	0.385%
51	13.640	2056	2059	2061	rVV	9323	13877	2.06%	0.250%
52	13.664	2061	2063	2070	rVB2	16055	22011	3.26%	0.396%
53	13.774	2074	2081	2091	rBV	72673	94948	14.08%	1.708%
54	13.872	2091	2097	2102	rVV	8837	12061	1.79%	0.217%
55	14.079	2125	2131	2137	rBV	7313	8630	1.28%	0.155%
56	14.213	2149	2153	2161	rVB	7018	9814	1.46%	0.177%
57	14.640	2219	2223	2232	rVB	22542	27983	4.15%	0.503%
58	14.780	2240	2246	2254	rVB	21264	26982	4.00%	0.485%

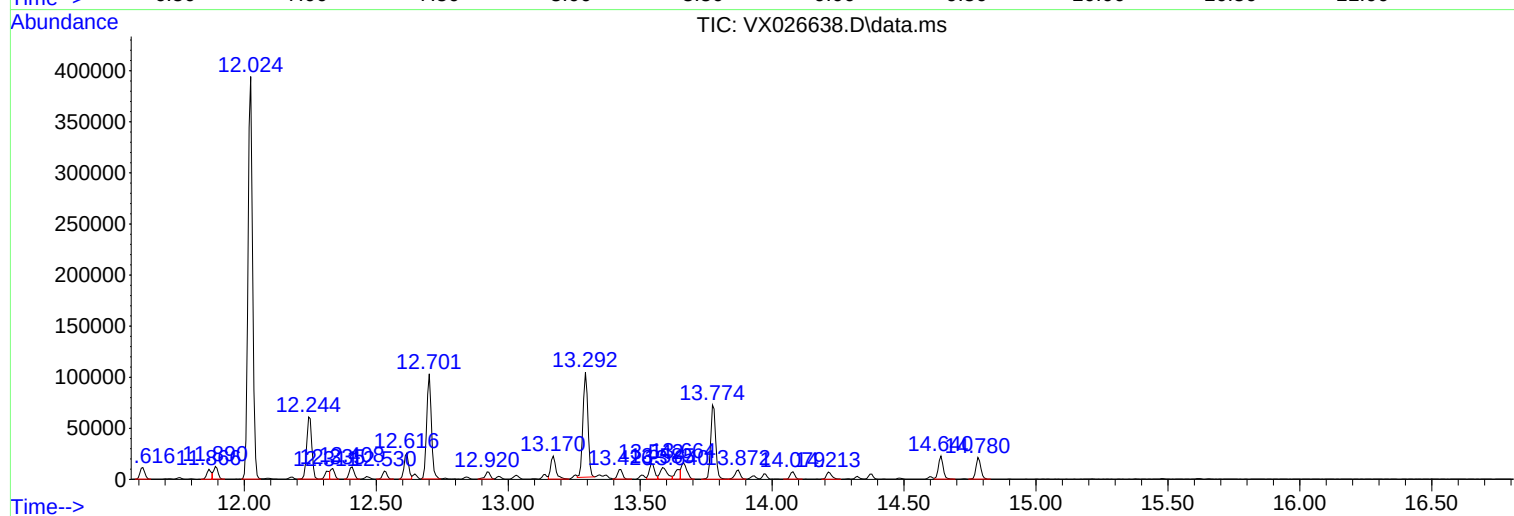
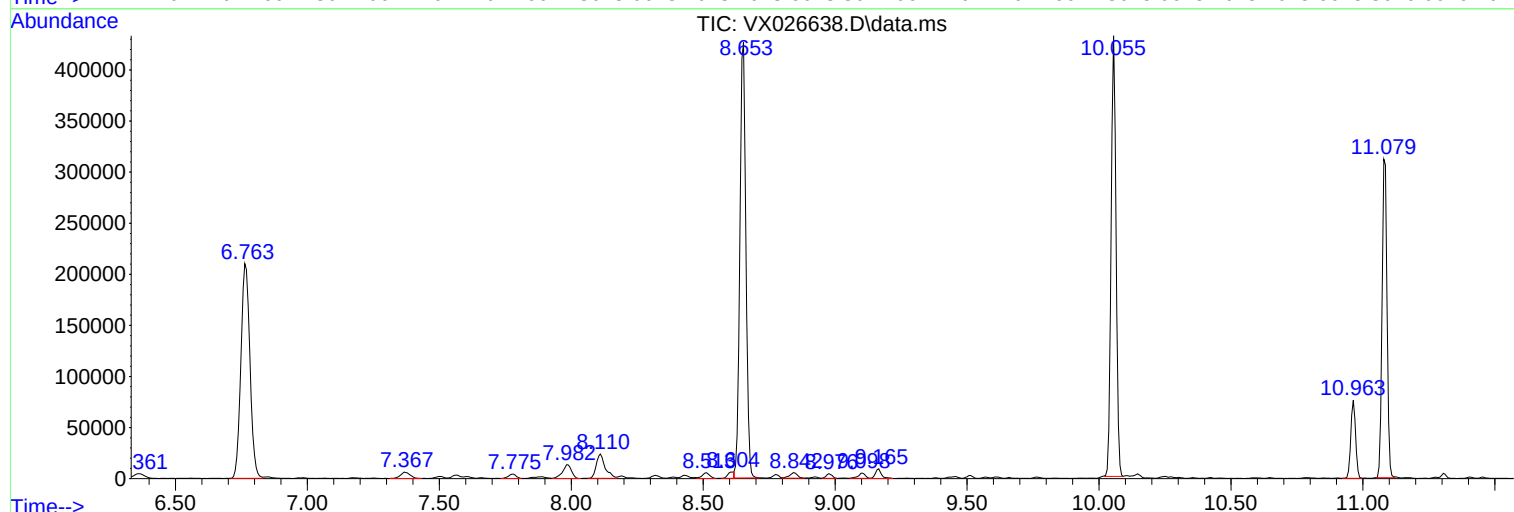
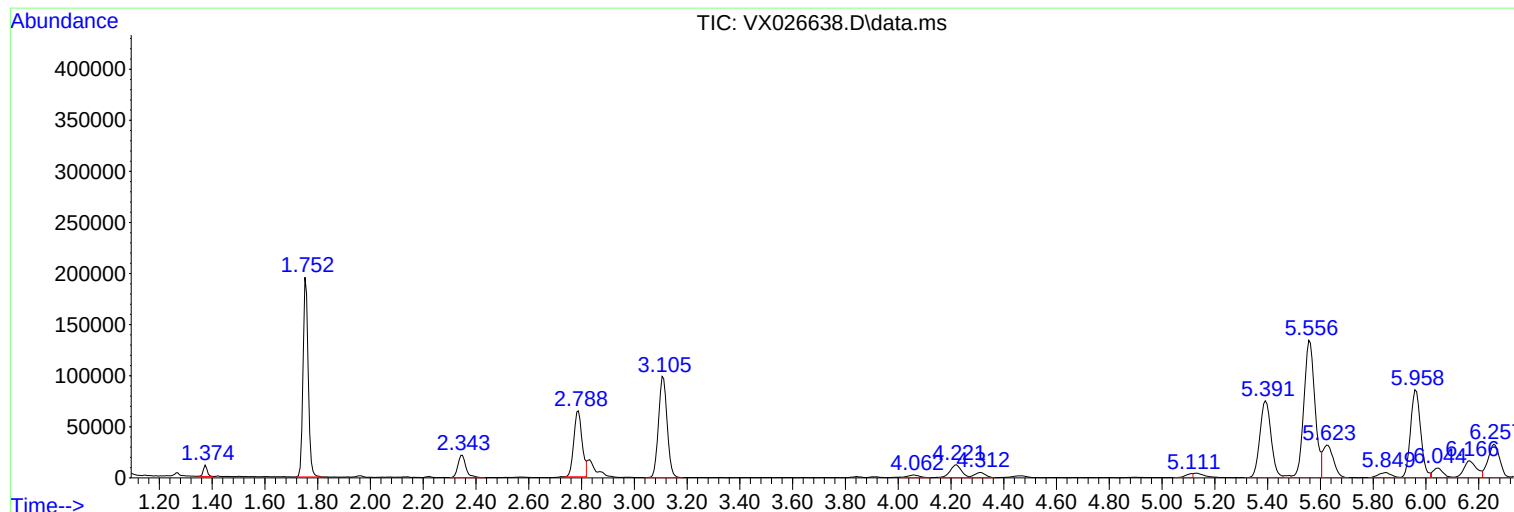
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Quant Title : SW846 8260

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



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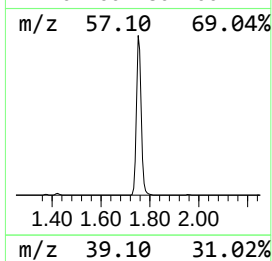
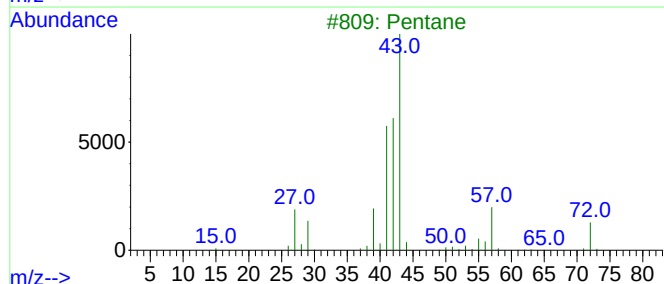
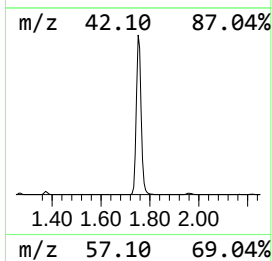
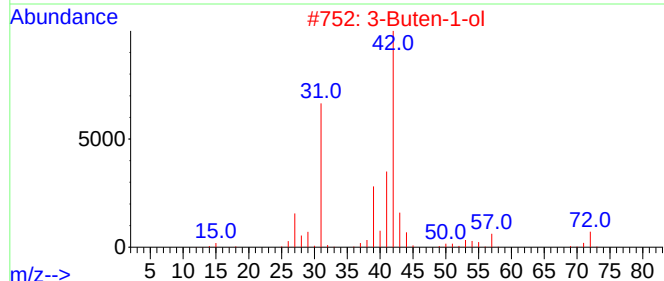
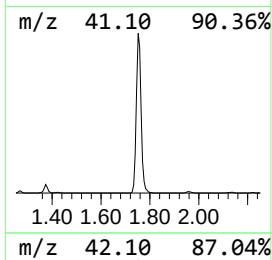
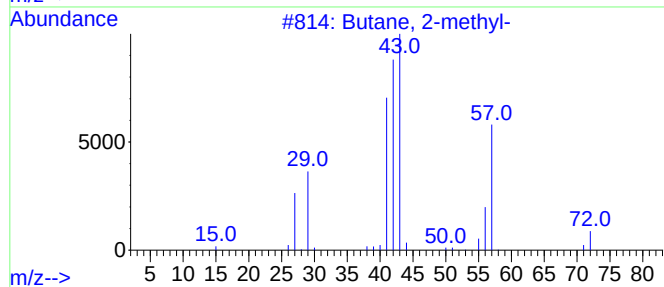
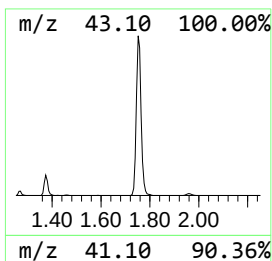
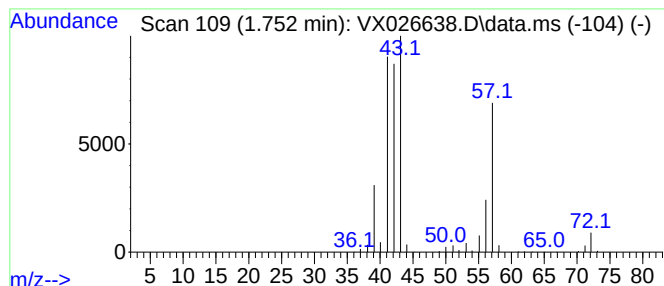
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Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	33.44 ug/l	265496	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	33
4			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28
5			1-Butene	56	C4H8	000106-98-9	10



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Instrument :
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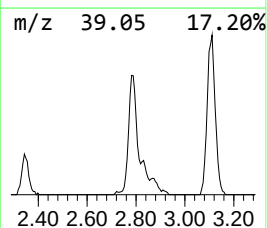
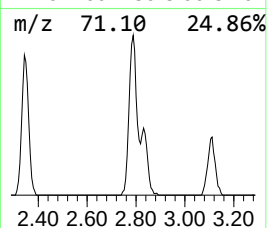
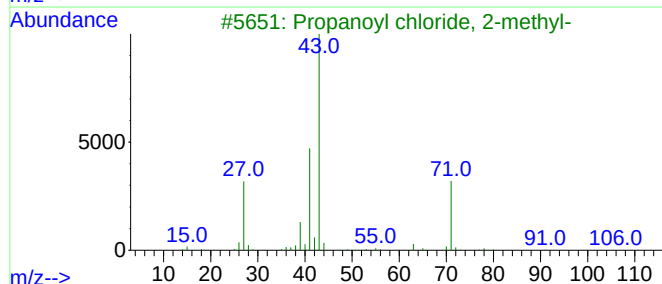
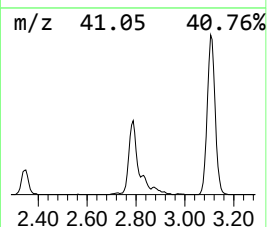
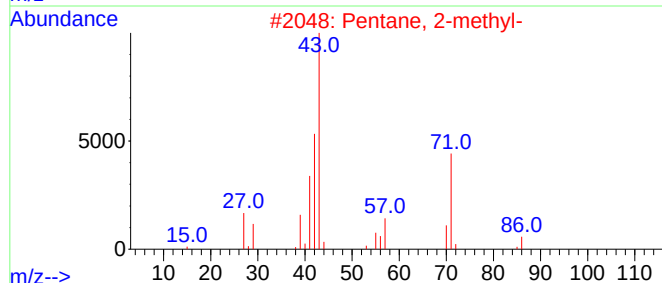
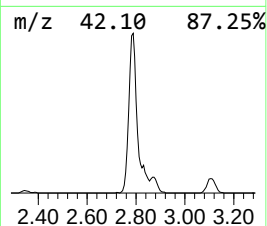
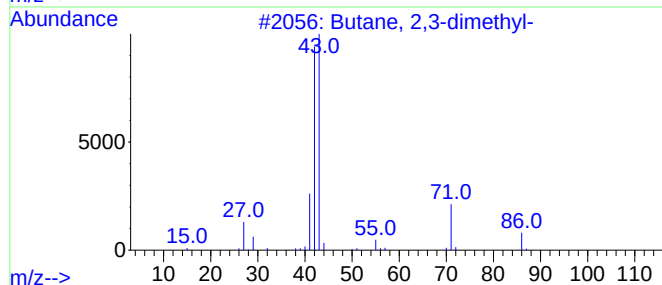
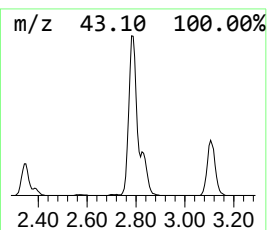
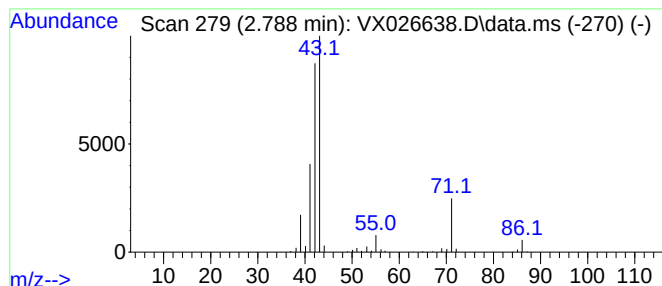
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.788	18.10 ug/l	143725	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	37
3			Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	16
4			C2H5C(CH3)2COCH3	114	C7H14O	020669-04-9	10
5			Pyrrolidine	71	C4H9N	000123-75-1	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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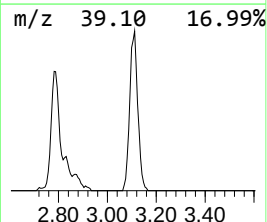
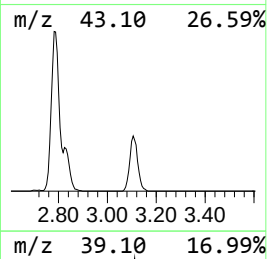
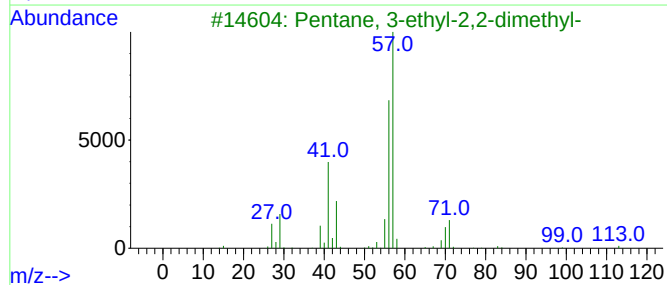
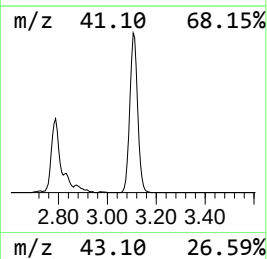
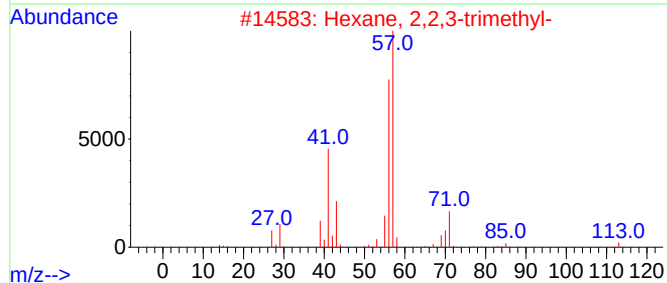
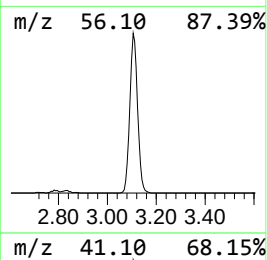
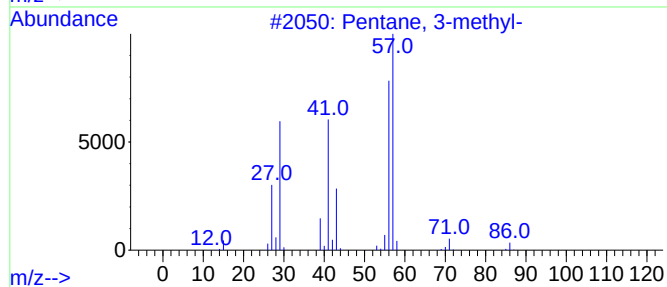
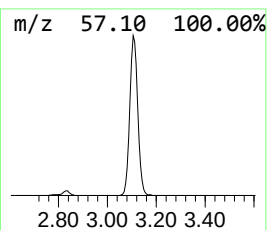
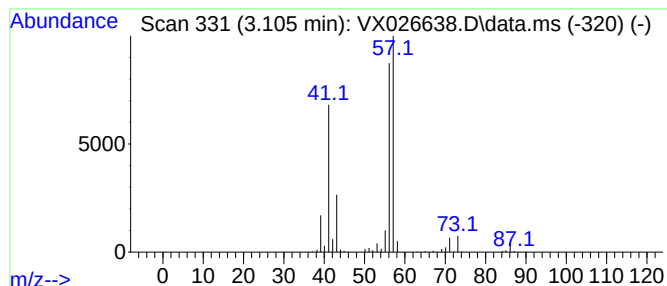
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	28.40 ug/l	225451	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	59
5			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40



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ALS Vial : 28 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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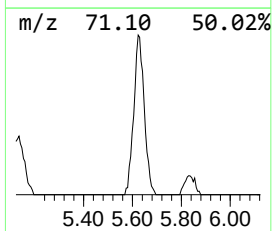
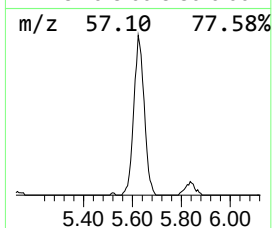
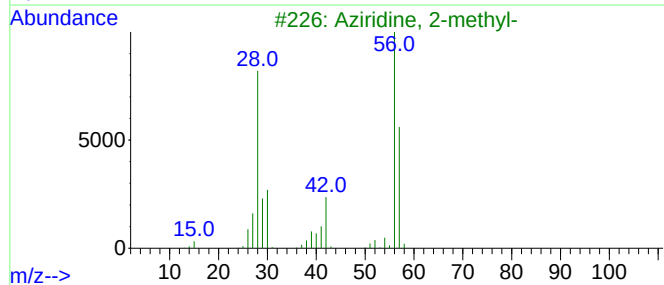
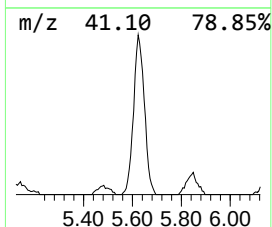
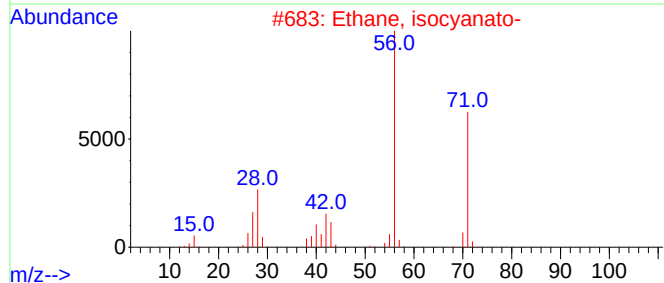
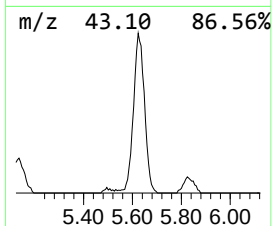
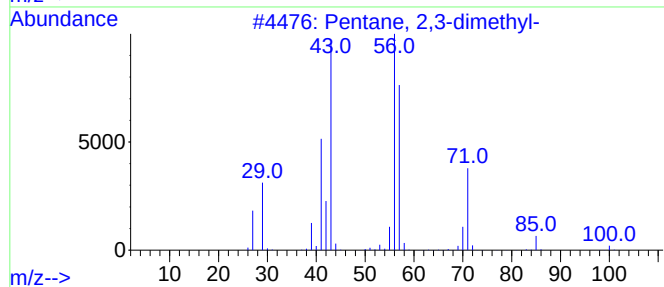
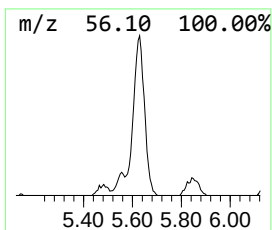
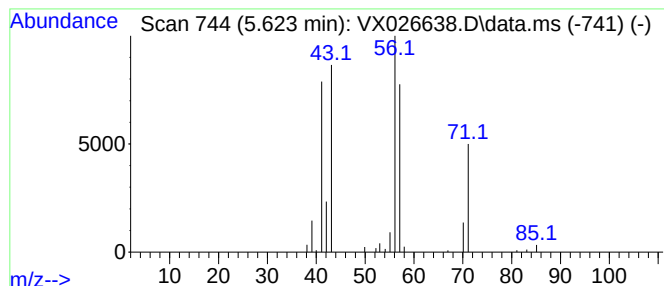
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.623	10.62 ug/l	84343	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	78
2			Ethane, isocyanato-	71	C3H5NO	000109-90-0	40
3			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	37
4			Oxirane, (3-methylbutyl)-	114	C7H14O	053229-41-7	36
5			1-Octene, 3,7-dimethyl-	140	C10H20	004984-01-4	33



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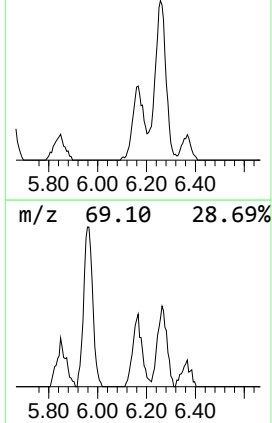
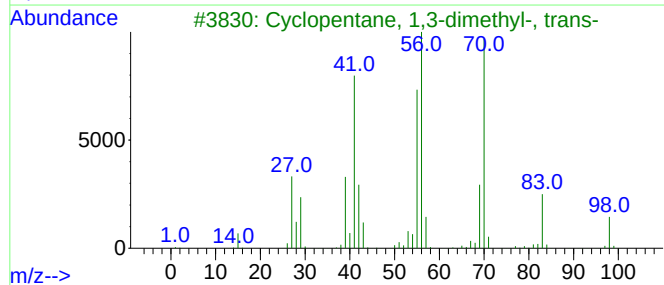
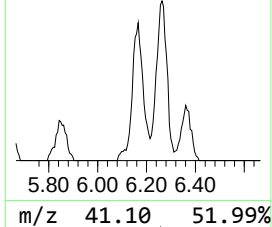
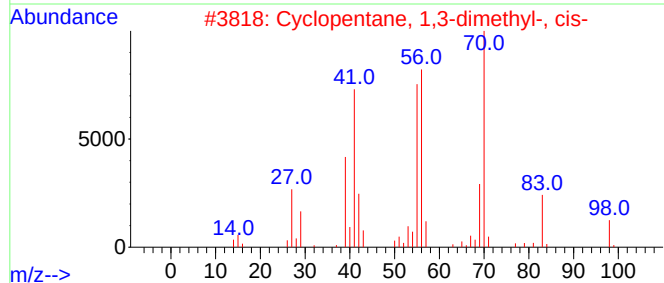
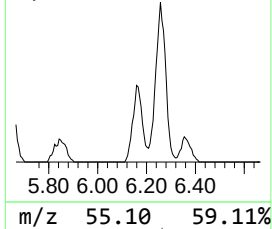
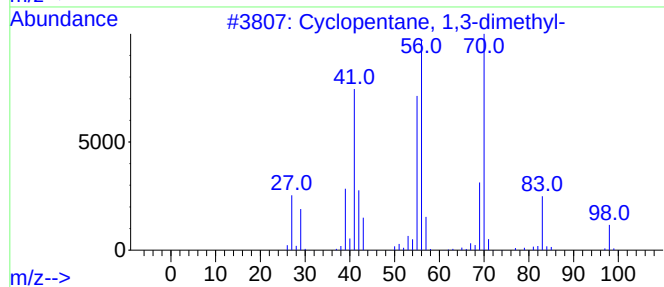
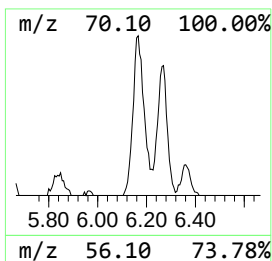
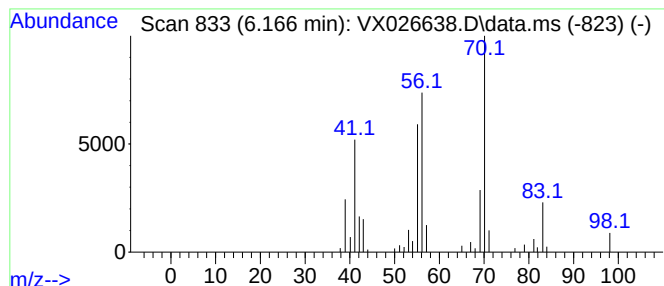
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, 1,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.166	5.65 ug/l	56268	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	91
2			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	91
3			Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	58
4			Cyclobutanone, 2,2-dimethyl-	98	C6H10O	001192-14-9	50
5			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026638.D
Acq On : 27 Jan 2022 20:30
Operator : JC/MD
Sample : N1297-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DB

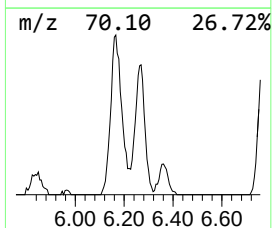
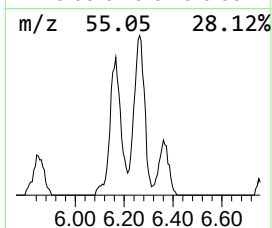
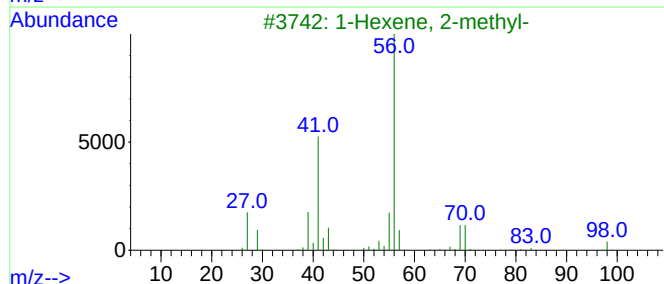
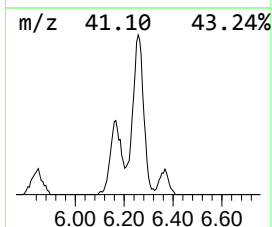
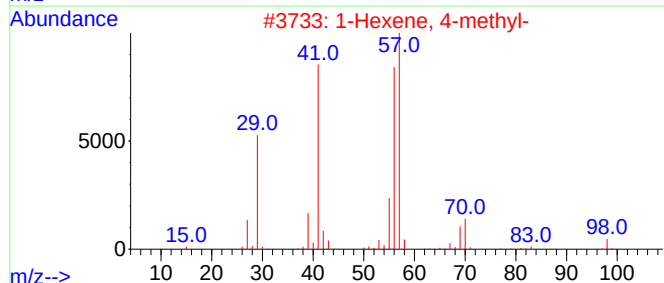
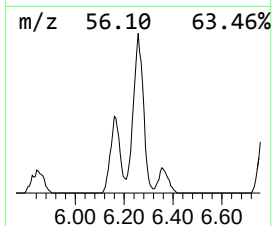
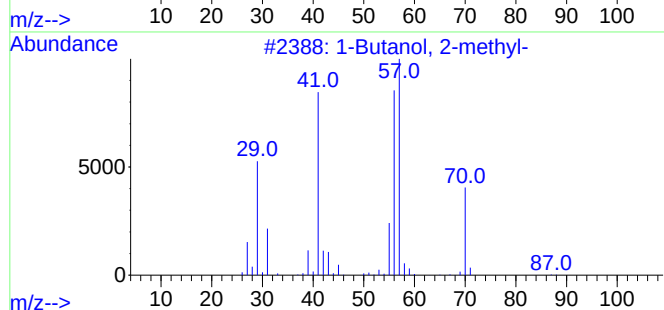
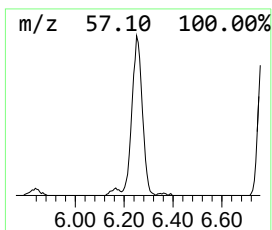
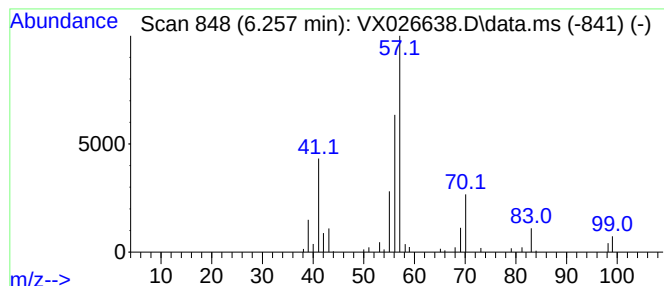
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Quant Title : SW846 8260

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

Peak Number 6 1-Butanol, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.257	9.88 ug/l	98355	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 2-methyl-			88	C5H12O	000137-32-6	53
2	1-Hexene, 4-methyl-			98	C7H14	003769-23-1	47
3	1-Hexene, 2-methyl-			98	C7H14	006094-02-6	46
4	Acetamide, N-2-propenyl-			99	C5H9NO	000692-33-1	43
5	1-Pentanol, 2-ethyl-4-methyl-			130	C8H18O	000106-67-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026638.D
Acq On : 27 Jan 2022 20:30
Operator : JC/MD
Sample : N1297-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DB

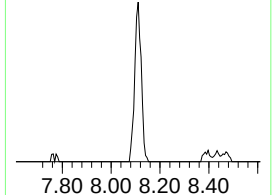
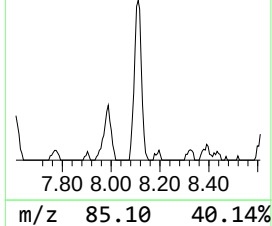
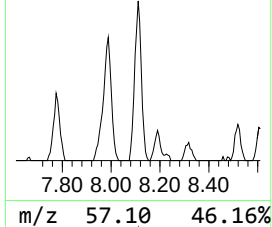
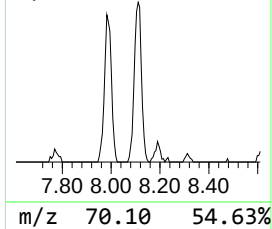
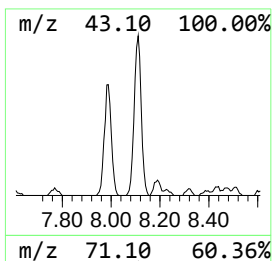
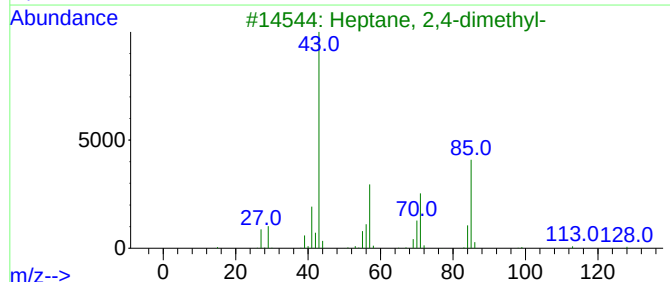
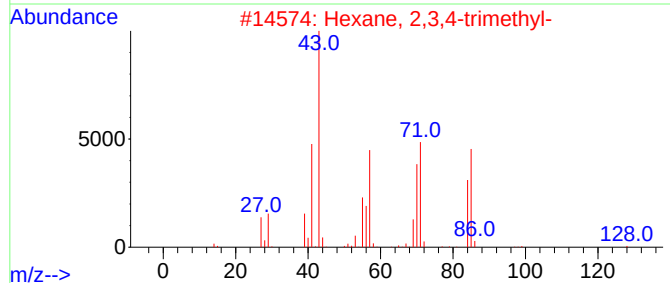
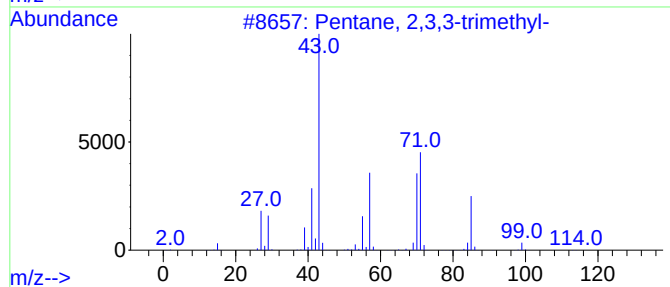
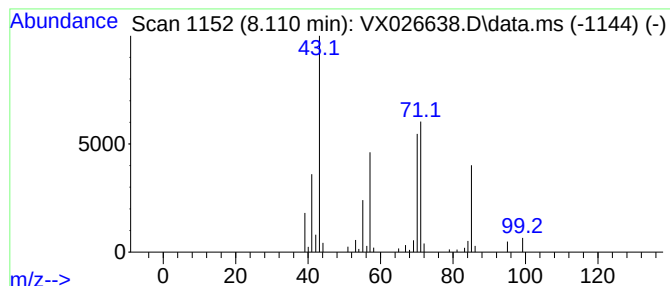
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	5.62 ug/l	55929	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, 2,3,4-trimethyl-	128	C9H20	000921-47-1	78
3			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026638.D
Acq On : 27 Jan 2022 20:30
Operator : JC/MD
Sample : N1297-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DB

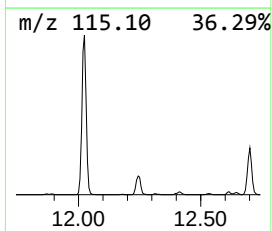
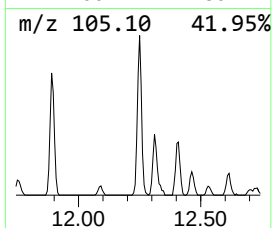
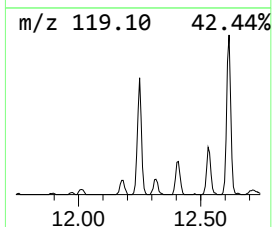
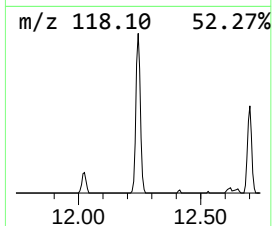
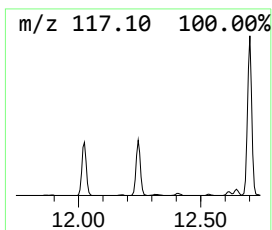
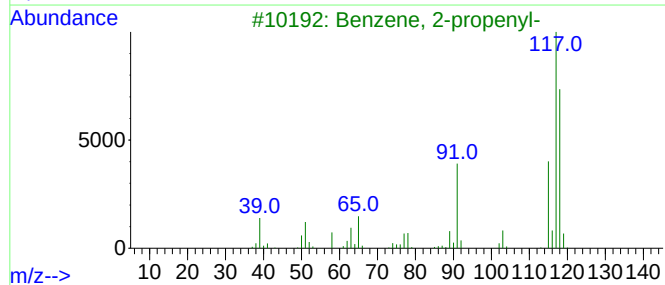
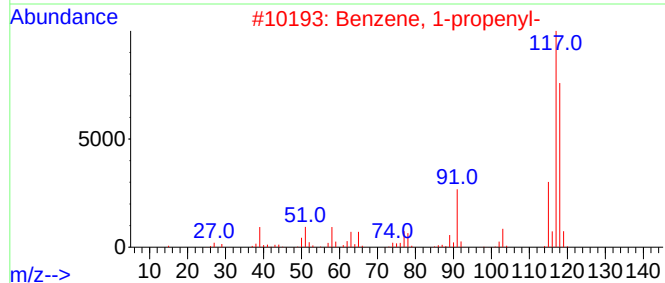
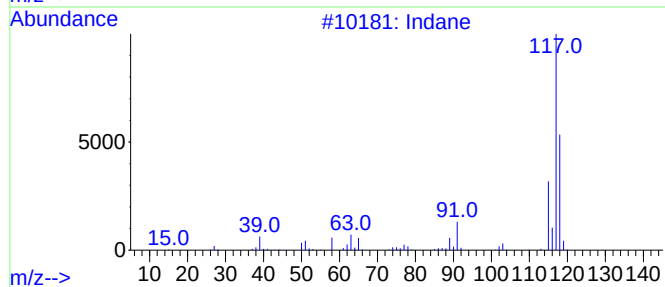
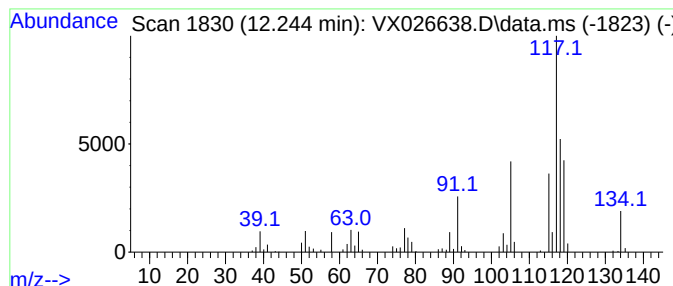
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Quant Title : SW846 8260

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

Peak Number 8 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	8.64 ug/l	81966	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, 1-propenyl-	118	C9H10	000637-50-3	60
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
4			Delta-cyclene	118	C9H10	007785-10-6	60
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026638.D
Acq On : 27 Jan 2022 20:30
Operator : JC/MD
Sample : N1297-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DB

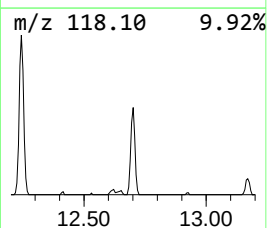
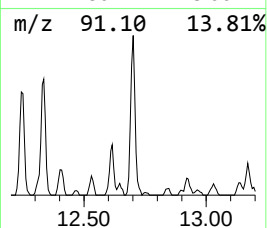
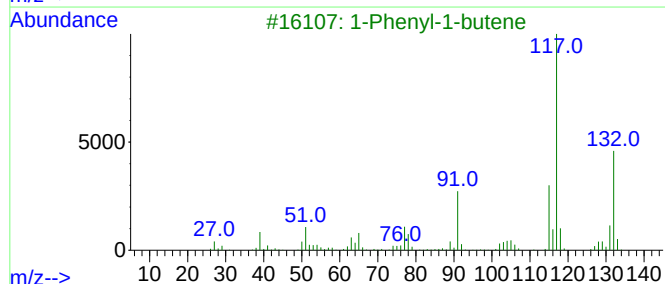
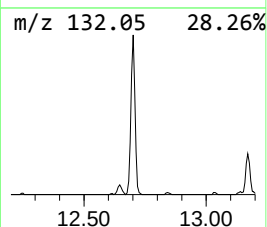
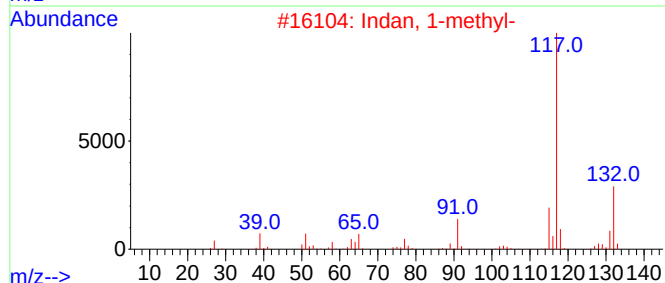
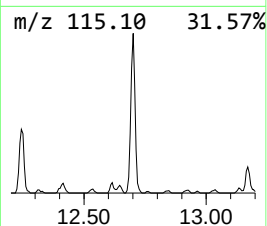
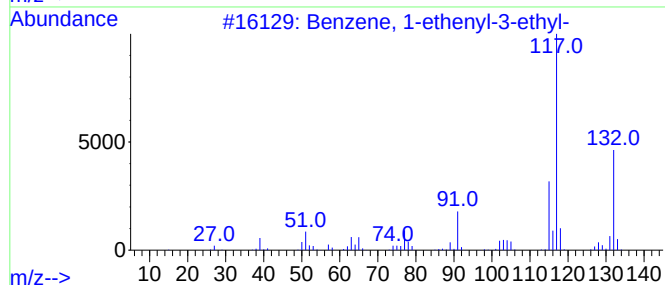
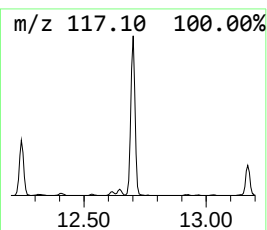
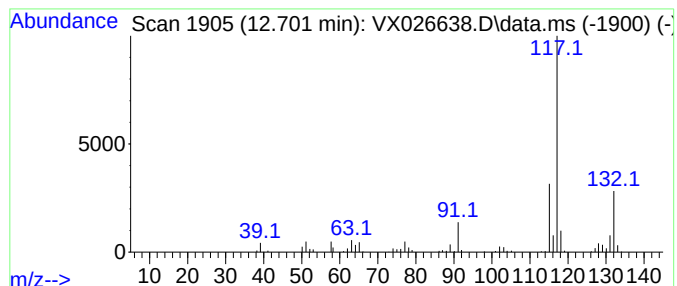
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	13.42 ug/l	127324	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2			Indan, 1-methyl-	132	C10H12	000767-58-8	90
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
5			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026638.D
Acq On : 27 Jan 2022 20:30
Operator : JC/MD
Sample : N1297-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DB

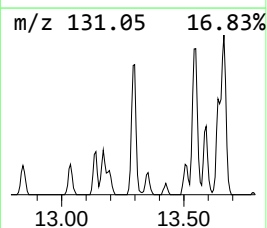
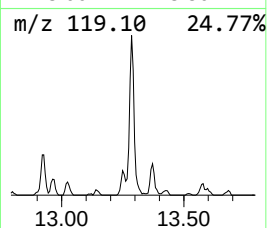
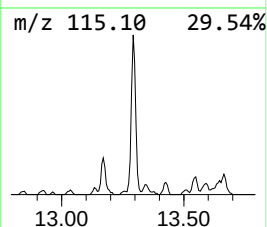
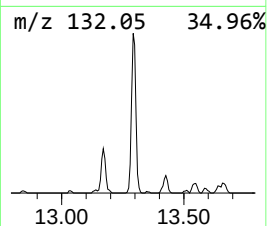
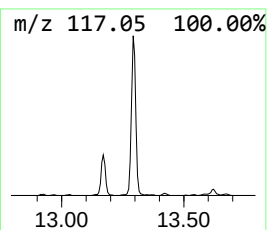
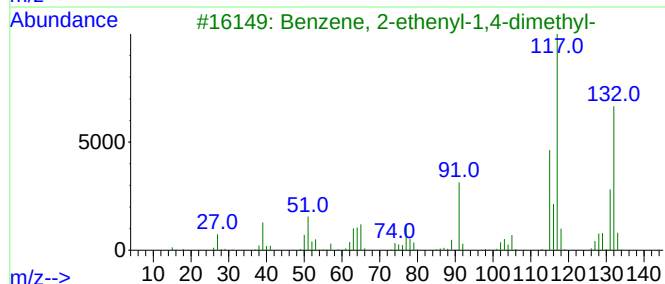
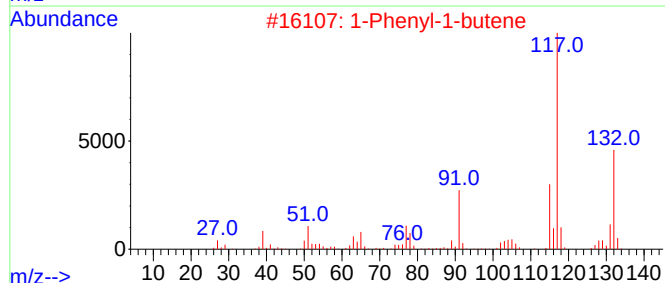
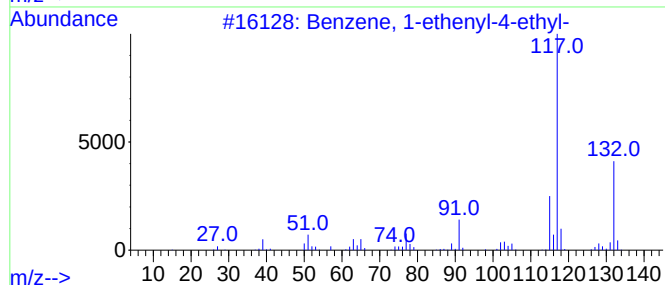
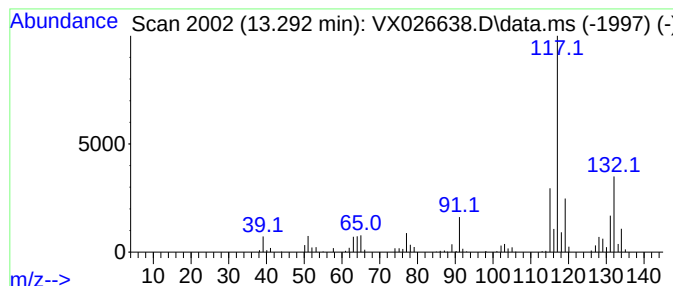
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	13.93 ug/l	132219	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	91
3			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026638.D
Acq On : 27 Jan 2022 20:30
Operator : JC/MD
Sample : N1297-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.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...	2.788	18.1	ug/l	143725	1	5.556	396965	50.0
Pentane, 3-methyl-	3.105	28.4	ug/l	225451	1	5.556	396965	50.0
Pentane, 2,3-di...	5.623	10.6	ug/l	84343	1	5.556	396965	50.0
Cyclopentane, 1...	6.166	5.7	ug/l	56268	2	6.763	497912	50.0
1-Butanol, 2-me...	6.257	9.9	ug/l	98355	2	6.763	497912	50.0
Pentane, 2,3,3-...	8.110	5.6	ug/l	55929	2	6.763	497912	50.0
Indane	12.244	8.6	ug/l	81966	4	12.024	474545	50.0
Benzene, 1-ethe...	12.701	13.4	ug/l	127324	4	12.024	474545	50.0
Benzene, 1-ethe...	13.292	13.9	ug/l	132219	4	12.024	474545	50.0