

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
 Data File : VX041275.D
 Acq On : 29 Apr 2024 14:40
 Operator : JC/MD
 Sample : P2183-02
 Misc : 1.28g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1233

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\82X042224W.M
 Title : SW846 8260

Signal : TIC: VX041275.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.422	209	219	300	rBV	4604753	20727966	34.60%	20.209%
2	5.483	710	721	733	rBV2	829965	2763763	4.61%	2.695%
3	5.599	734	740	759	rVB	360064	1151757	1.92%	1.123%
4	5.806	761	774	790	rBV	1419085	4142276	6.91%	4.039%
5	6.166	819	833	841	rBV6	189594	764309	1.28%	0.745%
6	6.598	892	904	922	rBV	1234771	2989808	4.99%	2.915%
7	7.367	1017	1030	1042	rBV2	334421	883063	1.47%	0.861%
8	8.732	1245	1254	1279	rVB	30118584	59903760	100.00%	58.404%
9	10.299	1501	1511	1518	rBV	1359319	1833798	3.06%	1.788%
10	10.640	1562	1567	1574	rVB	624546	806886	1.35%	0.787%
11	11.378	1683	1688	1695	rBV	481863	799617	1.33%	0.780%
12	11.750	1745	1749	1759	rVB	781629	1001244	1.67%	0.976%
13	12.024	1789	1794	1799	rVV	501227	649622	1.08%	0.633%
14	12.987	1946	1952	1957	rVB	660038	1033635	1.73%	1.008%
15	15.560	2368	2374	2380	rBV	2205437	3116581	5.20%	3.039%

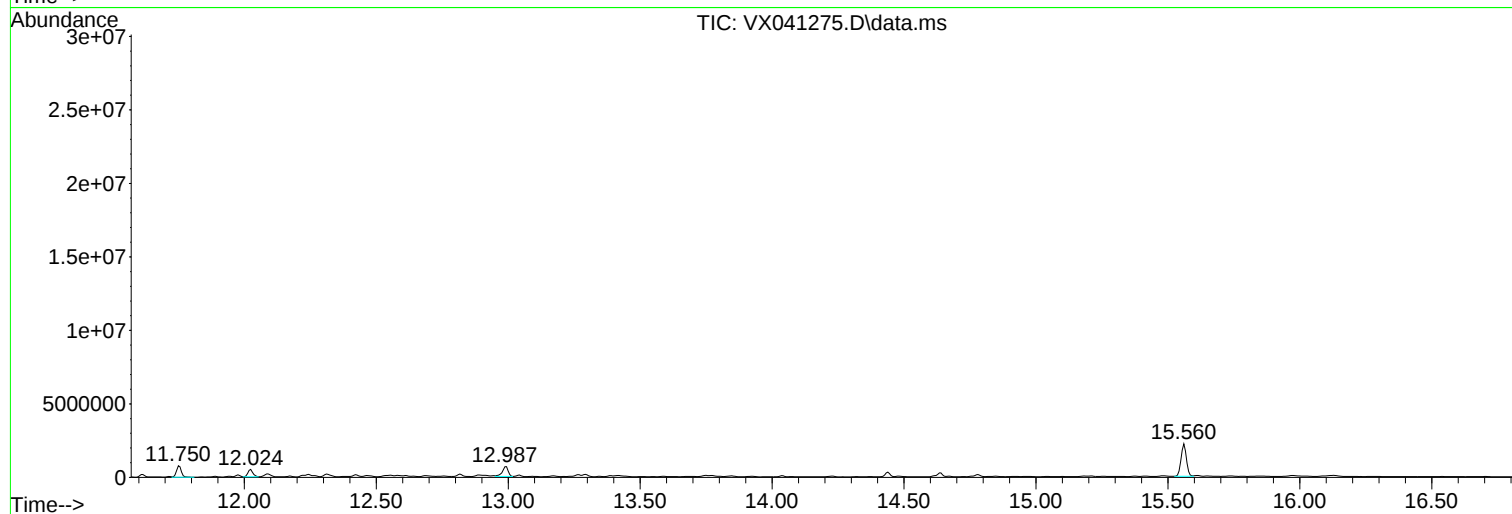
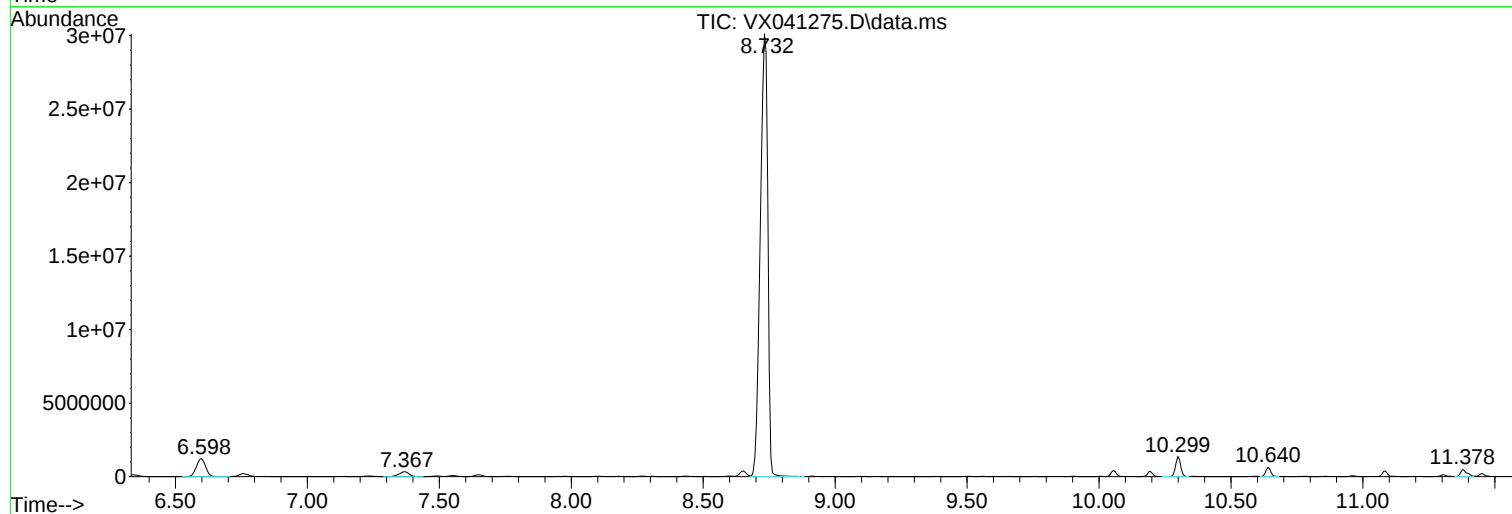
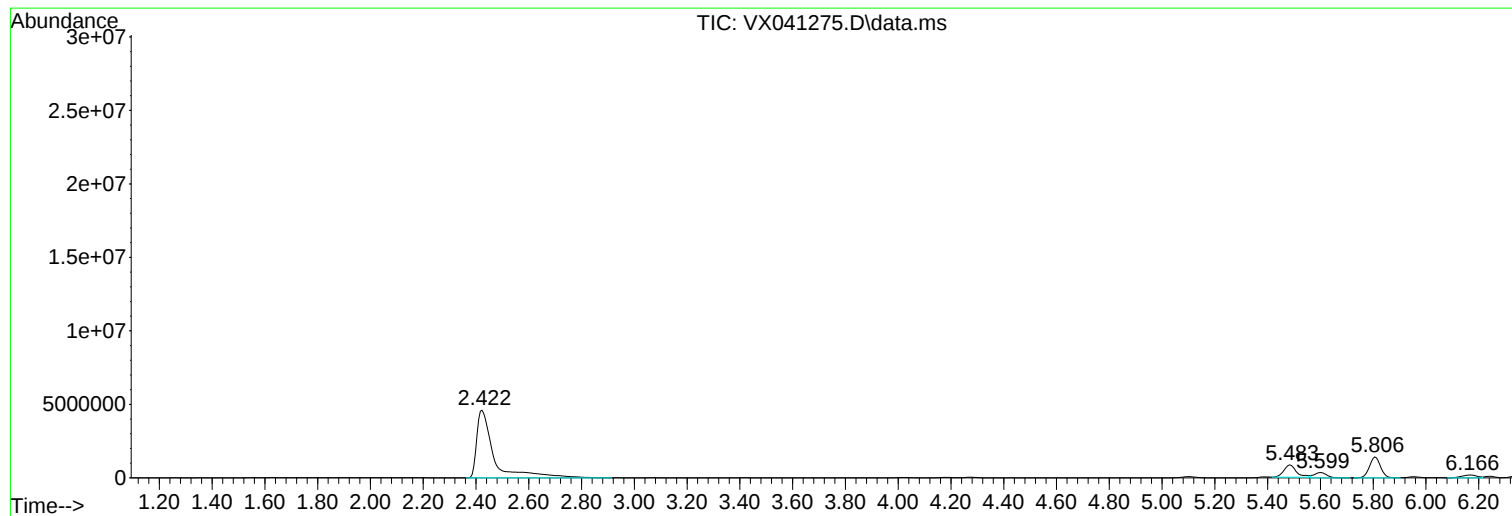
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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



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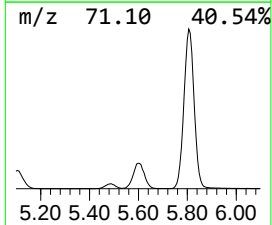
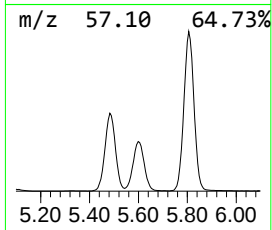
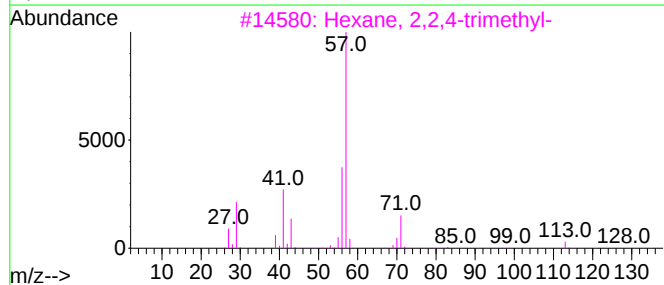
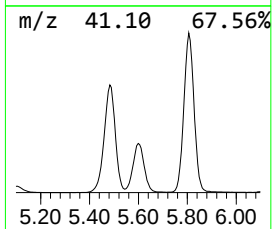
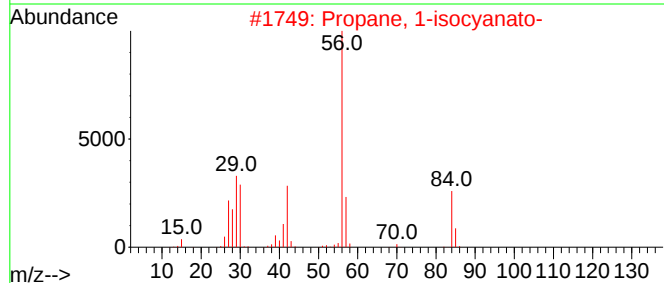
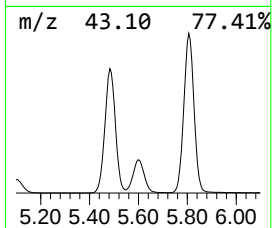
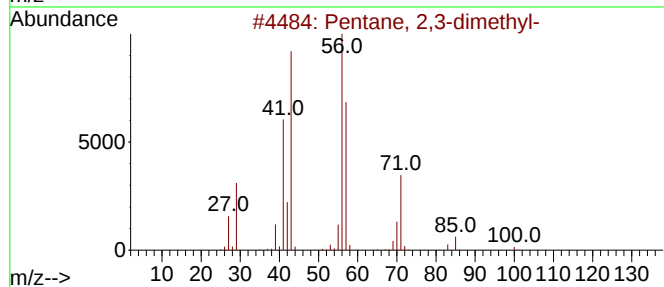
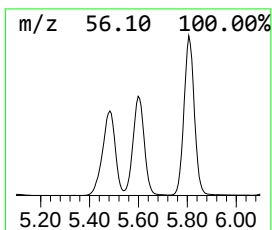
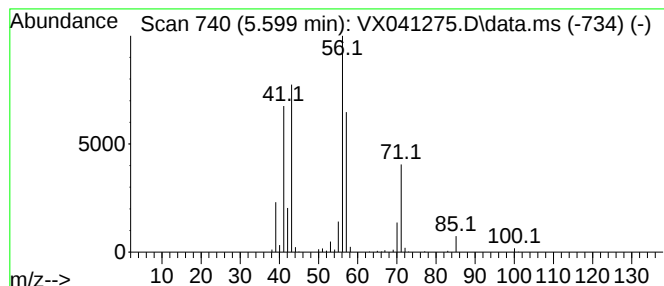
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Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.599	50.00 ug/l	1151760	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	47
3			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	38
4			Heptane	100	C7H16	000142-82-5	37
5			Pentane, 2-methyl-	86	C6H14	000107-83-5	35



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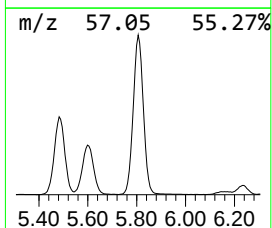
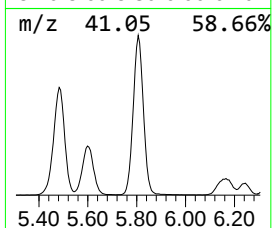
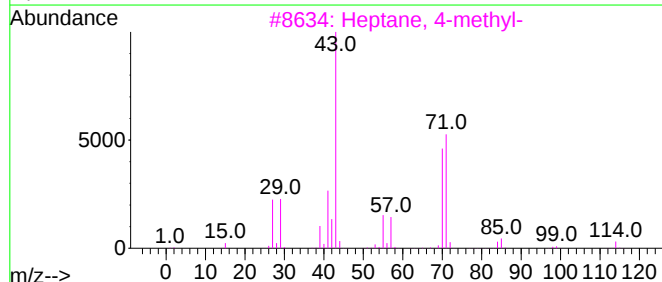
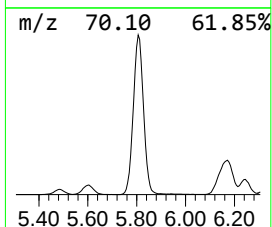
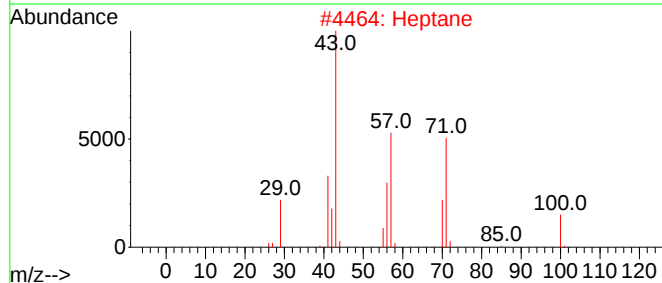
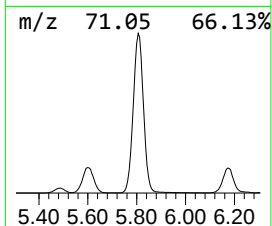
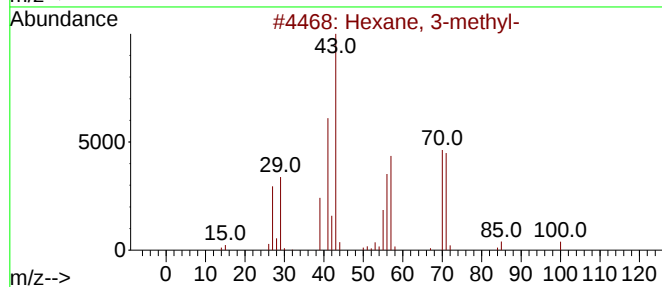
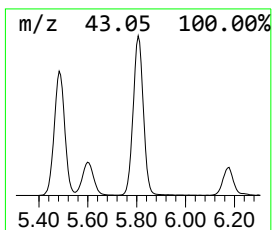
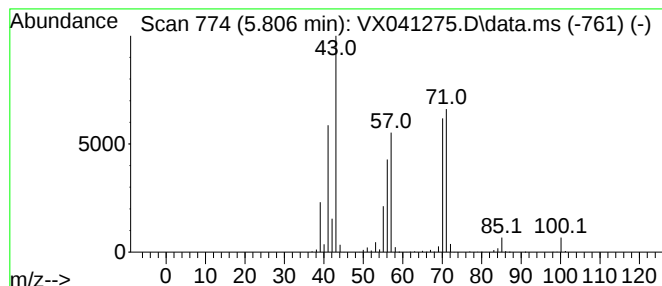
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.806	179.82 ug/l	4142280	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2			Heptane	100	C7H16	000142-82-5	64
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	53



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Instrument :
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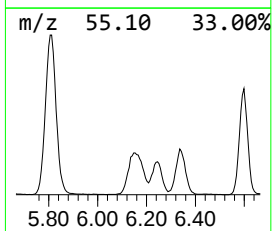
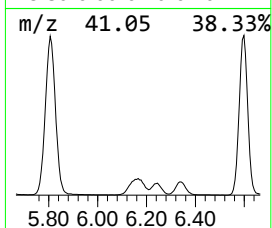
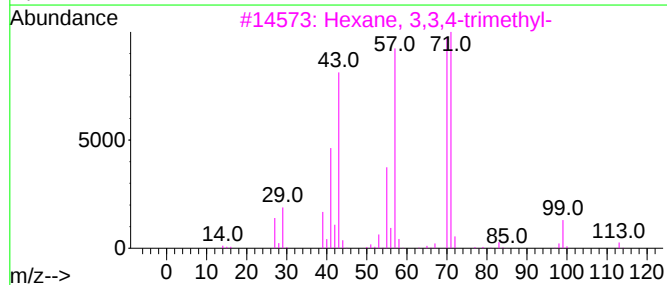
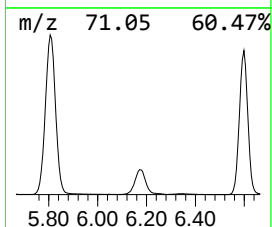
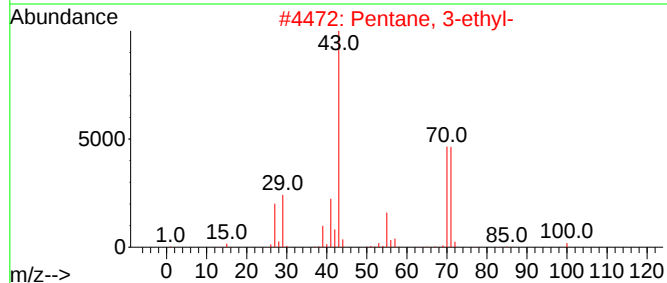
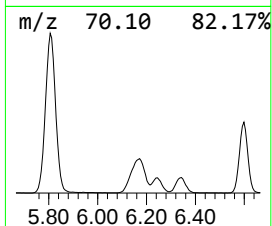
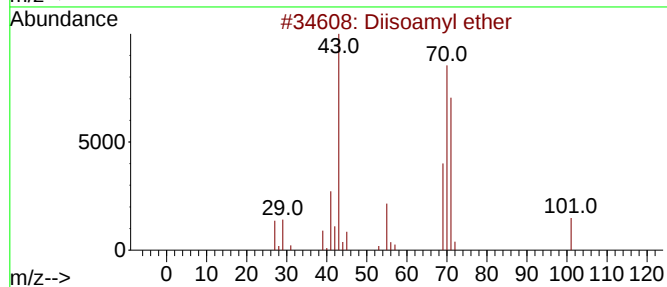
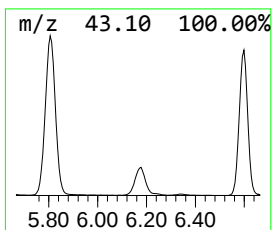
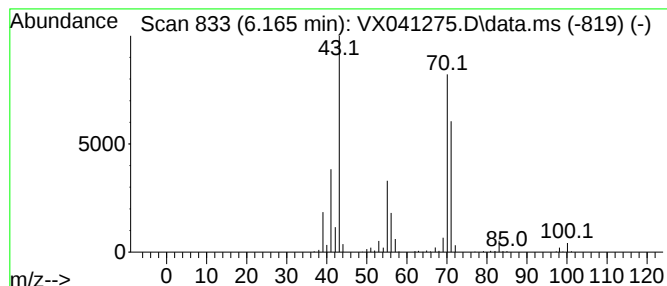
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Peak Number 3 Diisoamyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.165	12.78 ug/l	764309	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diisoamyl ether	158	C10H22O	000544-01-4	72
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	64
3			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
4			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	64
5			Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	56



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ALS Vial : 9 Sample Multiplier: 1

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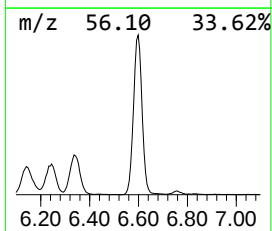
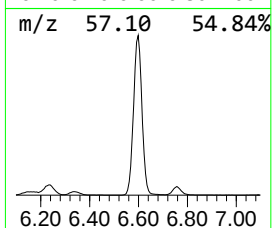
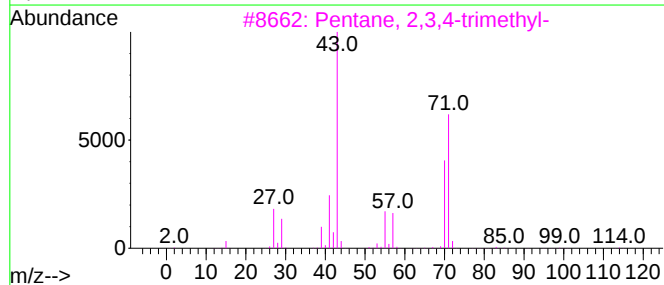
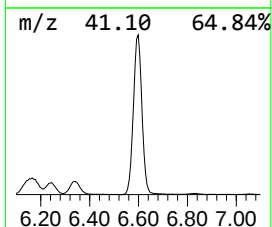
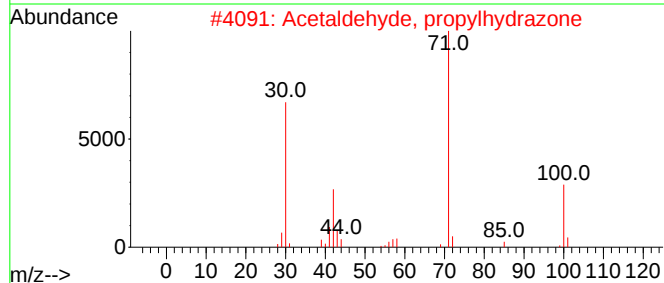
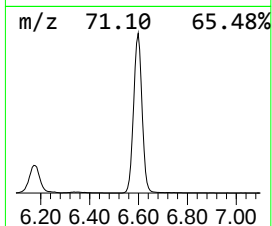
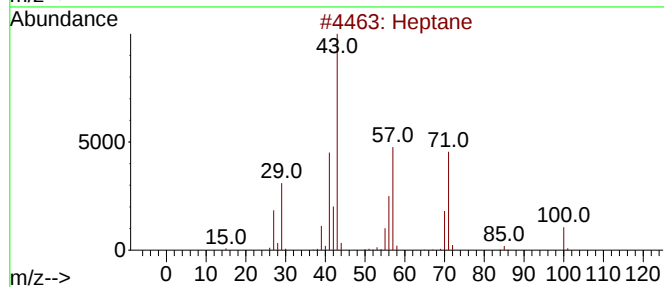
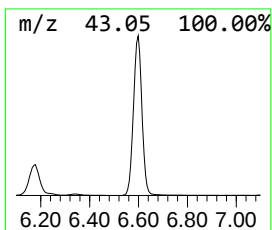
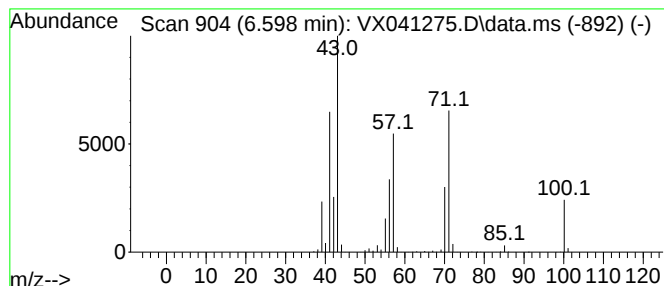
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.598	50.00 ug/l	2989810	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	47
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	40
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	40
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38



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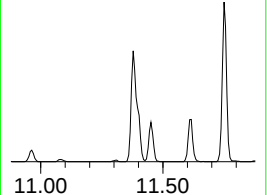
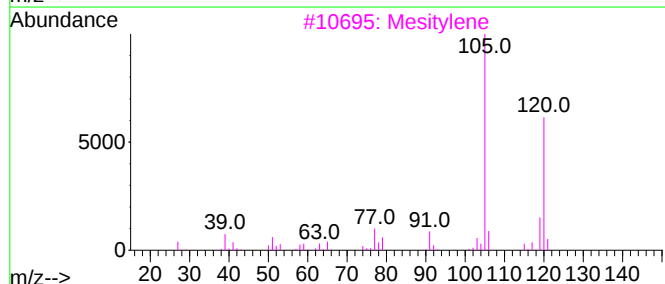
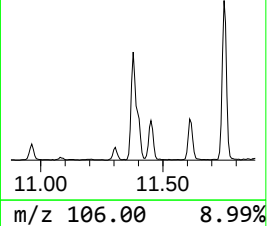
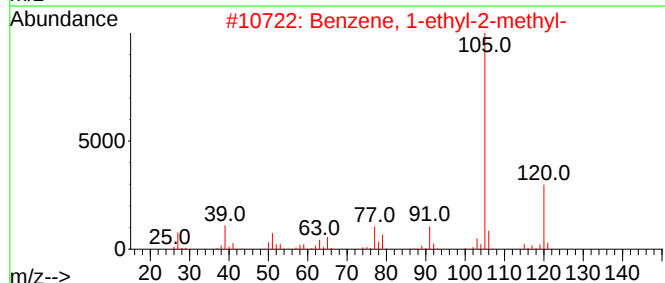
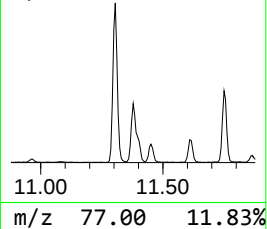
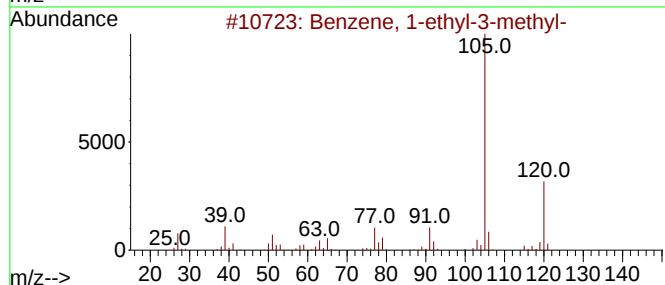
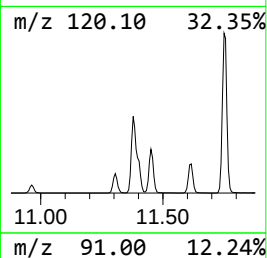
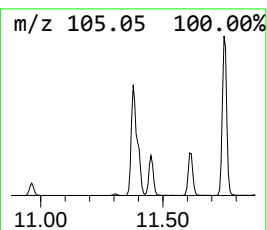
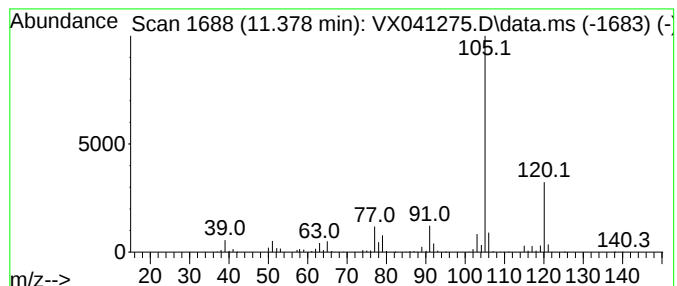
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	61.54 ug/l	799617	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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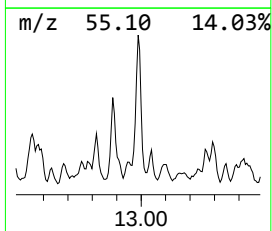
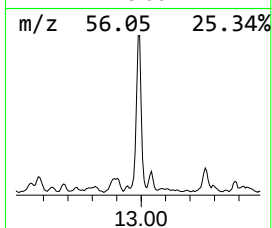
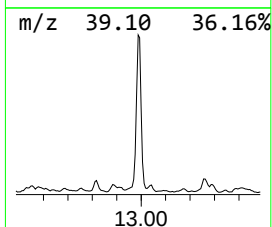
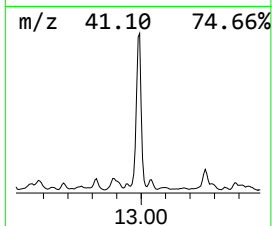
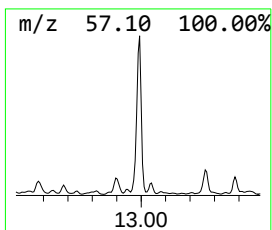
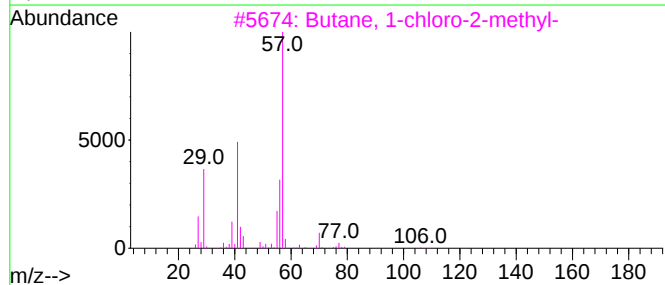
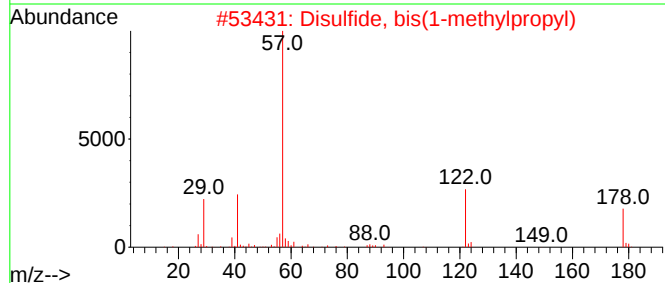
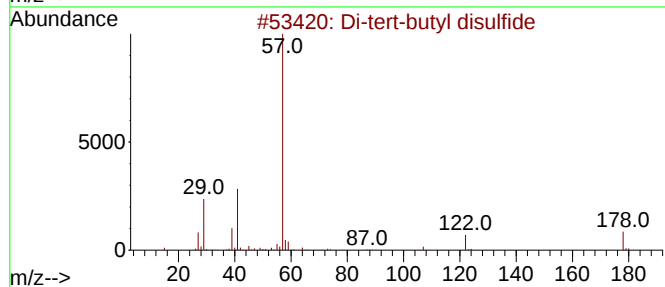
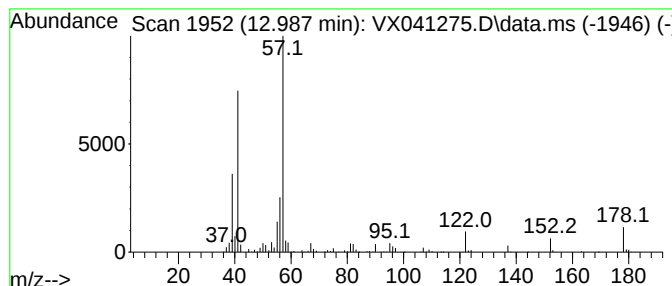
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Quant Title : SW846 8260

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

Peak Number 6 unknown12.988 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.988	79.56 ug/l	1033640	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	46
2			Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	43
3			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	38
4			Disulfide, bis(2-methylpropyl)	178	C8H18S2	001518-72-5	37
5			Butane, 1-bromo-	136	C4H9Br	000109-65-9	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041275.D
Acq On : 29 Apr 2024 14:40
Operator : JC/MD
Sample : P2183-02
Misc : 1.28g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1233

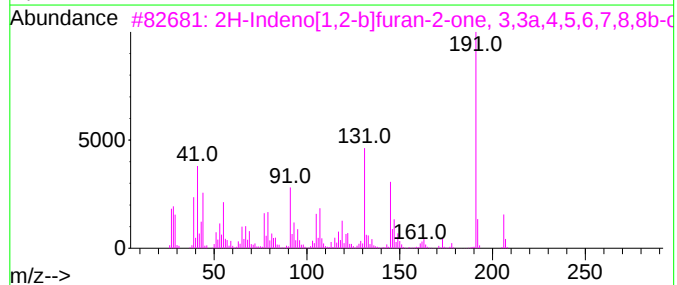
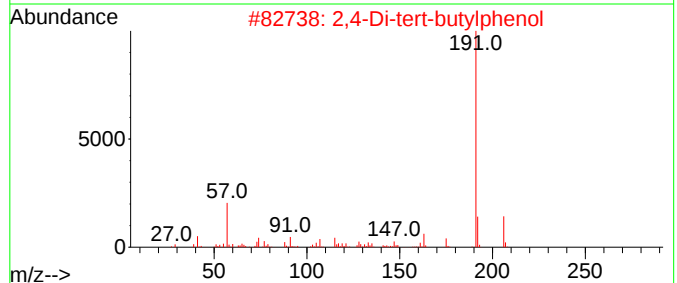
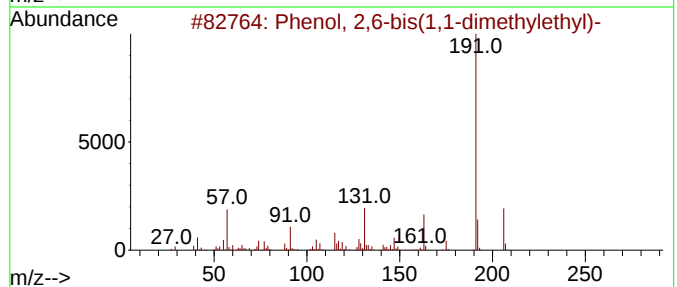
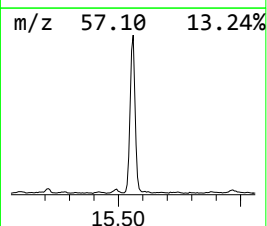
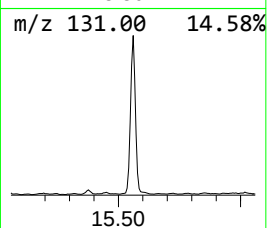
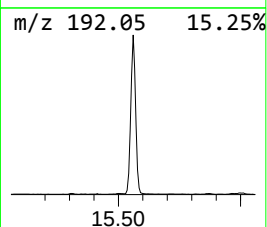
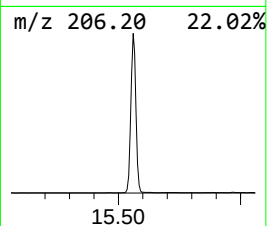
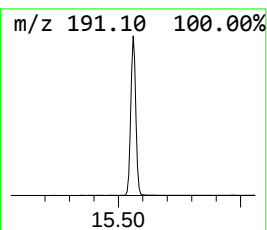
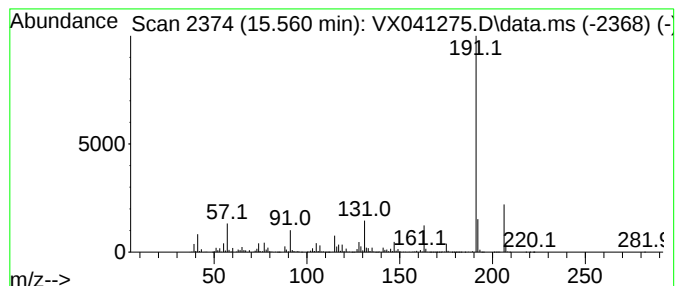
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Quant Title : SW846 8260

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

Peak Number 7 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	239.88 ug/l	3116580	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	96
2			2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	87
3			2H-Indeno[1,2-b]furan-2-one, 3,3...	206	C13H18O2	1000196-74-3	80
4			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	80
5			Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041275.D
Acq On : 29 Apr 2024 14:40
Operator : JC/MD
Sample : P2183-02
Misc : 1.28g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1233

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.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
Pentane, 2,3-di...	5.599	50.0	ug/l	1151760	1	5.544	1151760	50.0
Hexane, 3-methyl-	5.806	179.8	ug/l	4142280	1	5.544	1151760	50.0
Diisoamyl ether	6.165	12.8	ug/l	764309	2	6.757	2989810	50.0
Heptane	6.598	50.0	ug/l	2989810	2	6.757	2989810	50.0
Benzene, 1-ethy...	11.378	61.5	ug/l	799617	4	12.024	649622	50.0
unknown12.988	12.988	79.6	ug/l	1033640	4	12.024	649622	50.0
Phenol, 2,6-bis...	15.560	239.9	ug/l	3116580	4	12.024	649622	50.0