

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039950.D
Acq On : 25 Jan 2024 13:47
Operator : JC/MD
Sample : P1235-07
Misc : 5.07g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
131

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\82X011024W.M
Title : SW846 8260

Signal : TIC: VX039950.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	691	705	714	rBV2	53028	164765	3.78%	1.500%
2	5.489	714	722	727	rVV	102412	312560	7.18%	2.846%
3	5.544	727	731	755	rVB3	103817	377529	8.67%	3.437%
4	5.812	762	775	789	rBV2	155344	446742	10.26%	4.067%
5	5.952	789	798	816	rVB	70587	198938	4.57%	1.811%
6	6.178	821	835	842	rBV3	17934	65722	1.51%	0.598%
7	6.598	893	904	922	rBV	251338	609896	14.00%	5.553%
8	6.757	922	930	945	rVV	159115	397601	9.13%	3.620%
9	7.366	1021	1030	1040	rVB2	30479	77815	1.79%	0.708%
10	8.647	1234	1240	1246	rBV	321736	513303	11.79%	4.673%
11	8.720	1246	1252	1264	rVB	2761198	4355459	100.00%	39.654%
12	10.055	1466	1471	1478	rVB	337911	467846	10.74%	4.259%
13	10.195	1487	1494	1499	rBV	30227	48506	1.11%	0.442%
14	10.299	1499	1511	1517	rVV	98666	182821	4.20%	1.664%
15	10.360	1517	1521	1531	rVB	101857	137876	3.17%	1.255%
16	10.640	1561	1567	1577	rVB	37264	65114	1.49%	0.593%
17	10.854	1594	1602	1607	rBV3	27970	50457	1.16%	0.459%
18	11.085	1634	1640	1650	rVB	300919	454751	10.44%	4.140%
19	11.378	1684	1688	1694	rVV	89851	165422	3.80%	1.506%
20	11.475	1697	1704	1710	rVB2	157269	239203	5.49%	2.178%
21	11.616	1722	1727	1734	rVB	45617	74033	1.70%	0.674%
22	11.750	1746	1749	1759	rVB	135020	189201	4.34%	1.723%
23	12.024	1788	1794	1800	rBV	391173	525228	12.06%	4.782%
24	12.091	1800	1805	1810	rVB3	37937	79055	1.82%	0.720%
25	12.244	1825	1830	1832	rBV2	49882	66987	1.54%	0.610%
26	12.268	1832	1834	1837	rVB	42469	43953	1.01%	0.400%
27	12.317	1837	1842	1849	rVB3	60026	119021	2.73%	1.084%
28	12.420	1849	1859	1863	rBV	152658	189126	4.34%	1.722%
29	12.969	1945	1949	1955	rVB3	26859	46555	1.07%	0.424%
30	13.268	1992	1998	2000	rBV	71564	95957	2.20%	0.874%
31	13.292	2000	2002	2007	rVB2	49767	58422	1.34%	0.532%
32	13.420	2019	2023	2032	rVB	38121	68039	1.56%	0.619%
33	14.036	2120	2124	2127	rBV	49578	51646	1.19%	0.470%
34	15.188	2306	2313	2320	rBV6	21391	44238	1.02%	0.403%

Sum of corrected areas: 10983787

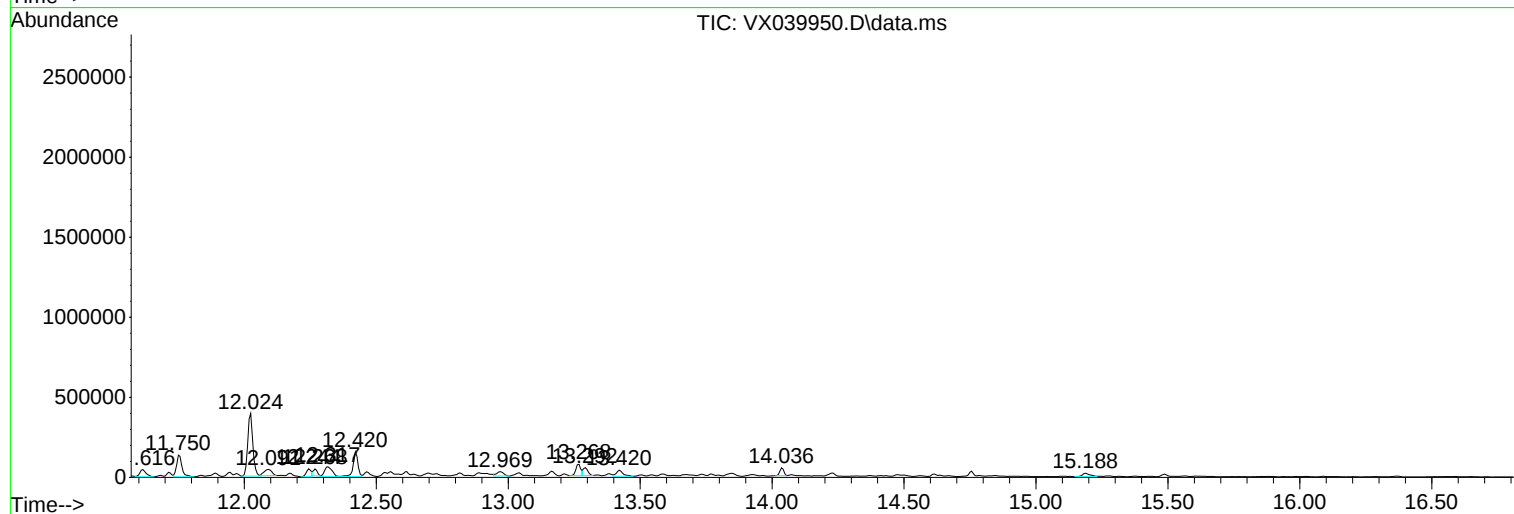
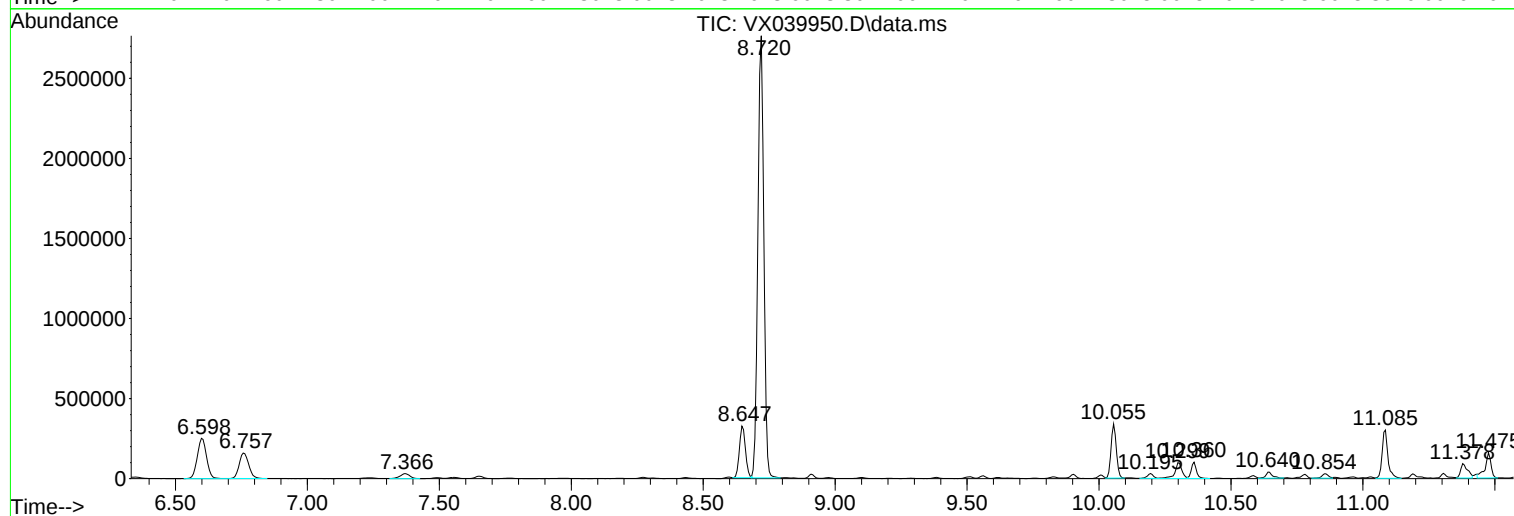
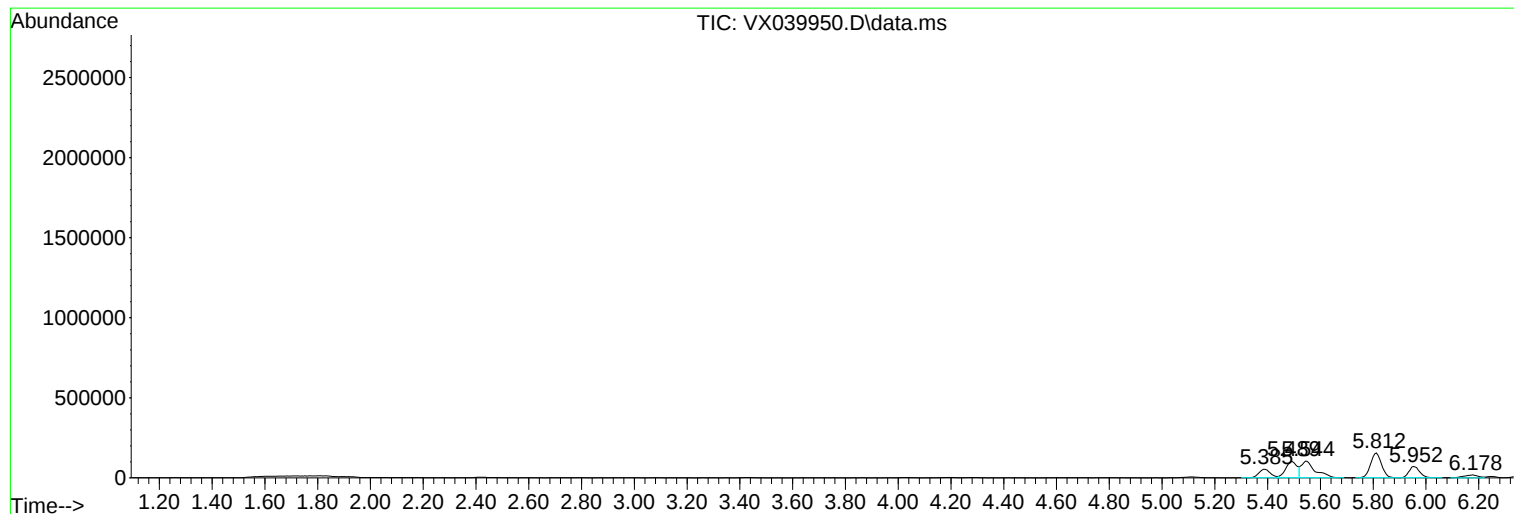
Instrument :
MSVOA_X
ClientSampleId :
131

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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



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Misc : 5.07g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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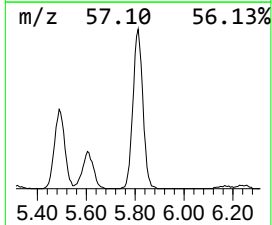
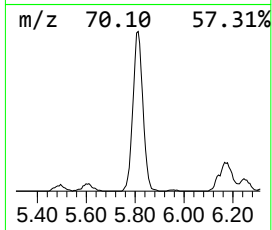
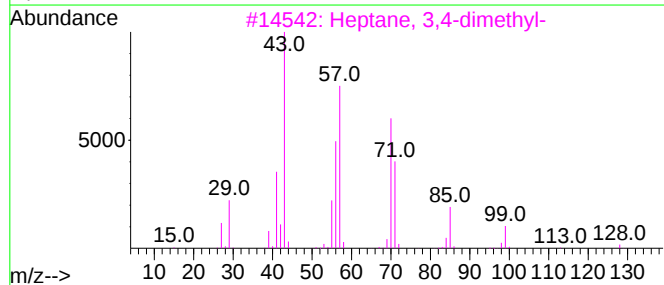
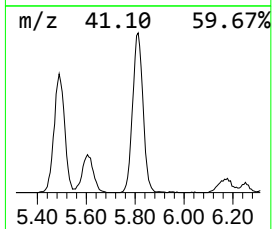
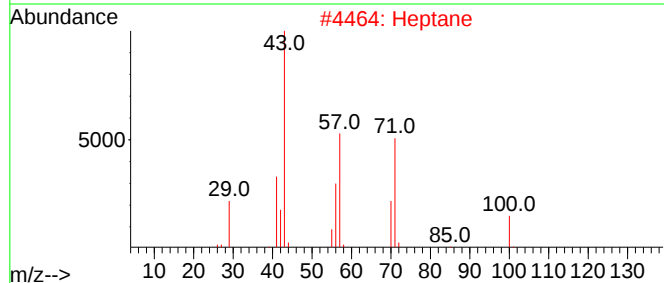
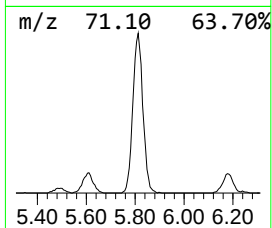
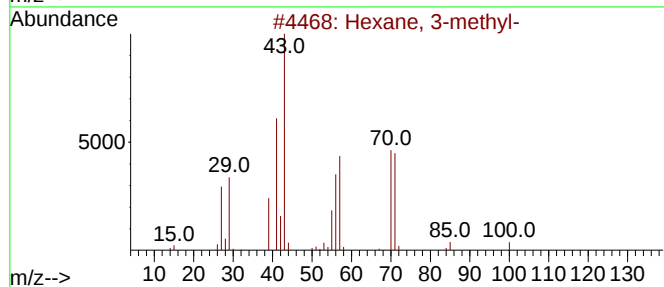
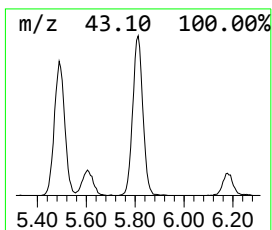
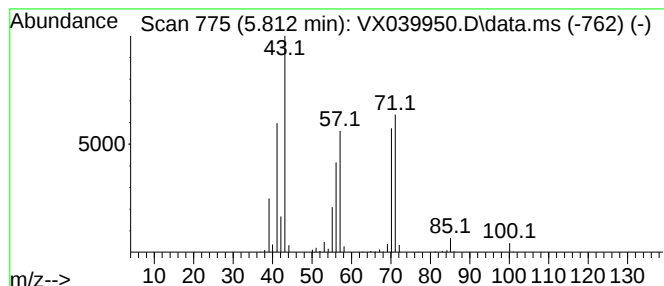
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.812	59.17 ug/l	446742	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	80
3			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	64
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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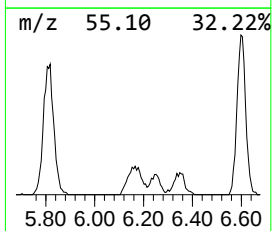
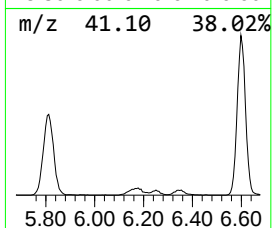
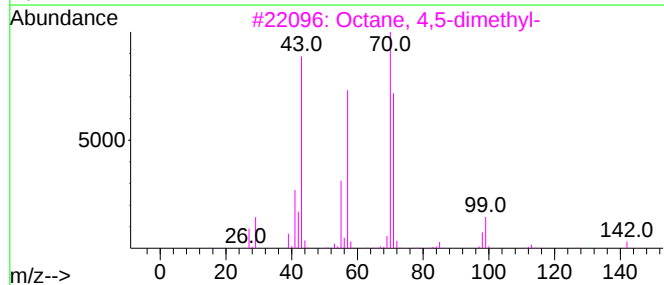
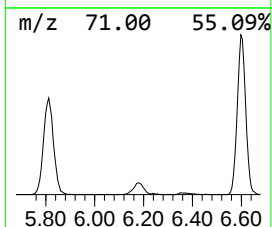
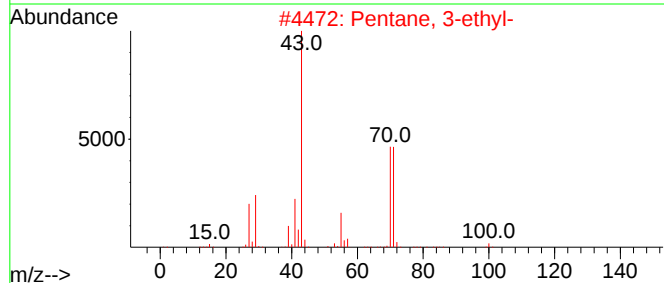
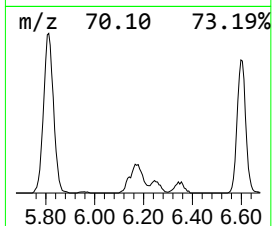
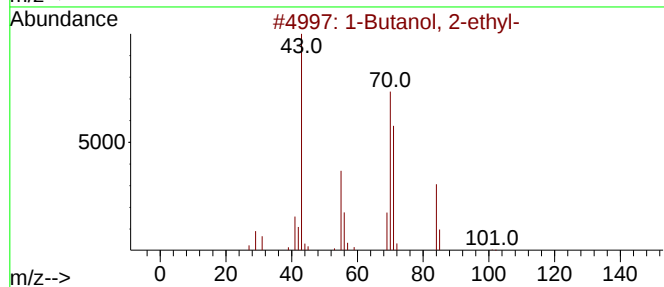
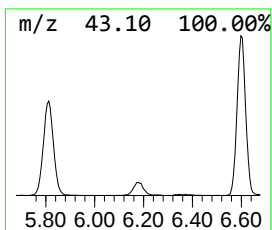
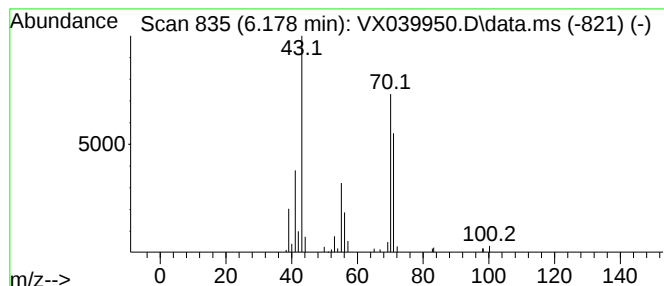
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Butanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.178	8.26 ug/l	65722	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 2-ethyl-			102	C6H14O	000097-95-0	64
2	Pentane, 3-ethyl-			100	C7H16	000617-78-7	59
3	Octane, 4,5-dimethyl-			142	C10H22	015869-96-2	56
4	Propanoic acid, 2-methyl-, 3-met...			158	C9H18O2	002050-01-3	56
5	Pyrrolidine			71	C4H9N	000123-75-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
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Misc : 5.07g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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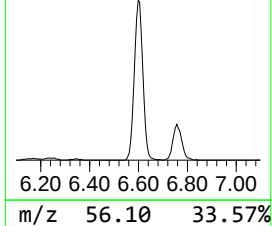
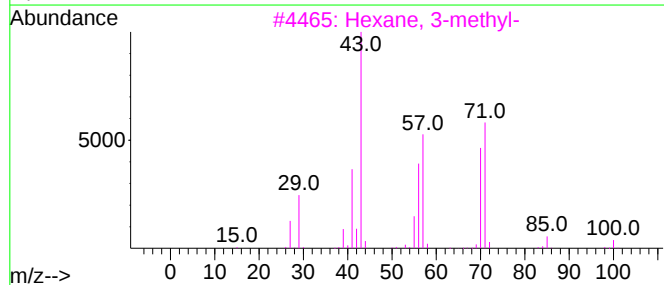
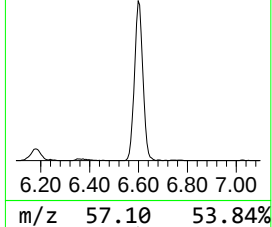
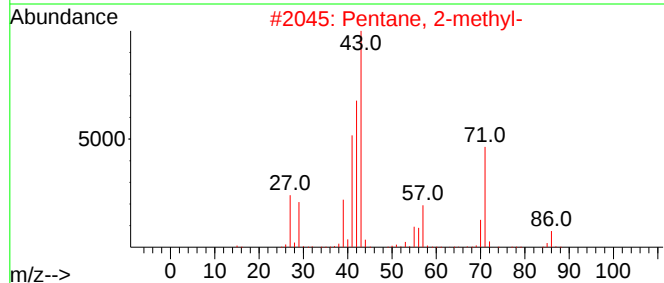
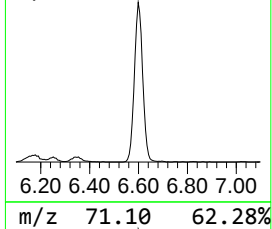
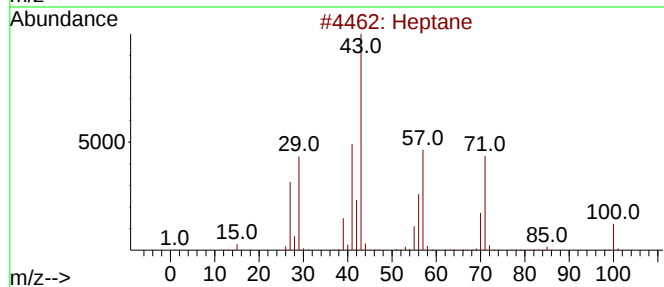
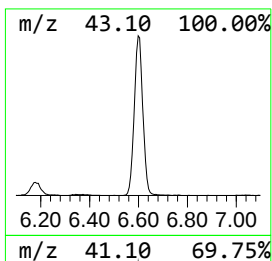
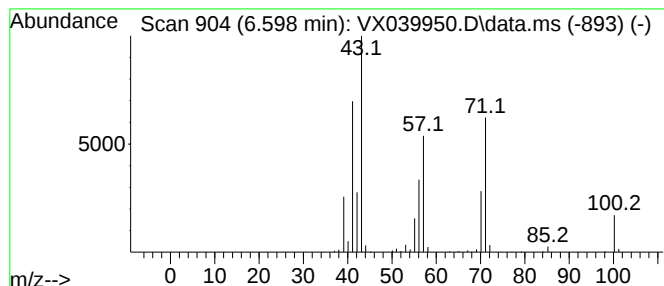
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 3 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.598	76.70 ug/l	609896	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	90
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	47
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	40
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
5			3-Hexanone	100	C6H12O	000589-38-8	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
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Sample : P1235-07
Misc : 5.07g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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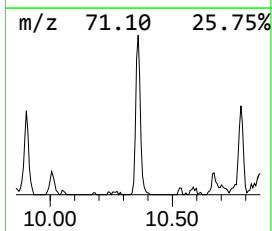
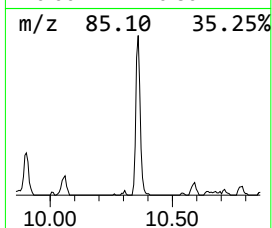
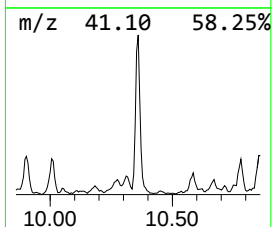
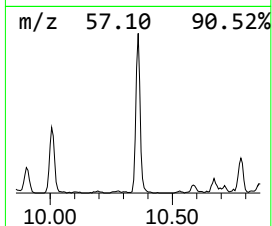
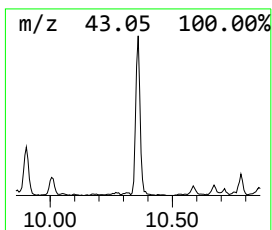
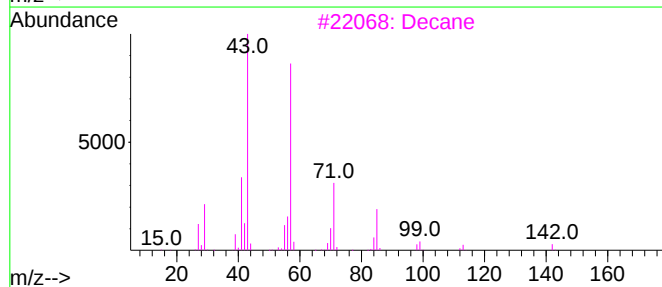
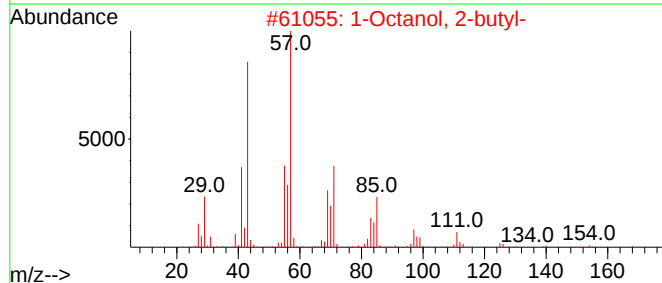
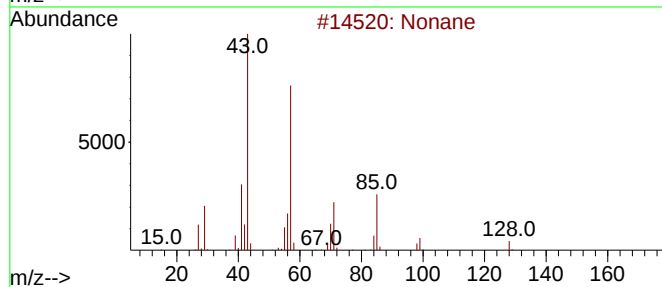
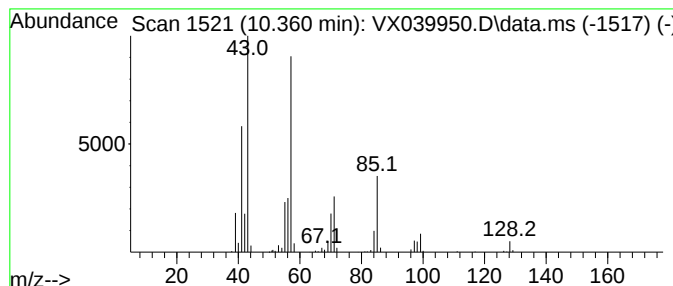
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Nonane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.360	14.74 ug/l	137876	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane	128	C9H20	000111-84-2	97
2			1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	72
3			Decane	142	C10H22	000124-18-5	59
4			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	53
5			Octane	114	C8H18	000111-65-9	53



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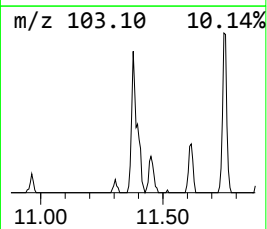
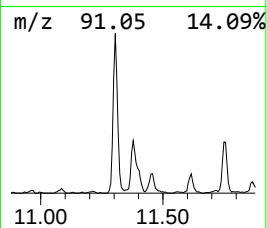
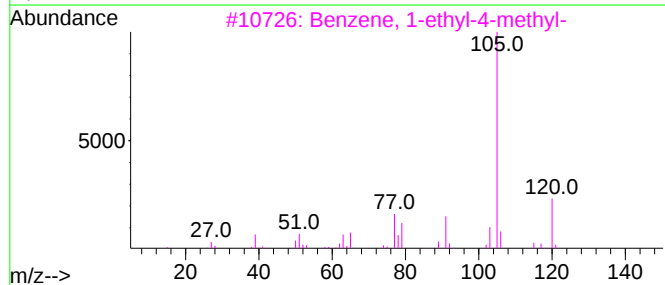
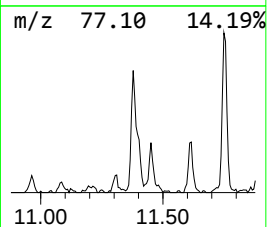
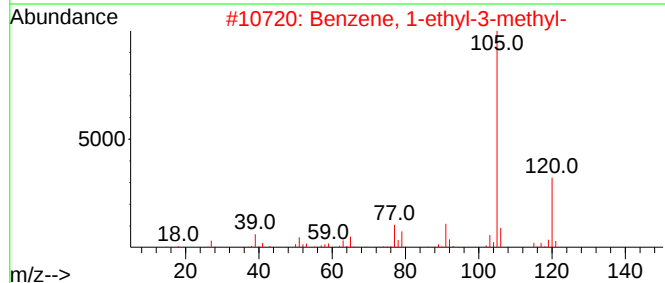
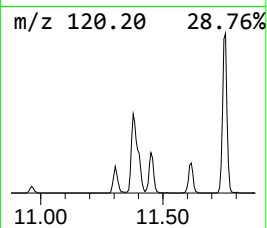
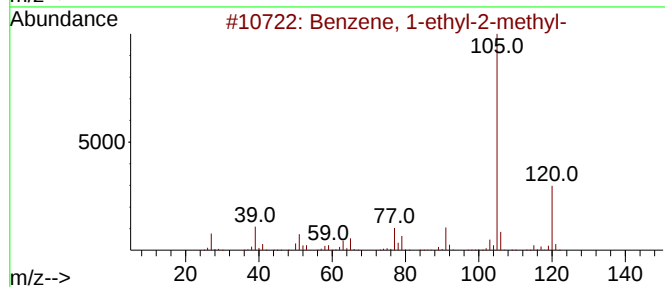
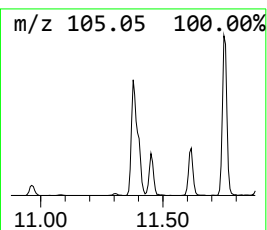
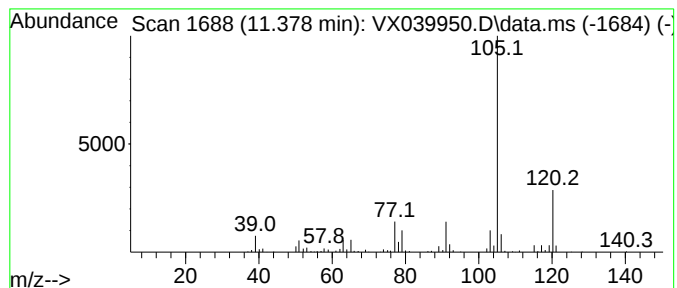
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	15.75 ug/l	165422	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	94
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



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Misc : 5.07g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
131

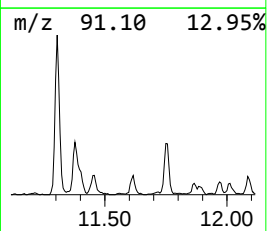
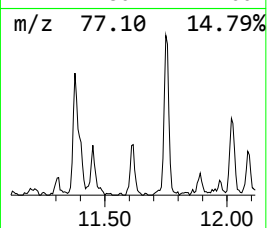
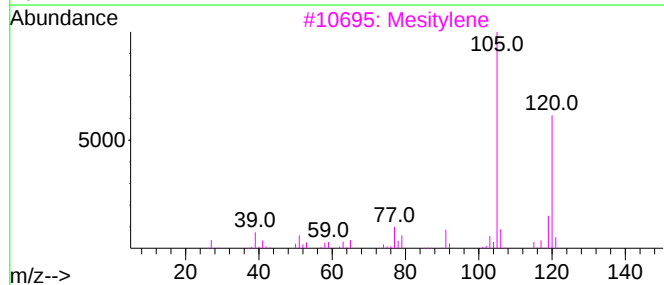
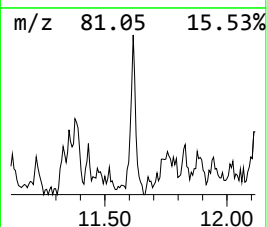
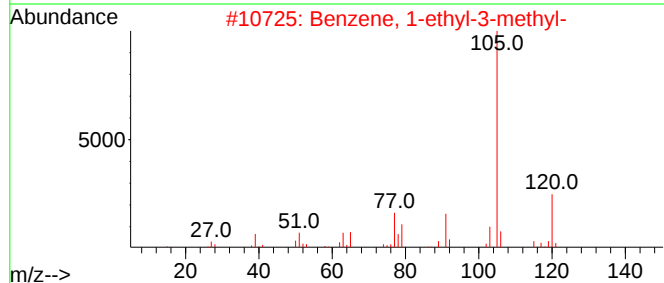
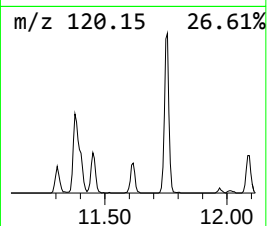
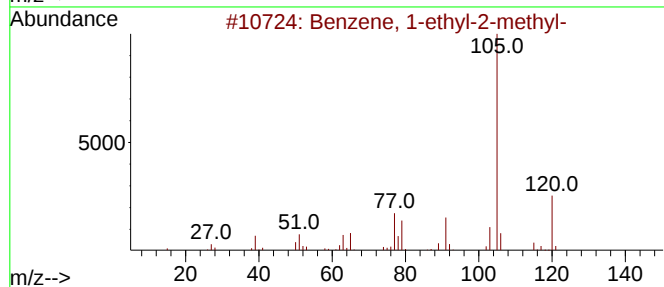
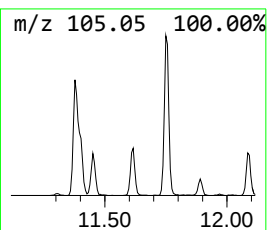
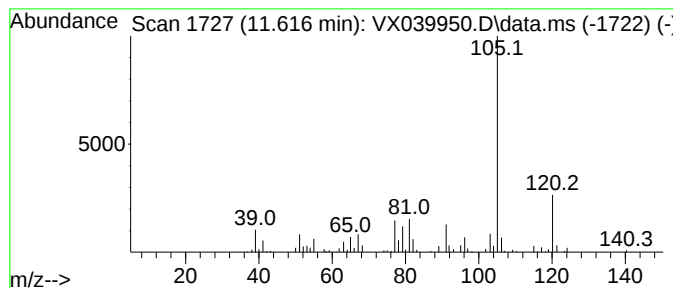
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	7.05 ug/l	74033	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	94
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
3			Mesitylene	120	C9H12	000108-67-8	81
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	81
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039950.D
Acq On : 25 Jan 2024 13:47
Operator : JC/MD
Sample : P1235-07
Misc : 5.07g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
131

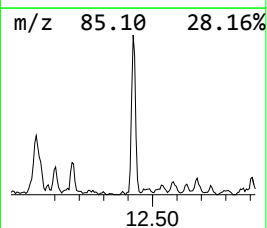
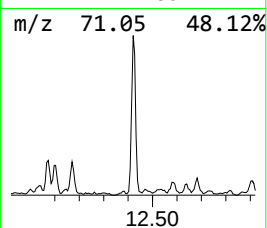
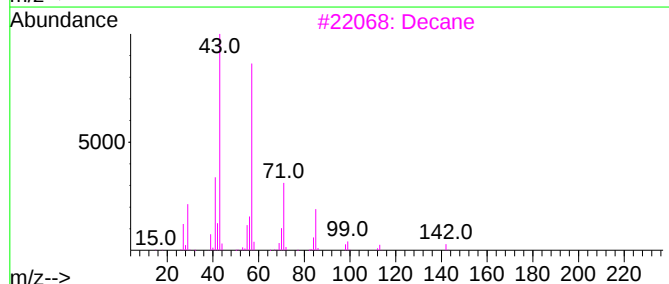
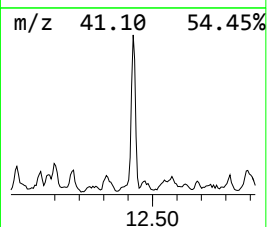
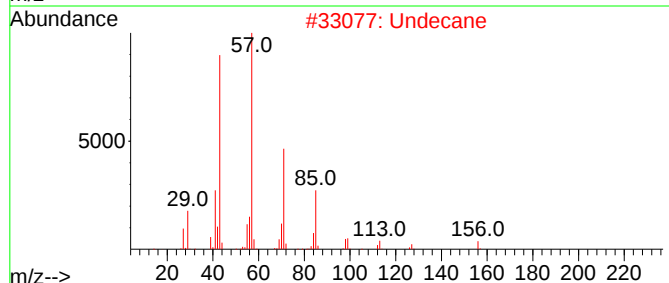
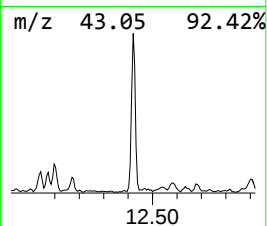
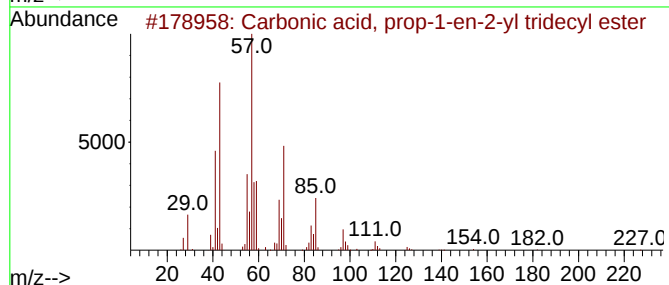
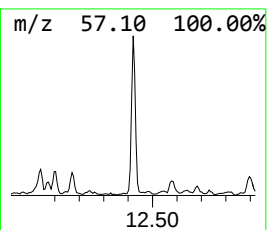
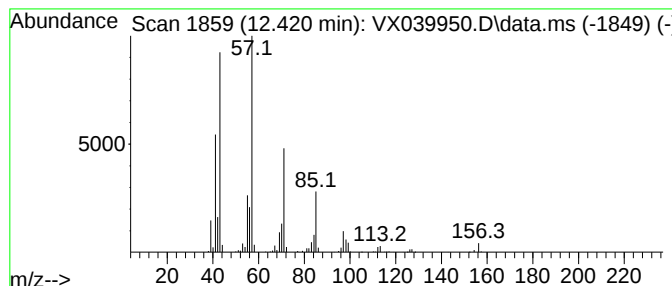
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Quant Title : SW846 8260

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

Peak Number 8 Carbonic acid, prop-1-en-2-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.420	18.00 ug/l	189126	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	90
2			Undecane	156	C11H24	001120-21-4	87
3			Decane	142	C10H22	000124-18-5	86
4			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	78
5			Tridecane	184	C13H28	000629-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039950.D
Acq On : 25 Jan 2024 13:47
Operator : JC/MD
Sample : P1235-07
Misc : 5.07g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
131

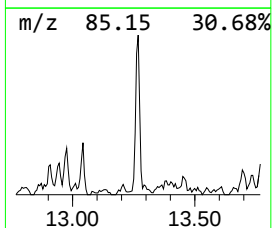
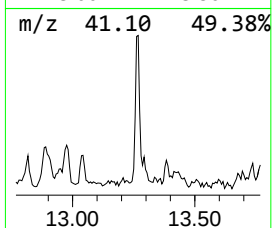
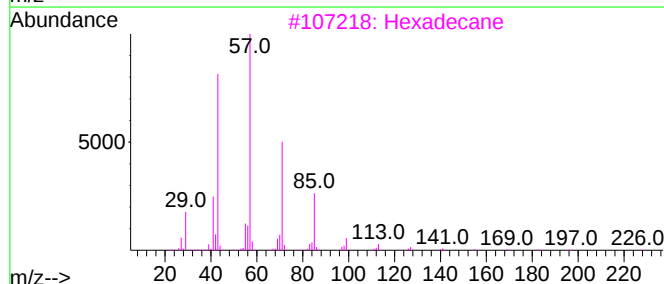
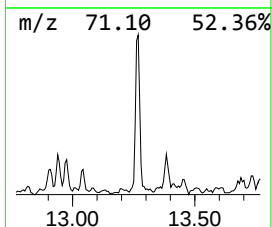
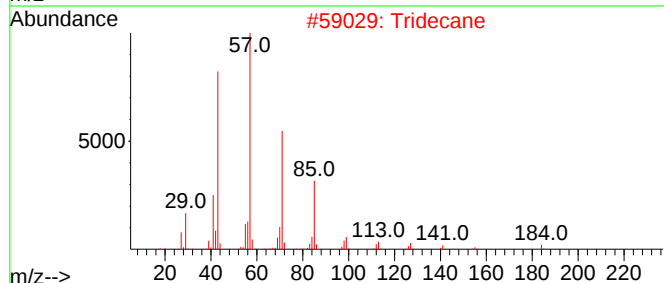
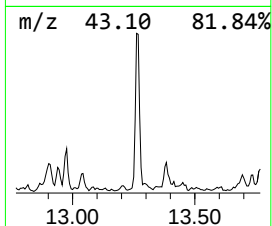
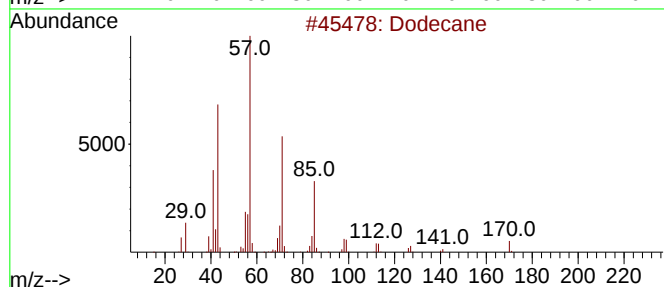
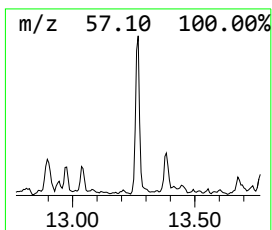
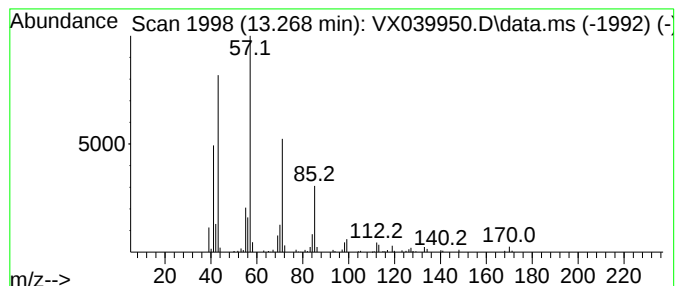
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Quant Title : SW846 8260

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

Peak Number 9 Dodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	9.13 ug/l	95957	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	95
2			Tridecane	184	C13H28	000629-50-5	90
3			Hexadecane	226	C16H34	000544-76-3	90
4			Tetradecane	198	C14H30	000629-59-4	90
5			Undecane	156	C11H24	001120-21-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039950.D
Acq On : 25 Jan 2024 13:47
Operator : JC/MD
Sample : P1235-07
Misc : 5.07g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
131

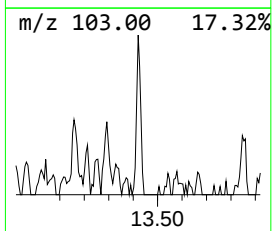
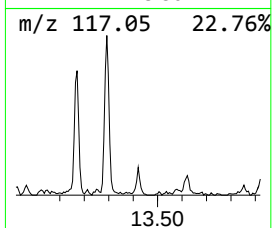
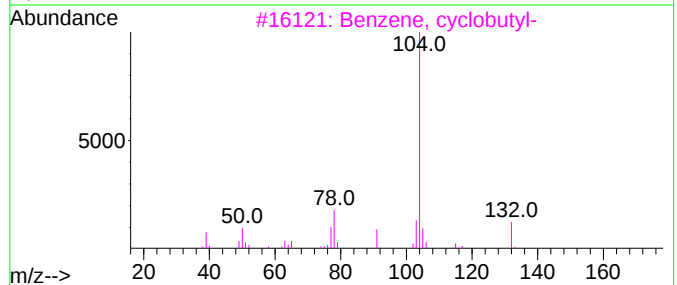
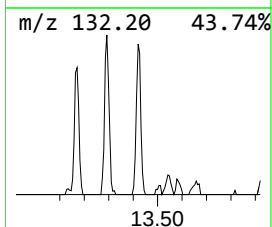
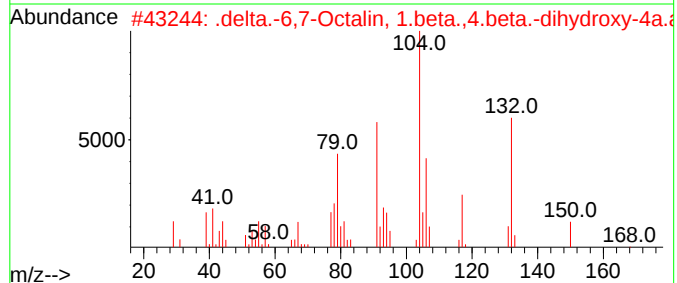
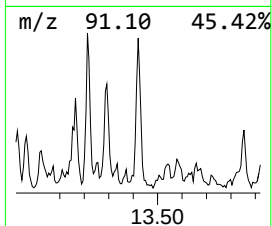
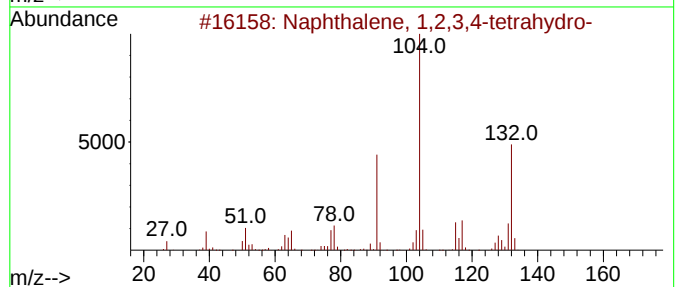
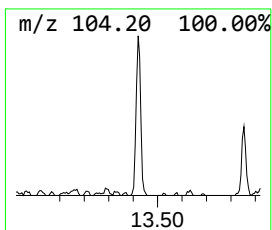
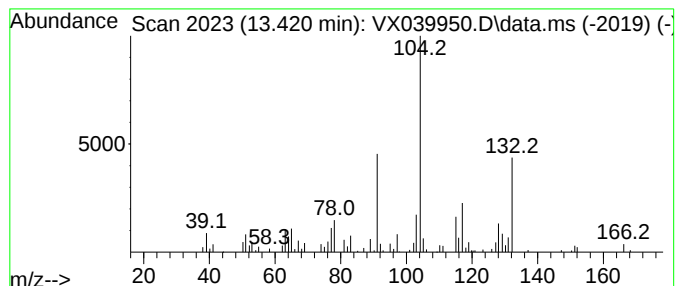
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	6.48 ug/l	68039	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	76
2			.delta.-6,7-Octalin, 1.beta.,4.b...	168	C10H16O2	051921-13-2	59
3			Benzene, cyclobutyl-	132	C10H12	004392-30-7	53
4			Indan, epoxide	132	C9H8O	000768-22-9	40
5			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
Data File : VX039950.D
Acq On : 25 Jan 2024 13:47
Operator : JC/MD
Sample : P1235-07
Misc : 5.07g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
131

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.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
Hexane, 3-methyl-	5.812	59.2	ug/l	446742	1	5.544	377529	50.0
1-Butanol, 2-et...	6.178	8.3	ug/l	65722	2	6.757	397601	50.0
Heptane	6.598	76.7	ug/l	609896	2	6.757	397601	50.0
Nonane	10.360	14.7	ug/l	137876	3	10.055	467846	50.0
Benzene, 1-ethy...	11.378	15.8	ug/l	165422	4	12.024	525228	50.0
Benzene, 1-ethy...	11.616	7.0	ug/l	74033	4	12.024	525228	50.0
Carbonic acid, ...	12.420	18.0	ug/l	189126	4	12.024	525228	50.0
Dodecane	13.268	9.1	ug/l	95957	4	12.024	525228	50.0
Naphthalene, 1,...	13.420	6.5	ug/l	68039	4	12.024	525228	50.0