

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041525\
 Data File : VX045790.D
 Acq On : 15 Apr 2025 11:40
 Operator : JC/MD
 Sample : Q1795-02 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31125

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\82X040225W.M
 Title : SW846 8260

Signal : TIC: VX045790.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	55	59	67	rBV	10841	14522	1.01%	0.276%
2	1.624	70	88	92	rBV5	5897	24485	1.70%	0.466%
3	2.075	154	162	170	rBV	17215	27283	1.90%	0.519%
4	2.380	207	212	225	rVB	12531	23419	1.63%	0.446%
5	5.379	692	704	720	rBV2	55833	166799	11.60%	3.175%
6	5.544	721	731	747	rVV2	81341	230623	16.04%	4.389%
7	5.952	788	798	809	rBV	66061	178506	12.41%	3.397%
8	6.757	921	930	944	rBV	142935	342833	23.84%	6.525%
9	7.458	1040	1045	1060	rBV	15192	36360	2.53%	0.692%
10	7.580	1060	1065	1079	rVB3	8672	20606	1.43%	0.392%
11	8.647	1233	1240	1249	rBV	301540	475162	33.05%	9.043%
12	10.049	1465	1470	1485	rBV	312260	429995	29.90%	8.184%
13	10.305	1507	1512	1524	rVB3	17425	38575	2.68%	0.734%
14	10.409	1524	1529	1540	rBV	43034	65209	4.54%	1.241%
15	10.585	1554	1558	1564	rBV2	10058	17498	1.22%	0.333%
16	10.652	1564	1569	1580	rVB2	24550	40998	2.85%	0.780%
17	10.902	1605	1610	1614	rBV	18834	25758	1.79%	0.490%
18	10.945	1614	1617	1620	rBV	11837	17943	1.25%	0.341%
19	11.079	1633	1639	1649	rBV	262494	330435	22.98%	6.289%
20	11.165	1649	1653	1663	rVB	17593	30135	2.10%	0.574%
21	11.482	1699	1705	1716	rVB5	22301	46521	3.24%	0.885%
22	11.756	1746	1750	1755	rVV	21245	28379	1.97%	0.540%
23	12.018	1788	1793	1800	rVB	307081	382429	26.60%	7.278%
24	12.219	1821	1826	1833	rBV	33151	57402	3.99%	1.092%
25	12.408	1853	1857	1866	rBV	121156	158616	11.03%	3.019%
26	12.804	1915	1922	1930	rBV3	20911	44257	3.08%	0.842%
27	12.890	1930	1936	1942	rVV5	10751	26924	1.87%	0.512%
28	12.969	1946	1949	1954	rVV4	20022	32130	2.23%	0.612%
29	13.292	1994	2002	2007	rBV5	15988	31182	2.17%	0.593%
30	13.347	2007	2011	2014	rVV5	12065	17731	1.23%	0.337%
31	13.384	2014	2017	2020	rVV	35015	44066	3.06%	0.839%
32	13.414	2020	2022	2032	rVB6	16590	41544	2.89%	0.791%
33	13.682	2060	2066	2067	rBV2	10933	16740	1.16%	0.319%
34	13.731	2071	2074	2076	rVV2	18206	24058	1.67%	0.458%
35	13.774	2076	2081	2088	rVV	1167971	1437878	100.00%	27.366%
36	13.841	2088	2092	2094	rVV3	30120	46799	3.25%	0.891%

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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

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Title : SW846 8260

37	13.865	2094	2096	2100	rVB	41885	47415	3.30%	0.902%
38	14.633	2214	2222	2231	rVB	89512	133483	9.28%	2.540%
39	14.780	2239	2246	2253	rVB	72749	99557	6.92%	1.895%

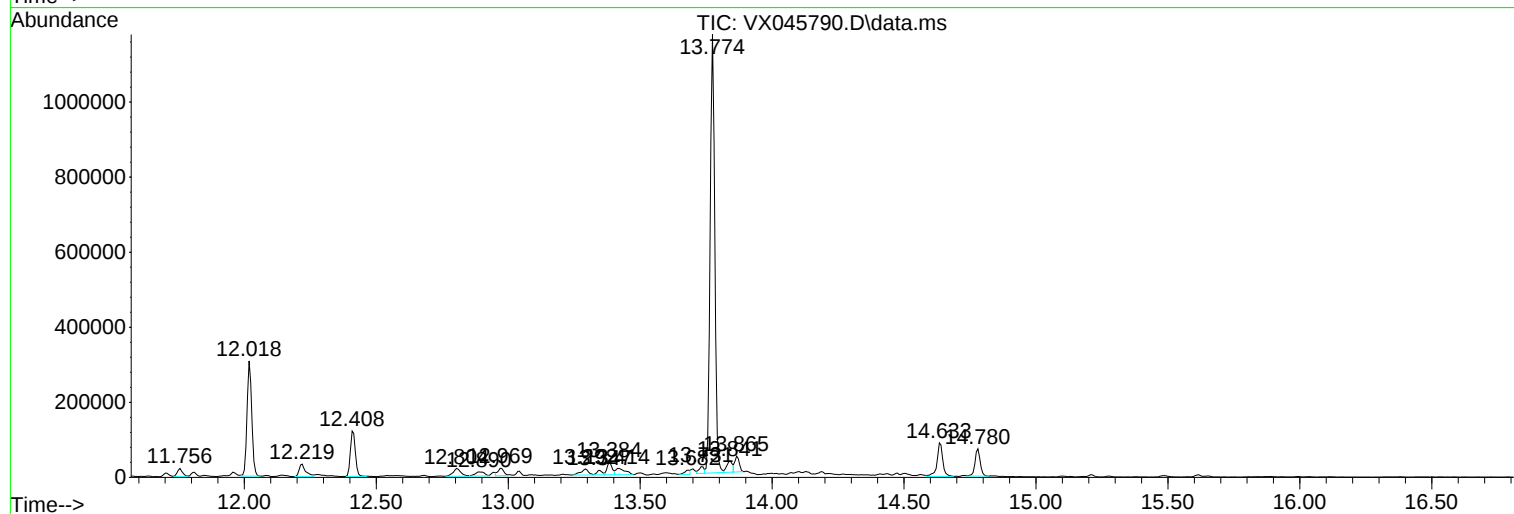
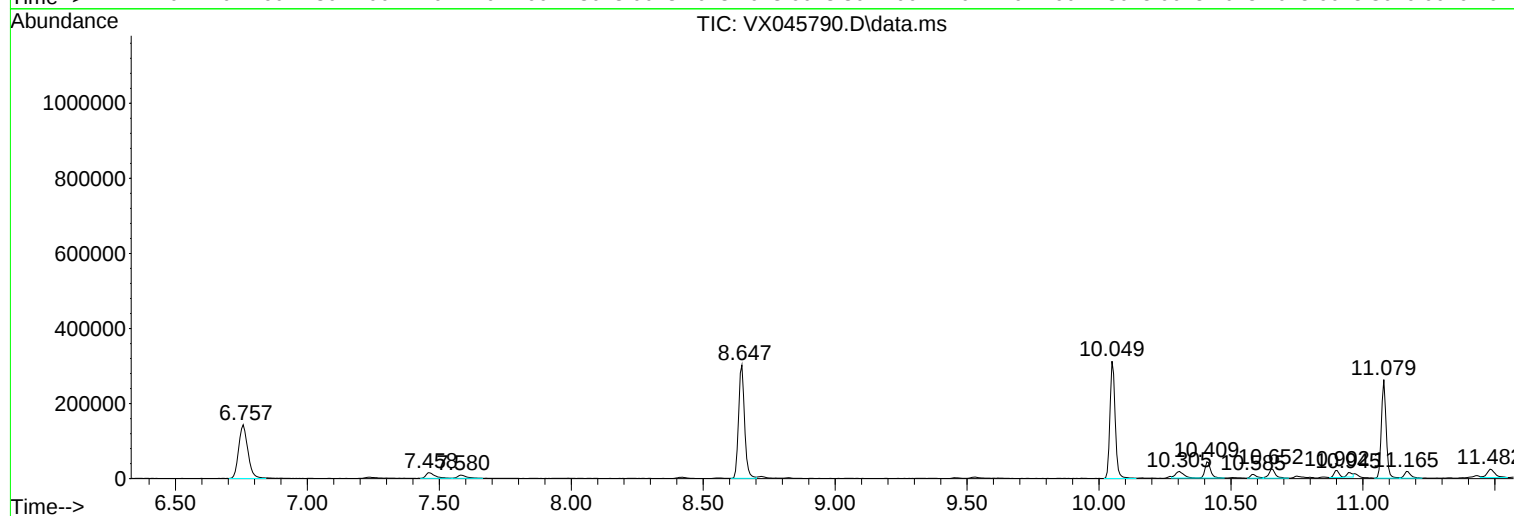
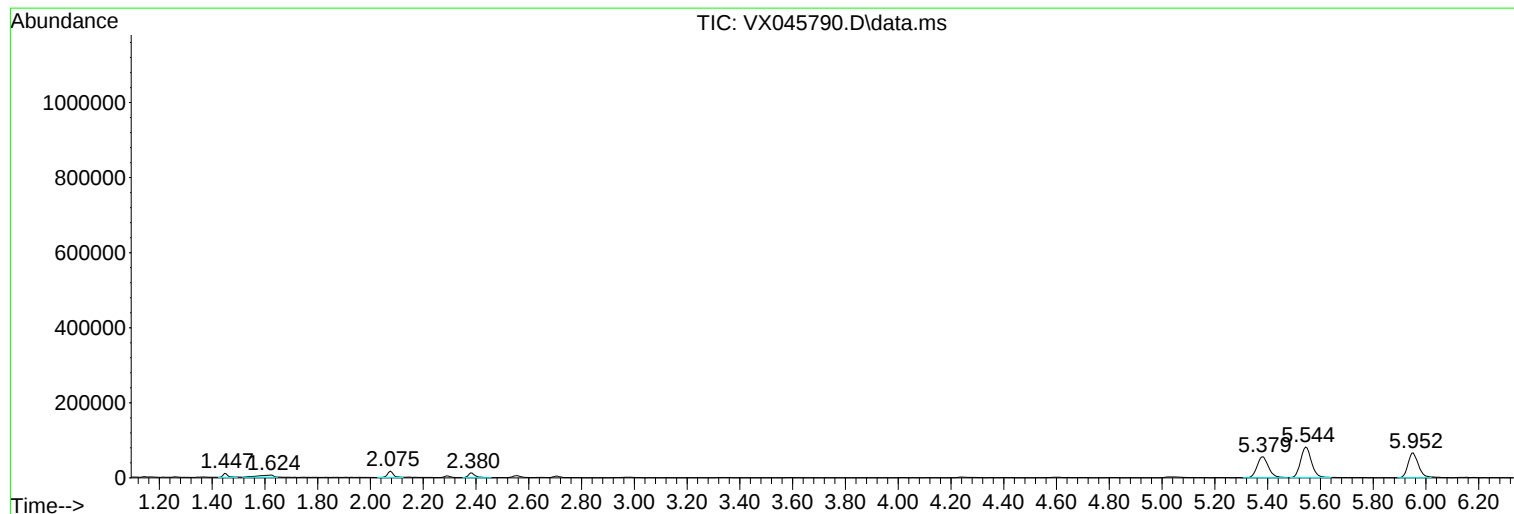
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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



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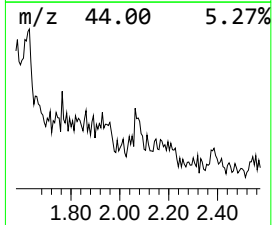
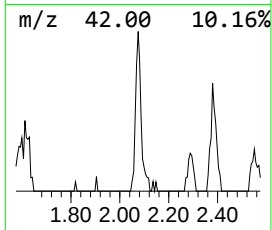
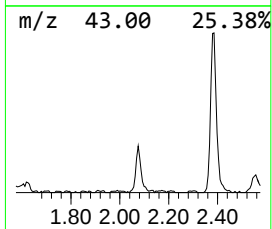
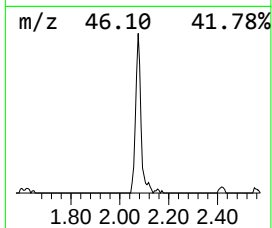
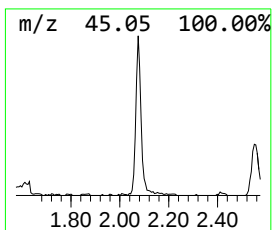
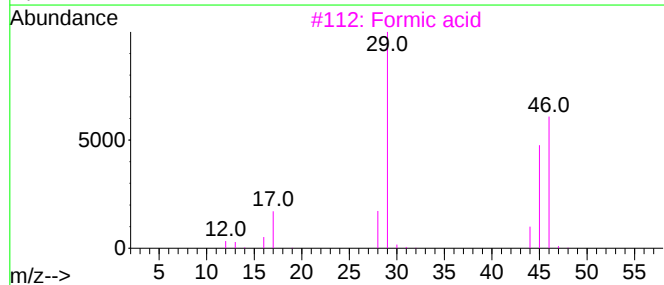
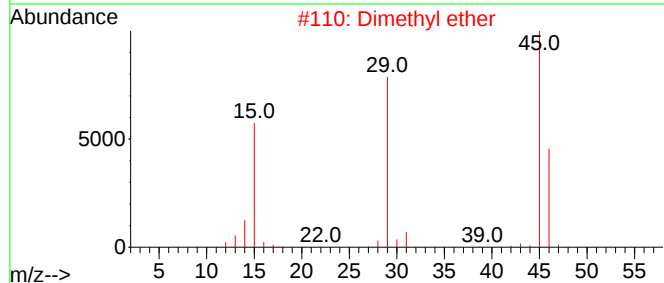
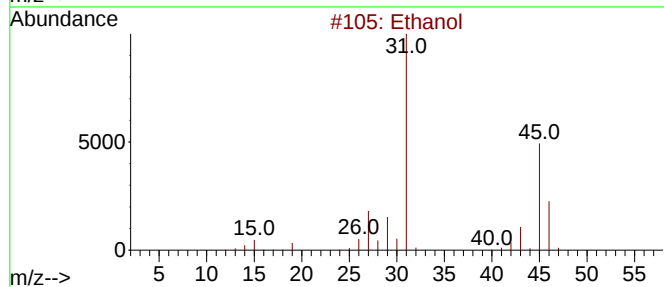
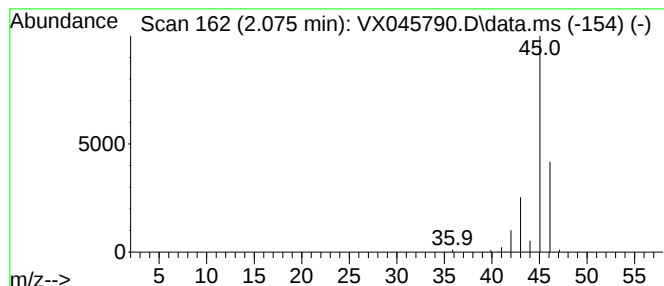
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.075	5.92 ug/l	27283	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Formic acid	46	CH2O2	000064-18-6	5
4			Methane, nitroso-	45	CH3NO	000865-40-7	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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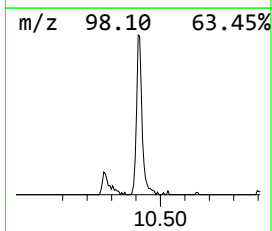
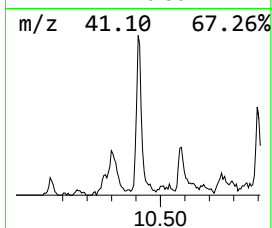
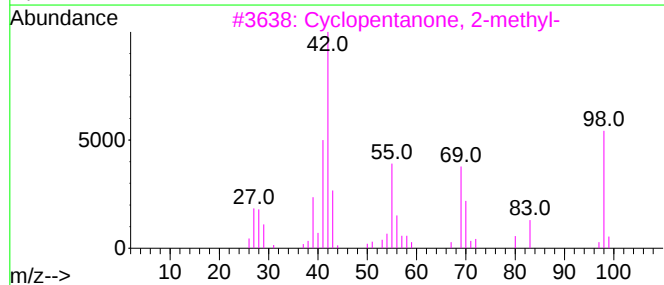
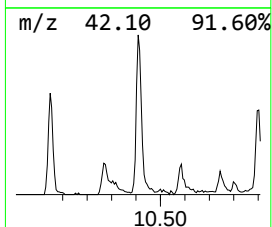
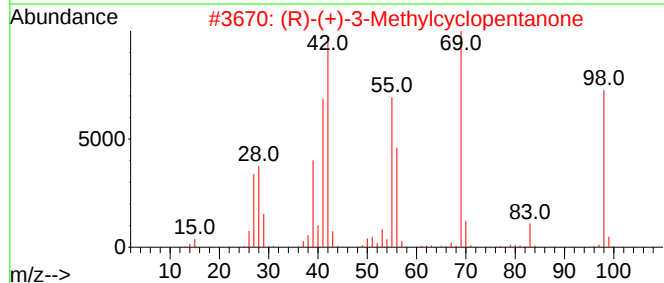
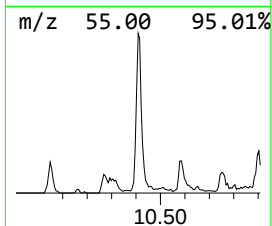
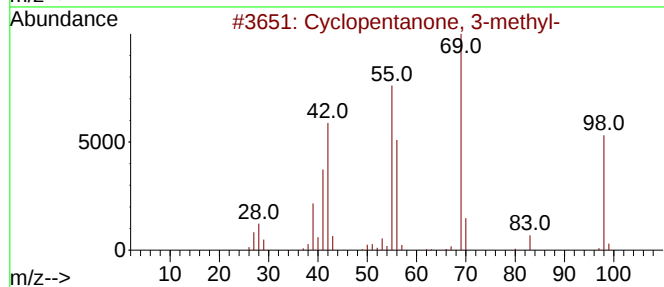
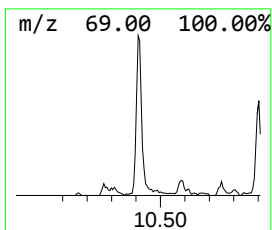
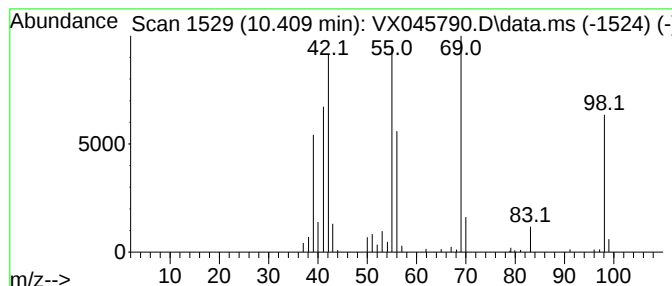
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Quant Title : SW846 8260

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

Peak Number 2 Cyclopentanone, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.409	7.58 ug/l	65209	Chlorobenzene-d5	10.049

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	87
2			(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	87
3			Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	53
4			1H-Tetrazole, 1,5-dimethyl-	98	C3H6N4	005144-11-6	53
5			Cyclobutanone, 2-ethyl-	98	C6H10O	010374-14-8	53



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ClientSampleId :
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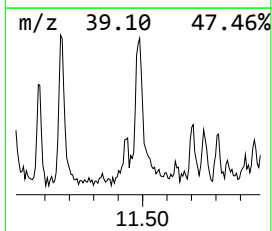
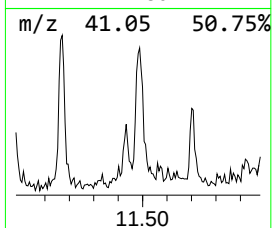
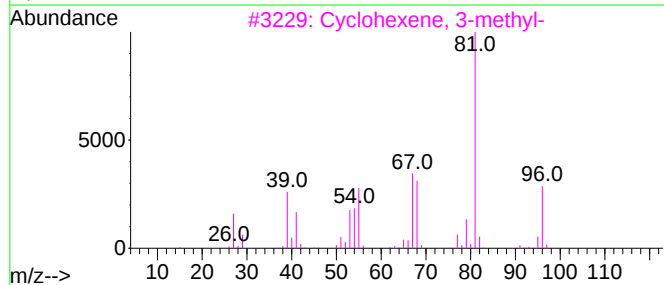
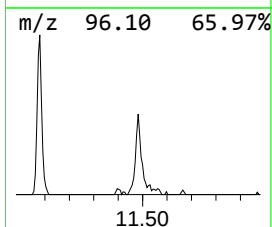
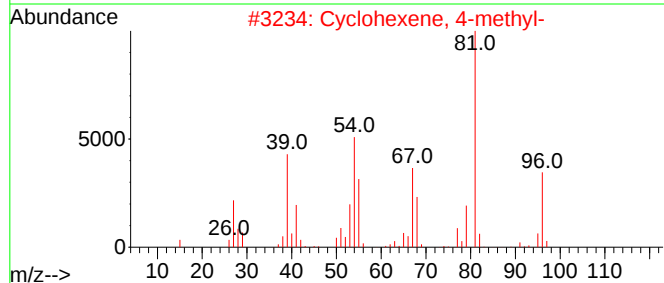
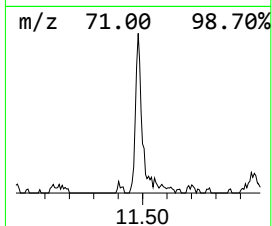
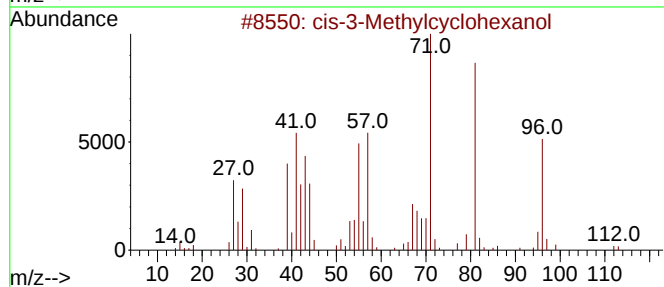
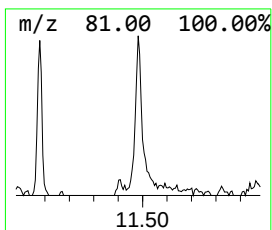
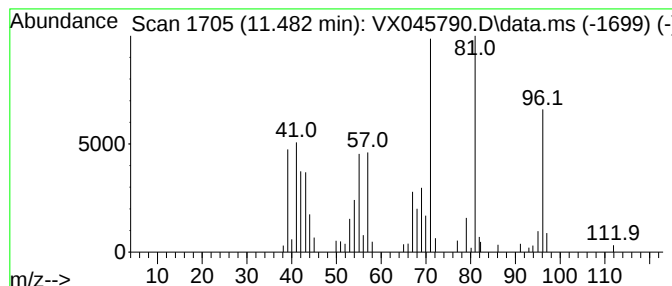
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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

Peak Number 3 cis-3-Methylcyclohexanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.482	6.08 ug/l	46521	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-3-Methylcyclohexanol	114	C7H14O	005454-79-5	90
2			Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	53
3			Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	45
4			Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	41
5			Cyclohexanol, 3-methyl-	114	C7H14O	000591-23-1	38



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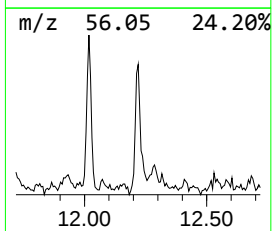
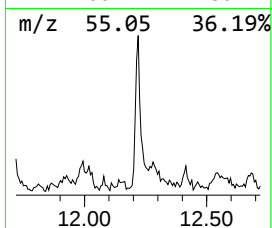
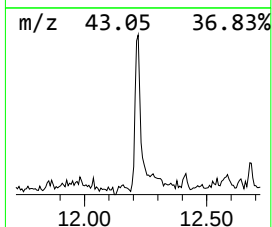
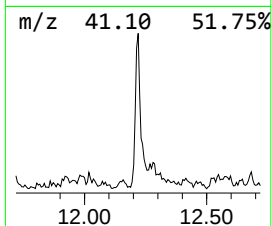
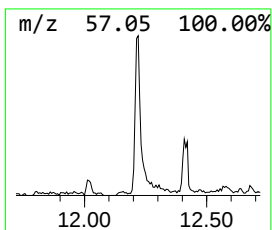
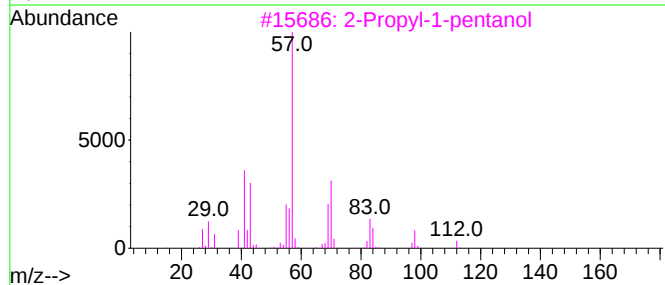
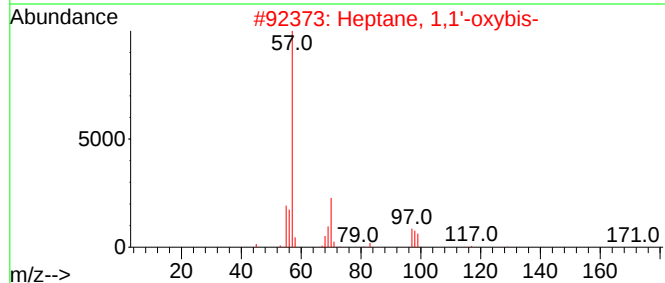
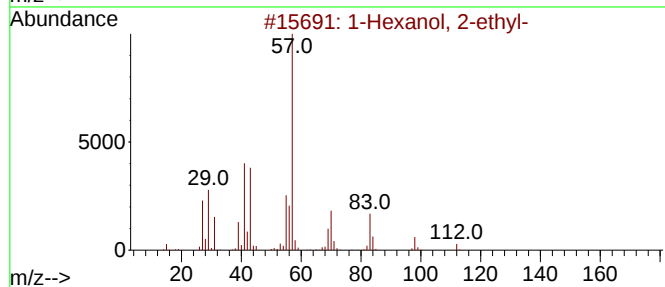
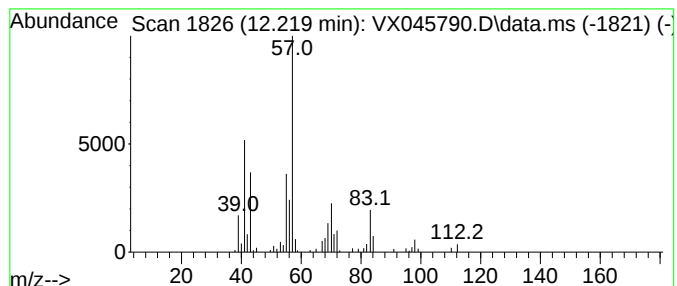
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	7.50 ug/l	57402	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4			Cycloheptane	98	C7H14	000291-64-5	43
5			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	43



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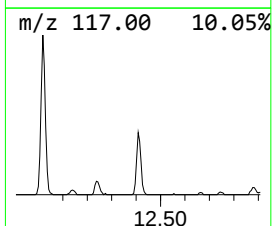
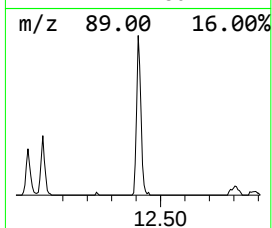
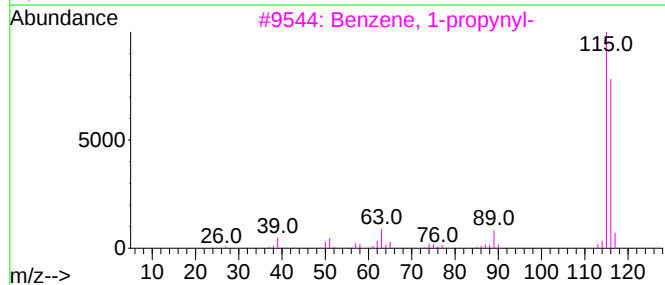
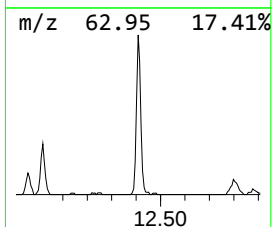
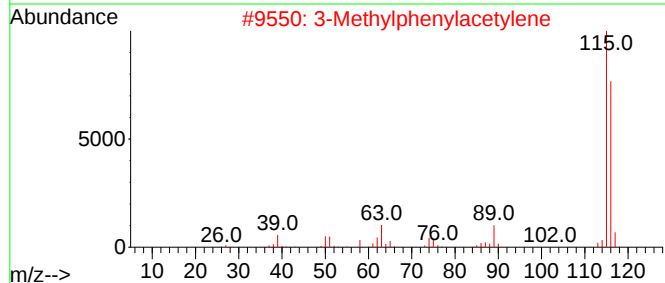
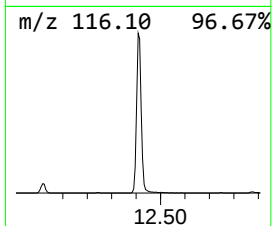
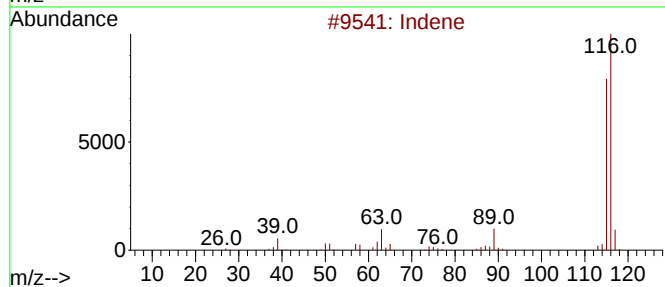
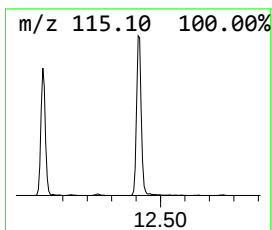
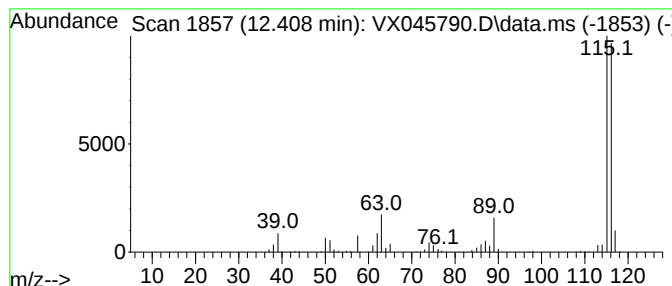
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Quant Title : SW846 8260

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

Peak Number 5 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.408	20.74 ug/l	158616	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	94
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041525\
Data File : VX045790.D
Acq On : 15 Apr 2025 11:40
Operator : JC/MD
Sample : Q1795-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31125

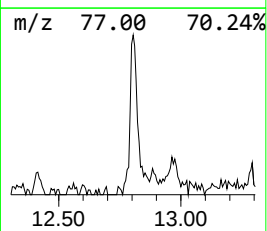
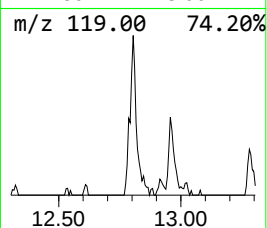
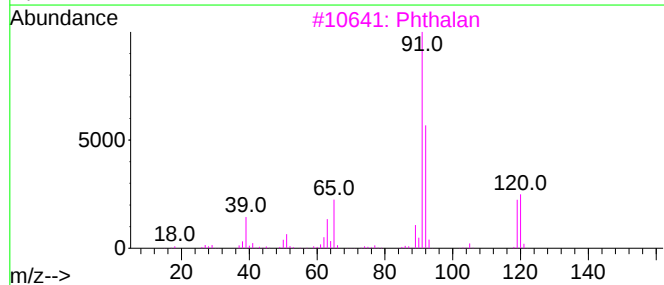
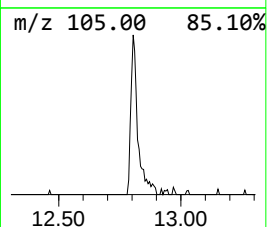
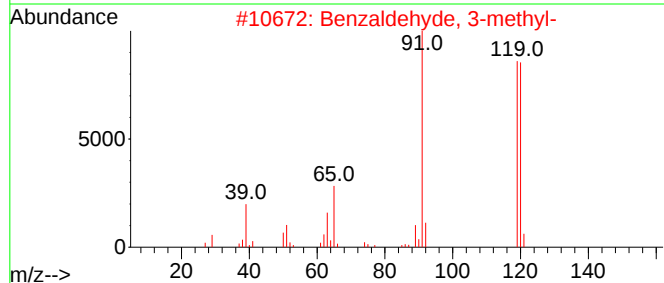
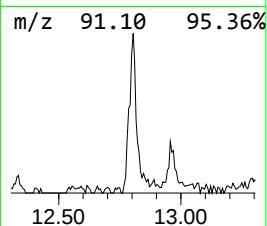
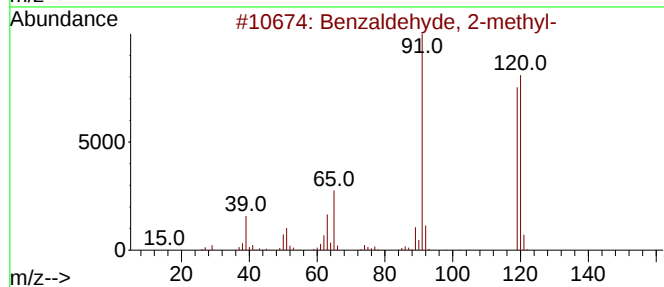
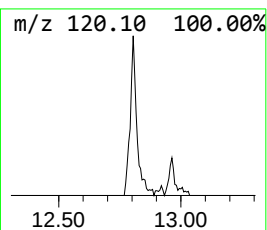
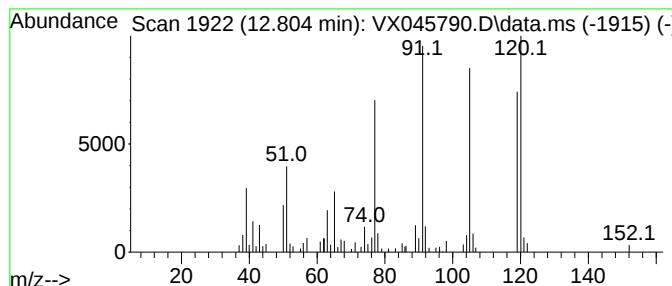
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Quant Title : SW846 8260

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

Peak Number 6 Benzaldehyde, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.805	5.79 ug/l	44257	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 2-methyl-	120	C8H8O	000529-20-4	94
2			Benzaldehyde, 3-methyl-	120	C8H8O	000620-23-5	90
3			Phthalan	120	C8H8O	000496-14-0	86
4			Benzaldehyde, 4-methyl-	120	C8H8O	000104-87-0	60
5			Benzofuran, 2,3-dihydro-	120	C8H8O	000496-16-2	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041525\
Data File : VX045790.D
Acq On : 15 Apr 2025 11:40
Operator : JC/MD
Sample : Q1795-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31125

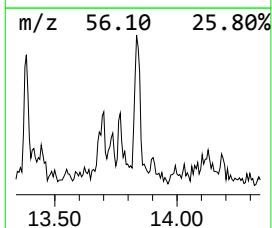
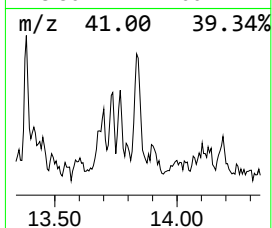
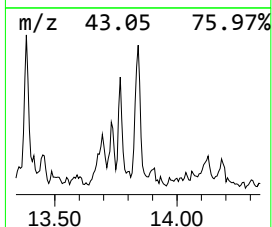
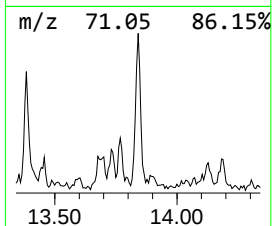
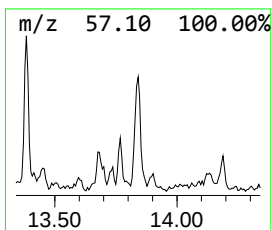
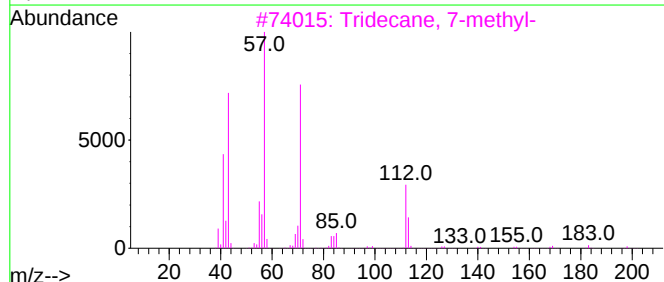
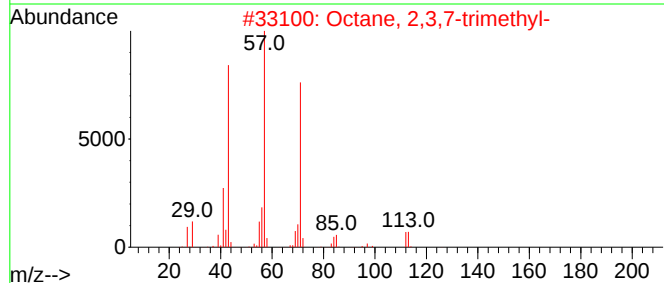
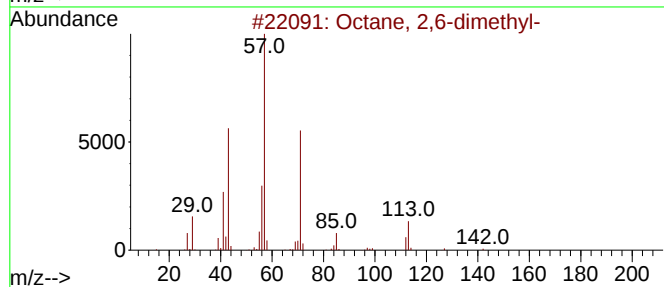
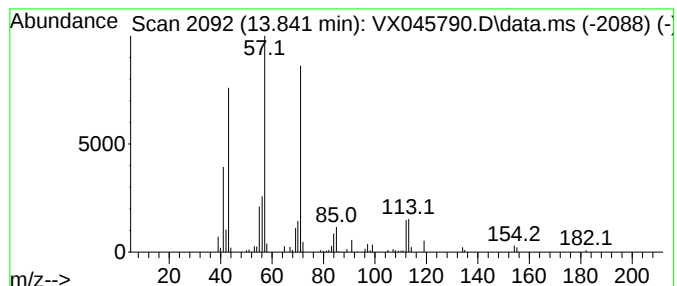
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Quant Title : SW846 8260

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

Peak Number 7 Octane, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.841	6.12 ug/l	46799	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	78
2			Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	72
3			Tridecane, 7-methyl-	198	C14H30	026730-14-3	64
4			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
5			Tetradecane	198	C14H30	000629-59-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041525\
Data File : VX045790.D
Acq On : 15 Apr 2025 11:40
Operator : JC/MD
Sample : Q1795-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31125

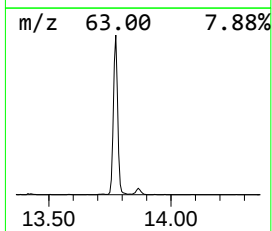
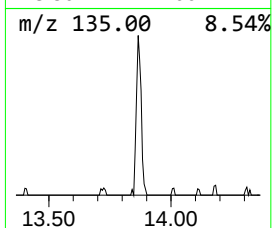
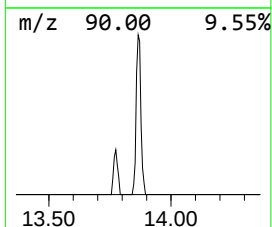
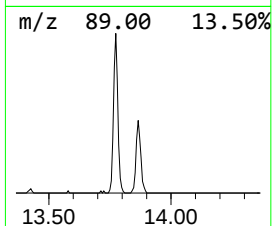
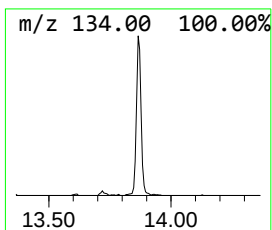
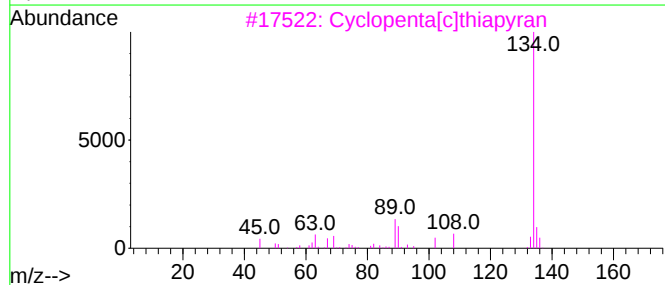
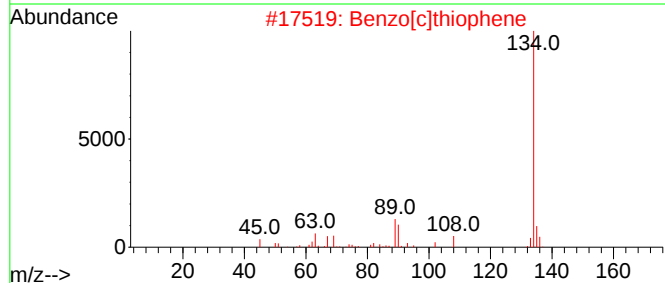
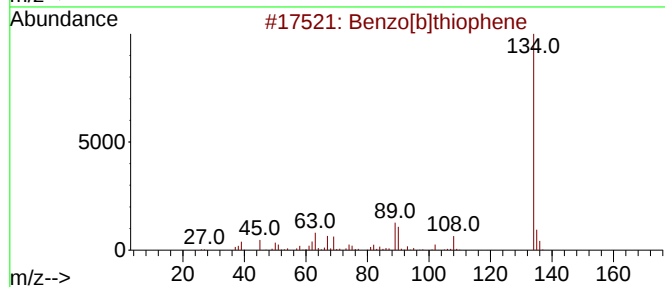
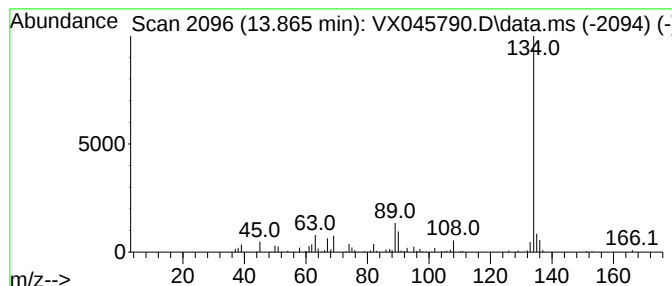
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Quant Title : SW846 8260

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

Peak Number 8 Benzo[b]thiophene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.865	6.20 ug/l	47415	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene	134	C8H6S	000095-15-8	95
2			Benzo[c]thiophene	134	C8H6S	000270-82-6	94
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	91
4			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	56
5			5-Phenyl-1,2,3-thiadiazole	162	C8H6N2S	018212-29-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041525\
Data File : VX045790.D
Acq On : 15 Apr 2025 11:40
Operator : JC/MD
Sample : Q1795-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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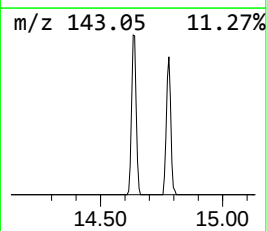
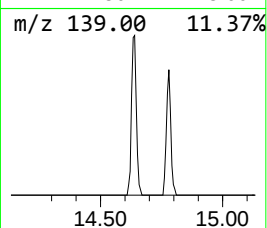
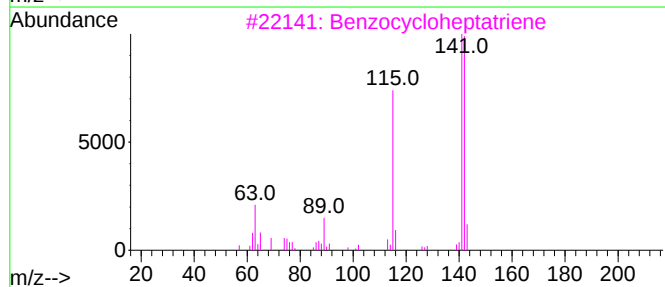
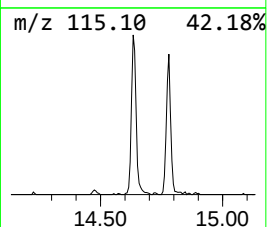
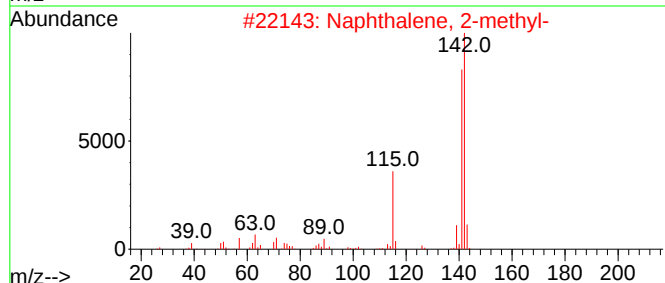
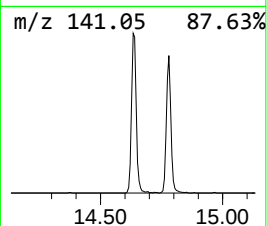
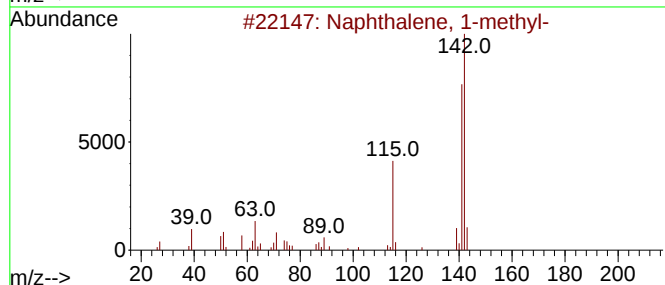
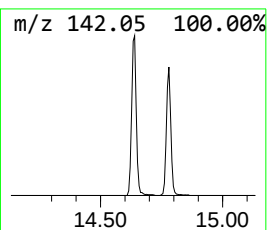
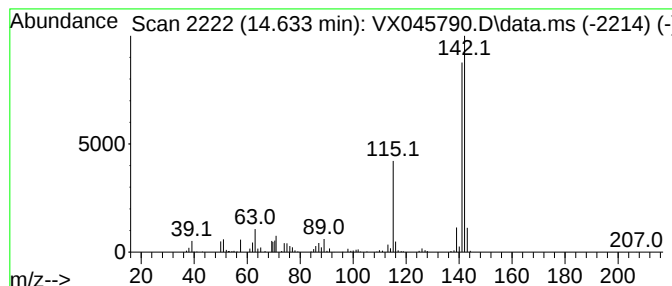
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	17.45 ug/l	133483	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041525\
Data File : VX045790.D
Acq On : 15 Apr 2025 11:40
Operator : JC/MD
Sample : Q1795-02 10X
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31125

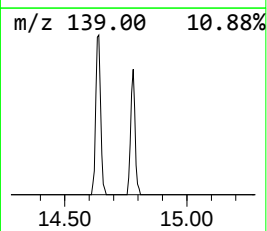
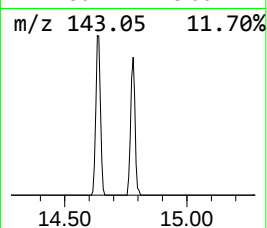
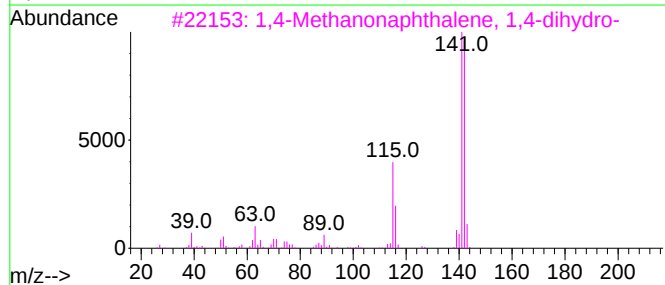
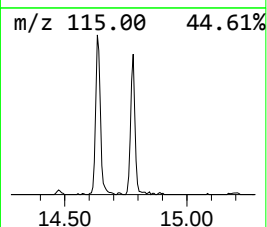
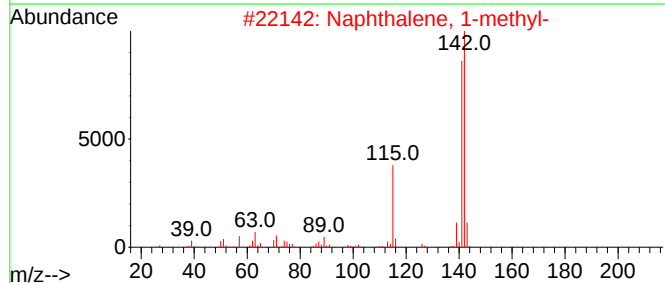
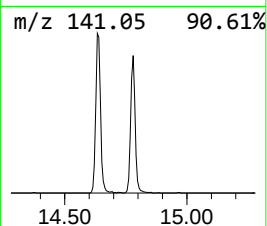
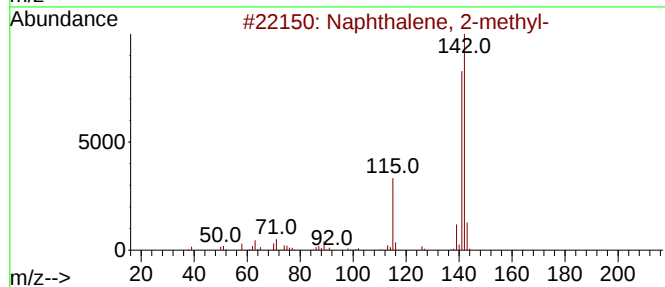
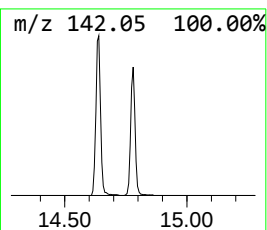
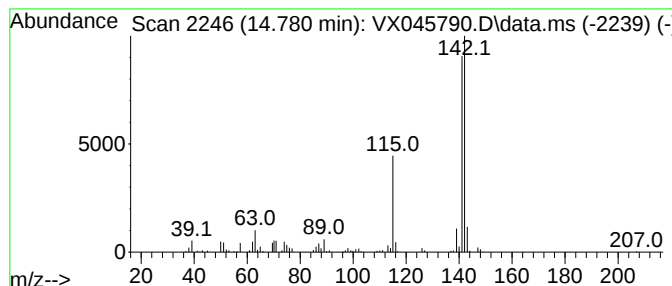
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	13.02 ug/l	99557	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041525\
Data File : VX045790.D
Acq On : 15 Apr 2025 11:40
Operator : JC/MD
Sample : Q1795-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31125

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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

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					#	RT	Resp	Conc
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Cyclopentanone,...	10.409	7.6	ug/l	65209	3	10.049	429995	50.0
cis-3-Methylcyc...	11.482	6.1	ug/l	46521	4	12.018	382429	50.0
1-Hexanol, 2-et...	12.219	7.5	ug/l	57402	4	12.018	382429	50.0
Indene	12.408	20.7	ug/l	158616	4	12.018	382429	50.0
Benzaldehyde, 2...	12.805	5.8	ug/l	44257	4	12.018	382429	50.0
Octane, 2,6-dim...	13.841	6.1	ug/l	46799	4	12.018	382429	50.0
Benzo[b]thiophene	13.865	6.2	ug/l	47415	4	12.018	382429	50.0
Naphthalene, 1-...	14.633	17.4	ug/l	133483	4	12.018	382429	50.0
Naphthalene, 2-...	14.780	13.0	ug/l	99557	4	12.018	382429	50.0