

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
 Data File : VX034759.D
 Acq On : 27 Mar 2023 18:55
 Operator : JC/MD
 Sample : 02073-01 400X
 Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TRE-1715

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\82X031023W.M
 Title : SW846 8260

Signal : TIC: VX034759.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	692	705	719	rBV	168911	487919	31.44%	3.445%
2	5.550	719	732	751	rVB2	303764	874944	56.38%	6.178%
3	5.952	788	798	815	rBV	199123	546794	35.23%	3.861%
4	6.763	921	931	955	rBV	471567	1150186	74.11%	8.122%
5	8.647	1233	1240	1249	rBV	1016038	1551969	100.00%	10.959%
6	8.720	1249	1252	1258	rVB4	13115	22148	1.43%	0.156%
7	10.055	1465	1471	1485	rVB	963078	1320612	85.09%	9.325%
8	10.360	1517	1521	1527	rVB	25760	32853	2.12%	0.232%
9	10.780	1582	1590	1594	rBV	42217	55501	3.58%	0.392%
10	10.853	1599	1602	1605	rVV3	15061	23586	1.52%	0.167%
11	10.896	1605	1609	1613	rVV	24678	34609	2.23%	0.244%
12	11.030	1628	1631	1634	rBV	18108	19686	1.27%	0.139%
13	11.079	1634	1639	1650	rVB	869287	1177762	75.89%	8.316%
14	11.189	1650	1657	1660	rBV	59518	87520	5.64%	0.618%
15	11.341	1677	1682	1685	rBV4	11269	19031	1.23%	0.134%
16	11.384	1686	1689	1693	rVV4	11747	17610	1.13%	0.124%
17	11.433	1693	1697	1700	rVV2	57957	89255	5.75%	0.630%
18	11.475	1700	1704	1711	rVB	491714	589549	37.99%	4.163%
19	11.634	1727	1730	1734	rVB2	29316	34897	2.25%	0.246%
20	11.683	1734	1738	1740	rBV2	34752	44008	2.84%	0.311%
21	11.713	1740	1743	1747	rVV	195895	213619	13.76%	1.508%
22	11.750	1747	1749	1753	rVV2	18800	25667	1.65%	0.181%
23	11.835	1758	1763	1766	rBV2	29159	46944	3.02%	0.331%
24	11.890	1766	1772	1777	rVV2	84101	131470	8.47%	0.928%
25	11.945	1777	1781	1784	rBV	93299	124277	8.01%	0.878%
26	11.975	1784	1786	1789	rVV2	43400	46118	2.97%	0.326%
27	12.018	1789	1793	1799	rVV	969043	1355234	87.32%	9.570%
28	12.073	1799	1802	1804	rVV	82759	90234	5.81%	0.637%
29	12.103	1804	1807	1811	rVB2	108089	130389	8.40%	0.921%
30	12.170	1811	1818	1825	rVB2	102033	183003	11.79%	1.292%
31	12.268	1825	1834	1837	rBV	48647	111071	7.16%	0.784%
32	12.317	1837	1842	1848	rBV5	80309	166554	10.73%	1.176%
33	12.420	1848	1859	1864	rBV	715897	946533	60.99%	6.684%
34	12.463	1864	1866	1873	rVB5	90302	149281	9.62%	1.054%
35	12.554	1874	1881	1883	rBV4	85872	161529	10.41%	1.141%
36	12.585	1883	1886	1890	rVB2	51482	73639	4.74%	0.520%

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Integrator: RTE

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Stop Thrs : 0

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

Peak separation: 5

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37	12.682	1898	1902	1905	rBV2	95013	116477	7.51%	0.822%
38	12.725	1905	1909	1913	rVV2	70724	130766	8.43%	0.923%
39	12.762	1913	1915	1917	rVV2	29296	36534	2.35%	0.258%
40	12.792	1917	1920	1922	rVV3	49769	78416	5.05%	0.554%
41	12.817	1922	1924	1930	rVB5	70518	98782	6.36%	0.698%
42	12.884	1930	1935	1943	rBV5	166071	371640	23.95%	2.624%
43	12.945	1943	1945	1946	rVV	36149	35798	2.31%	0.253%
44	12.975	1946	1950	1954	rVB3	81468	140228	9.04%	0.990%
45	13.042	1954	1961	1964	rBV4	61135	109113	7.03%	0.770%
46	13.158	1974	1980	1983	rVV4	57343	95110	6.13%	0.672%
47	13.213	1985	1989	1992	rVV2	54660	68717	4.43%	0.485%
48	13.268	1992	1998	2000	rVV3	107014	196316	12.65%	1.386%
49	13.292	2000	2002	2006	rVV3	91185	140369	9.04%	0.991%
50	13.329	2006	2008	2012	rVB	39265	46167	2.97%	0.326%
51	13.371	2012	2015	2020	rBV3	26961	30961	1.99%	0.219%
52	13.432	2020	2025	2032	rVB5	44264	108343	6.98%	0.765%
53	13.505	2032	2037	2040	rBV4	24021	39223	2.53%	0.277%
54	13.579	2045	2049	2055	rBV3	46204	92913	5.99%	0.656%
55	13.676	2060	2065	2074	rVB2	24610	49462	3.19%	0.349%
56	13.792	2079	2084	2088	rVV3	20330	40434	2.61%	0.286%

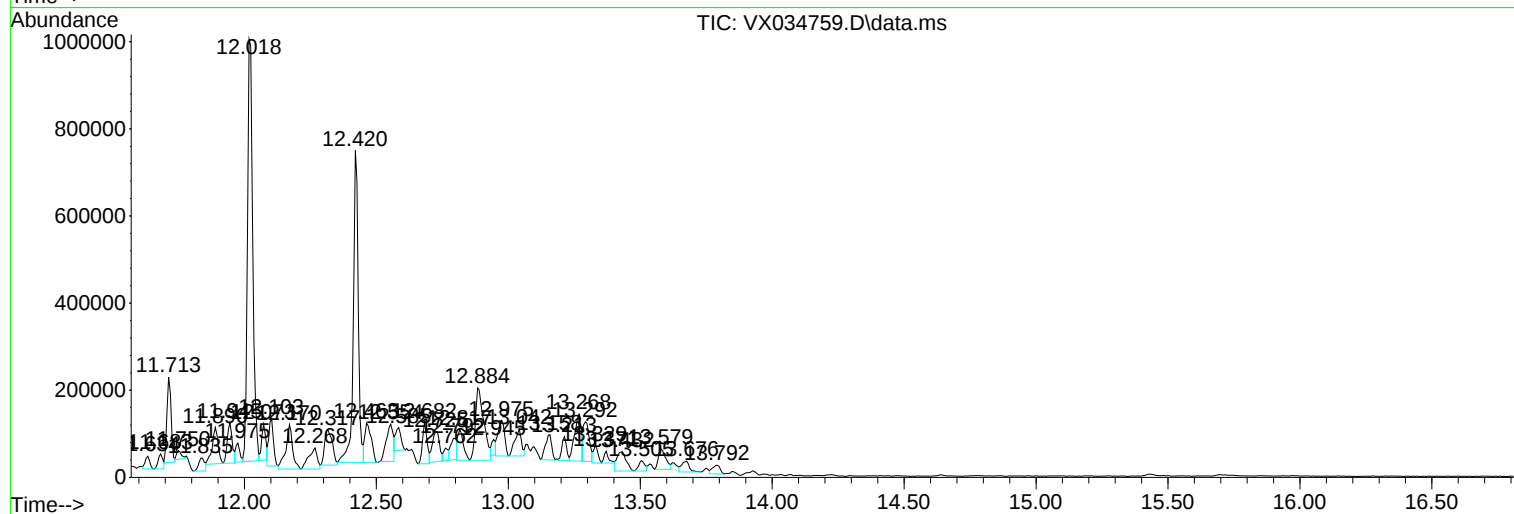
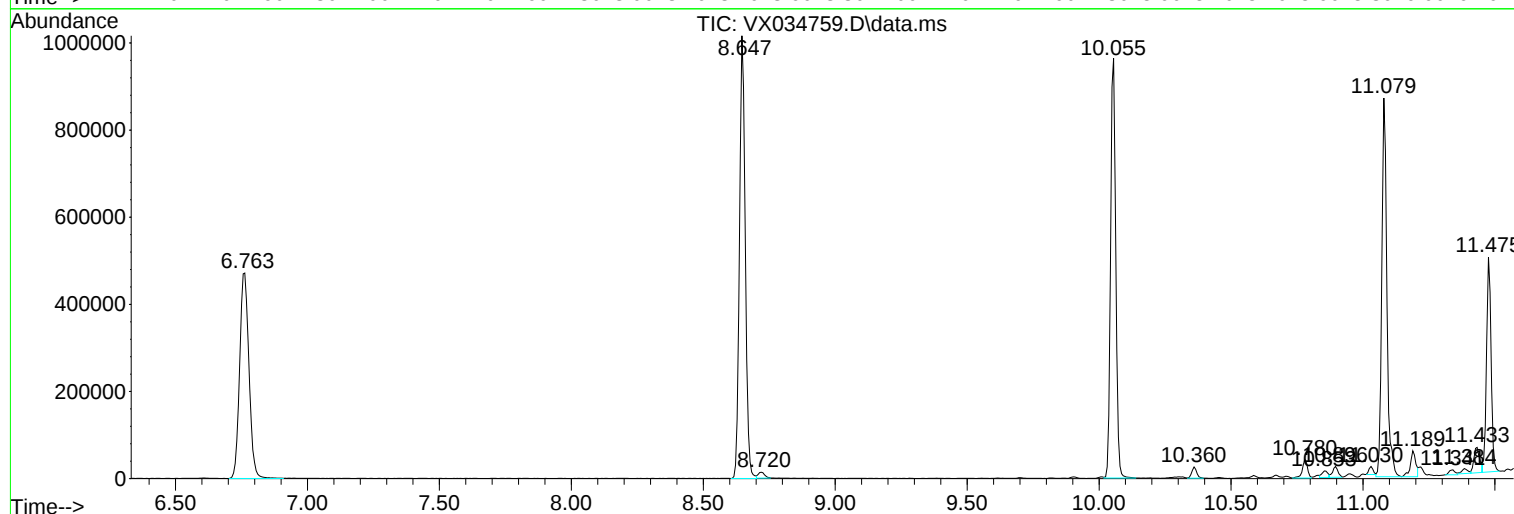
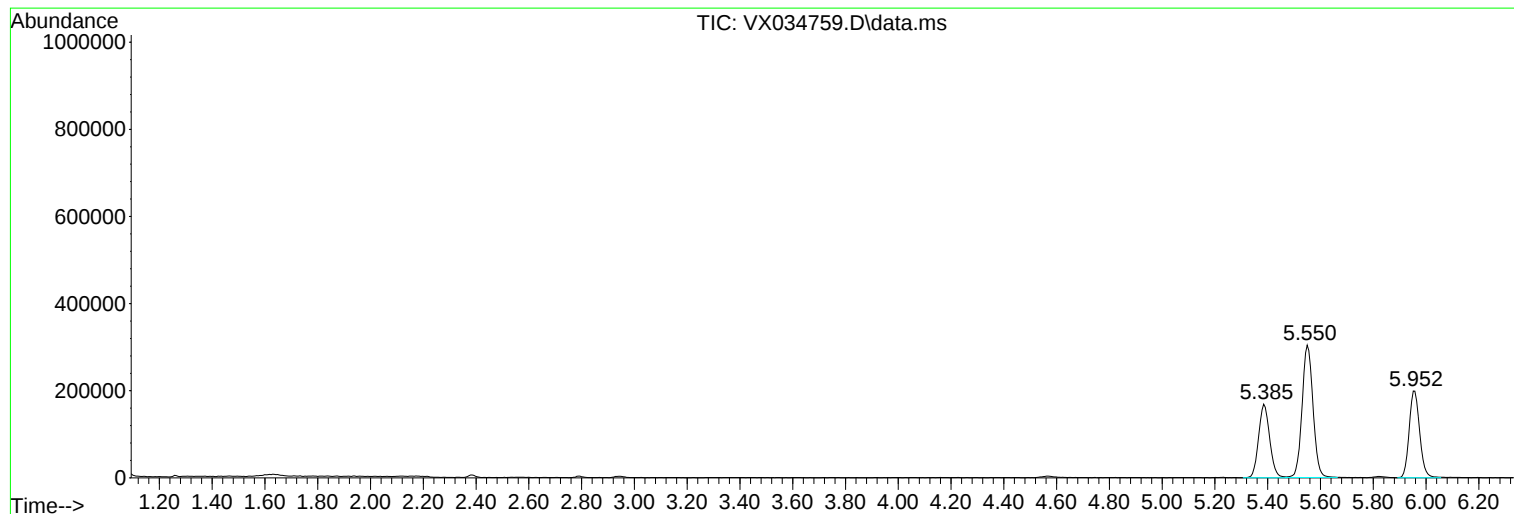
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_X
ClientSampleId :
TRE-1715

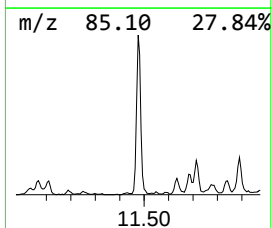
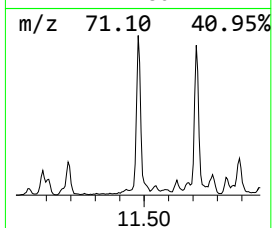
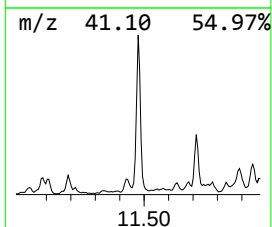
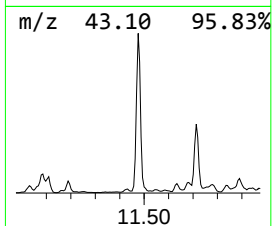
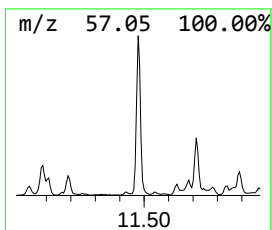
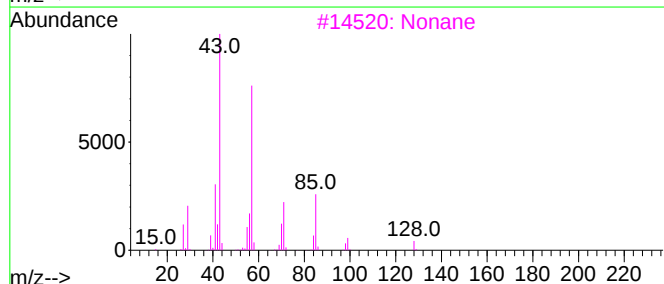
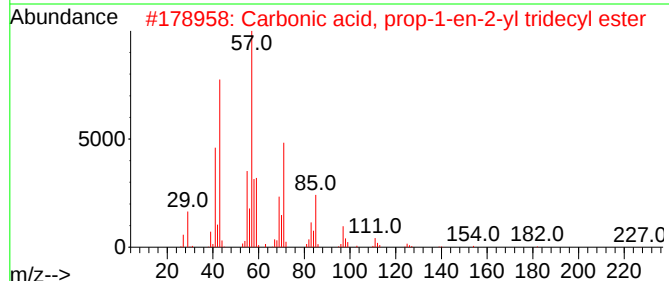
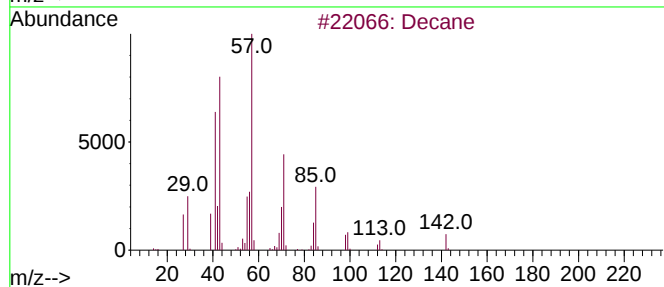
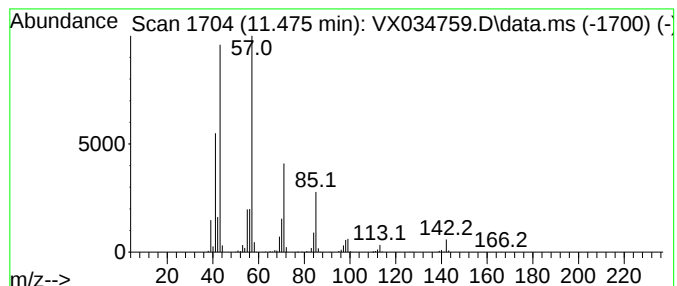
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

Peak Number 1 Decane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.475	21.75 ug/l	589549	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	94
2			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	83
3			Nonane	128	C9H20	000111-84-2	72
4			Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	64
5			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	64



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Instrument :
MSVOA_X
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TRE-1715

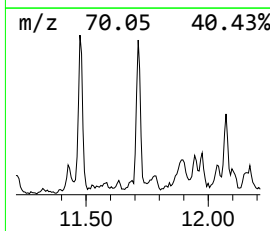
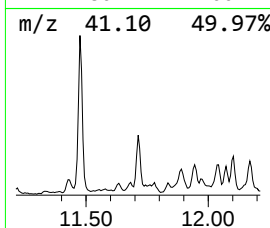
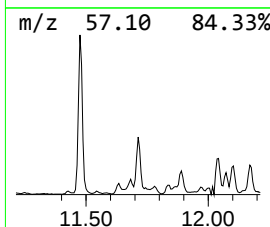
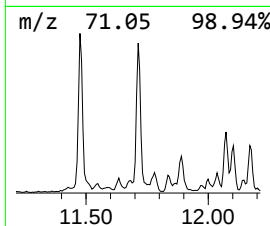
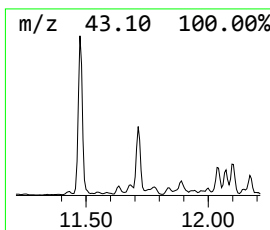
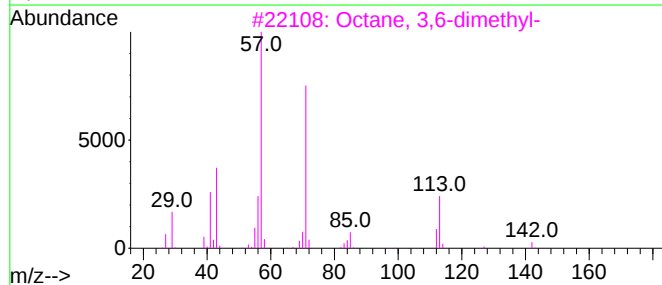
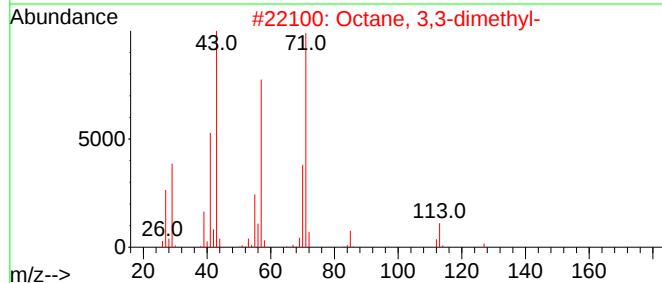
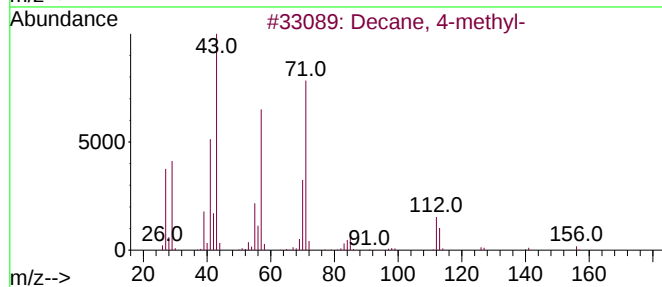
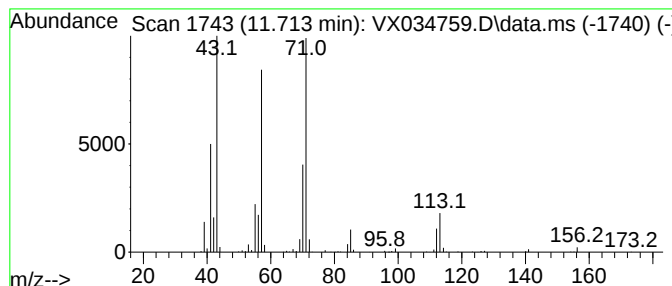
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

Peak Number 2 Decane, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.713	7.88 ug/l	213619	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 4-methyl-	156	C11H24	002847-72-5	87
2			Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	78
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
5			Dodecane, 4-methyl-	184	C13H28	006117-97-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
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Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-1715

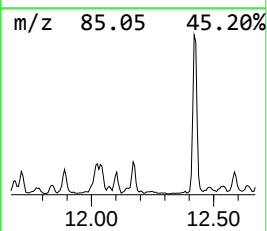
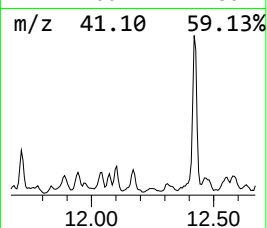
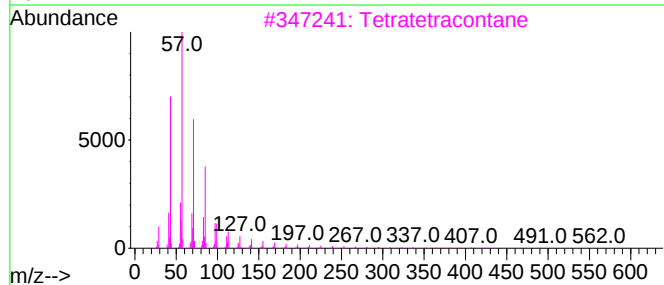
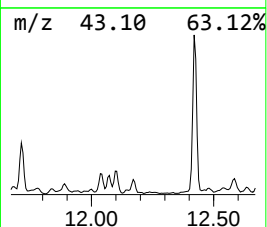
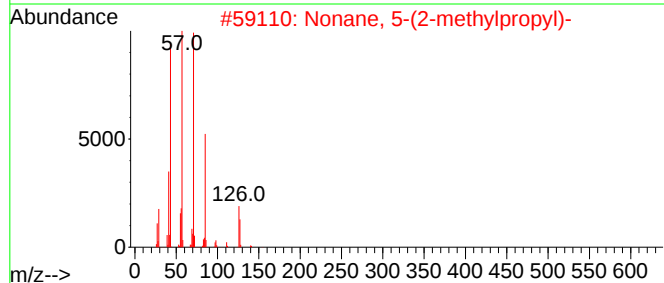
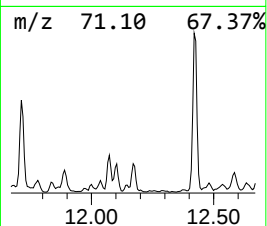
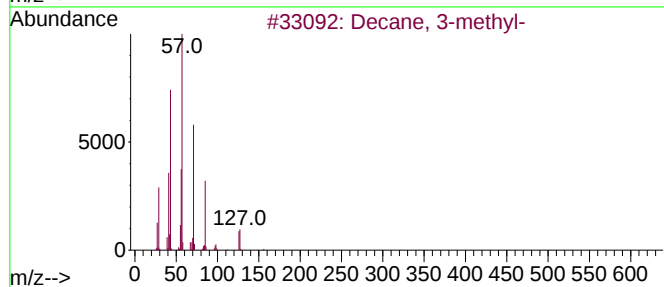
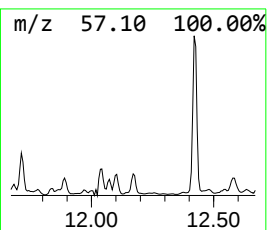
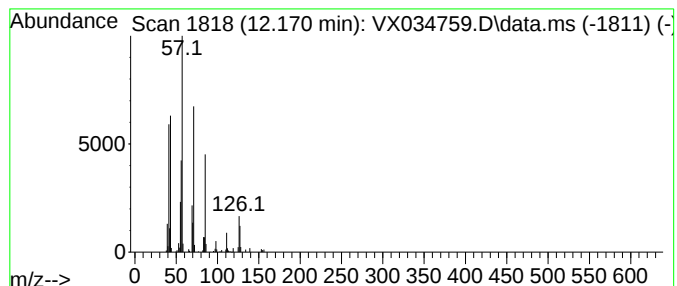
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

Peak Number 3 Decane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.170	6.75 ug/l	183003	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3-methyl-	156	C11H24	013151-34-3	87
2			Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	53
3			Tetratetracontane	619	C44H90	007098-22-8	53
4			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	47
5			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	46



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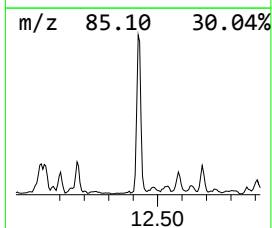
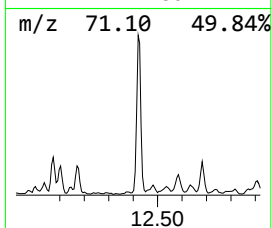
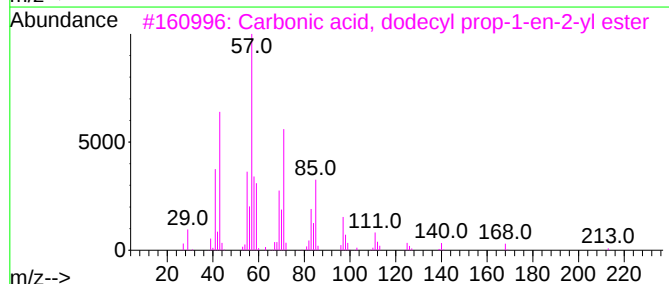
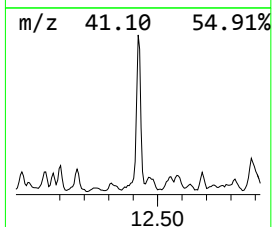
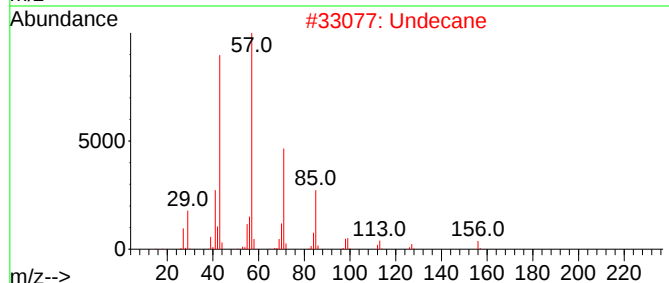
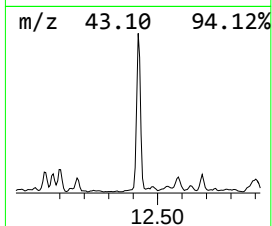
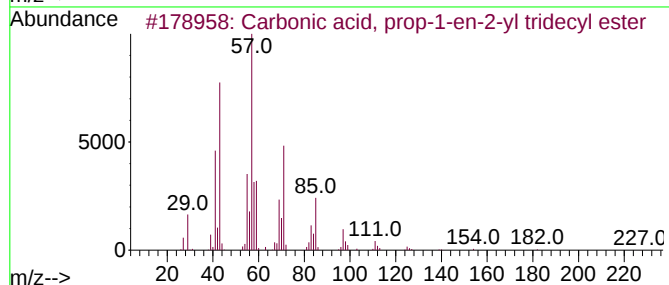
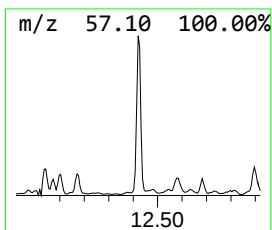
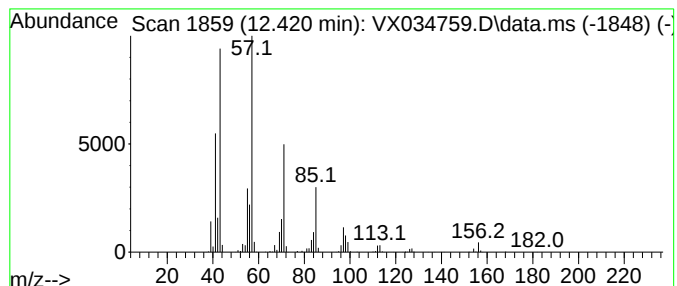
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

Peak Number 4 Carbonic acid, prop-1-en-2-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.420	34.92 ug/l	946533	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			Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	86
4			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	86
5			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	78



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ClientSampleId :
TRE-1715

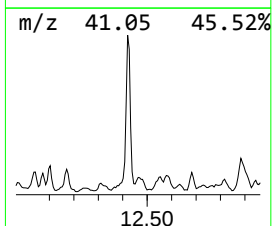
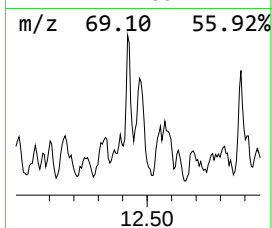
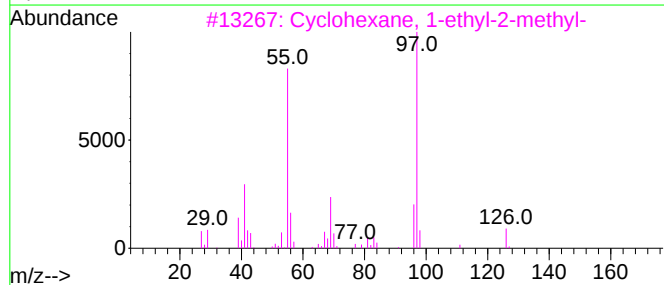
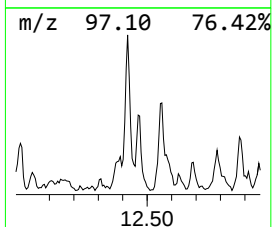
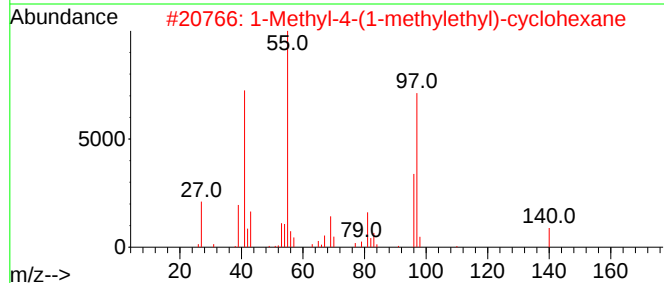
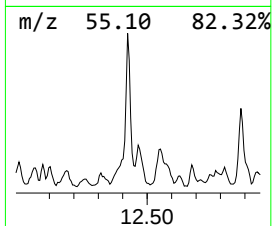
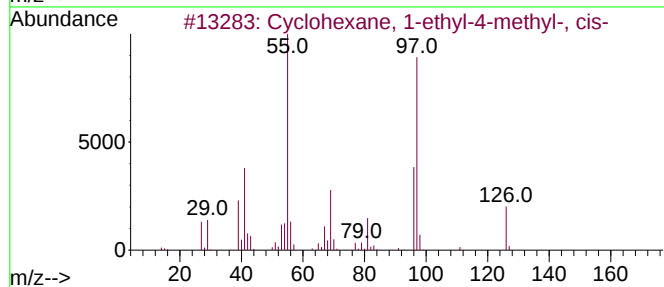
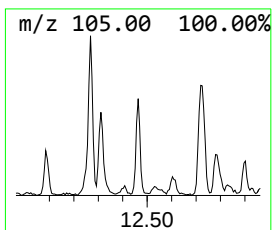
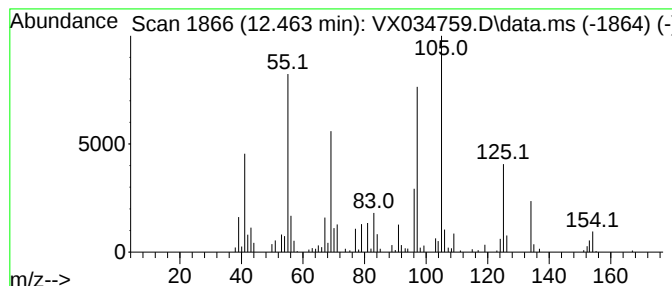
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Quant Title : SW846 8260

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

Peak Number 5 unknown12.463 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	5.51 ug/l	149281	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	45
2			1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	38
3			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	38
4			1'-Methyl-1,4'-bipiperidin-4-ami...	343	C14H22F5N3O	1000469-28-7	27
5			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034759.D
Acq On : 27 Mar 2023 18:55
Operator : JC/MD
Sample : 02073-01 400X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-1715

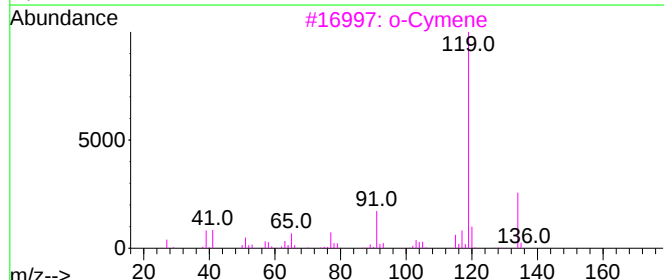
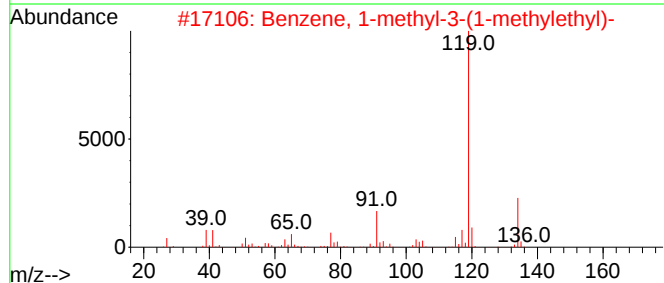
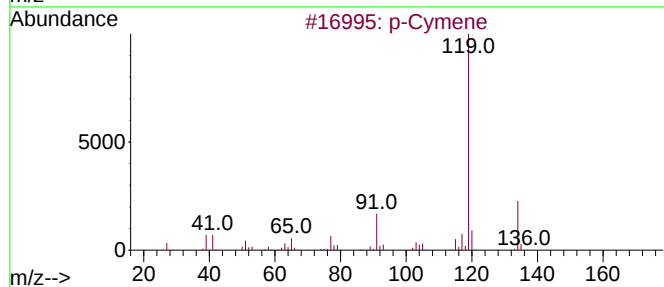
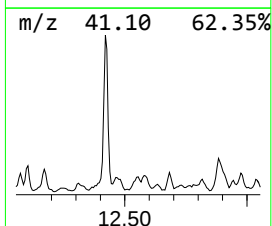
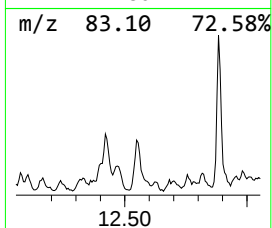
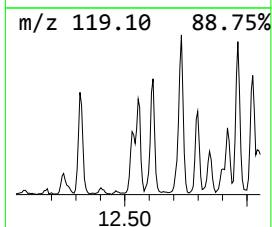
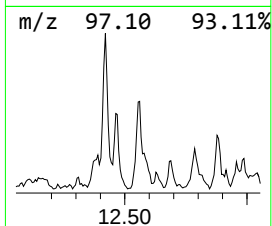
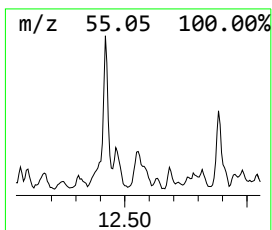
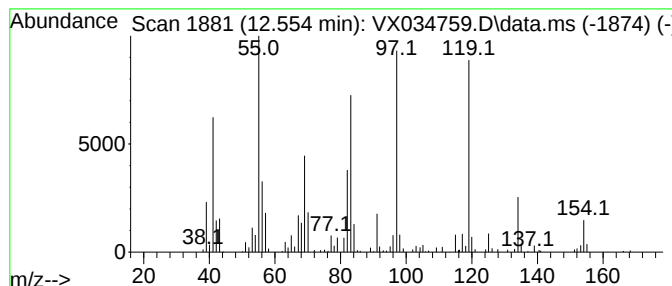
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Quant Title : SW846 8260

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

Peak Number 6 p-Cymene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.554	5.96 ug/l	161529	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		p-Cymene	134	C10H14	000099-87-6	68
2		Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	64
3		o-Cymene	134	C10H14	000527-84-4	64
4		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	35
5		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034759.D
Acq On : 27 Mar 2023 18:55
Operator : JC/MD
Sample : 02073-01 400X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-1715

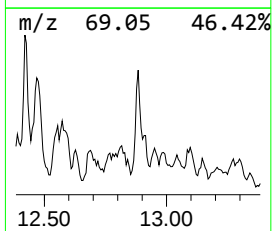
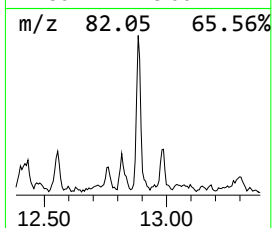
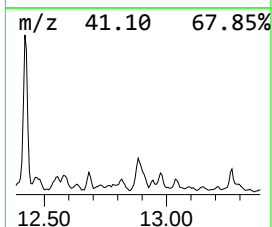
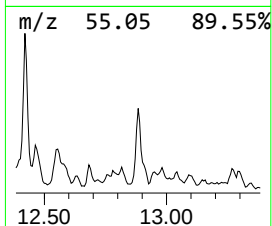
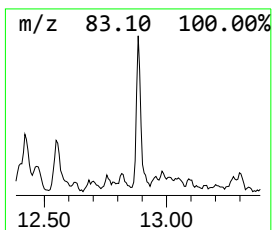
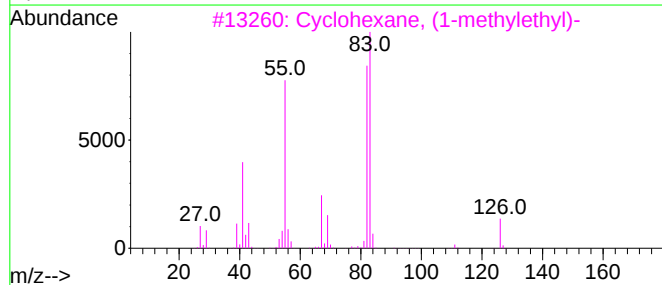
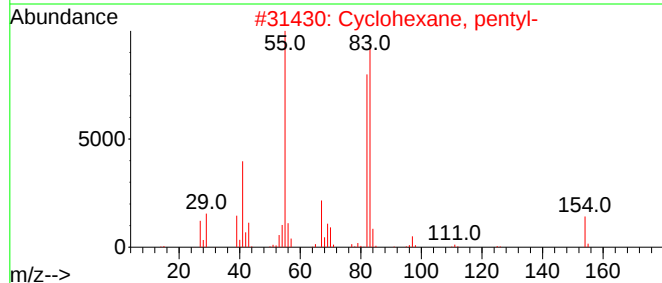
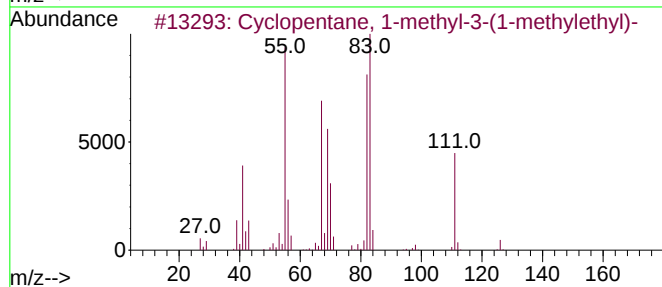
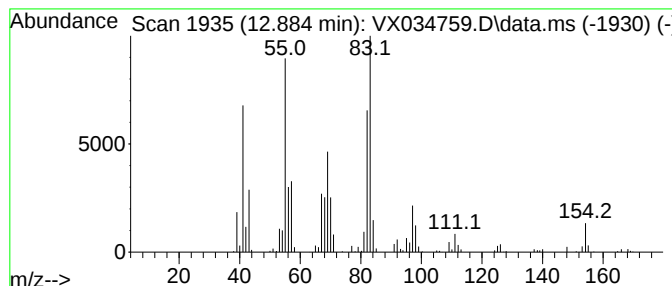
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, 1-methyl-3-(1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.884	13.71 ug/l	371640	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-methyl-3-(1-meth...	126	C9H18	053771-88-3	64
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	52
3			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	49
4			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	47
5			Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034759.D
Acq On : 27 Mar 2023 18:55
Operator : JC/MD
Sample : 02073-01 400X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-1715

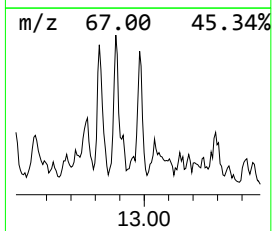
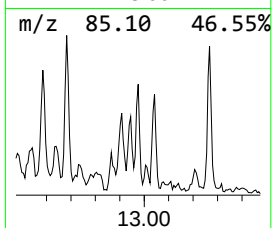
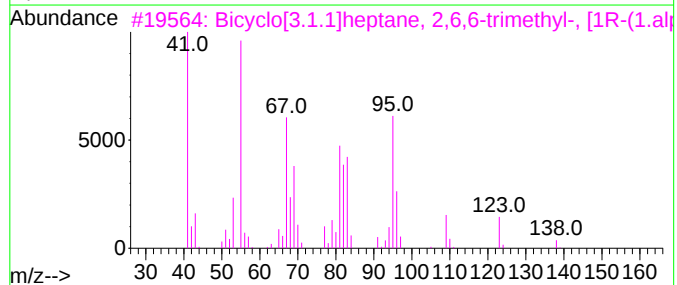
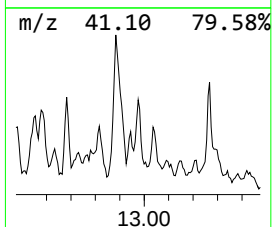
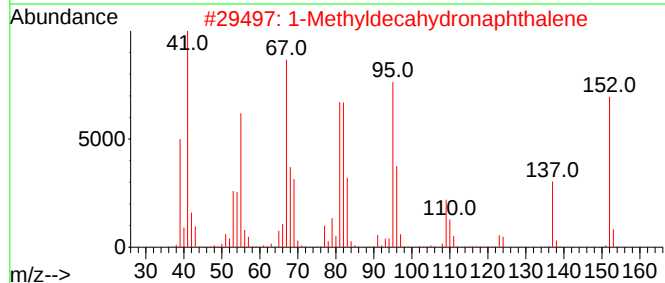
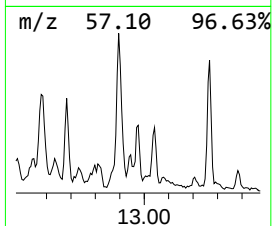
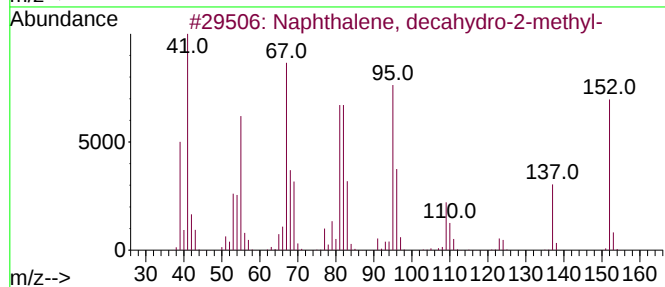
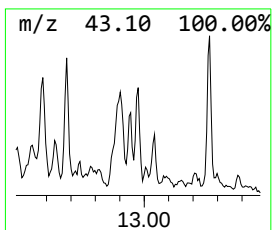
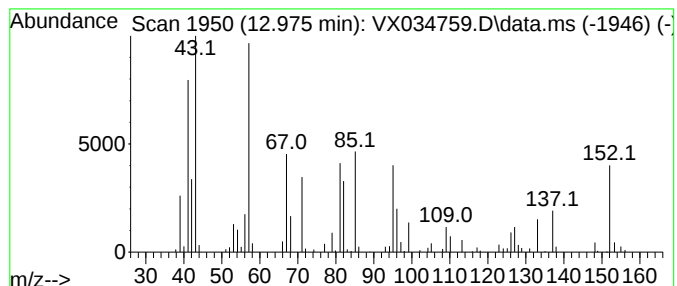
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, decahydro-2-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.975	5.17 ug/l	140228	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	93
2			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	93
3			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004863-59-6	41
4			Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	38
5			4-Pyridinol, acetate (ester)	137	C7H7NO2	014210-20-9	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034759.D
Acq On : 27 Mar 2023 18:55
Operator : JC/MD
Sample : 02073-01 400X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-1715

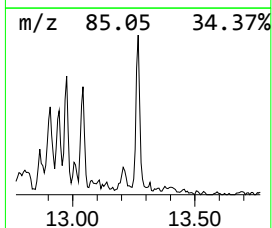
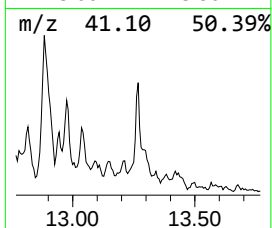
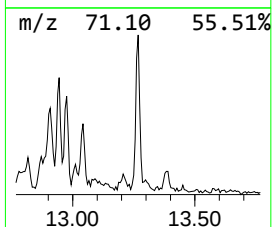
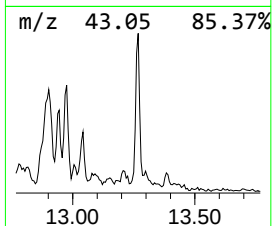
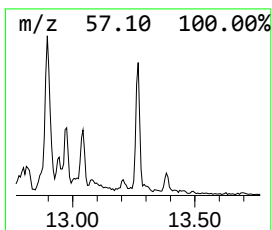
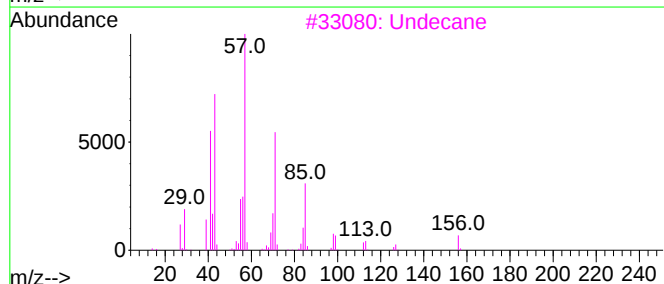
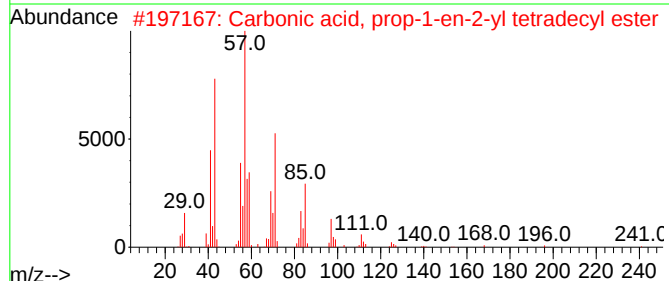
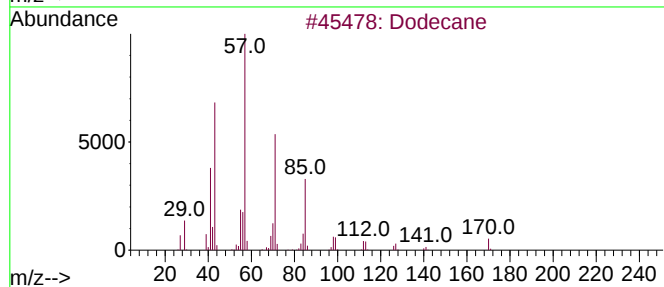
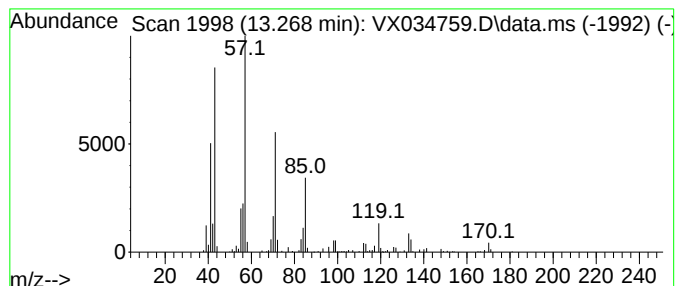
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Quant Title : SW846 8260

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

Peak Number 9 Dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	7.24 ug/l	196316	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	94
2			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	72
3			Undecane	156	C11H24	001120-21-4	64
4			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	59
5			Hexadecane	226	C16H34	000544-76-3	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034759.D
Acq On : 27 Mar 2023 18:55
Operator : JC/MD
Sample : 02073-01 400X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-1715

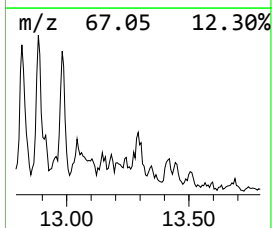
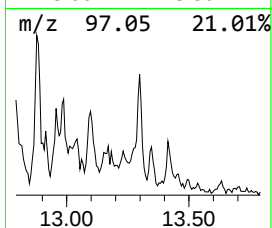
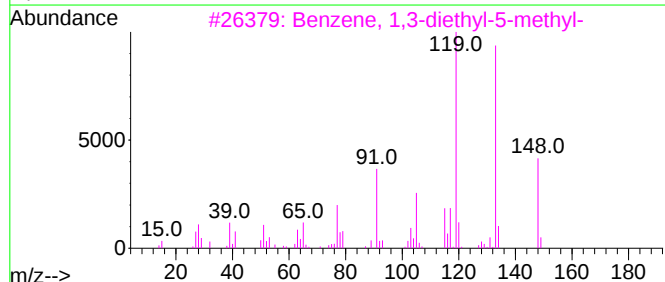
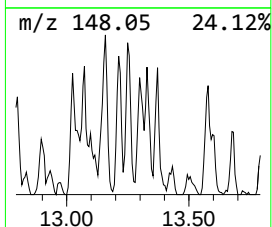
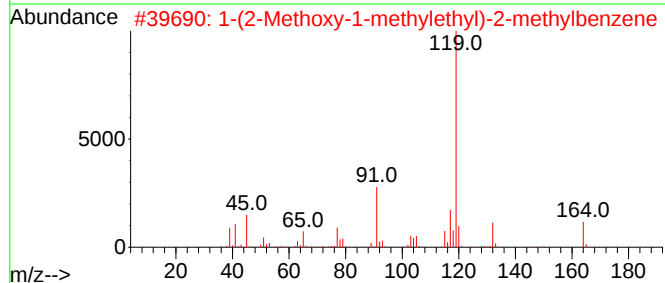
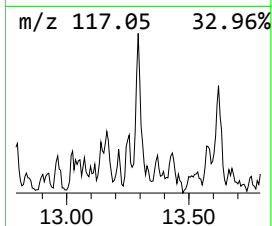
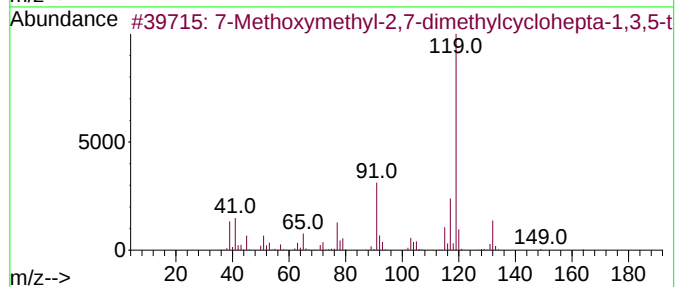
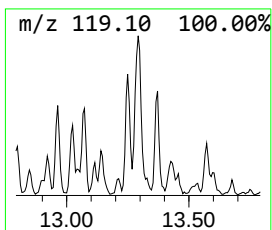
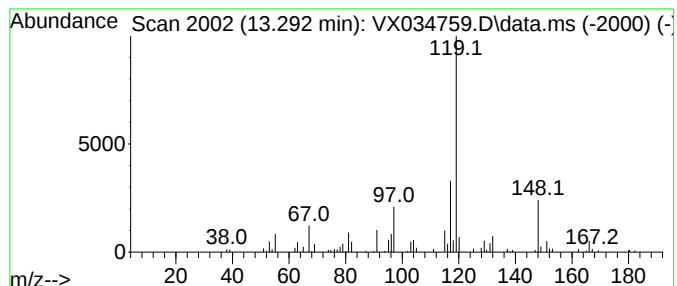
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Quant Title : SW846 8260

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

Peak Number 10 unknown13.292 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	5.18 ug/l	140369	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Methoxymethyl-2,7-dimethylcycl...	164	C11H16O	073992-48-0	47
2			1-(2-Methoxy-1-methylethyl)-2-me...	164	C11H16O	1000210-02-1	43
3			Benzene, 1,3-diethyl-5-methyl-	148	C11H16	002050-24-0	38
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	38
5			o-Cymene	134	C10H14	000527-84-4	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034759.D
Acq On : 27 Mar 2023 18:55
Operator : JC/MD
Sample : 02073-01 400X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-1715

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.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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Decane, 4-methyl-	11.713	7.9	ug/l	213619	4	12.024	1355230	50.0
Decane, 3-methyl-	12.170	6.8	ug/l	183003	4	12.024	1355230	50.0
Carbonic acid, ...	12.420	34.9	ug/l	946533	4	12.024	1355230	50.0
unknown12.463	12.463	5.5	ug/l	149281	4	12.024	1355230	50.0
p-Cymene	12.554	6.0	ug/l	161529	4	12.024	1355230	50.0
Cyclopentane, 1...	12.884	13.7	ug/l	371640	4	12.024	1355230	50.0
Naphthalene, de...	12.975	5.2	ug/l	140228	4	12.024	1355230	50.0
Dodecane	13.268	7.2	ug/l	196316	4	12.024	1355230	50.0
unknown13.292	13.292	5.2	ug/l	140369	4	12.024	1355230	50.0