

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
 Data File : VX034343.D
 Acq On : 06 Mar 2023 12:36
 Operator : JC/MD
 Sample : 01758-01DL 10X
 Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FMC-0081DL

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\82X021723W.M
 Title : SW846 8260

Signal : TIC: VX034343.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	694	705	716	rBV	164389	479432	12.25%	2.060%
2	5.550	716	732	753	rVB	284503	900648	23.02%	3.870%
3	5.824	765	777	789	rBV2	34164	103873	2.65%	0.446%
4	5.952	789	798	814	rBV2	185033	490333	12.53%	2.107%
5	6.610	896	906	915	rBV2	42891	100450	2.57%	0.432%
6	6.763	921	931	947	rBV	439534	1070794	27.37%	4.602%
7	7.379	1020	1032	1043	rBV	54745	124987	3.19%	0.537%
8	8.647	1233	1240	1246	rBV	954674	1490476	38.09%	6.405%
9	8.720	1246	1252	1269	rVB	1039991	1598399	40.85%	6.869%
10	10.055	1465	1471	1487	rVB	931220	1272284	32.52%	5.468%
11	10.360	1517	1521	1529	rVB	42294	55861	1.43%	0.240%
12	11.079	1634	1639	1652	rVV	771266	1045841	26.73%	4.494%
13	11.189	1652	1657	1660	rBV3	32204	45545	1.16%	0.196%
14	11.433	1692	1697	1700	rBV2	39520	61666	1.58%	0.265%
15	11.475	1700	1704	1709	rVB	283055	334056	8.54%	1.436%
16	11.573	1716	1720	1723	rBV	41066	53739	1.37%	0.231%
17	11.713	1740	1743	1746	rBV	108660	122984	3.14%	0.529%
18	11.835	1759	1763	1766	rBV3	48004	77979	1.99%	0.335%
19	11.890	1766	1772	1776	rVV3	76853	114739	2.93%	0.493%
20	11.939	1776	1780	1784	rBV2	137607	211486	5.41%	0.909%
21	11.975	1784	1786	1789	rVB2	41282	41447	1.06%	0.178%
22	12.024	1789	1794	1799	rBV	905806	1293734	33.06%	5.560%
23	12.073	1799	1802	1804	rVV2	85049	71851	1.84%	0.309%
24	12.103	1804	1807	1812	rBV	110803	109532	2.80%	0.471%
25	12.152	1812	1815	1816	rBV2	43876	46935	1.20%	0.202%
26	12.170	1816	1818	1825	rVB2	143250	194202	4.96%	0.835%
27	12.262	1825	1833	1836	rBV4	66268	156382	4.00%	0.672%
28	12.311	1836	1841	1848	rBV6	147676	305210	7.80%	1.312%
29	12.384	1848	1853	1854	rBV3	77812	120969	3.09%	0.520%
30	12.420	1855	1859	1864	rVB	1173374	1373345	35.10%	5.902%
31	12.469	1864	1867	1873	rVB3	192886	343513	8.78%	1.476%
32	12.555	1874	1881	1883	rBV4	196091	354661	9.06%	1.524%
33	12.634	1891	1894	1898	rVB2	59514	81713	2.09%	0.351%
34	12.683	1898	1902	1905	rBV2	130692	174802	4.47%	0.751%
35	12.762	1911	1915	1917	rBV3	102881	140118	3.58%	0.602%
36	12.817	1921	1924	1930	rVB	286021	379455	9.70%	1.631%

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37	12.884	1930	1935	1943	rBV2	444908	765168	19.56%	3.288%
38	12.945	1943	1945	1947	rBV2	61250	76517	1.96%	0.329%
39	12.987	1947	1952	1957	rVB	1146143	1522279	38.91%	6.542%
40	13.042	1957	1961	1965	rVB3	138478	156545	4.00%	0.673%
41	13.097	1967	1970	1975	rVB2	68783	121224	3.10%	0.521%
42	13.158	1975	1980	1981	rBV5	50933	82232	2.10%	0.353%
43	13.268	1993	1998	2000	rVV	314314	474431	12.13%	2.039%
44	13.292	2000	2002	2008	rVB4	239359	329202	8.41%	1.415%
45	13.347	2008	2011	2015	rVB4	82441	96799	2.47%	0.416%
46	13.414	2018	2022	2032	rVB5	165920	416388	10.64%	1.789%
47	13.499	2032	2036	2041	rVB6	57227	96181	2.46%	0.413%
48	13.591	2047	2051	2055	rVB6	36299	50747	1.30%	0.218%
49	13.676	2061	2065	2068	rBV4	41214	75406	1.93%	0.324%
50	13.798	2082	2085	2089	rVB2	39399	45795	1.17%	0.197%
51	14.438	2185	2190	2206	rVB	3376797	3912747	100.00%	16.815%
52	14.981	2274	2279	2285	rVB	48666	63721	1.63%	0.274%
53	15.194	2308	2314	2320	rBV4	21515	40882	1.04%	0.176%

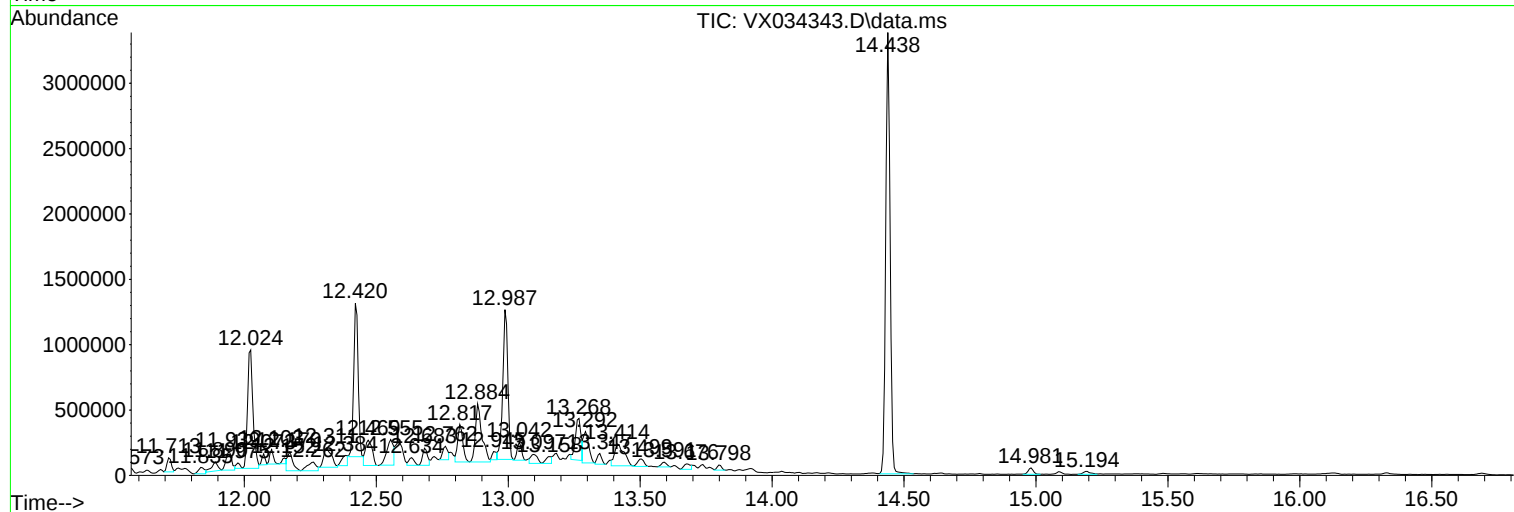
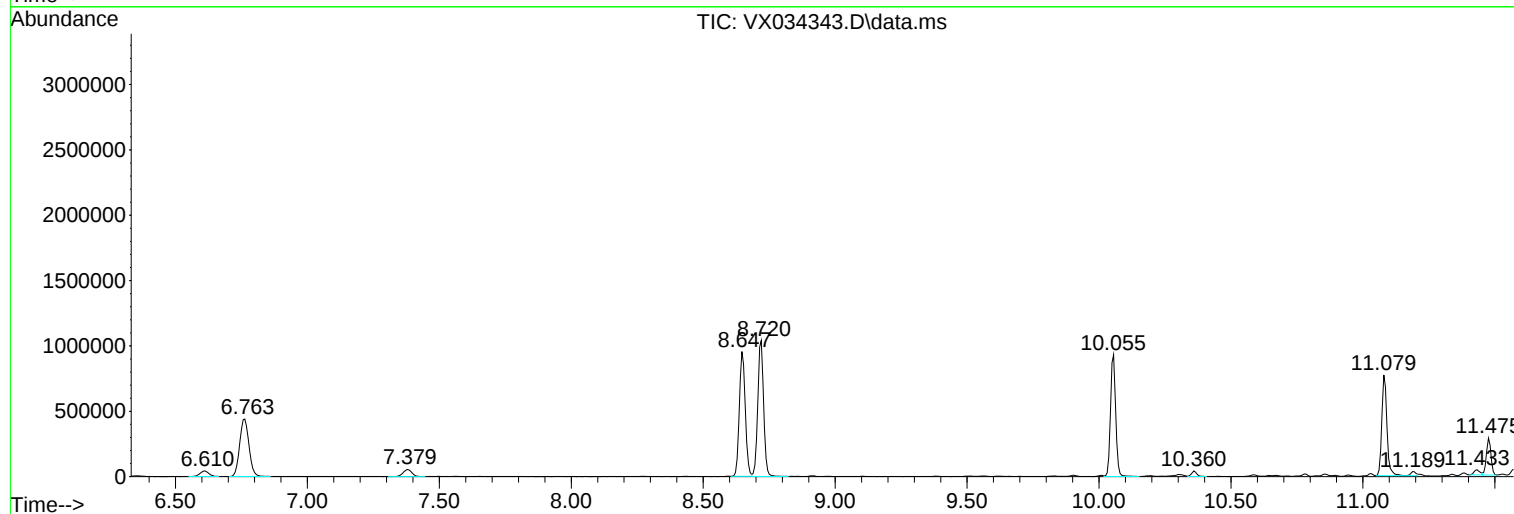
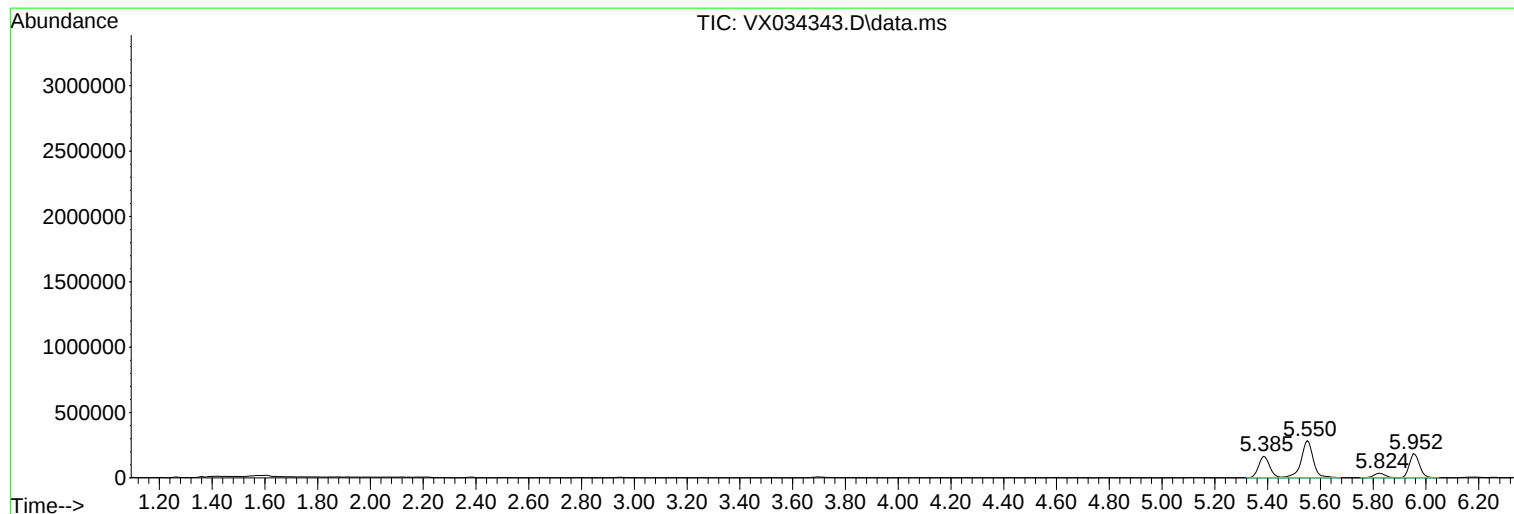
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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ClientSampleId :
FMC-0081DL

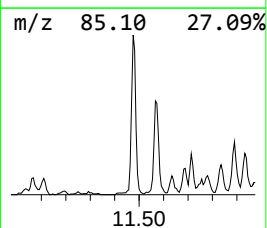
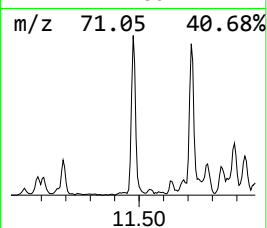
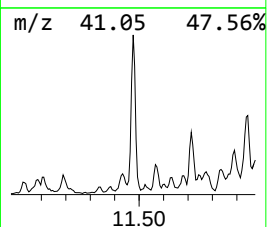
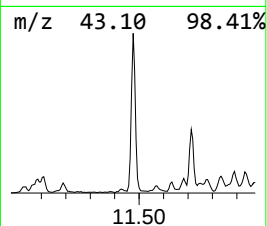
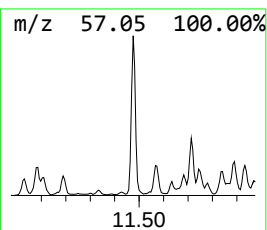
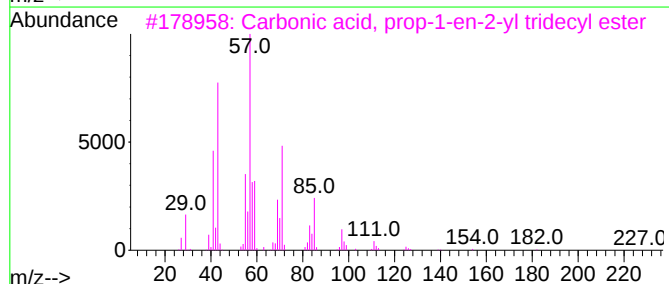
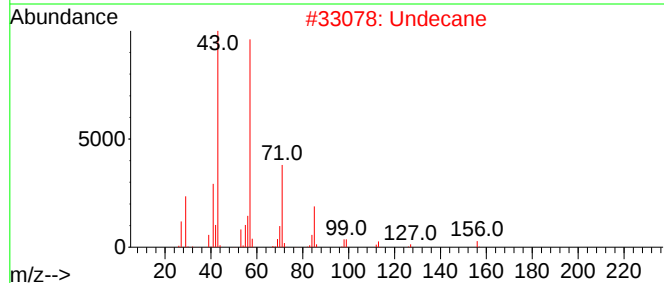
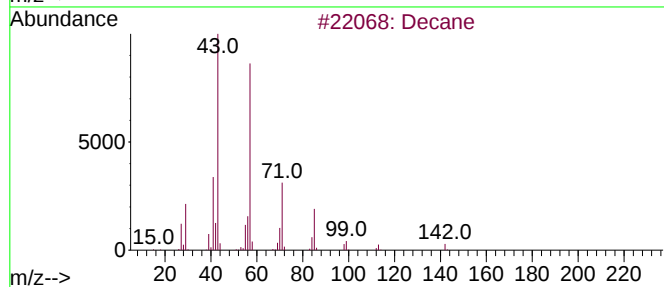
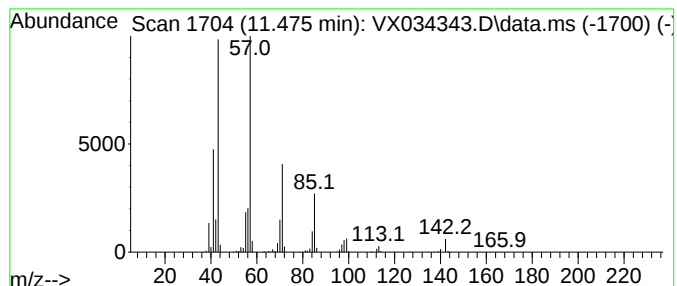
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 1 Decane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.475	12.91 ug/l	334056	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	95
2			Undecane	156	C11H24	001120-21-4	78
3			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	78
4			Nonane	128	C9H20	000111-84-2	64
5			Tridecane	184	C13H28	000629-50-5	59



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Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0081DL

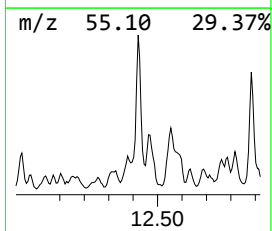
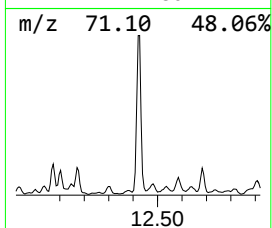
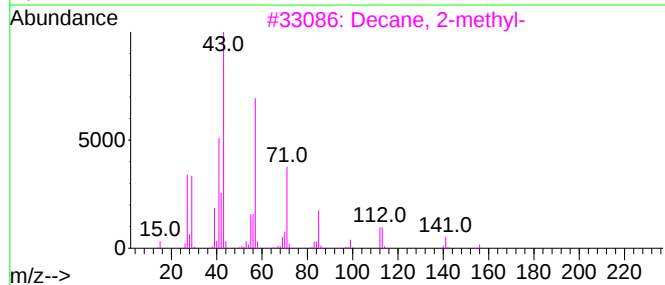
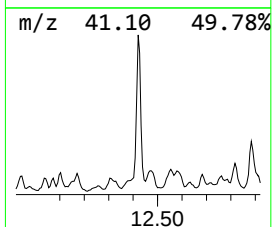
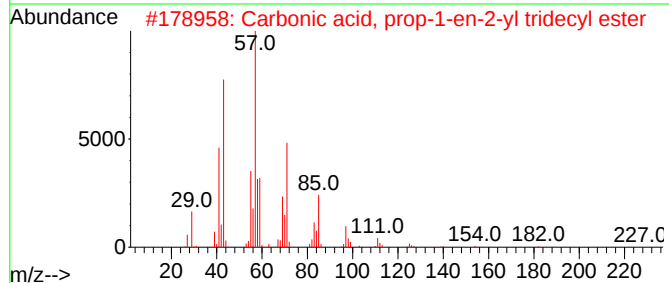
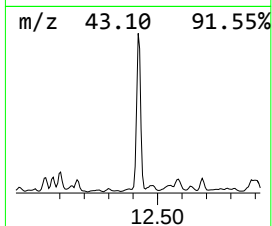
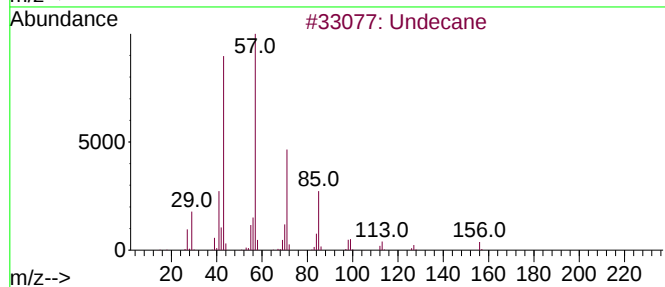
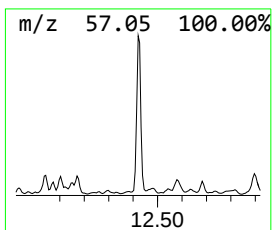
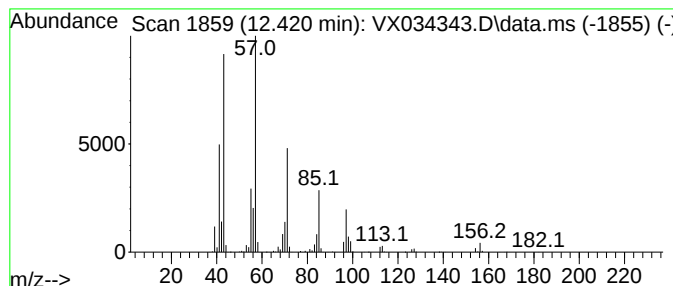
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 2 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.420	53.08 ug/l	1373350	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	81
2			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	80
3			Decane, 2-methyl-	156	C11H24	006975-98-0	72
4			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	72
5			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
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Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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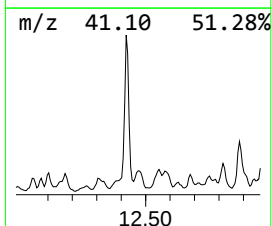
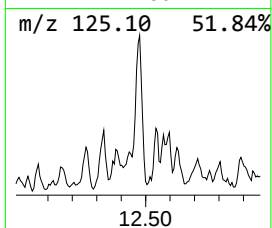
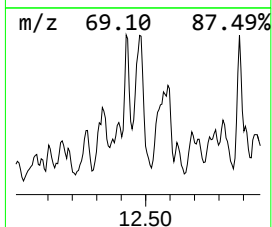
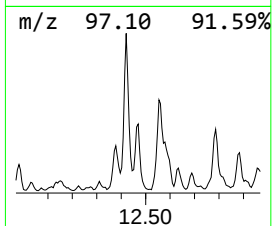
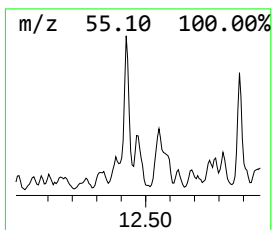
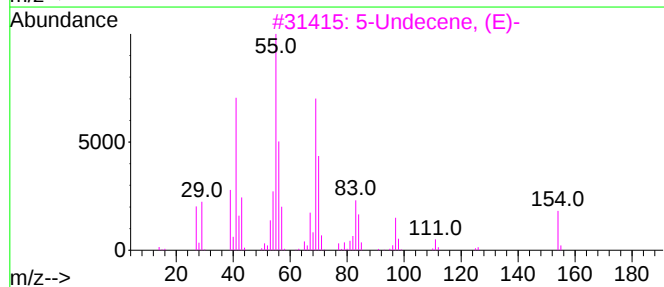
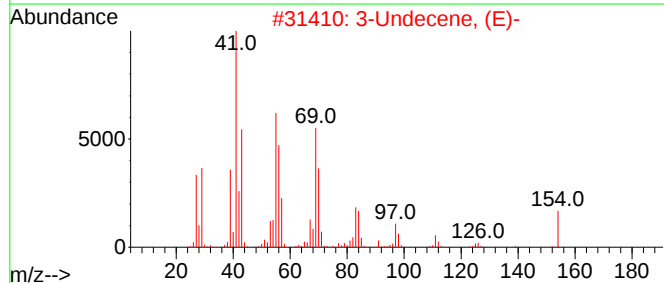
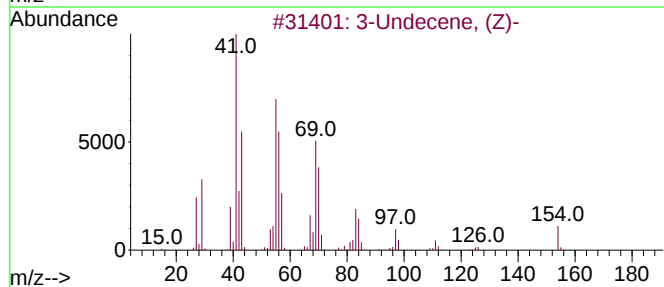
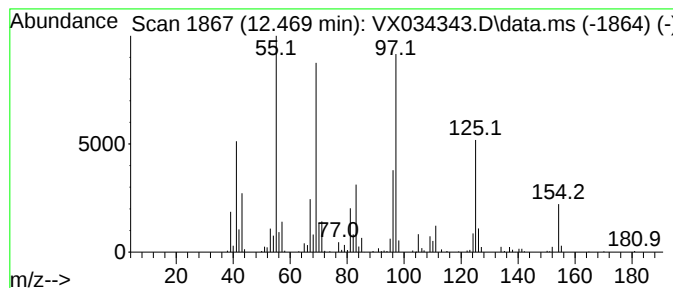
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.469 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	13.28 ug/l	343513	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Undecene, (Z)-	154	C11H22	000821-97-6	43	
2	3-Undecene, (E)-	154	C11H22	001002-68-2	43	
3	5-Undecene, (E)-	154	C11H22	000764-97-6	43	
4	4-Hepten-3-one, 4-methyl-	126	C8H14O	022319-31-9	43	
5	Cyclohexane, 1,1,4,4-tetramethyl-	140	C10H20	002223-52-1	38	



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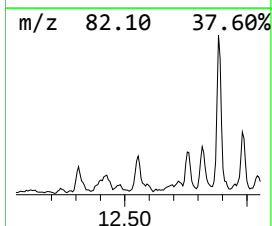
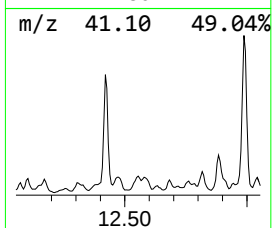
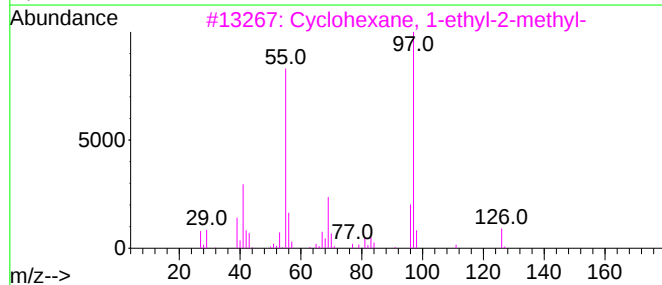
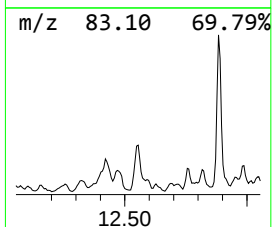
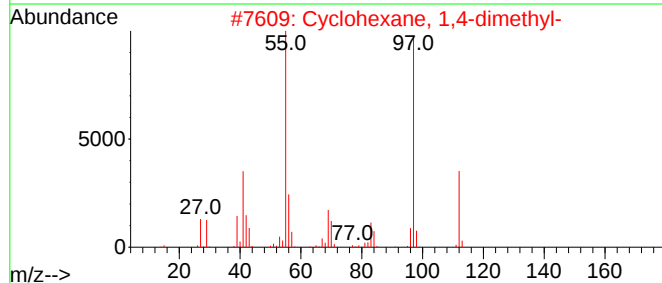
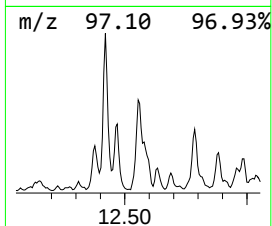
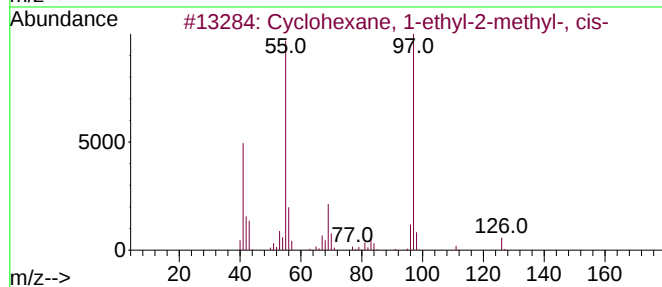
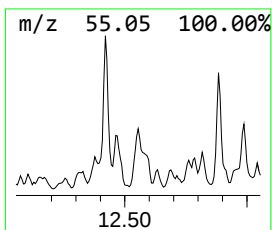
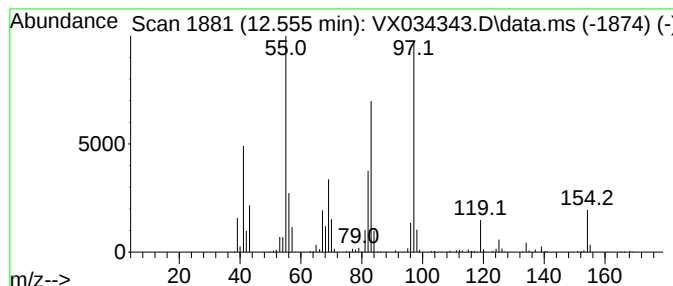
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown12.555 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.555	13.71 ug/l	354661	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	49
2			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	47
3			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	43
4			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	43
5			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	38



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FMC-0081DL

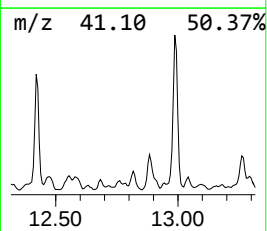
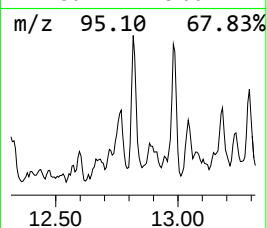
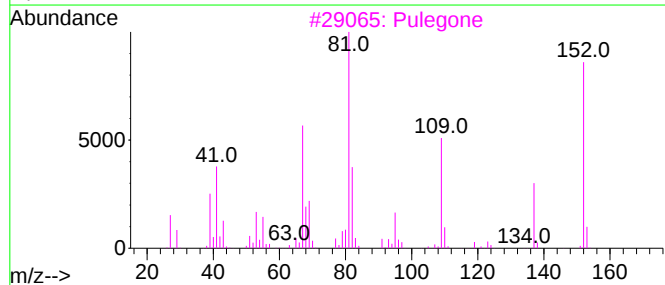
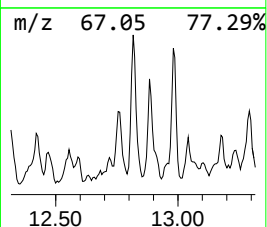
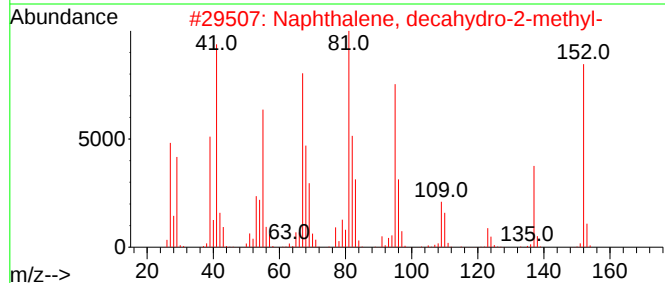
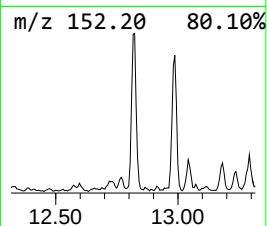
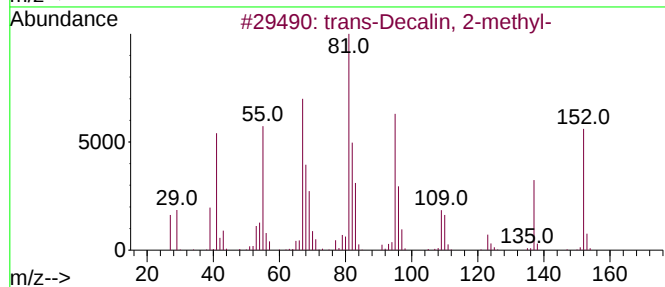
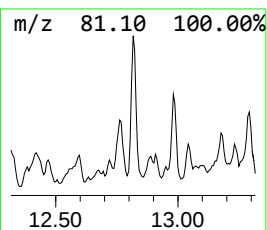
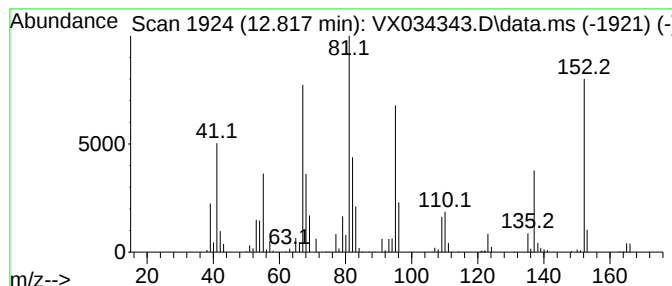
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Quant Title : SW846 8260

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

Peak Number 5 trans-Decalin, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.817	14.67 ug/l	379455	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	94
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	93
3			Pulegone	152	C10H16O	000089-82-7	87
4			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	83
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VOX030623\
Data File : VX034343.D
Acq On : 06 Mar 2023 12:36
Operator : JC/MD
Sample : 01758-01DL 10X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0081DL

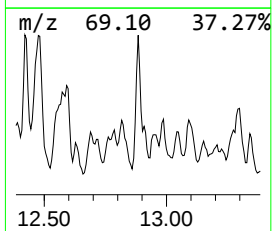
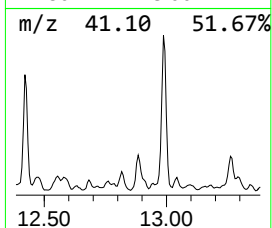
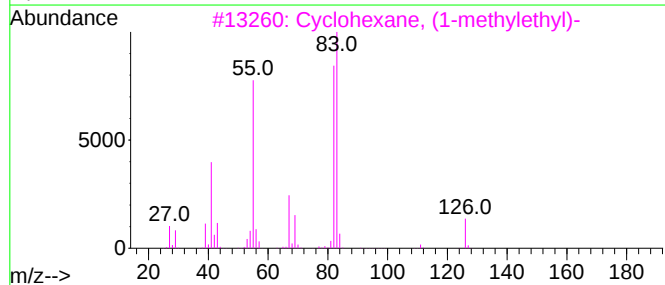
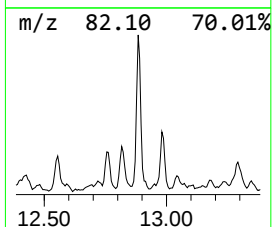
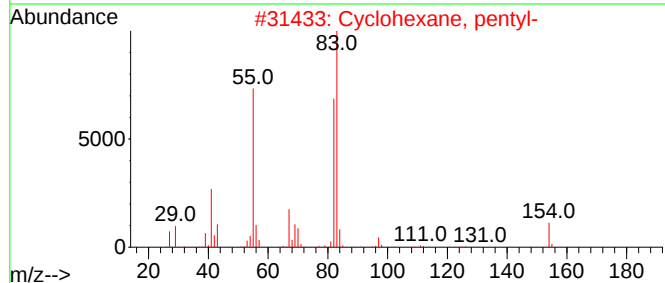
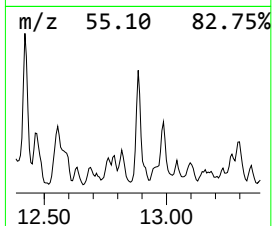
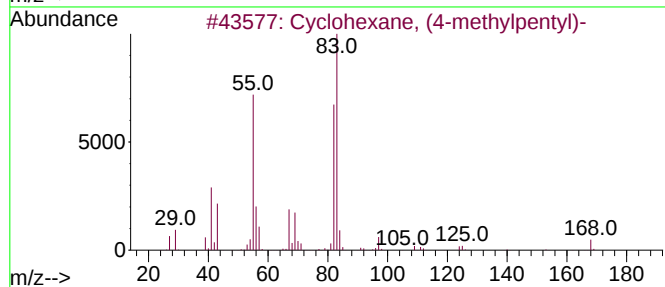
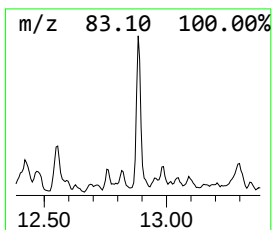
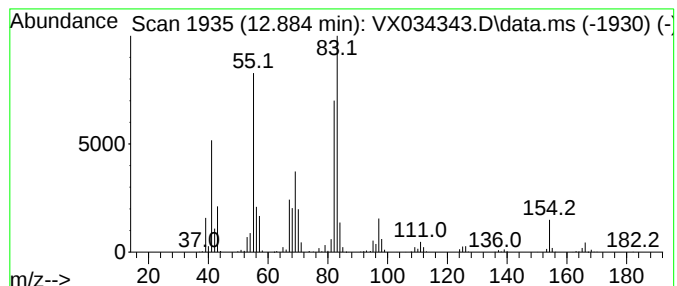
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Quant Title : SW846 8260

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

Peak Number 6 Cyclohexane, (4-methylpentyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.884	29.57 ug/l	765168	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	76
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	74
3			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	52
4			1-Butanone, 1-cyclohexyl-	154	C10H18O	001462-27-7	43
5			5-Undecene	154	C11H22	004941-53-1	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034343.D
Acq On : 06 Mar 2023 12:36
Operator : JC/MD
Sample : 01758-01DL 10X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0081DL

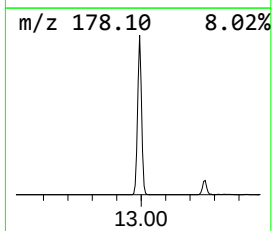
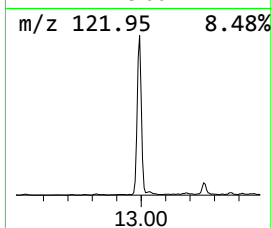
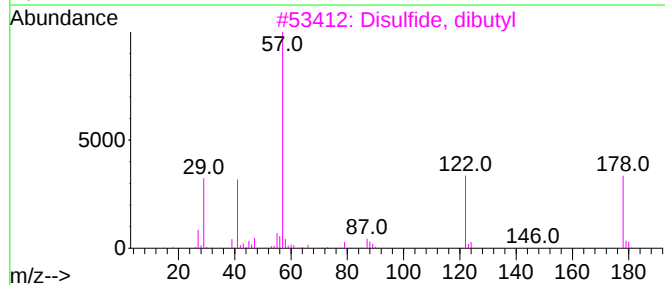
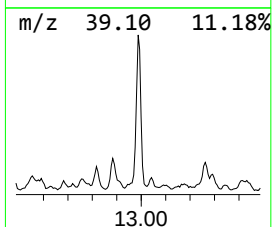
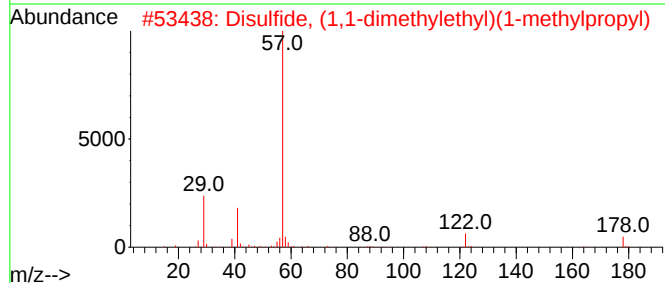
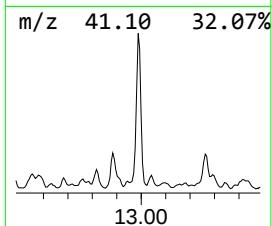
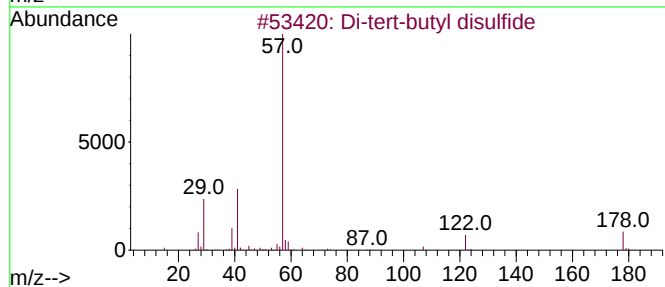
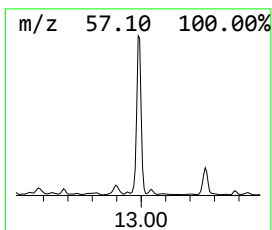
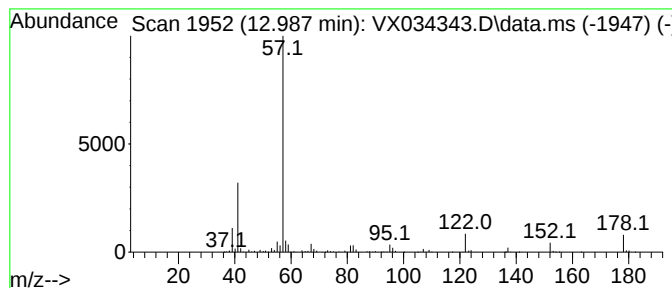
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Quant Title : SW846 8260

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

Peak Number 7 Di-tert-butyl disulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.987	58.83 ug/l	1522280	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	62
2			Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	49
3			Disulfide, dibutyl	178	C8H18S2	000629-45-8	47
4			Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	47
5			Phosphinous chloride, (chloromet...	172	C5H11Cl2P	078055-63-7	16



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034343.D
Acq On : 06 Mar 2023 12:36
Operator : JC/MD
Sample : 01758-01DL 10X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0081DL

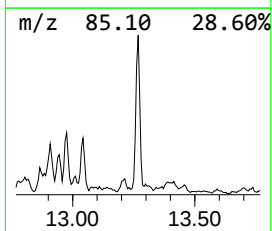
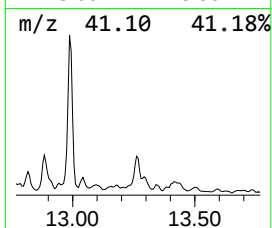
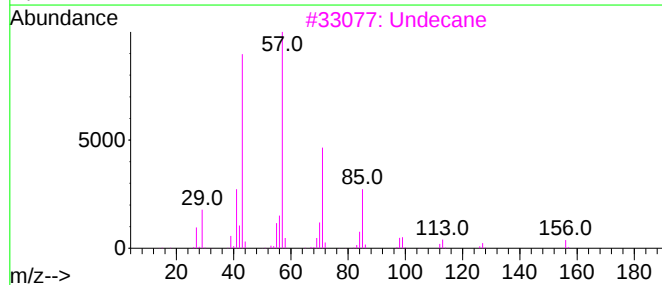
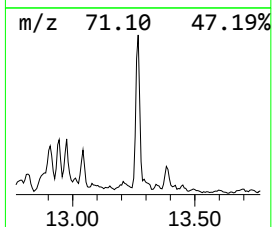
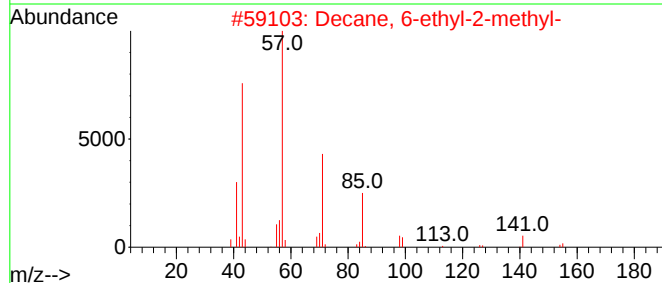
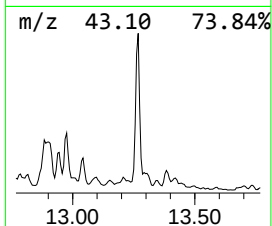
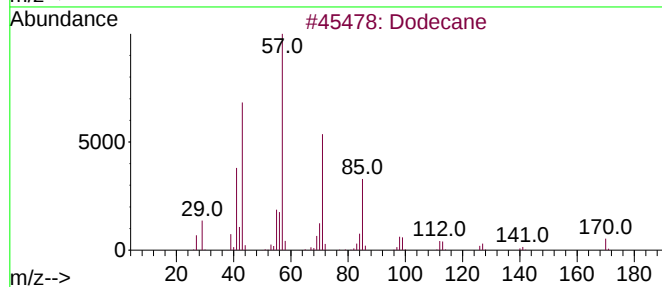
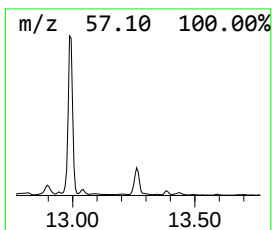
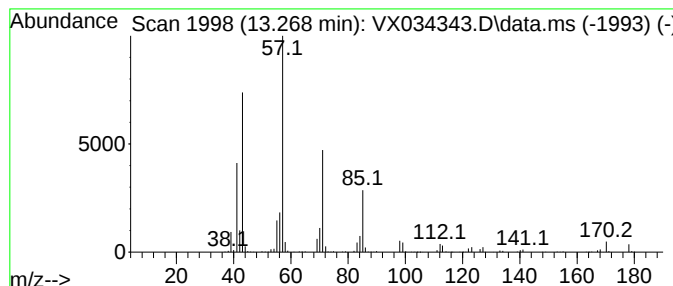
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Quant Title : SW846 8260

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

Peak Number 8 Dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	18.34 ug/l	474431	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	95
2			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	80
3			Undecane	156	C11H24	001120-21-4	80
4			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	78
5			Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034343.D
Acq On : 06 Mar 2023 12:36
Operator : JC/MD
Sample : 01758-01DL 10X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0081DL

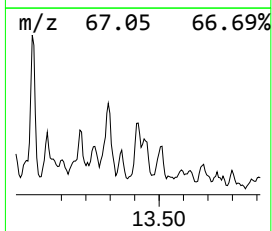
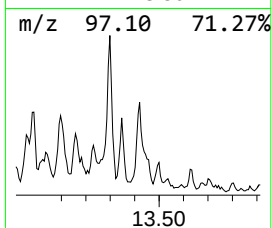
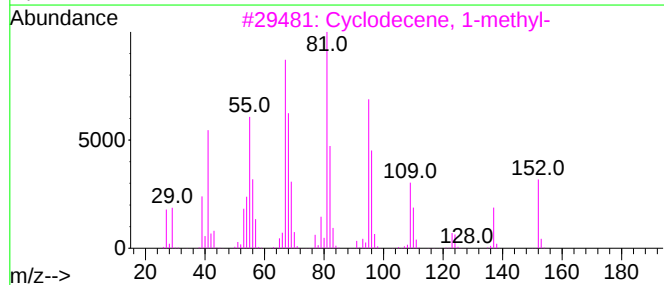
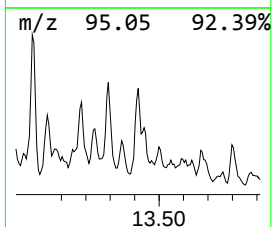
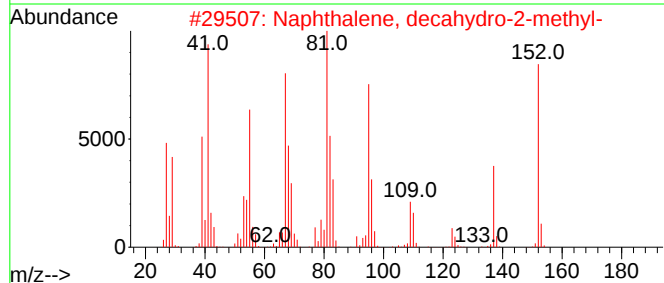
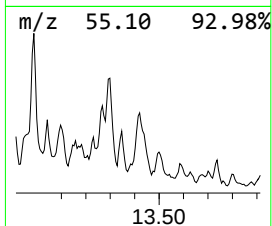
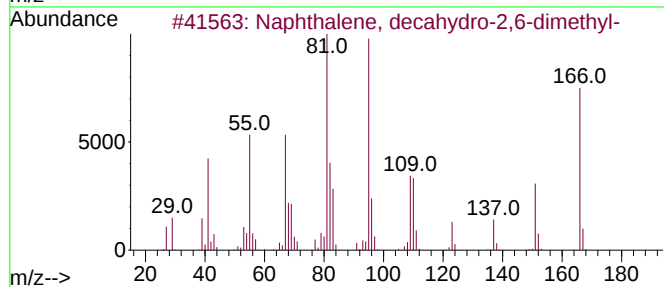
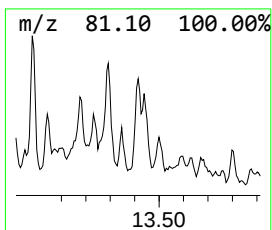
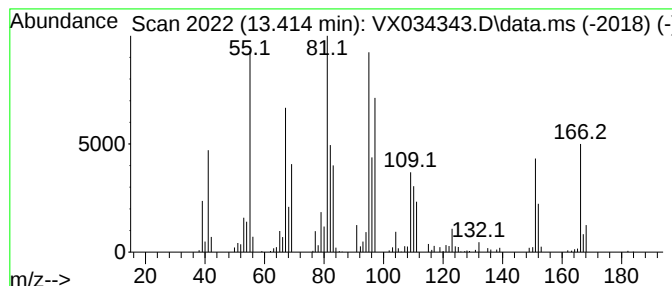
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, decahydro-2,6-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.414	16.09 ug/l	416388	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	92
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	60
3			Cyclodecene, 1-methyl-	152	C11H20	066633-38-3	55
4			Cyclohexene, 1,6-dimethyl-	110	C8H14	001759-64-4	46
5			Cyclohexanol, 1-ethynyl-	124	C8H12O	000078-27-3	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034343.D
Acq On : 06 Mar 2023 12:36
Operator : JC/MD
Sample : 01758-01DL 10X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0081DL

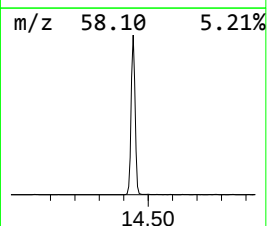
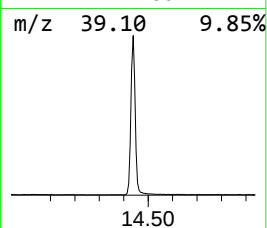
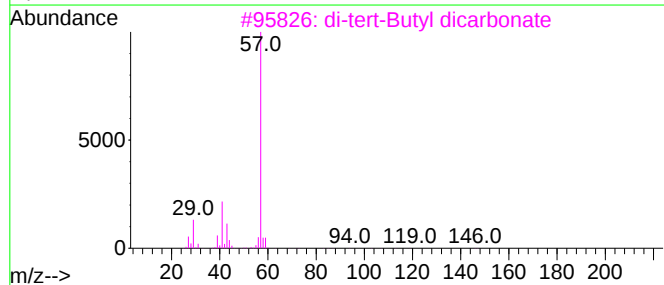
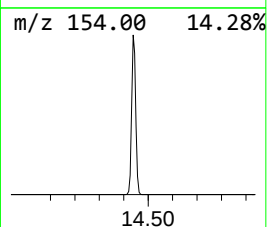
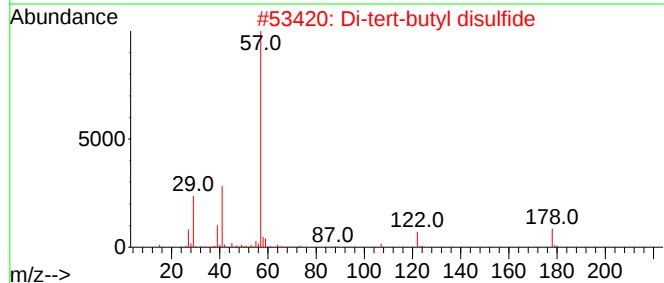
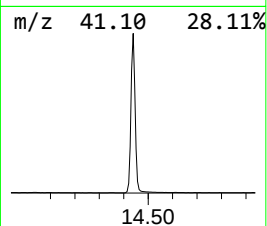
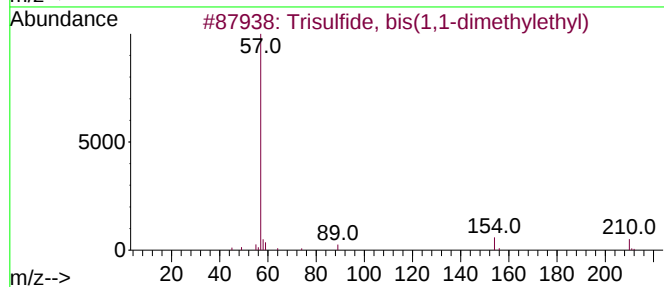
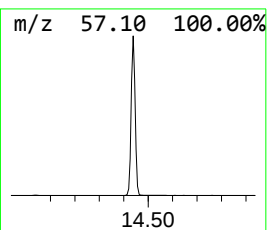
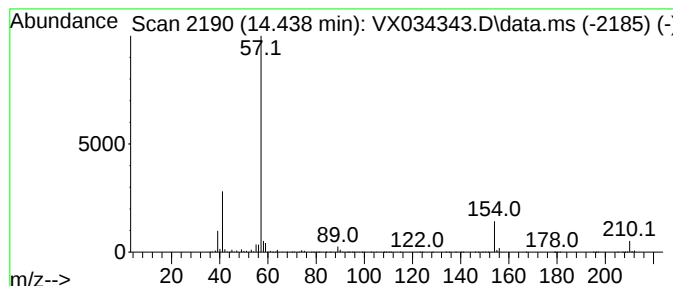
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Quant Title : SW846 8260

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

Peak Number 10 unknown14.438 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.438	151.22 ug/l	3912750	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	49
2			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	37
3			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	17
4			Hypophosphonous dichloride, bis(...	246	C8H18Cl2P2	079898-85-4	12
5			Propane, 2-[(1,1-dimethylethyl)s...	178	C8H18O2S	001886-75-5	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034343.D
Acq On : 06 Mar 2023 12:36
Operator : JC/MD
Sample : 01758-01DL 10X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0081DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.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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Undecane	12.420	53.1	ug/l	1373350	4	12.024	1293730	50.0
unknown12.469	12.469	13.3	ug/l	343513	4	12.024	1293730	50.0
unknown12.555	12.555	13.7	ug/l	354661	4	12.024	1293730	50.0
trans-Decalin, ...	12.817	14.7	ug/l	379455	4	12.024	1293730	50.0
Cyclohexane, (4...	12.884	29.6	ug/l	765168	4	12.024	1293730	50.0
Di-tert-butyl d...	12.987	58.8	ug/l	1522280	4	12.024	1293730	50.0
Dodecane	13.268	18.3	ug/l	474431	4	12.024	1293730	50.0
Naphthalene, de...	13.414	16.1	ug/l	416388	4	12.024	1293730	50.0
unknown14.438	14.438	151.2	ug/l	3912750	4	12.024	1293730	50.0