

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020623\
 Data File : VN076549.D
 Acq On : 06 Feb 2023 18:12
 Operator : JC\MD
 Sample : 01407-01
 Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 30984

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_N\methods\82N020623W.M
 Title : SW846 8260

Signal : TIC: VN076549.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.171	1030	1040	1044	rBV	324259	786975	13.42%	1.783%
2	8.224	1044	1049	1063	rVB	662681	1477416	25.18%	3.347%
3	8.582	1099	1110	1119	rBV	332004	758587	12.93%	1.718%
4	9.100	1188	1198	1211	rBV	876702	1811566	30.88%	4.104%
5	10.565	1438	1447	1455	rBV	1274500	2371512	40.43%	5.372%
6	11.865	1660	1668	1682	rBV	1086715	1967998	33.55%	4.458%
7	12.853	1829	1836	1845	rVB	809127	1376844	23.47%	3.119%
8	13.706	1976	1981	1987	rVV5	61346	144099	2.46%	0.326%
9	13.794	1990	1996	2002	rVV	1043611	1784438	30.42%	4.042%
10	13.859	2002	2007	2015	rVB2	73163	173873	2.96%	0.394%
11	14.006	2026	2032	2039	rBV4	46842	114061	1.94%	0.258%
12	14.112	2045	2050	2055	rBV5	131253	276943	4.72%	0.627%
13	14.159	2055	2058	2062	rVB3	59389	77881	1.33%	0.176%
14	14.217	2064	2068	2071	rBV3	87939	123700	2.11%	0.280%
15	14.264	2071	2076	2080	rBV3	151169	262696	4.48%	0.595%
16	14.323	2081	2086	2089	rBV6	107640	186711	3.18%	0.423%
17	14.370	2090	2094	2100	rVB	310927	534540	9.11%	1.211%
18	14.429	2100	2104	2108	rBV2	143943	264534	4.51%	0.599%
19	14.506	2110	2117	2122	rBV5	286794	627598	10.70%	1.422%
20	14.588	2122	2131	2134	rBV3	882336	1955662	33.34%	4.430%
21	14.629	2134	2138	2142	rVV2	1685860	2469596	42.10%	5.594%
22	14.664	2142	2144	2149	rVB	809358	900286	15.35%	2.039%
23	14.735	2152	2156	2161	rBV3	984890	1395095	23.78%	3.160%
24	14.794	2162	2166	2171	rVB2	721952	1055360	17.99%	2.391%
25	14.847	2171	2175	2180	rVB3	447126	760357	12.96%	1.722%
26	14.900	2181	2184	2186	rBV4	223921	310893	5.30%	0.704%
27	14.935	2187	2190	2192	rBV2	246947	307383	5.24%	0.696%
28	15.047	2204	2209	2211	rBV	992104	1688738	28.79%	3.825%
29	15.082	2211	2215	2226	rVB4	2151702	5866360	100.00%	13.289%
30	15.182	2227	2232	2236	rBV4	552116	1090354	18.59%	2.470%
31	15.235	2237	2241	2244	rBV4	740932	1210435	20.63%	2.742%
32	15.317	2251	2255	2262	rVB7	564818	1105689	18.85%	2.505%
33	15.535	2285	2292	2297	rVB3	1095837	2804206	47.80%	6.352%
34	15.594	2298	2302	2310	rVB3	1146532	2599519	44.31%	5.889%
35	15.676	2311	2316	2328	rBV7	590454	1900400	32.39%	4.305%
36	15.923	2355	2358	2362	rBV5	206172	390018	6.65%	0.883%

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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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37	16.505	2454	2457	2470	rVB2	394252	1212833	20.67%	2.747%
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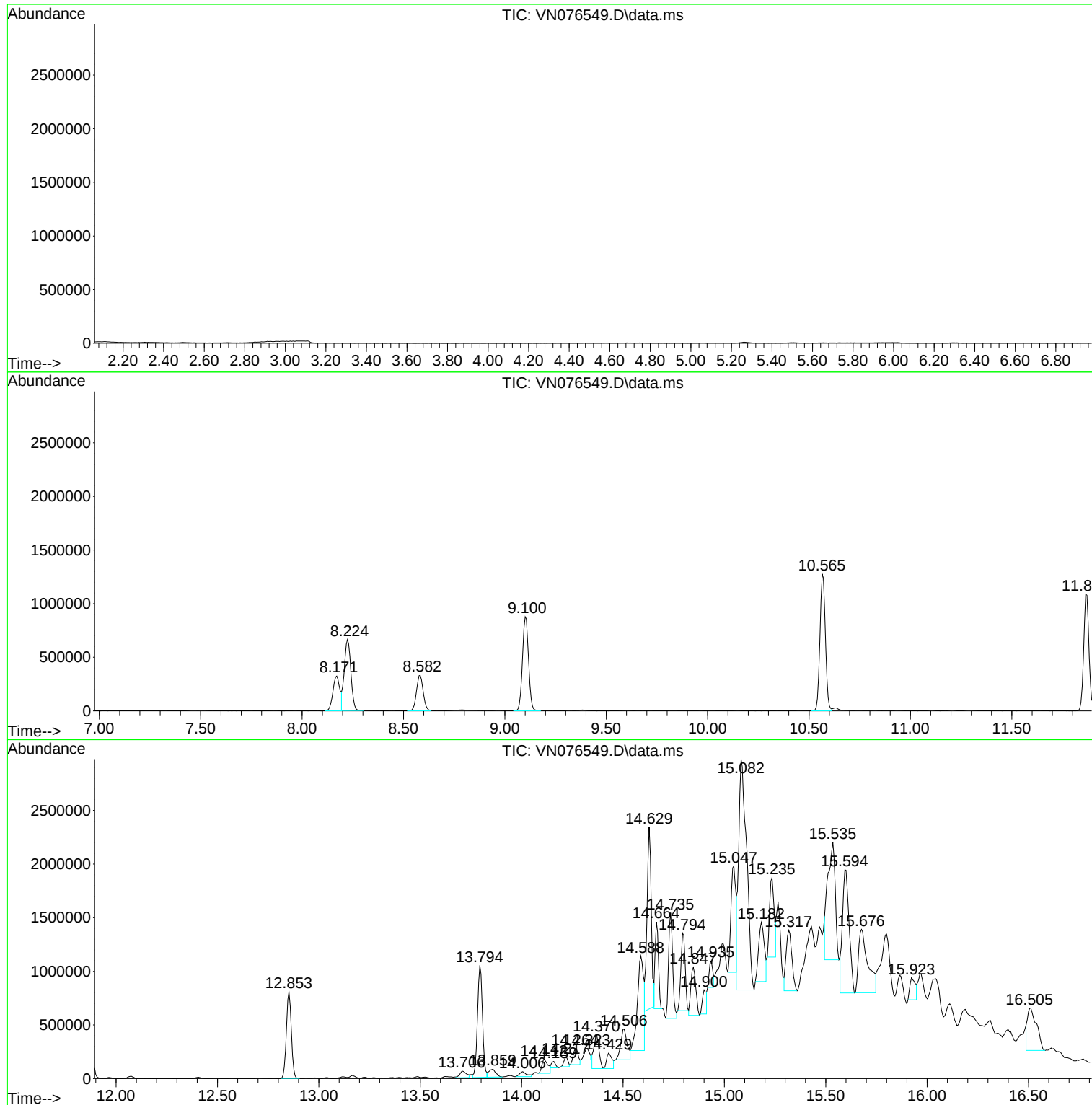
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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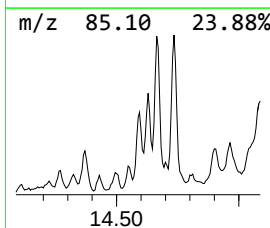
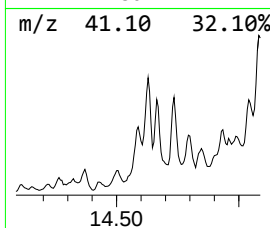
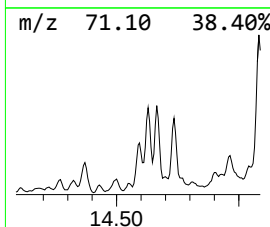
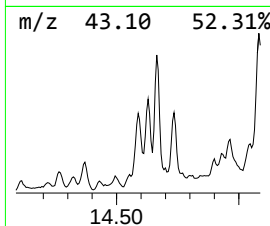
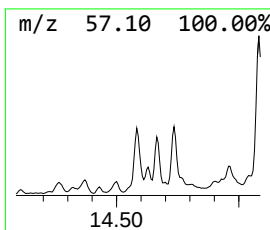
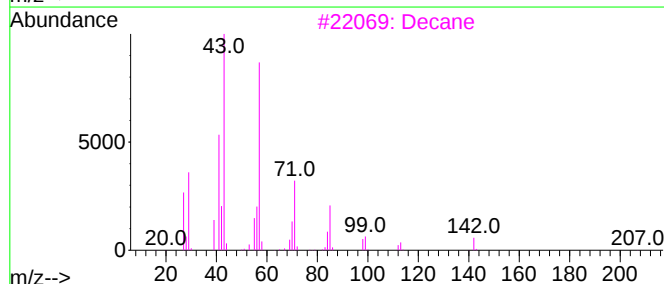
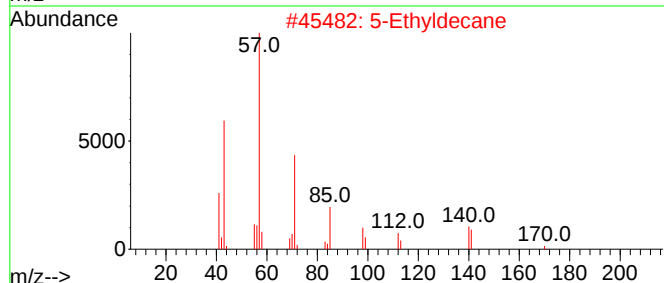
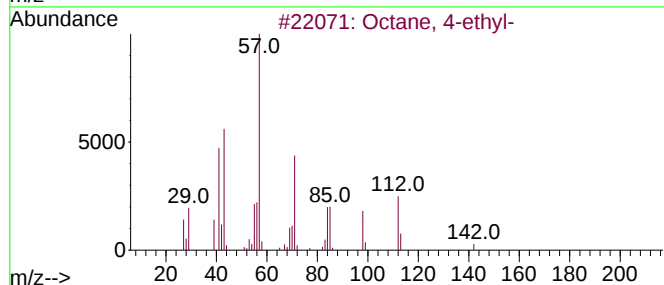
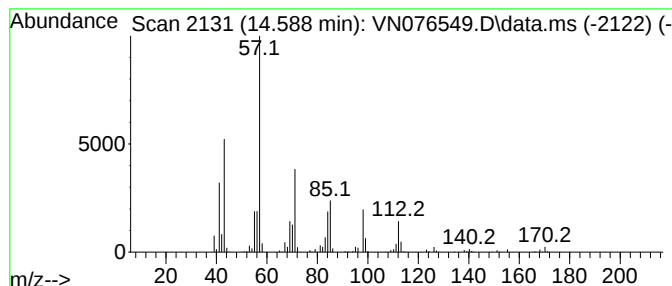
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020623W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Octane, 4-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.588	54.80 ug/l	1955660	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octane, 4-ethyl-	142	C10H22	015869-86-0	78
2		5-Ethyldecane	170	C12H26	017302-36-2	72
3		Decane	142	C10H22	000124-18-5	58
4		Dodecane	170	C12H26	000112-40-3	53
5		Undecane, 5-methyl-	170	C12H26	001632-70-8	53



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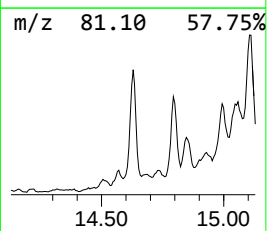
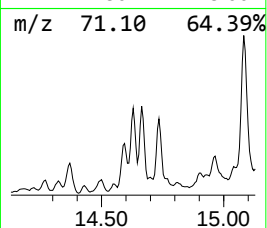
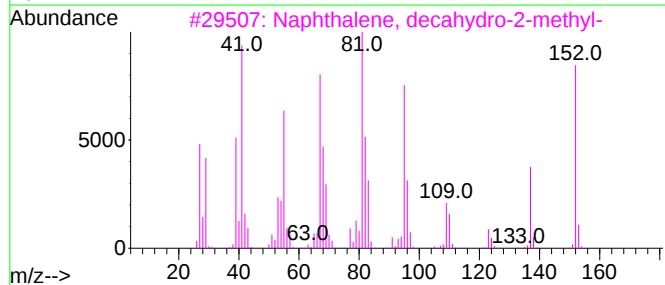
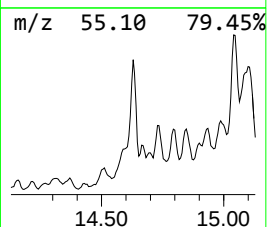
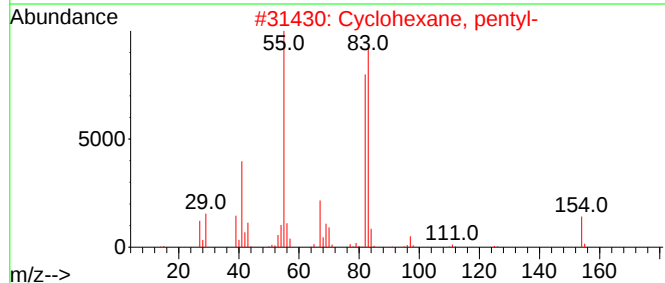
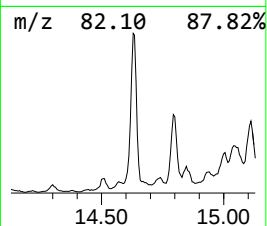
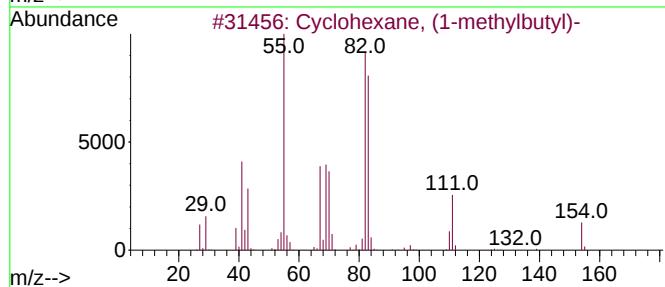
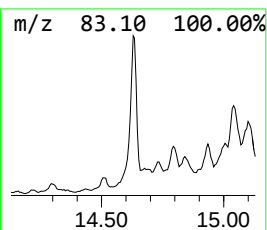
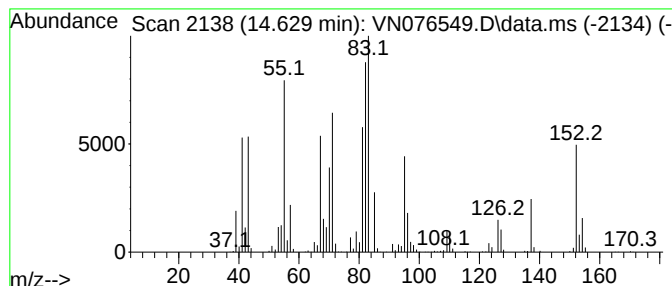
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Cyclohexane, (1-methylbutyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.629	69.20 ug/l	2469600	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	53
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	41
3			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	38
4			(Z)-Hex-3-enyl (E)-2-methylbut-2...	182	C11H18O2	067883-79-8	35
5			Cyclohexane, 1,1'-(1,4-butanediyl...	222	C16H30	006165-44-2	35



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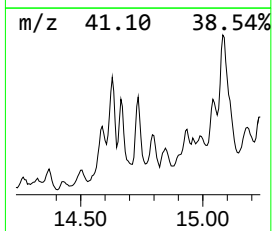
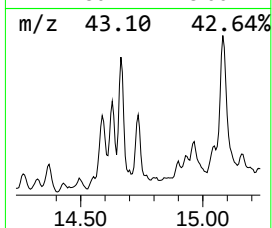
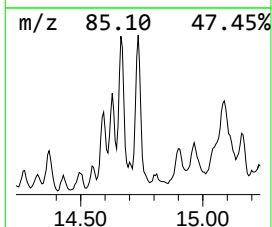
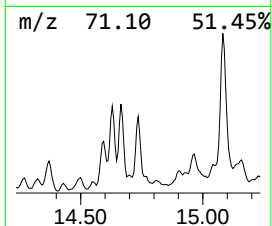
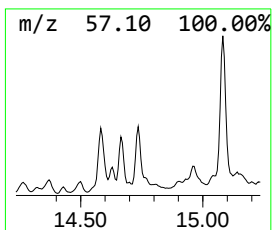
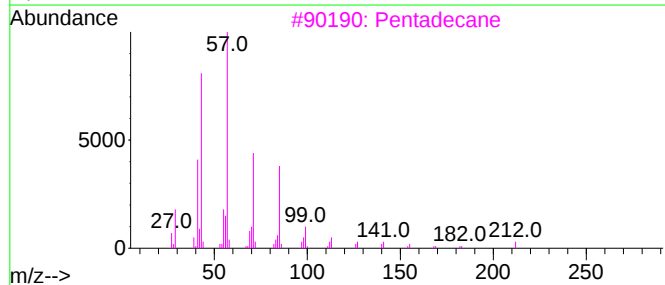
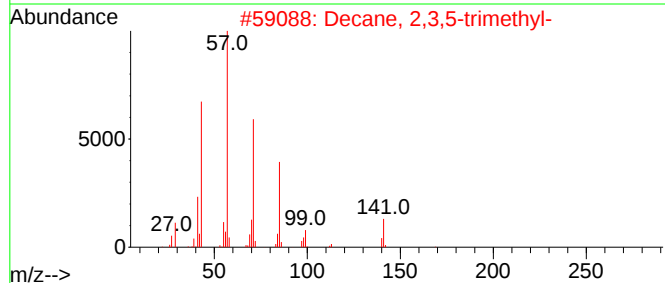
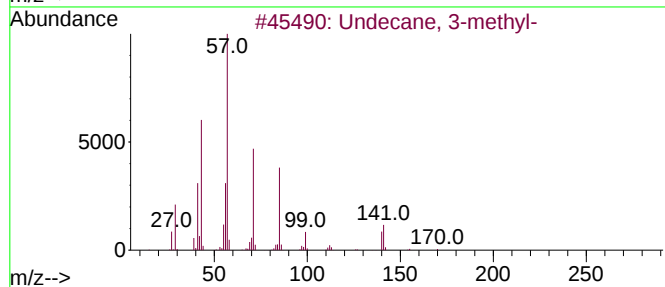
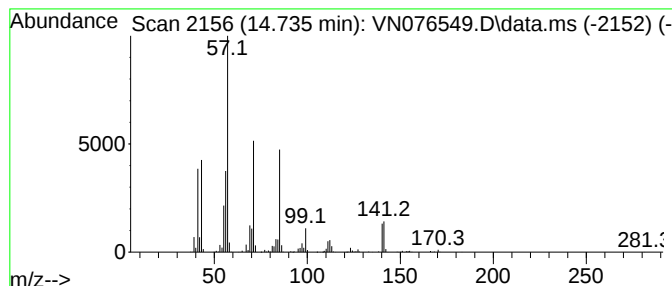
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Undecane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.735	39.09 ug/l	1395100	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3-methyl-	170	C12H26	001002-43-3	91
2			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72
3			Pentadecane	212	C15H32	000629-62-9	64
4			Oxalic acid, 6-ethyloct-3-yl iso...	286	C16H30O4	1010309-34-1	59
5			Oxalic acid, bis(6-ethyloct-3-yl...	370	C22H42O4	1000309-34-6	59



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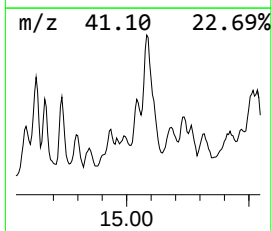
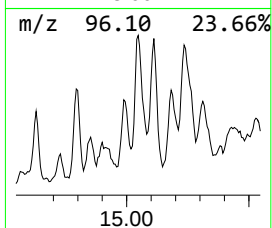
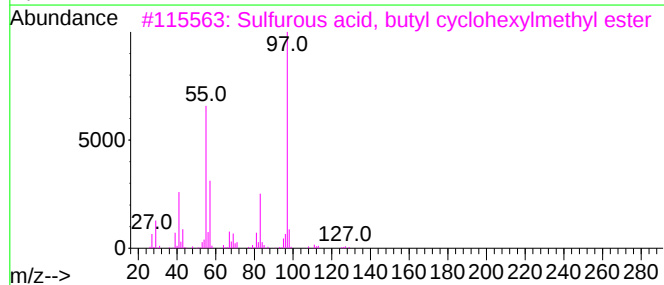
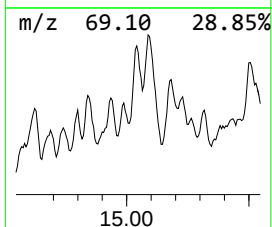
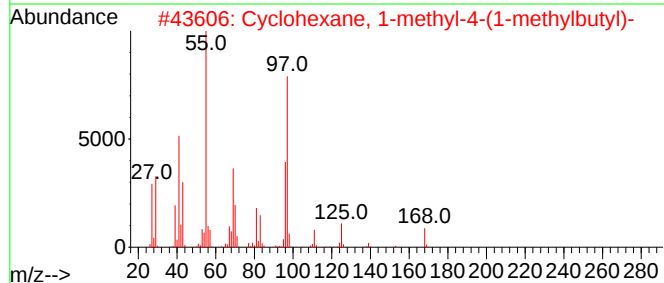
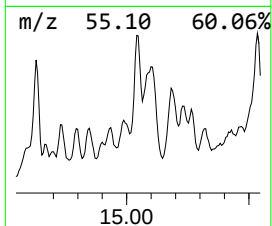
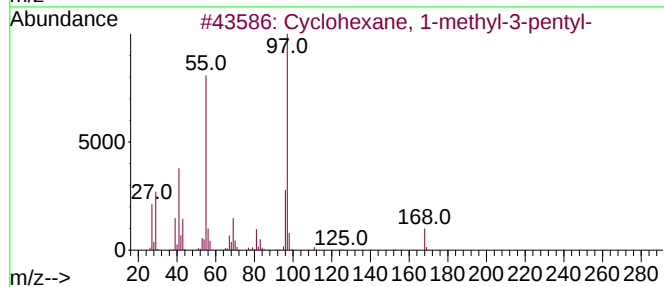
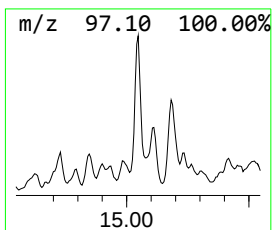
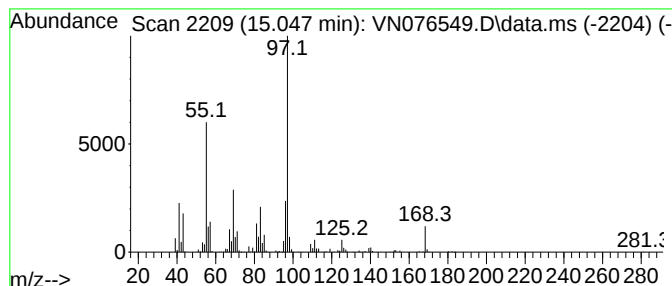
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Cyclohexane, 1-methyl-3-pen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	47.32 ug/l	1688740	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-3-pentyl-	168	C12H24	054411-02-8	64
2			Cyclohexane, 1-methyl-4-(1-methy...	168	C12H24	054411-00-6	59
3			Sulfurous acid, butyl cyclohexyl...	234	C11H22O3S	1000309-21-4	59
4			2,2,3,3-Tetramethylcyclopropanec...	238	C15H26O2	1010221-97-5	59
5			Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	53



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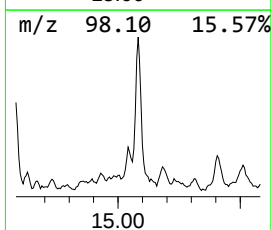
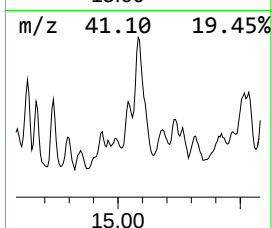
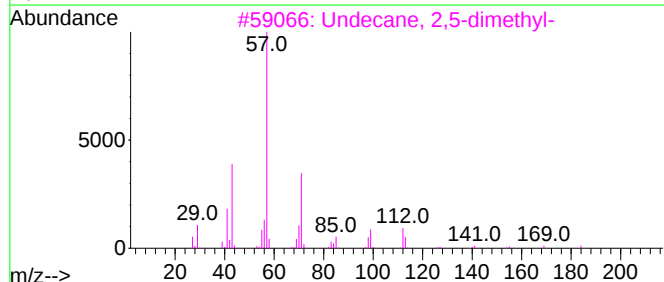
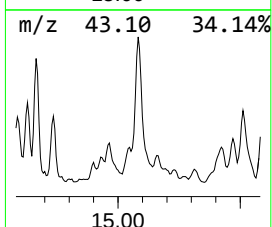
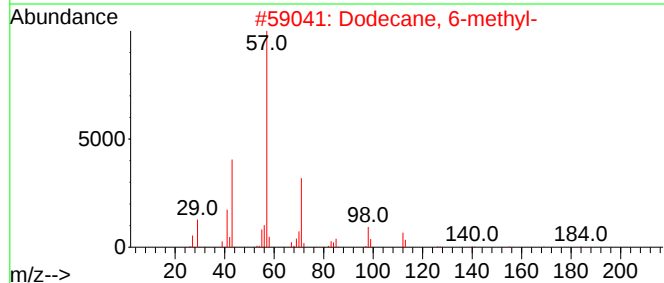
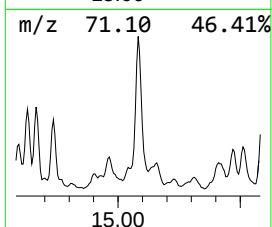
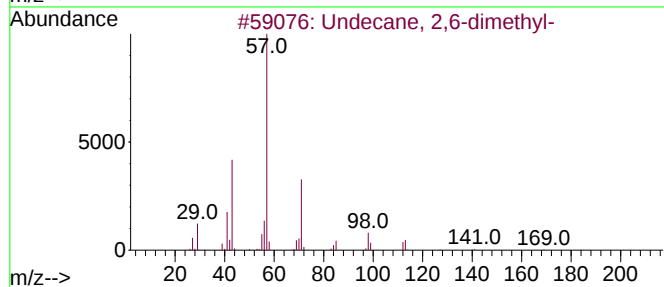
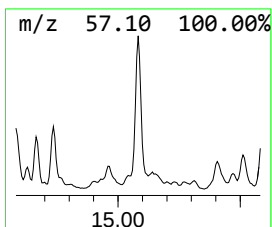
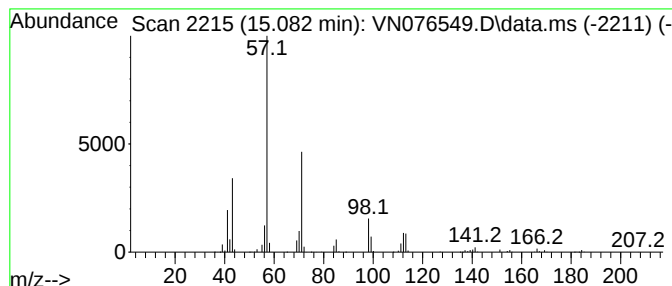
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Quant Title : SW846 8260

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

Peak Number 5 Undecane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.082	164.38 ug/l	5866360	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	95
2			Dodecane, 6-methyl-	184	C13H28	006044-71-9	76
3			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	70
4			Tridecane, 6-methyl-	198	C14H30	013287-21-3	64
5			Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020623\
Data File : VN076549.D
Acq On : 06 Feb 2023 18:12
Operator : JC\MD
Sample : 01407-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30984

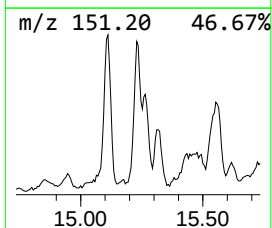
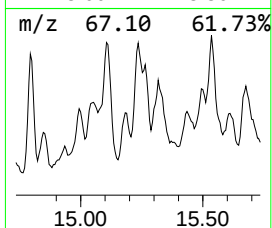
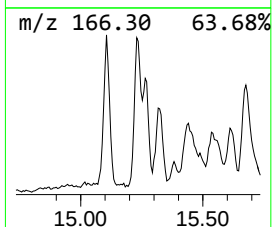
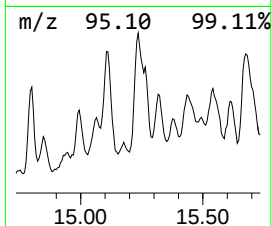
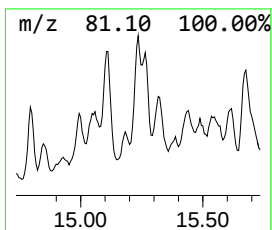
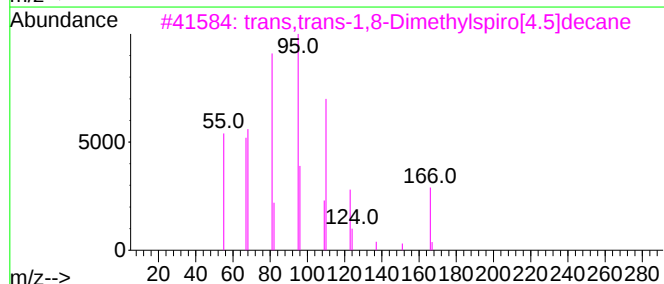
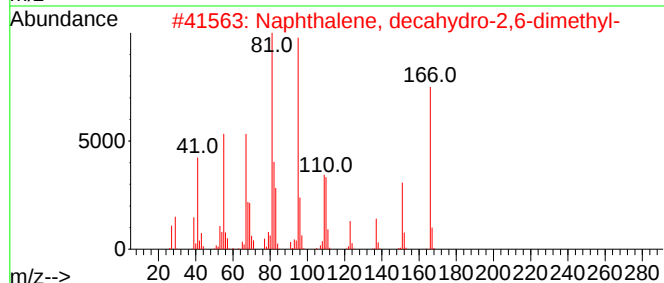
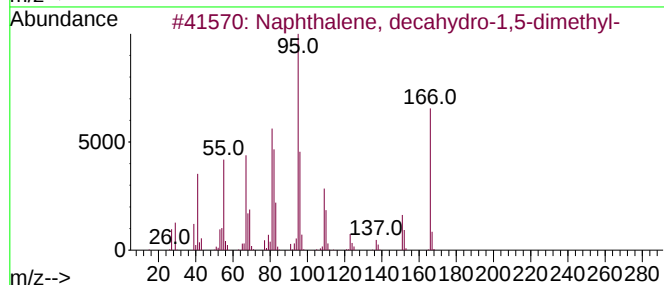
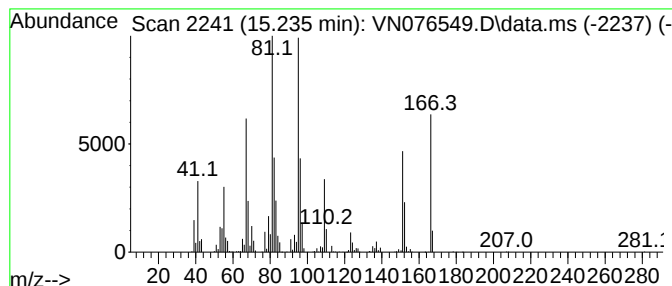
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, decahydro-1,5-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.235	33.92 ug/l	1210440	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-1,5-dimet...	166	C12H22	066552-62-3	86
2			Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	83
3			trans,trans-1,8-Dimethylspiro[4...	166	C12H22	1000111-72-8	74
4			9-Methylbicyclo[3.3.1]nonane	138	C10H18	025107-01-1	70
5			cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020623\
Data File : VN076549.D
Acq On : 06 Feb 2023 18:12
Operator : JC\MD
Sample : 01407-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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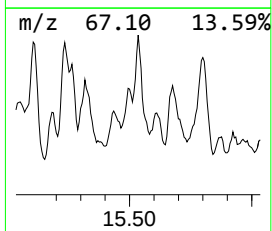
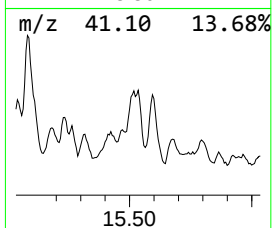
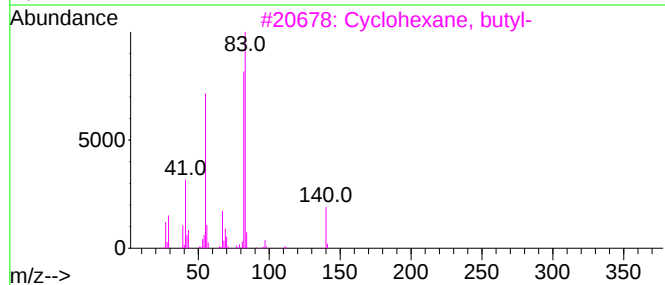
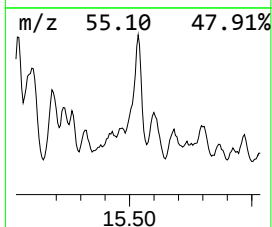
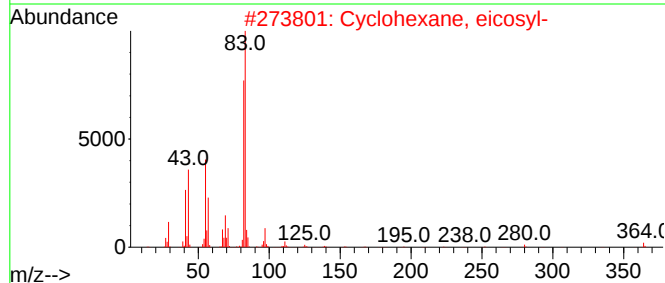
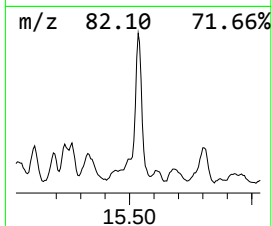
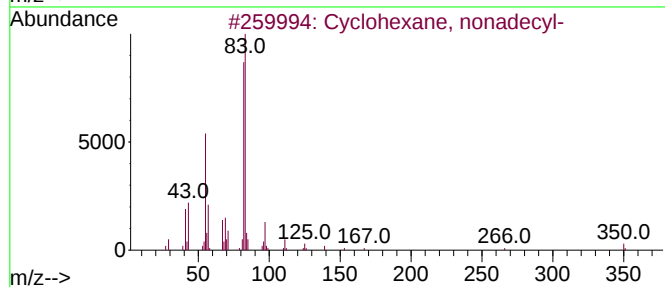
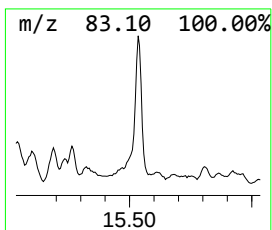
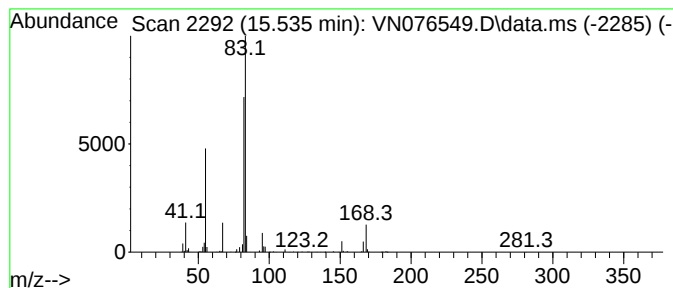
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexane, nonadecyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.535	78.57 ug/l	2804210	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, nonadecyl-	350	C25H50	022349-03-7	72
2			Cyclohexane, eicosyl-	364	C26H52	004443-55-4	72
3			Cyclohexane, butyl-	140	C10H20	001678-93-9	72
4			Cyclohexane, hexyl-	168	C12H24	004292-75-5	72
5			Cyclohexane, decyl-	224	C16H32	001795-16-0	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020623\
Data File : VN076549.D
Acq On : 06 Feb 2023 18:12
Operator : JC\MD
Sample : 01407-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30984

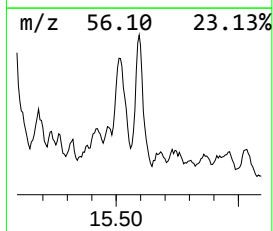
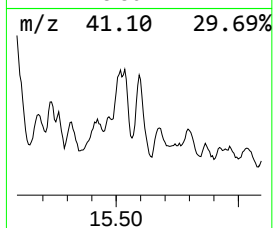
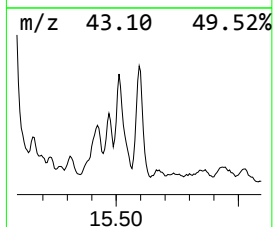
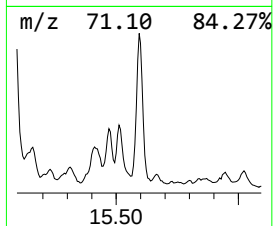
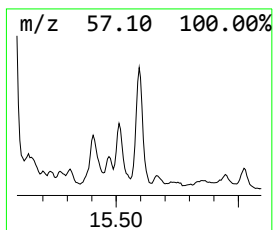
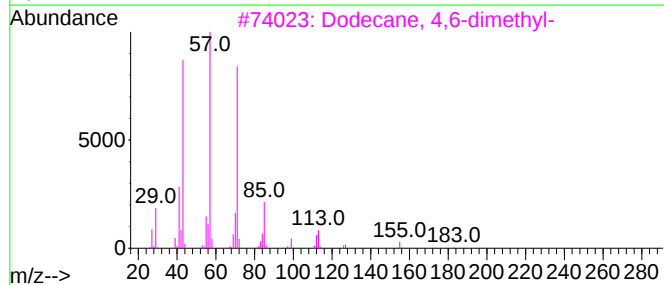
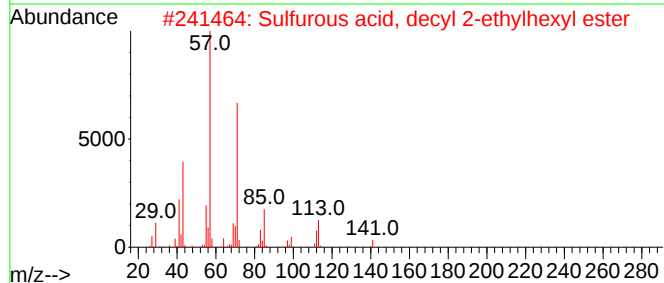
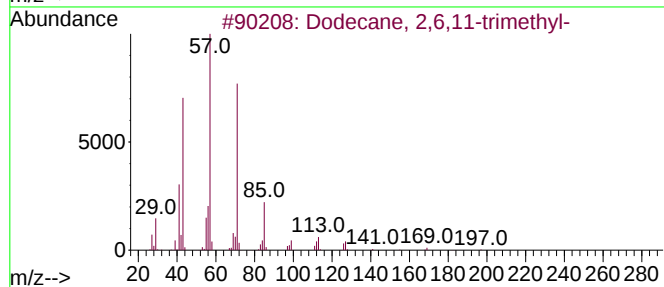
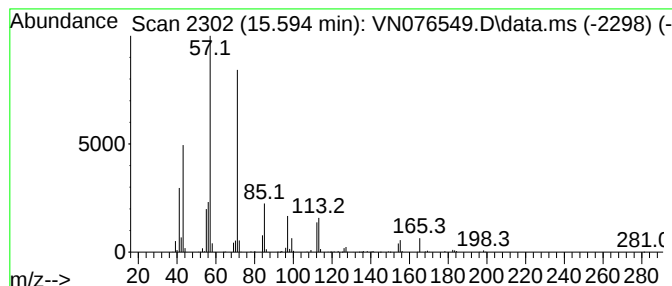
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Quant Title : SW846 8260

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

Peak Number 8 Dodecane, 2,6,11-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.594	72.84 ug/l	2599520	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
2			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	64
3			Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	64
4			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
5			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020623\
Data File : VN076549.D
Acq On : 06 Feb 2023 18:12
Operator : JC\MD
Sample : 01407-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30984

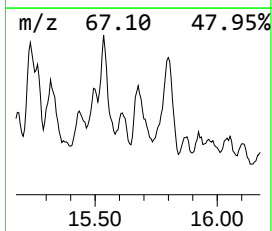
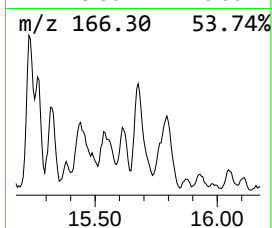
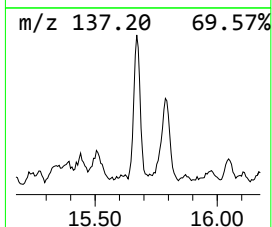
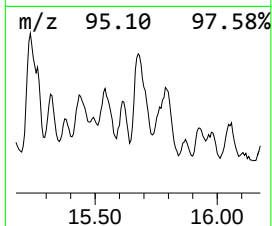
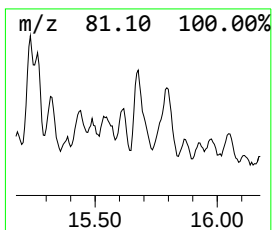
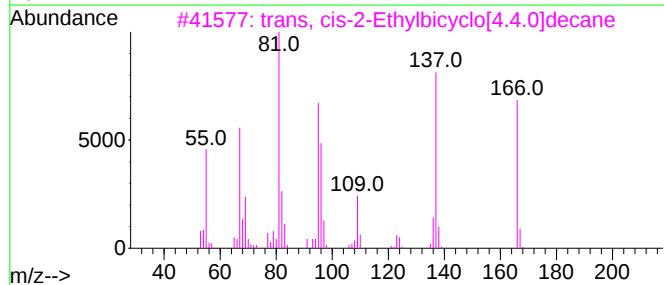
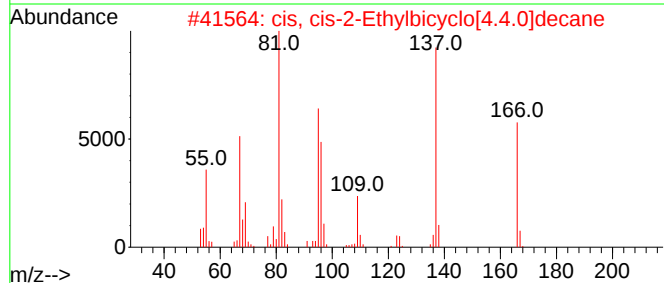
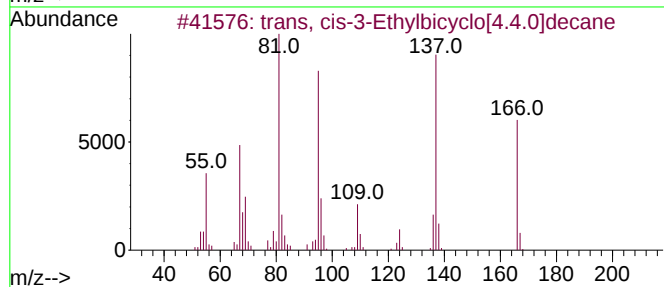
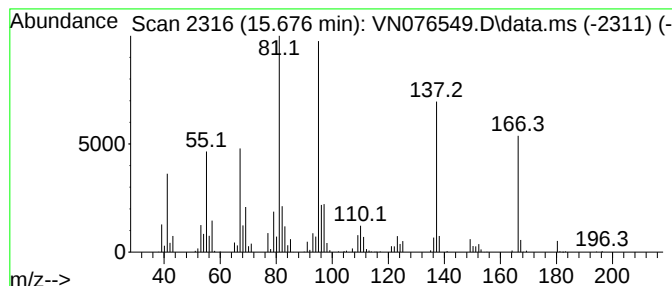
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Quant Title : SW846 8260

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

Peak Number 9 trans, cis-3-Ethylbicyclo[4... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.676	53.25 ug/l	1900400	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	91
2			cis, cis-2-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-40-0	68
3			trans, cis-2-Ethylbicyclo[4.4.0]...	166	C12H22	066660-39-7	68
4			trans,trans-3-Ethylbicyclo[4.4.0]...	166	C12H22	058462-32-1	64
5			Cyclohexene, 4-methyl-1-(1-methy...	138	C10H18	000500-00-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020623\
Data File : VN076549.D
Acq On : 06 Feb 2023 18:12
Operator : JC\MD
Sample : 01407-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30984

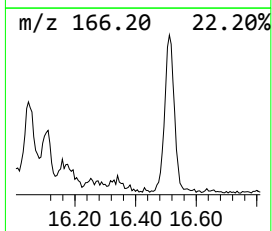
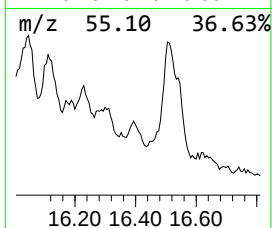
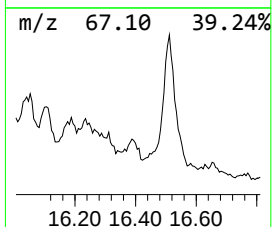
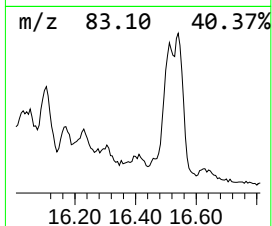
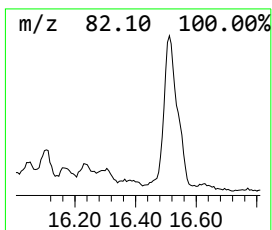
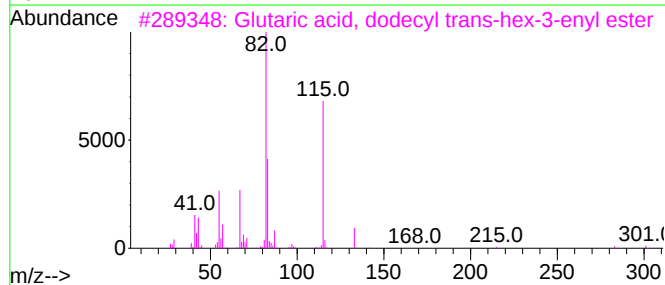
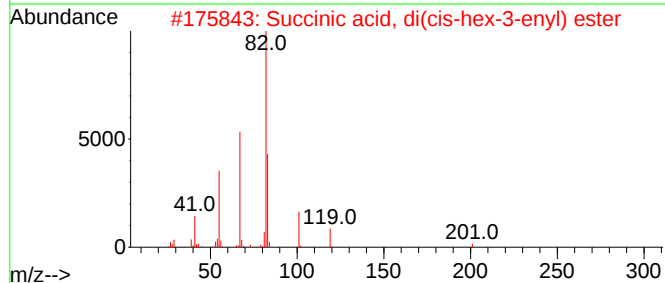
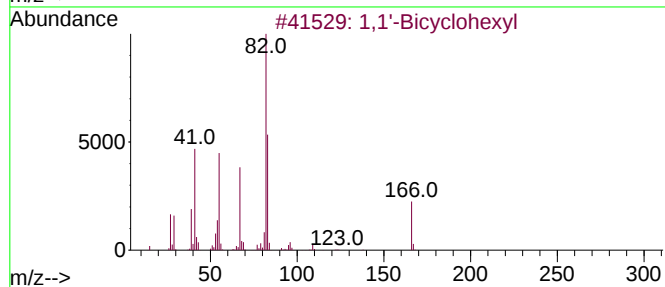
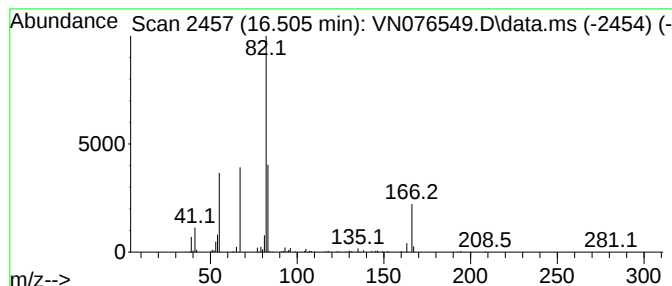
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020623W.M
Quant Title : SW846 8260

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

Peak Number 10 1,1'-Bicyclohexyl Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.506	33.98 ug/l	1212830	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1'-Bicyclohexyl	166	C12H22	000092-51-3	78
2			Succinic acid, di(cis-hex-3-enyl...)	282	C16H26O4	1000353-42-2	50
3			Glutaric acid, dodecyl trans-hex...	382	C23H42O4	1010359-93-2	50
4			Succinic acid, di(trans-hex-3-en...	282	C16H26O4	1000353-43-7	39
5			Glutaric acid, nonyl trans-hex-3...	340	C20H36O4	1000359-92-9	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020623\
Data File : VN076549.D
Acq On : 06 Feb 2023 18:12
Operator : JC\MD
Sample : 01407-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020623W.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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Cyclohexane, (1...	14.629	69.2	ug/l	2469600	4	13.794	1784440	50.0
Undecane, 3-met...	14.735	39.1	ug/l	1395100	4	13.794	1784440	50.0
Cyclohexane, 1-...	15.047	47.3	ug/l	1688740	4	13.794	1784440	50.0
Undecane, 2,6-d...	15.082	164.4	ug/l	5866360	4	13.794	1784440	50.0
Naphthalene, de...	15.235	33.9	ug/l	1210440	4	13.794	1784440	50.0
Cyclohexane, no...	15.535	78.6	ug/l	2804210	4	13.794	1784440	50.0
Dodecane, 2,6,1...	15.594	72.8	ug/l	2599520	4	13.794	1784440	50.0
trans, cis-3-Et...	15.676	53.3	ug/l	1900400	4	13.794	1784440	50.0
1,1'-Bicyclohexyl	16.506	34.0	ug/l	1212830	4	13.794	1784440	50.0