

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100724\
 Data File : VN084329.D
 Acq On : 07 Oct 2024 13:09
 Operator : JC\MD
 Sample : P4278-01
 Misc : 1.40g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 BUR-1300

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\82N093024W.M
 Title : SW846 8260

Signal : TIC: VN084329.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	47	57	63	rBV3	10854	23896	2.25%	0.239%
2	2.889	133	159	160	rBV5	18103	72664	6.84%	0.728%
3	5.024	511	522	534	rBV3	3696	13012	1.22%	0.130%
4	8.165	1046	1056	1060	rBV	129747	310705	29.23%	3.113%
5	8.218	1060	1065	1080	rVB	237015	526397	49.52%	5.273%
6	8.577	1117	1126	1135	rBV	143867	326919	30.75%	3.275%
7	9.100	1205	1215	1225	rBV	335566	690087	64.92%	6.913%
8	10.565	1455	1464	1472	rBV	516769	929946	87.48%	9.316%
9	11.865	1678	1685	1695	rBV	437107	767203	72.17%	7.686%
10	12.612	1808	1812	1817	rVB3	10430	14982	1.41%	0.150%
11	12.847	1843	1852	1861	rBV	314685	537761	50.59%	5.387%
12	13.788	2005	2012	2021	rBV	385560	661523	62.23%	6.627%
13	13.865	2021	2025	2033	rVB4	6600	11670	1.10%	0.117%
14	14.453	2115	2125	2132	rBV5	36346	121345	11.42%	1.216%
15	14.529	2132	2138	2151	rBV2	283340	514459	48.40%	5.154%
16	14.629	2151	2155	2159	rBV	70322	107068	10.07%	1.073%
17	14.670	2159	2162	2164	rBV4	9790	13647	1.28%	0.137%
18	14.741	2169	2174	2175	rVV	122406	190725	17.94%	1.911%
19	14.770	2175	2179	2194	rVV2	344579	1063027	100.00%	10.649%
20	14.888	2194	2199	2221	rVB	212335	385657	36.28%	3.863%
21	15.106	2229	2236	2254	rBV	398892	702549	66.09%	7.038%
22	15.323	2270	2273	2279	rVB4	8568	12621	1.19%	0.126%
23	15.429	2286	2291	2293	rBV3	40064	63783	6.00%	0.639%
24	15.459	2293	2296	2304	rVB4	90071	159953	15.05%	1.602%
25	15.594	2313	2319	2322	rBV	92788	171791	16.16%	1.721%
26	15.635	2322	2326	2340	rVB2	208109	404059	38.01%	4.048%
27	16.011	2383	2390	2407	rBV	267757	560475	52.72%	5.615%
28	16.341	2434	2446	2451	rVV5	97001	254644	23.95%	2.551%
29	16.400	2451	2456	2469	rVB6	51331	138309	13.01%	1.386%
30	16.564	2472	2484	2489	rBV5	41958	119450	11.24%	1.197%
31	16.617	2489	2493	2501	rVB3	51903	111887	10.53%	1.121%

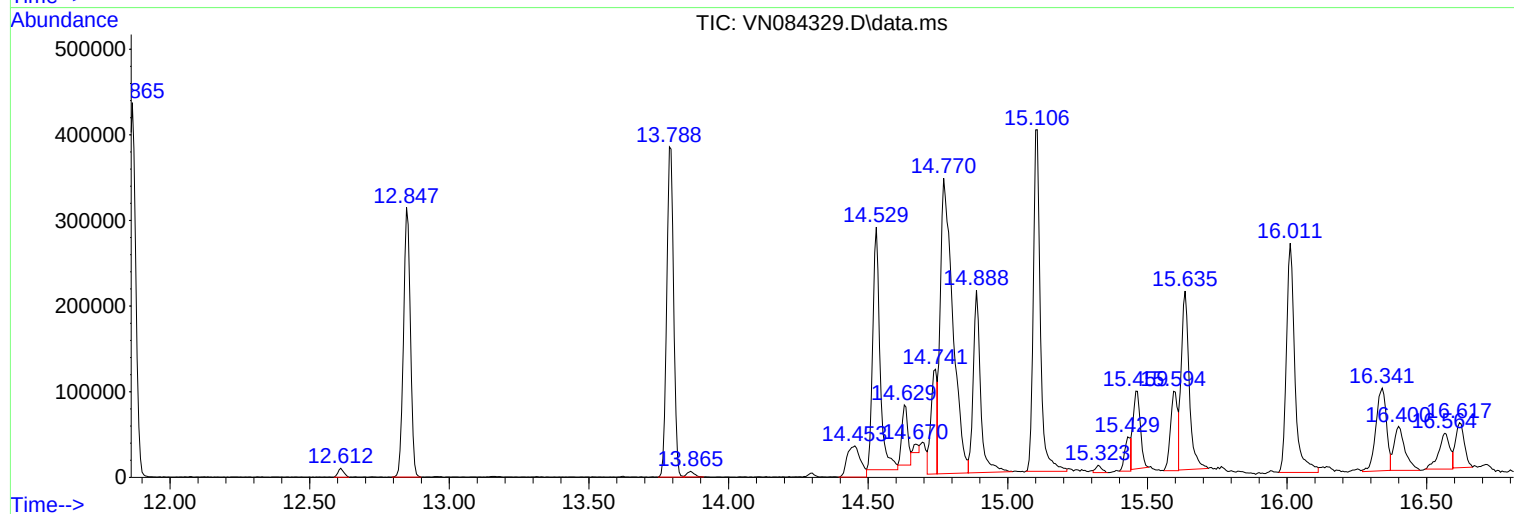
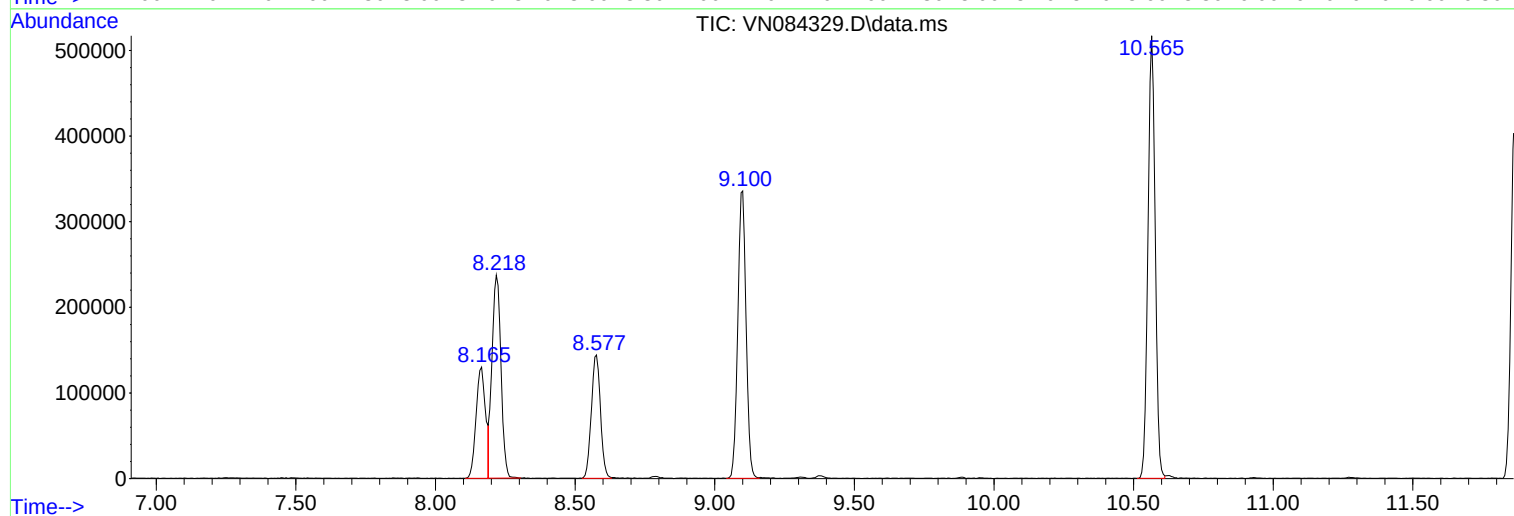
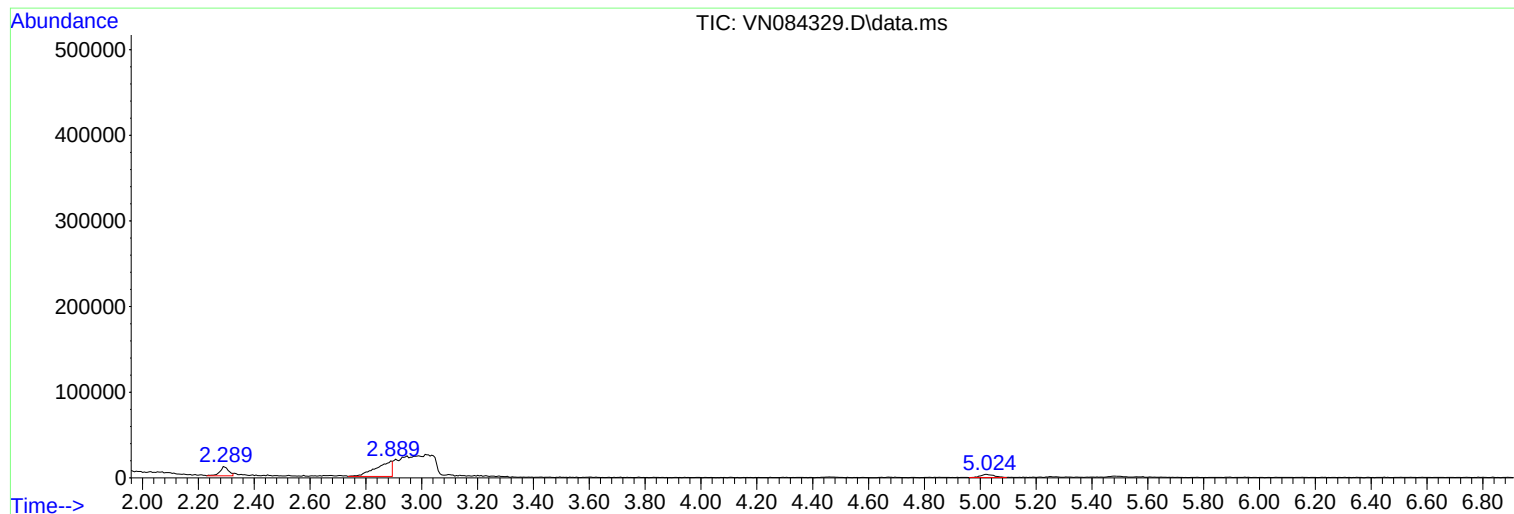
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Quant Title : SW846 8260

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



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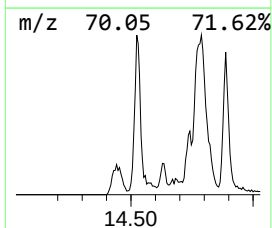
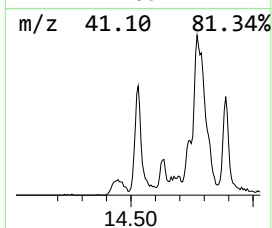
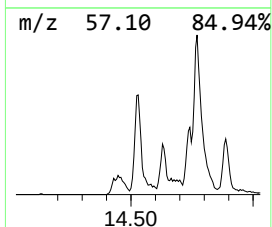
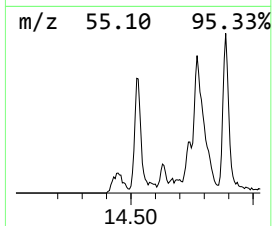
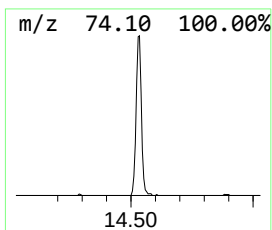
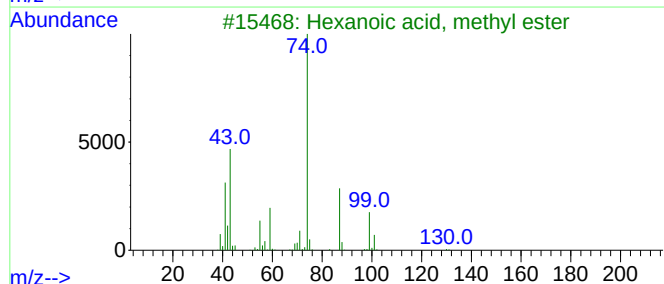
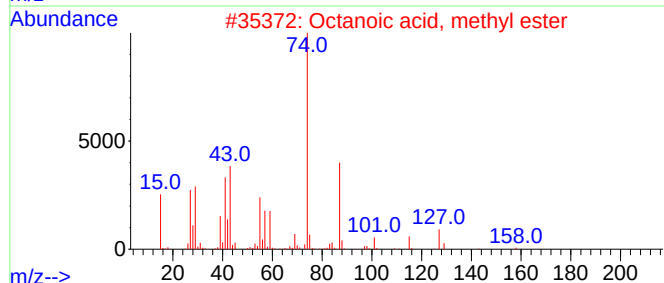
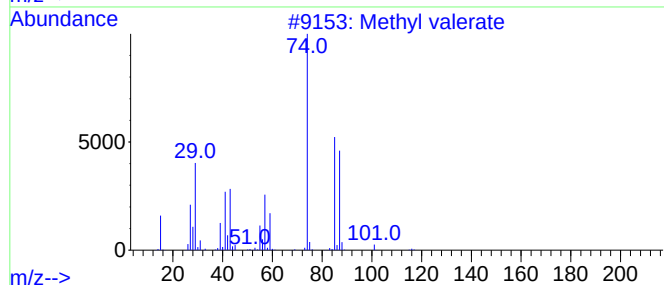
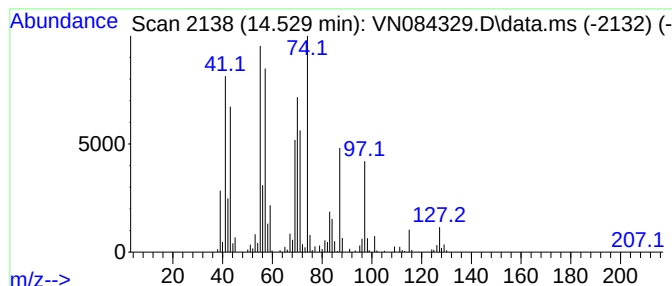
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N093024W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown14.529 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.529	38.88 ug/l	514459	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl valerate	116	C6H12O2	000624-24-8	38
2			Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	38
3			Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	30
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	22
5			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	22



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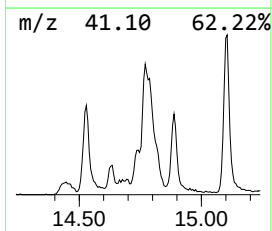
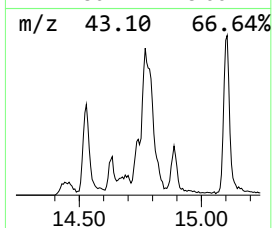
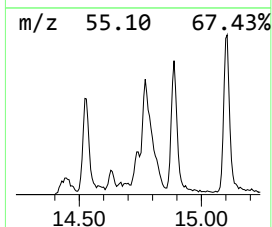
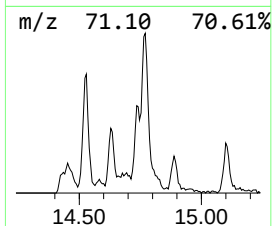
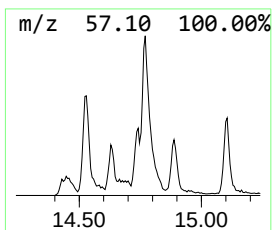
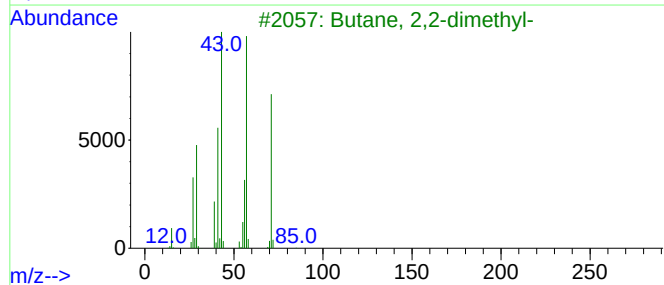
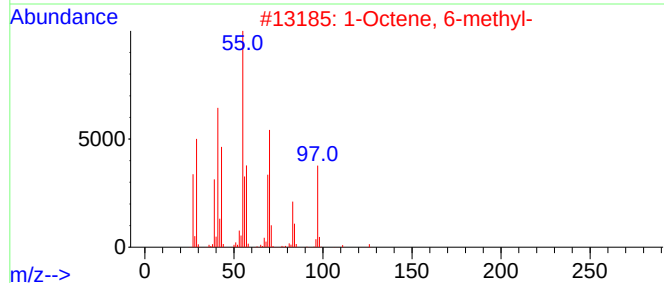
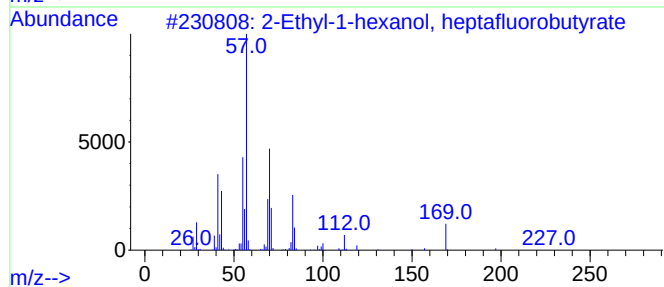
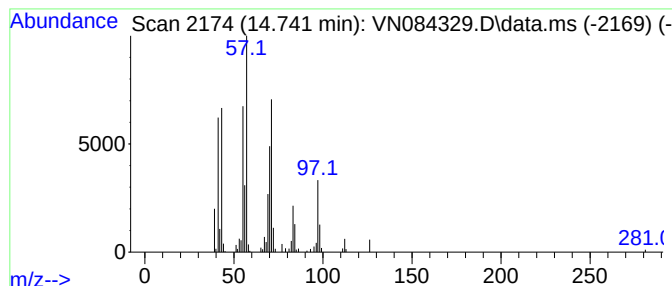
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N093024W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown14.741 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.741	14.42 ug/l	190725	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-1-hexanol, heptafluorobu...	326	C12H17F7O2	1000365-16-0	43
2			1-Octene, 6-methyl-	126	C9H18	013151-10-5	43
3			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	35
4			2-Octene, (E)-	112	C8H16	013389-42-9	30
5			2-Nonene, (E)-	126	C9H18	006434-78-2	30



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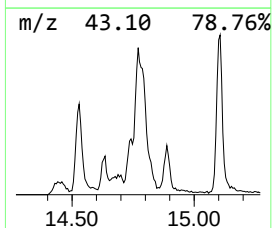
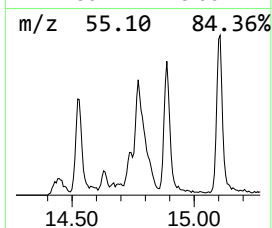
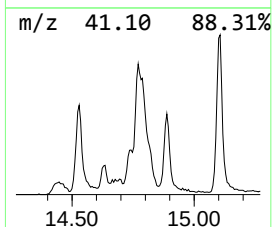
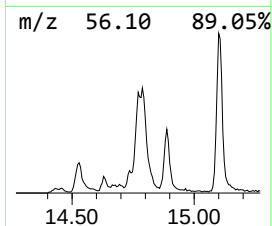
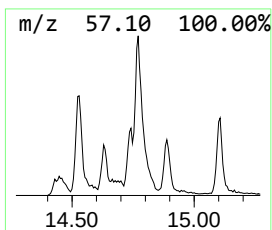
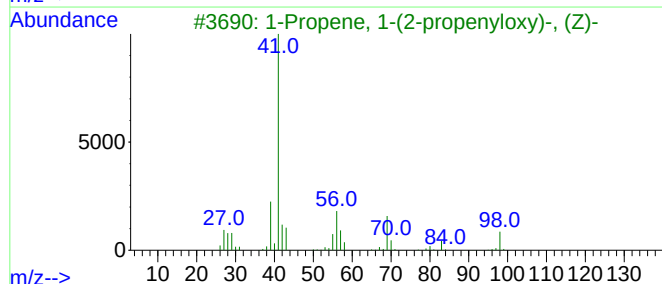
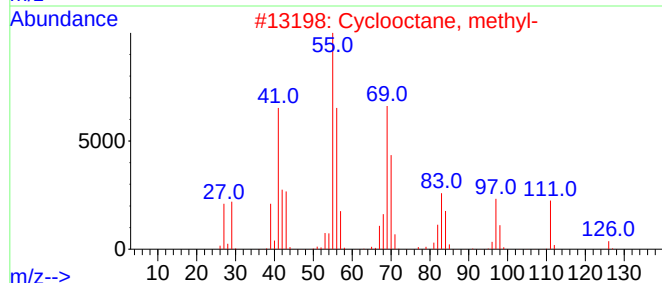
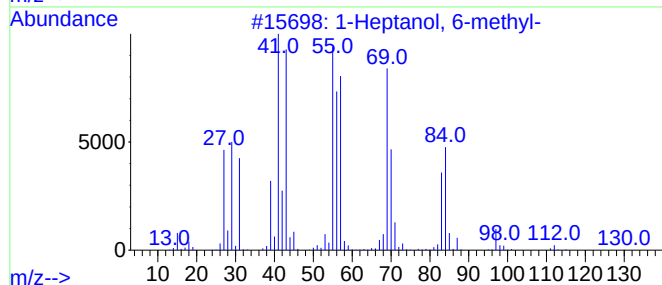
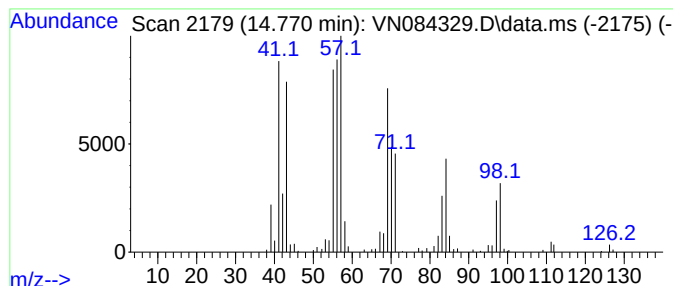
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1-Heptanol, 6-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.770	80.35 ug/l	1063030	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	59
2			Cyclooctane, methyl-	126	C9H18	001502-38-1	53
3			1-Propene, 1-(2-propenyloxy)-, (Z)-	98	C6H10O	061142-12-9	53
4			3-Heptene, (E)-	98	C7H14	014686-14-7	46
5			(Z)-3-Heptene	98	C7H14	007642-10-6	46



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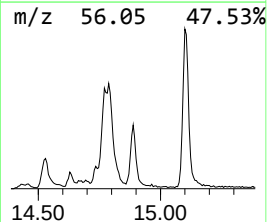
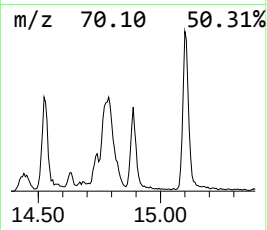
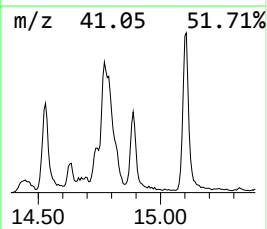
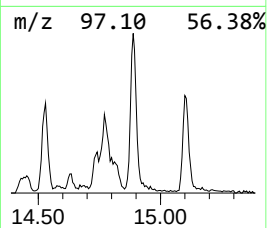
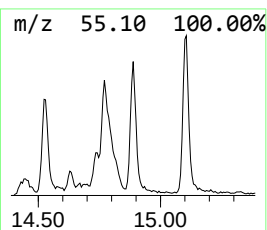
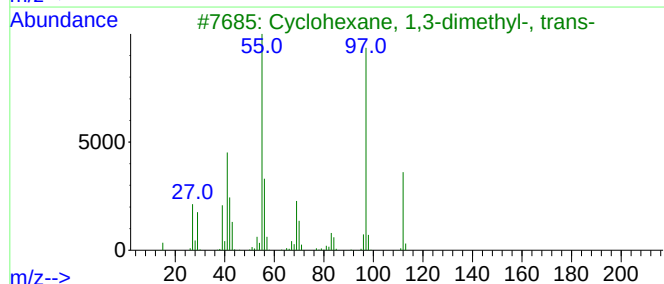
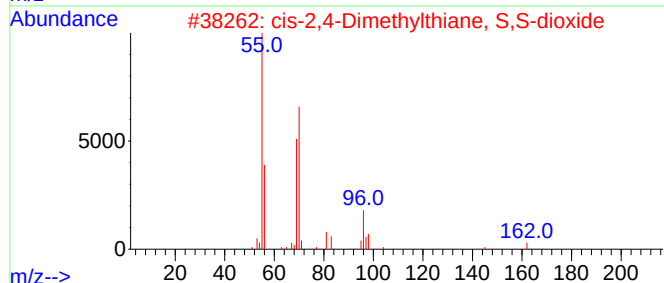
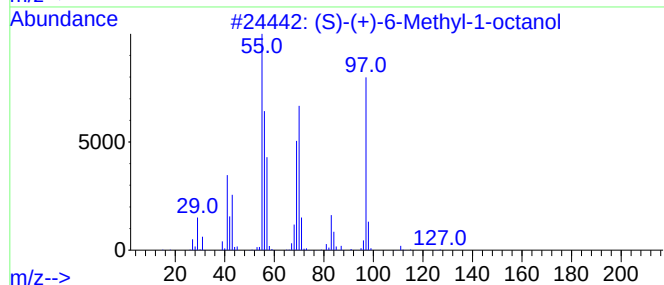
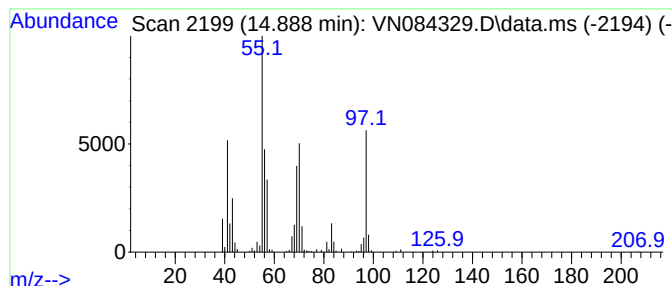
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Peak Number 4 (S)-(+)-6-Methyl-1-octanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.888	29.15 ug/l	385657	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	86
2			cis-2,4-Dimethylthiane, S,S-dioxide	162	C7H14O2S	1000215-67-5	50
3			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	47
4			Cyclopropane, 1-methyl-2-(3-meth...	140	C10H20	062238-07-7	47
5			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	47



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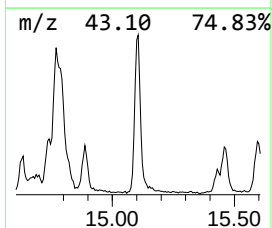
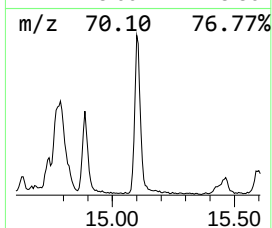
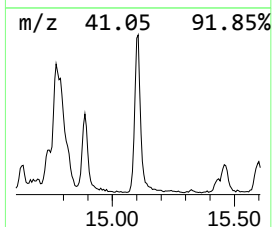
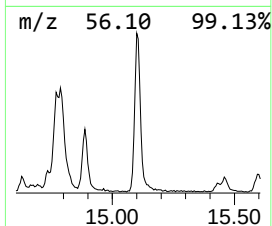
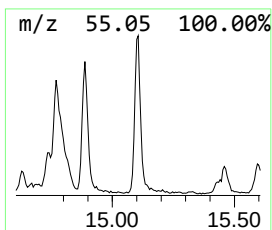
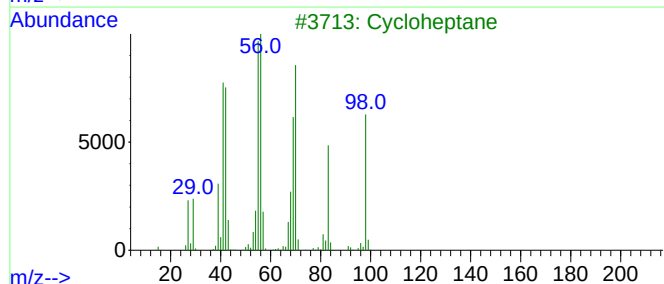
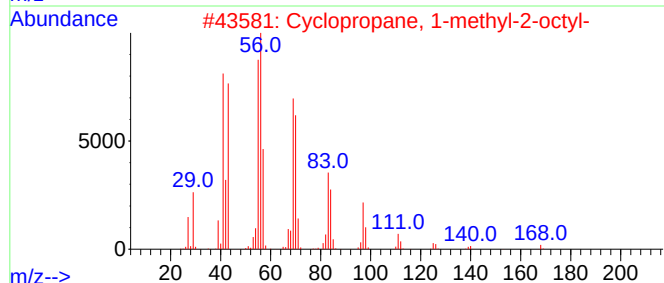
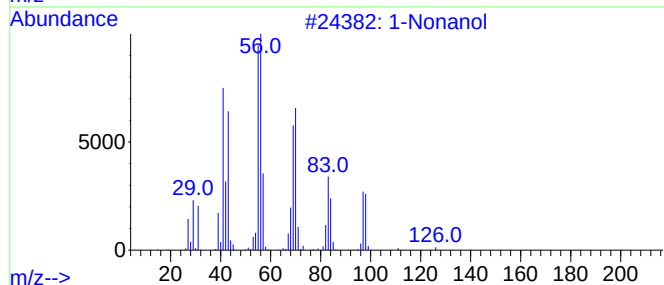
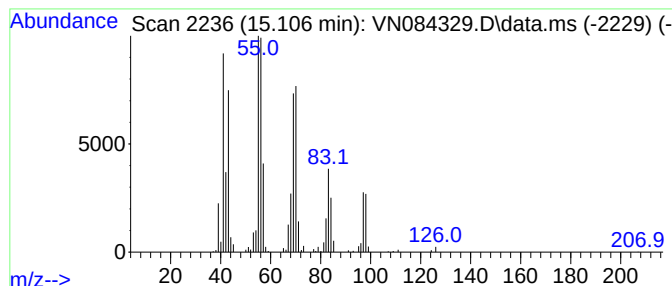
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Peak Number 5 1-Nonanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.106	53.10 ug/l	702549	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonanol	144	C9H20O	000143-08-8	91
2			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	86
3			Cycloheptane	98	C7H14	000291-64-5	83
4			1-Decanol	158	C10H22O	000112-30-1	72
5			Isopropylcyclobutane	98	C7H14	000872-56-0	53



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BUR-1300

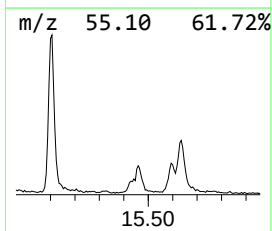
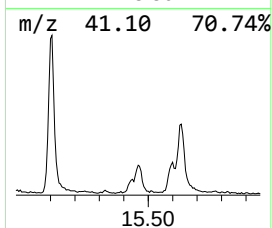
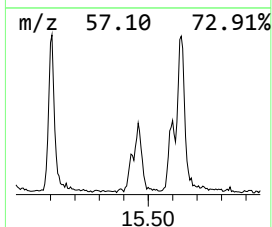
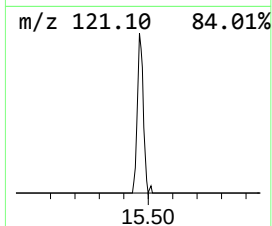
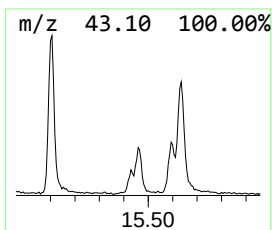
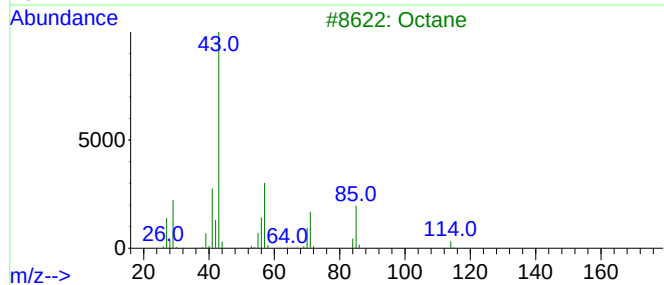
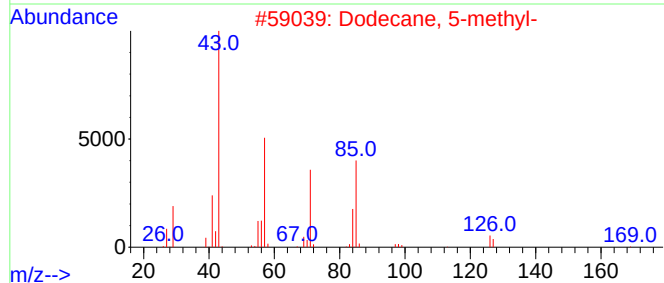
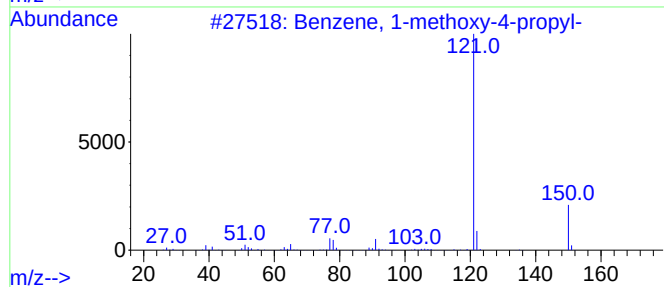
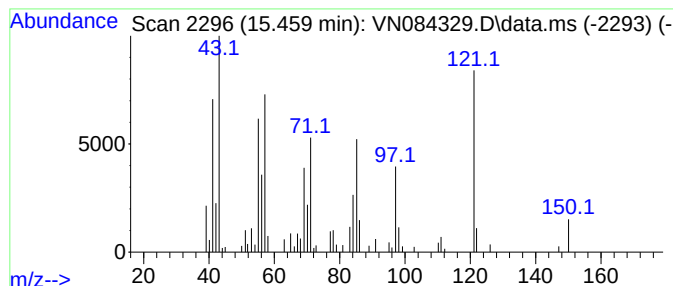
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Quant Title : SW846 8260

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

Peak Number 6 unknown15.459 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.459	12.09 ug/l	159953	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	30
2			Dodecane, 5-methyl-	184	C13H28	017453-93-9	27
3			Octane	114	C8H18	000111-65-9	27
4			5-Eicosene, (E)-	280	C20H40	074685-30-6	27
5			Nonane	128	C9H20	000111-84-2	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100724\
Data File : VN084329.D
Acq On : 07 Oct 2024 13:09
Operator : JC\MD
Sample : P4278-01
Misc : 1.40g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1300

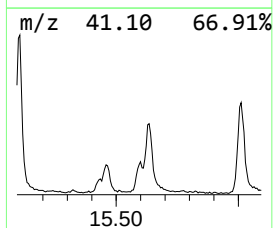
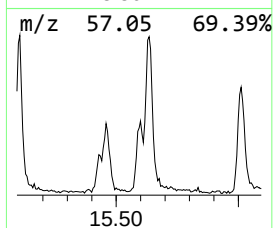
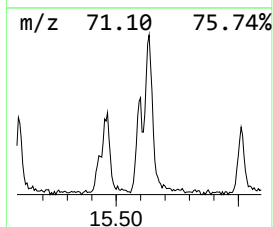
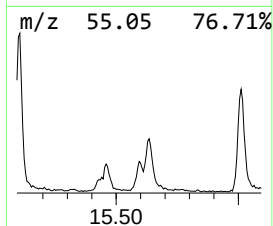
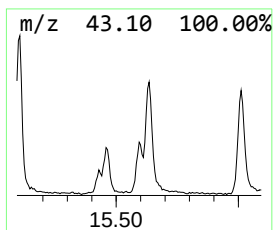
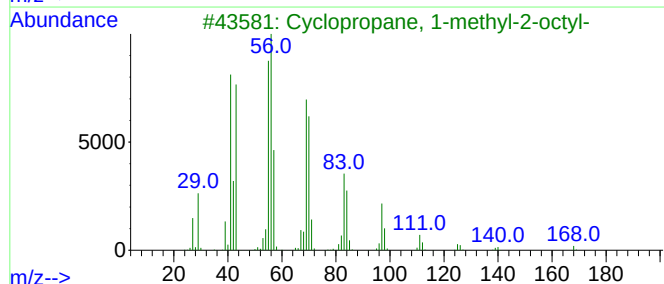
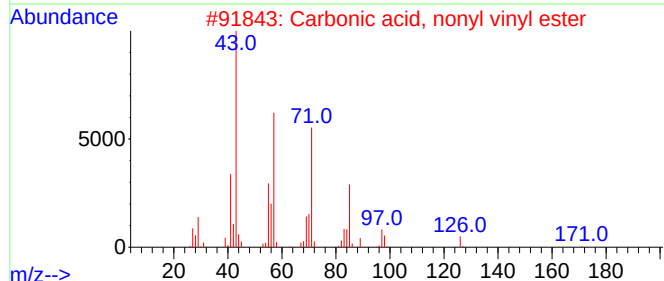
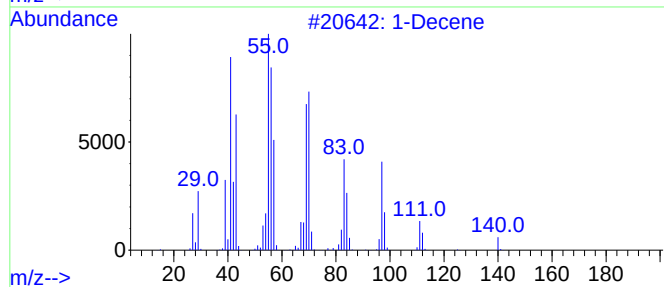
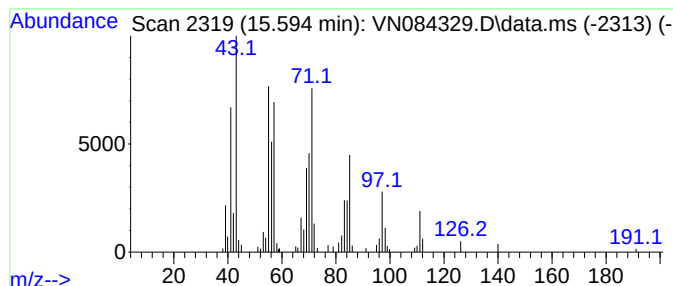
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Quant Title : SW846 8260

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

Peak Number 7 1-Decene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.594	12.98 ug/l	171791	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decene	140	C10H20	000872-05-9	89
2			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	53
3			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	46
4			2-Dodecene, (Z)-	168	C12H24	007206-26-0	38
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100724\
Data File : VN084329.D
Acq On : 07 Oct 2024 13:09
Operator : JC\MD
Sample : P4278-01
Misc : 1.40g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1300

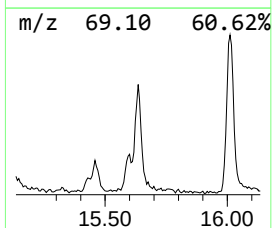
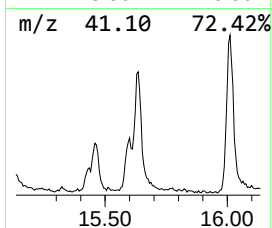
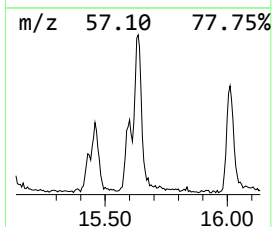
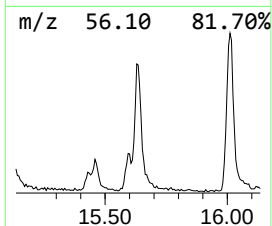
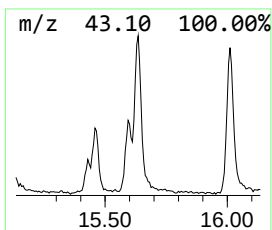
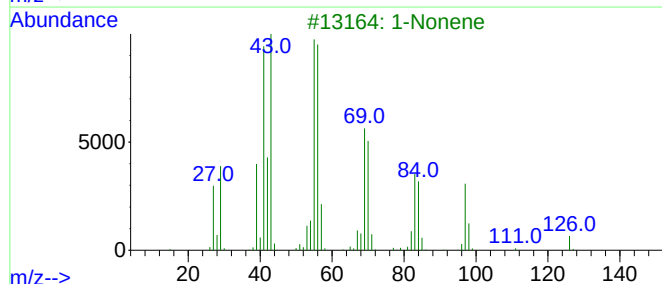
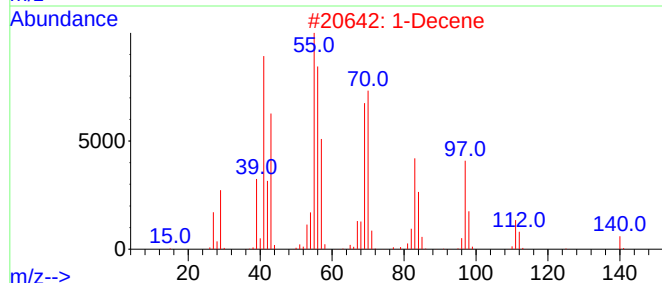
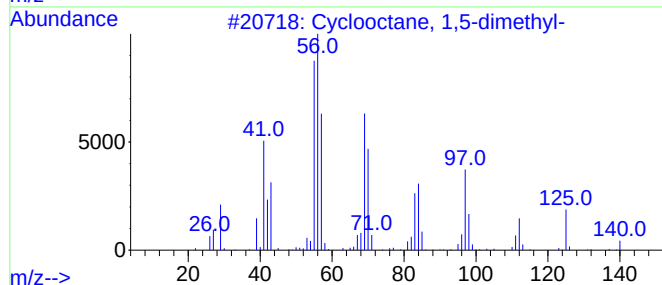
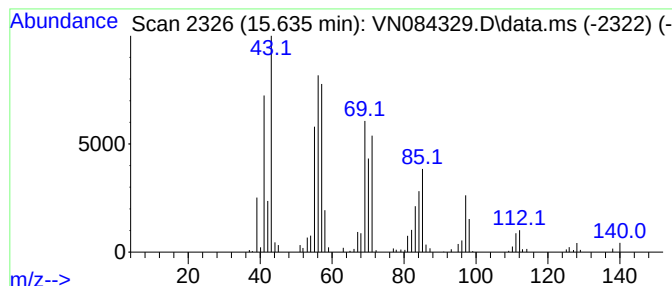
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Quant Title : SW846 8260

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

Peak Number 8 Cyclooctane, 1,5-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.635	30.54 ug/l	404059	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctane, 1,5-dimethyl-	140	C10H20	021328-57-4	93
2			1-Decene	140	C10H20	000872-05-9	50
3			1-Nonene	126	C9H18	000124-11-8	49
4			Cyclopentane, 1,1,2-trimethyl-	112	C8H16	004259-00-1	45
5			1,3-Cyclohexanedione, 4,5-dimethyl-	140	C8H12O2	042824-00-0	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100724\
Data File : VN084329.D
Acq On : 07 Oct 2024 13:09
Operator : JC\MD
Sample : P4278-01
Misc : 1.40g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1300

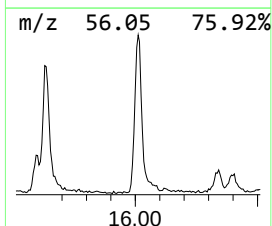
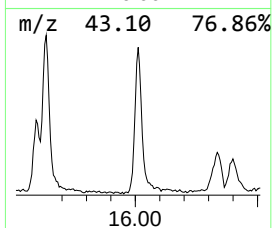
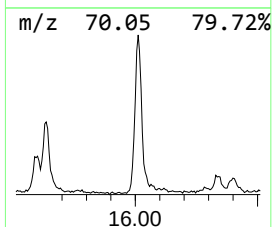
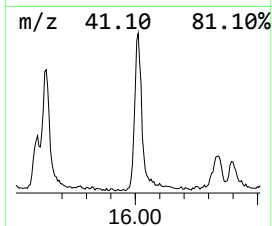
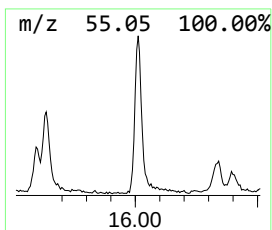
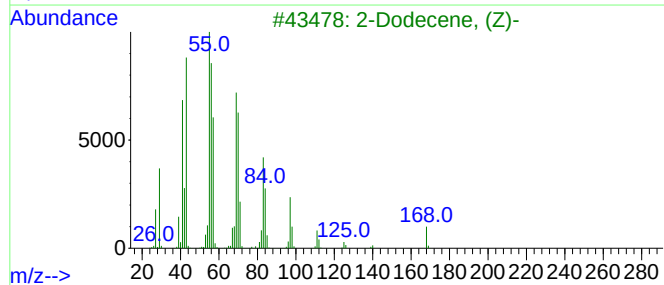
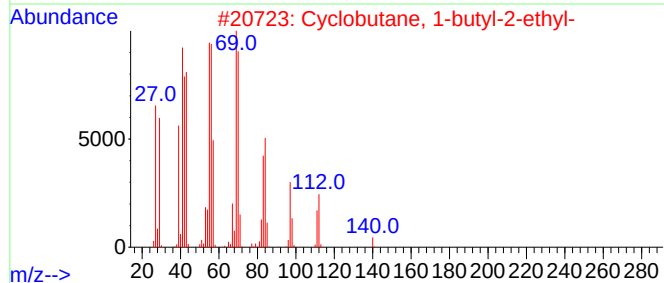
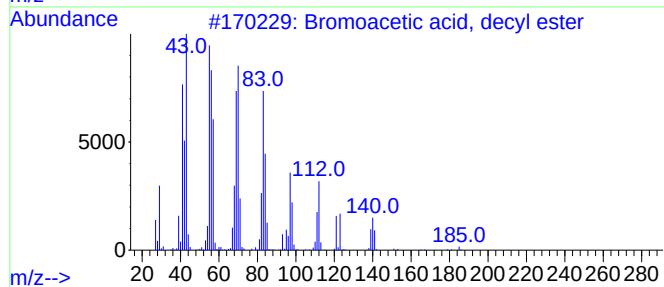
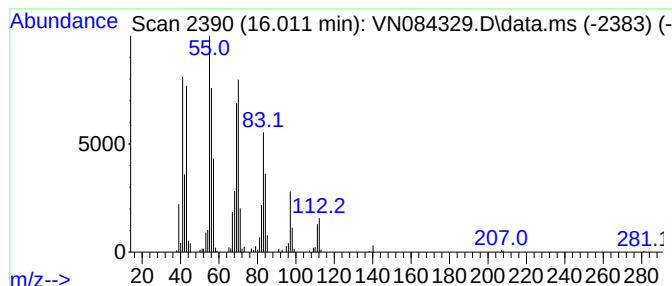
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Quant Title : SW846 8260

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

Peak Number 9 Bromoacetic acid, decyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.012	42.36 ug/l	560475	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, decyl ester	278	C12H23BrO2	005436-93-1	91
2			Cyclobutane, 1-butyl-2-ethyl-	140	C10H20	1010150-67-3	89
3			2-Dodecene, (Z)-	168	C12H24	007206-26-0	87
4			1-Decanol	158	C10H22O	000112-30-1	87
5			1-Undecanol	172	C11H24O	000112-42-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100724\
Data File : VN084329.D
Acq On : 07 Oct 2024 13:09
Operator : JC\MD
Sample : P4278-01
Misc : 1.40g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1300

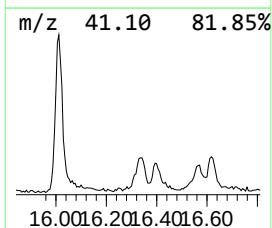
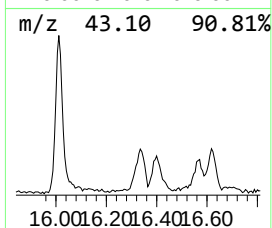
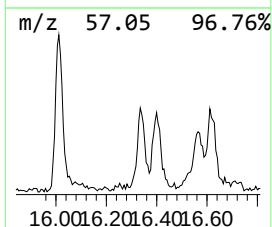
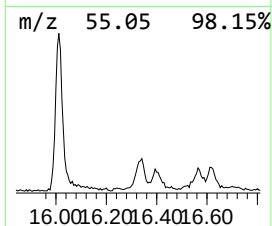
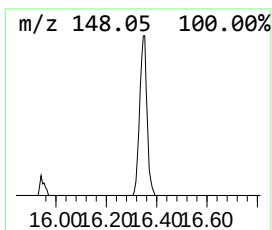
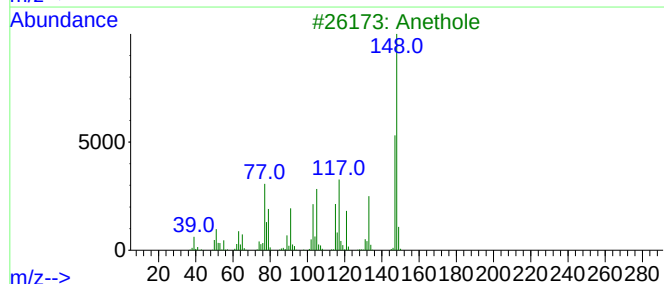
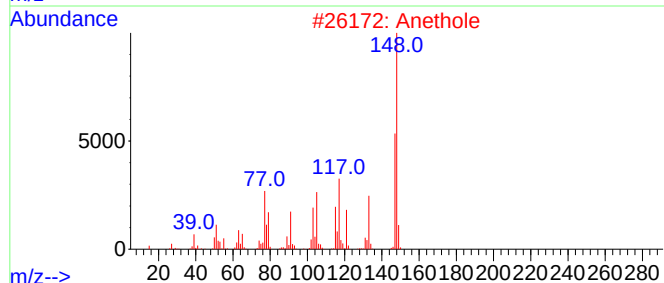
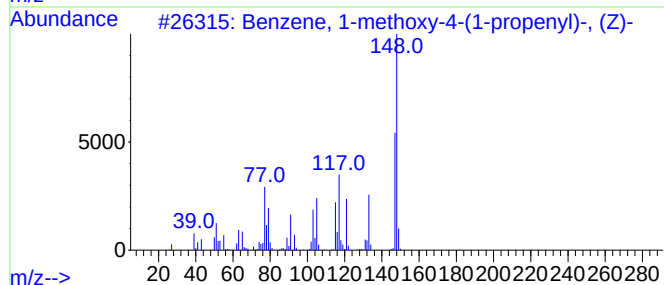
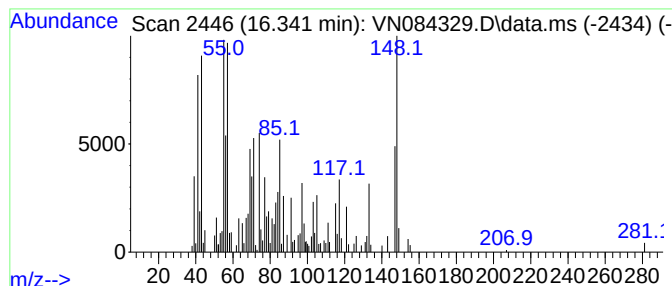
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-methoxy-4-(1-pro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.341	19.25 ug/l	254644	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methoxy-4-(1-propenyl...	148	C10H12O	025679-28-1	96
2			Anethole	148	C10H12O	000104-46-1	96
3			Anethole	148	C10H12O	004180-23-8	96
4			Estragole	148	C10H12O	000140-67-0	64
5			N-Acetyl-D-phenylalanine	207	C11H13NO3	010172-89-1	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100724\
Data File : VN084329.D
Acq On : 07 Oct 2024 13:09
Operator : JC\MD
Sample : P4278-01
Misc : 1.40g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1300

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N093024W.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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unknown14.741	14.741	14.4	ug/l	190725	4	13.794	661523	50.0
1-Heptanol, 6-m...	14.770	80.3	ug/l	1063030	4	13.794	661523	50.0
(S)-(+)-6-Methy...	14.888	29.1	ug/l	385657	4	13.794	661523	50.0
1-Nonanol	15.106	53.1	ug/l	702549	4	13.794	661523	50.0
unknown15.459	15.459	12.1	ug/l	159953	4	13.794	661523	50.0
1-Decene	15.594	13.0	ug/l	171791	4	13.794	661523	50.0
Cyclooctane, 1,...	15.635	30.5	ug/l	404059	4	13.794	661523	50.0
Bromoacetic aci...	16.012	42.4	ug/l	560475	4	13.794	661523	50.0
Benzene, 1-meth...	16.341	19.3	ug/l	254644	4	13.794	661523	50.0