

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
 Data File : VN071324.D
 Acq On : 16 Mar 2022 16:48
 Operator : JC\MD
 Sample : N1886-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 2822-A

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\82N030722W.M
 Title : SW846 8260

Signal : TIC: VN071324.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.281	380	390	402	rBV	978114	2847280	15.29%	2.343%
2	4.569	424	439	454	rBV	382253	1259447	6.76%	1.036%
3	4.851	477	487	500	rVB	98626	312552	1.68%	0.257%
4	7.063	850	863	874	rBV3	138604	445941	2.39%	0.367%
5	7.334	895	909	921	rBV2	129323	396375	2.13%	0.326%
6	8.022	1014	1026	1031	rBV	606763	1519857	8.16%	1.250%
7	8.081	1031	1036	1053	rVB	1205825	2731282	14.67%	2.247%
8	8.434	1085	1096	1110	rBV	728312	1728744	9.28%	1.422%
9	8.963	1177	1186	1197	rBV	1770368	3615507	19.42%	2.975%
10	9.151	1210	1218	1236	rBV	519098	1244930	6.69%	1.024%
11	9.410	1254	1262	1273	rVB	158545	322184	1.73%	0.265%
12	10.328	1411	1418	1426	rBV	388895	704294	3.78%	0.579%
13	10.439	1429	1437	1445	rVV	2846454	5158999	27.71%	4.244%
14	10.533	1449	1453	1460	rVB	99706	188486	1.01%	0.155%
15	10.945	1514	1523	1537	rBV	1361639	2542107	13.65%	2.091%
16	11.127	1549	1554	1559	rVV	215830	376419	2.02%	0.310%
17	11.457	1604	1610	1625	rVB	242963	467228	2.51%	0.384%
18	11.739	1647	1658	1668	rBV	2541719	4668692	25.07%	3.841%
19	11.945	1686	1693	1706	rVB	309712	624859	3.36%	0.514%
20	12.727	1819	1826	1835	rVB	2091420	3495557	18.77%	2.876%
21	12.816	1835	1841	1848	rBV	475087	908663	4.88%	0.748%
22	12.927	1855	1860	1867	rBV	299178	476778	2.56%	0.392%
23	13.051	1877	1881	1894	rVB2	159109	292382	1.57%	0.241%
24	13.304	1911	1924	1937	rBV7	80348	327909	1.76%	0.270%
25	13.516	1955	1960	1966	rVB4	108227	195001	1.05%	0.160%
26	13.580	1966	1971	1978	rBV2	300345	497165	2.67%	0.409%
27	13.668	1979	1986	1993	rBV	2124219	3714200	19.95%	3.056%
28	13.763	1993	2002	2010	rVV	2206659	4553199	24.45%	3.746%
29	13.833	2010	2014	2024	rVB4	183366	428846	2.30%	0.353%
30	13.986	2035	2040	2044	rBV	234134	369266	1.98%	0.304%
31	14.027	2044	2047	2056	rVB3	152945	234561	1.26%	0.193%
32	14.133	2059	2065	2073	rBV	661616	1168415	6.28%	0.961%
33	14.339	2088	2100	2106	rBV3	674570	2078026	11.16%	1.710%
34	14.416	2106	2113	2122	rBV	8301742	13376114	71.84%	11.005%
35	14.521	2126	2131	2135	rBV	941750	1422208	7.64%	1.170%
36	14.563	2135	2138	2139	rBV2	184639	212980	1.14%	0.175%

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Peak Location: TOP

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

Peak separation: 5

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37	14.586	2139	2142	2144	rBV	342335	410284	2.20%	0.338%
38	14.627	2144	2149	2151	rBV	3306383	5073590	27.25%	4.174%
39	14.668	2151	2156	2161	rBV3	7247488	18620025	100.00%	15.319%
40	14.780	2170	2175	2181	rVB	4120478	6134765	32.95%	5.047%
41	14.992	2201	2211	2218	rBV4	1261038	3437482	18.46%	2.828%
42	15.104	2219	2230	2231	rVV5	847913	2160163	11.60%	1.777%
43	15.133	2232	2235	2237	rVV2	1264167	2028408	10.89%	1.669%
44	15.163	2238	2240	2244	rVV2	1559263	2778667	14.92%	2.286%
45	15.198	2244	2246	2255	rVV3	1298932	3274817	17.59%	2.694%
46	15.286	2255	2261	2265	rVV	1406528	3205220	17.21%	2.637%
47	15.333	2266	2269	2274	rVV2	1104190	2204924	11.84%	1.814%
48	15.398	2274	2280	2282	rVV	835283	1960485	10.53%	1.613%
49	15.439	2284	2287	2295	rVV	1149838	2823780	15.17%	2.323%
50	15.527	2296	2302	2317	rVB4	657443	2068992	11.11%	1.702%
51	15.880	2357	2362	2373	rVB2	120738	247714	1.33%	0.204%
52	16.192	2411	2415	2422	rVB3	109559	212040	1.14%	0.174%

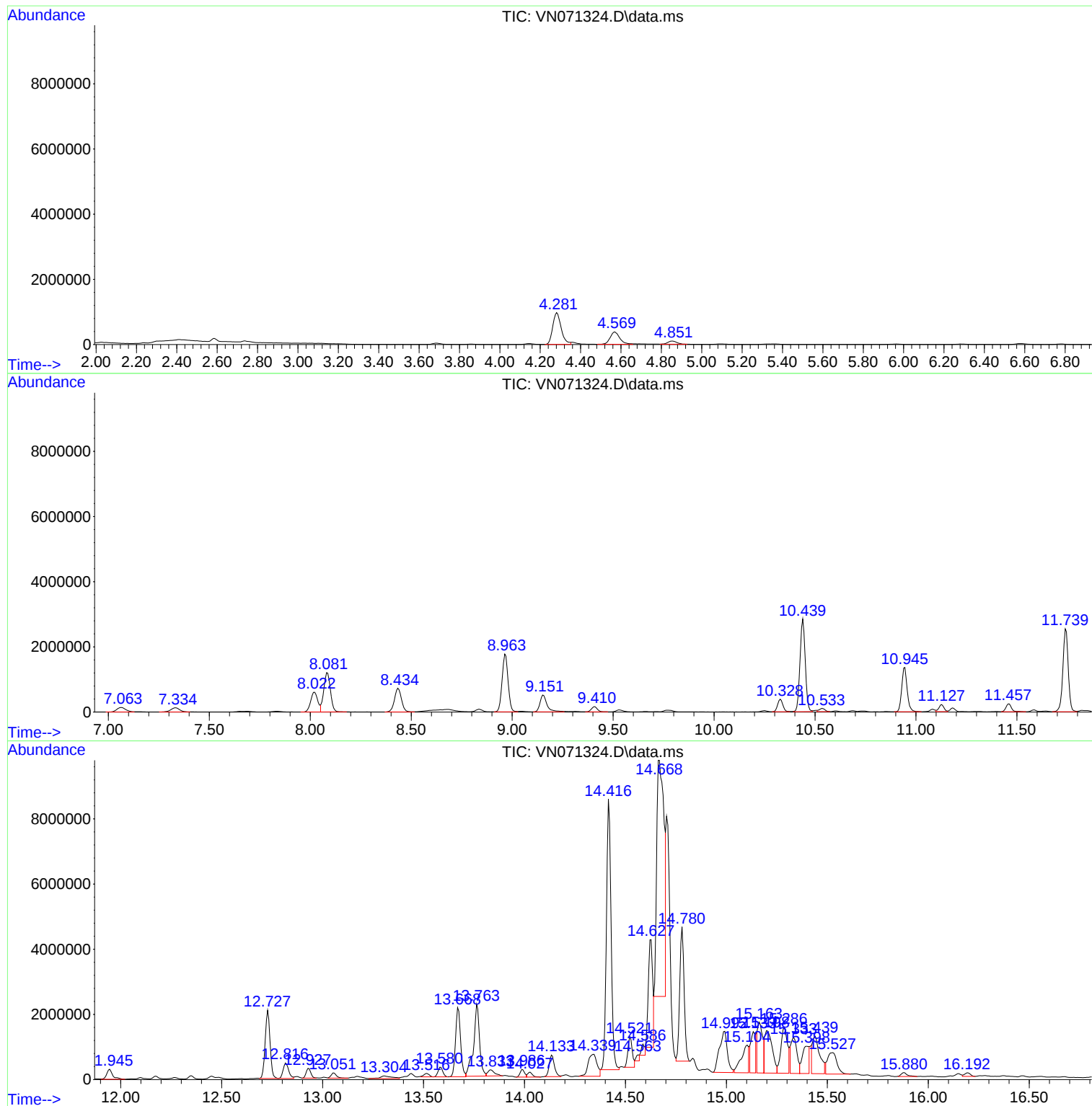
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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



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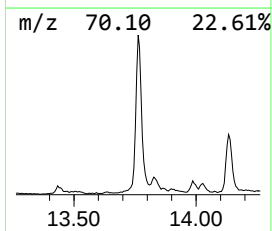
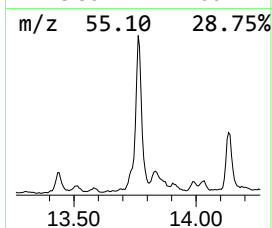
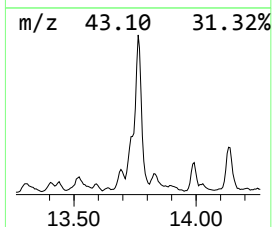
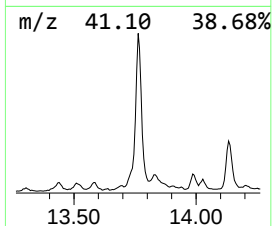
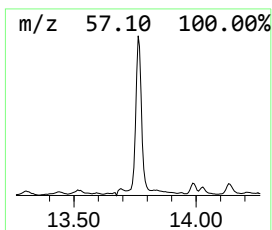
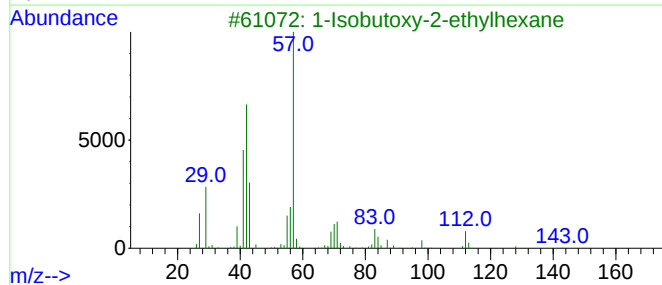
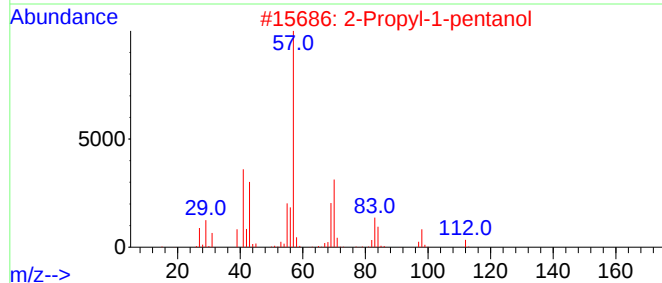
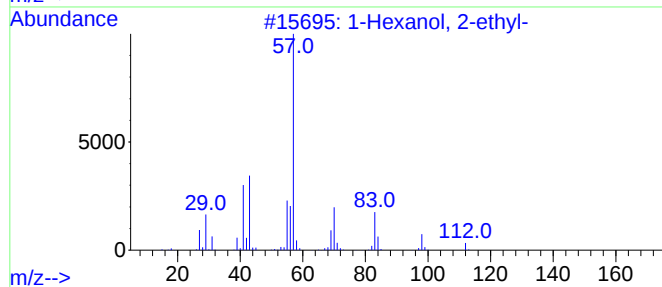
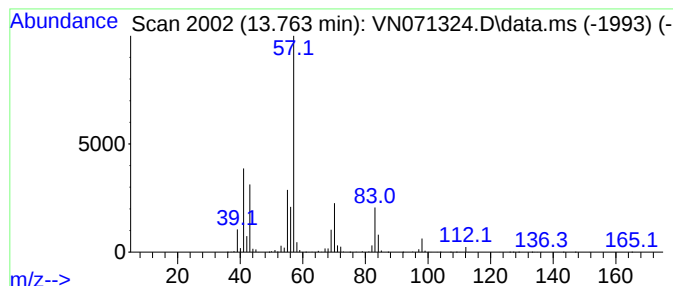
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.763	61.29 ug/l	4553200	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	42
5			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	38



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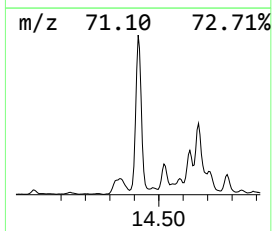
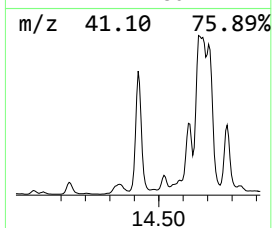
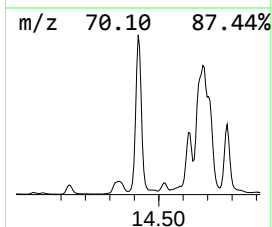
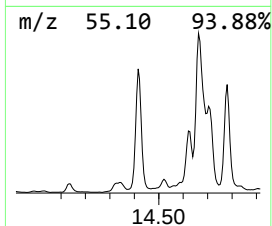
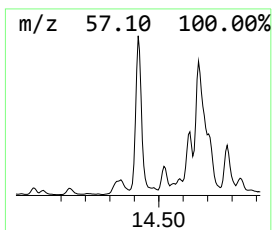
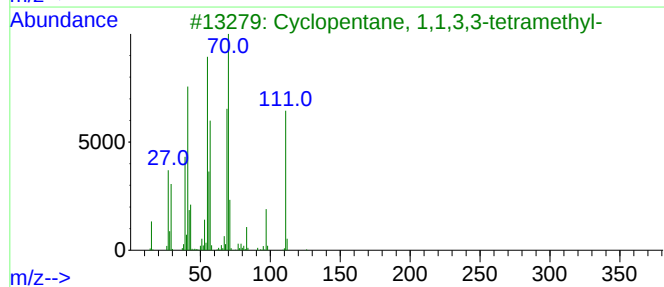
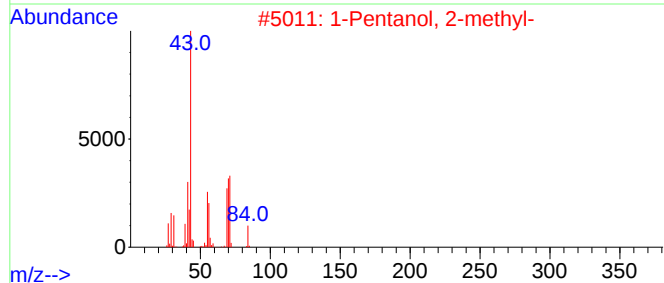
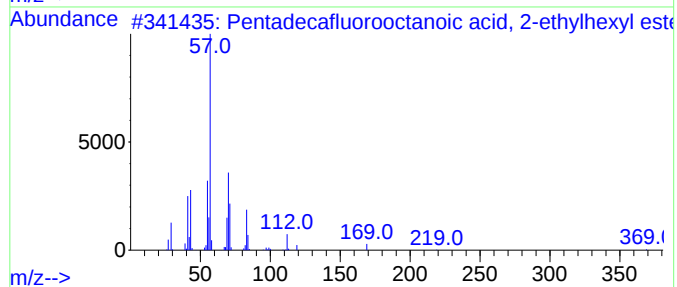
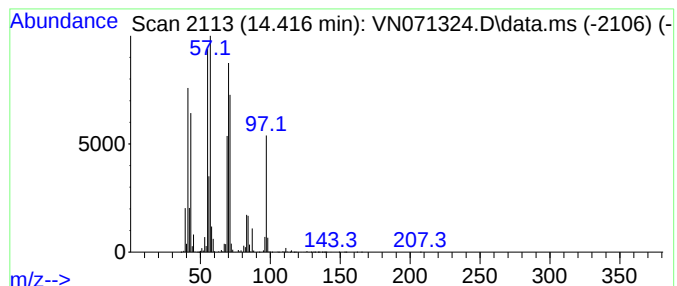
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.416	180.07 ug/l	13376100	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
2			1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	50
3			Cyclopentane, 1,1,3,3-tetramethyl-	126	C9H18	050876-33-0	50
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	47
5			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	47



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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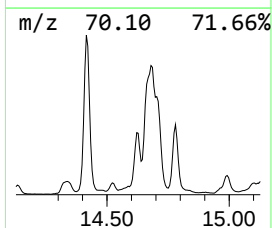
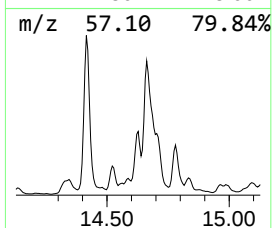
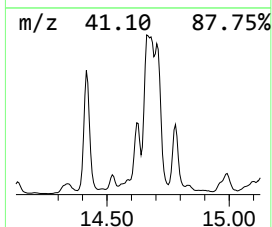
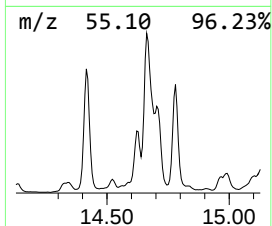
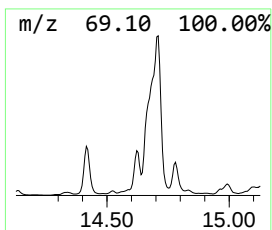
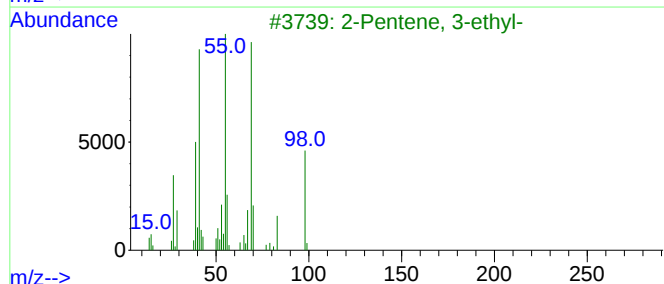
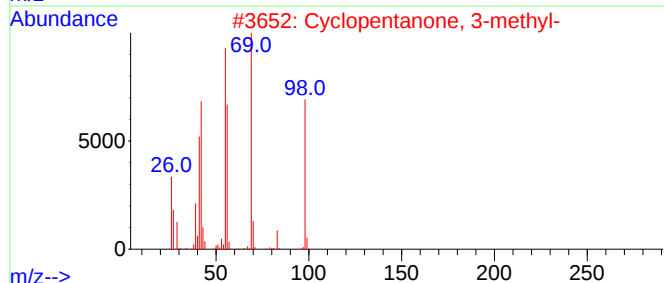
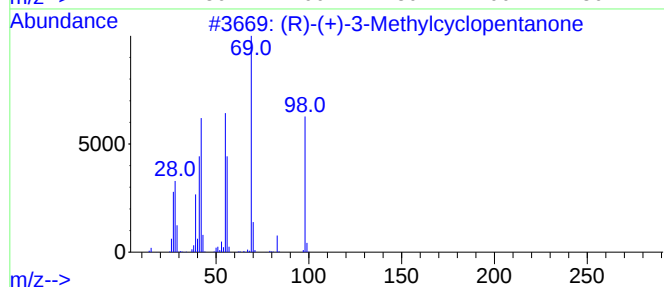
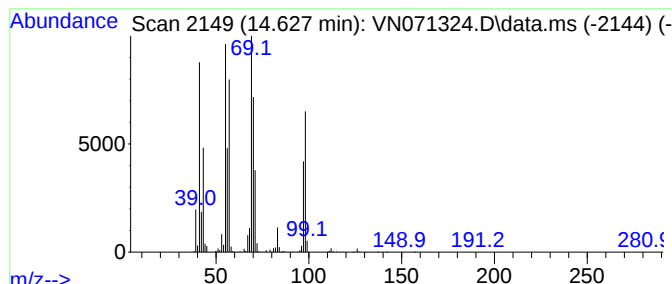
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 3 (R)-(+)-3-Methylcyclopentanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.627	68.30 ug/l	5073590	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	52		
2	Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	52		
3	2-Pentene, 3-ethyl-	98	C7H14	000816-79-5	43		
4	3-Heptene	98	C7H14	000592-78-9	43		
5	Cyclopentanecarboxaldehyde	98	C6H10O	000872-53-7	38		



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Instrument :
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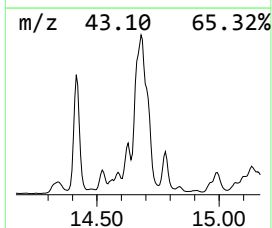
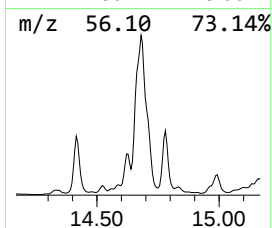
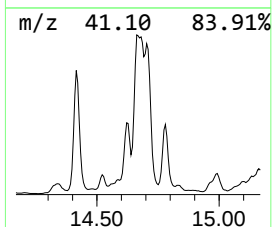
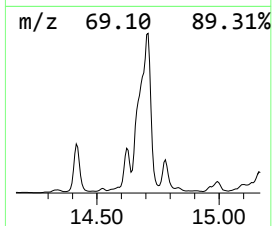
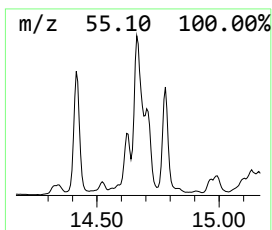
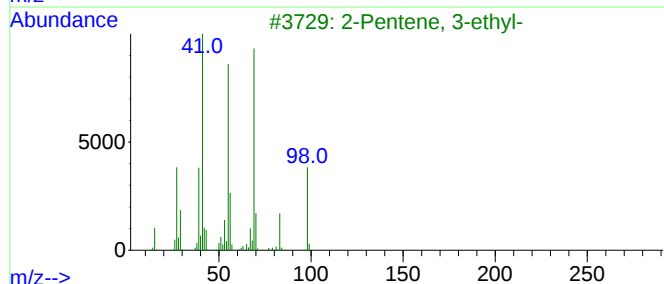
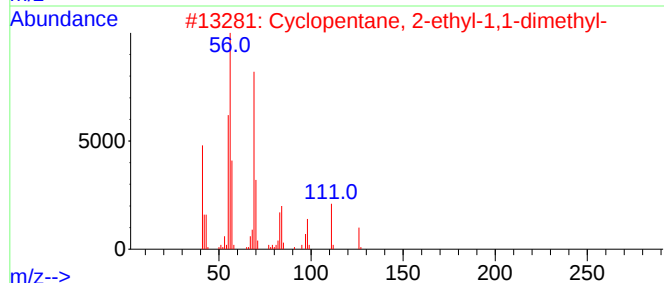
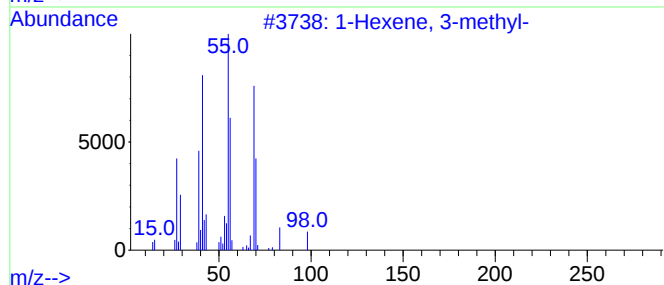
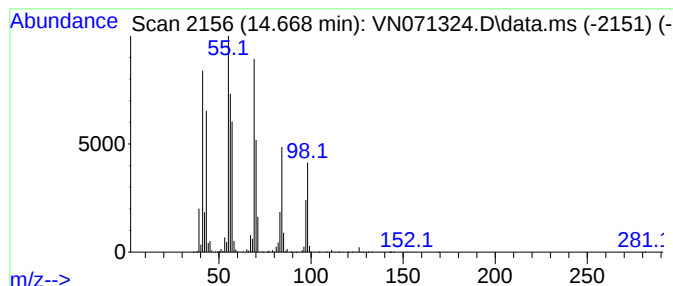
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Hexene, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.668	250.66 ug/l	18620000	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexene, 3-methyl-	98	C7H14	003404-61-3	53
2			Cyclopentane, 2-ethyl-1,1-dimethyl-	126	C9H18	054549-80-3	52
3			2-Pentene, 3-ethyl-	98	C7H14	000816-79-5	43
4			Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	43
5			5-Nonanol, trifluoroacetate	240	C11H19F3O2	1000463-48-1	38



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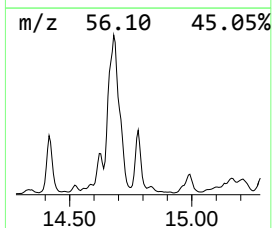
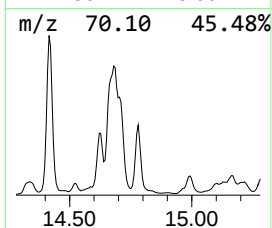
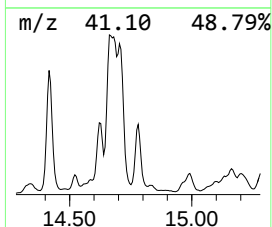
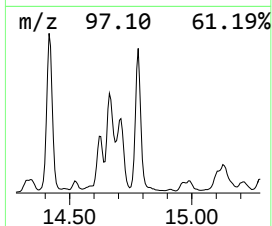
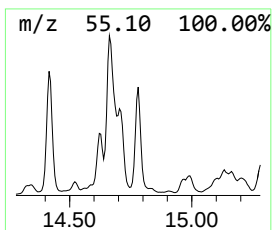
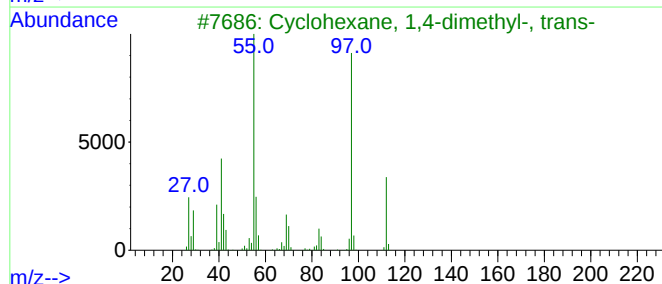
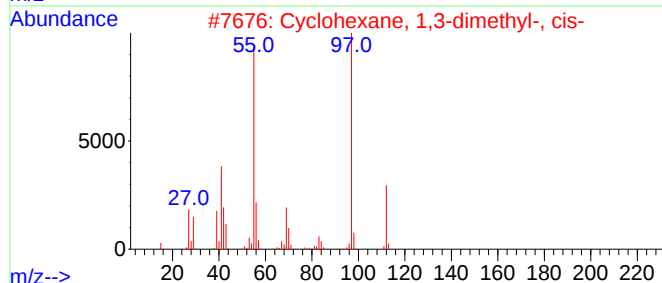
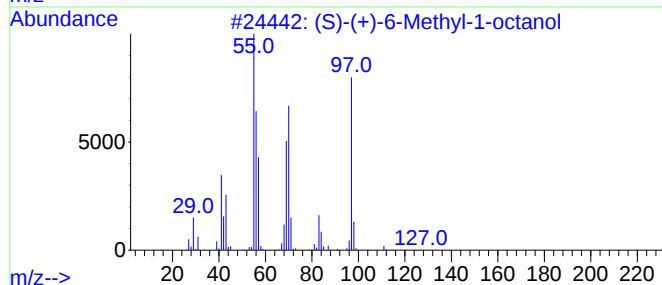
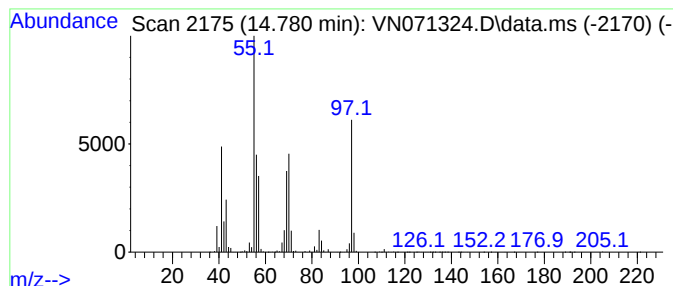
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Quant Title : SW846 8260

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

Peak Number 5 (S)-(+)-6-Methyl-1-octanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	82.59 ug/l	6134770	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	91
2			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	47
3			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	47
4			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	47
5			Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071324.D
Acq On : 16 Mar 2022 16:48
Operator : JC\MD
Sample : N1886-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-A

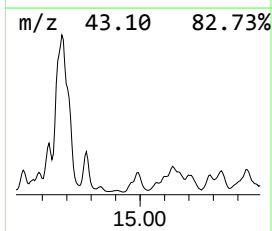
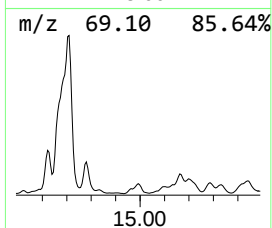
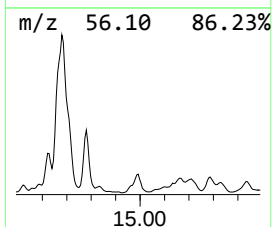
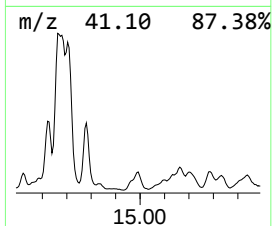
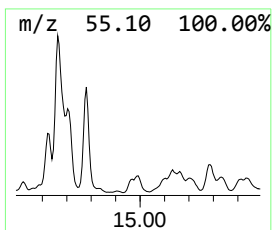
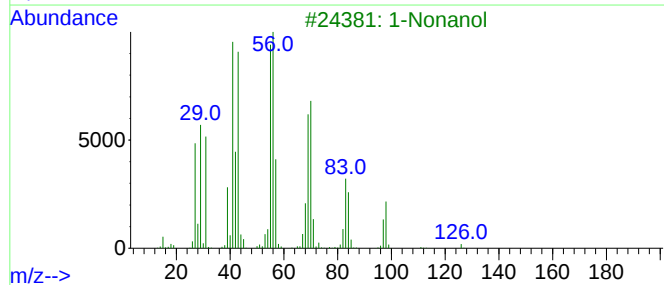
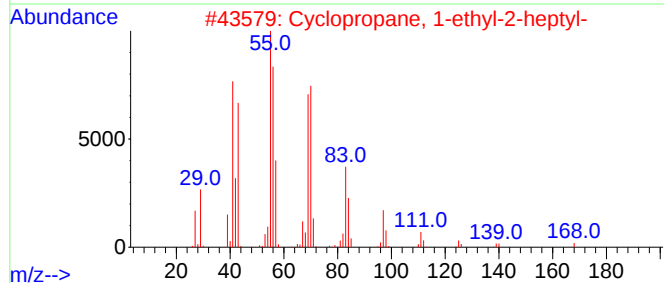
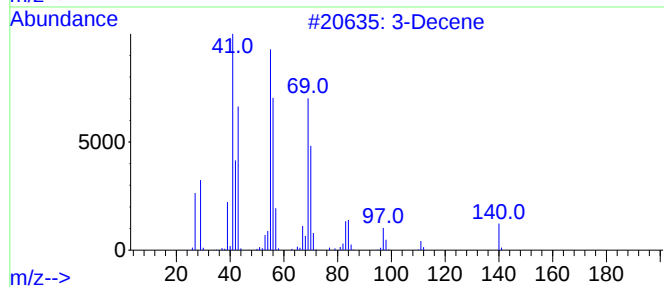
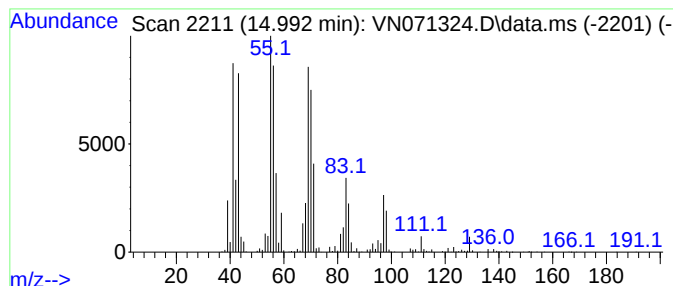
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Quant Title : SW846 8260

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

Peak Number 6 3-Decene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.992	46.27 ug/l	3437480	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Decene	140	C10H20	019398-37-9	70
2			Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	64
3			1-Nonanol	144	C9H20O	000143-08-8	58
4			Cycloheptane	98	C7H14	000291-64-5	55
5			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071324.D
Acq On : 16 Mar 2022 16:48
Operator : JC\MD
Sample : N1886-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-A

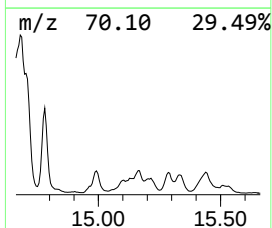
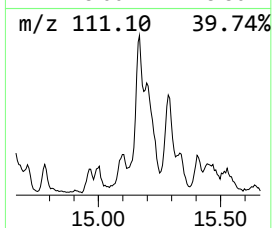
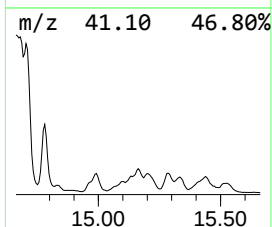
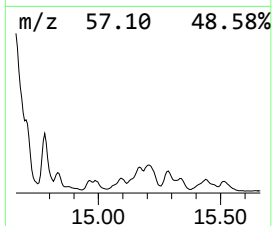
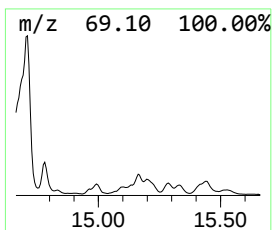
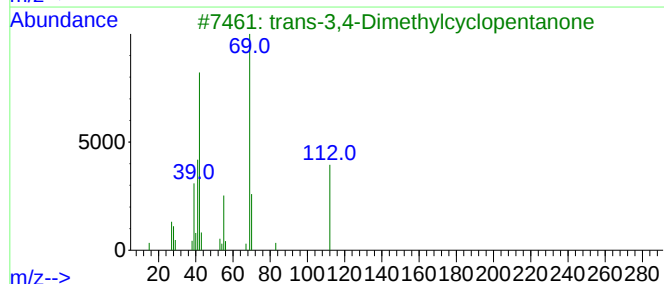
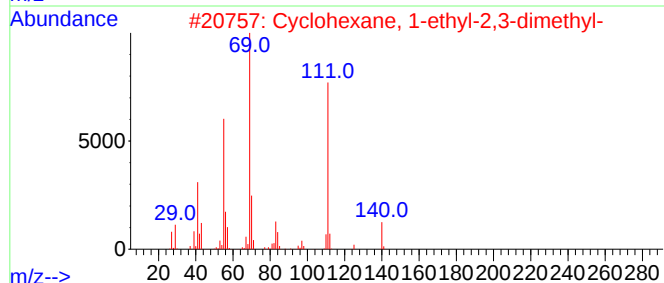
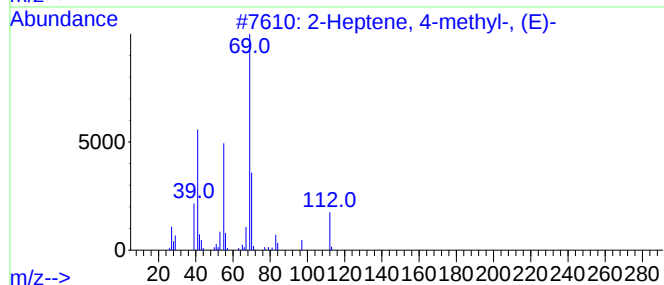
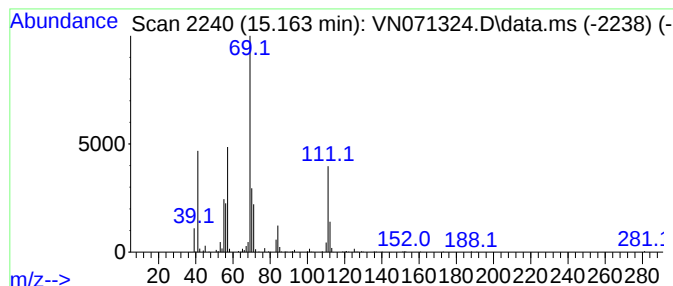
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Quant Title : SW846 8260

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

Peak Number 7 unknown15.163 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	37.41 ug/l	2778670	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptene, 4-methyl-, (E)-			112	C8H16	066225-17-0	43
2	Cyclohexane, 1-ethyl-2,3-dimethyl-			140	C10H20	007058-05-1	39
3	trans-3,4-Dimethylcyclopentanone			112	C7H12O	019550-73-3	38
4	3-Cyclopropylcarboxy-6-ethyldecane			254	C16H30O2	1000245-65-6	38
5	2-Hexene, 2,5-dimethyl-			112	C8H16	003404-78-2	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071324.D
Acq On : 16 Mar 2022 16:48
Operator : JC\MD
Sample : N1886-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-A

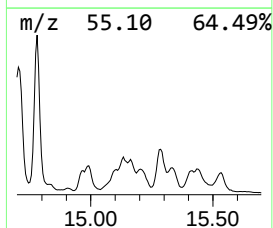
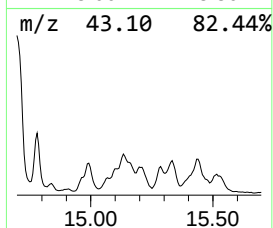
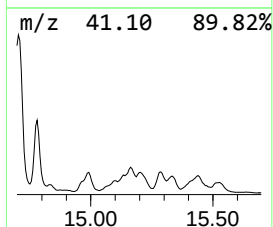
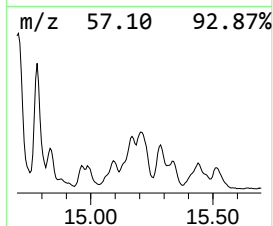
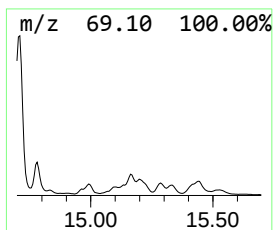
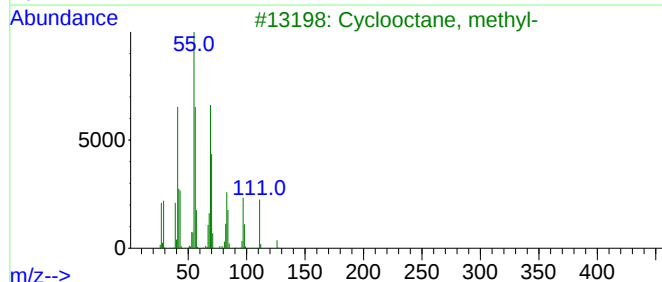
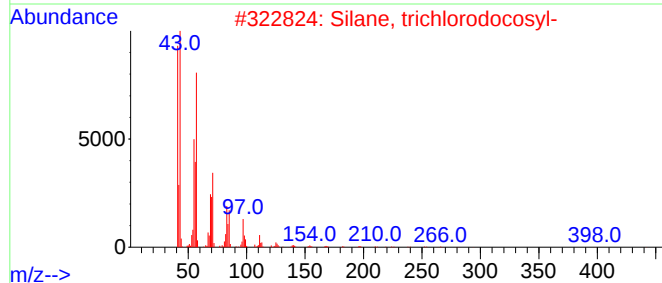
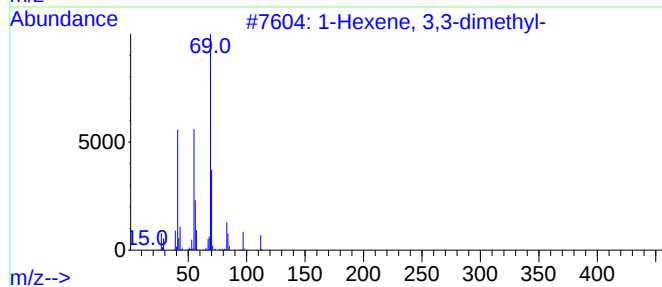
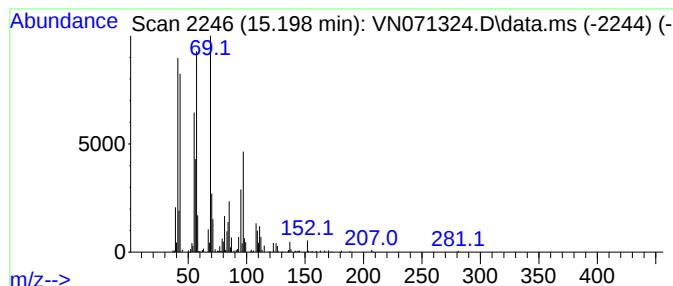
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Quant Title : SW846 8260

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

Peak Number 8 unknown15.198 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	44.09 ug/l	3274820	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	35
2			Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	30
3			Cyclooctane, methyl-	126	C9H18	001502-38-1	30
4			Cycloheptane, methyl-	112	C8H16	004126-78-7	30
5			1,5-Heptadiene, 2,3,6-trimethyl-	138	C10H18	033501-88-1	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071324.D
Acq On : 16 Mar 2022 16:48
Operator : JC\MD
Sample : N1886-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-A

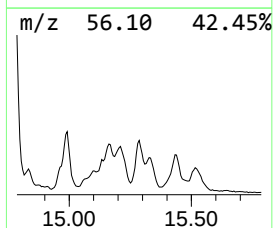
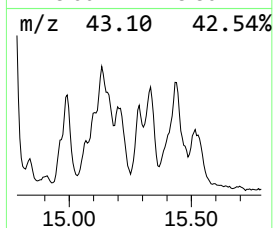
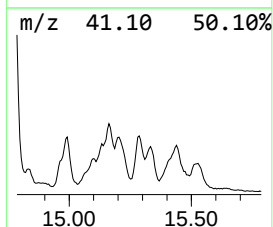
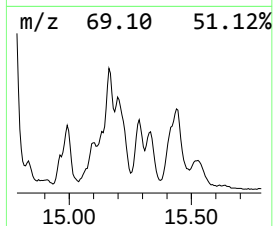
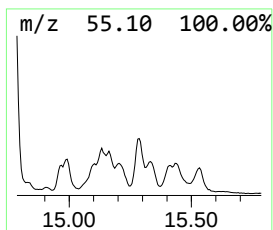
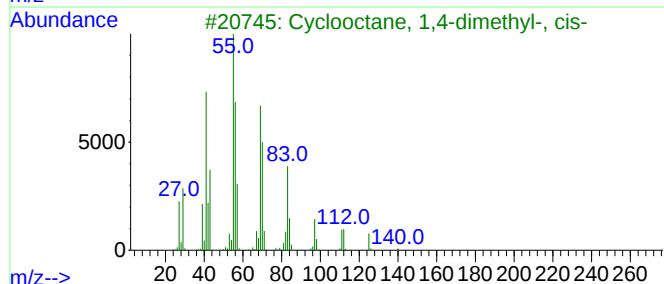
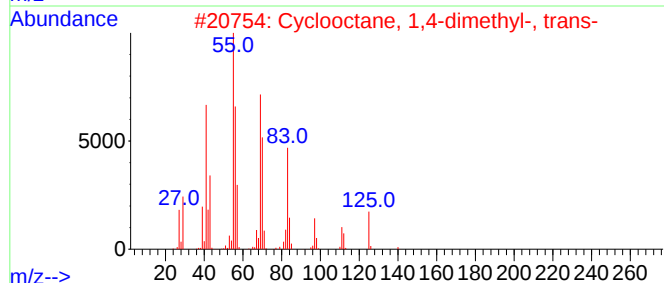
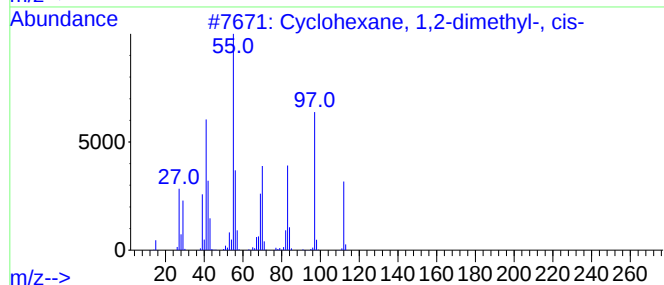
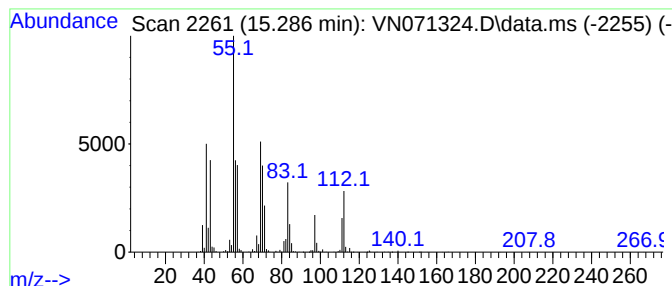
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Quant Title : SW846 8260

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

Peak Number 9 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.286	43.15 ug/l	3205220	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	002207-01-4	74
2			Cyclooctane, 1,4-dimethyl-, trans-	140	C10H20	013151-98-9	68
3			Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	68
4			2-Octene, (E)-	112	C8H16	013389-42-9	64
5			4-Octene, (E)-	112	C8H16	014850-23-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071324.D
Acq On : 16 Mar 2022 16:48
Operator : JC\MD
Sample : N1886-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-A

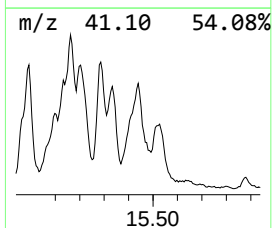
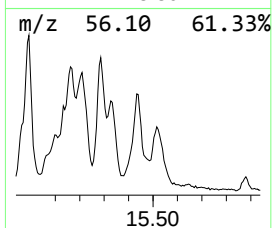
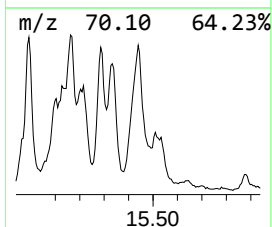
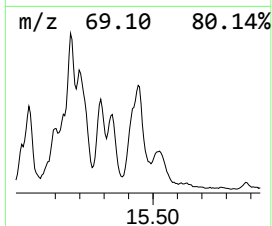
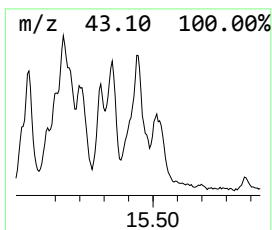
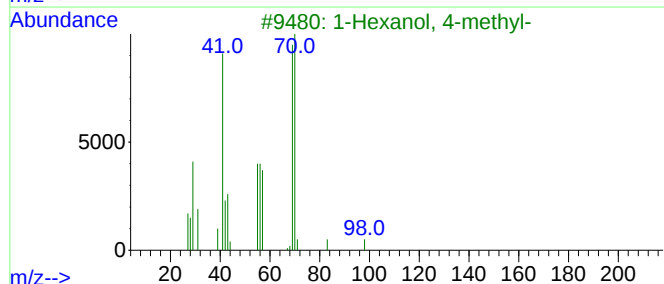
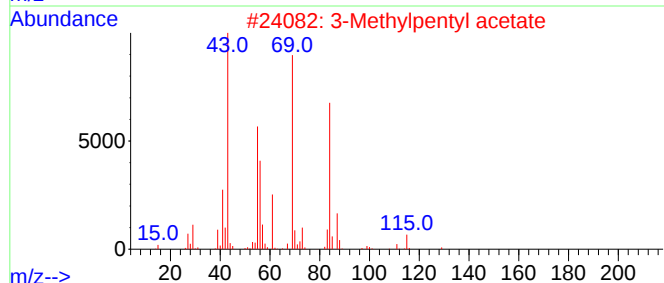
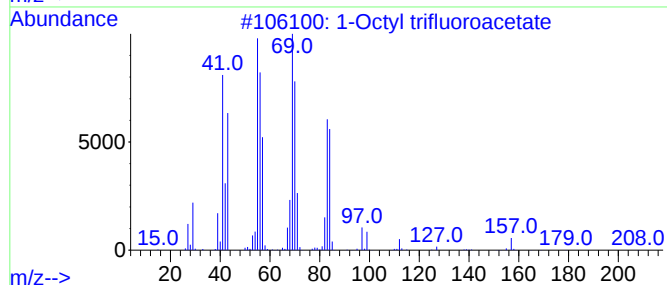
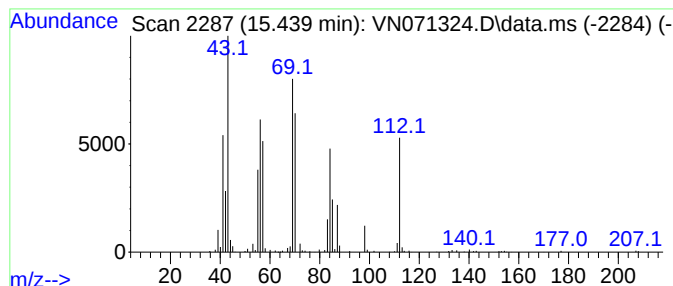
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Quant Title : SW846 8260

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

Peak Number 10 1-Octyl trifluoroacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.439	38.01 ug/l	2823780	1,4-Dichlorobenzene-d4	13.669

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octyl trifluoroacetate	226	C10H17F3O2	002561-21-9	53
2		3-Methylpentyl acetate	144	C8H16O2	035897-13-3	38
3		1-Hexanol, 4-methyl-	116	C7H16O	000818-49-5	35
4		Cyclopropane, 1,2,3-trimethyl-	84	C6H12	042984-19-0	35
5		Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071324.D
Acq On : 16 Mar 2022 16:48
Operator : JC\MD
Sample : N1886-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.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
1-Hexanol, 2-et...	13.763	61.3	ug/l	4553200	4	13.669	3714200	50.0
Pentadecafluoro...	14.416	180.1	ug/l	13376100	4	13.669	3714200	50.0
(R)-(+)-3-Methy...	14.627	68.3	ug/l	5073590	4	13.669	3714200	50.0
1-Hexene, 3-met...	14.668	250.7	ug/l	18620000	4	13.669	3714200	50.0
(S)-(+)-6-Methy...	14.780	82.6	ug/l	6134770	4	13.669	3714200	50.0
3-Decene	14.992	46.3	ug/l	3437480	4	13.669	3714200	50.0
unknown15.163	15.163	37.4	ug/l	2778670	4	13.669	3714200	50.0
unknown15.198	15.198	44.1	ug/l	3274820	4	13.669	3714200	50.0
Cyclohexane, 1,...	15.286	43.1	ug/l	3205220	4	13.669	3714200	50.0
1-Octyl trifluo...	15.439	38.0	ug/l	2823780	4	13.669	3714200	50.0