

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041422\
 Data File : VY008330.D
 Acq On : 14 Apr 2022 16:13
 Operator : KP/MD
 Sample : N2423-05
 Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 D2460-D2462

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_Y\methods\82Y040822S.M
 Title : SW846 8260

Signal : TIC: VY008330.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.217	59	65	78	rBV2	25056	48323	1.94%	0.263%
2	4.704	464	473	493	rVB3	9884	32102	1.29%	0.175%
3	6.978	835	846	859	rBV	12366	38028	1.52%	0.207%
4	7.716	955	967	972	rBV	83360	192116	7.69%	1.046%
5	7.789	972	979	990	rVB	128877	301687	12.08%	1.643%
6	8.136	1022	1036	1047	rBV3	95371	285469	11.43%	1.555%
7	8.685	1118	1126	1135	rBV	211957	407832	16.33%	2.221%
8	10.179	1364	1371	1377	rBV	339355	573265	22.96%	3.122%
9	10.240	1377	1381	1393	rVB	47614	81399	3.26%	0.443%
10	10.581	1426	1437	1443	rBV	26352	48379	1.94%	0.263%
11	11.489	1579	1586	1592	rBV	312404	493416	19.76%	2.687%
12	11.697	1614	1620	1632	rVB	24226	48120	1.93%	0.262%
13	12.337	1718	1725	1738	rBV	93742	150156	6.01%	0.818%
14	12.483	1742	1749	1759	rVB	233082	379494	15.20%	2.067%
15	12.806	1797	1802	1810	rVB2	43306	66492	2.66%	0.362%
16	13.367	1883	1894	1899	rBV	307320	450372	18.04%	2.452%
17	13.422	1899	1903	1908	rVV	242800	375498	15.04%	2.045%
18	13.489	1908	1914	1921	rVB	1668648	2497165	100.00%	13.598%
19	13.751	1952	1957	1961	rBV2	21661	31116	1.25%	0.169%
20	13.873	1972	1977	1988	rBV3	61316	107861	4.32%	0.587%
21	13.965	1988	1992	1999	rVB2	15744	26820	1.07%	0.146%
22	14.093	2006	2013	2014	rBV	137861	214305	8.58%	1.167%
23	14.111	2014	2016	2023	rVV3	166533	337407	13.51%	1.837%
24	14.184	2023	2028	2034	rVV	797450	1232803	49.37%	6.713%
25	14.239	2034	2037	2041	rVV2	70213	145850	5.84%	0.794%
26	14.294	2041	2046	2049	rVV	343239	556163	22.27%	3.029%
27	14.324	2049	2051	2054	rVV3	127571	216246	8.66%	1.178%
28	14.397	2058	2063	2065	rVV	412804	678185	27.16%	3.693%
29	14.428	2065	2068	2083	rVV2	855701	2186000	87.54%	11.904%
30	14.550	2083	2088	2095	rVV	303288	500938	20.06%	2.728%
31	14.611	2095	2098	2105	rVB4	32462	51601	2.07%	0.281%
32	14.757	2117	2122	2140	rBV	371080	581448	23.28%	3.166%
33	14.946	2146	2153	2165	rBV	308486	521407	20.88%	2.839%
34	15.092	2168	2177	2191	rBV	1408495	2249681	90.09%	12.251%
35	15.227	2193	2199	2201	rBV2	142119	226282	9.06%	1.232%
36	15.257	2201	2204	2216	rVB	230337	412480	16.52%	2.246%

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37	15.538	2245	2250	2256	rBV	29476	52844	2.12%	0.288%
38	15.611	2256	2262	2277	rBV	224531	413155	16.54%	2.250%
39	15.909	2304	2311	2317	rBV	406761	723789	28.98%	3.941%
40	15.970	2317	2321	2329	rVB2	48337	95437	3.82%	0.520%
41	16.123	2341	2346	2350	rBV5	29784	58569	2.35%	0.319%
42	16.172	2350	2354	2361	rVB2	46137	83797	3.36%	0.456%
43	16.476	2400	2404	2413	rVB8	22381	46580	1.87%	0.254%
44	16.598	2419	2424	2441	rVB9	32987	103677	4.15%	0.565%
45	16.763	2447	2451	2455	rBV7	21865	40143	1.61%	0.219%

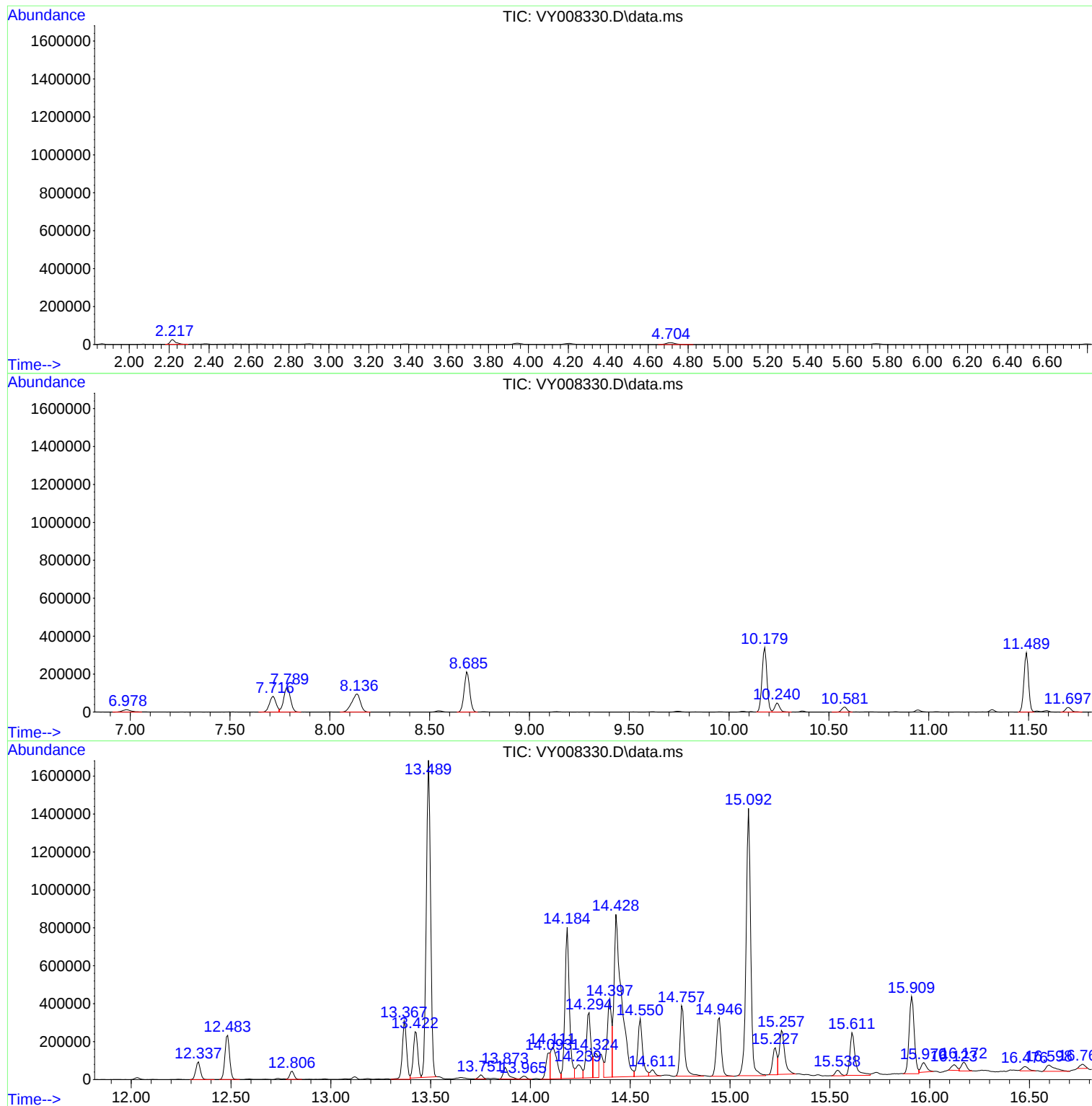
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y040822S.M
Quant Title : SW846 8260

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



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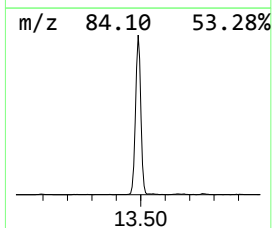
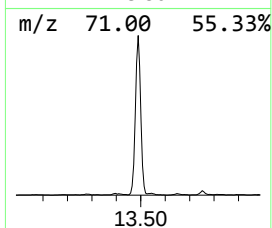
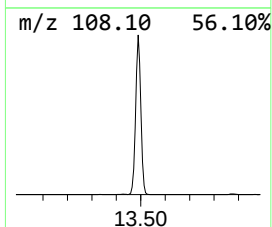
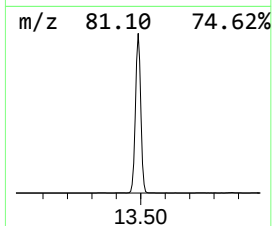
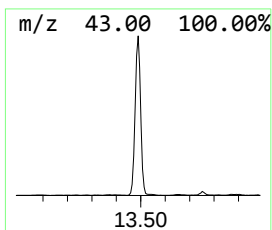
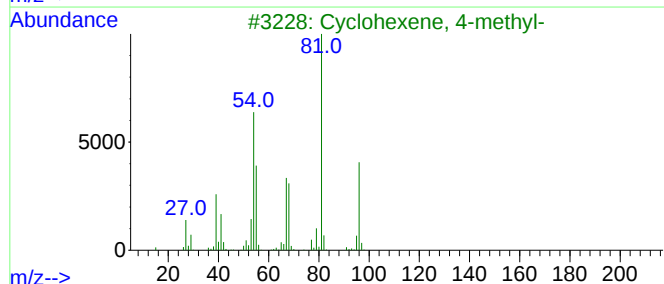
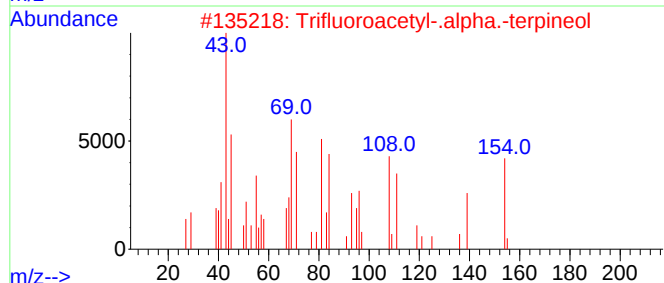
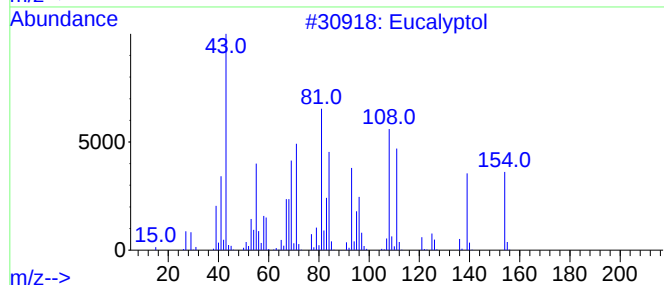
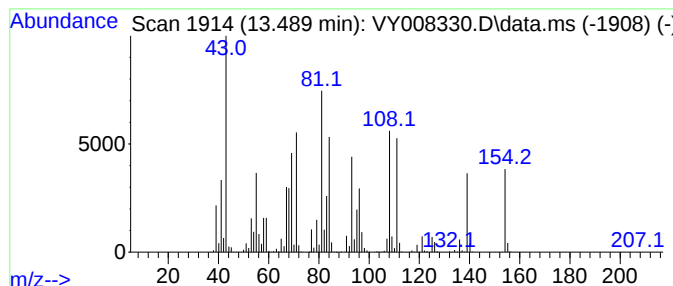
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y040822S.M
Quant Title : SW846 8260

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

Peak Number 1 Eucalyptol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.489	332.51 ug/l	2497170	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	99
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	53
3			Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	25
4			3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25
5			2,4-Hexadiene, 3-methyl-	96	C7H12	028823-42-9	15



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D2460-D2462

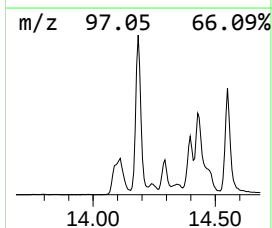
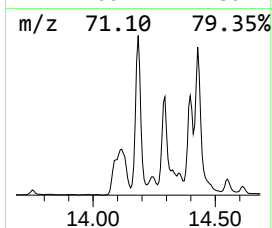
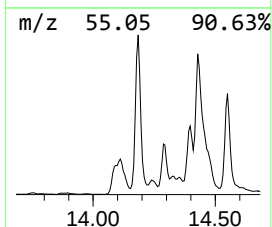
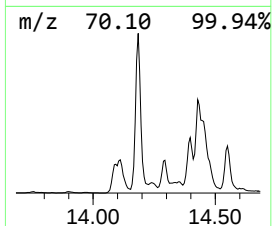
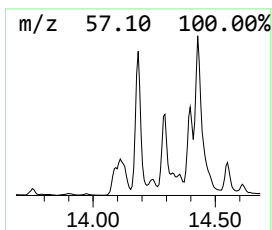
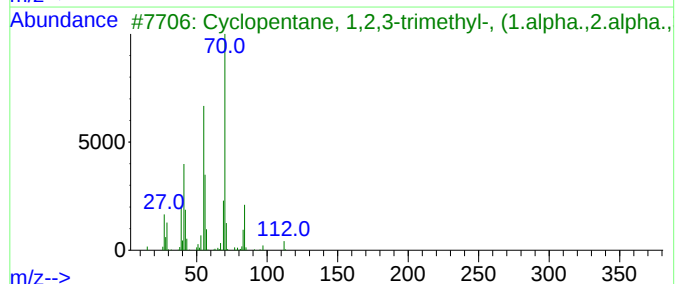
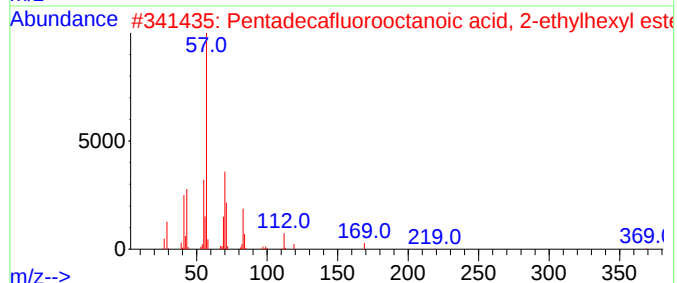
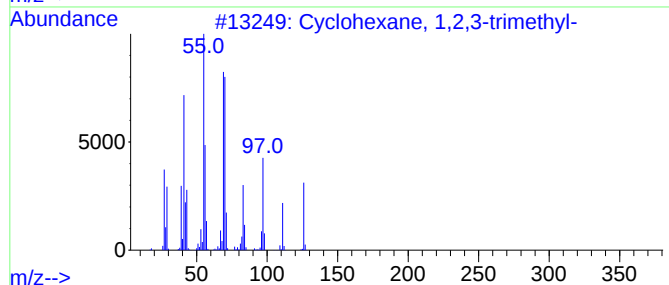
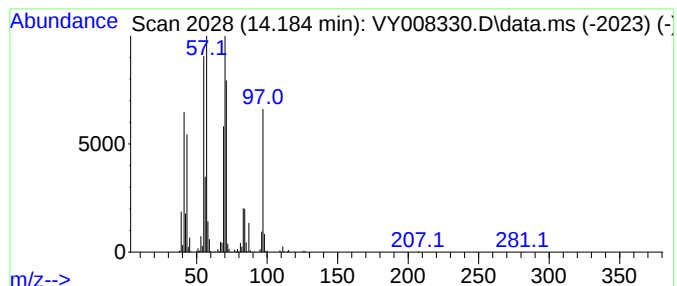
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y040822S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown14.184 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.184	164.16 ug/l	1232800	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	47
2			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	43
3			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	38
4			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	38
5			1-Heptene, 5-methyl-	112	C8H16	013151-04-7	38



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ALS Vial : 10 Sample Multiplier: 1

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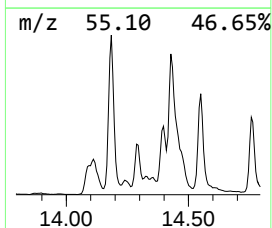
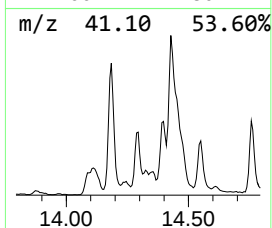
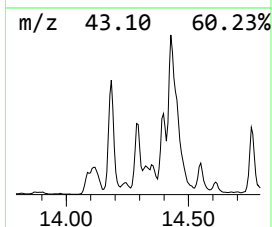
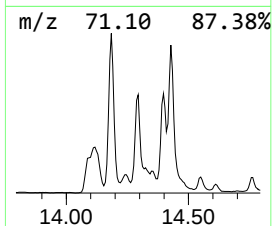
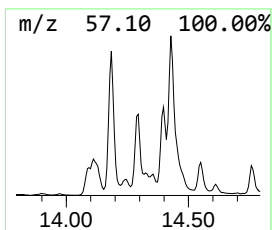
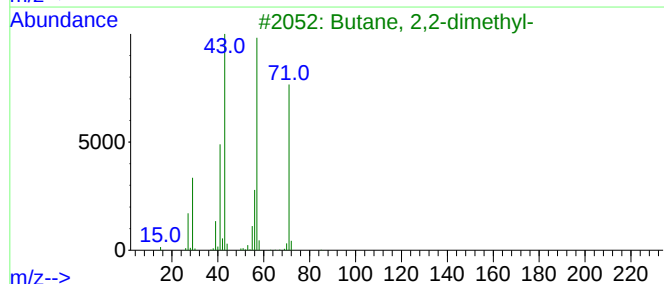
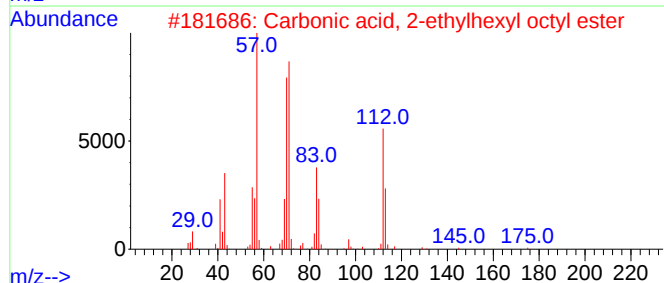
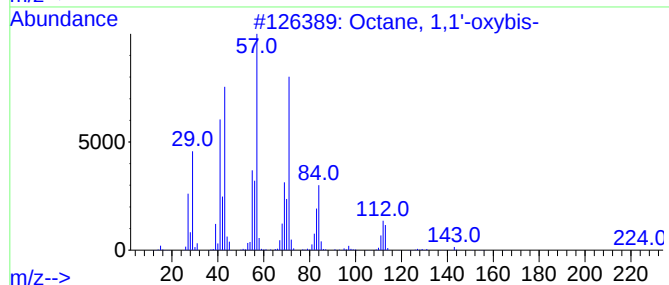
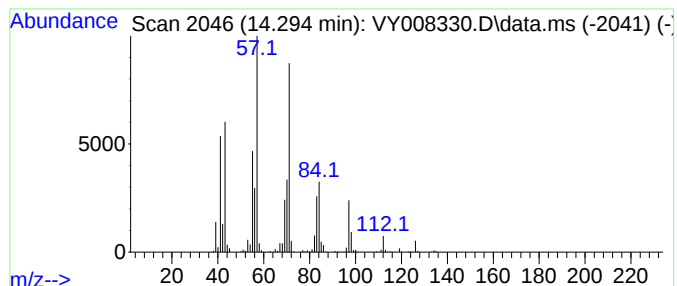
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octane, 1,1'-oxybis- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.294	74.06 ug/l	556163	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	72
2			Carbonic acid, 2-ethylhexyl octyl ester	286	C17H34O3	1000383-13-5	53
3			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	43
4			1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	43
5			Acetic acid, octyl ester	172	C10H20O2	000112-14-1	35



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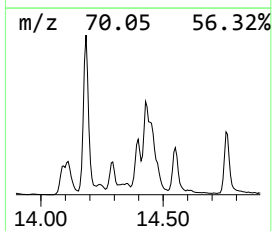
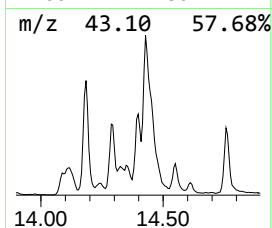
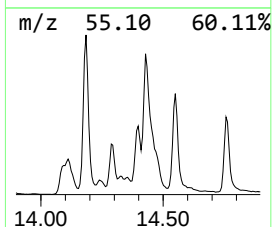
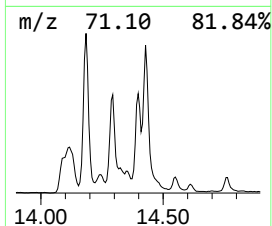
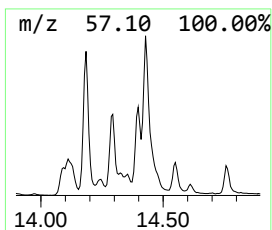
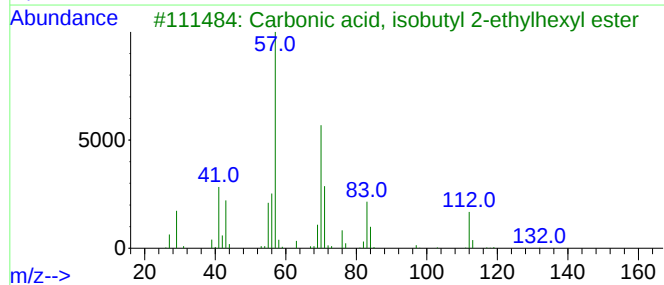
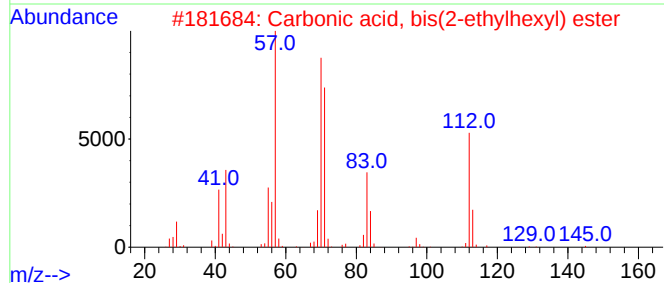
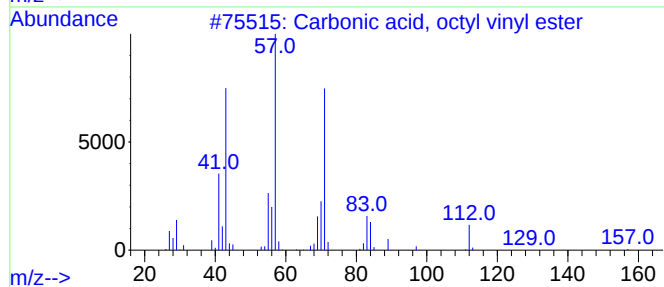
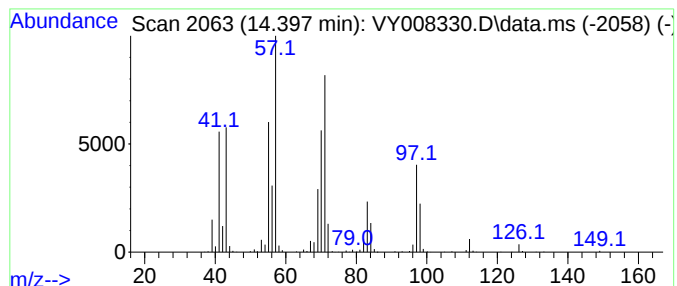
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.398 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.398	90.30 ug/l	678185	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	47
2			Carbonic acid, bis(2-ethylhexyl)...	286	C17H34O3	014858-73-2	43
3			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	38
4			Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	002207-01-4	38
5			Carbonic acid, butyl 2-ethylhexy...	230	C13H26O3	1000357-84-4	38



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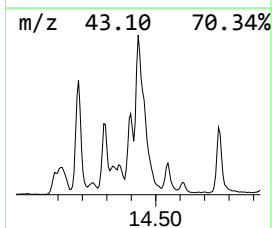
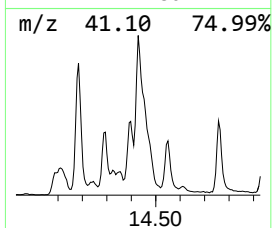
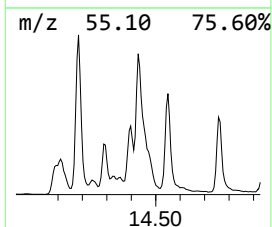
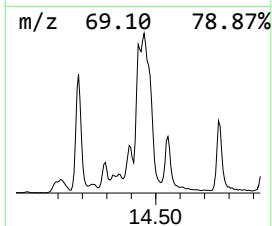
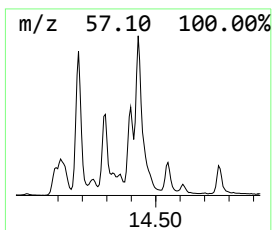
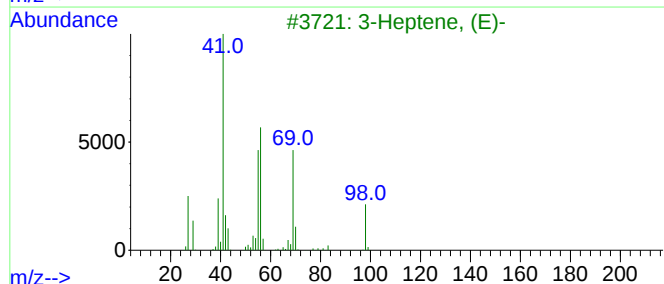
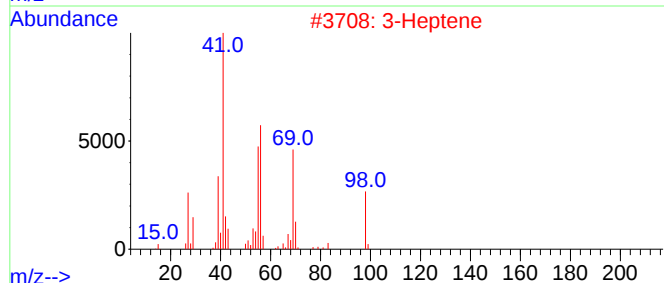
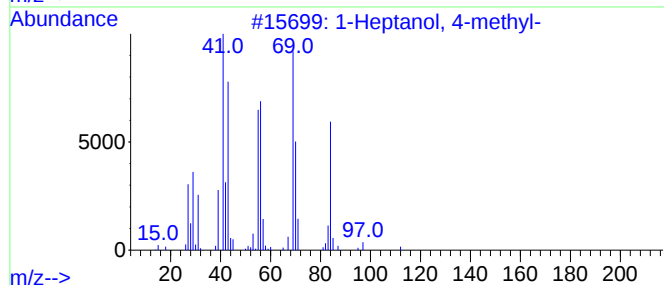
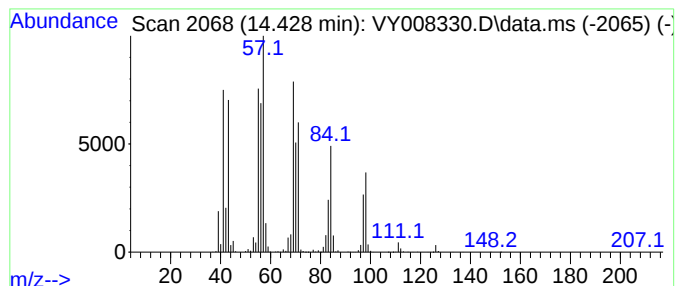
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Quant Title : SW846 8260

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

Peak Number 5 1-Heptanol, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.428	291.08 ug/l	2186000	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	58
2			3-Heptene	98	C7H14	000592-78-9	43
3			3-Heptene, (E)-	98	C7H14	014686-14-7	43
4			1-Propene, 1-(2-propenyloxy)-, (Z)-	98	C6H10O	061142-12-9	43
5			1H-Tetrazole, 1,5-dimethyl-	98	C3H6N4	005144-11-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041422\
Data File : VY008330.D
Acq On : 14 Apr 2022 16:13
Operator : KP/MD
Sample : N2423-05
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D2460-D2462

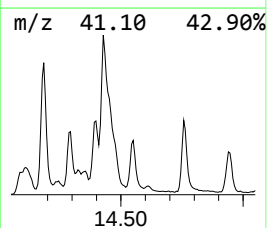
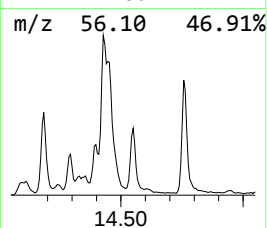
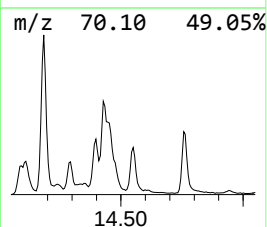
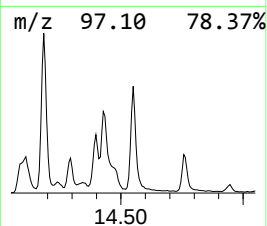
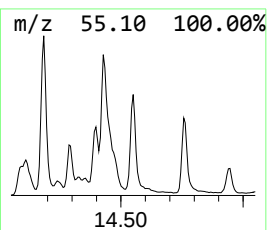
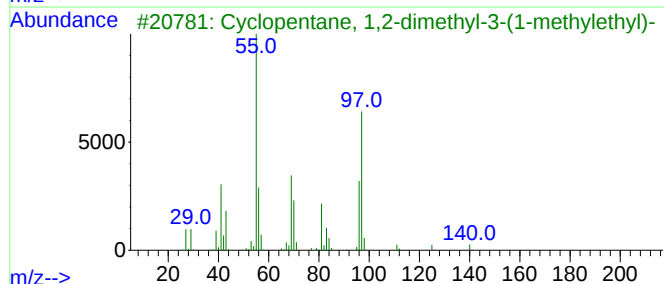
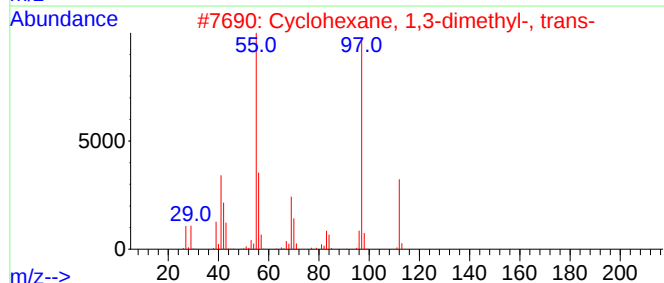
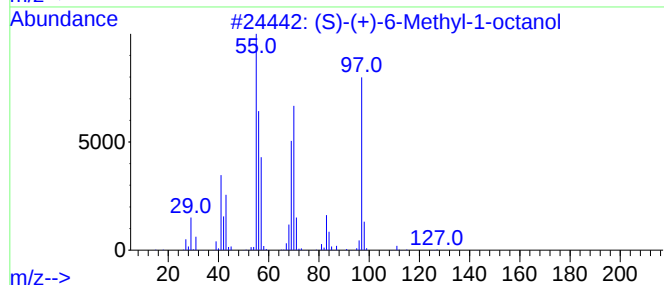
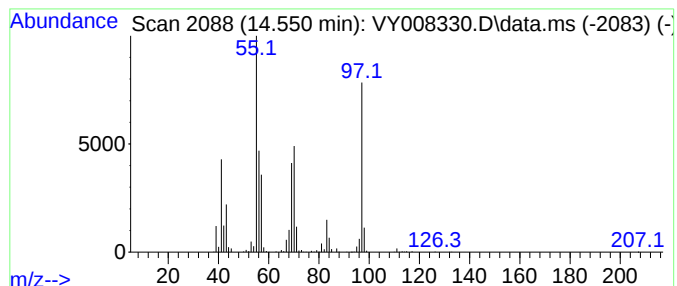
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Quant Title : SW846 8260

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

Peak Number 6 (S)-(+)-6-Methyl-1-octanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.550	66.70 ug/l	500938	1,4-Dichlorobenzene-d4	13.428

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-, trans-	112	C8H16	002207-03-6	64		
3	Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-	140	C10H20	000489-20-3	53		
4	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	50		
5	6-Methyloctyl acetate	186	C11H22O2	1000439-66-5	50		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041422\
Data File : VY008330.D
Acq On : 14 Apr 2022 16:13
Operator : KP/MD
Sample : N2423-05
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D2460-D2462

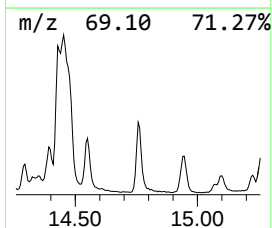
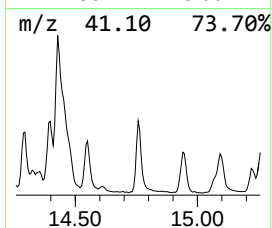
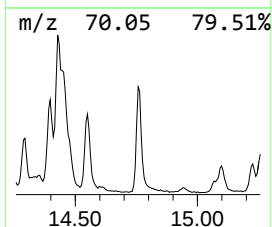
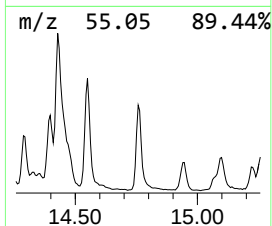
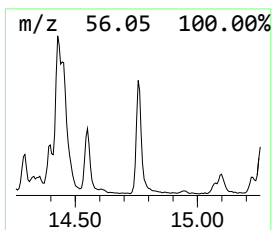
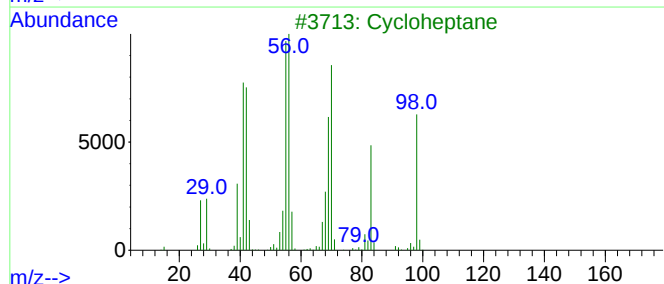
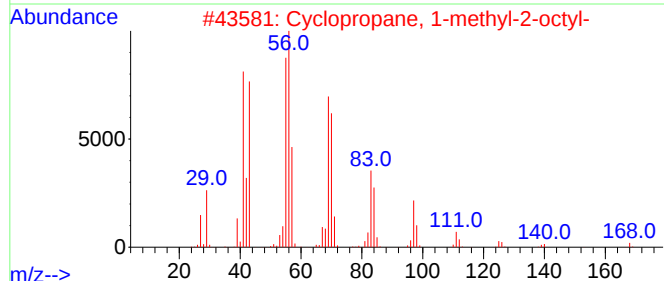
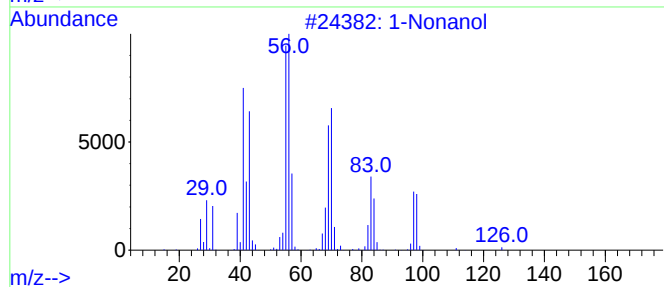
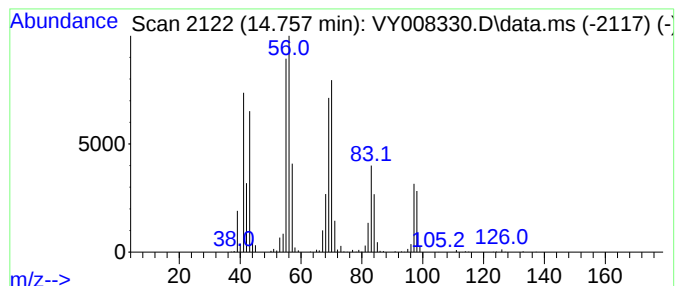
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Quant Title : SW846 8260

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

Peak Number 7 1-Nonanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.757	77.42 ug/l	581448	1,4-Dichlorobenzene-d4	13.428

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	78
3			Cycloheptane	98	C7H14	000291-64-5	72
4			Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	72
5			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041422\
Data File : VY008330.D
Acq On : 14 Apr 2022 16:13
Operator : KP/MD
Sample : N2423-05
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D2460-D2462

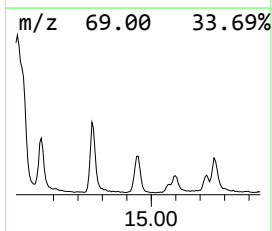
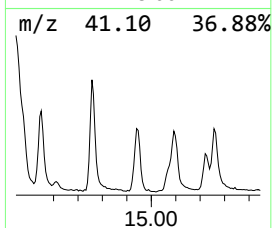
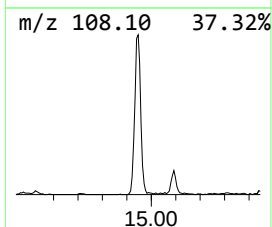
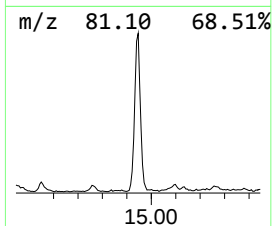
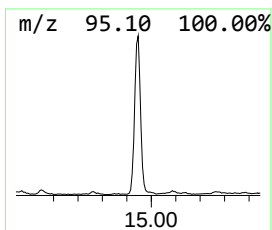
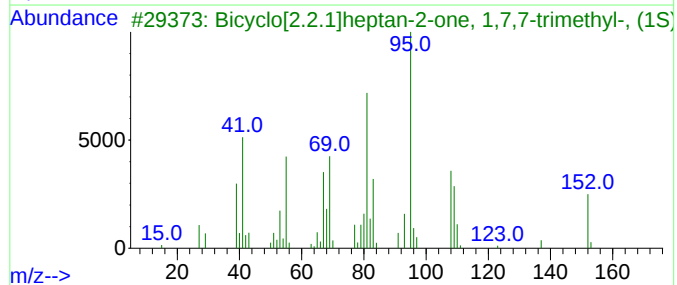
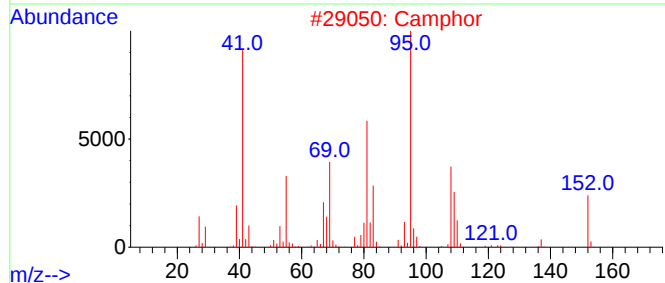
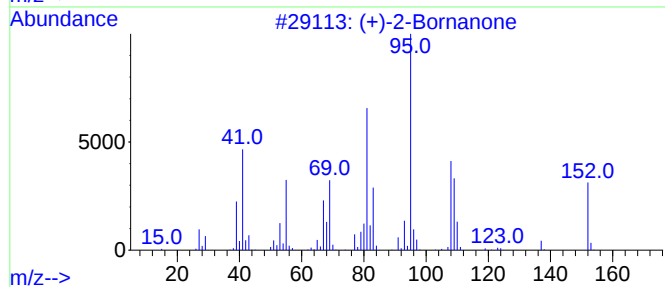
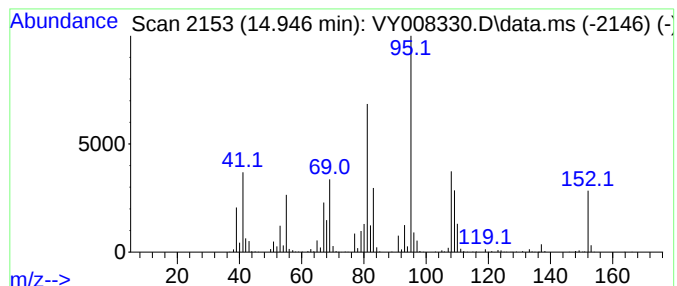
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Quant Title : SW846 8260

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

Peak Number 8 (+)-2-Bornanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.946	69.43 ug/l	521407	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2			Camphor	152	C10H16O	000076-22-2	98
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	96
4			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	52
5			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041422\
Data File : VY008330.D
Acq On : 14 Apr 2022 16:13
Operator : KP/MD
Sample : N2423-05
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D2460-D2462

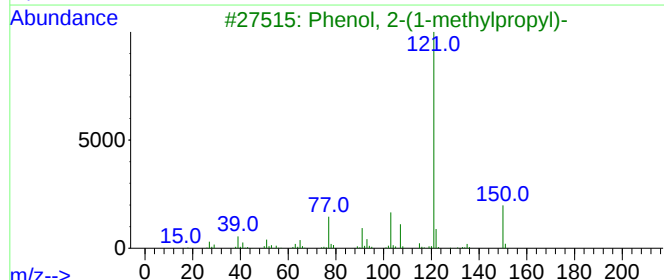
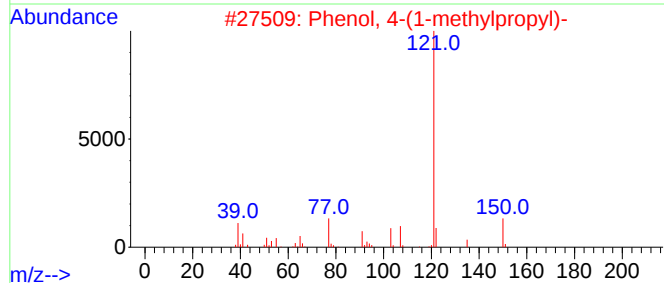
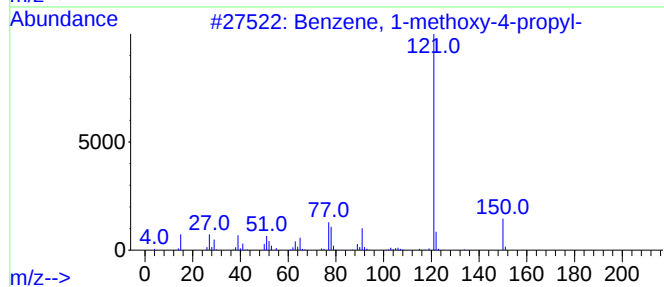
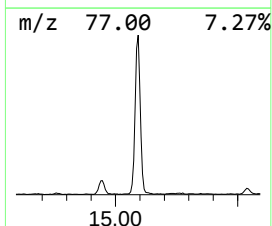
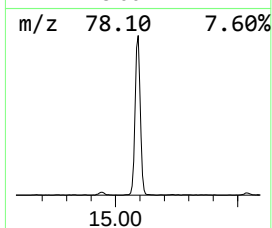
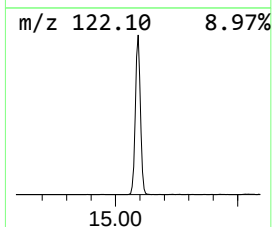
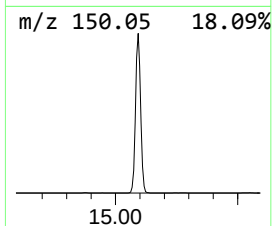
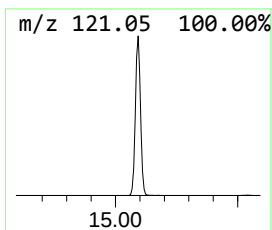
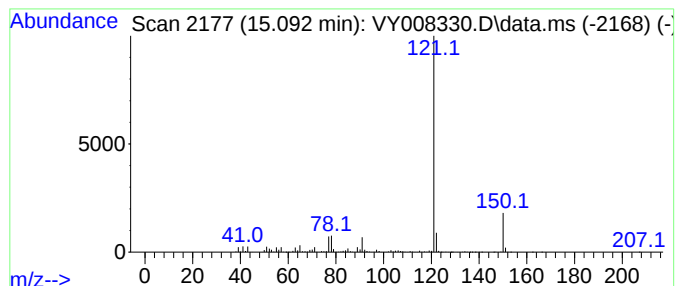
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-methoxy-4-propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	299.56 ug/l	2249680	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	91
2			Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	78
3			Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	78
4			Succinic acid, 3-chlorophenyl 4-...	348	C18H17ClO5	1000389-69-3	64
5			5-(p-Anisylthio)-3H-1,3,4-thiadi...	270	C10H10N2OS3	136384-20-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041422\
Data File : VY008330.D
Acq On : 14 Apr 2022 16:13
Operator : KP/MD
Sample : N2423-05
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D2460-D2462

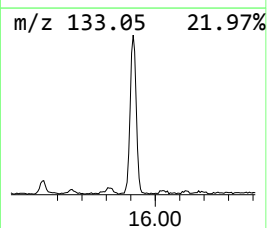
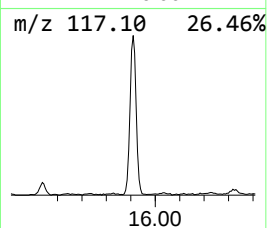
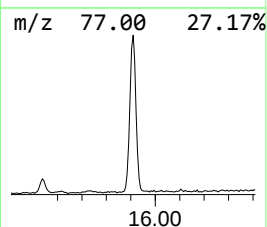
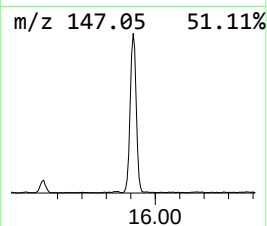
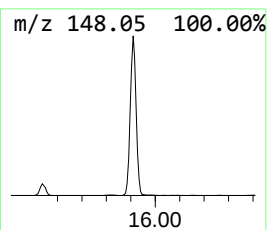
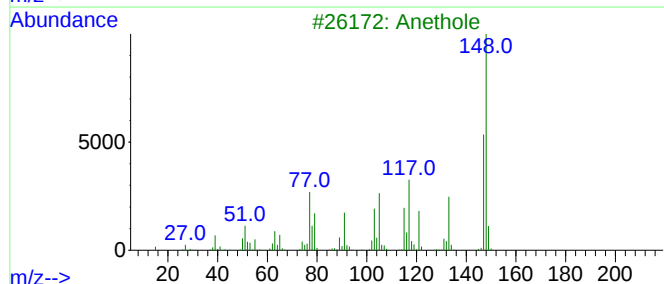
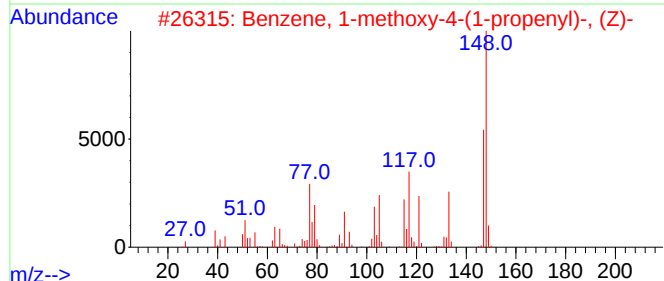
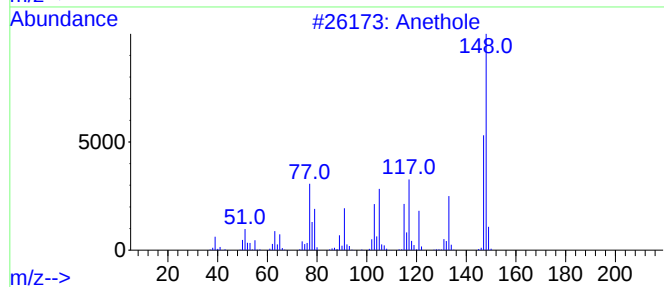
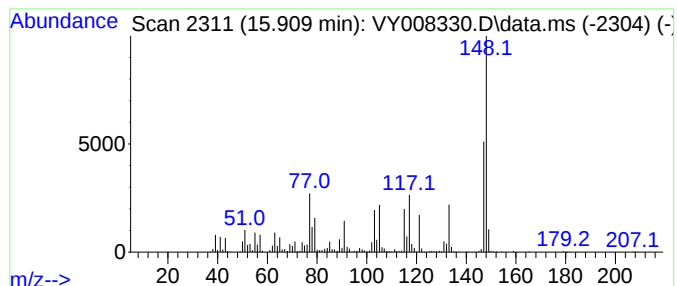
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Quant Title : SW846 8260

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

Peak Number 10 Anethole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.909	96.38 ug/l	723789	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anethole			148	C10H12O	004180-23-8	98
2	Benzene, 1-methoxy-4-(1-propenyl)-			148	C10H12O	025679-28-1	98
3	Anethole			148	C10H12O	000104-46-1	98
4	Estragole			148	C10H12O	000140-67-0	91
5	8,9-Dehydrothymol			148	C10H12O	018612-99-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041422\
Data File : VY008330.D
Acq On : 14 Apr 2022 16:13
Operator : KP/MD
Sample : N2423-05
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D2460-D2462

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y040822S.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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unknown14.184	14.184	164.2	ug/l	1232800	4	13.428	375498	50.0
Octane, 1,1'-ox...	14.294	74.1	ug/l	556163	4	13.428	375498	50.0
unknown14.398	14.398	90.3	ug/l	678185	4	13.428	375498	50.0
1-Heptanol, 4-m...	14.428	291.1	ug/l	2186000	4	13.428	375498	50.0
(S)-(+)-6-Methy...	14.550	66.7	ug/l	500938	4	13.428	375498	50.0
1-Nonanol	14.757	77.4	ug/l	581448	4	13.428	375498	50.0
(+)-2-Bornanone	14.946	69.4	ug/l	521407	4	13.428	375498	50.0
Benzene, 1-meth...	15.092	299.6	ug/l	2249680	4	13.428	375498	50.0
Anethole	15.909	96.4	ug/l	723789	4	13.428	375498	50.0