

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082423\
 Data File : VY015317.D
 Acq On : 24 Aug 2023 17:18
 Operator : SY/MD
 Sample : 04112-01
 Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 RBR-22282

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\82Y081423S.M

Title : SW846 8260

Signal : TIC: VY015317.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.716	465	475	485	rVB3	5407	15916	2.23%	0.238%
2	5.753	632	645	655	rBV3	10225	32153	4.50%	0.480%
3	6.972	835	845	858	rBV2	20656	62178	8.70%	0.929%
4	7.716	957	967	973	rBV	65080	152572	21.36%	2.279%
5	7.789	973	979	990	rVB	116912	260409	36.46%	3.890%
6	8.143	1029	1037	1045	rBV	62819	143336	20.07%	2.141%
7	8.691	1119	1127	1136	rBV	169022	337053	47.19%	5.035%
8	10.179	1365	1371	1379	rBV	275774	478525	66.99%	7.148%
9	11.490	1580	1586	1596	rVB	246604	401433	56.20%	5.996%
10	12.124	1679	1690	1697	rBV4	99307	400193	56.03%	5.978%
11	12.483	1744	1749	1754	rBV	182001	284376	39.81%	4.248%
12	12.806	1797	1802	1807	rVB3	76598	131430	18.40%	1.963%
13	13.044	1837	1841	1843	rBV2	53684	82164	11.50%	1.227%
14	13.422	1899	1903	1913	rVB3	343515	714290	100.00%	10.670%
15	13.751	1951	1957	1962	rBV3	249342	472419	66.14%	7.057%
16	13.965	1990	1992	1997	rVB2	57264	81353	11.39%	1.215%
17	14.074	2006	2010	2016	rBV2	106252	190459	26.66%	2.845%
18	14.215	2028	2033	2034	rBV5	37834	61915	8.67%	0.925%
19	14.257	2036	2040	2046	rVB6	75273	174475	24.43%	2.606%
20	14.379	2056	2060	2063	rBV2	76650	111772	15.65%	1.670%
21	14.422	2063	2067	2078	rVB3	100227	195733	27.40%	2.924%
22	14.611	2094	2098	2103	rBV2	133037	178146	24.94%	2.661%
23	14.672	2103	2108	2114	rVV4	149865	371089	51.95%	5.543%
24	14.727	2114	2117	2124	rVB2	132186	233123	32.64%	3.482%
25	14.940	2149	2152	2156	rBV4	59828	87804	12.29%	1.312%
26	15.050	2165	2170	2176	rBV4	68932	147194	20.61%	2.199%
27	15.208	2191	2196	2205	rBV4	122025	227380	31.83%	3.396%
28	15.434	2230	2233	2239	rBV4	60503	85138	11.92%	1.272%
29	15.727	2278	2281	2287	rVB3	54989	87561	12.26%	1.308%
30	16.031	2326	2331	2337	rVB5	56271	99785	13.97%	1.491%
31	16.153	2347	2351	2356	rVB2	52634	84895	11.89%	1.268%
32	16.226	2359	2363	2370	rVB4	56416	108474	15.19%	1.620%
33	16.483	2399	2405	2419	rVB4	53239	199900	27.99%	2.986%

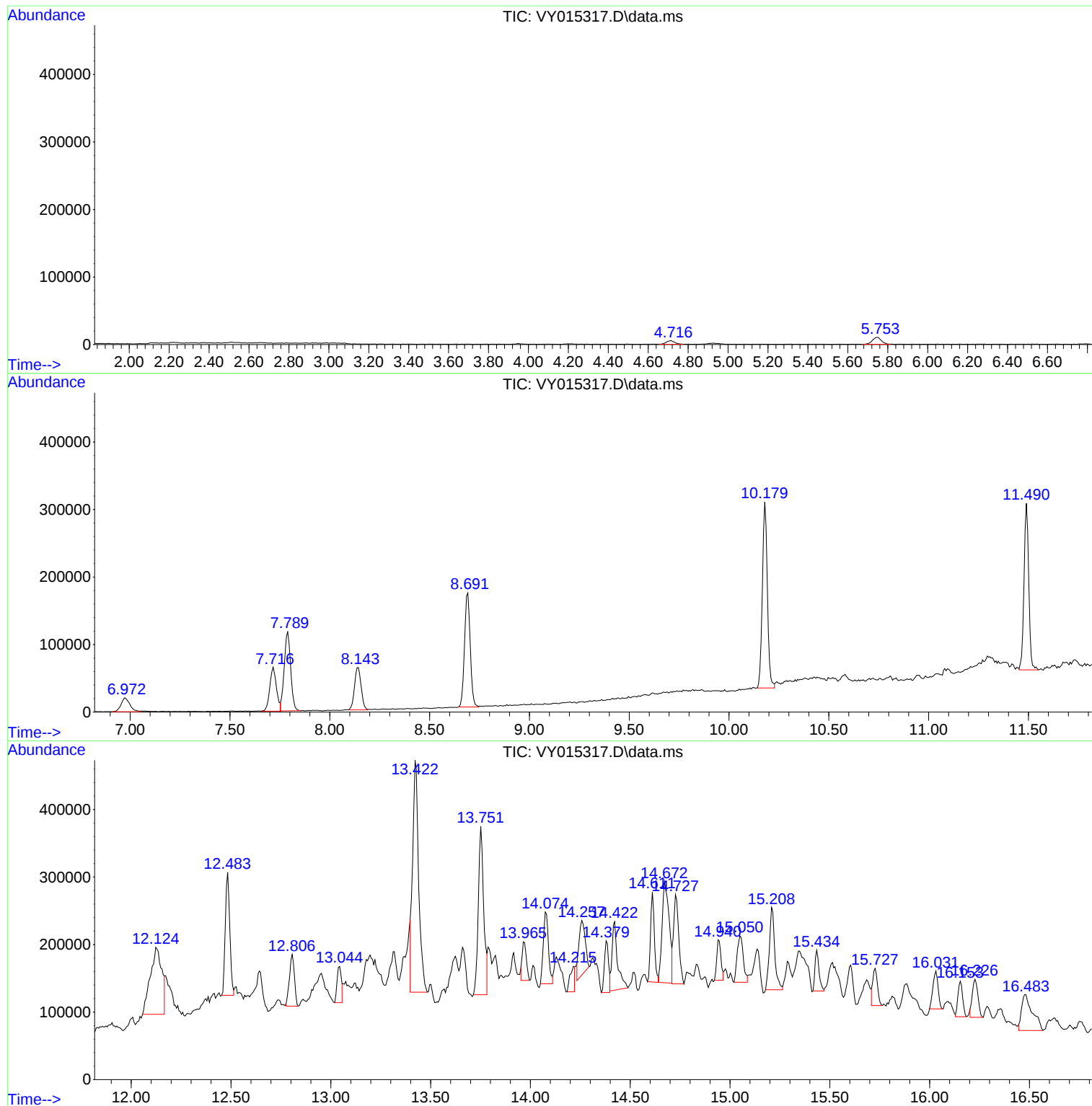
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ClientSampleId :
RBR-22282

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.M
Quant Title : SW846 8260

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



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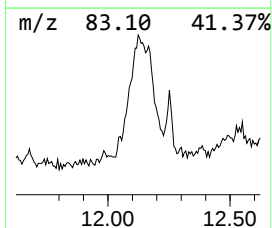
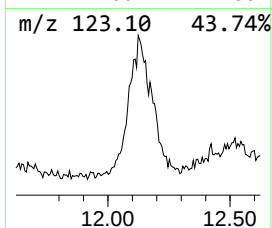
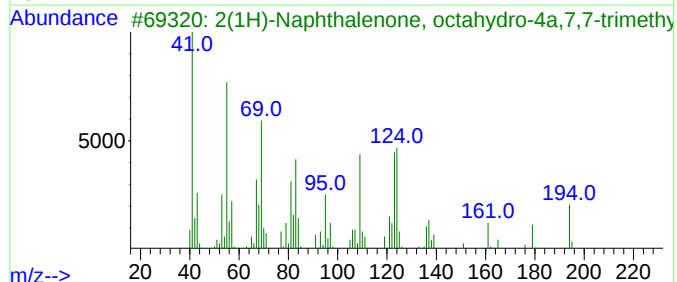
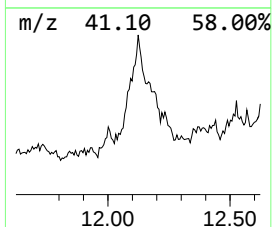
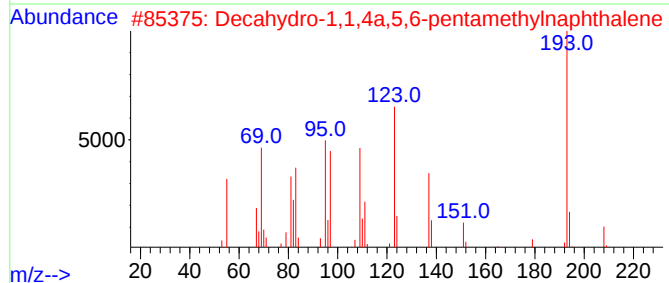
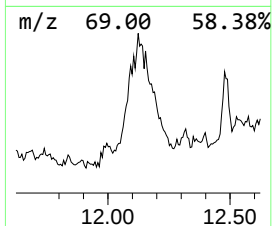
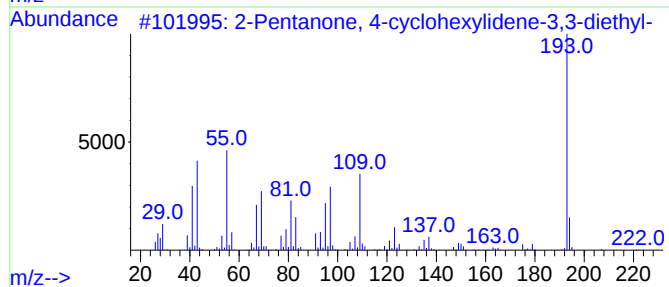
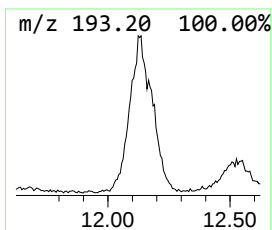
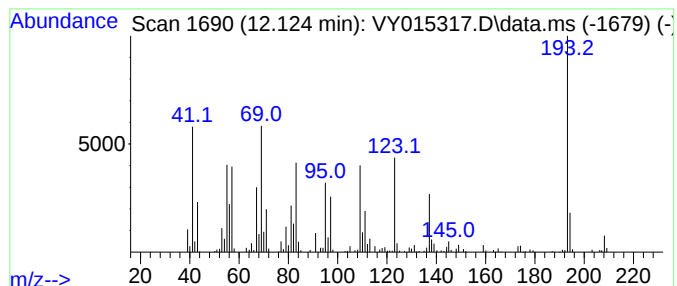
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.M
Quant Title : SW846 8260

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

Peak Number 1 2-Pentanone, 4-cyclohexylidene... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.124	49.85 ug/l	400193	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	50		
2	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	49		
3	2(1H)-Naphthalenone, octahydro-4...	194	C13H22O	007056-56-6	49		
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38		
5	Fumaric acid, di(2-fluorophenyl)...	304	C16H10F2O4	1000345-22-9	27		



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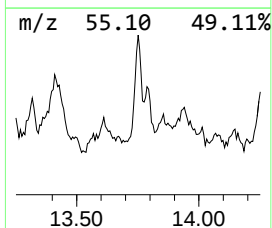
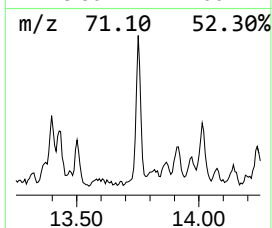
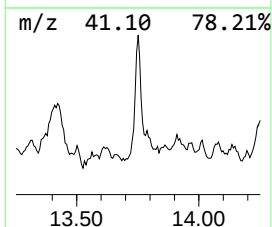
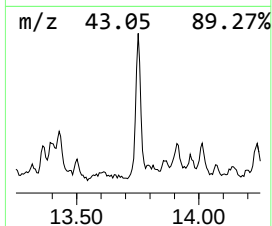
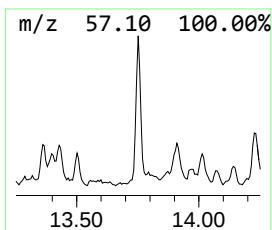
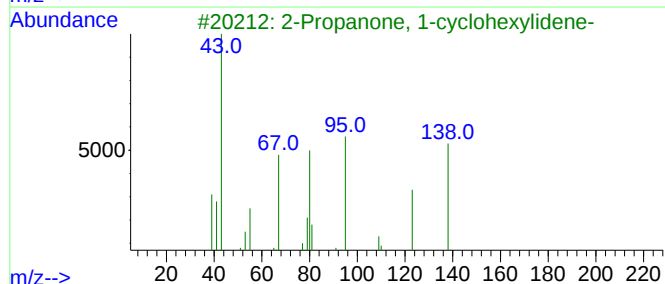
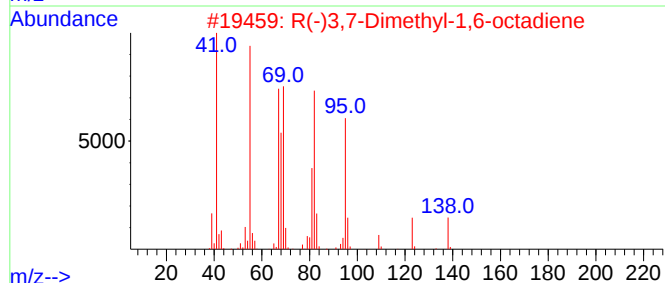
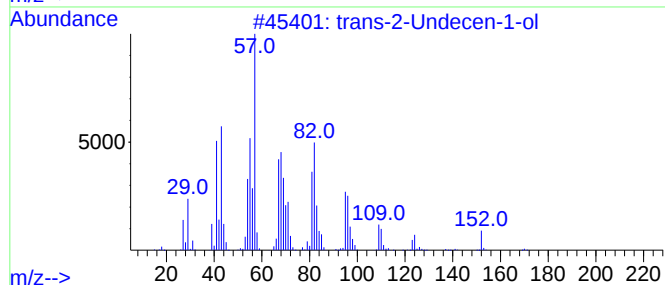
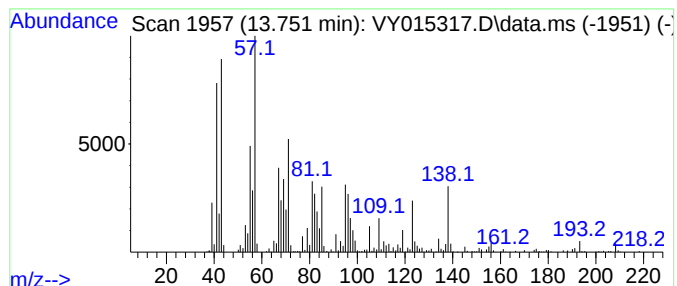
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Quant Title : SW846 8260

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

Peak Number 2 unknown13.751 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	33.07 ug/l	472419	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2-Undecen-1-ol	170	C11H22O	075039-84-8	45
2			R(-)3,7-Dimethyl-1,6-octadiene	138	C10H18	010281-56-8	42
3			2-Propanone, 1-cyclohexylidene-	138	C9H14O	000874-68-0	42
4			Cyclooctene, 1,2-dimethyl-	138	C10H18	054299-96-6	38
5			2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	38



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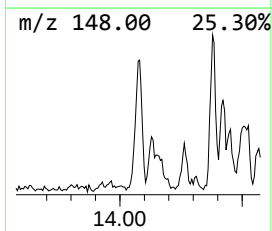
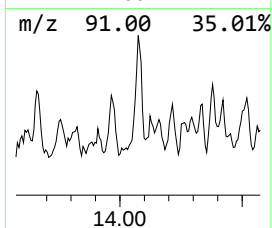
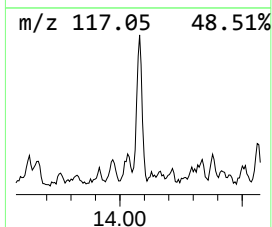
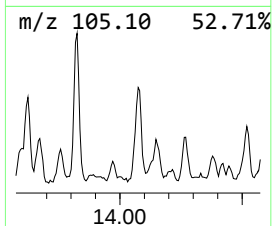
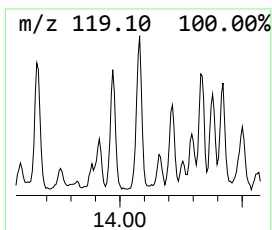
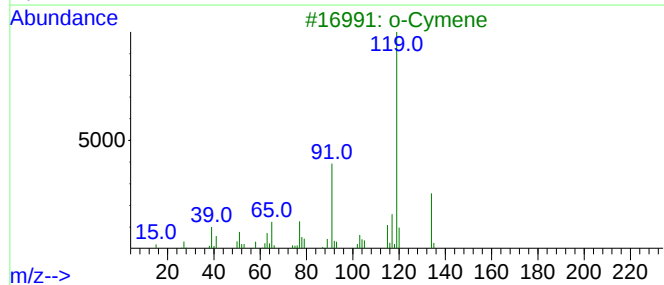
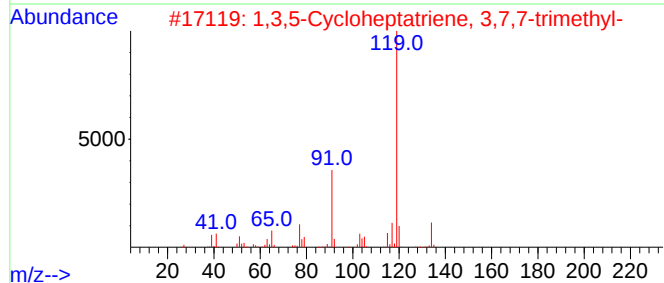
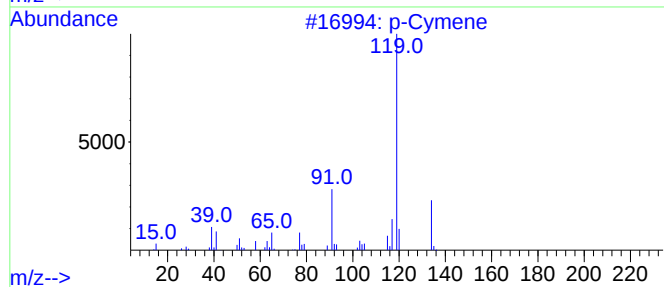
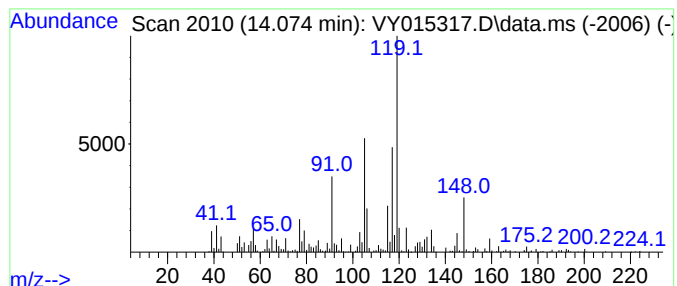
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown14.074 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	13.33 ug/l	190459	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Cymene	134	C10H14	000099-87-6	49
2			1,3,5-Cycloheptatriene, 3,7,7-tr...	134	C10H14	003479-89-8	46
3			o-Cymene	134	C10H14	000527-84-4	46
4			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	46
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	46



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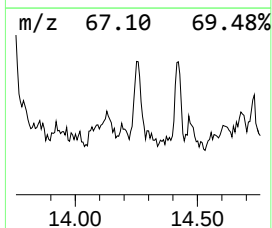
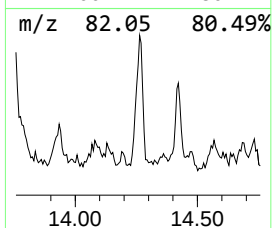
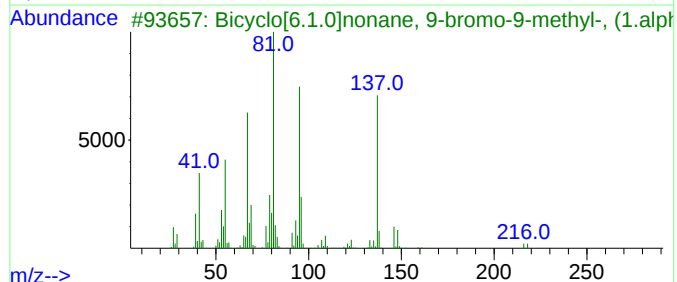
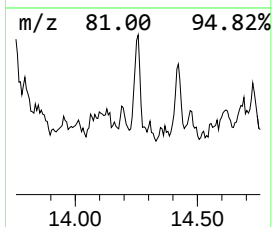
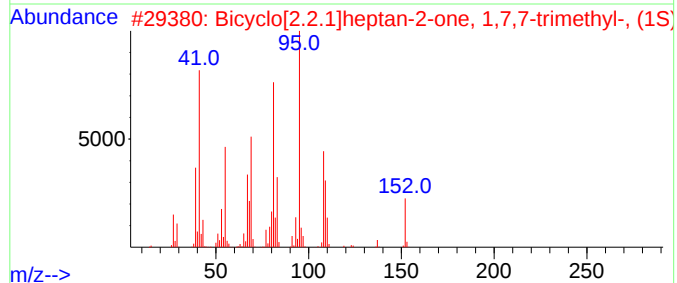
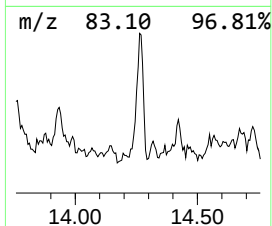
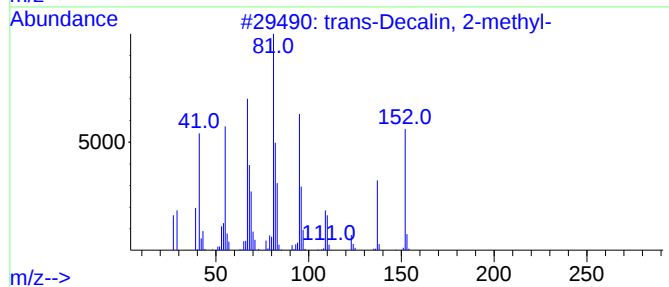
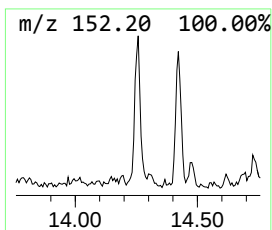
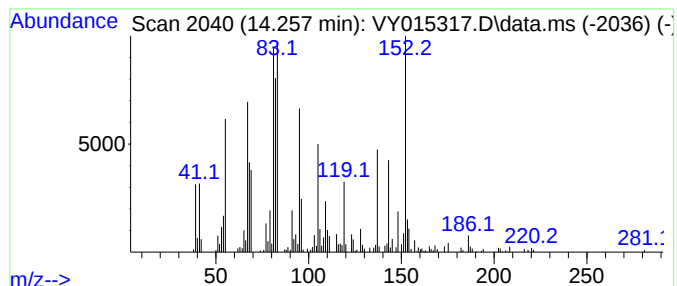
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Peak Number 4 trans-Decalin, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	12.21 ug/l	174475	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	53
2			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	50
3			Bicyclo[6.1.0]nonane, 9-bromo-9-...	216	C10H17Br	059474-03-2	30
4			5-Dodecyne	166	C12H22	019780-12-2	30
5			Pulegone	152	C10H16O	000089-82-7	30



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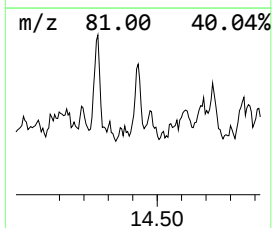
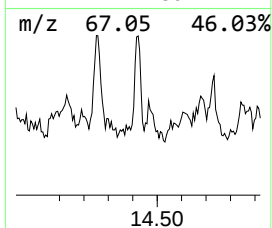
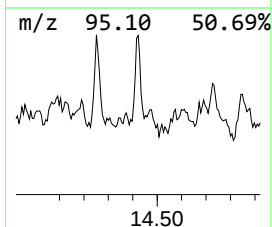
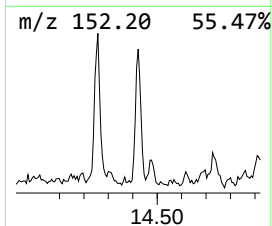
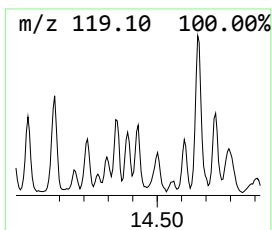
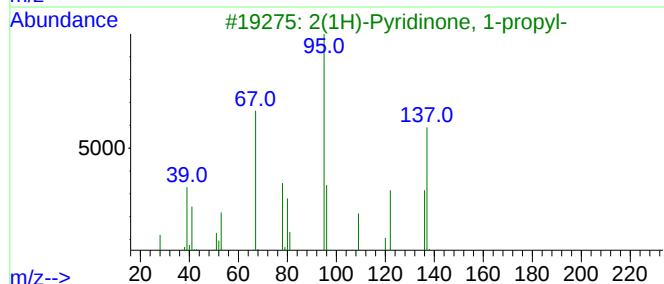
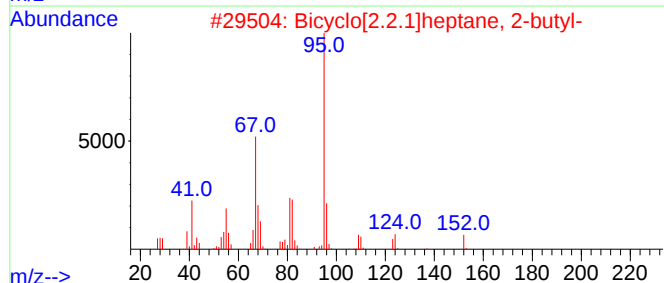
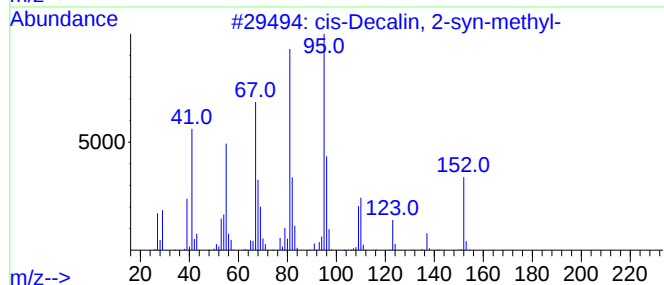
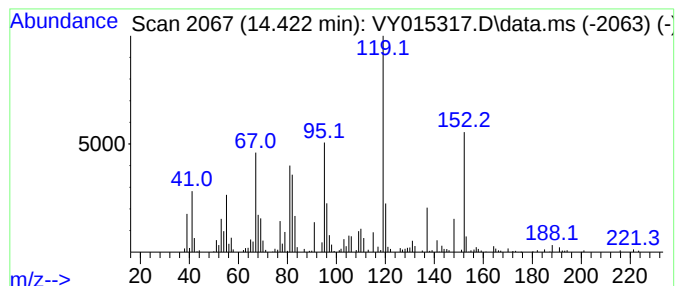
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Peak Number 5 cis-Decalin, 2-syn-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.422	13.70 ug/l	195733	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	87
2			Bicyclo[2.2.1]heptane, 2-butyl-	152	C11H20	061177-16-0	38
3			2(1H)-Pyridinone, 1-propyl-	137	C8H11NO	019006-63-4	38
4			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	35
5			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	27



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ClientSampleId :
RBR-22282

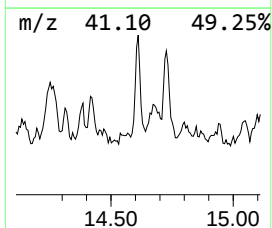
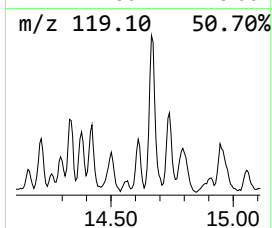
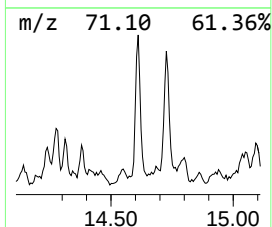
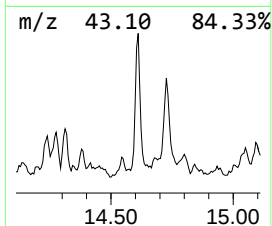
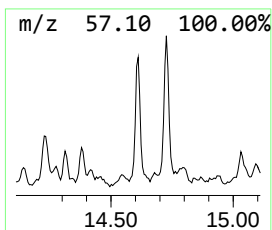
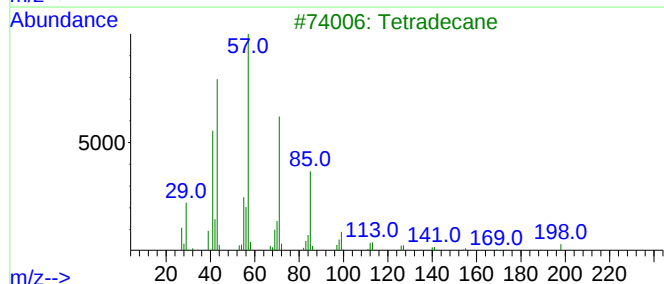
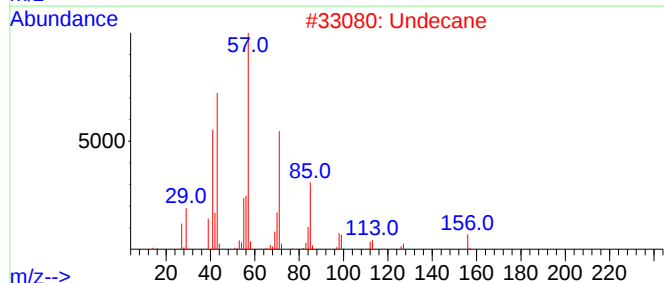
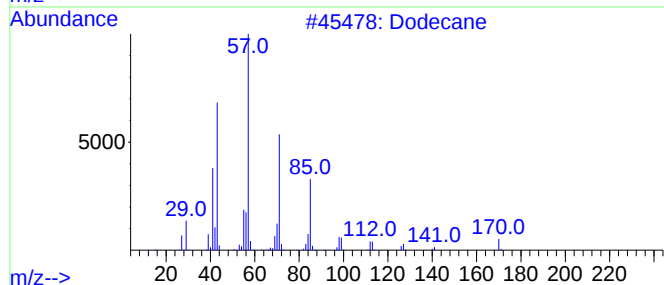
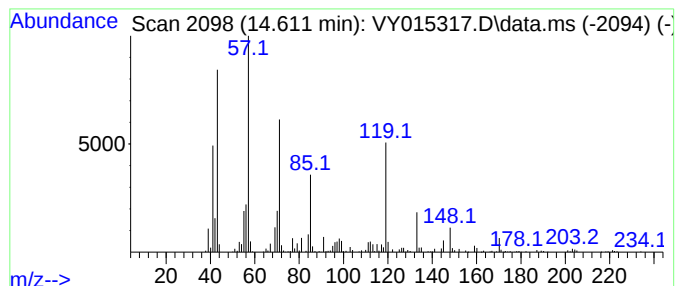
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Quant Title : SW846 8260

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

Peak Number 6 Dodecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.611	12.47 ug/l	178146	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	60
2			Undecane	156	C11H24	001120-21-4	49
3			Tetradecane	198	C14H30	000629-59-4	46
4			Nonane	128	C9H20	000111-84-2	43
5			Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082423\
Data File : VY015317.D
Acq On : 24 Aug 2023 17:18
Operator : SY/MD
Sample : 04112-01
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RBR-22282

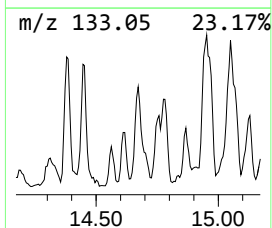
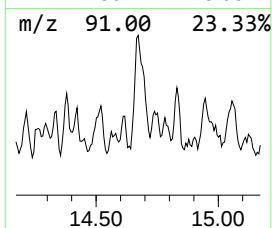
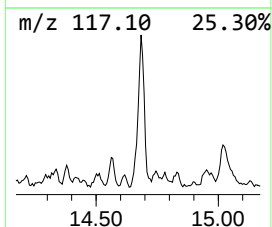
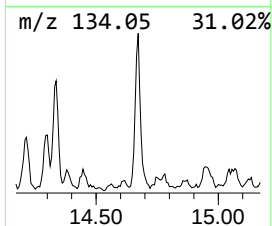
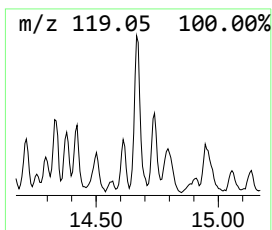
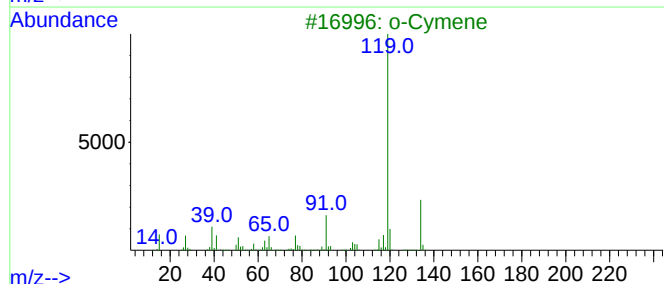
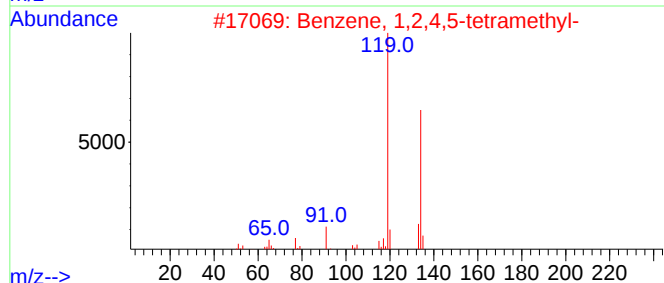
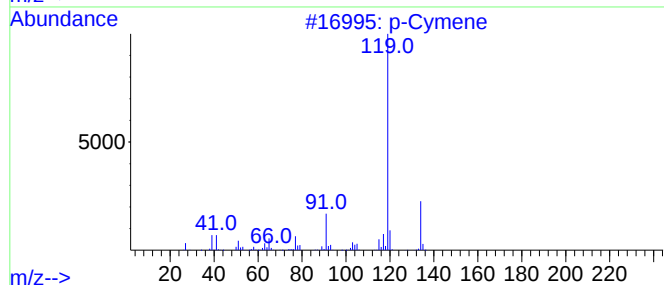
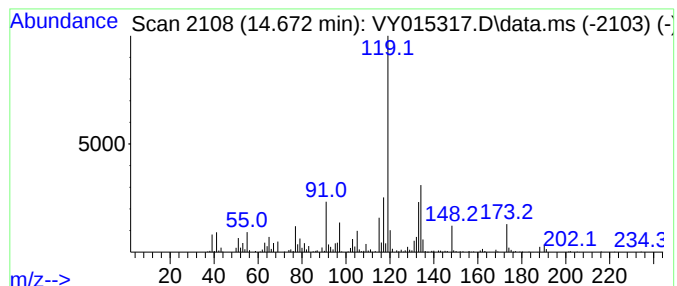
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Quant Title : SW846 8260

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

Peak Number 7 p-Cymene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.672	25.98 ug/l	371089	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Cymene	134	C10H14	000099-87-6	60
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	60
3			o-Cymene	134	C10H14	000527-84-4	60
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	60
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082423\
Data File : VY015317.D
Acq On : 24 Aug 2023 17:18
Operator : SY/MD
Sample : 04112-01
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RBR-22282

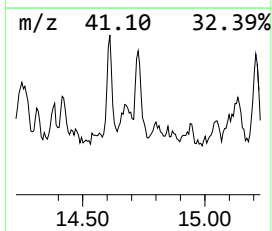
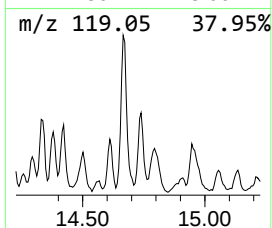
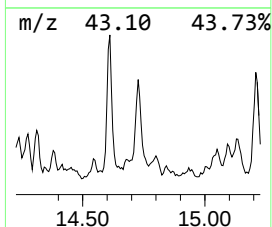
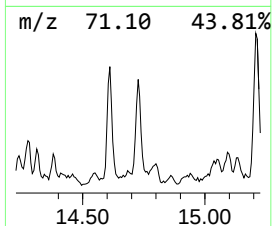
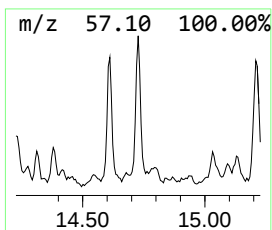
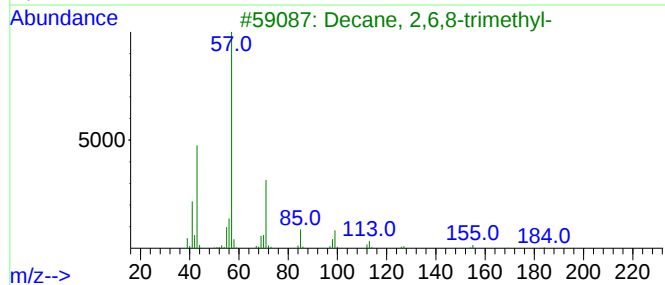
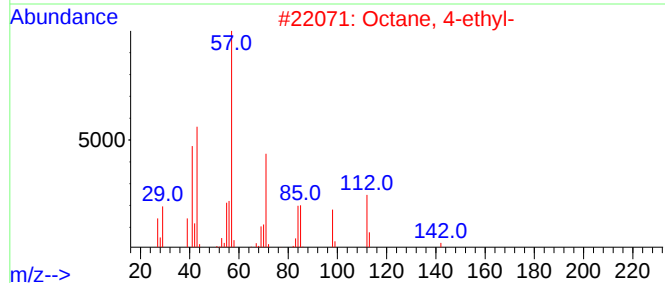
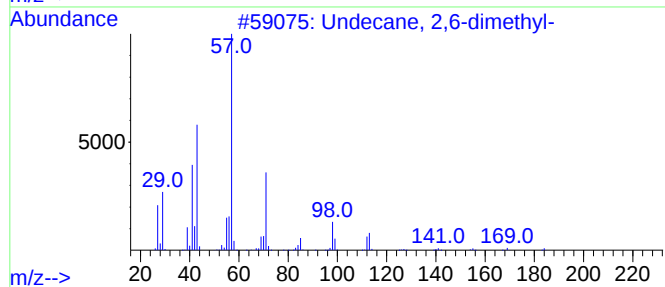
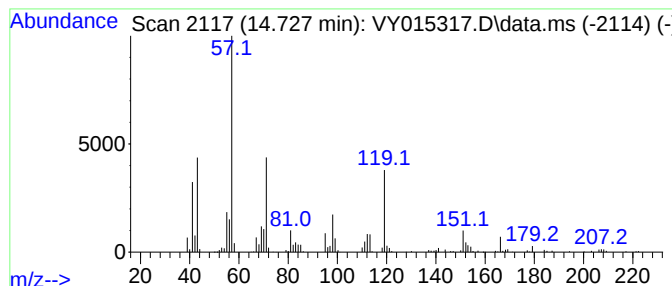
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Quant Title : SW846 8260

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

Peak Number 8 Undecane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	16.32 ug/l	233123	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	60
2			Octane, 4-ethyl-	142	C10H22	015869-86-0	47
3			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	46
4			Tridecane, 6-methyl-	198	C14H30	013287-21-3	43
5			Dodecane, 6-methyl-	184	C13H28	006044-71-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082423\
Data File : VY015317.D
Acq On : 24 Aug 2023 17:18
Operator : SY/MD
Sample : 04112-01
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RBR-22282

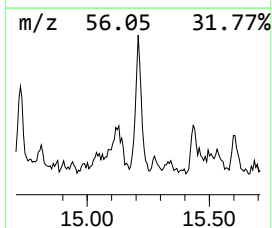
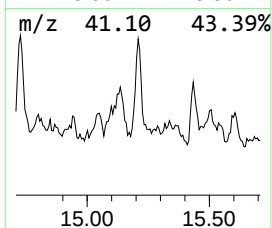
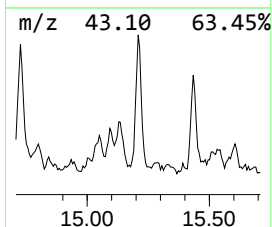
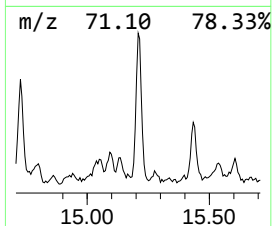
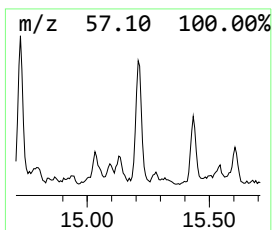
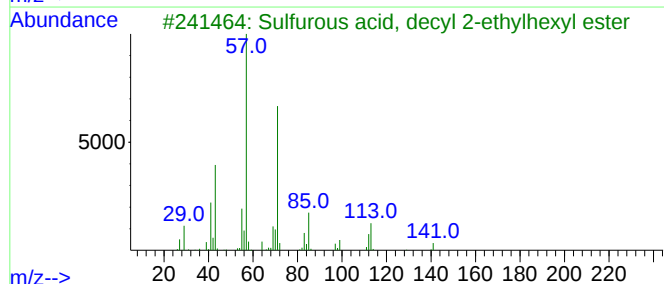
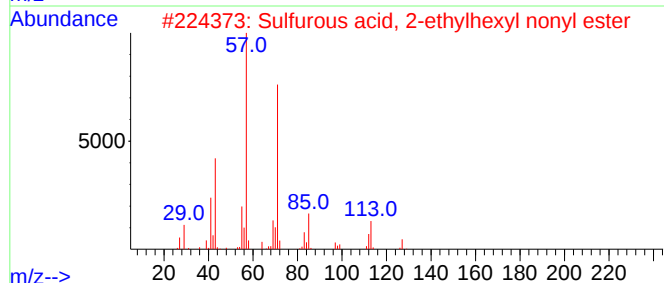
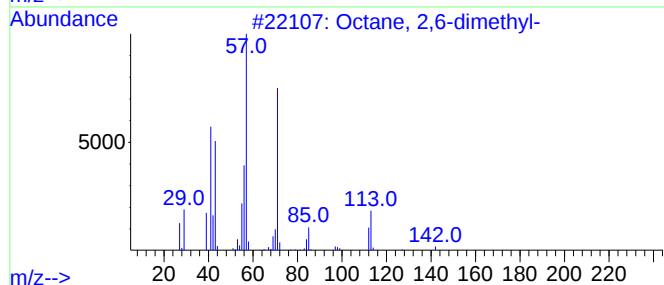
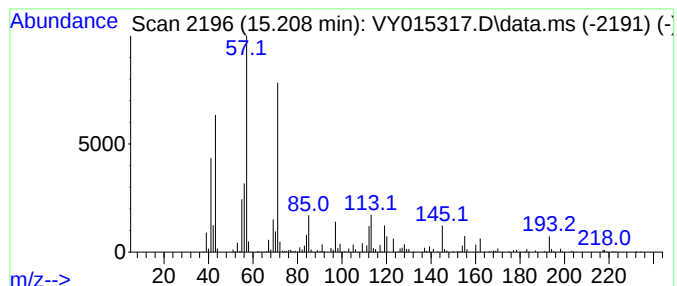
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Quant Title : SW846 8260

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

Peak Number 9 Octane, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.208	15.92 ug/l	227380	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
2			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	64
3			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	64
4			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	64
5			Tridecane, 7-methyl-	198	C14H30	026730-14-3	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082423\
Data File : VY015317.D
Acq On : 24 Aug 2023 17:18
Operator : SY/MD
Sample : 04112-01
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RBR-22282

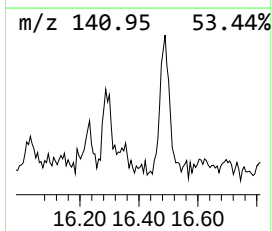
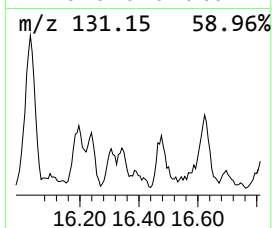
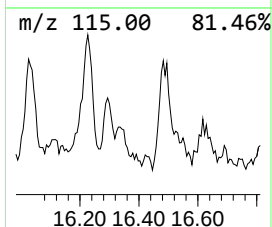
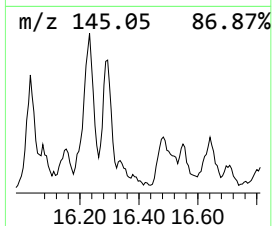
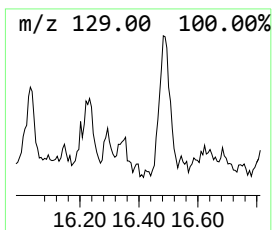
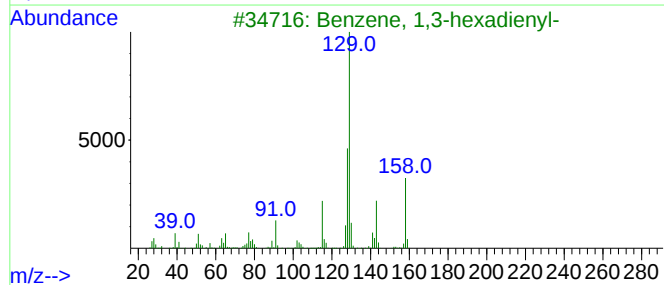
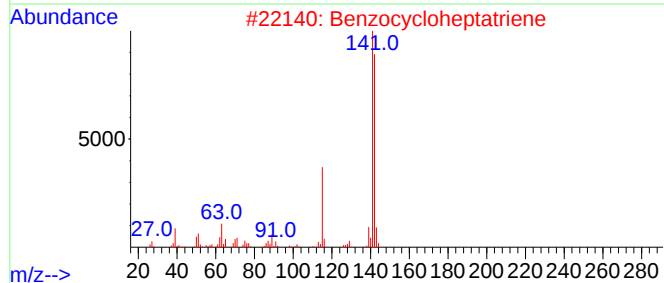
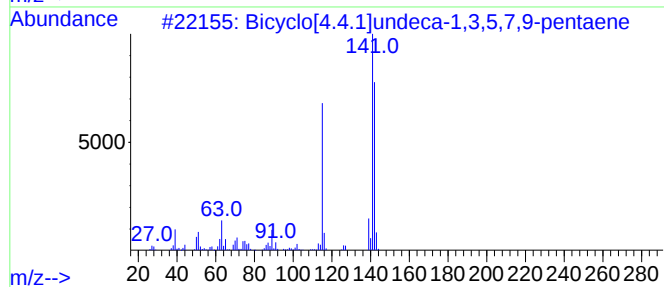
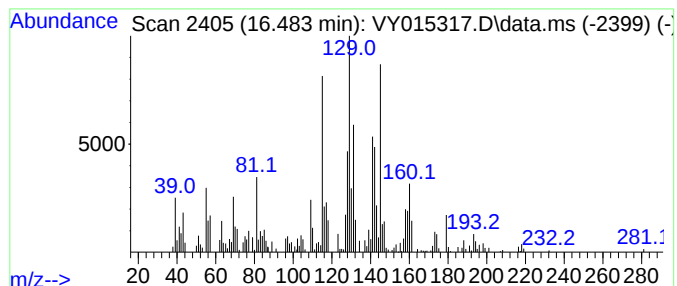
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Quant Title : SW846 8260

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

Peak Number 10 unknown16.483 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.483	13.99 ug/l	199900	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	38
2			Benzocycloheptatriene	142	C11H10	000264-09-5	25
3			Benzene, 1,3-hexadienyl-	158	C12H14	041635-77-2	22
4			Bicyclo[4.2.0]oct-1-ene, exo-7-(...	188	C14H20	1000142-22-1	20
5			1,4-Methanonaphthalen-9-ol, 1,4-...	158	C11H10O	004796-33-2	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082423\
Data File : VY015317.D
Acq On : 24 Aug 2023 17:18
Operator : SY/MD
Sample : 04112-01
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RBR-22282

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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					#	RT	Resp	Conc
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unknown13.751	13.751	33.1	ug/l	472419	4	13.422	714290	50.0
unknown14.074	14.074	13.3	ug/l	190459	4	13.422	714290	50.0
trans-Decalin, ...	14.257	12.2	ug/l	174475	4	13.422	714290	50.0
cis-Decalin, 2-...	14.422	13.7	ug/l	195733	4	13.422	714290	50.0
Dodecane	14.611	12.5	ug/l	178146	4	13.422	714290	50.0
p-Cymene	14.672	26.0	ug/l	371089	4	13.422	714290	50.0
Undecane, 2,6-d...	14.727	16.3	ug/l	233123	4	13.422	714290	50.0
Octane, 2,6-dim...	15.208	15.9	ug/l	227380	4	13.422	714290	50.0
unknown16.483	16.483	14.0	ug/l	199900	4	13.422	714290	50.0