

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD022624\
 Data File : VD078550.D
 Acq On : 26 Feb 2024 13:30
 Operator : RP/MD
 Sample : P1588-01
 Misc : 5.08G/5ml/MSVOA_D/SOIL/A
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 1838

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_D\Method\82D021324S.M

Title : SW846 8260

Signal : TIC: VD078550.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.740	19	26	39	rVB	442685	710155	35.13%	4.435%
2	4.805	533	547	558	rBV3	9601	29620	1.47%	0.185%
3	7.810	1047	1058	1063	rBV	92141	218803	10.82%	1.366%
4	7.881	1063	1070	1078	rVB2	144906	337059	16.67%	2.105%
5	8.234	1122	1130	1141	rVB2	62683	146054	7.22%	0.912%
6	8.781	1213	1223	1233	rBV	239577	488654	24.17%	3.052%
7	10.269	1464	1476	1485	rBV	401089	706190	34.93%	4.410%
8	11.581	1690	1699	1712	rBV	437879	746229	36.91%	4.660%
9	12.428	1837	1843	1849	rBV2	32007	57676	2.85%	0.360%
10	12.575	1861	1868	1878	rVB	345915	567511	28.07%	3.544%
11	12.892	1914	1922	1930	rVB2	57812	85959	4.25%	0.537%
12	13.457	2013	2018	2023	rBV	135303	217991	10.78%	1.361%
13	13.516	2023	2028	2033	rVV	461330	737397	36.48%	4.605%
14	13.581	2033	2039	2053	rVB	1039346	1699481	84.07%	10.613%
15	13.745	2063	2067	2077	rVB7	9014	24539	1.21%	0.153%
16	13.963	2099	2104	2115	rBV7	22406	53252	2.63%	0.333%
17	14.175	2134	2140	2141	rBV	146557	196481	9.72%	1.227%
18	14.269	2151	2156	2162	rBV	656888	994371	49.19%	6.210%
19	14.322	2162	2165	2170	rVB3	27791	43832	2.17%	0.274%
20	14.375	2170	2174	2178	rBV	297391	433736	21.46%	2.709%
21	14.410	2178	2180	2183	rVV3	21396	26584	1.32%	0.166%
22	14.481	2188	2192	2194	rVV2	335130	512789	25.37%	3.202%
23	14.516	2194	2198	2212	rVV3	718733	1868335	92.42%	11.668%
24	14.634	2212	2218	2225	rVV	300526	492246	24.35%	3.074%
25	14.692	2226	2228	2235	rVB5	26397	35753	1.77%	0.223%
26	14.839	2247	2253	2263	rBV	263158	431577	21.35%	2.695%
27	15.034	2278	2286	2296	rBV	165392	311540	15.41%	1.946%
28	15.181	2301	2311	2326	rVV	1222304	2021540	100.00%	12.624%
29	15.310	2326	2333	2336	rBV	151158	262893	13.00%	1.642%
30	15.345	2336	2339	2352	rVB2	203769	366331	18.12%	2.288%
31	15.528	2365	2370	2377	rVB6	15138	27297	1.35%	0.170%
32	15.704	2393	2400	2408	rBV	129961	230656	11.41%	1.440%
33	15.816	2416	2419	2431	rVB	11849	26658	1.32%	0.166%
34	16.010	2441	2452	2458	rBV	370777	685513	33.91%	4.281%
35	16.063	2458	2461	2467	rVB2	46122	78280	3.87%	0.489%
36	16.222	2480	2488	2492	rBV7	29710	61579	3.05%	0.385%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Title : SW846 8260

37	16.269	2492	2496	2502	rVB3	31184	54993	2.72%	0.343%
38	16.463	2525	2529	2536	rVB6	14446	23473	1.16%	0.147%

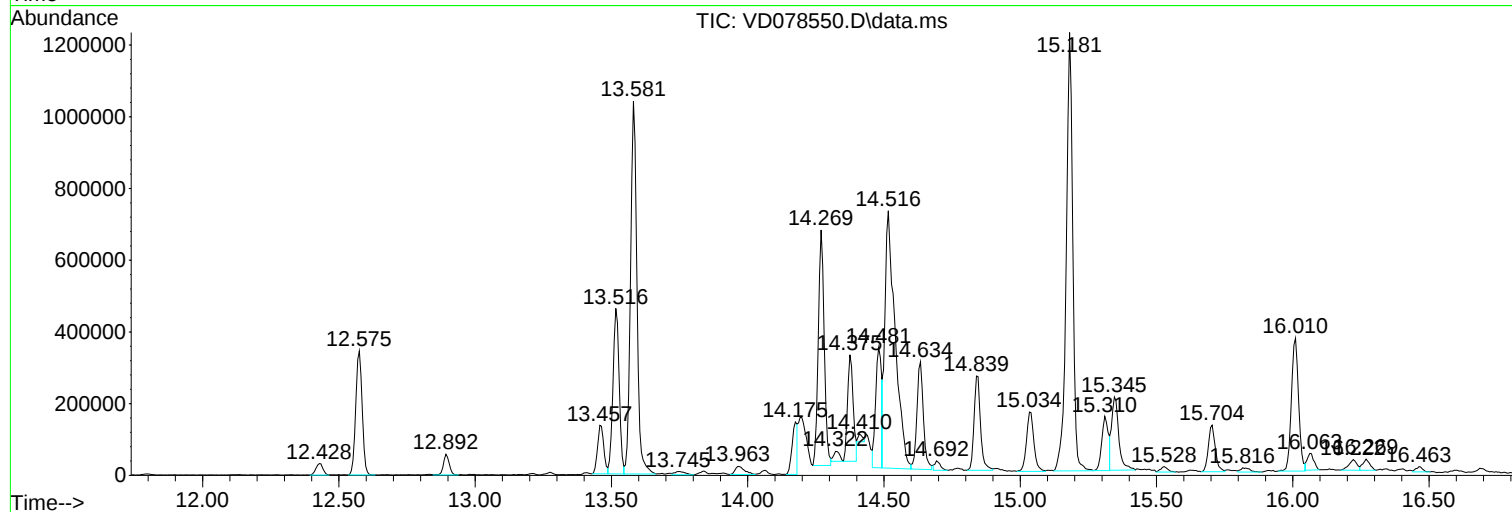
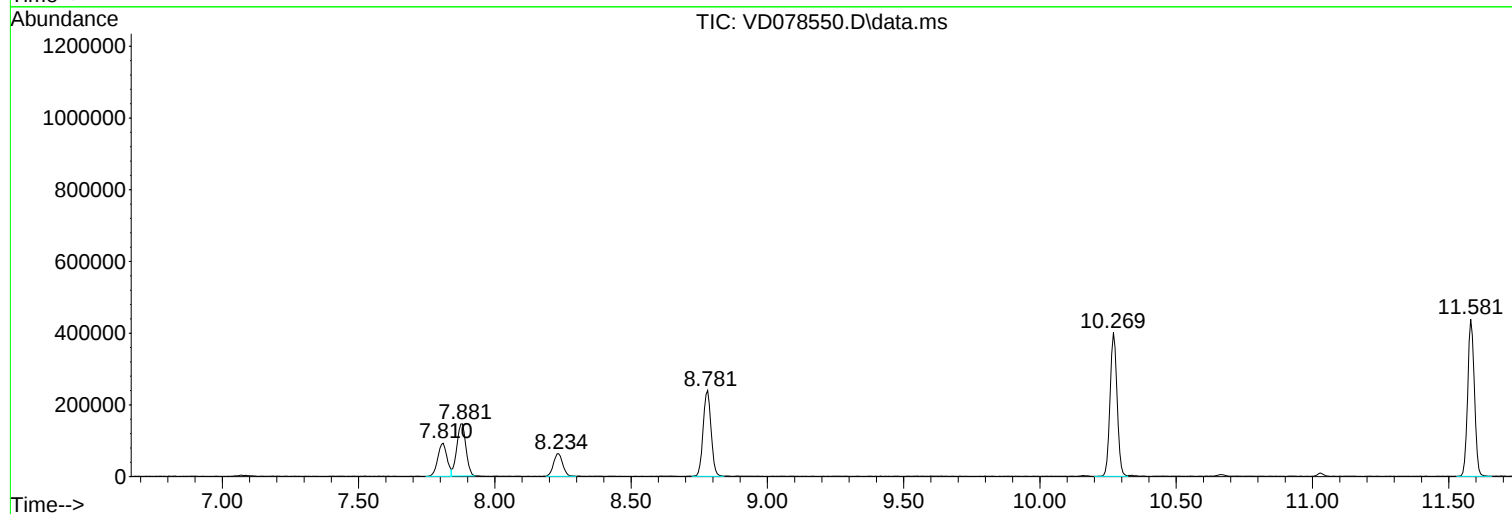
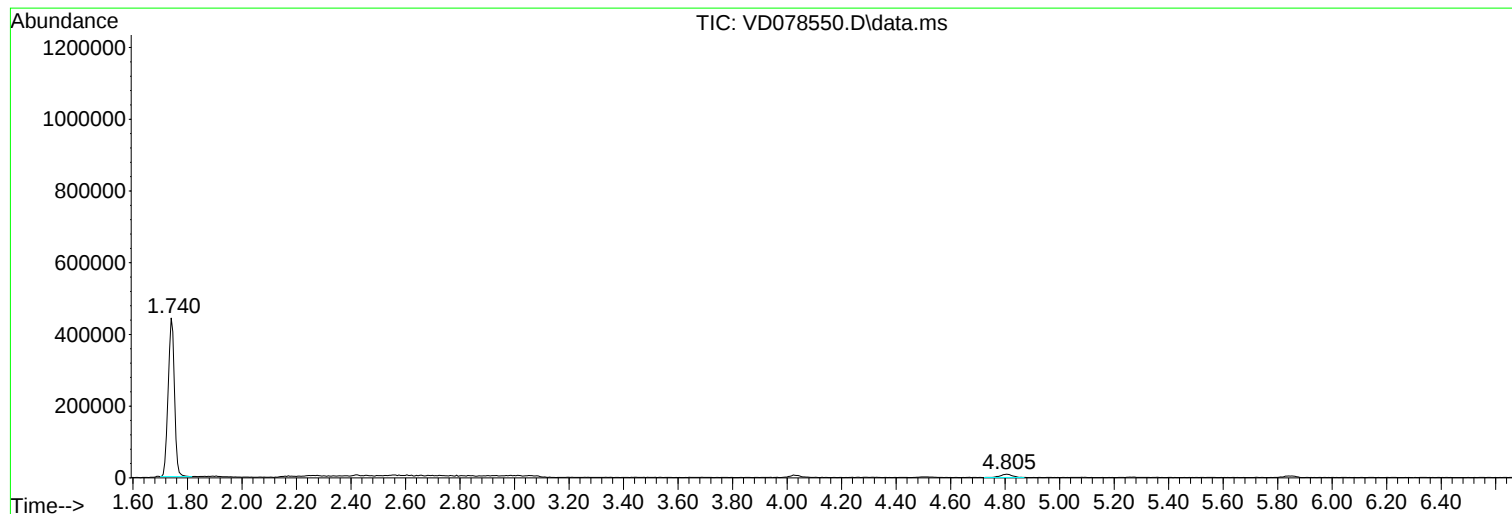
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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



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Misc : 5.08G/5ml/MSVOA_D/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
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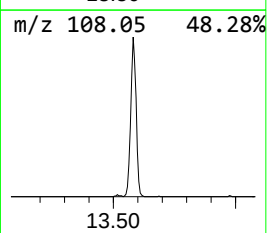
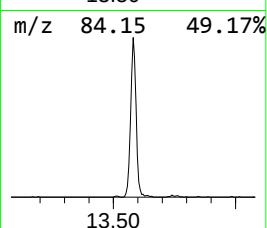
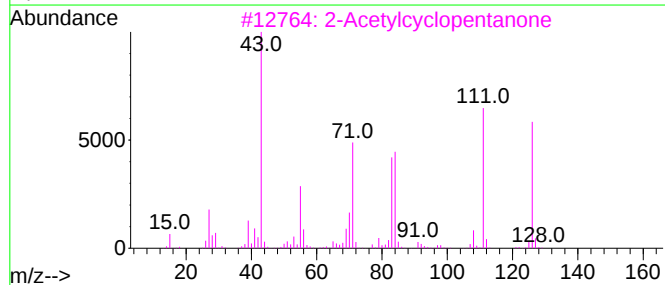
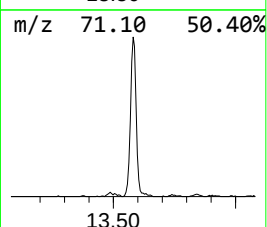
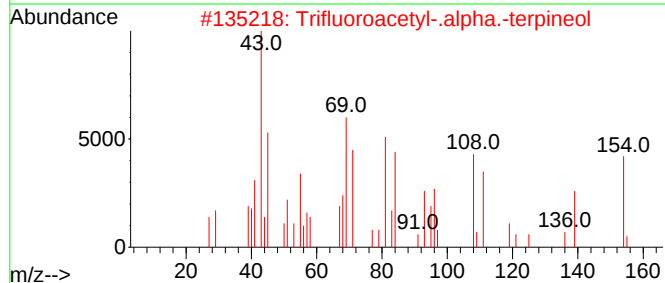
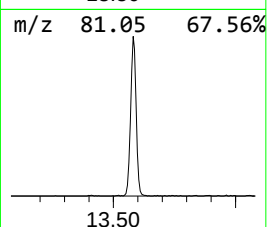
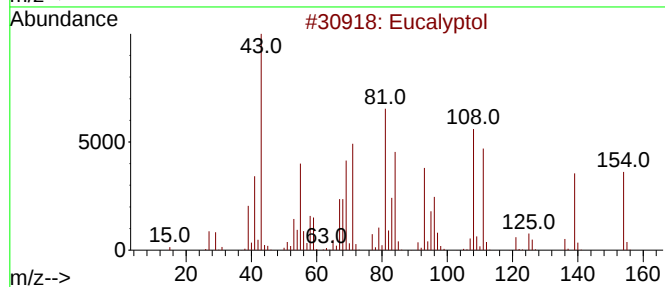
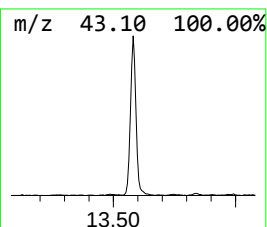
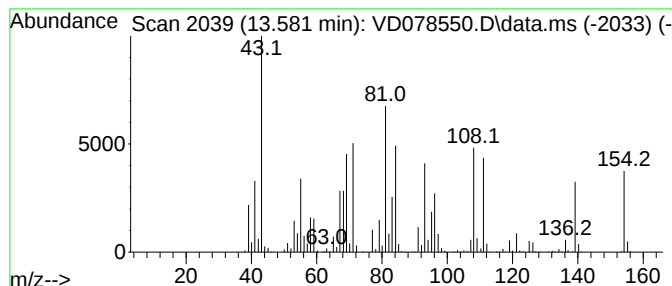
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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

Peak Number 2 Eucalyptol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.581	115.24 ug/l	1699480	1,4-Dichlorobenzene-d4	13.516

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	74
3			2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	27
4			5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	22
5			2-Acetylcylohexanone	154	C9H14O2	006126-53-0	22



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Misc : 5.08G/5ml/MSVOA_D/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
1838

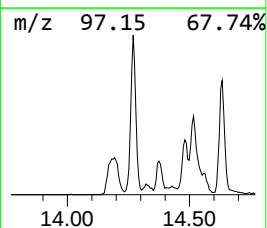
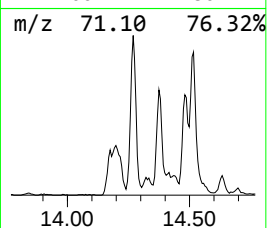
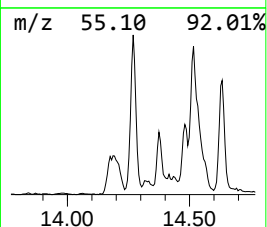
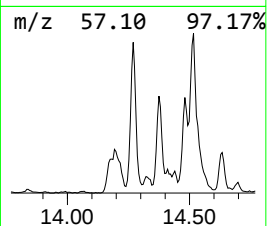
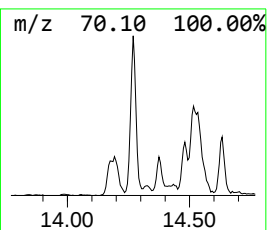
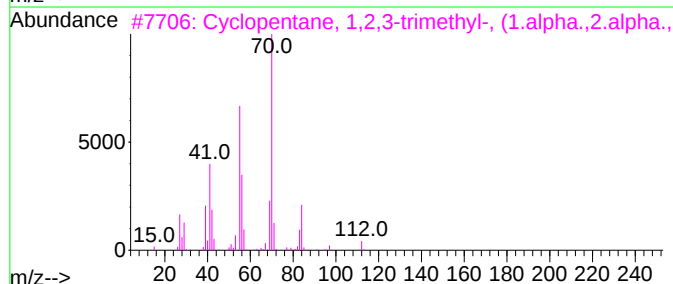
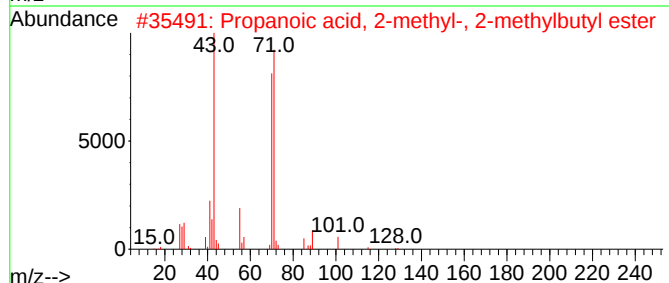
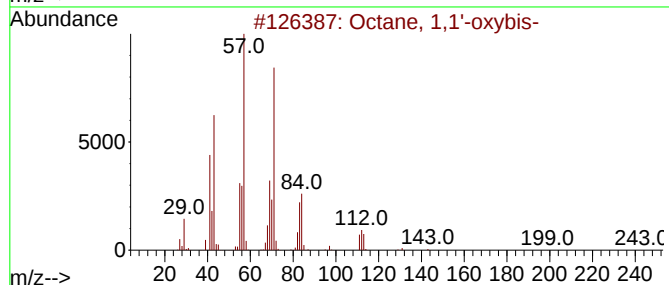
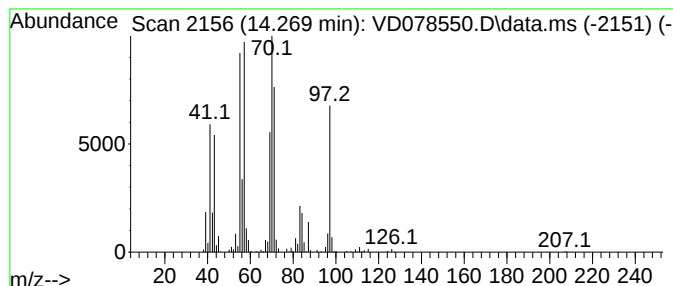
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown14.269 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	67.42 ug/l	994371	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	43
2			Propanoic acid, 2-methyl-, 2-met...	158	C9H18O2	002445-69-4	43
3			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	38
4			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	38
5			Allyl n-octyl ether	170	C11H22O	003295-97-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD022624\
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Misc : 5.08G/5ml/MSVOA_D/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
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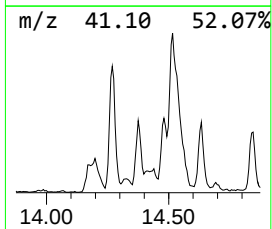
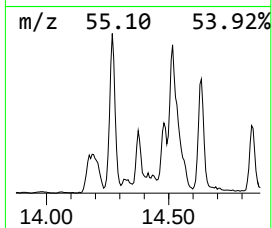
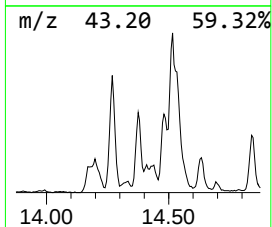
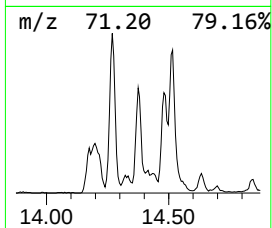
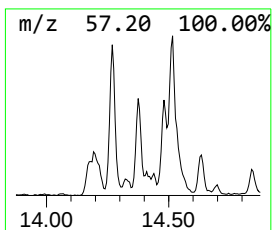
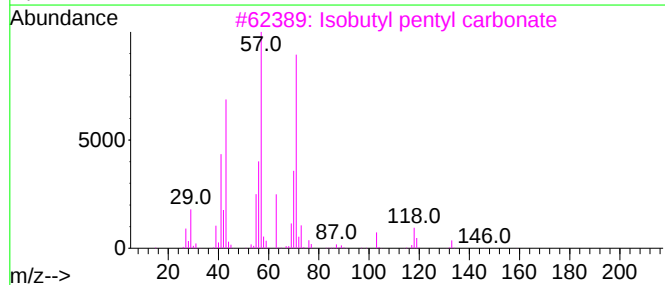
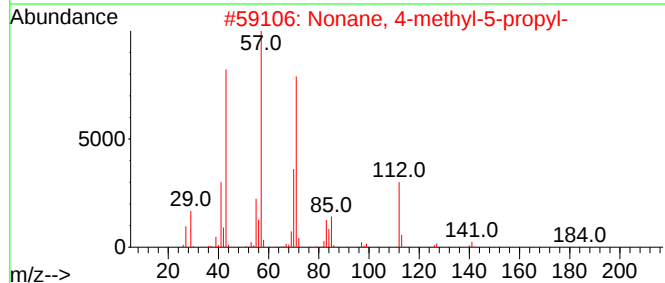
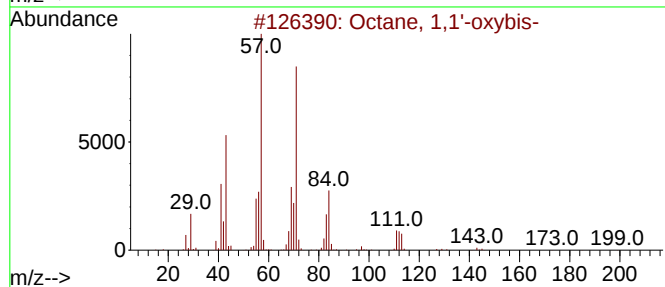
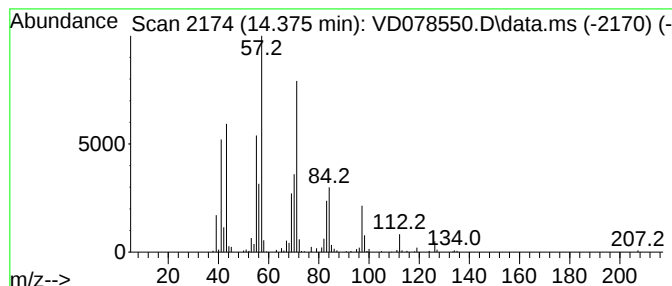
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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

Peak Number 4 Octane, 1,1'-oxybis- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.375	29.41 ug/l	433736	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	64
2			Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	53
3			Isobutyl pentyl carbonate	188	C10H20O3	178442-32-5	50
4			4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	47
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	43



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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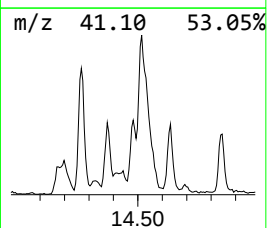
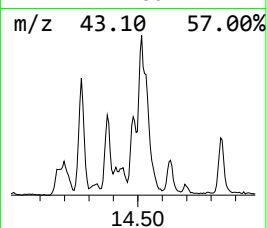
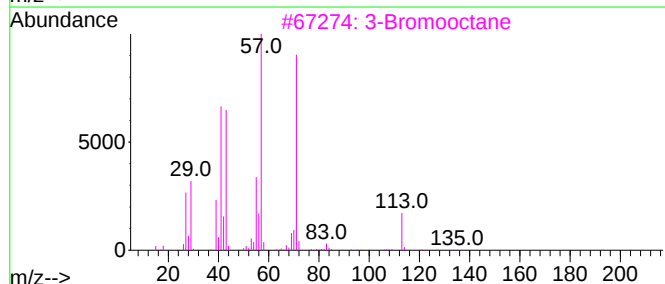
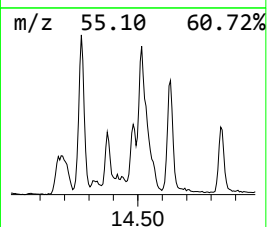
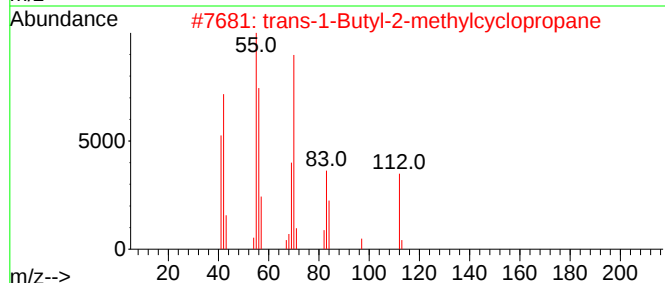
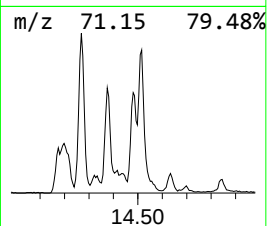
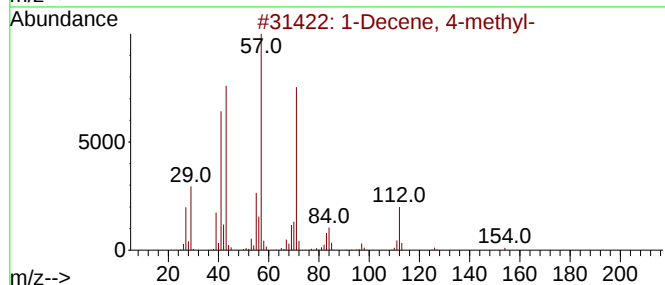
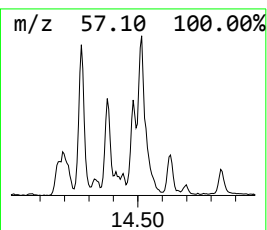
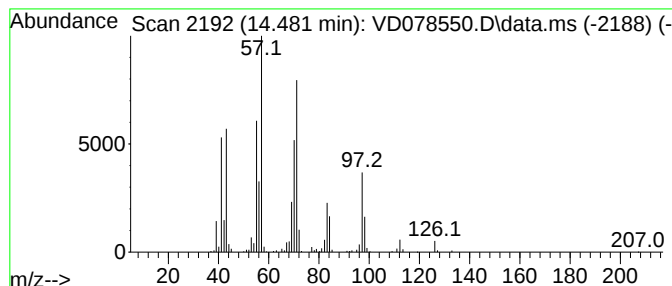
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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

Peak Number 5 unknown14.481 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.481	34.77 ug/l	512789	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decene, 4-methyl-	154	C11H22	013151-29-6	43
2			trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	41
3			3-Bromooctane	192	C8H17Br	000999-64-4	38
4			Dichloroacetic acid, 2-ethylhexy...	240	C10H18Cl2O2	068144-72-9	38
5			cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	38



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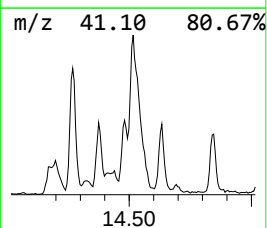
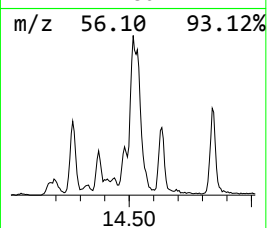
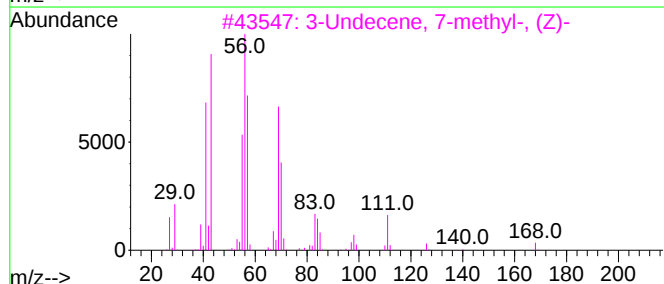
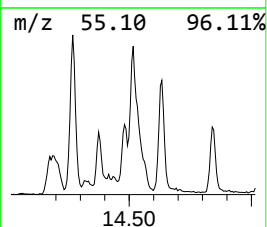
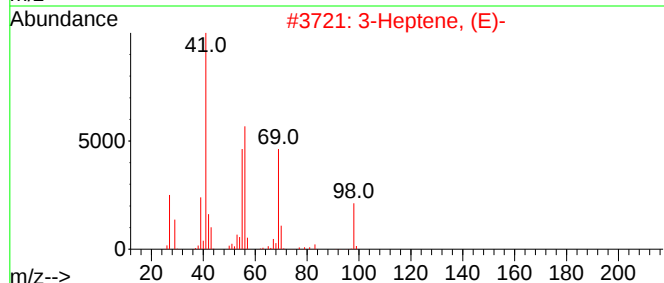
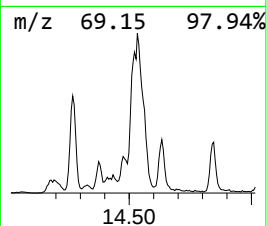
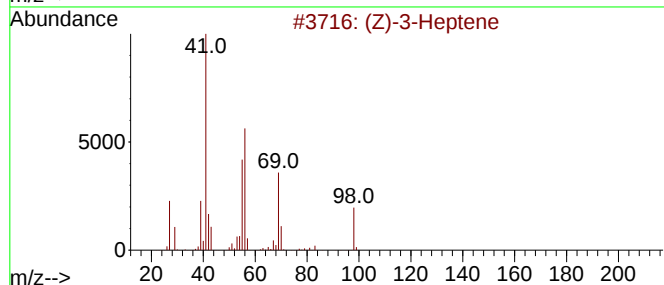
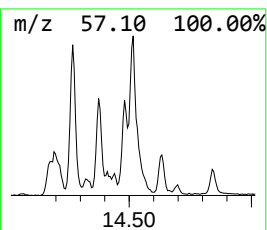
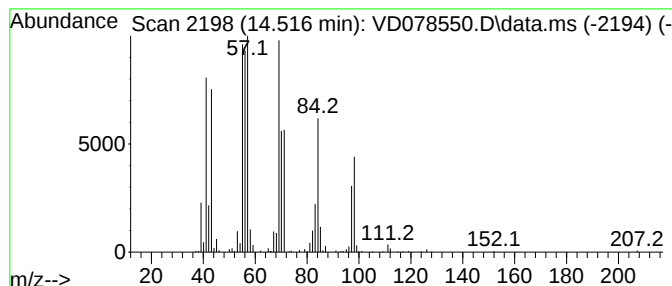
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Quant Title : SW846 8260

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

Peak Number 6 (Z)-3-Heptene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.516	126.68 ug/l	1868340	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(Z)-3-Heptene	98	C7H14	007642-10-6	60
2			3-Heptene, (E)-	98	C7H14	014686-14-7	55
3			3-Undecene, 7-methyl-, (Z)-	168	C12H24	074630-49-2	53
4			1-Hexene, 3-methyl-	98	C7H14	003404-61-3	47
5			3-Heptene	98	C7H14	000592-78-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD022624\
Data File : VD078550.D
Acq On : 26 Feb 2024 13:30
Operator : RP/MD
Sample : P1588-01
Misc : 5.08G/5ml/MSVOA_D/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
1838

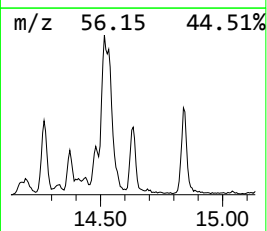
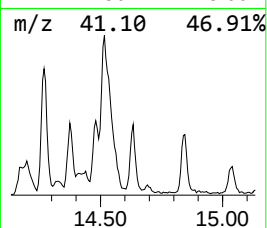
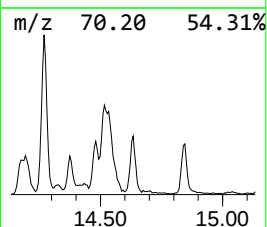
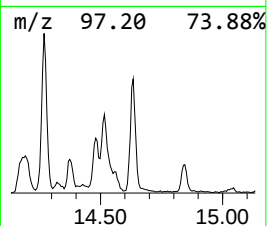
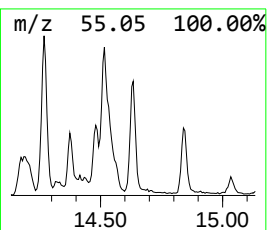
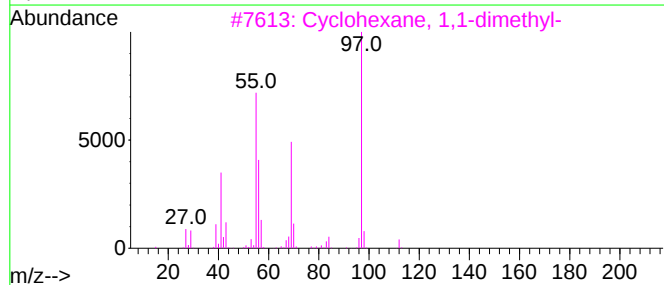
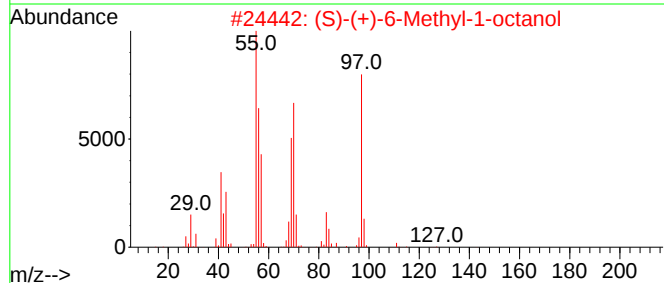
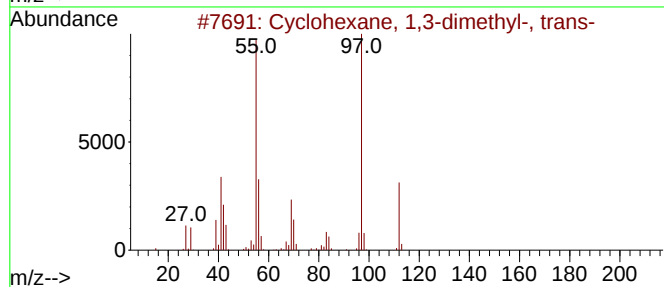
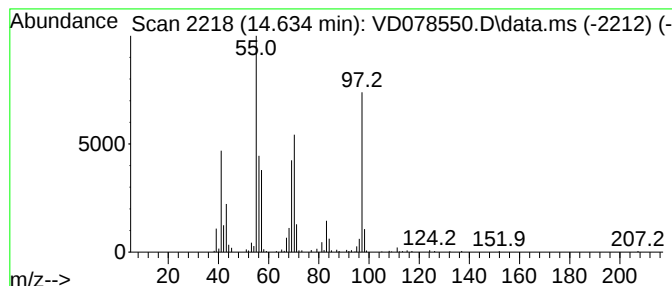
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	33.38 ug/l	492246	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	72
2			(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	64
3			Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	53
4			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	50
5			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD022624\
Data File : VD078550.D
Acq On : 26 Feb 2024 13:30
Operator : RP/MD
Sample : P1588-01
Misc : 5.08G/5ml/MSVOA_D/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

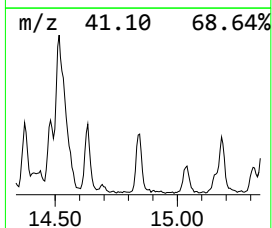
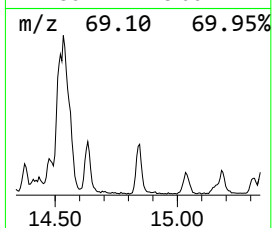
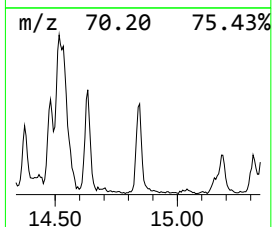
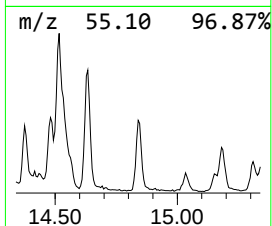
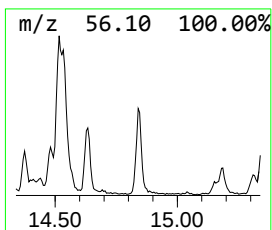
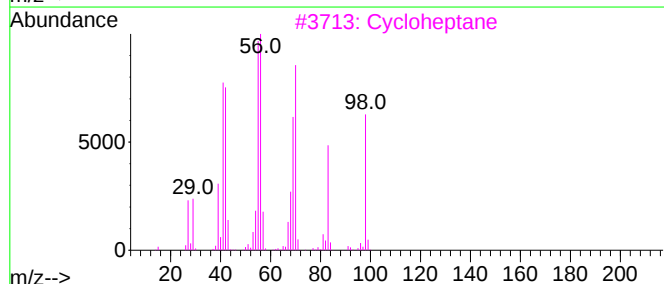
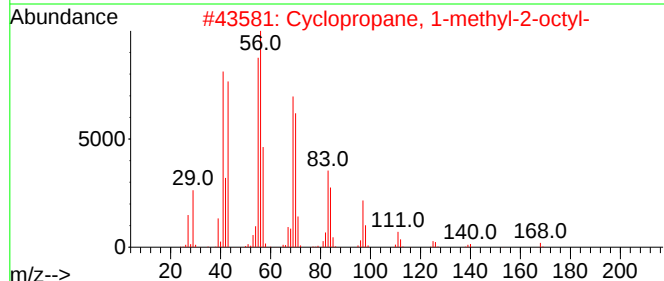
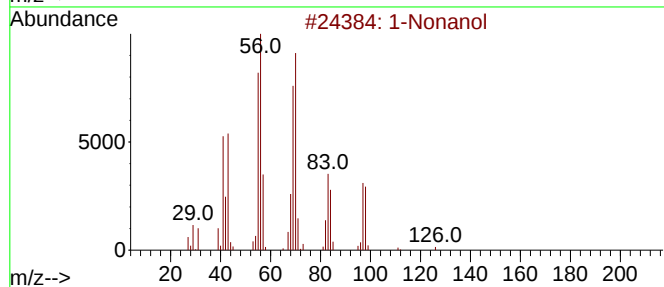
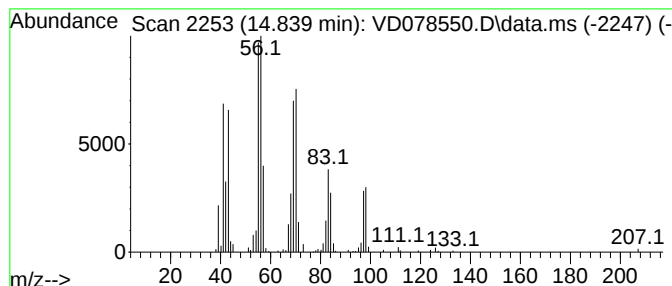
Instrument :
MSVOA_D
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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

Peak Number 8 1-Nonanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.839	29.26 ug/l	431577	1,4-Dichlorobenzene-d4	13.516	
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	80
3	Cycloheptane	98	C7H14	000291-64-5	74
4	1-Octanol	130	C8H18O	000111-87-5	64
5	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD022624\
Data File : VD078550.D
Acq On : 26 Feb 2024 13:30
Operator : RP/MD
Sample : P1588-01
Misc : 5.08G/5ml/MSVOA_D/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
1838

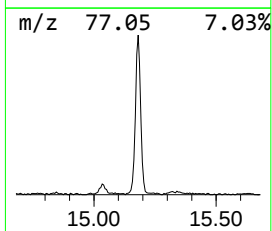
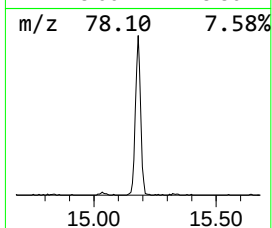
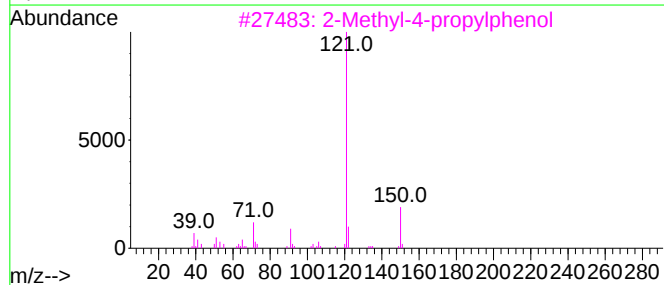
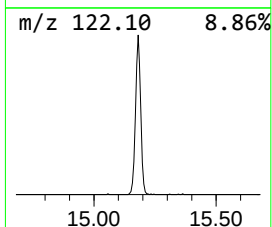
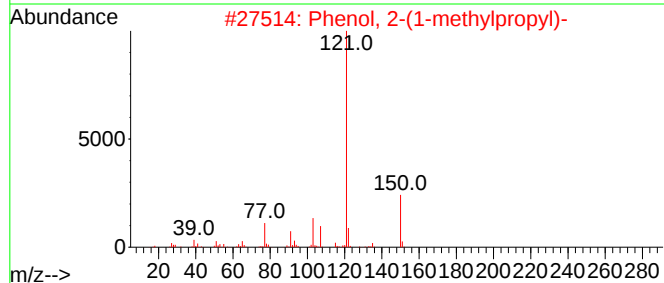
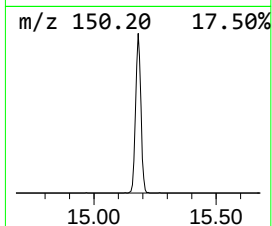
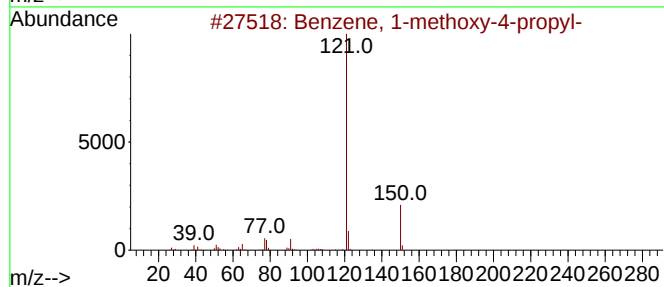
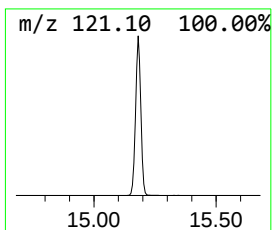
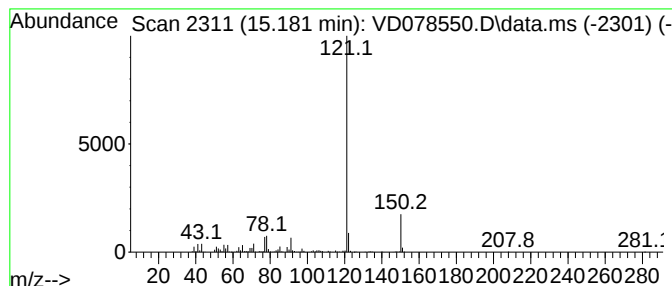
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.181	137.07 ug/l	2021540	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	90
2			Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	86
3			2-Methyl-4-propylphenol	150	C10H14O	018441-56-0	72
4			Propanedinitrile, [3-(4-methoxypropyl)-	226	C14H14N2O	069244-84-4	64
5			(Z)-Ethyl 2-(2-(4-methoxybenzyl)-	387	C20H21NO5S	1135696-36-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD022624\
Data File : VD078550.D
Acq On : 26 Feb 2024 13:30
Operator : RP/MD
Sample : P1588-01
Misc : 5.08G/5ml/MSVOA_D/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
1838

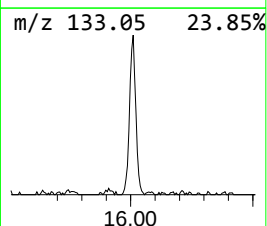
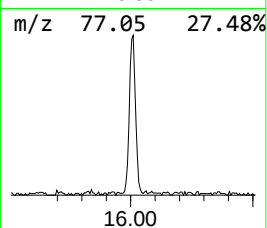
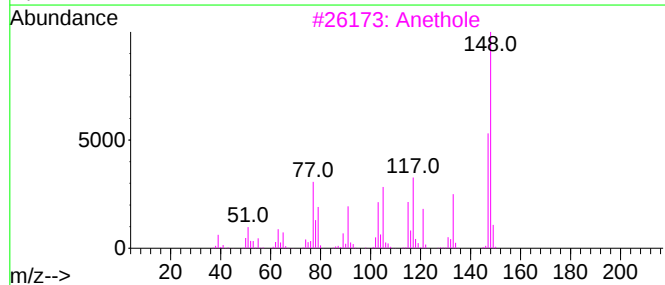
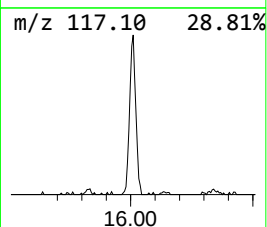
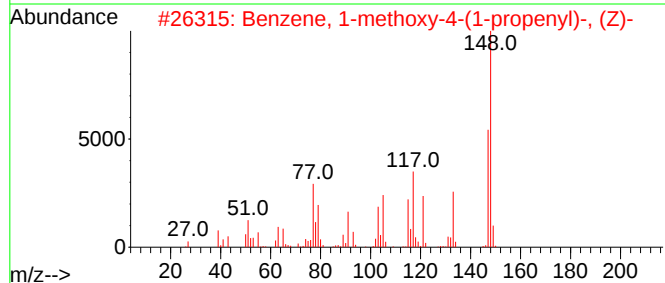
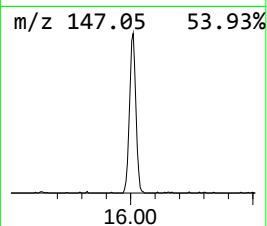
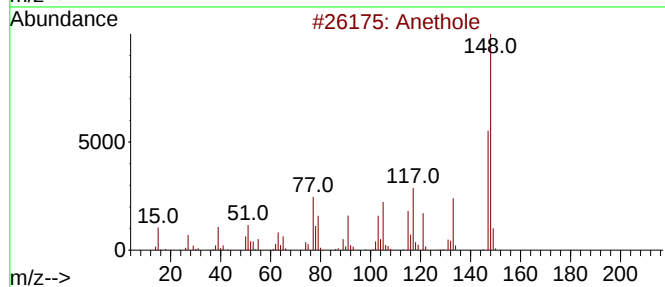
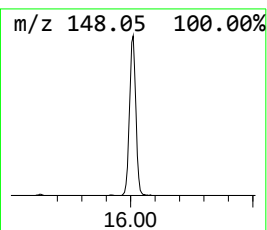
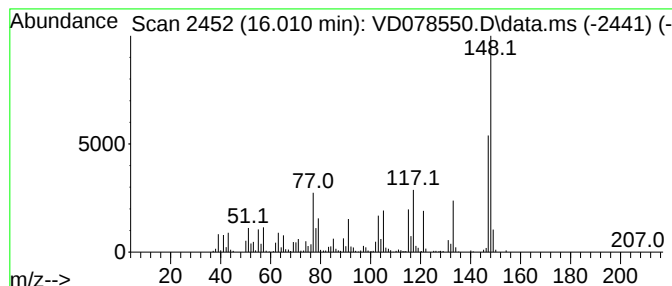
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Quant Title : SW846 8260

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

Peak Number 10 Anethole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.010	46.48 ug/l	685513	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anethole			148	C10H12O	000104-46-1	98
2	Benzene, 1-methoxy-4-(1-propenyl)-			148	C10H12O	025679-28-1	97
3	Anethole			148	C10H12O	004180-23-8	96
4	Estragole			148	C10H12O	000140-67-0	94
5	8,9-Dehydrothymol			148	C10H12O	018612-99-2	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD022624\
Data File : VD078550.D
Acq On : 26 Feb 2024 13:30
Operator : RP/MD
Sample : P1588-01
Misc : 5.08G/5ml/MSVOA_D/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
1838

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.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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unknown14.269	14.269	67.4	ug/l	994371	4	13.516	737397	50.0
Octane, 1,1'-ox...	14.375	29.4	ug/l	433736	4	13.516	737397	50.0
unknown14.481	14.481	34.8	ug/l	512789	4	13.516	737397	50.0
(Z)-3-Heptene	14.516	126.7	ug/l	1868340	4	13.516	737397	50.0
Cyclohexane, 1,...	14.634	33.4	ug/l	492246	4	13.516	737397	50.0
1-Nonanol	14.839	29.3	ug/l	431577	4	13.516	737397	50.0
Benzene, 1-meth...	15.181	137.1	ug/l	2021540	4	13.516	737397	50.0
Anethole	16.010	46.5	ug/l	685513	4	13.516	737397	50.0