

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110824\
 Data File : VY020232.D
 Acq On : 08 Nov 2024 14:48
 Operator : SY/MD
 Sample : P4771-05
 Misc : 7.55g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 P-1

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\82Y103024S.M

Title : SW846 8260

Signal : TIC: VY020232.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.616	464	475	488	rBV3	18851	61155	4.34%	0.600%
2	7.634	959	970	976	rBV	199579	473909	33.66%	4.648%
3	7.707	976	982	994	rVB	282361	657055	46.67%	6.445%
4	8.061	1030	1040	1053	rBV	180068	407754	28.96%	4.000%
5	8.616	1120	1131	1146	rBV	545794	1056490	75.05%	10.363%
6	9.670	1296	1304	1312	rBV3	32352	66569	4.73%	0.653%
7	10.109	1368	1376	1390	rBV	804318	1407796	100.00%	13.809%
8	11.414	1583	1590	1597	rBV	819828	1311390	93.15%	12.863%
9	12.408	1741	1753	1763	rBV	576217	973292	69.14%	9.547%
10	12.962	1834	1844	1846	rBV2	37366	64207	4.56%	0.630%
11	12.993	1846	1849	1856	rVB2	52043	83317	5.92%	0.817%
12	13.103	1859	1867	1873	rVB	24579	43095	3.06%	0.423%
13	13.206	1873	1884	1890	rBV	314730	506599	35.99%	4.969%
14	13.279	1892	1896	1899	rVV3	22224	34542	2.45%	0.339%
15	13.346	1899	1907	1912	rVV	639562	1032766	73.36%	10.130%
16	13.395	1912	1915	1928	rVB	217463	434233	30.84%	4.259%
17	13.566	1933	1943	1947	rBV2	59479	119313	8.48%	1.170%
18	13.712	1963	1967	1971	rBV7	10647	23284	1.65%	0.228%
19	13.883	1984	1995	2011	rVB3	123382	295882	21.02%	2.902%
20	14.054	2016	2023	2026	rBV6	16810	39447	2.80%	0.387%
21	14.084	2026	2028	2033	rVB4	15688	20908	1.49%	0.205%
22	14.310	2057	2065	2074	rBV3	164787	339075	24.09%	3.326%
23	14.444	2082	2087	2092	rBV3	18017	36675	2.61%	0.360%
24	14.554	2098	2105	2113	rBV9	7189	23234	1.65%	0.228%
25	14.639	2114	2119	2128	rVB4	16095	33154	2.36%	0.325%
26	14.773	2138	2141	2151	rVB7	9684	26721	1.90%	0.262%
27	14.852	2151	2154	2158	rBV5	8270	15761	1.12%	0.155%
28	15.084	2185	2192	2195	rBV6	16261	40948	2.91%	0.402%
29	15.133	2195	2200	2206	rVB2	50303	90871	6.45%	0.891%
30	15.297	2219	2227	2233	rBV2	26422	54844	3.90%	0.538%
31	15.450	2250	2252	2258	rVB6	8987	14593	1.04%	0.143%
32	15.742	2293	2300	2304	rBV4	39267	82196	5.84%	0.806%
33	15.797	2304	2309	2315	rVB2	48235	85790	6.09%	0.841%
34	16.023	2336	2346	2358	rVB5	45851	155295	11.03%	1.523%
35	16.145	2360	2366	2370	rBV8	9517	21452	1.52%	0.210%
36	16.200	2372	2375	2380	rVB7	11406	16729	1.19%	0.164%

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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_Y\methods\82Y103024S.M
Title : SW846 8260

37	16.358	2397	2401	2408	rBV8	5547	14098	1.00%	0.138%
38	16.639	2441	2447	2455	rVB8	10530	30542	2.17%	0.300%

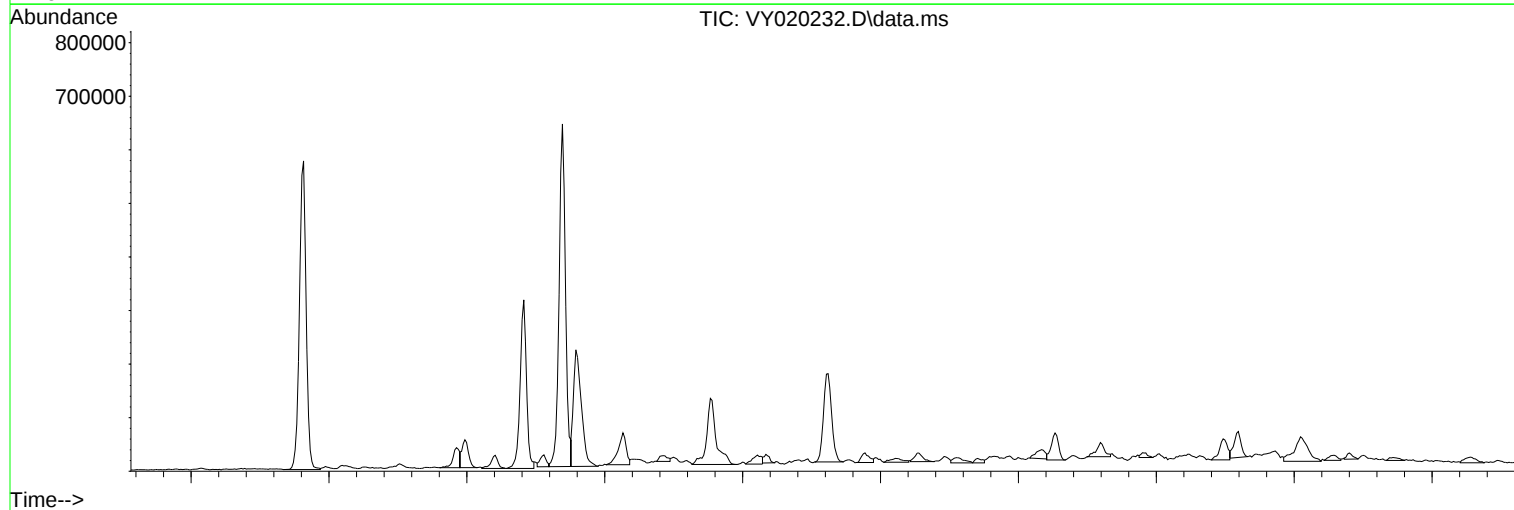
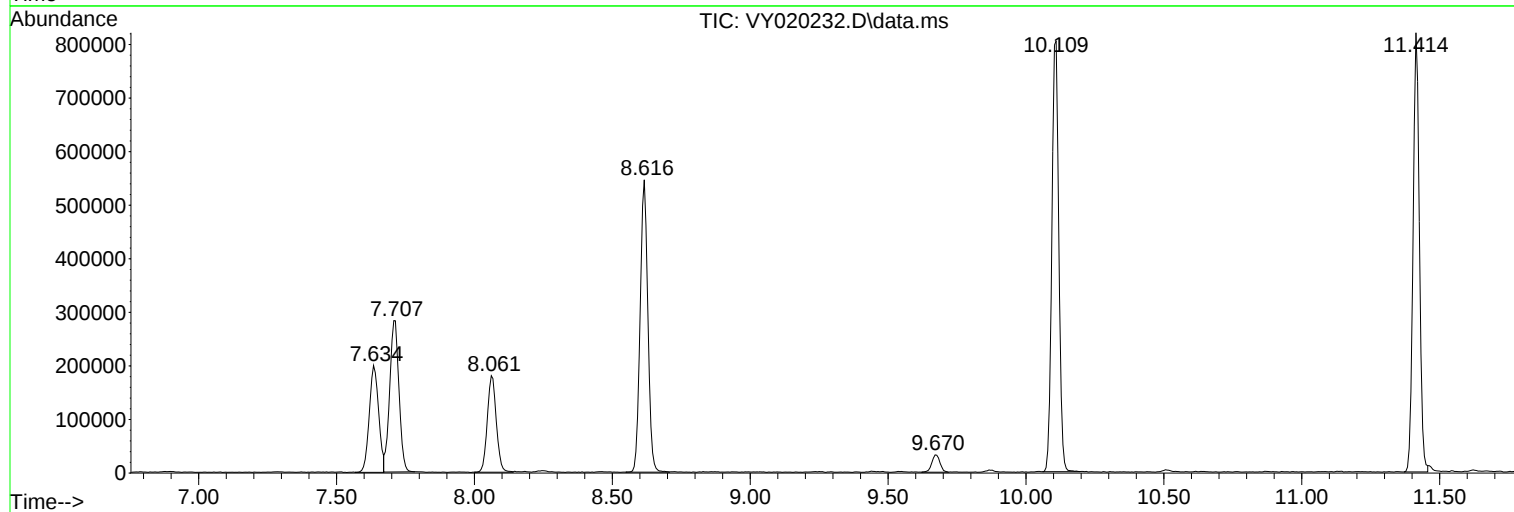
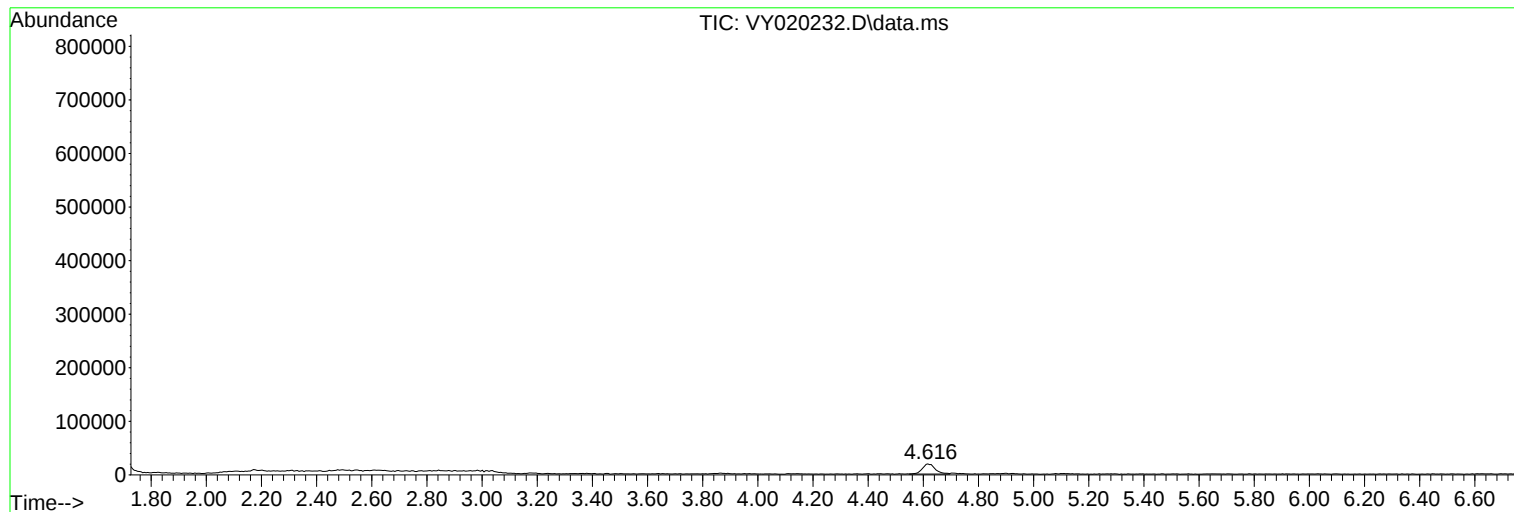
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y103024S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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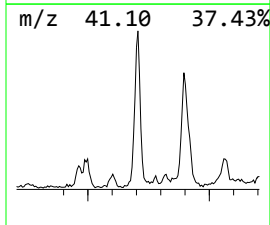
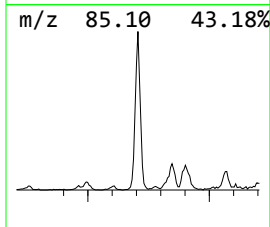
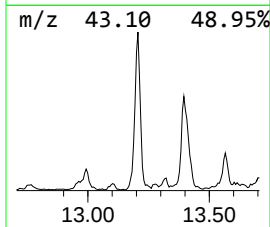
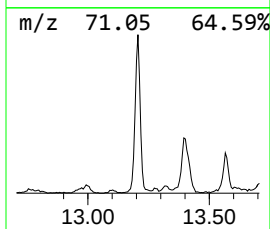
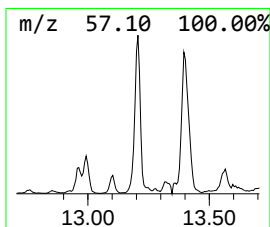
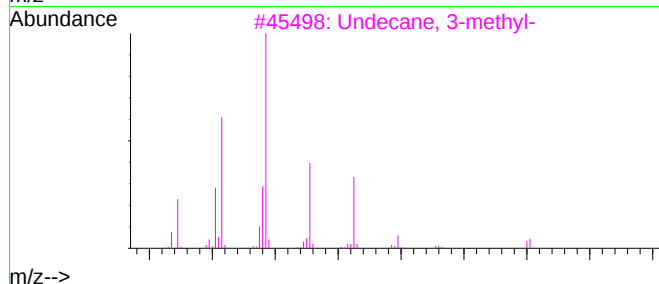
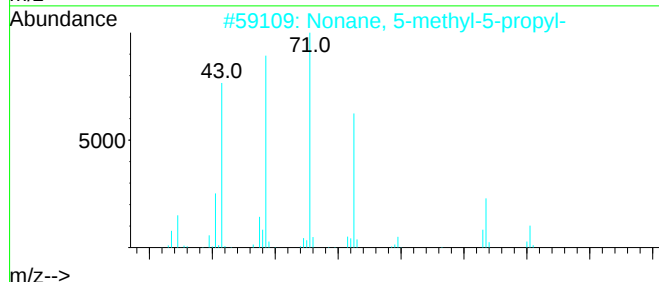
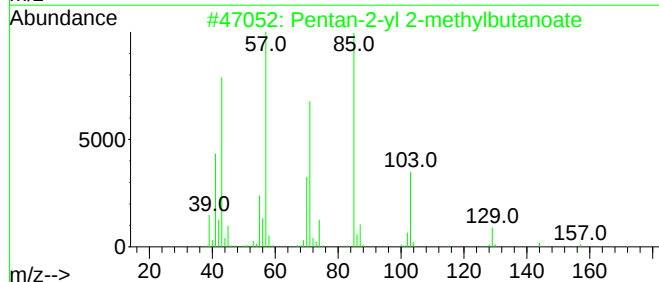
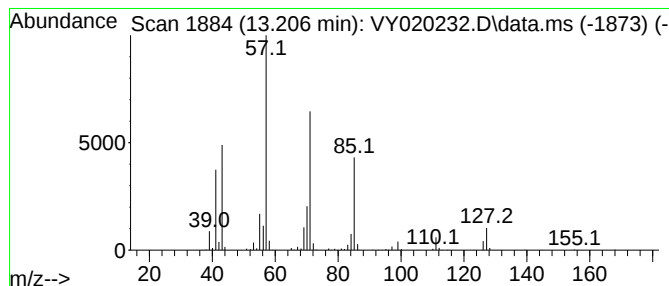
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Pentan-2-yl 2-methylbutanoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.206	24.53 ug/l	506599	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	59
2	Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	58
3	Undecane, 3-methyl-	170	C12H26	001002-43-3	50
4	Nonane, 5-butyl-	184	C13H28	017312-63-9	50
5	Tridecane, 6-methyl-	198	C14H30	013287-21-3	50



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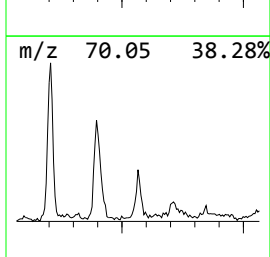
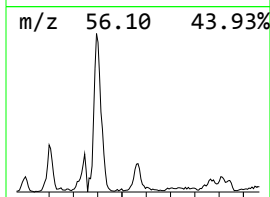
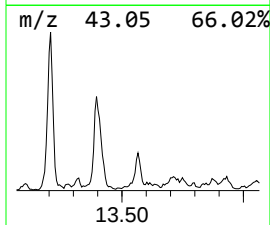
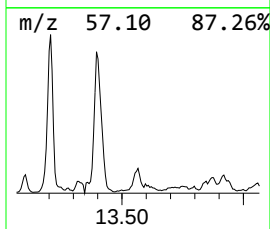
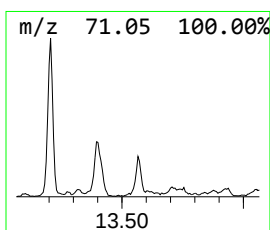
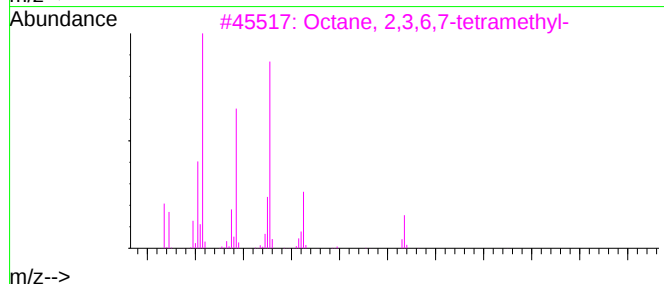
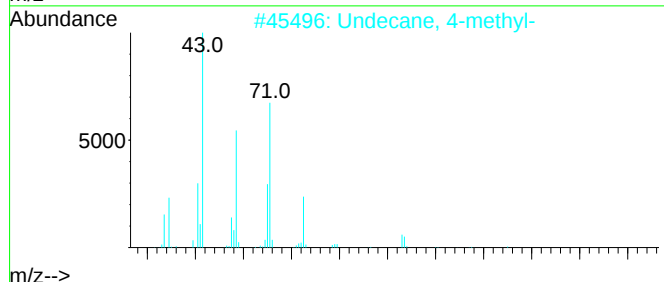
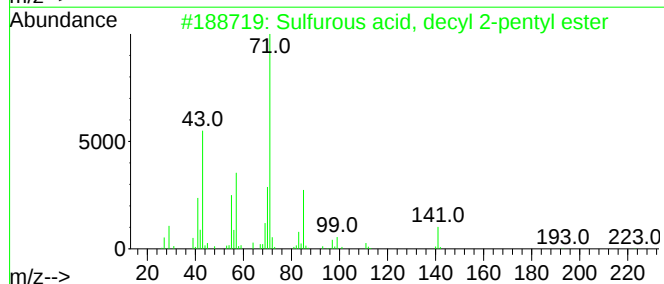
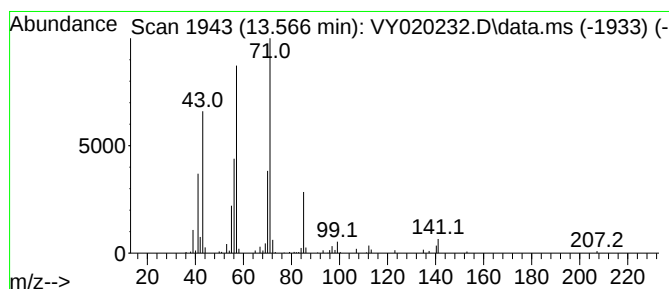
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y103024S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Sulfurous acid, decyl 2-pen... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.566	5.78 ug/l	119313	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, decyl 2-pentyl e...	292	C15H32O3S	1000309-15-9	59
2	Undecane, 4-methyl-	170	C12H26	002980-69-0	53
3	Octane, 2,3,6,7-tetramethyl-	170	C12H26	052670-34-5	53
4	Sulfurous acid, decyl pentyl ester	292	C15H32O3S	1000309-14-3	53
5	Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	50



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Instrument :
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ClientSampleId :
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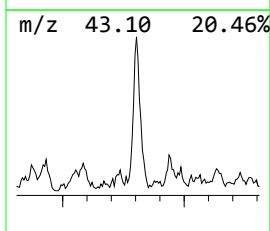
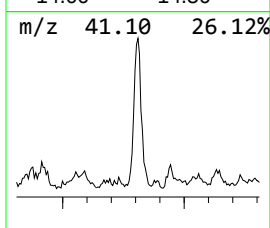
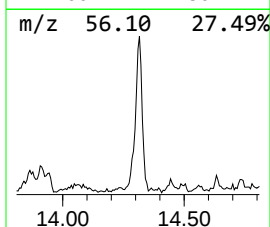
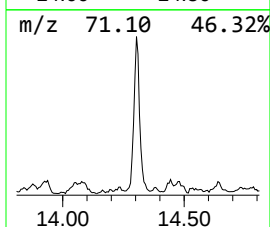
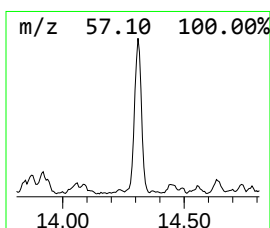
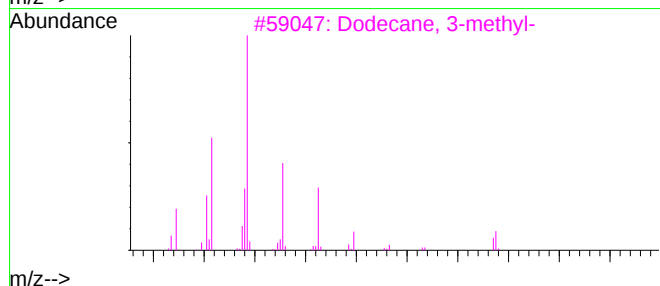
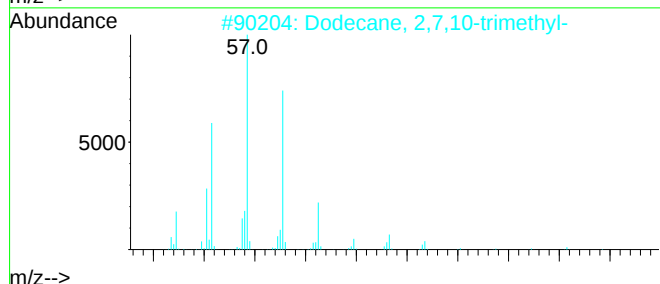
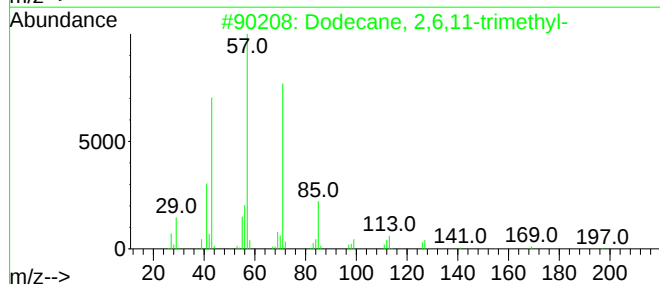
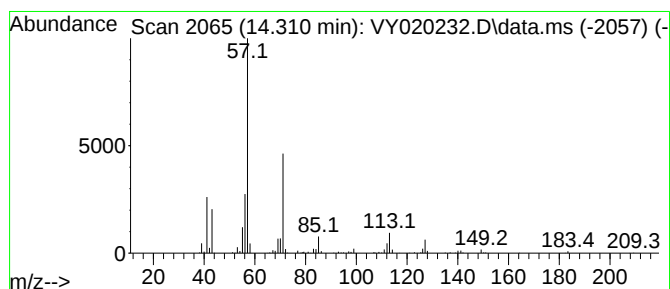
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y103024S.M
Quant Title : SW846 8260

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

Peak Number 4 Dodecane, 2,6,11-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.310	16.42 ug/l	339075	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	59
3	Dodecane, 3-methyl-	184	C13H28	017312-57-1	59
4	Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	59
5	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	53



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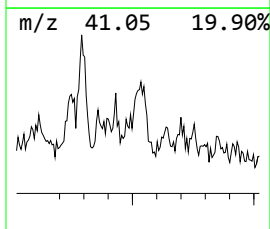
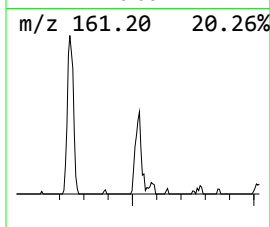
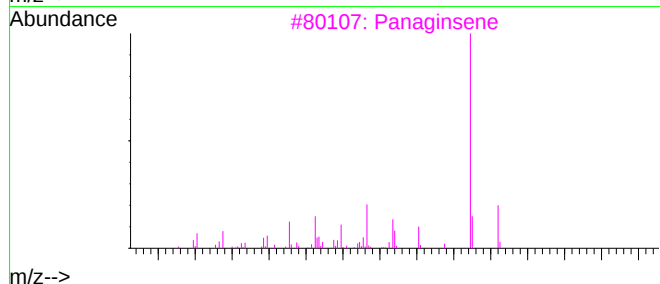
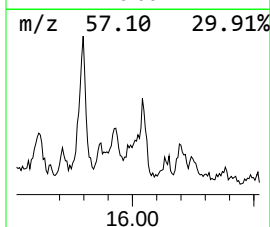
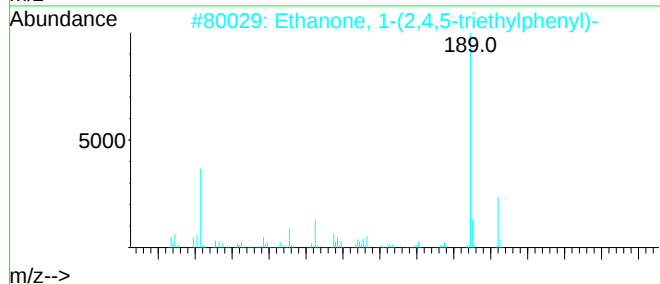
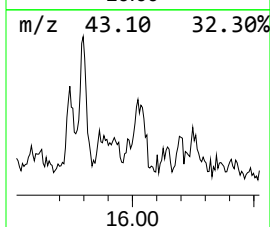
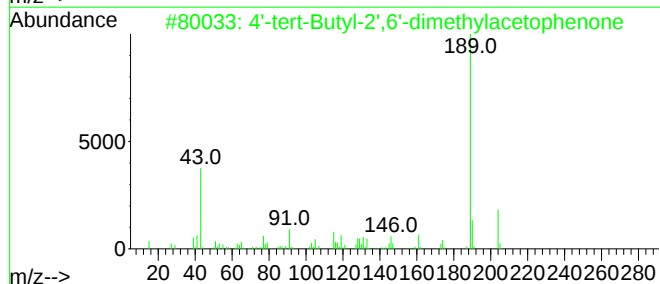
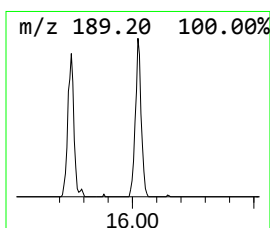
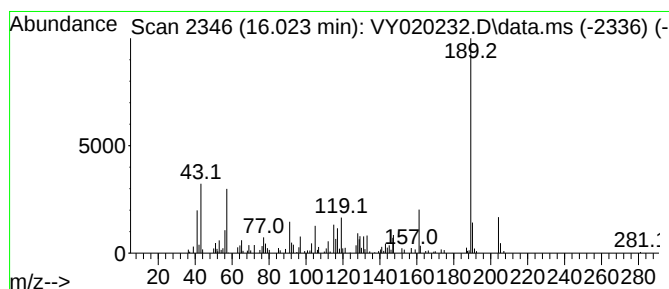
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4'-tert-Butyl-2',6'-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.023	7.52 ug/l	155295	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4'-tert-Butyl-2',6'-dimethylacet...	204	C14H20O	002040-10-0	76
2	Ethanone, 1-(2,4,5-triethylphenyl)-	204	C14H20O	002715-54-0	76
3	Panaginsene	204	C15H24	871660-96-7	68
4	6S-2,3,8,8-Tetramethyltricyclo[5...	204	C15H24	137235-48-4	64
5	2-Acetyl-3,5-dimethylbenzo(b)thi...	204	C12H12OS	006179-05-1	59



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentan-2-yl 2-m...	13.206	24.5	ug/l	506599	4	13.347	1032770	50.0
Sulfurous acid,...	13.566	5.8	ug/l	119313	4	13.347	1032770	50.0
Dodecane, 2,6,1...	14.310	16.4	ug/l	339075	4	13.347	1032770	50.0
4'-tert-Butyl-2...	16.023	7.5	ug/l	155295	4	13.347	1032770	50.0