

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110122\
 Data File : VY011227.D
 Acq On : 01 Nov 2022 17:13
 Operator : KP/MD
 Sample : N5380-01
 Misc : 5.51g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 TP-E

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\82Y110122S.M
 Title : SW846 8260

Signal : TIC: VY011227.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.710	461	474	487	rBV	41852	128472	8.35%	1.269%
2	4.930	497	510	517	rBV2	5253	19185	1.25%	0.190%
3	5.746	633	644	657	rVB2	7209	20092	1.31%	0.198%
4	6.972	833	845	861	rBV	34152	106301	6.91%	1.050%
5	7.710	956	966	972	rBV	221316	531890	34.55%	5.254%
6	7.783	972	978	997	rVB	300238	688082	44.70%	6.797%
7	8.136	1019	1036	1050	rBV2	223358	555627	36.10%	5.488%
8	8.685	1118	1126	1140	rVB	477085	928584	60.32%	9.173%
9	9.179	1197	1207	1213	rBV3	10270	24123	1.57%	0.238%
10	9.612	1271	1278	1285	rBV4	7717	15960	1.04%	0.158%
11	9.746	1293	1300	1306	rBV2	11351	25078	1.63%	0.248%
12	10.179	1363	1371	1382	rBV	887307	1539334	100.00%	15.206%
13	10.362	1393	1401	1407	rVB6	7742	22322	1.45%	0.220%
14	10.514	1422	1426	1431	rVB2	9512	15617	1.01%	0.154%
15	10.575	1431	1436	1441	rBV	18969	34343	2.23%	0.339%
16	10.941	1491	1496	1504	rVV	56157	109788	7.13%	1.084%
17	11.032	1507	1511	1515	rVV2	14987	25603	1.66%	0.253%
18	11.087	1515	1520	1526	rVV	37370	63149	4.10%	0.624%
19	11.203	1533	1539	1543	rBV3	16547	28352	1.84%	0.280%
20	11.288	1543	1553	1562	rVB6	22890	86402	5.61%	0.853%
21	11.380	1562	1568	1572	rBV	16773	28270	1.84%	0.279%
22	11.489	1578	1586	1595	rBV	682031	1125633	73.12%	11.119%
23	11.709	1611	1622	1624	rBV6	25919	64894	4.22%	0.641%
24	11.733	1624	1626	1631	rVV	24195	37889	2.46%	0.374%
25	11.776	1631	1633	1638	rVB	16579	21420	1.39%	0.212%
26	12.001	1662	1670	1677	rBV5	39339	109377	7.11%	1.080%
27	12.117	1686	1689	1693	rVB	28107	38182	2.48%	0.377%
28	12.203	1693	1703	1705	rBV5	38107	82424	5.35%	0.814%
29	12.233	1705	1708	1714	rVB3	43174	81705	5.31%	0.807%
30	12.373	1725	1731	1735	rBV5	18602	41337	2.69%	0.408%
31	12.410	1735	1737	1739	rVV2	15500	17748	1.15%	0.175%
32	12.477	1742	1748	1754	rVV	686981	1074450	69.80%	10.613%
33	12.568	1758	1763	1767	rVB5	11566	19774	1.28%	0.195%
34	12.642	1768	1775	1782	rVB7	54203	132600	8.61%	1.310%
35	12.727	1782	1789	1793	rBV5	30086	75426	4.90%	0.745%
36	12.806	1795	1802	1808	rBV5	112637	221791	14.41%	2.191%

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37	12.946	1821	1825	1829	rBV5	29180	46385	3.01%	0.458%
38	13.001	1831	1834	1836	rVV3	17918	24826	1.61%	0.245%
39	13.038	1836	1840	1842	rVV	63323	88707	5.76%	0.876%
40	13.062	1842	1844	1849	rVB	56505	73353	4.77%	0.725%
41	13.117	1849	1853	1857	rVB3	25927	40715	2.64%	0.402%
42	13.172	1857	1862	1867	rBV2	33327	53271	3.46%	0.526%
43	13.282	1872	1880	1883	rBV	71324	133072	8.64%	1.314%
44	13.361	1889	1893	1896	rBV4	19975	26817	1.74%	0.265%
45	13.422	1896	1903	1909	rVV	723577	1140377	74.08%	11.265%
46	13.477	1909	1912	1919	rVB3	56236	116167	7.55%	1.148%
47	13.641	1932	1939	1950	rVB5	25568	82322	5.35%	0.813%
48	13.745	1951	1956	1961	rBV3	42513	65997	4.29%	0.652%
49	13.965	1988	1992	2005	rVB6	21909	51863	3.37%	0.512%
50	14.074	2005	2010	2015	rBV3	12872	19724	1.28%	0.195%
51	15.312	2205	2213	2220	rBV	10695	18664	1.21%	0.184%

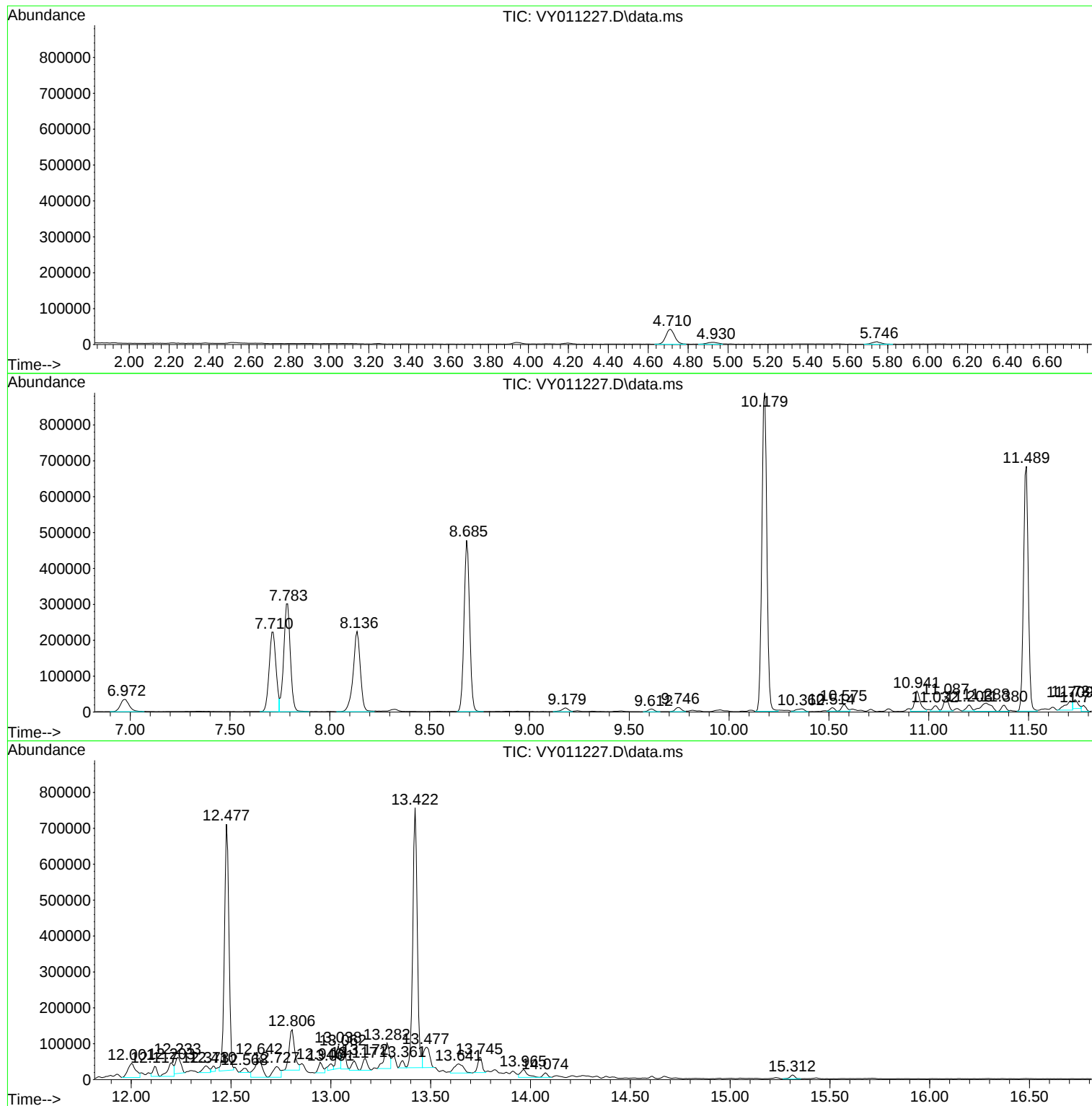
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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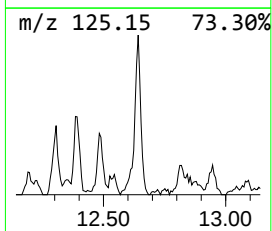
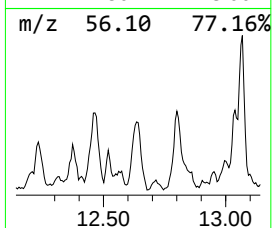
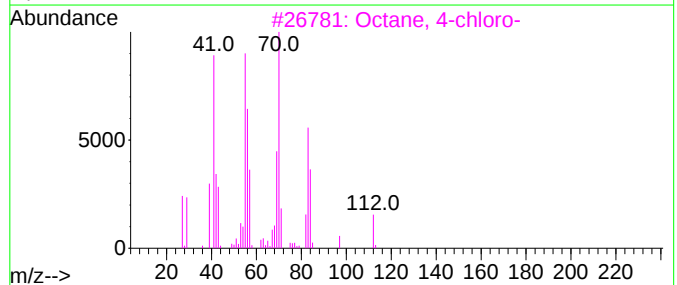
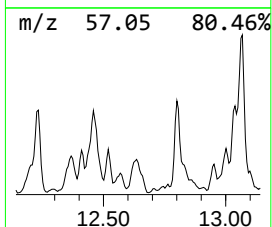
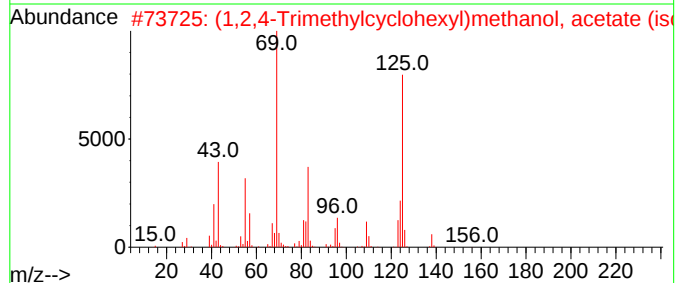
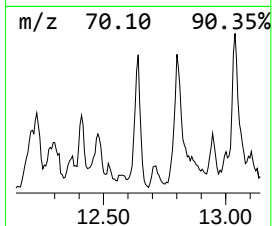
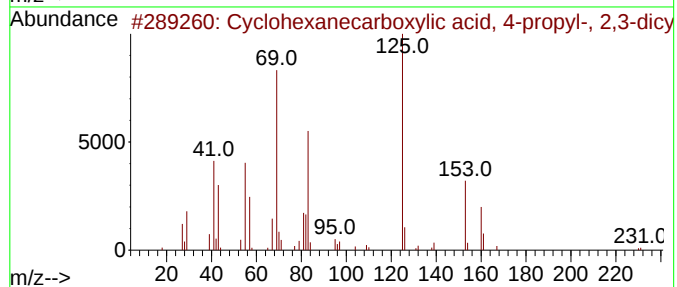
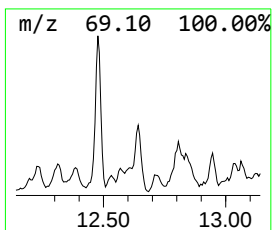
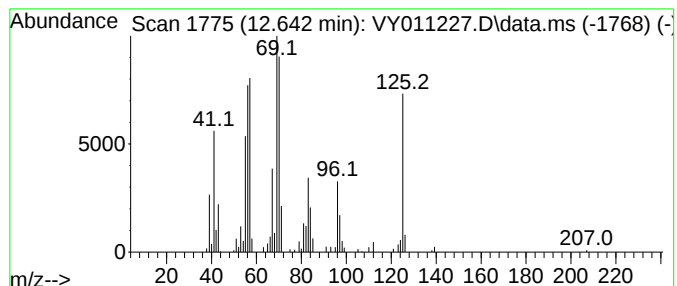
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y110122S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.642 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.642	5.81 ug/l	132600	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanecarboxylic acid, 4-pr...	382	C23H30N2O3	075941-50-3	27
2			(1,2,4-Trimethylcyclohexyl)metha...	198	C12H22O2	1010499-04-6	27
3			Octane, 4-chloro-	148	C8H17Cl	000999-07-5	22
4			3-Undecene, 9-methyl-, (Z)-	168	C12H24	074630-50-5	22
5			1-Undecene, 10-methyl-	168	C12H24	022370-55-4	22



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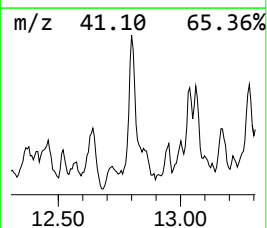
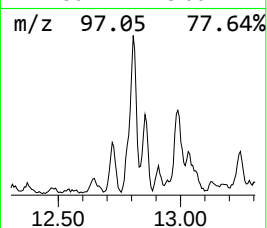
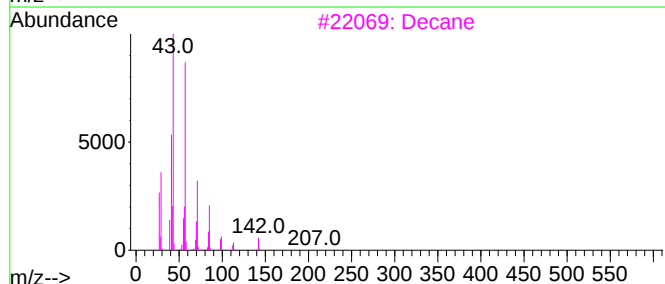
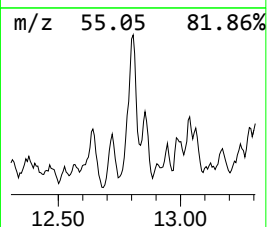
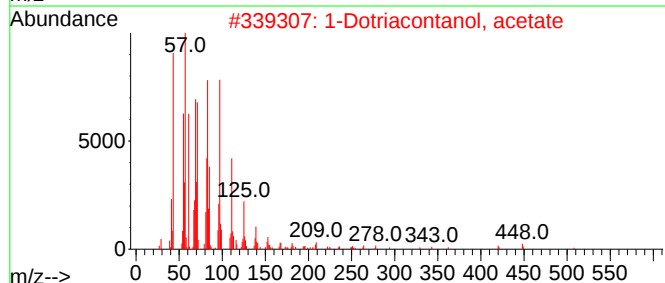
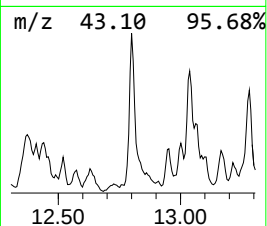
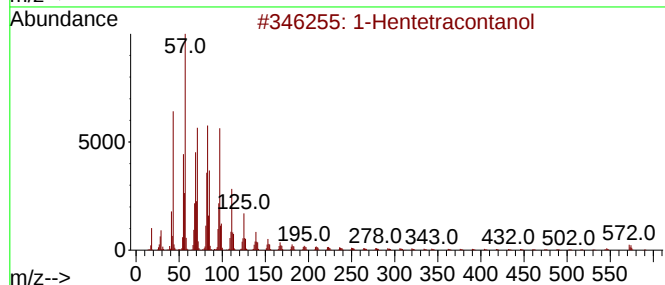
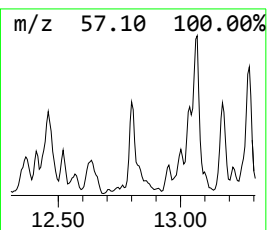
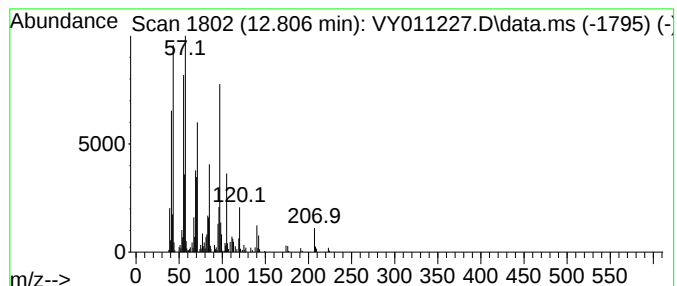
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y110122S.M
Quant Title : SW846 8260

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

Peak Number 3 1-Hentetracontanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.806	9.72 ug/l	221791	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hentetracontanol	593	C41H84O	040710-42-7	59
2			1-Dotriacontanol, acetate	509	C34H68O2	023811-94-1	53
3			Decane	142	C10H22	000124-18-5	30
4			3-Hexene, 3-ethyl-2,5-dimethyl-	140	C10H20	062338-08-3	30
5			Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	27



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Misc : 5.51g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

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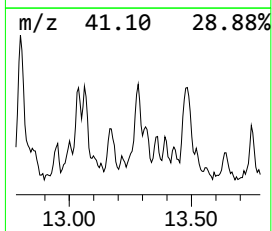
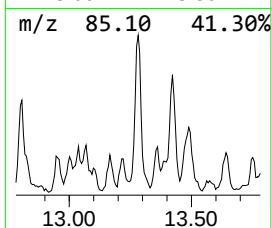
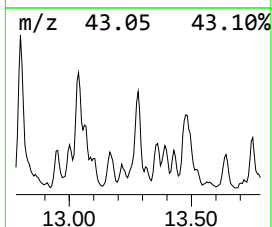
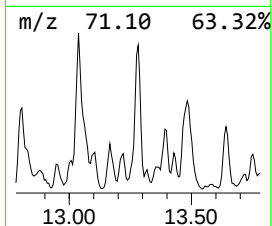
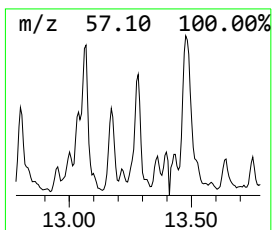
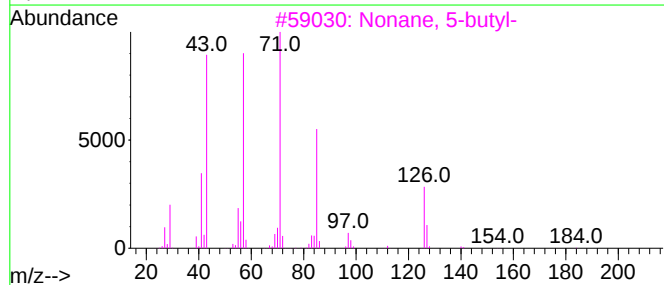
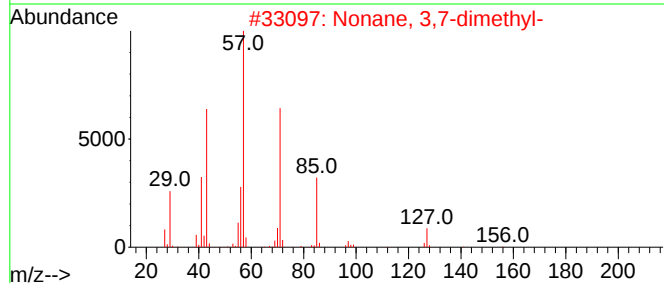
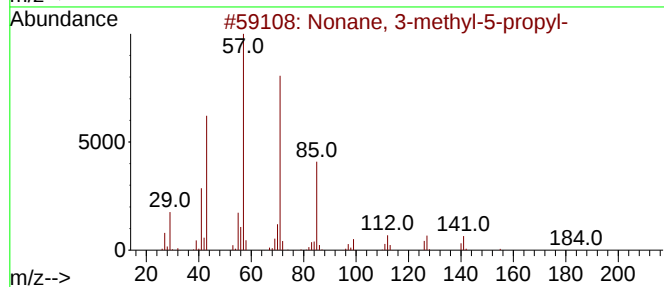
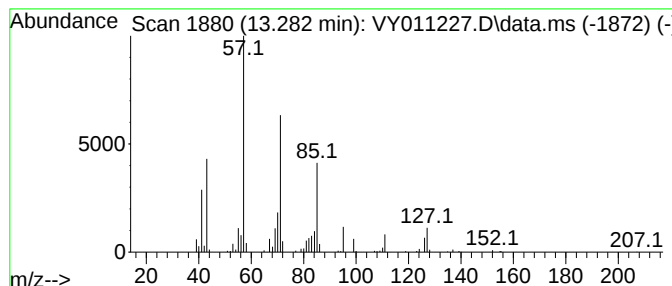
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Nonane, 3-methyl-5-propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	5.83 ug/l	133072	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	64
2			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	64
3			Nonane, 5-butyl-	184	C13H28	017312-63-9	53
4			Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	53
5			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	50



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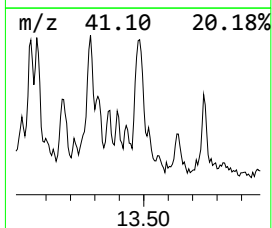
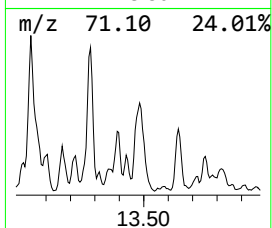
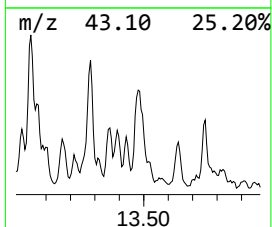
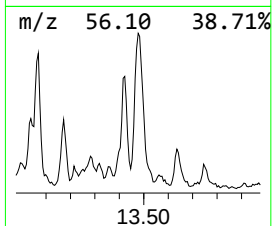
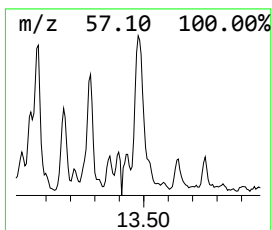
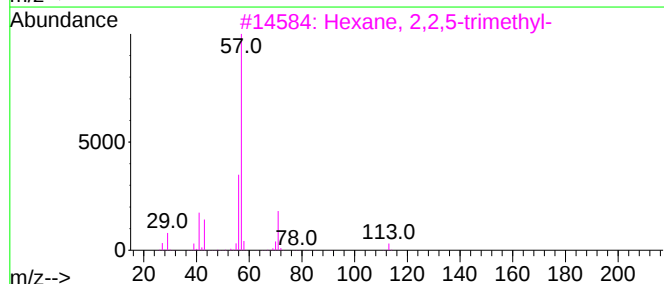
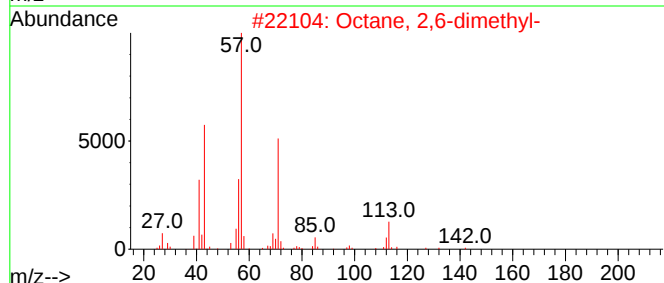
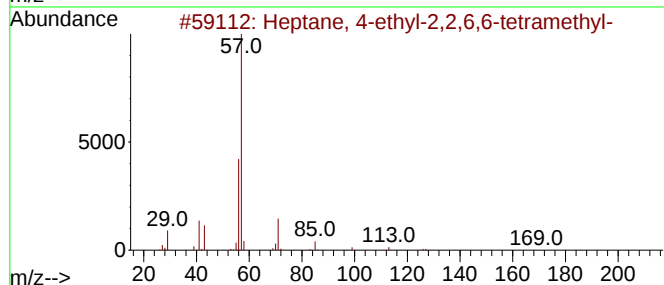
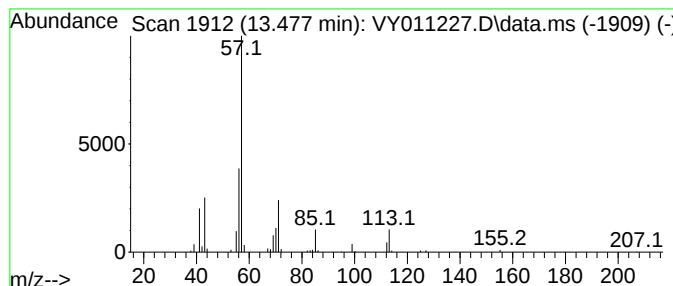
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Peak Number 5 Heptane, 4-ethyl-2,2,6,6-te... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.477	5.09 ug/l	116167	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 4-ethyl-2,2,6,6-tetrame...	184	C13H28	062108-31-0	72
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
3			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	59
4			Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	53
5			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	50



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown12.642	12.642	5.8	ug/l	132600	4	13.422	1140380	50.0
1-Hentetracontanol	12.806	9.7	ug/l	221791	4	13.422	1140380	50.0
Nonane, 3-methy...	13.282	5.8	ug/l	133072	4	13.422	1140380	50.0
Heptane, 4-ethy...	13.477	5.1	ug/l	116167	4	13.422	1140380	50.0