

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
 Data File : VY020635.D
 Acq On : 18 Dec 2024 14:54
 Operator : SY/MD
 Sample : P5299-04
 Misc : 6.77g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SB-02

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y121724S.M

Title : SW846 8260

Signal : TIC: VY020635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.812	9	15	35	rVB	286229	413266	16.75%	1.107%
2	4.610	465	474	484	rBV3	10353	33561	1.36%	0.090%
3	7.628	958	969	976	rBV	121653	300775	12.19%	0.806%
4	7.707	976	982	994	rVB	208867	472636	19.16%	1.266%
5	8.061	1030	1040	1049	rBV	129197	279089	11.31%	0.747%
6	8.610	1120	1130	1145	rBV	369438	733369	29.73%	1.964%
7	10.103	1367	1375	1396	rBV	587913	1000913	40.58%	2.681%
8	11.219	1548	1558	1568	rBV4	13880	37862	1.53%	0.101%
9	11.414	1582	1590	1600	rBV	529449	845111	34.26%	2.263%
10	11.603	1616	1621	1624	rBV	23203	42078	1.71%	0.113%
11	11.640	1624	1627	1635	rVB4	29793	62975	2.55%	0.169%
12	11.926	1667	1674	1686	rBV6	24391	78451	3.18%	0.210%
13	12.170	1709	1714	1722	rVB5	21891	46625	1.89%	0.125%
14	12.402	1747	1752	1758	rVV	396388	640084	25.95%	1.714%
15	12.450	1758	1760	1766	rVB3	33960	52903	2.14%	0.142%
16	12.566	1776	1779	1786	rVB2	41508	68667	2.78%	0.184%
17	12.652	1786	1793	1796	rBV3	33107	67688	2.74%	0.181%
18	12.731	1796	1806	1811	rBV2	290971	547849	22.21%	1.467%
19	12.786	1811	1815	1819	rVB2	93063	149665	6.07%	0.401%
20	12.841	1819	1824	1826	rBV3	39458	62714	2.54%	0.168%
21	12.871	1826	1829	1832	rVB3	40755	53020	2.15%	0.142%
22	12.926	1832	1838	1840	rBV2	60754	110195	4.47%	0.295%
23	12.962	1840	1844	1851	rVB2	188083	306615	12.43%	0.821%
24	13.036	1851	1856	1861	rBV4	26624	64711	2.62%	0.173%
25	13.115	1861	1869	1871	rBV3	58306	149385	6.06%	0.400%
26	13.243	1881	1890	1893	rBV3	233624	570925	23.15%	1.529%
27	13.286	1893	1897	1900	rVV2	152041	233734	9.48%	0.626%
28	13.347	1900	1907	1914	rVB3	587640	1061690	43.04%	2.843%
29	13.426	1915	1920	1923	rBV2	158987	240806	9.76%	0.645%
30	13.529	1934	1937	1939	rBV3	36311	48079	1.95%	0.129%
31	13.560	1940	1942	1945	rVB2	55610	60347	2.45%	0.162%
32	13.627	1945	1953	1954	rBV4	79894	168735	6.84%	0.452%
33	13.676	1954	1961	1965	rVV2	1467892	2465291	99.94%	6.602%
34	13.712	1965	1967	1971	rVV2	230600	312993	12.69%	0.838%
35	13.773	1971	1977	1983	rVV5	190162	442239	17.93%	1.184%
36	13.840	1983	1988	1992	rVV3	207799	495145	20.07%	1.326%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y121724S.M
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37	13.889	1993	1996	2000	rVV3	205591	358382	14.53%	0.960%
38	13.938	2001	2004	2008	rVB3	190785	259612	10.52%	0.695%
39	13.993	2009	2013	2018	rBV6	79616	159072	6.45%	0.426%
40	14.066	2019	2025	2029	rBV3	159593	321938	13.05%	0.862%
41	14.115	2029	2033	2036	rBV3	182511	248763	10.08%	0.666%
42	14.170	2036	2042	2050	rVB8	871922	1884599	76.40%	5.047%
43	14.237	2050	2053	2058	rVB3	251683	314873	12.76%	0.843%
44	14.304	2060	2064	2066	rBV3	177110	227711	9.23%	0.610%
45	14.340	2066	2070	2074	rVB2	550694	778329	31.55%	2.084%
46	14.395	2074	2079	2085	rVB3	280878	493394	20.00%	1.321%
47	14.474	2086	2092	2094	rBV5	74489	160559	6.51%	0.430%
48	14.529	2097	2101	2108	rBV	1642437	2274920	92.23%	6.093%
49	14.602	2108	2113	2116	rBV	385209	589701	23.91%	1.579%
50	14.645	2116	2120	2127	rVB	1161709	1830302	74.20%	4.902%
51	14.724	2128	2133	2136	rBV4	182622	344421	13.96%	0.922%
52	14.767	2136	2140	2148	rVB2	465290	1044816	42.36%	2.798%
53	14.852	2149	2154	2159	rVB4	262178	519142	21.05%	1.390%
54	14.907	2159	2163	2165	rBV3	111866	184935	7.50%	0.495%
55	14.950	2166	2170	2176	rBV5	272529	581243	23.56%	1.557%
56	15.011	2176	2180	2182	rBV3	165942	277147	11.24%	0.742%
57	15.054	2183	2187	2193	rVB3	554324	1052416	42.66%	2.819%
58	15.121	2193	2198	2203	rBV	1040980	1638153	66.41%	4.387%
59	15.169	2203	2206	2215	rVB4	188149	445584	18.06%	1.193%
60	15.249	2216	2219	2221	rBV4	96079	140119	5.68%	0.375%
61	15.346	2230	2235	2241	rBV	1696318	2466700	100.00%	6.606%
62	15.450	2249	2252	2256	rVB2	223210	341319	13.84%	0.914%
63	15.511	2257	2262	2268	rVB2	465130	816678	33.11%	2.187%
64	15.864	2317	2320	2323	rVV3	105258	148626	6.03%	0.398%
65	15.919	2324	2329	2335	rVV4	306099	748845	30.36%	2.006%
66	15.980	2335	2339	2345	rVB3	280811	618679	25.08%	1.657%
67	16.047	2345	2350	2358	rVB	582565	1045287	42.38%	2.799%
68	16.248	2378	2383	2389	rBV	1194703	2113456	85.68%	5.660%
69	16.358	2397	2401	2404	rBV2	108507	189297	7.67%	0.507%

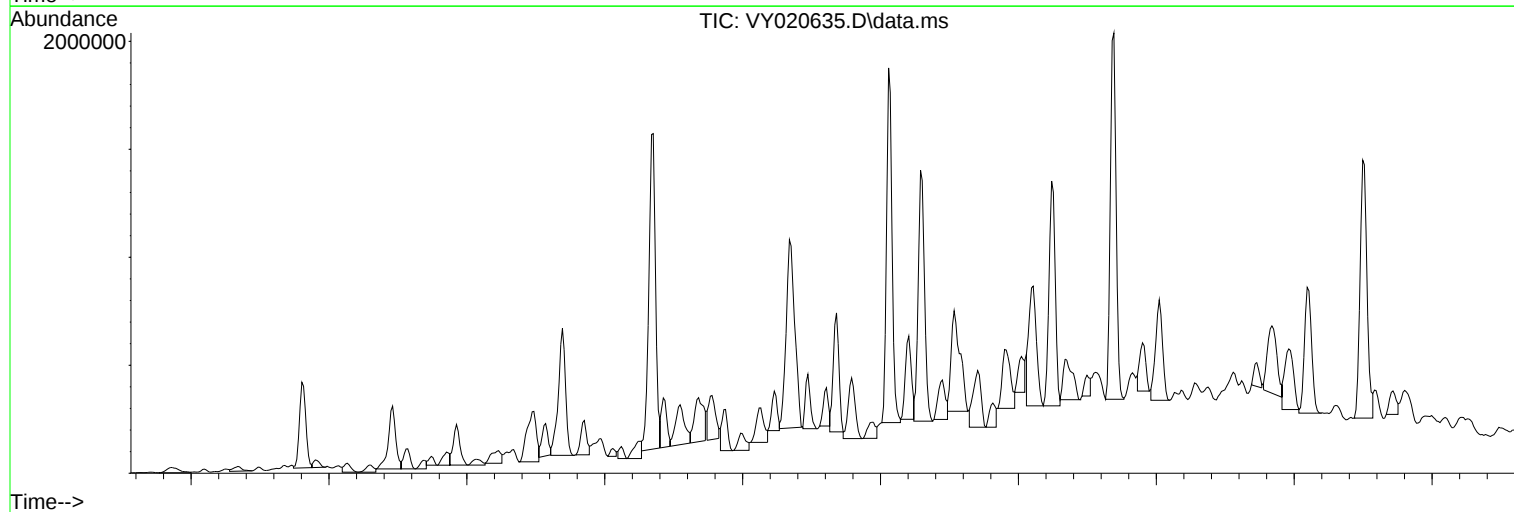
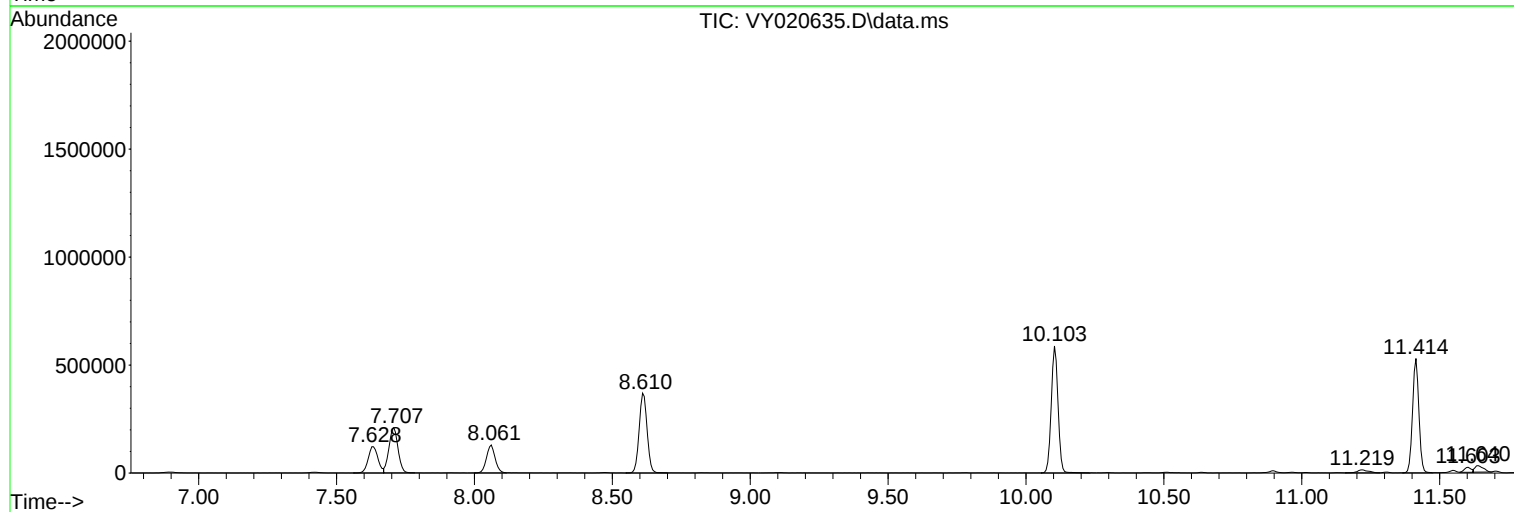
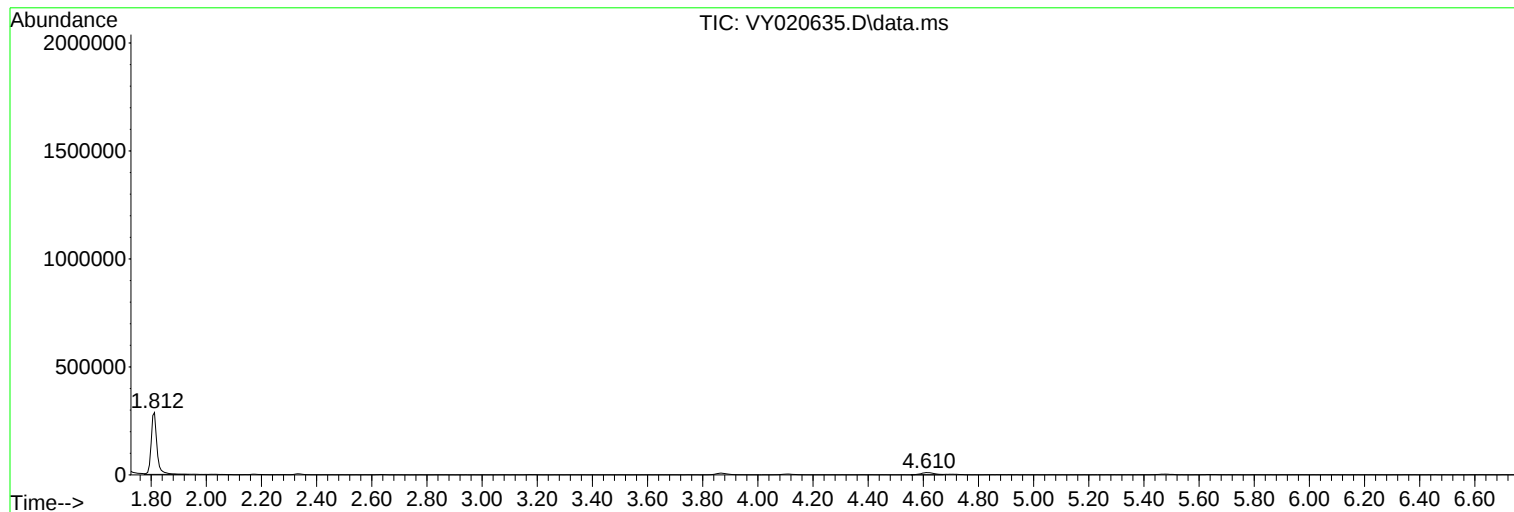
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Instrument :
MSVOA_Y
ClientSampleId :
SB-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y121724S.M
Quant Title : SW846 8260

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



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Misc : 6.77g/5.0mL/MSVOA_Y/SOIL/A
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Instrument :
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ClientSampleId :
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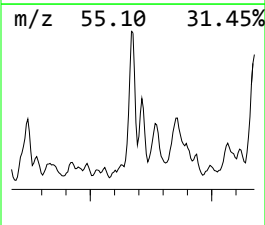
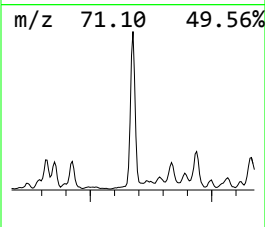
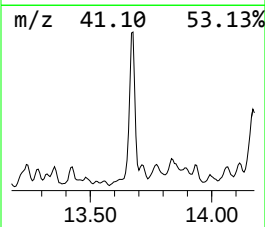
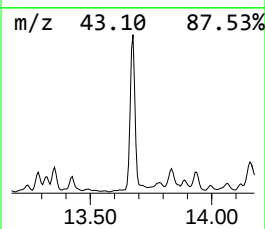
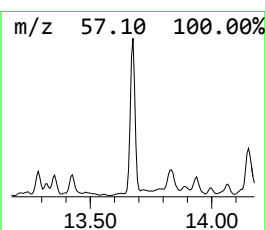
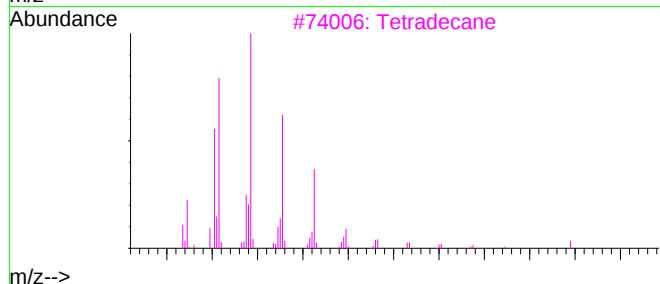
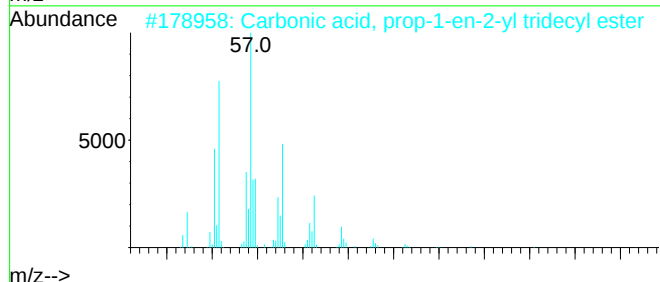
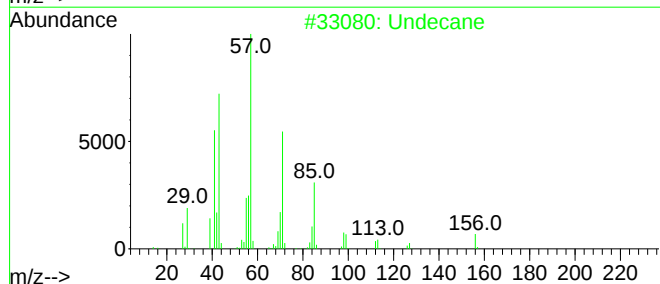
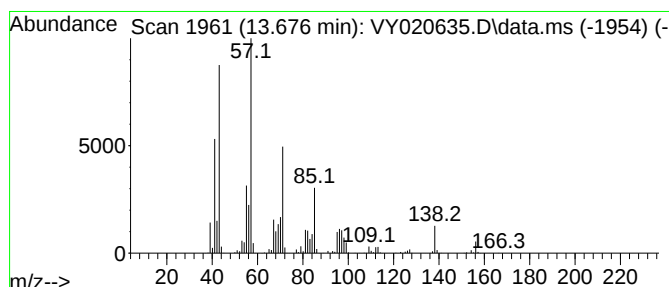
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y121724S.M
Quant Title : SW846 8260

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

Peak Number 1 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	116.10 ug/l	2465290	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	64
2	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	64
3	Tetradecane	198	C14H30	000629-59-4	58
4	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	58
5	Decane	142	C10H22	000124-18-5	53



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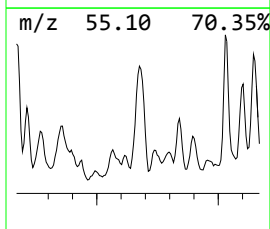
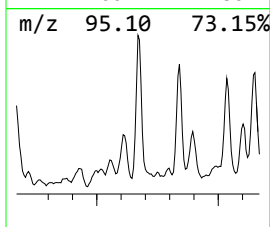
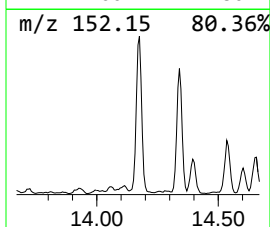
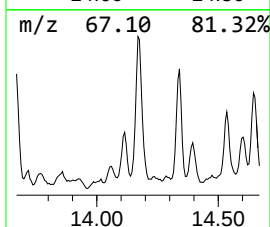
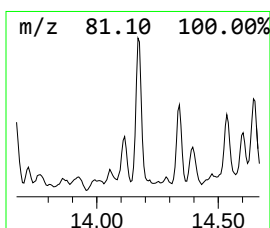
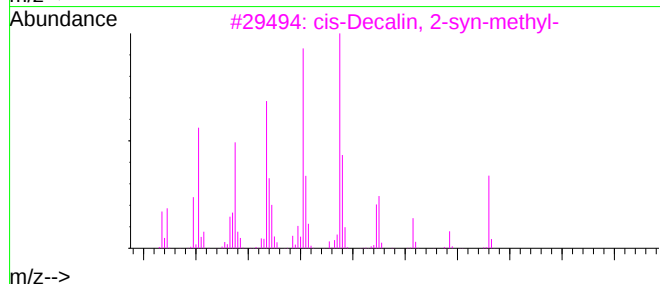
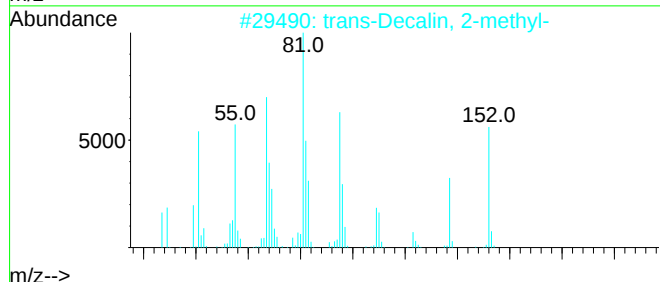
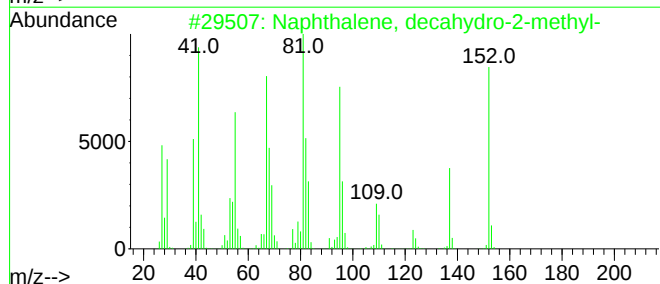
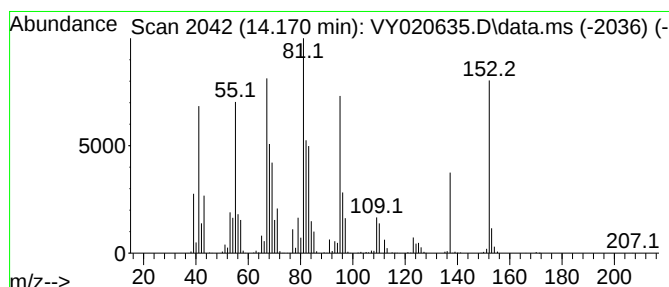
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y121724S.M
Quant Title : SW846 8260

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

Peak Number 2 Naphthalene, decahydro-2-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	88.75 ug/l	1884600	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	98
2	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	97
3	cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	83
4	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	70
5	Bicyclo[4.1.0]heptan-3-one, 4,7,...	152	C10H16O	004176-04-9	70



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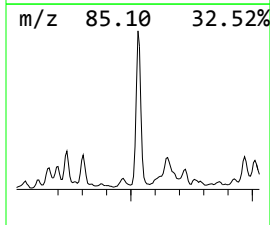
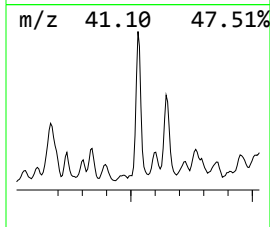
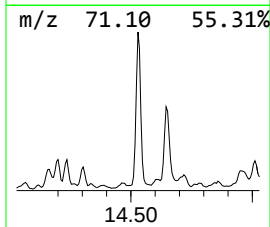
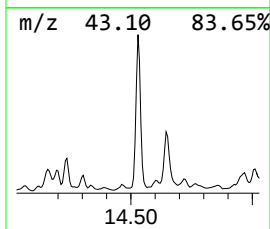
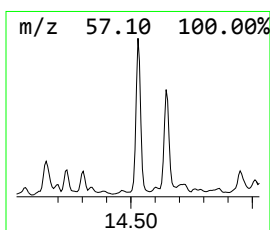
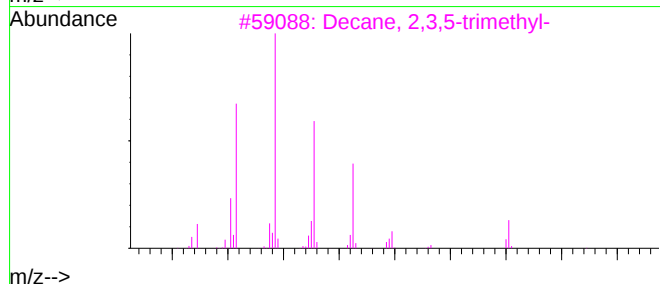
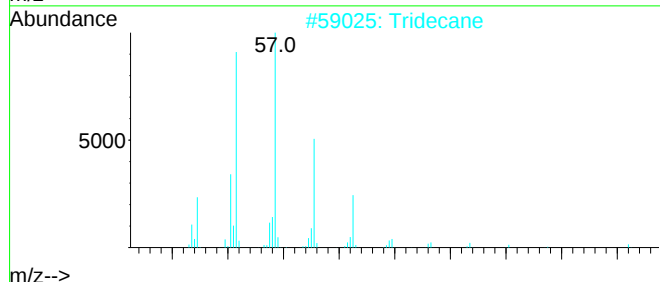
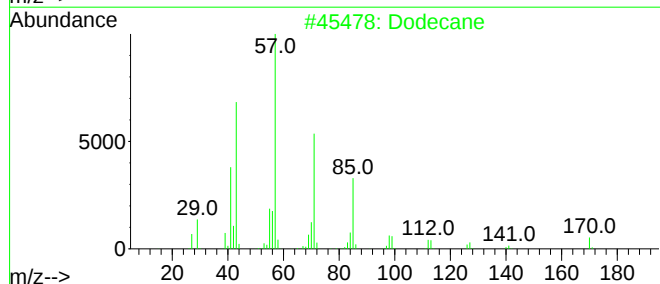
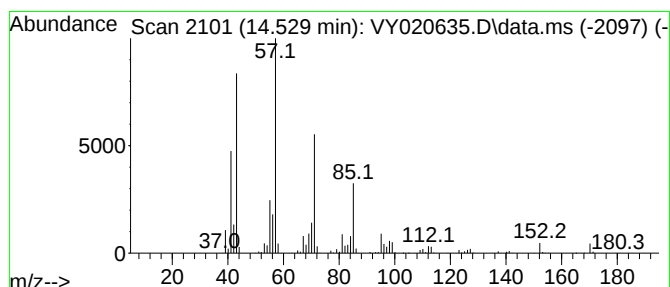
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.529	107.14 ug/l	2274920	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	93
2	Tridecane	184	C13H28	000629-50-5	72
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72
4	Undecane	156	C11H24	001120-21-4	72
5	Tetradecane	198	C14H30	000629-59-4	72



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Instrument :
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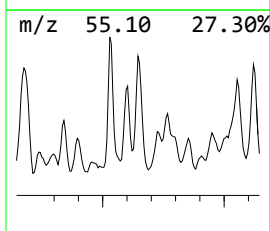
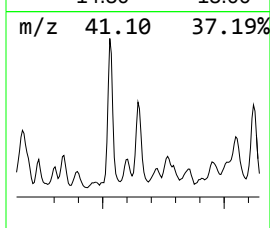
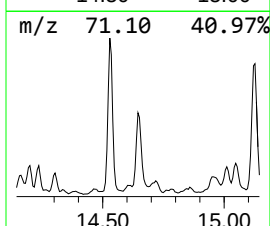
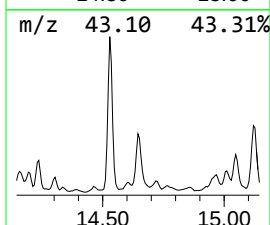
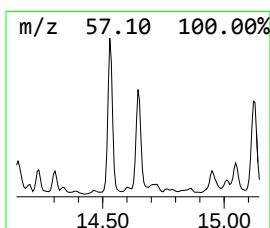
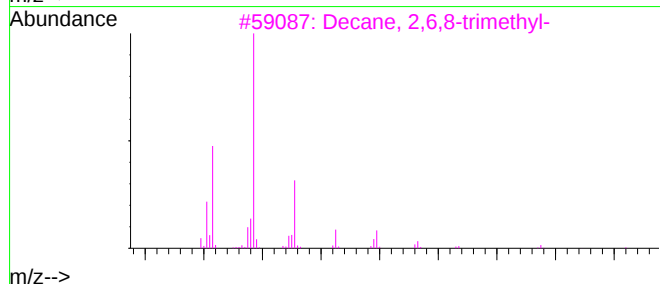
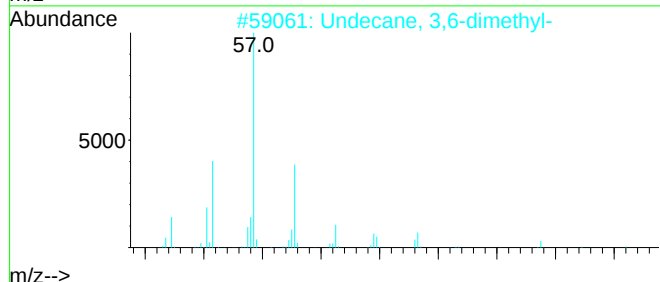
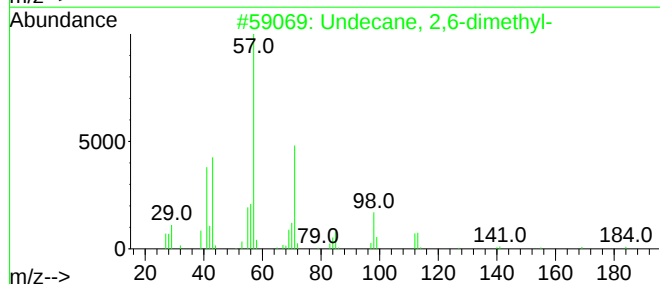
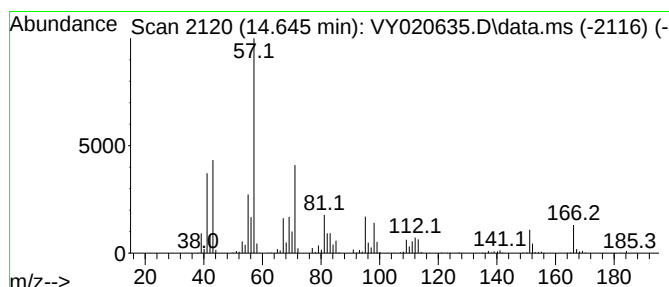
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y121724S.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.645	86.20 ug/l	1830300	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	96
2	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	60
3	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	47
4	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	43
5	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
Data File : VY020635.D
Acq On : 18 Dec 2024 14:54
Operator : SY/MD
Sample : P5299-04
Misc : 6.77g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-02

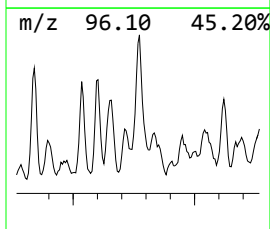
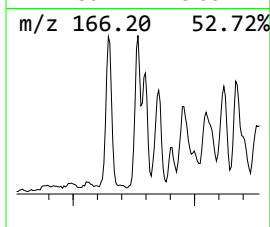
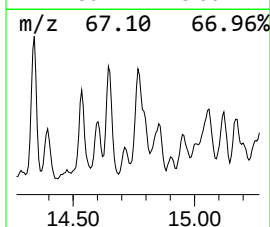
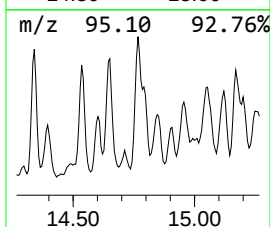
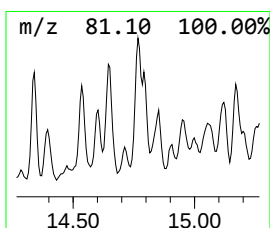
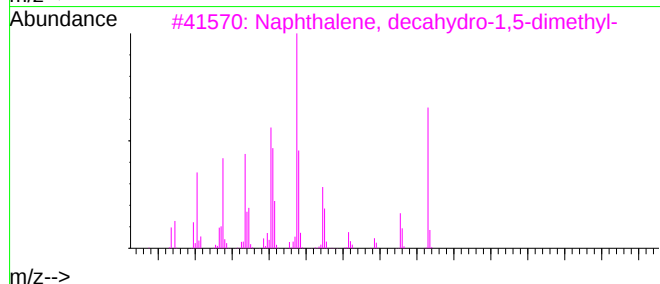
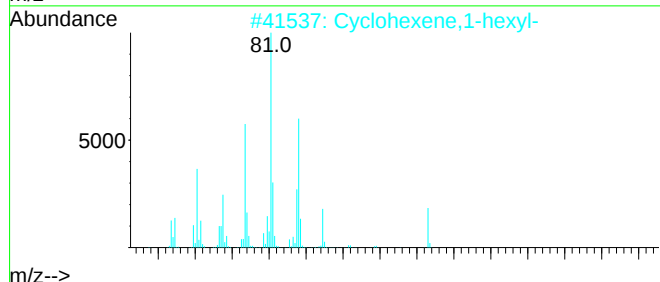
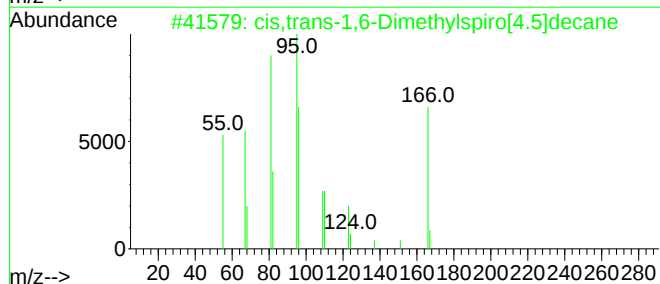
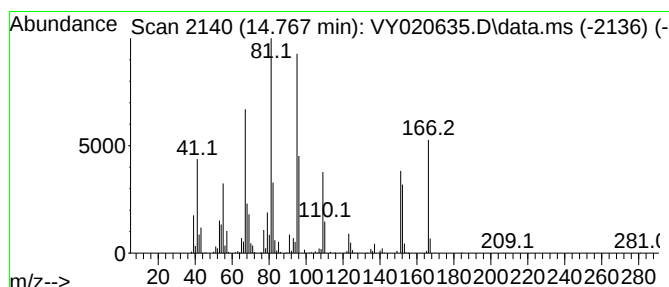
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Quant Title : SW846 8260

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

Peak Number 5 cis,trans-1,6-Dimethylspiro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.767	49.21 ug/l	1044820	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	70
2	Cyclohexene,1-hexyl-	166	C12H22	003964-66-7	60
3	Naphthalene, decahydro-1,5-dimet...	166	C12H22	066552-62-3	60
4	Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	58
5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
Data File : VY020635.D
Acq On : 18 Dec 2024 14:54
Operator : SY/MD
Sample : P5299-04
Misc : 6.77g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-02

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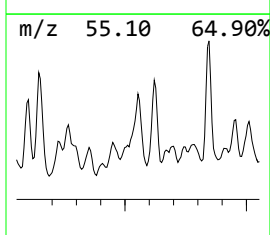
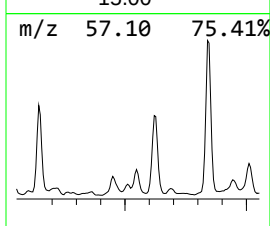
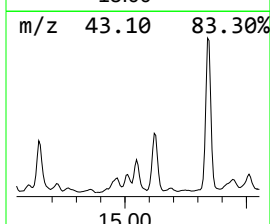
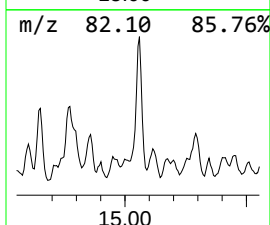
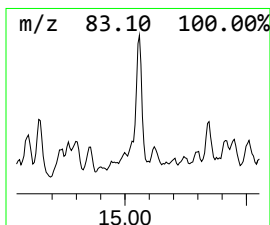
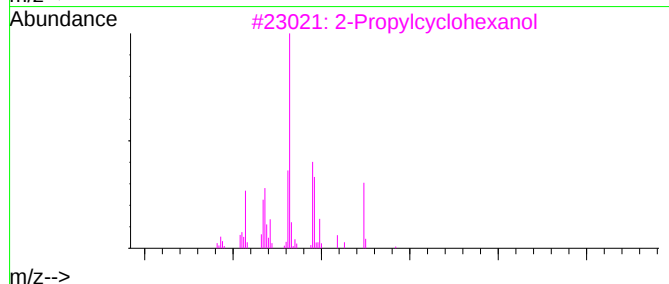
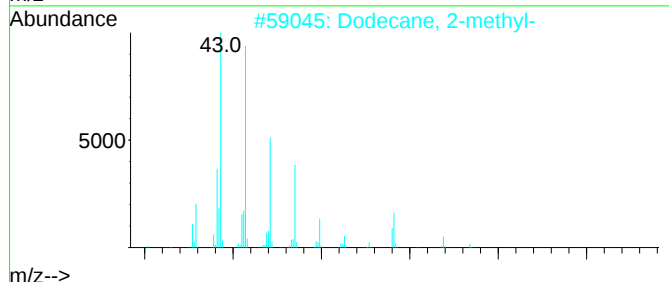
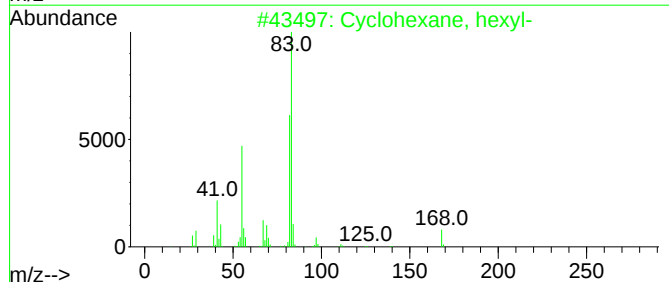
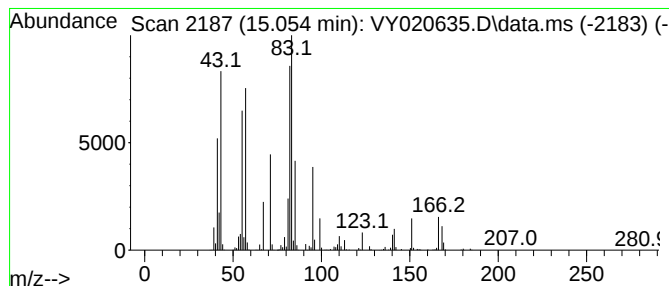
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TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown15.054 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.054	49.56 ug/l	1052420	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, hexyl-	168	C12H24	004292-75-5	38
2	Dodecane, 2-methyl-	184	C13H28	001560-97-0	35
3	2-Propylcyclohexanol	142	C9H18O	090676-25-8	35
4	3-Methyl-1-[(1H)-1,2,4-triazol-1...	153	C7H11N3O	064922-02-7	27
5	cis-3-Hexenyl 2-ethylbutyrate	198	C12H22O2	1000433-24-6	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
Data File : VY020635.D
Acq On : 18 Dec 2024 14:54
Operator : SY/MD
Sample : P5299-04
Misc : 6.77g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-02

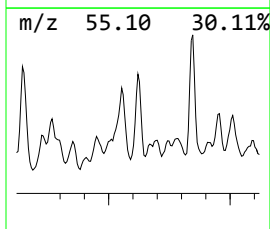
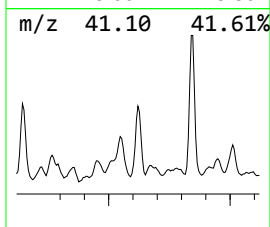
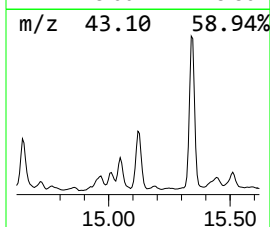
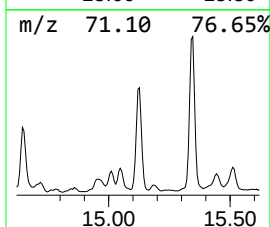
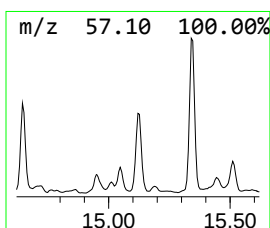
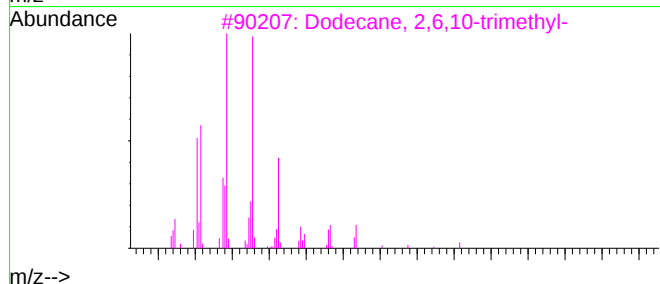
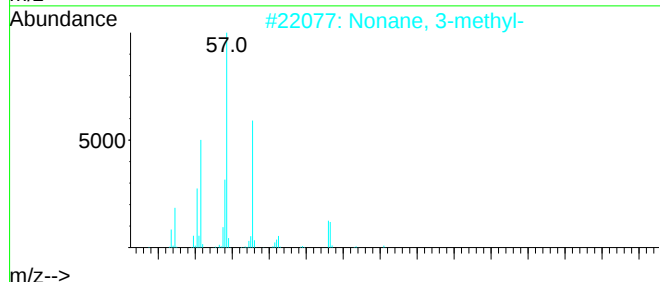
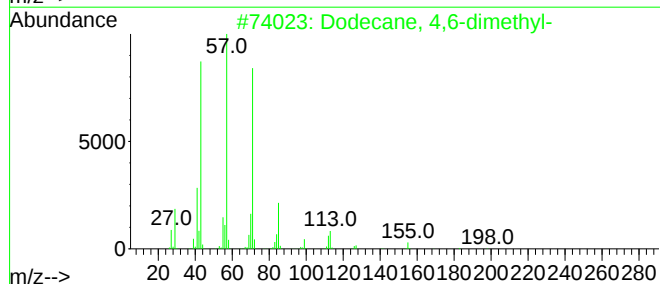
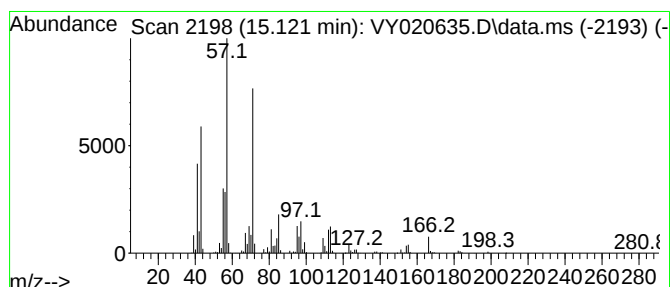
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Dodecane, 4,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.121	77.15 ug/l	1638150	1,4-Dichlorobenzene-d4	13.347	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	72
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	72
3	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64
4	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
5	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
Data File : VY020635.D
Acq On : 18 Dec 2024 14:54
Operator : SY/MD
Sample : P5299-04
Misc : 6.77g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-02

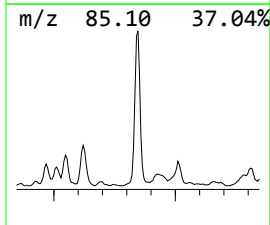
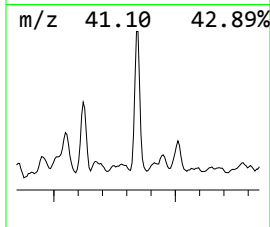
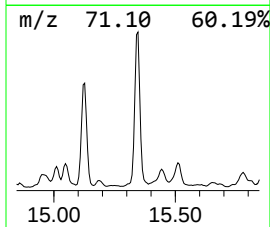
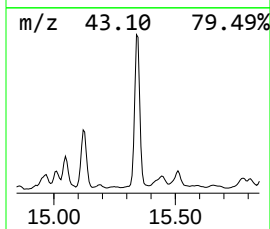
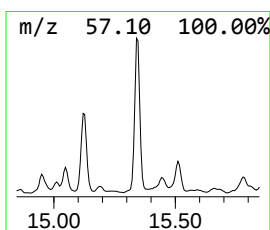
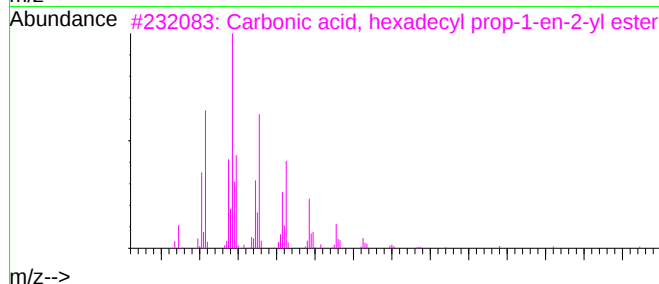
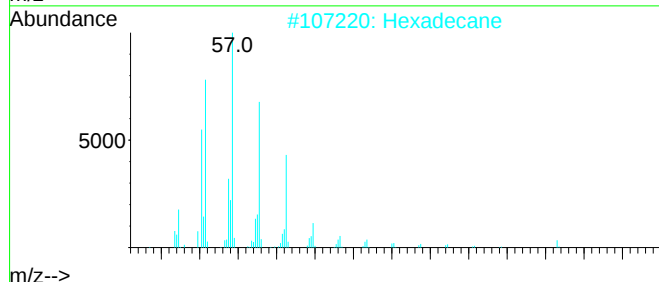
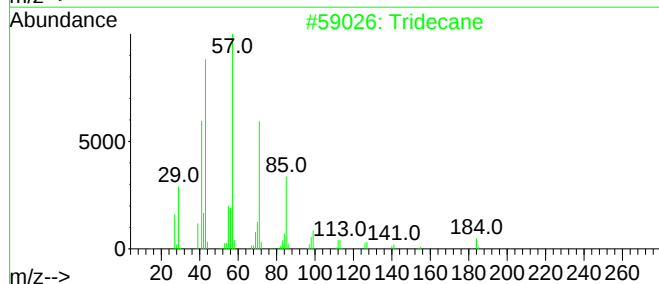
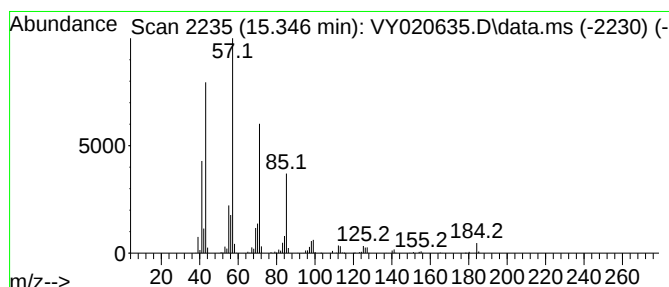
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Quant Title : SW846 8260

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

Peak Number 8 Tridecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.346	116.17 ug/l	2466700	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	96
2	Hexadecane	226	C16H34	000544-76-3	91
3	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	80
4	Dodecane	170	C12H26	000112-40-3	80
5	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
Data File : VY020635.D
Acq On : 18 Dec 2024 14:54
Operator : SY/MD
Sample : P5299-04
Misc : 6.77g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-02

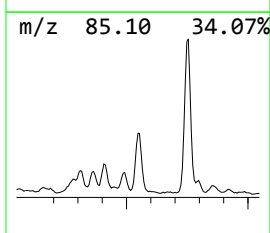
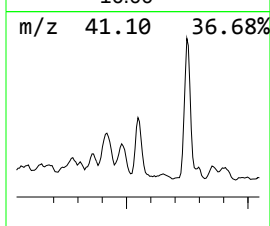
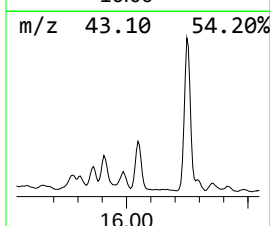
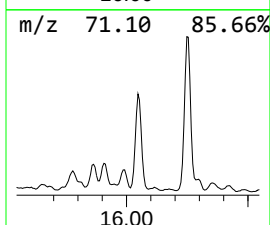
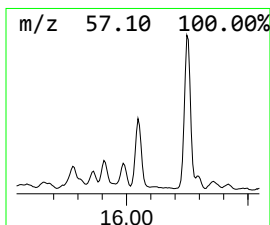
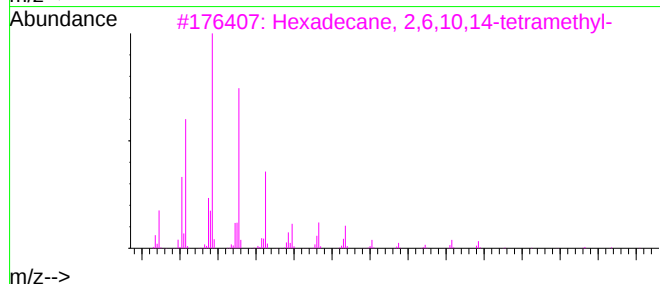
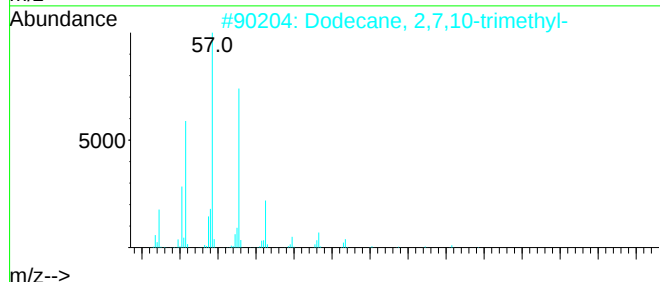
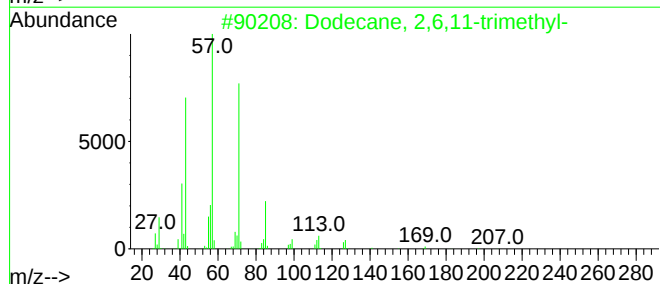
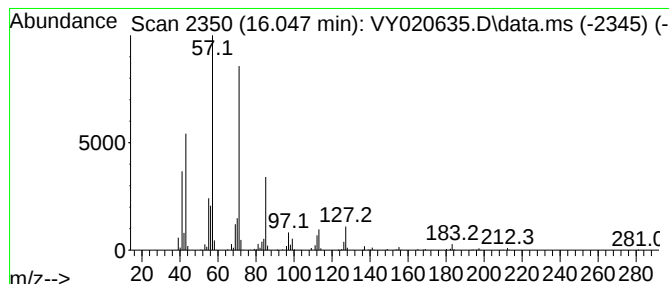
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Quant Title : SW846 8260

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

Peak Number 9 Dodecane, 2,6,11-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.047	49.23 ug/l	1045290	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	90
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	90
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
4	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	80
5	Tetradecane, 4-methyl-	212	C15H32	025117-24-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
Data File : VY020635.D
Acq On : 18 Dec 2024 14:54
Operator : SY/MD
Sample : P5299-04
Misc : 6.77g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-02

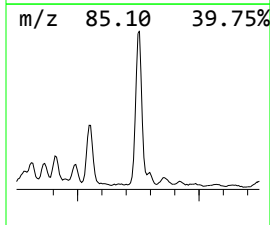
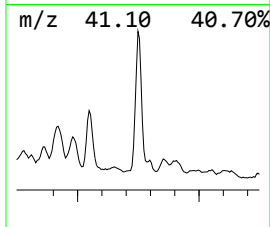
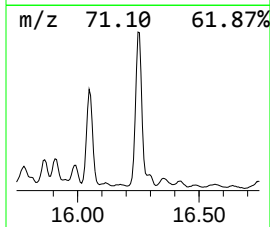
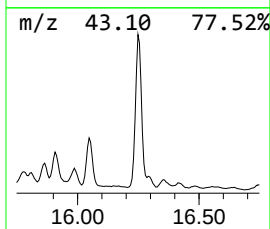
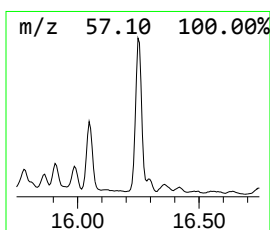
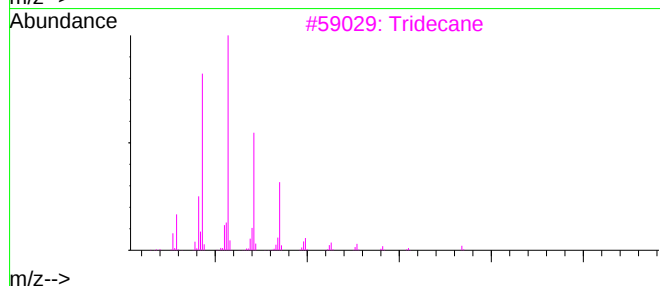
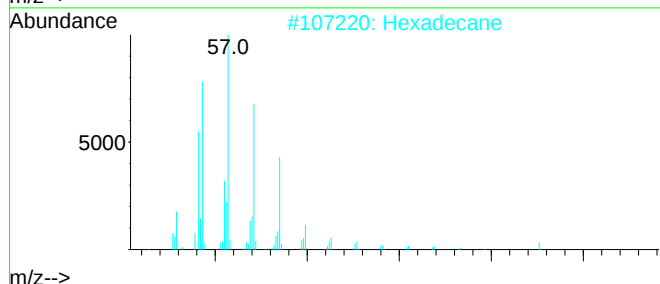
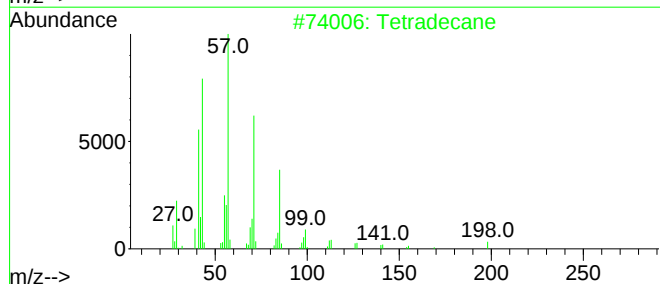
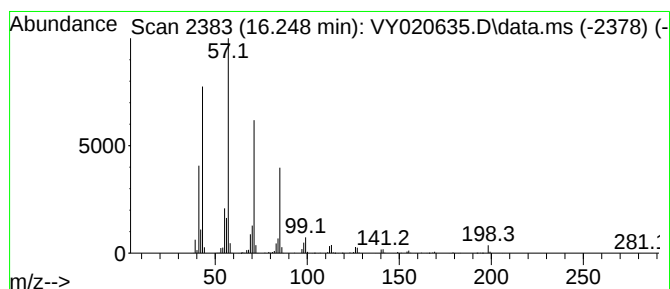
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Quant Title : SW846 8260

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

Peak Number 10 Tetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.248	99.53 ug/l	2113460	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	98
2	Hexadecane	226	C16H34	000544-76-3	91
3	Tridecane	184	C13H28	000629-50-5	86
4	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	86
5	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
Data File : VY020635.D
Acq On : 18 Dec 2024 14:54
Operator : SY/MD
Sample : P5299-04
Misc : 6.77g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y121724S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Naphthalene, de...	14.169	88.8	ug/l	1884600	4	13.347	1061690	50.0
Dodecane	14.529	107.1	ug/l	2274920	4	13.347	1061690	50.0
Undecane, 2,6-d...	14.645	86.2	ug/l	1830300	4	13.347	1061690	50.0
cis,trans-1,6-D...	14.767	49.2	ug/l	1044820	4	13.347	1061690	50.0
unknown15.054	15.054	49.6	ug/l	1052420	4	13.347	1061690	50.0
Dodecane, 4,6-d...	15.121	77.2	ug/l	1638150	4	13.347	1061690	50.0
Tridecane	15.346	116.2	ug/l	2466700	4	13.347	1061690	50.0
Dodecane, 2,6,1...	16.047	49.2	ug/l	1045290	4	13.347	1061690	50.0
Tetradecane	16.248	99.5	ug/l	2113460	4	13.347	1061690	50.0