

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
 Data File : VY020640.D
 Acq On : 18 Dec 2024 16:51
 Operator : SY/MD
 Sample : P5299-03
 Misc : 5.73g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SB-01

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: VY020640.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	10	15	33	rVB2	206063	317384	25.23%	3.343%
2	3.872	340	353	362	rBV2	19315	56615	4.50%	0.596%
3	4.104	381	391	405	rBV	12924	36387	2.89%	0.383%
4	4.616	465	475	487	rBV3	10526	34159	2.72%	0.360%
5	6.896	840	849	862	rBV2	9718	30541	2.43%	0.322%
6	7.634	961	970	976	rBV	167295	406450	32.32%	4.282%
7	7.707	976	982	997	rVB	285084	654529	52.04%	6.895%
8	8.061	1031	1040	1051	rBV	148407	335156	26.65%	3.531%
9	8.609	1123	1130	1143	rBV	450495	910242	72.37%	9.589%
10	10.103	1368	1375	1382	rBV	723615	1257732	100.00%	13.249%
11	11.414	1584	1590	1600	rVB	645467	1036391	82.40%	10.918%
12	12.249	1715	1727	1740	rBV2	159714	812599	64.61%	8.560%
13	12.401	1747	1752	1763	rVB2	484079	838079	66.63%	8.829%
14	13.346	1901	1907	1915	rBV	542633	851326	67.69%	8.968%
15	13.676	1957	1961	1965	rBV	45194	61063	4.86%	0.643%
16	13.889	1991	1996	2002	rVB	74994	125622	9.99%	1.323%
17	14.169	2039	2042	2050	rVB8	31675	71319	5.67%	0.751%
18	14.236	2050	2053	2055	rBV3	12247	15959	1.27%	0.168%
19	14.340	2067	2070	2075	rBV3	20812	31954	2.54%	0.337%
20	14.395	2076	2079	2086	rVB6	17003	32058	2.55%	0.338%
21	14.529	2097	2101	2109	rVB2	76056	112534	8.95%	1.185%
22	14.602	2109	2113	2116	rBV4	17562	29415	2.34%	0.310%
23	14.645	2116	2120	2126	rVB2	74489	120424	9.57%	1.269%
24	14.724	2128	2133	2135	rBV6	10998	19677	1.56%	0.207%
25	14.767	2135	2140	2143	rBV3	53238	91274	7.26%	0.962%
26	14.852	2148	2154	2159	rBV5	34884	69628	5.54%	0.733%
27	14.956	2166	2171	2175	rBV5	33518	67801	5.39%	0.714%
28	15.053	2182	2187	2193	rVB8	48521	100899	8.02%	1.063%
29	15.120	2193	2198	2203	rBV2	85609	135659	10.79%	1.429%
30	15.169	2203	2206	2209	rBV3	29169	45563	3.62%	0.480%
31	15.255	2216	2220	2222	rBV4	17660	27666	2.20%	0.291%
32	15.346	2230	2235	2240	rBV	134404	186768	14.85%	1.967%
33	15.450	2250	2252	2257	rVB4	23343	31988	2.54%	0.337%
34	15.511	2257	2262	2268	rVB3	48782	89461	7.11%	0.942%
35	15.925	2324	2330	2335	rBV4	41361	91126	7.25%	0.960%
36	15.974	2336	2338	2346	rVB5	30478	63177	5.02%	0.666%

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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\82Y121724S.M
Title : SW846 8260

37	16.053	2346	2351	2357	rVB4	49645	88765	7.06%	0.935%
38	16.254	2378	2384	2388	rBV	118156	205341	16.33%	2.163%

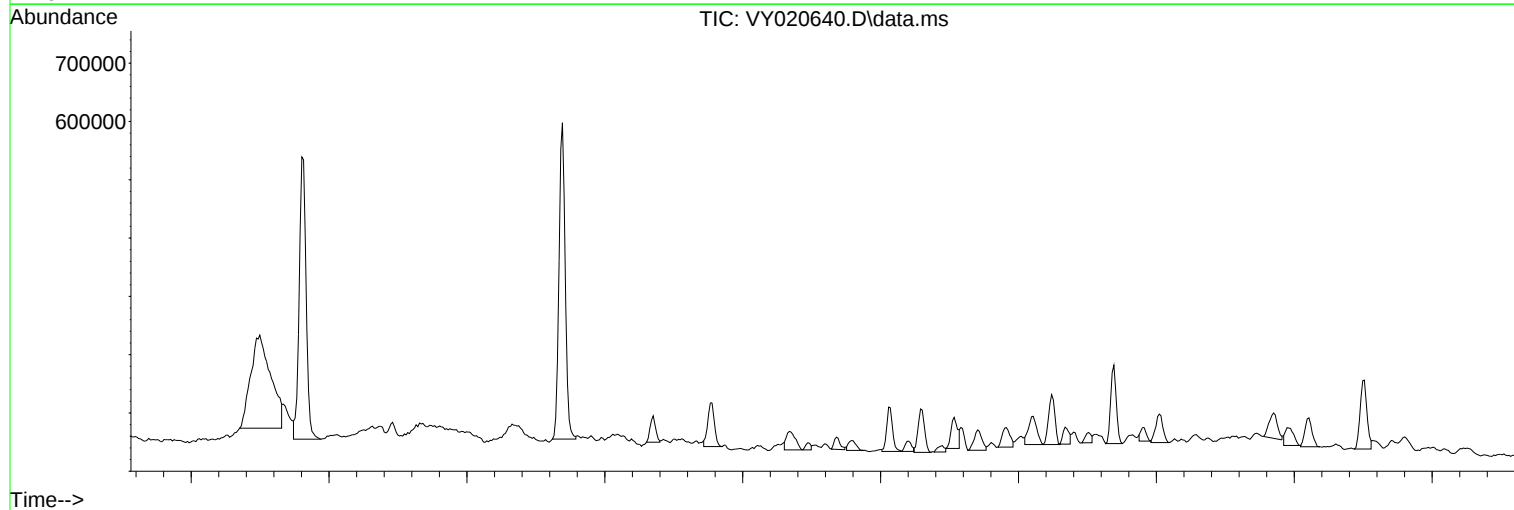
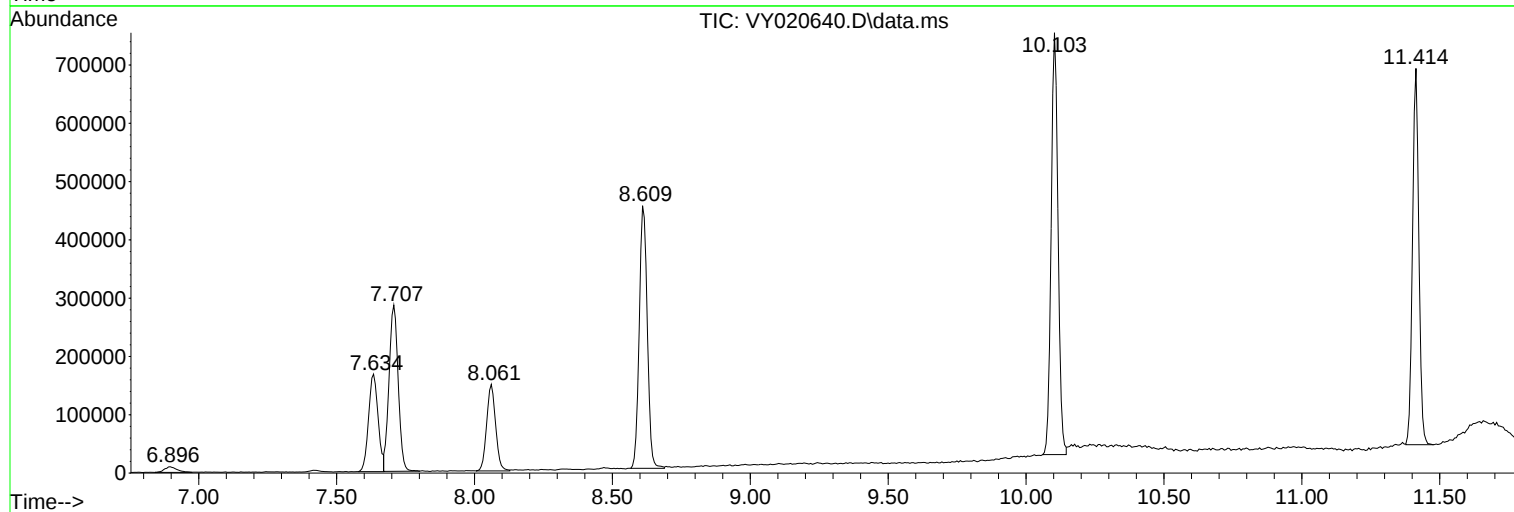
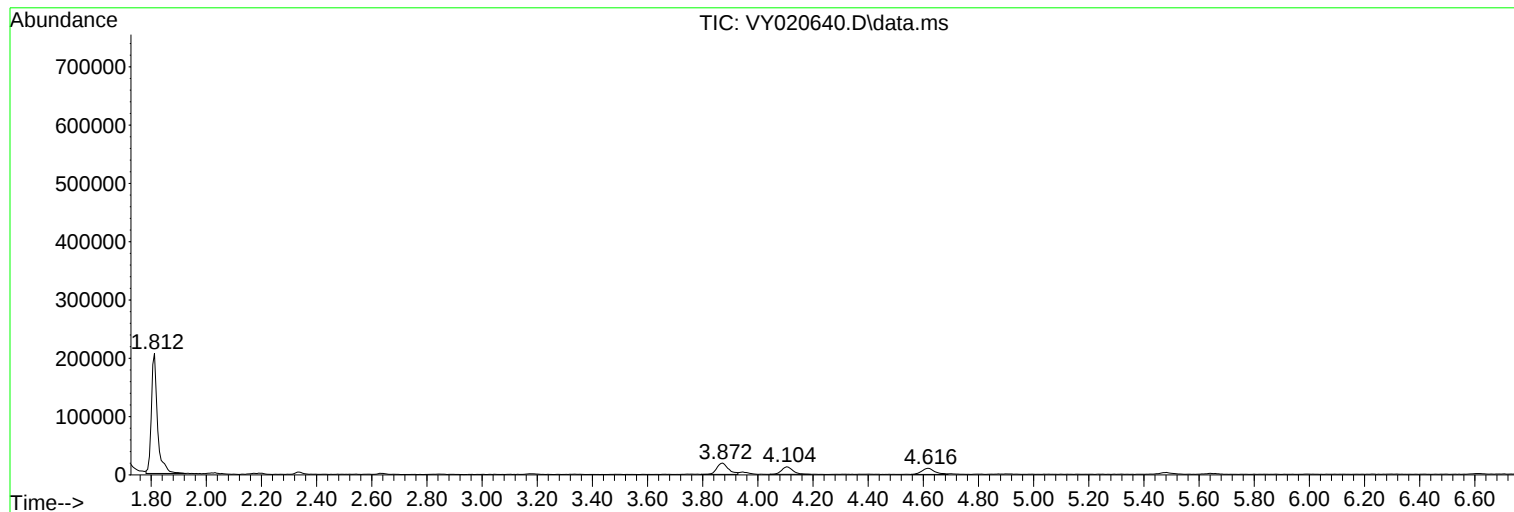
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Quant Title : SW846 8260

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



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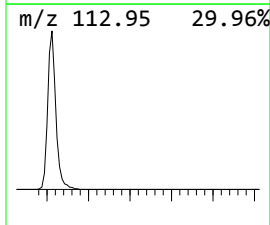
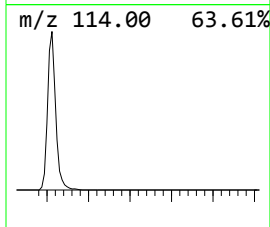
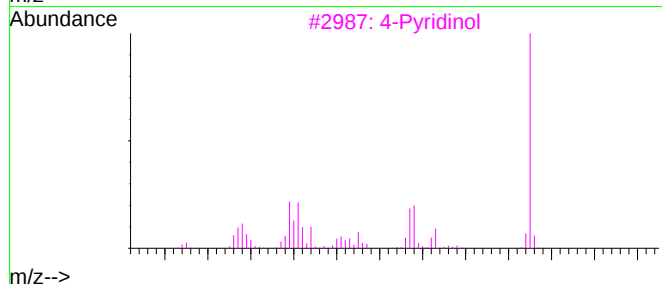
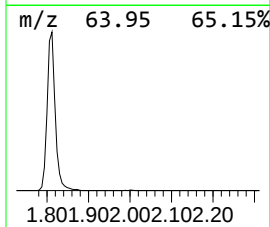
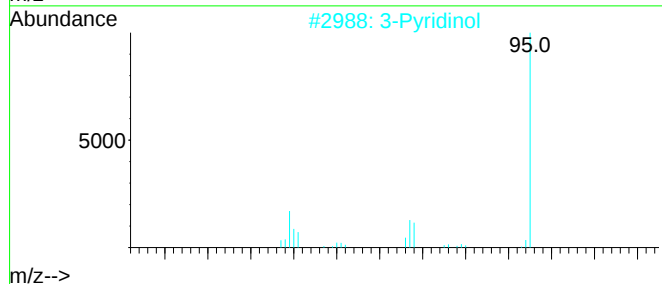
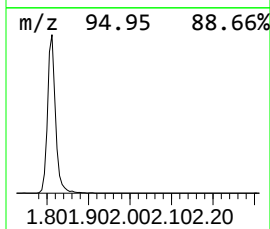
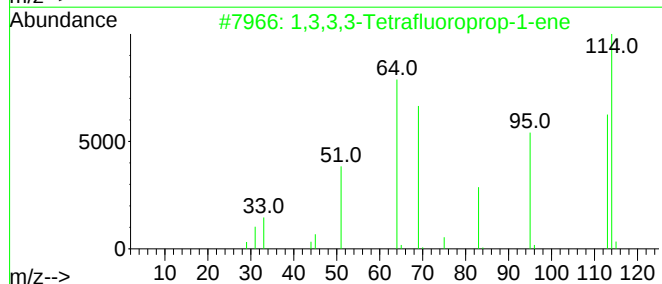
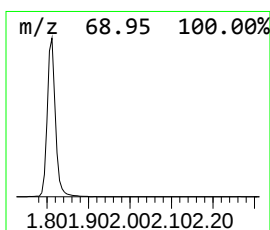
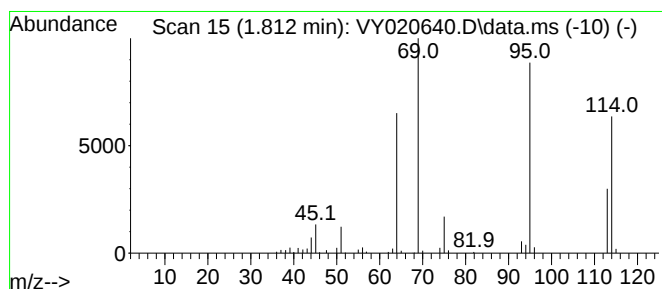
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y121724S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.812 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.812	24.25 ug/l	317384	Pentafluorobenzene	7.707

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,3,3-Tetrafluoroprop-1-ene	114	C3H2F4	1000389-53-0	28
2			3-Pyridinol	95	C5H5NO	000109-00-2	9
3			4-Pyridinol	95	C5H5NO	000626-64-2	9
4			Butenamide, N,N-dimethyl-	113	C6H11NO	023135-18-4	9
5			Ethyl diazoacetate	114	C4H6N2O2	000623-73-4	9



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MSVOA_Y
ClientSampleId :
SB-01

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

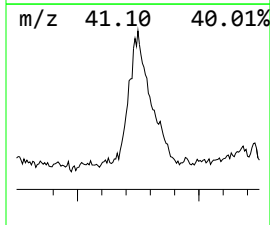
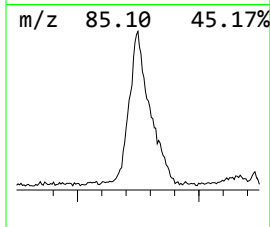
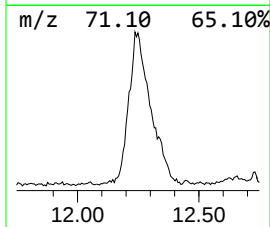
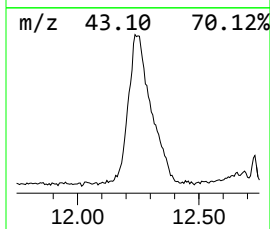
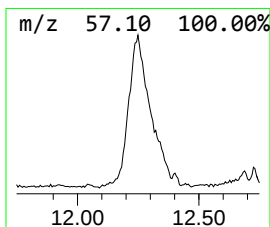
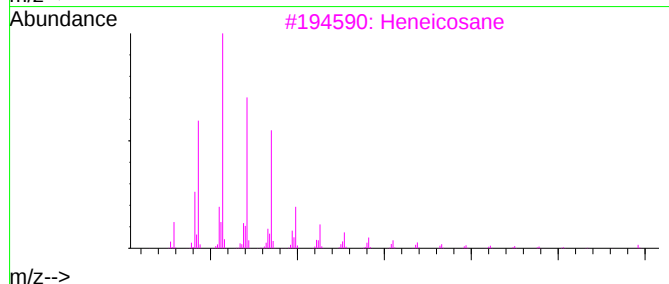
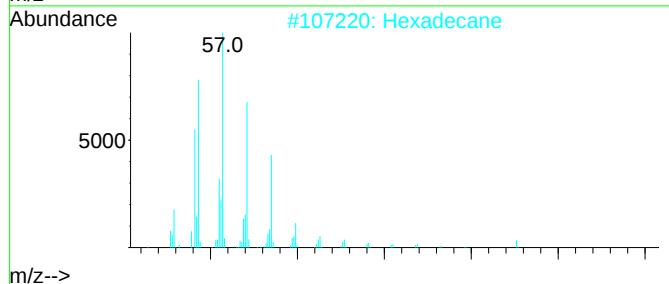
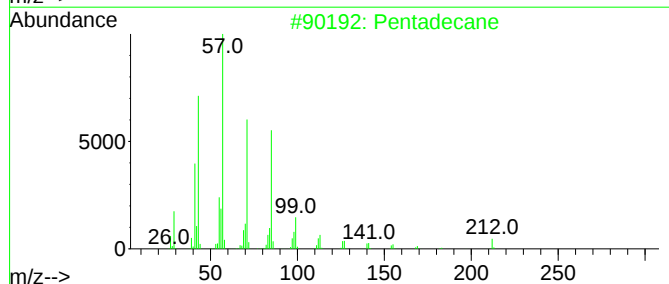
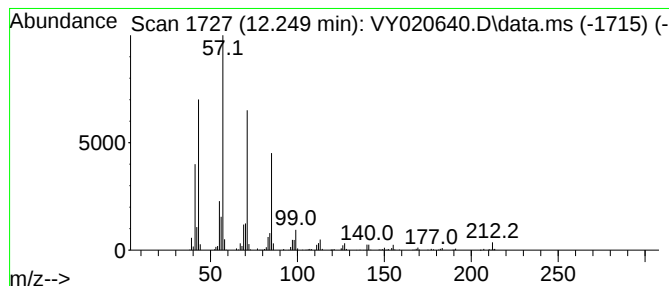
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.249	39.20 ug/l	812599	Chlorobenzene-d5	11.414

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	96
2	Hexadecane	226	C16H34	000544-76-3	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Nonadecane	268	C19H40	000629-92-5	87
5	Tetradecane	198	C14H30	000629-59-4	87



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

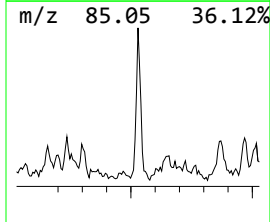
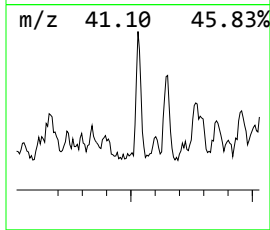
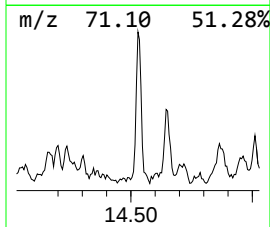
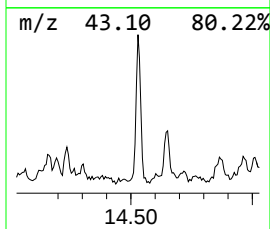
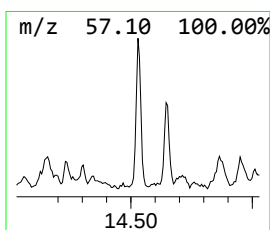
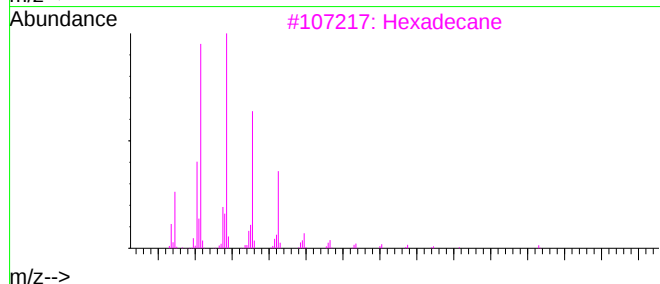
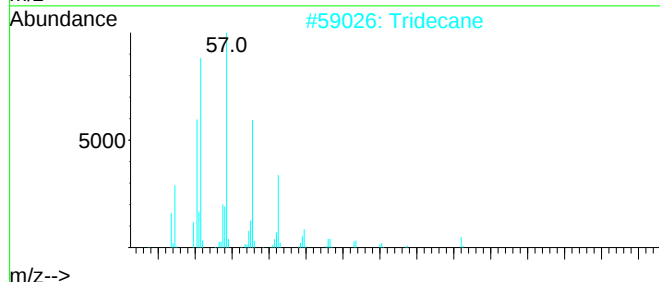
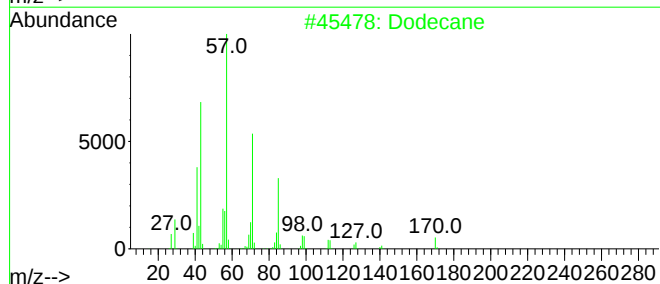
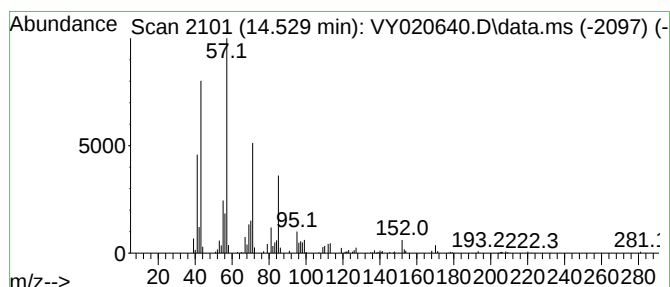
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.529	6.61 ug/l	112534	1,4-Dichlorobenzene-d4	13.346

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	Hexadecane	226	C16H34	000544-76-3	72
4	Tetradecane	198	C14H30	000629-59-4	72
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	64



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ClientSampleId :
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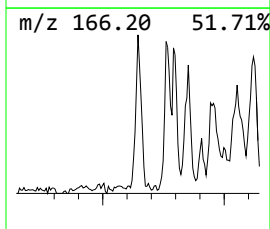
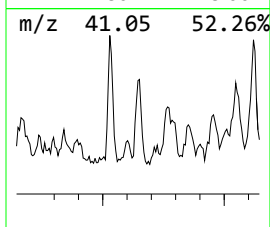
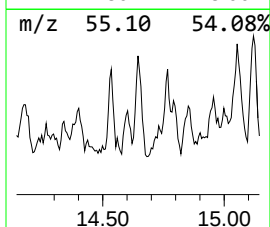
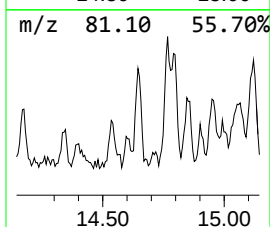
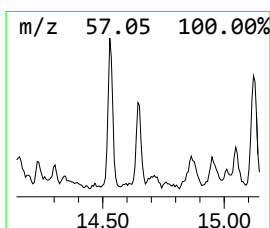
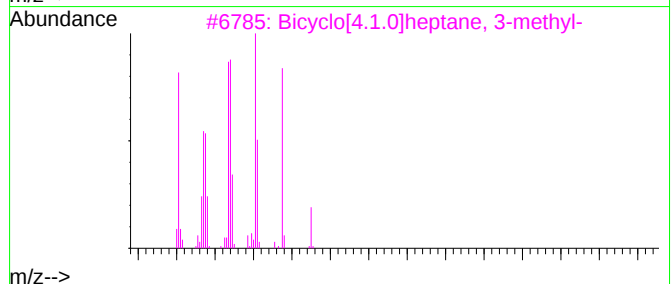
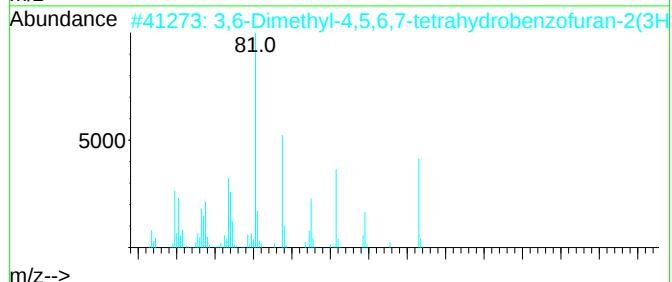
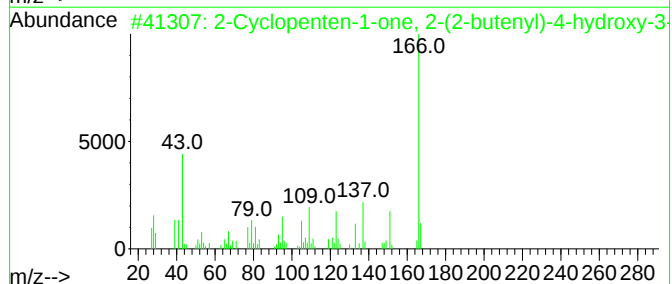
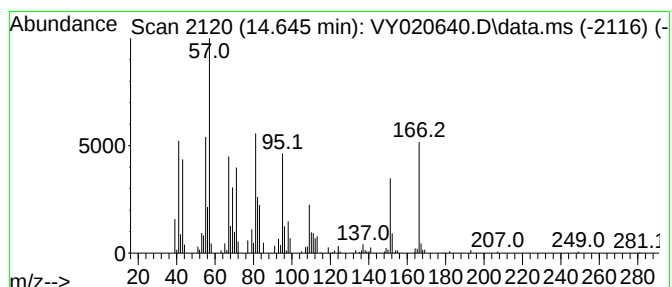
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Peak Number 5 unknown14.645 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.645	7.07 ug/l	120424	1,4-Dichlorobenzene-d4	13.346

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclopenten-1-one, 2-(2-butenyl)-	166	C10H14O2	017190-74-8	38
2	3,6-Dimethyl-4,5,6,7-tetrahydrobenzofuran-2(3H)-one	166	C10H14O2	016642-41-4	27
3	Bicyclo[4.1.0]heptane, 3-methyl-	110	C8H14	041977-47-3	25
4	2-(1-Hydroxycyclohexyl)-furan	166	C10H14O2	036169-67-2	22
5	8-Hexadecyne	222	C16H30	019781-86-3	22



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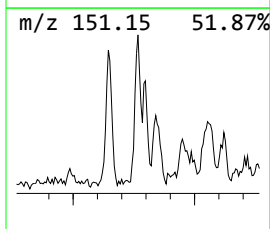
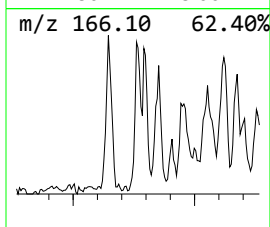
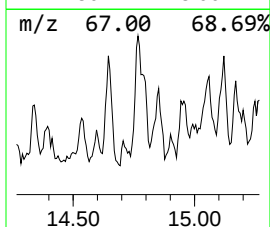
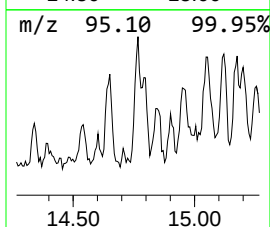
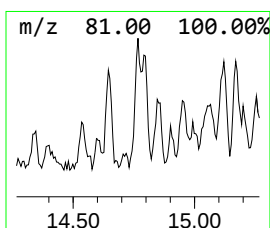
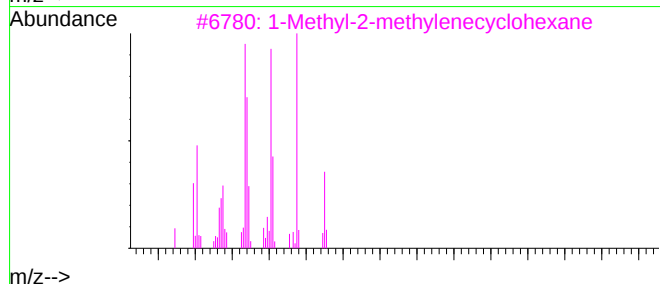
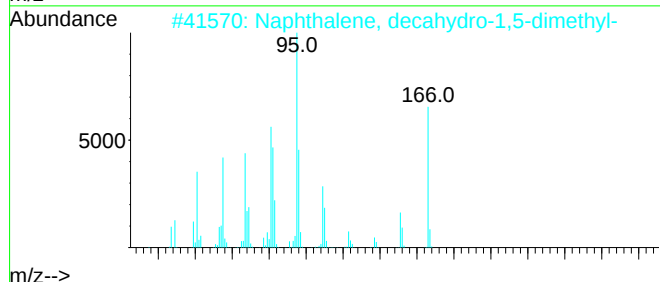
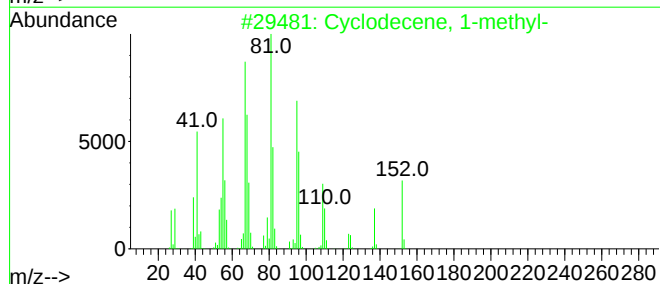
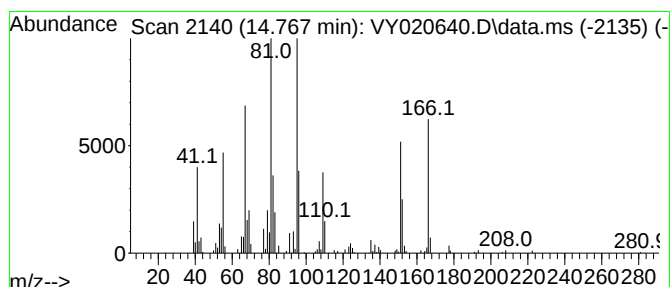
Instrument :
MSVOA_Y
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Quant Title : SW846 8260

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

Peak Number 6 Cyclodecene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.767	5.36 ug/l	91274	1,4-Dichlorobenzene-d4	13.346	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclodecene, 1-methyl-	152	C11H20	066633-38-3	58
2	Naphthalene, decahydro-1,5-dimet...	166	C12H22	066552-62-3	58
3	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	55
4	Cyclohexene,3-hexyl-	166	C12H22	015232-78-7	55
5	Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
Data File : VY020640.D
Acq On : 18 Dec 2024 16:51
Operator : SY/MD
Sample : P5299-03
Misc : 5.73g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-01

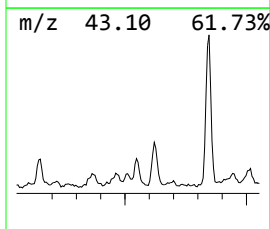
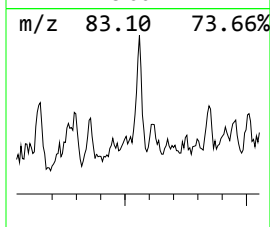
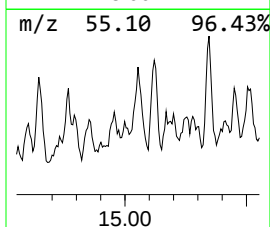
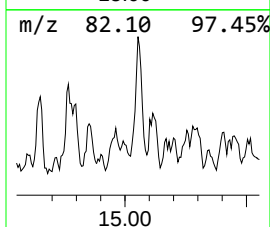
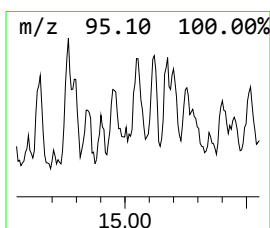
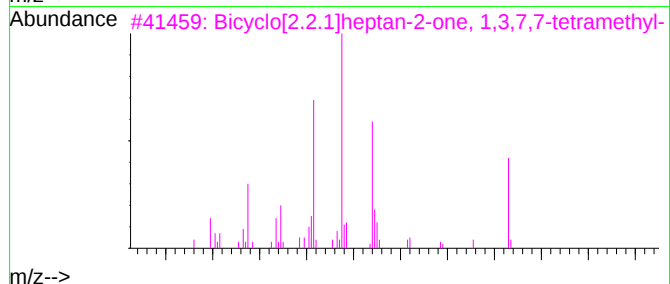
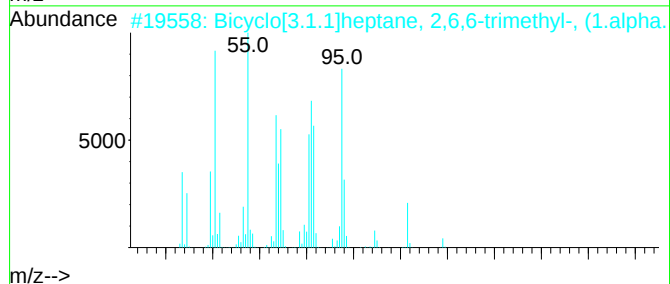
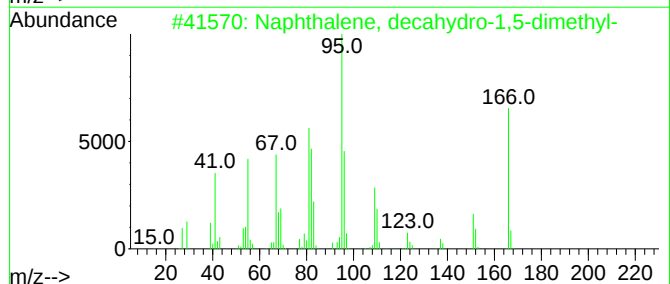
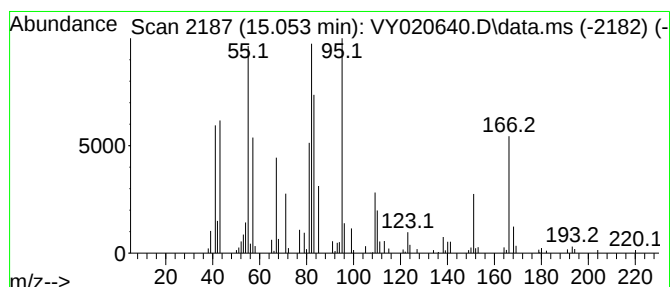
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Naphthalene, decahydro-1,5-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.053	5.93 ug/l	100899	1,4-Dichlorobenzene-d4	13.346	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-1,5-dimet...	166	C12H22	066552-62-3	53
2	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	006876-13-7	47
3	Bicyclo[2.2.1]heptan-2-one, 1,3,...	166	C11H18O	005811-48-3	43
4	Vinylcyclohexyl ether	126	C8H14O	002182-55-0	35
5	Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
Data File : VY020640.D
Acq On : 18 Dec 2024 16:51
Operator : SY/MD
Sample : P5299-03
Misc : 5.73g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-01

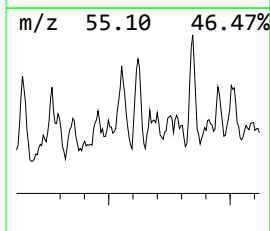
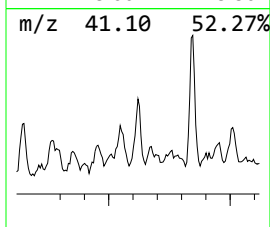
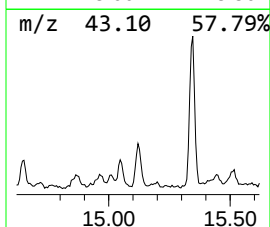
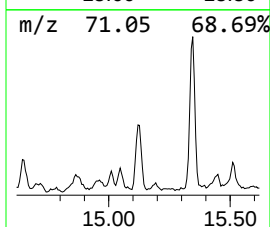
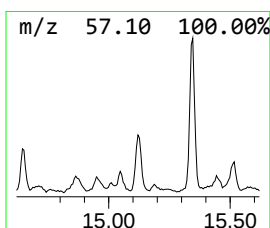
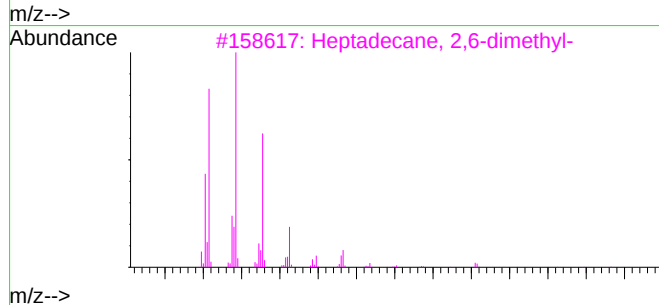
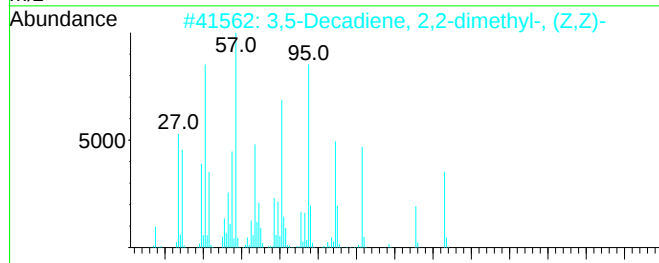
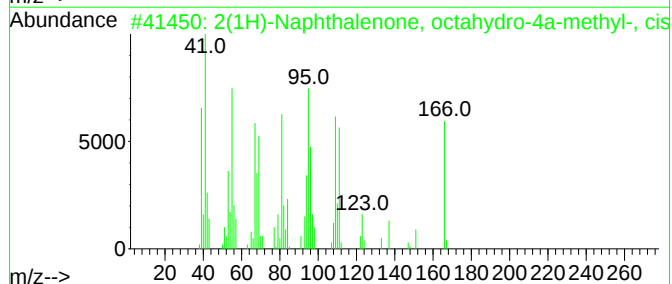
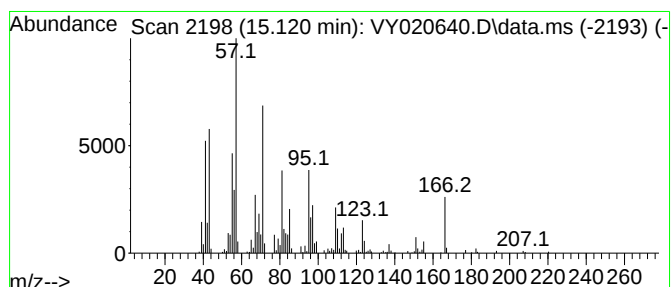
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Quant Title : SW846 8260

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

Peak Number 8 unknown15.120 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.120	7.97 ug/l	135659	1,4-Dichlorobenzene-d4	13.346

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, octahydro-4...	166	C11H18O	000938-06-7	38
2	3,5-Decadiene, 2,2-dimethyl-, (Z...	166	C12H22	055638-50-1	35
3	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	27
4	Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	27
5	Cyclohexanone, 2,2-dimethyl-5-(3...	182	C11H18O2	141033-65-0	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
Data File : VY020640.D
Acq On : 18 Dec 2024 16:51
Operator : SY/MD
Sample : P5299-03
Misc : 5.73g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-01

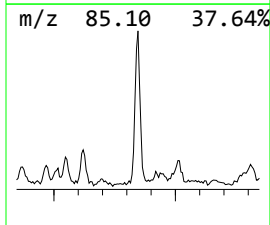
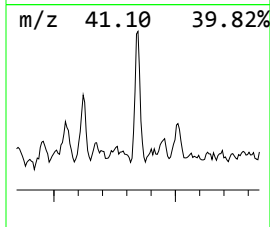
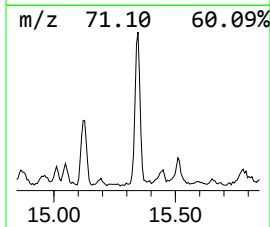
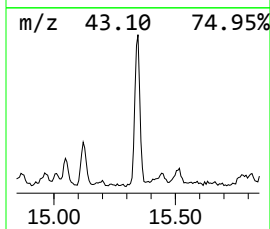
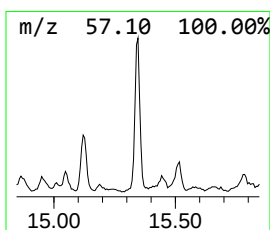
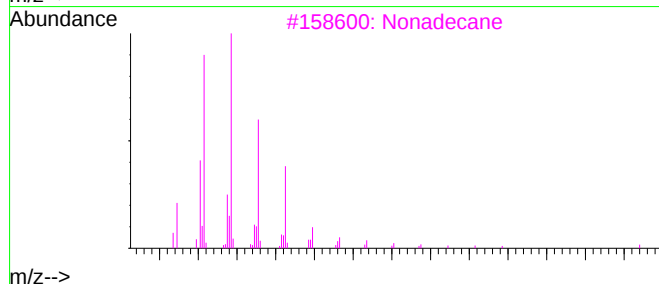
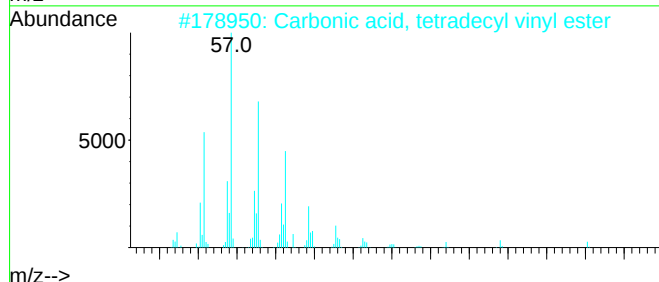
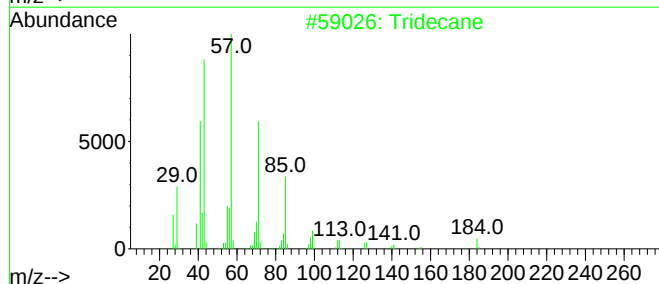
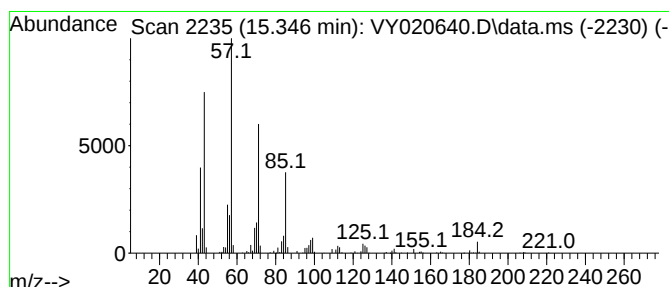
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Quant Title : SW846 8260

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

Peak Number 9 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.346	10.97 ug/l	186768	1,4-Dichlorobenzene-d4	13.346

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	96
2	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	80
3	Nonadecane	268	C19H40	000629-92-5	80
4	Pentadecane	212	C15H32	000629-62-9	80
5	Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
Data File : VY020640.D
Acq On : 18 Dec 2024 16:51
Operator : SY/MD
Sample : P5299-03
Misc : 5.73g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-01

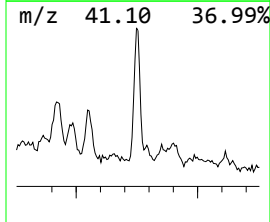
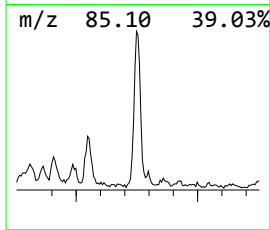
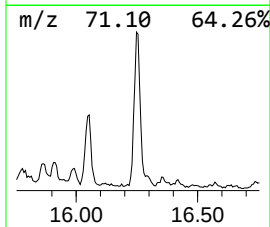
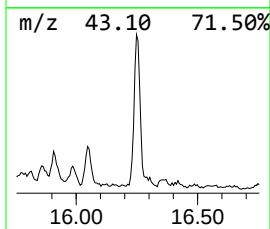
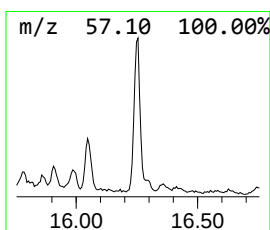
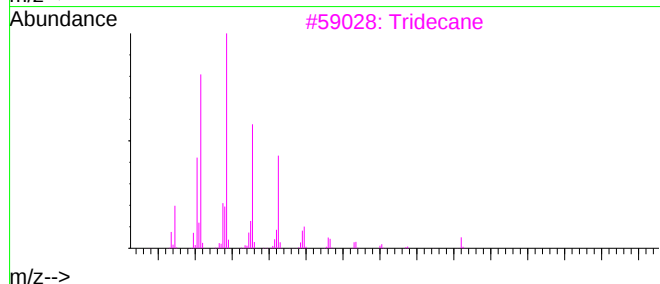
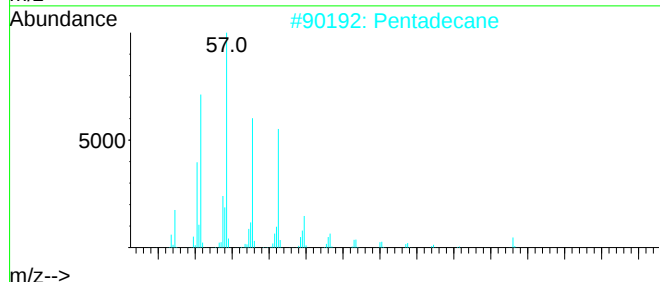
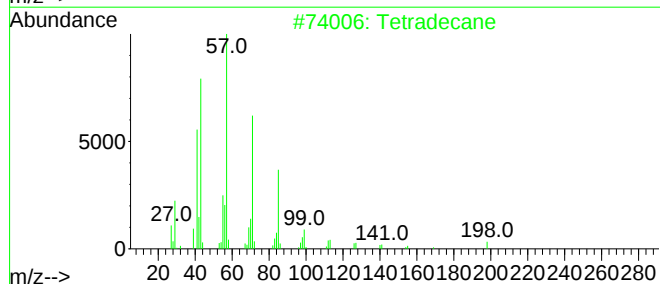
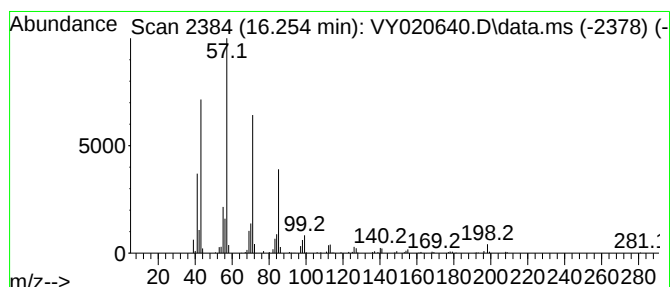
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Quant Title : SW846 8260

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

Peak Number 10 Tetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.254	12.06 ug/l	205341	1,4-Dichlorobenzene-d4	13.346

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	98
2	Pentadecane	212	C15H32	000629-62-9	86
3	Tridecane	184	C13H28	000629-50-5	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121824\
Data File : VY020640.D
Acq On : 18 Dec 2024 16:51
Operator : SY/MD
Sample : P5299-03
Misc : 5.73g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-01

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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Pentadecane	12.249	39.2	ug/l	812599	3	11.414	1036390	50.0
Dodecane	14.529	6.6	ug/l	112534	4	13.346	851326	50.0
unknown14.645	14.645	7.1	ug/l	120424	4	13.346	851326	50.0
Cyclodecene, 1-...	14.767	5.4	ug/l	91274	4	13.346	851326	50.0
Naphthalene, de...	15.053	5.9	ug/l	100899	4	13.346	851326	50.0
unknown15.120	15.120	8.0	ug/l	135659	4	13.346	851326	50.0
Tridecane	15.346	11.0	ug/l	186768	4	13.346	851326	50.0
Tetradecane	16.254	12.1	ug/l	205341	4	13.346	851326	50.0