

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111324\
 Data File : VN084820.D
 Acq On : 13 Nov 2024 12:01
 Operator : JC\MD
 Sample : P4793-01
 Misc : 1.35g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 M00-24-00345

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_N\methods\82N103024W.M

Title : SW846 8260

Signal : TIC: VN084820.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	50	57	69	rBV	38686	72024	1.97%	0.707%
2	2.506	86	94	110	rBV5	15589	66867	1.83%	0.656%
3	2.895	145	160	161	rBV9	14279	45763	1.25%	0.449%
4	8.159	1046	1055	1059	rBV	123022	298441	8.16%	2.930%
5	8.212	1059	1064	1075	rVV2	304626	697200	19.06%	6.845%
6	8.312	1075	1081	1091	rVB2	32024	75085	2.05%	0.737%
7	8.436	1093	1102	1113	rBV2	126505	288362	7.88%	2.831%
8	8.571	1118	1125	1134	rVB	133481	292552	8.00%	2.872%
9	8.694	1134	1146	1155	rBV5	19060	58491	1.60%	0.574%
10	8.959	1182	1191	1200	rVB	129854	251708	6.88%	2.471%
11	9.094	1205	1214	1223	rBV	328186	660362	18.05%	6.483%
12	10.565	1455	1464	1468	rBV	454888	842216	23.02%	8.268%
13	10.624	1468	1474	1490	rVB	1956185	3658780	100.00%	35.920%
14	11.865	1677	1685	1696	rBV	409669	732220	20.01%	7.189%
15	12.065	1712	1719	1730	rVB2	20576	38984	1.07%	0.383%
16	12.847	1845	1852	1864	rVB	307261	514772	14.07%	5.054%
17	13.159	1900	1905	1912	rVB4	19724	38986	1.07%	0.383%
18	13.535	1963	1969	1979	rVB	41794	63545	1.74%	0.624%
19	13.788	2006	2012	2021	rBV	389774	652685	17.84%	6.408%
20	13.870	2021	2026	2032	rVB	31688	51355	1.40%	0.504%
21	14.100	2061	2065	2073	rBV4	29732	48091	1.31%	0.472%
22	14.923	2199	2205	2215	rBV	509810	737494	20.16%	7.240%

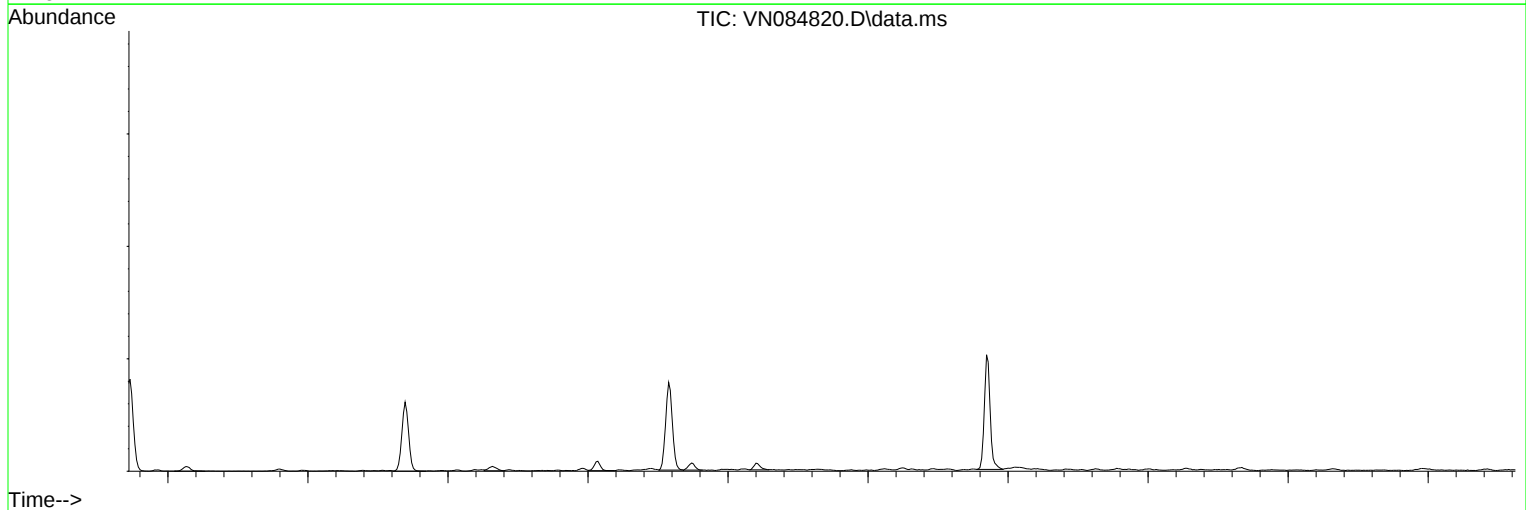
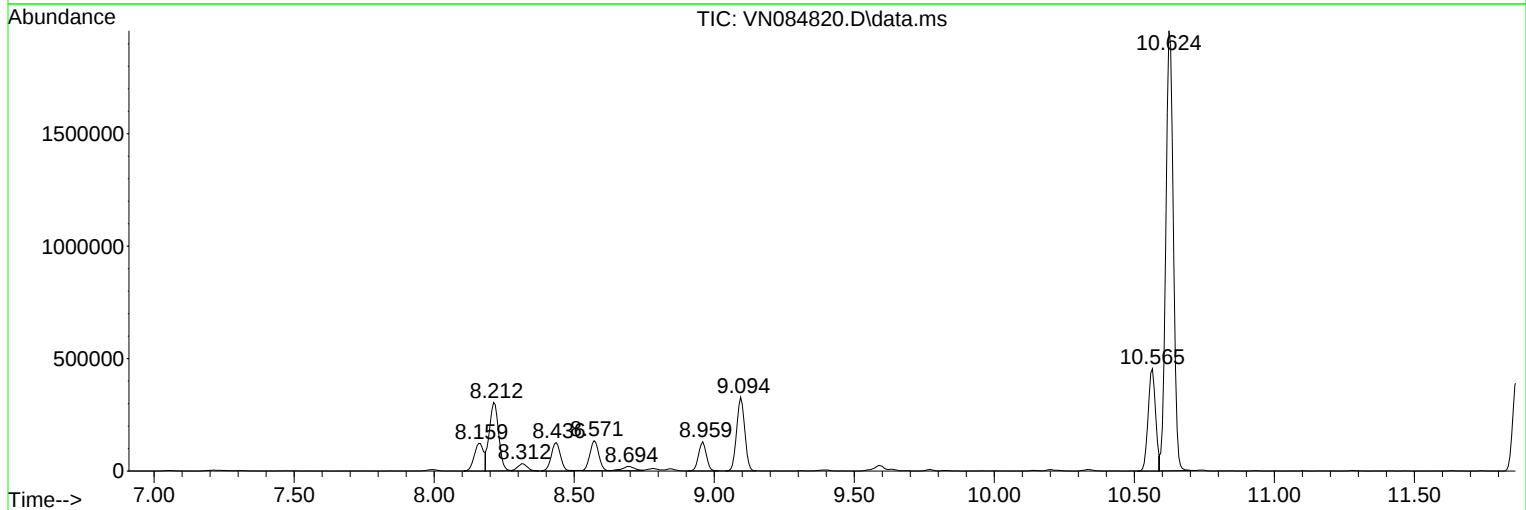
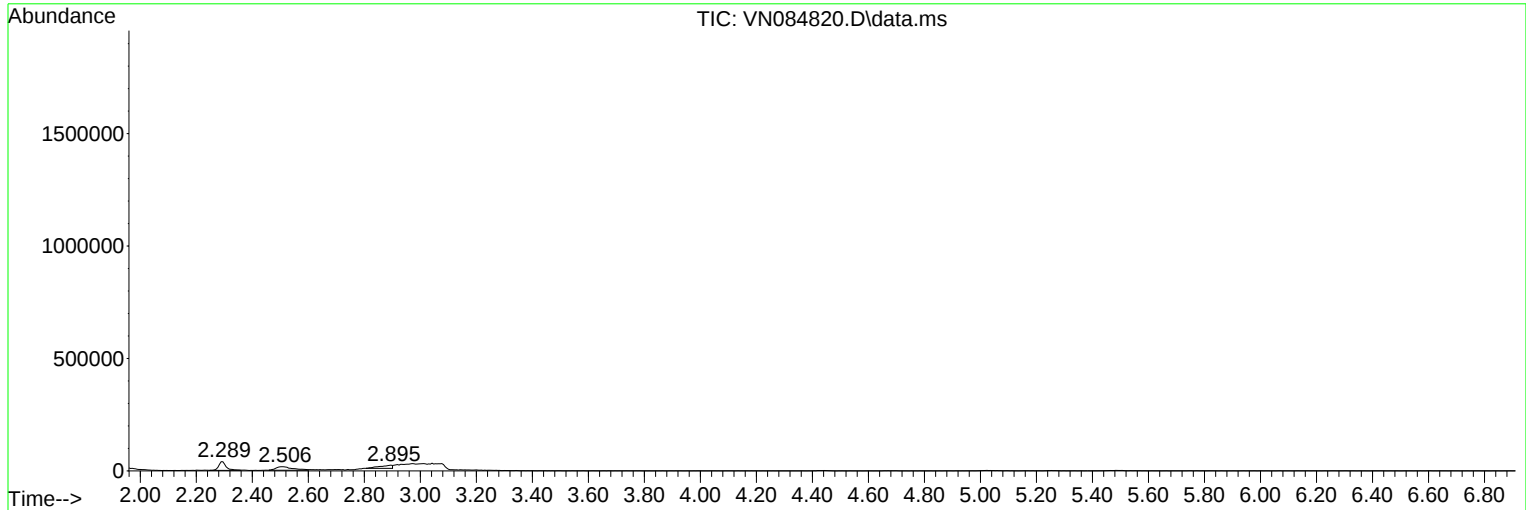
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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



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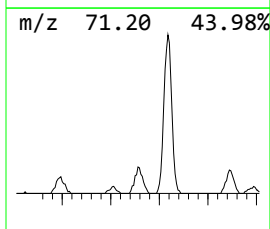
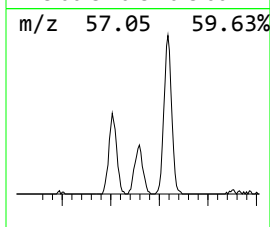
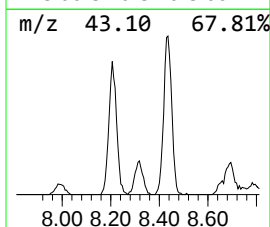
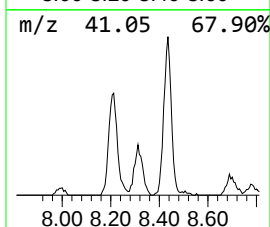
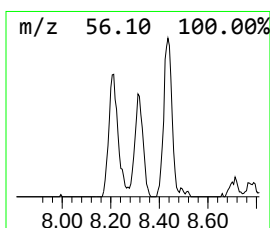
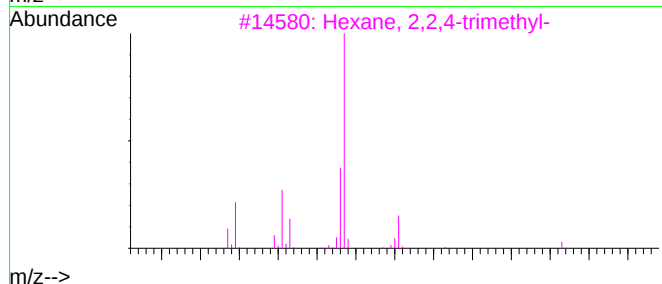
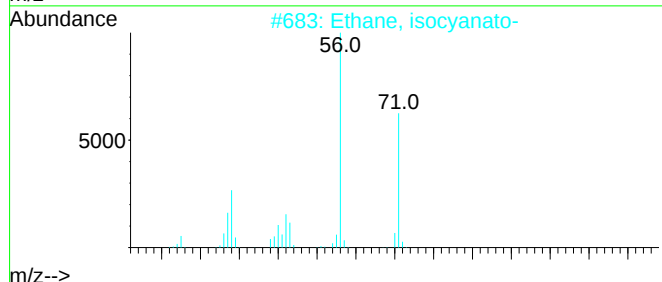
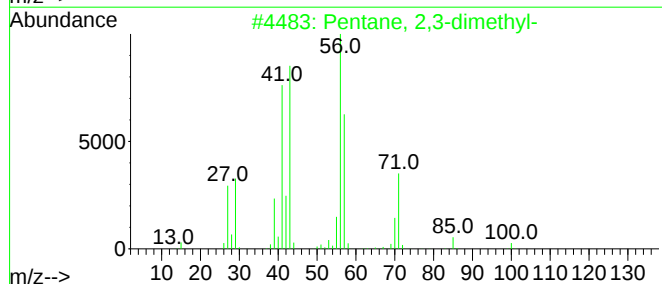
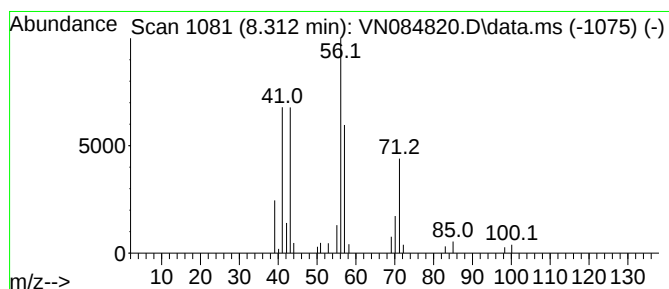
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.312	5.38 ug/l	75085	Pentafluorobenzene	8.218	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	87
2	Ethane, isocyanato-	71	C3H5NO	000109-90-0	64
3	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	56
4	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	50
5	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	47



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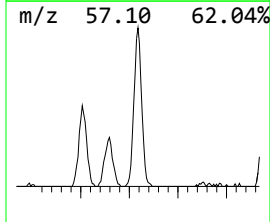
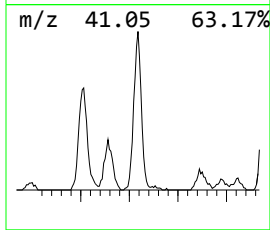
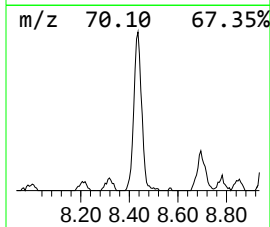
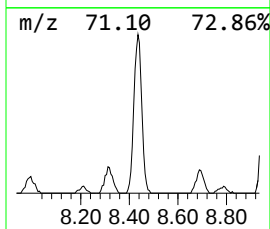
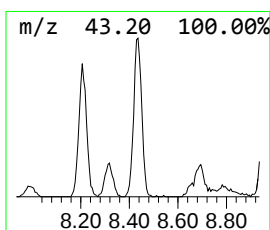
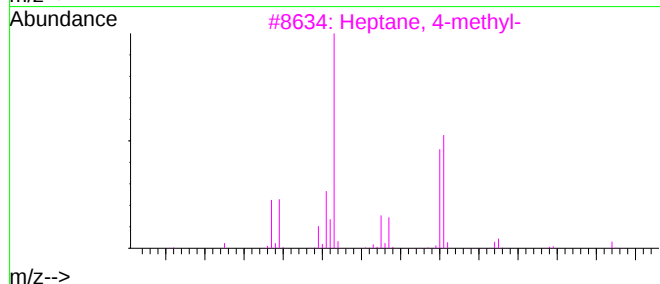
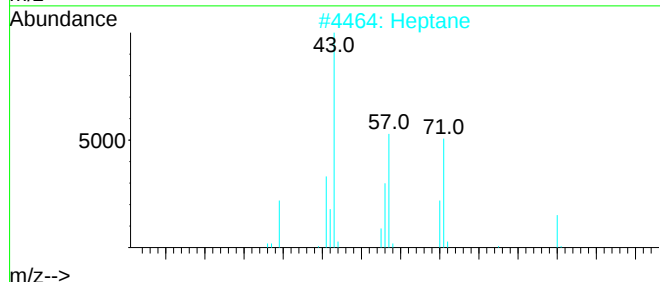
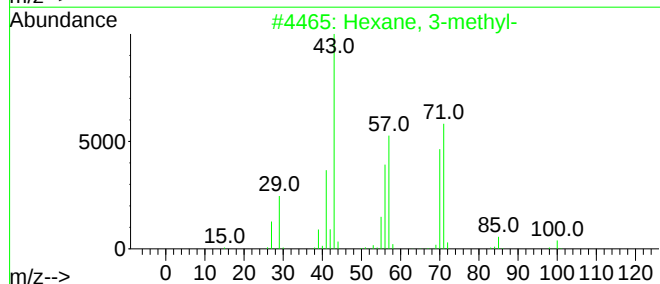
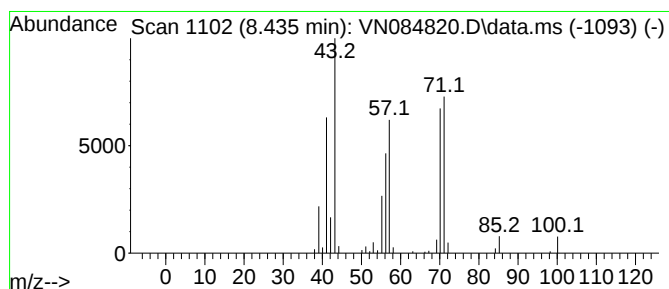
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.435	20.68 ug/l	288362	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2	Heptane	100	C7H16	000142-82-5	83
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	53
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	53



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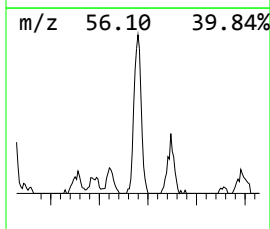
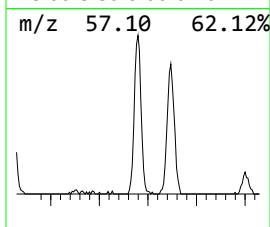
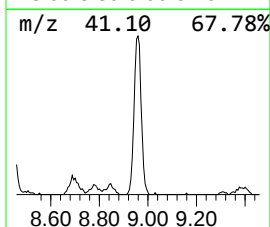
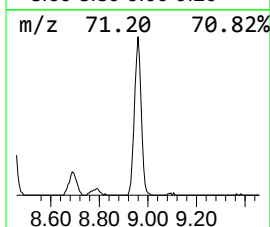
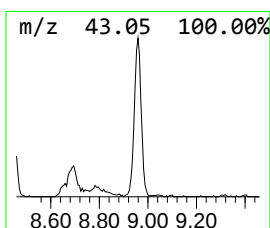
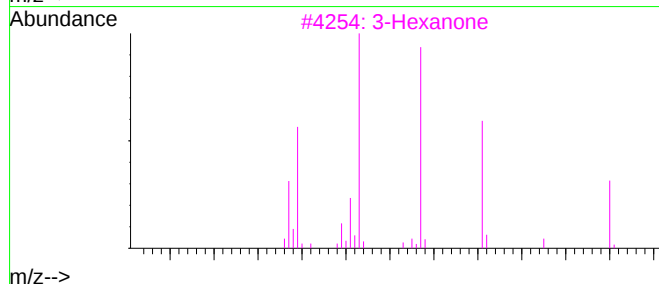
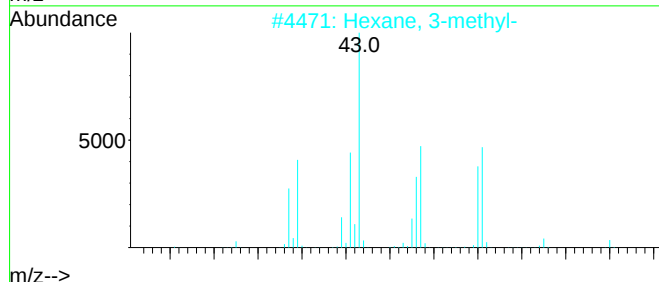
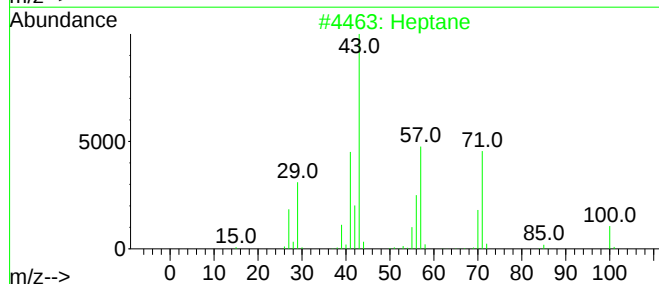
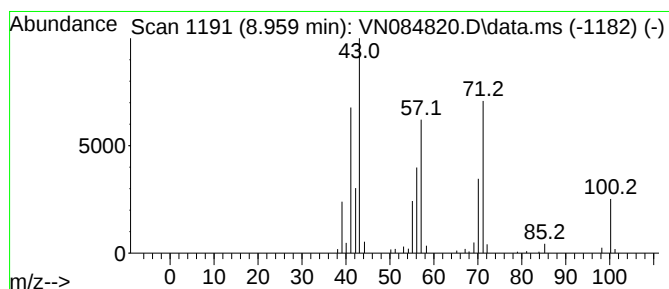
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.959	19.06 ug/l	251708	1,4-Difluorobenzene	9.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	53
3	3-Hexanone	100	C6H12O	000589-38-8	43
4	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	40
5	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	38



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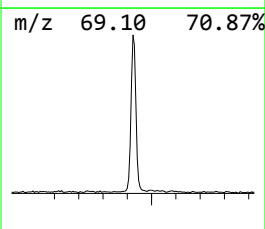
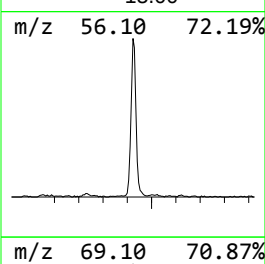
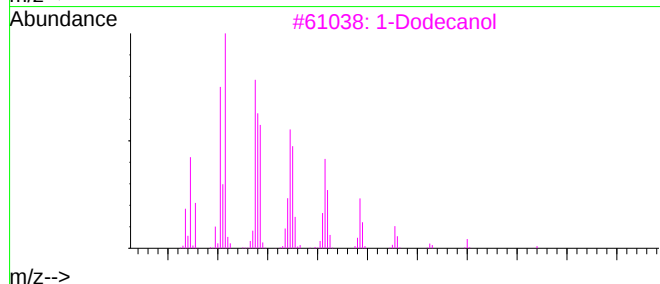
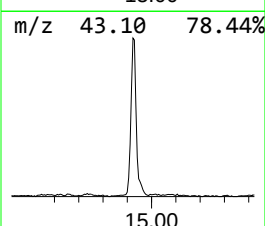
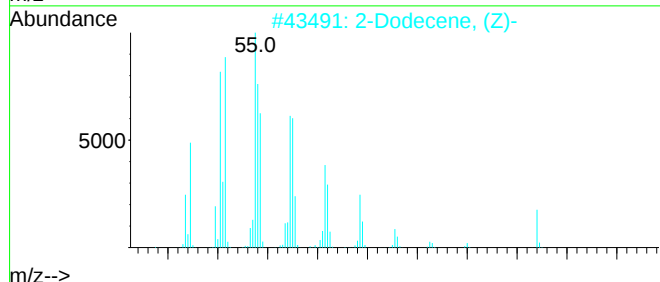
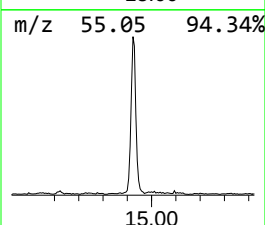
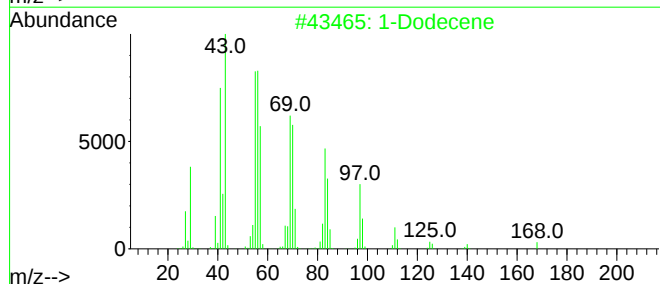
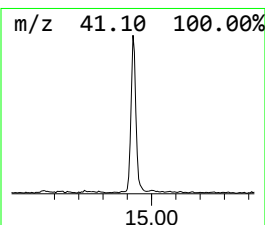
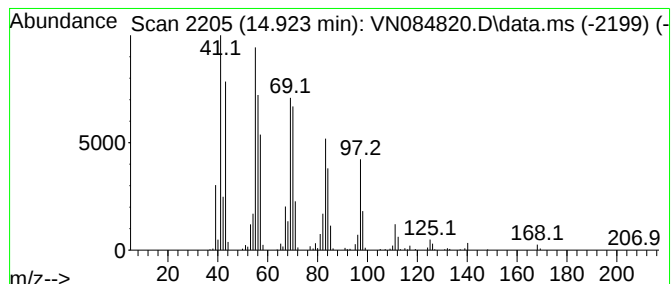
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TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Dodecene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.923	56.50 ug/l	737494	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecene	168	C12H24	000112-41-4	97
2	2-Dodecene, (Z)-	168	C12H24	007206-26-0	91
3	1-Dodecanol	186	C12H26O	000112-53-8	83
4	Cyclooctane, methyl-	126	C9H18	001502-38-1	83
5	1-Tridecene	182	C13H26	002437-56-1	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,3-di...	8.312	5.4	ug/l	75085	1	8.218	697200	50.0
Hexane, 3-methyl-	8.435	20.7	ug/l	288362	1	8.218	697200	50.0
Heptane	8.959	19.1	ug/l	251708	2	9.094	660362	50.0
1-Dodecene	14.923	56.5	ug/l	737494	4	13.788	652685	50.0