

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040125\
 Data File : VN086198.D
 Acq On : 01 Apr 2025 16:01
 Operator : JC\MD
 Sample : Q1690-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW112010

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\82N031825W.M
 Title : SW846 8260

Signal : TIC: VN086198.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.665	119	121	127	rVB3	7142	10530	1.15%	0.163%
2	2.812	141	146	154	rVB7	10224	26034	2.85%	0.404%
3	4.430	410	421	435	rBV2	12745	44101	4.83%	0.684%
4	5.030	514	523	525	rBV3	7283	16670	1.83%	0.259%
5	8.165	1046	1056	1060	rBV	132728	312268	34.20%	4.845%
6	8.224	1060	1066	1077	rVV	223277	506141	55.43%	7.853%
7	8.318	1077	1082	1089	rVB7	4653	11603	1.27%	0.180%
8	8.577	1117	1126	1134	rBV2	142283	397291	43.51%	6.164%
9	9.100	1206	1215	1227	rBV	328472	676260	74.06%	10.493%
10	10.141	1387	1392	1399	rBV6	5331	11416	1.25%	0.177%
11	10.441	1439	1443	1449	rVB5	5747	10340	1.13%	0.160%
12	10.565	1455	1464	1473	rBV	499420	913093	100.00%	14.167%
13	11.865	1676	1685	1697	rVB	445766	789115	86.42%	12.244%
14	12.659	1816	1820	1827	rBV4	7148	14327	1.57%	0.222%
15	12.847	1845	1852	1861	rBV	369218	631611	69.17%	9.800%
16	13.065	1879	1889	1890	rBV6	10382	20275	2.22%	0.315%
17	13.618	1979	1983	1989	rVB6	7234	12980	1.42%	0.201%
18	13.788	2004	2012	2021	rBV	430323	722882	79.17%	11.216%
19	13.988	2042	2046	2054	rVB2	11590	18894	2.07%	0.293%
20	14.241	2079	2089	2093	rBV	90319	173042	18.95%	2.685%
21	14.312	2093	2101	2112	rVB5	109088	378179	41.42%	5.868%
22	14.441	2120	2123	2129	rVB5	12743	20793	2.28%	0.323%
23	14.553	2137	2142	2150	rVV9	7113	18537	2.03%	0.288%
24	14.653	2154	2159	2167	rVB3	15579	32109	3.52%	0.498%
25	14.876	2192	2197	2202	rBV4	9308	16848	1.85%	0.261%
26	15.429	2283	2291	2300	rVB9	15836	34134	3.74%	0.530%
27	15.694	2330	2336	2342	rBV3	13227	27779	3.04%	0.431%
28	15.776	2344	2350	2356	rVB4	11304	25111	2.75%	0.390%
29	16.006	2382	2389	2402	rBV2	147660	330404	36.19%	5.126%
30	16.253	2426	2431	2434	rBV7	6723	12823	1.40%	0.199%
31	16.329	2434	2444	2452	rVV6	11726	40658	4.45%	0.631%
32	16.488	2463	2471	2472	rBV5	10897	22318	2.44%	0.346%
33	16.559	2474	2483	2497	rVB5	42507	166597	18.25%	2.585%

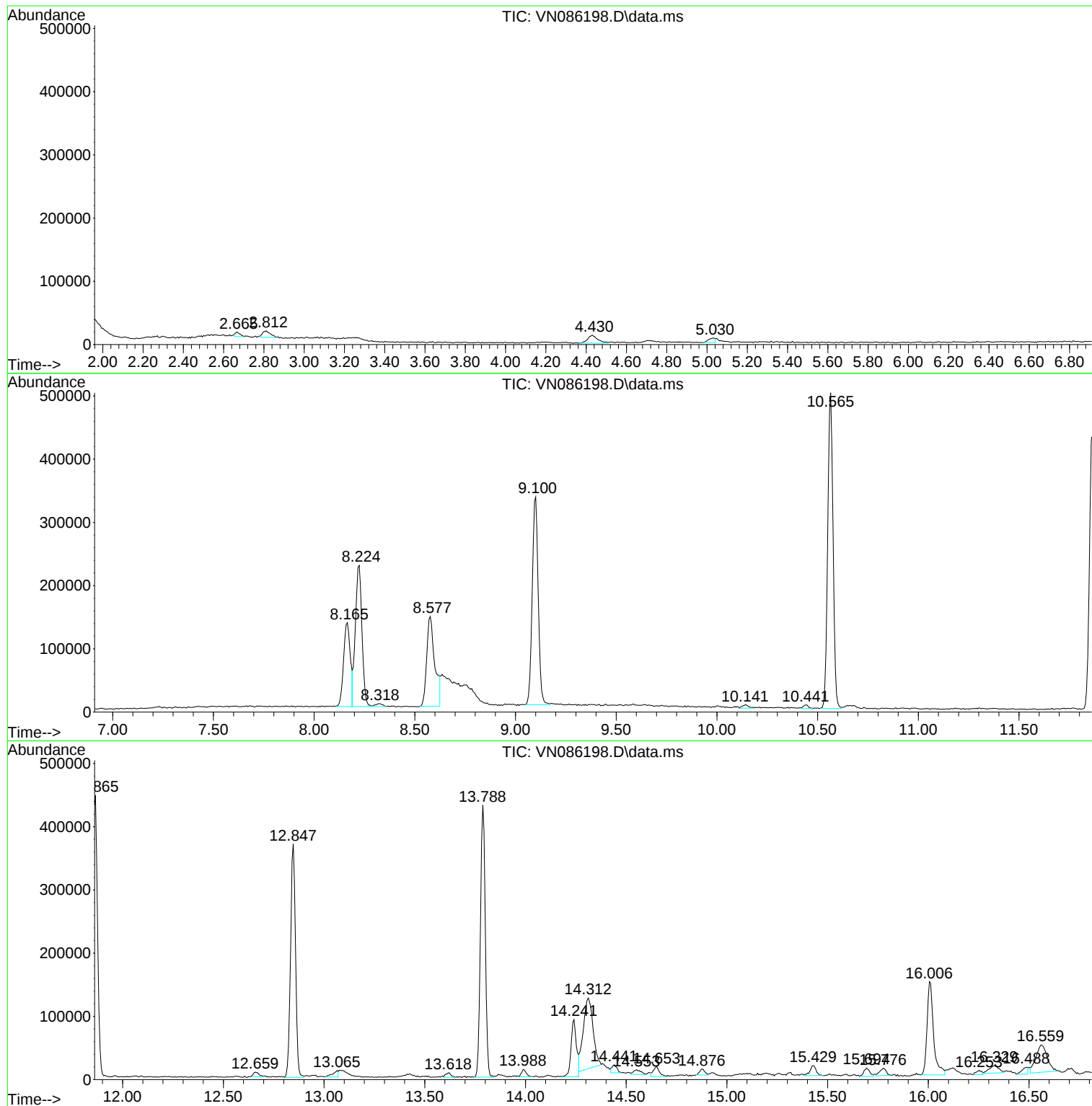
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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



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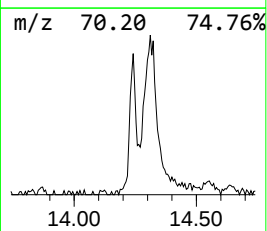
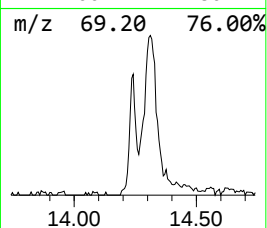
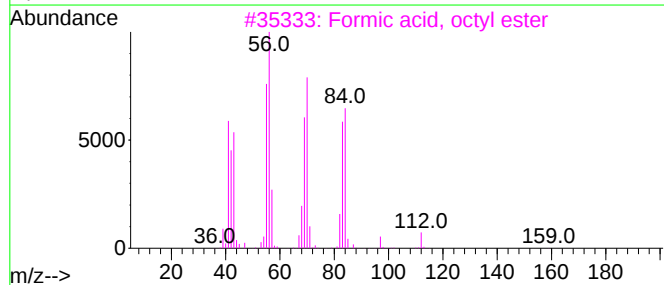
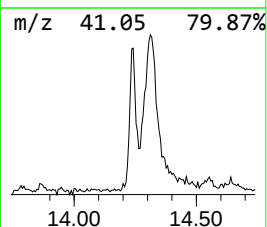
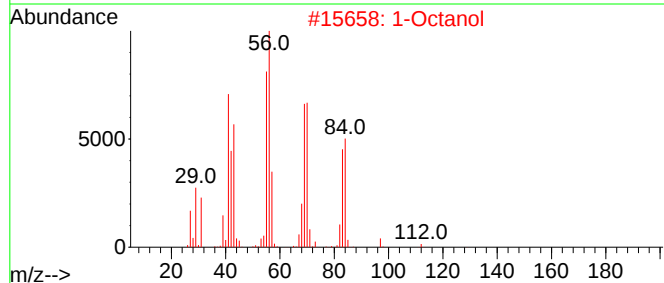
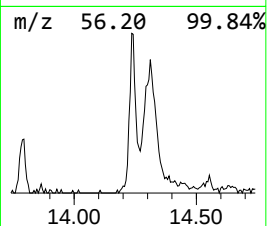
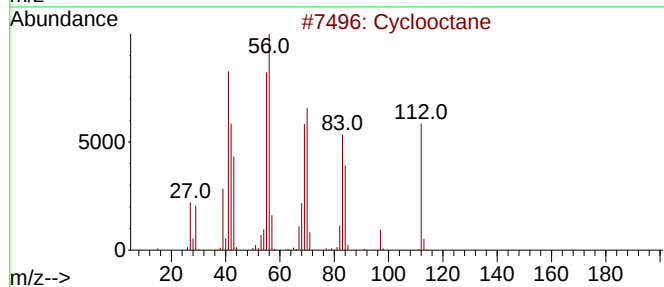
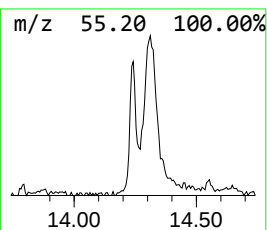
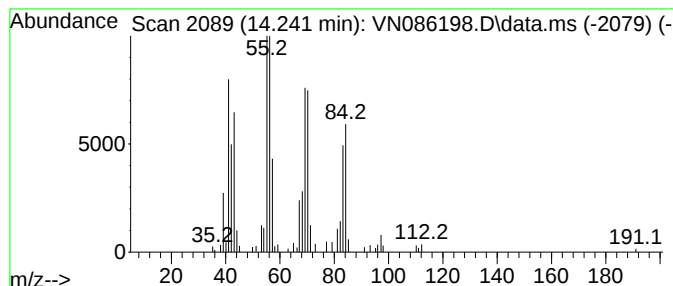
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclooctane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.241	11.97 ug/l	173042	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctane	112	C8H16	000292-64-8	90
2			1-Octanol	130	C8H18O	000111-87-5	90
3			Formic acid, octyl ester	158	C9H18O2	000112-32-3	78
4			1-Nonanol	144	C9H20O	000143-08-8	72
5			Acetic acid, trichloro-, octyl e...	274	C10H17Cl3O2	016958-78-4	72



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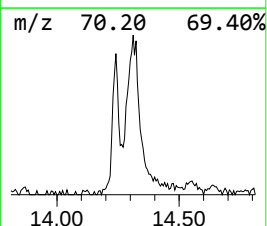
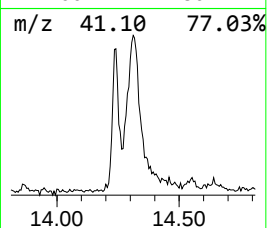
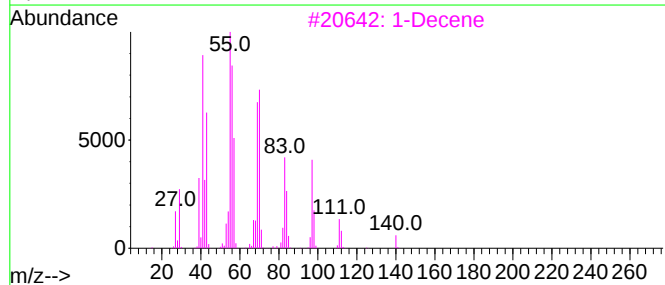
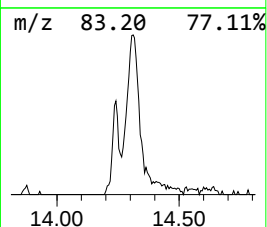
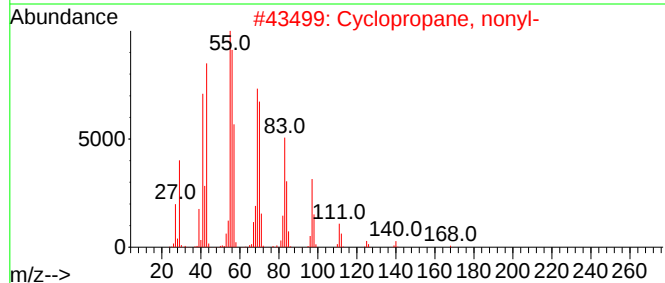
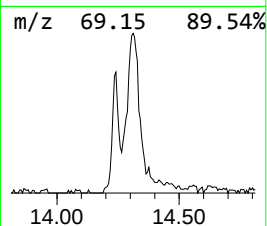
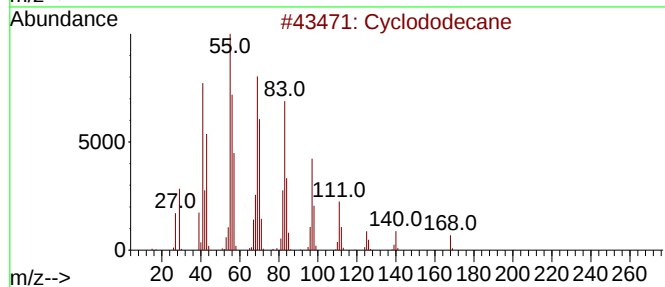
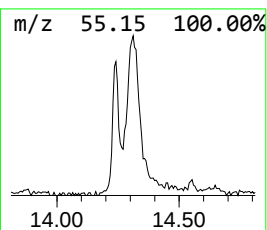
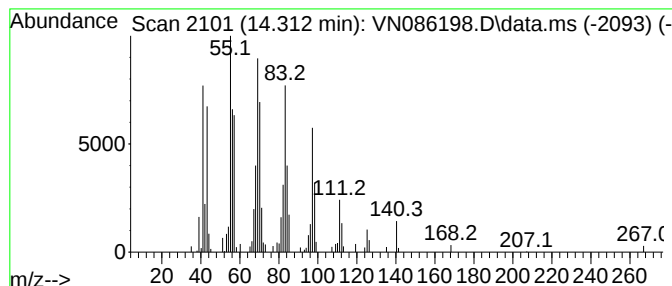
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclododecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.312	26.16 ug/l	378179	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclododecane	168	C12H24	000294-62-2	95
2			Cyclopropane, nonyl-	168	C12H24	074663-85-7	95
3			1-Decene	140	C10H20	000872-05-9	94
4			Cyclodecane	140	C10H20	000293-96-9	93
5			1-Tetradecanol	214	C14H30O	000112-72-1	91



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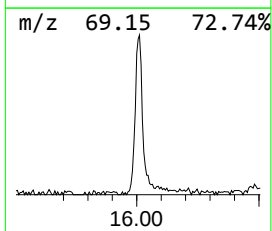
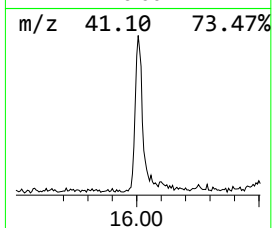
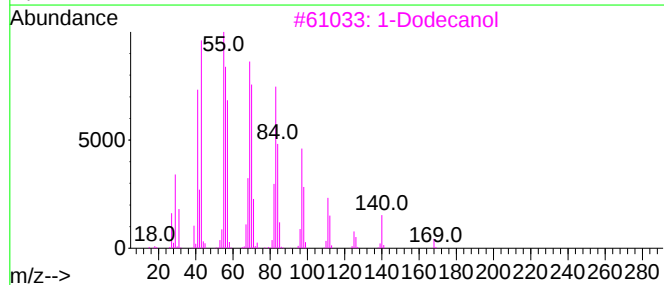
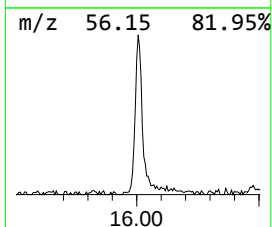
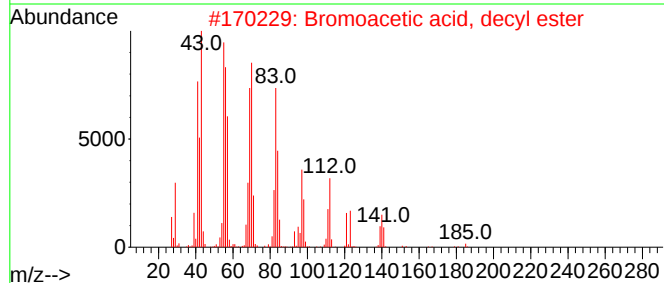
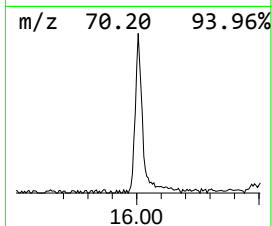
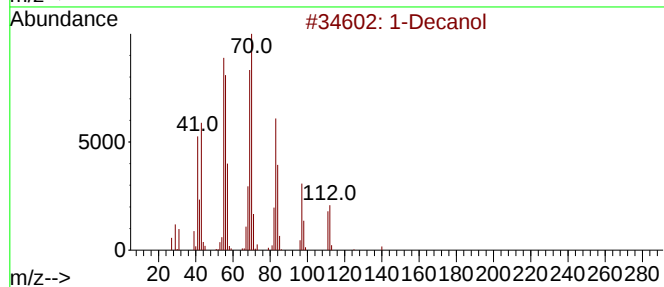
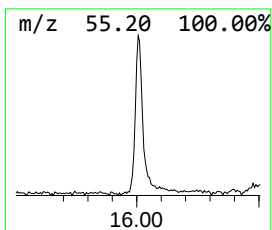
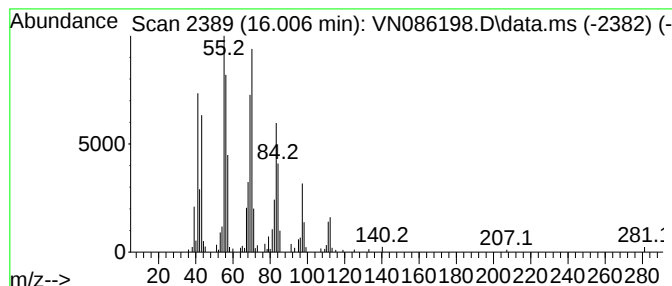
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1-Decanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.006	22.85 ug/l	330404	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decanol	158	C10H22O	000112-30-1	91
2			Bromoacetic acid, decyl ester	278	C12H23BrO2	005436-93-1	91
3			1-Dodecanol	186	C12H26O	000112-53-8	91
4			1-Undecanol	172	C11H24O	000112-42-5	90
5			Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	86



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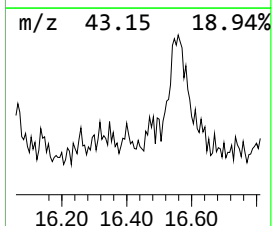
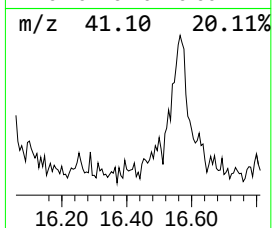
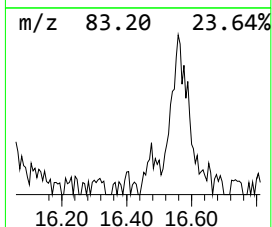
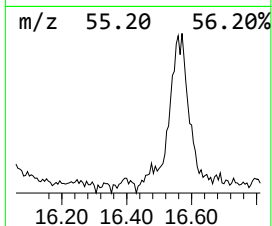
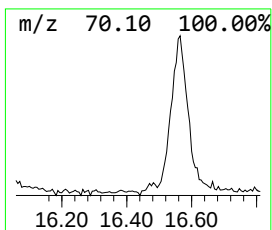
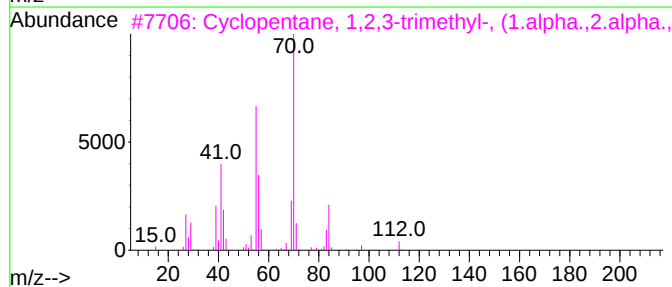
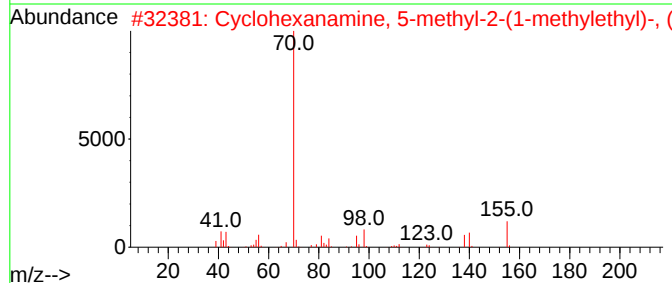
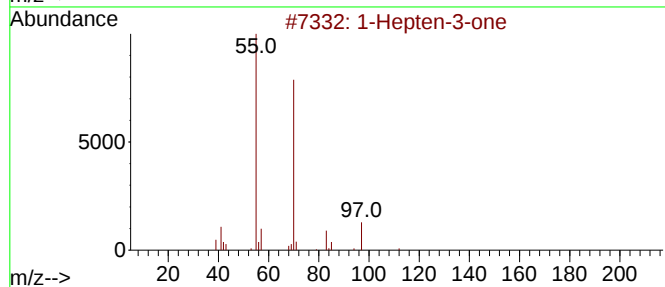
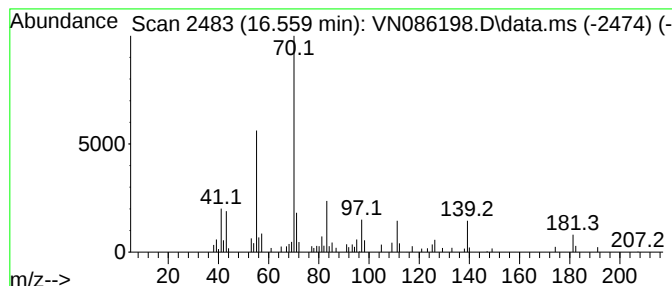
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TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown16.558 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.558	11.52 ug/l	166597	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hepten-3-one	112	C7H12O	002918-13-0	50
2			Cyclohexanamine, 5-methyl-2-(1-m...	155	C10H21N	023399-21-5	38
3			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	38
4			4-(4-Methyl-piperazin-1-yl)-1,5,...	182	C8H14N4O	1000287-66-9	35
5			Tetrahydrogeranyl formate	186	C11H22O2	1000429-39-6	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclooctane	14.241	12.0	ug/l	173042	4	13.788	722882	50.0
Cyclododecane	14.312	26.2	ug/l	378179	4	13.788	722882	50.0
1-Decanol	16.006	22.9	ug/l	330404	4	13.788	722882	50.0
unknown16.558	16.558	11.5	ug/l	166597	4	13.788	722882	50.0