LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091818\
Data File : VX004689.D
Acq On : 19 Sep 2018 06:02
Operator : JC/MD
Sample : J4957-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : N48966

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_X\METHOD\82X091118W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.440	205	211	223	rBV	95383	161173	12.80%	1.614%
2	2.611	233	239	250	rVB	39658	76991	6.12%	0.771%
3	2.928	285	291	299	rVB2	26051	50968	4.05%	0.510%
4	5.153	645	656	677	rBV	339035	996524	79.16%	9.980%
5	5.501	702	713	727	rBV2	176519	500961	39.80%	5.017%
6	5.659	728	739	757	rVB2	256479	715526	56.84%	7.166%
7	6.068	795	806	828	rBV2	178353	458461	36.42%	4.591%
8	6.860	925	936	951	rBV	344890	801643	63.68%	8.028%
9	8.713	1233	1240	1250	rBV	804603	1258823	100.00%	12.606%
10	10.116	1464	1470	1480	rBV	687134	942088	74.84%	9.434%
11	11.140	1632	1638	1652	rBV	700824	874956	69.51%	8.762%
12	12.079	1787	1792	1799	rBV	1006366	1213107	96.37%	12.149%
13	12.274	1819	1824	1827	rBV	10761	13422	1.07%	0.134%
14	12.822	1910	1914	1917	rBV2	11288	13192	1.05%	0.132%
15	13.834	2076	2080	2086	rVB	10591	16426	1.30%	0.164%
16	14.090	2119	2122	2127	rVB3	13123	15651	1.24%	0.157%
17	14.176	2131	2136	2141	rBV	385799	469221	37.27%	4.699%
18	14.286	2149	2154	2166	rVB9	14229	34219	2.72%	0.343%
19	14.426	2172	2177	2183	rBV3	54553	71043	5.64%	0.711%
20	14.542	2192	2196	2200	rBV2	10589	14341	1.14%	0.144%
21	14.590	2200	2204	2210	rVV5	9382	13253	1.05%	0.133%
22	14.670	2213	2217	2220	rVV2	18675	30277	2.41%	0.303%
23	14.834	2240	2244	2248	rBV3	10335	14795	1.18%	0.148%
24	15.145	2286	2295	2299	rBV	41243	63781	5.07%	0.639%
25	15.212	2299	2306	2320	rVV	393856	612743	48.68%	6.136%
26	15.334	2321	2326	2333	rVB	16414	32423	2.58%	0.325%
27	15.883	2411	2416	2421	rBV4	9648	17827	1.42%	0.179%
28	16.736	2546	2556	2564	rBV	233731	501750	39.86%	5.025%

Sum of corrected areas: 9985585

LSC Report - Integrated Chromatogram

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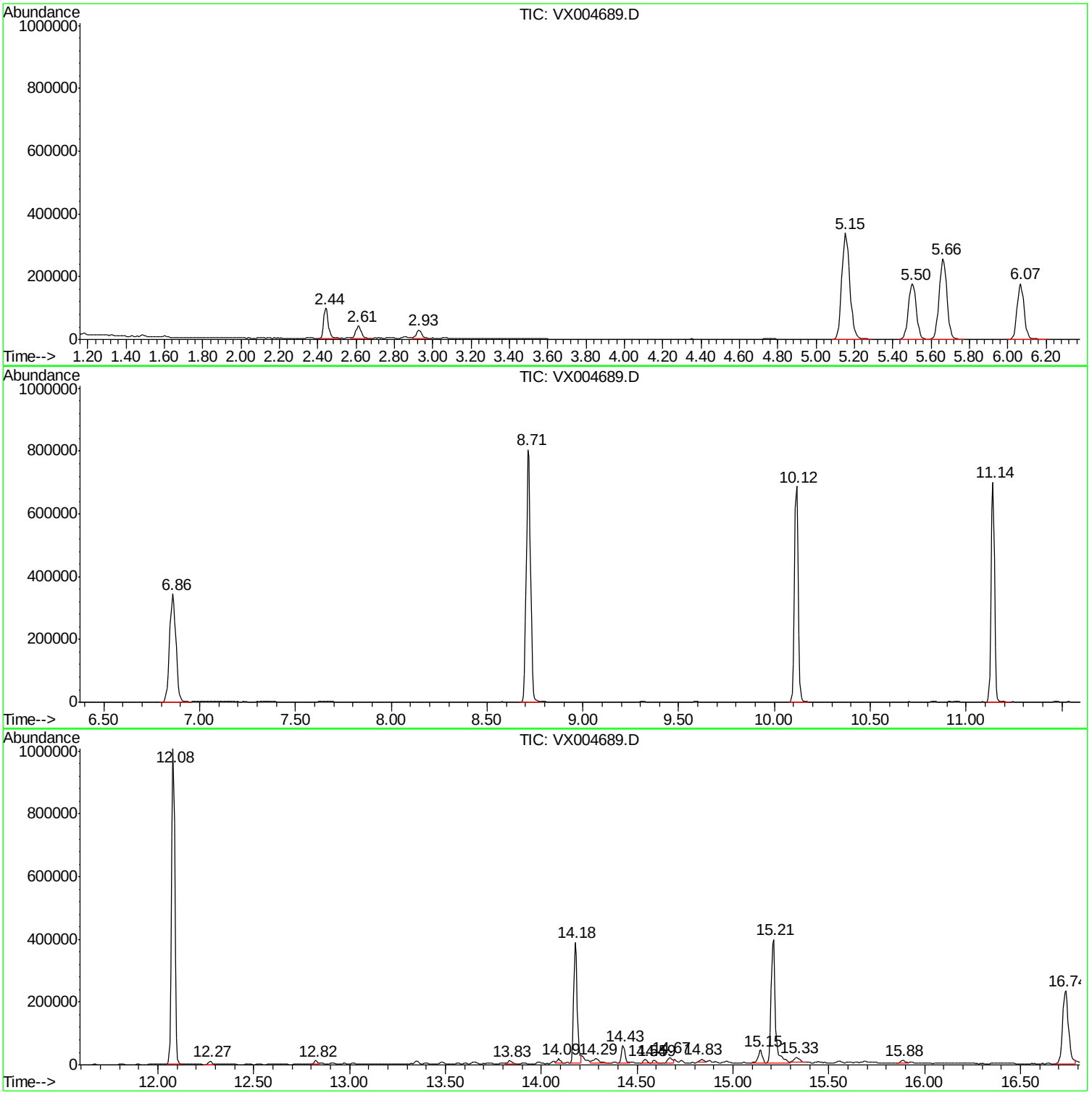
ClientSampleId : N48966

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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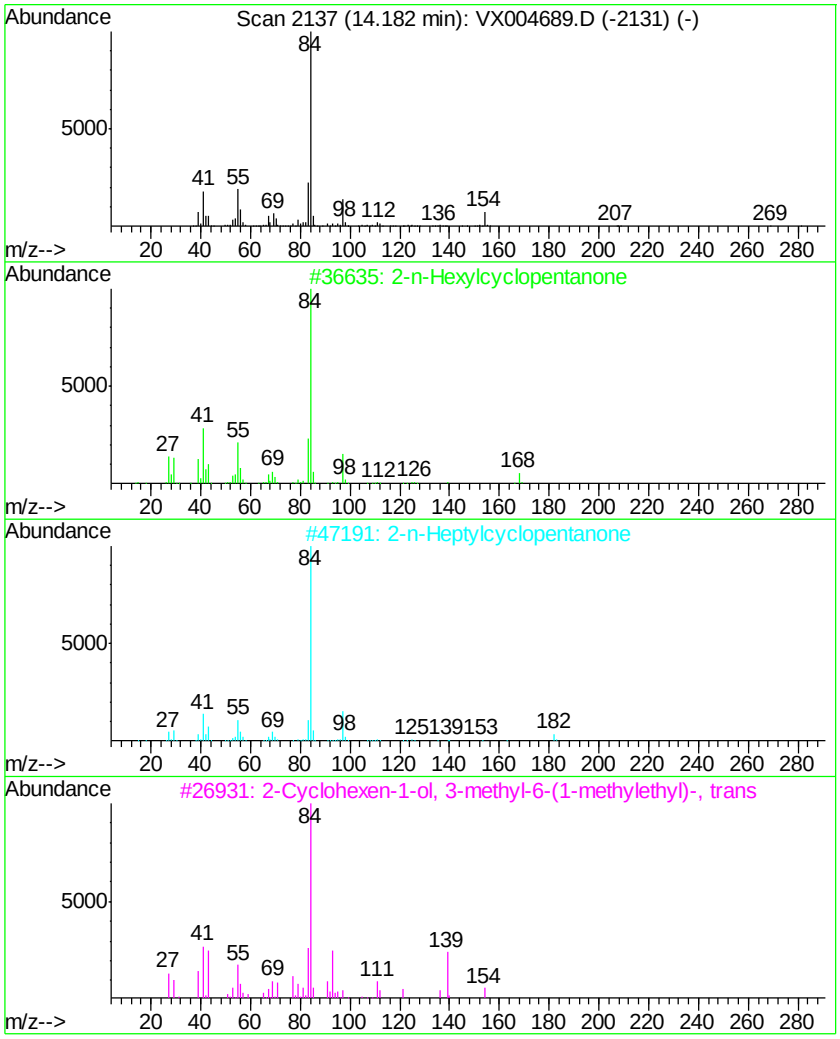
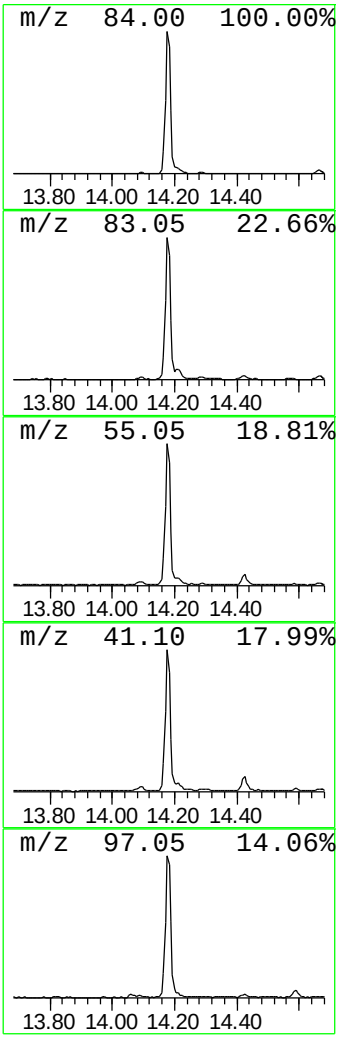
Peak Number 1 2-n-Hexylcyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	19.34 ug/l	469221	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-n-Hexylcyclopentanone	168	C11H20O	013074-65-2	78
2	2-n-Heptylcyclopentanone	182	C12H22O	000137-03-1	72
3	2-Cyclohexen-1-ol, 3-methyl-6-(1...	154	C10H18O	016721-39-4	64
4	2-Pentylcyclopentanone	154	C10H18O	1000191-05-3	64
5	Cyclopentanone, 2-octyl-	196	C13H24O	040566-23-2	59





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ALS Vial : 48 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : N48966

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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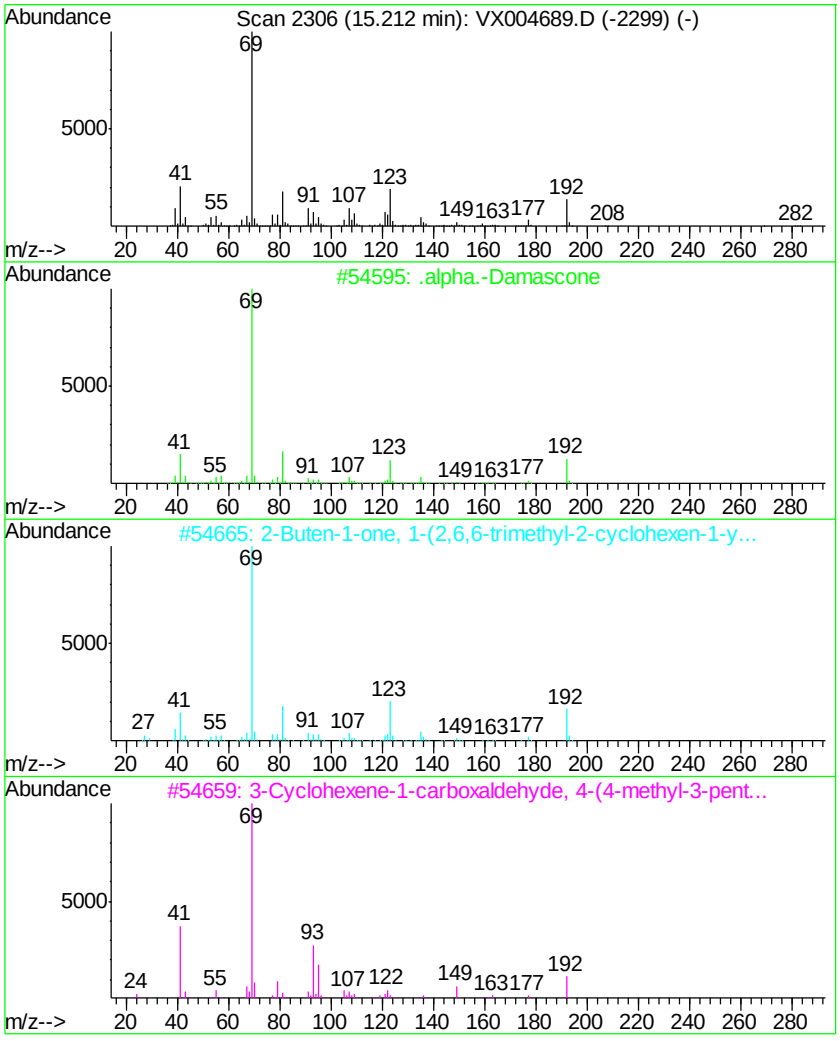
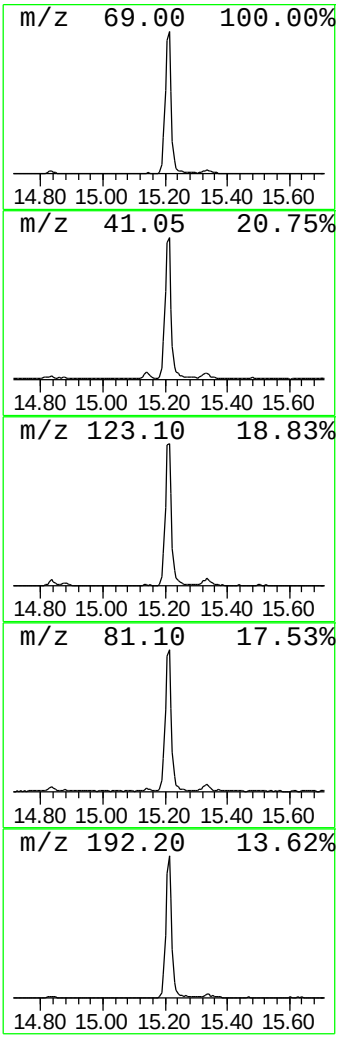
Peak Number 2 .alpha.-Damascone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	25.26 ug/l	612743	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Damascone	192	C13H20O	031089-90-4	90
2	2-Buten-1-one, 1-(2,6,6-trimethy...	192	C13H20O	024720-09-0	87
3	3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	037677-14-8	59
4	2-Buten-1-one, 1-(2,6,6-trimethy...	192	C13H20O	041436-42-4	56
5	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	47





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ALS Vial : 48 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : N48966

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

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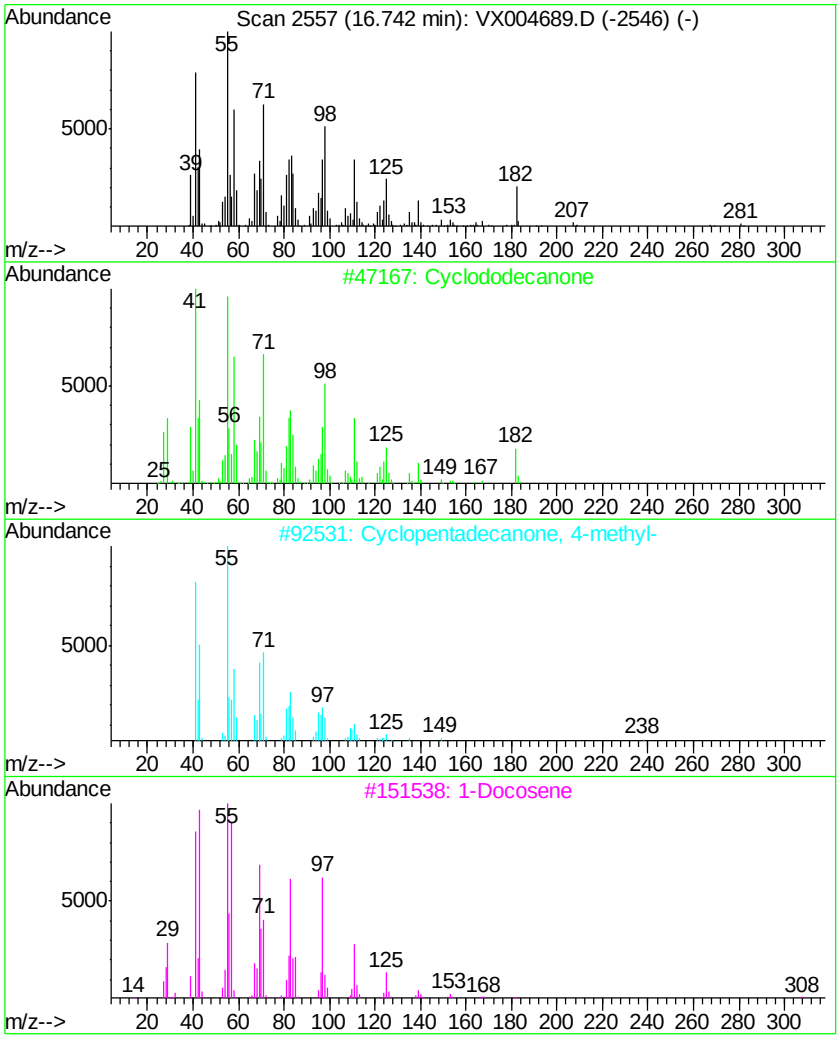
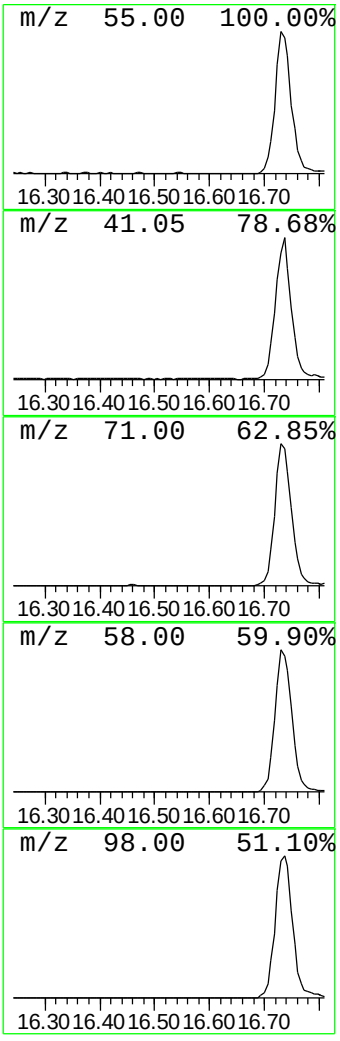
Peak Number 3 Cyclododecanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.74	20.68 ug/l	501750	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecanone	182	C12H22O	000830-13-7	99
2	Cyclopentadecanone, 4-methyl-	238	C16H30O	034894-60-5	47
3	1-Docosene	308	C22H44	001599-67-3	38
4	Cyclooctanone	126	C8H14O	000502-49-8	25
5	Cyclotridecane	182	C13H26	000295-02-3	22





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-n-Hexylcyclopen...	14.18	19.3	ug/l	469221	4	12.08	1213110	50.0
.alpha.-Damascone	15.21	25.3	ug/l	612743	4	12.08	1213110	50.0
Cyclododecanone	16.74	20.7	ug/l	501750	4	12.08	1213110	50.0