

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031225\
 Data File : VN085963.D
 Acq On : 12 Mar 2025 16:30
 Operator : JC\MD
 Sample : Q1528-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 22425

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\82N021825W.M
 Title : SW846 8260

Signal : TIC: VN085963.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	18	22	29	rVB3	8106	10935	1.26%	0.145%
2	2.295	54	58	66	rVB	11448	18583	2.14%	0.247%
3	2.665	115	121	130	rVB2	4523	9254	1.06%	0.123%
4	2.812	140	146	155	rVB6	7190	16574	1.91%	0.220%
5	3.789	303	312	330	rBV	78488	207358	23.84%	2.757%
6	4.424	409	420	438	rBV	145855	436855	50.24%	5.809%
7	4.712	460	469	470	rBV	10877	20277	2.33%	0.270%
8	5.030	515	523	531	rBV2	3861	10800	1.24%	0.144%
9	7.230	886	897	905	rBV4	13434	40172	4.62%	0.534%
10	8.165	1046	1056	1060	rBV2	140030	313829	36.09%	4.173%
11	8.224	1060	1066	1082	rVB	227788	521217	59.94%	6.930%
12	8.577	1112	1126	1139	rBV2	150457	439092	50.49%	5.838%
13	8.777	1152	1160	1163	rBV3	7586	19281	2.22%	0.256%
14	9.100	1205	1215	1232	rBV	343274	706640	81.26%	9.396%
15	9.271	1236	1244	1254	rVB2	4678	10544	1.21%	0.140%
16	10.565	1456	1464	1470	rBV	472224	869614	100.00%	11.563%
17	10.629	1470	1475	1489	rVB	312596	561482	64.57%	7.466%
18	11.300	1582	1589	1594	rBV2	14003	25689	2.95%	0.342%
19	11.865	1676	1685	1697	rBV	473136	829929	95.44%	11.035%
20	12.065	1712	1719	1729	rVB	113475	215717	24.81%	2.868%
21	12.394	1766	1775	1782	rBV2	54597	111502	12.82%	1.483%
22	12.847	1844	1852	1862	rBV	361765	608422	69.96%	8.090%
23	13.088	1888	1893	1898	rBV5	6601	13531	1.56%	0.180%
24	13.482	1955	1960	1965	rBV3	15587	24416	2.81%	0.325%
25	13.788	2004	2012	2020	rBV	440519	754642	86.78%	10.034%
26	13.870	2020	2026	2036	rVV	312764	509246	58.56%	6.771%
27	15.394	2278	2285	2292	rBV	71624	121531	13.98%	1.616%
28	15.641	2320	2327	2333	rVB	5241	10500	1.21%	0.140%
29	15.817	2350	2357	2363	rVB3	11751	24553	2.82%	0.326%
30	15.935	2370	2377	2383	rVB5	13168	23762	2.73%	0.316%
31	16.111	2398	2407	2413	rBV2	18367	34760	4.00%	0.462%

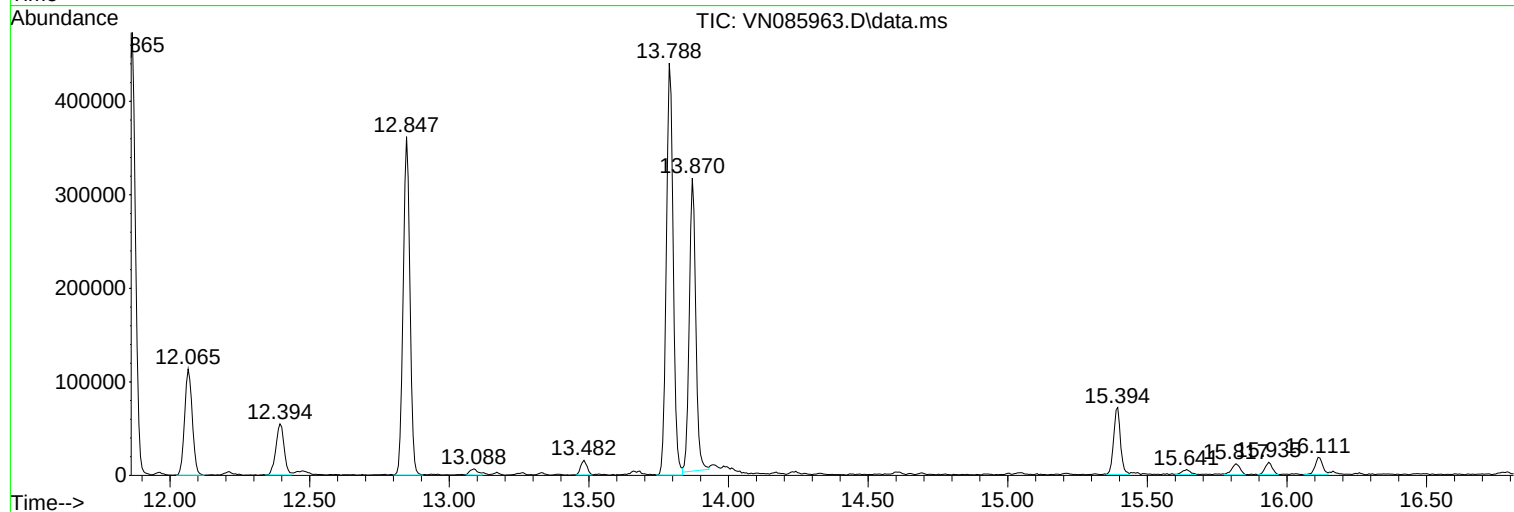
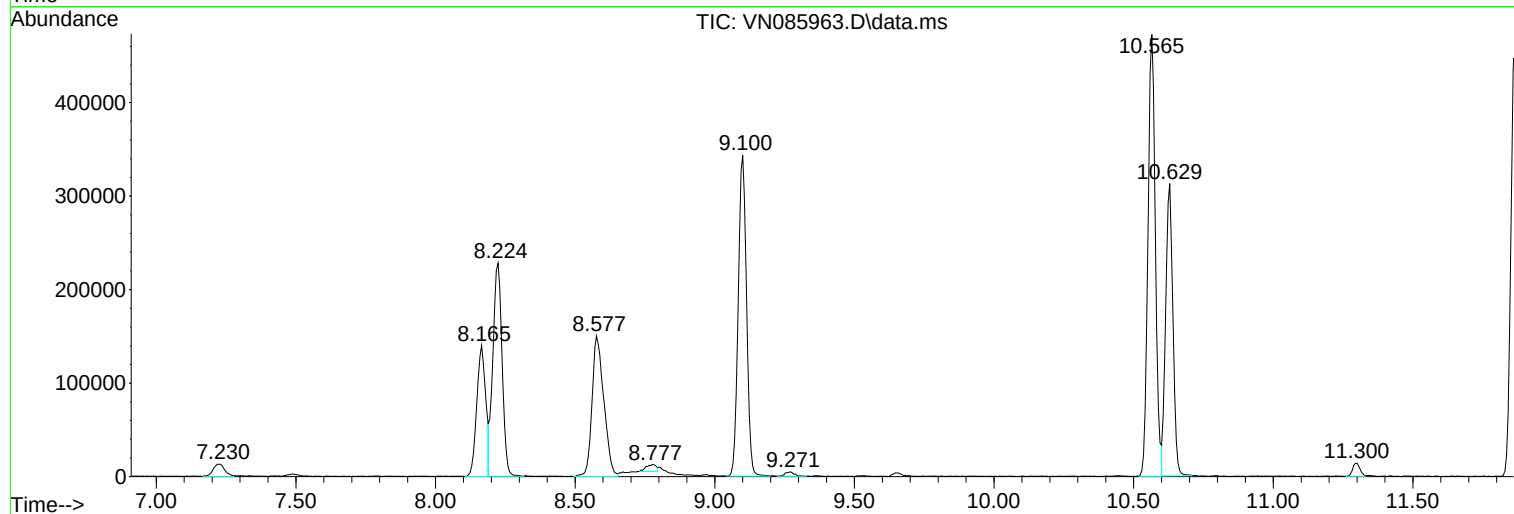
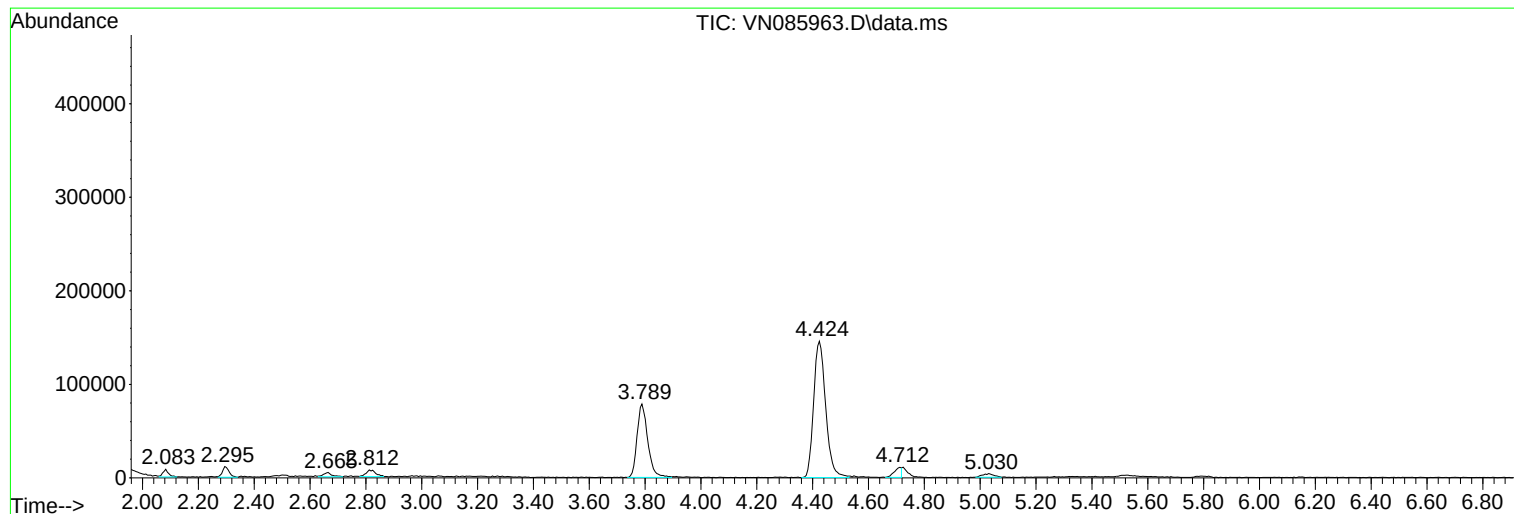
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021825W.M
Quant Title : SW846 8260

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



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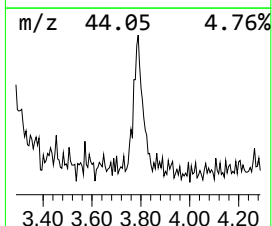
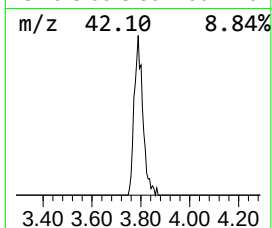
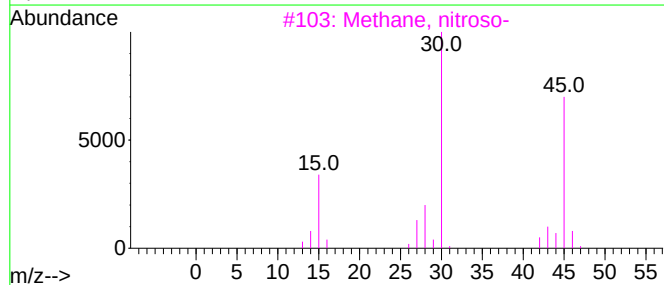
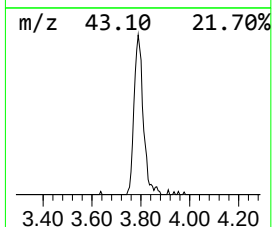
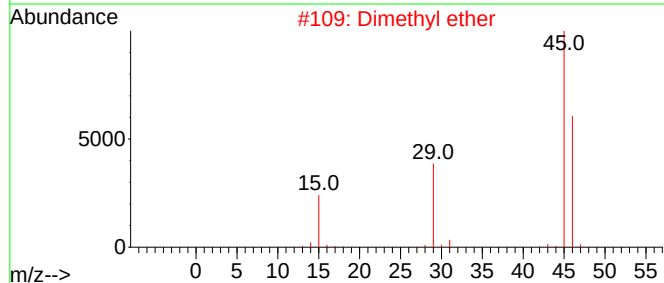
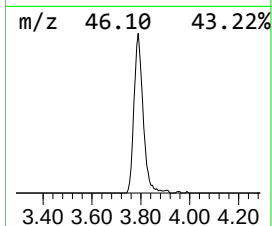
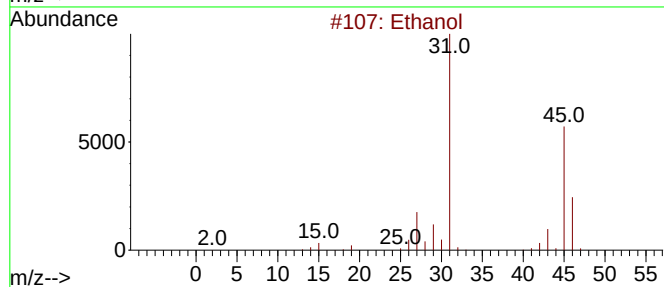
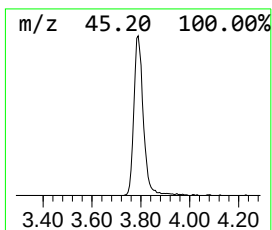
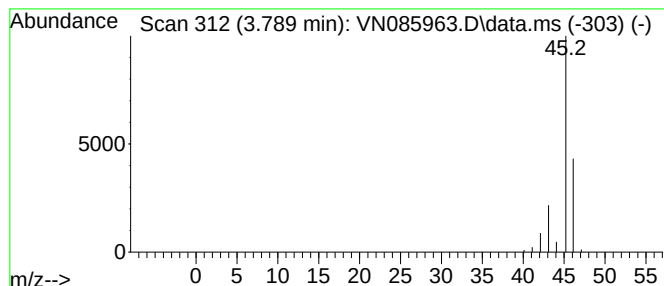
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021825W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.789	19.89 ug/l	207358	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	74
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	Formic acid			46	CH2O2	000064-18-6	4
5	Oxalic acid			90	C2H2O4	000144-62-7	4



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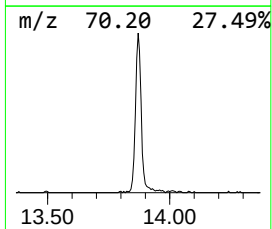
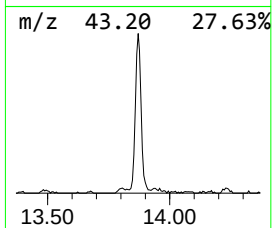
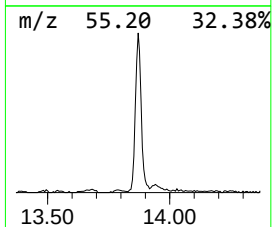
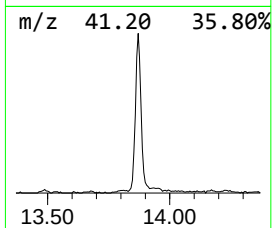
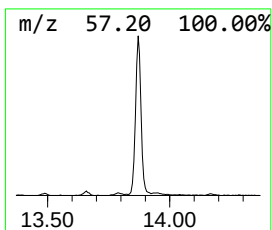
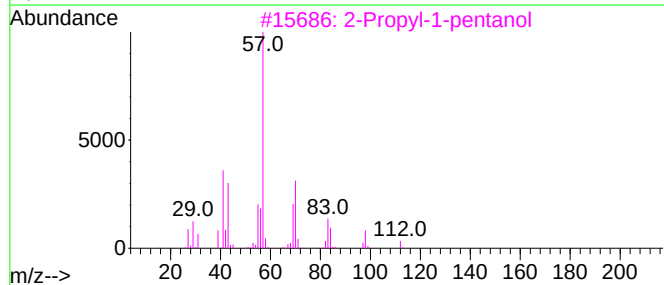
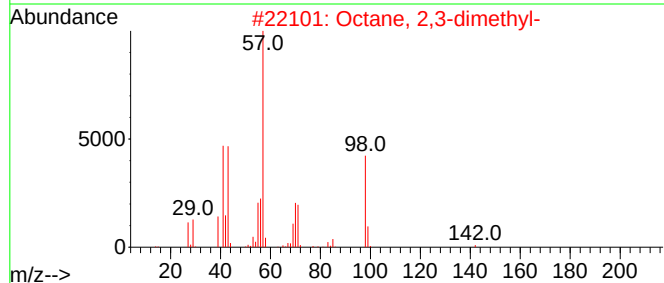
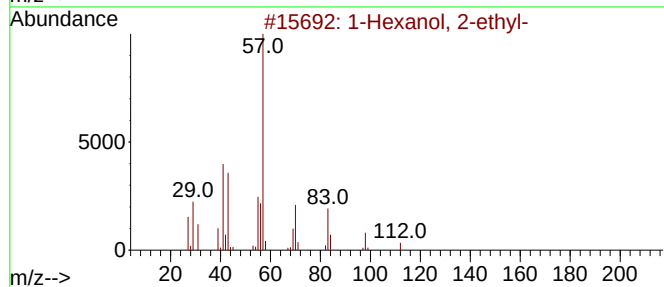
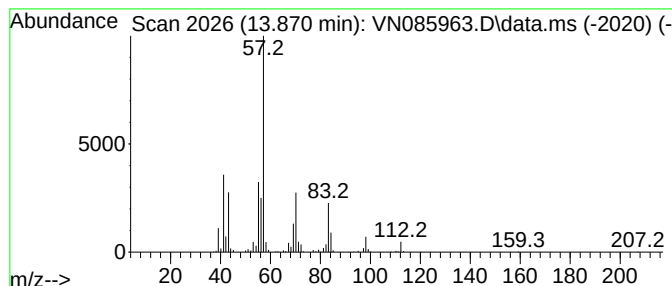
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.870	33.74 ug/l	509246	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	43
5			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	42



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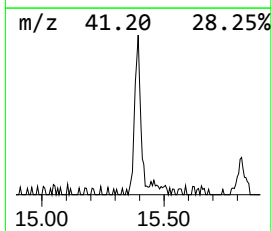
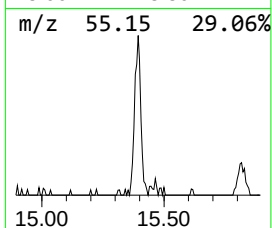
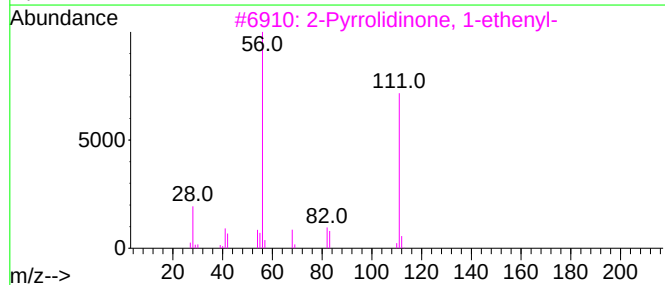
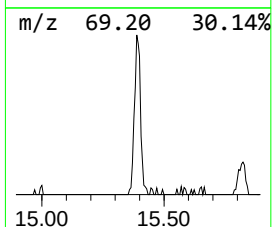
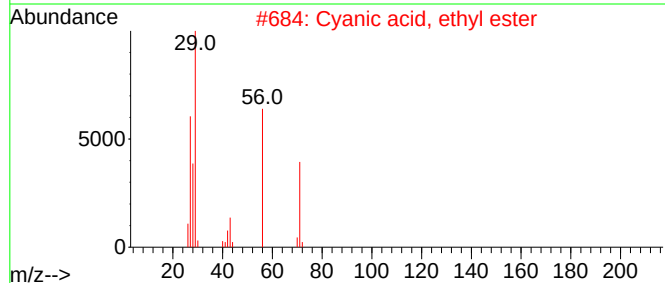
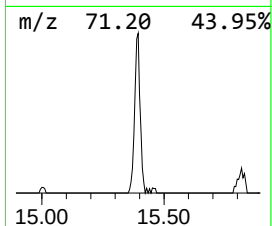
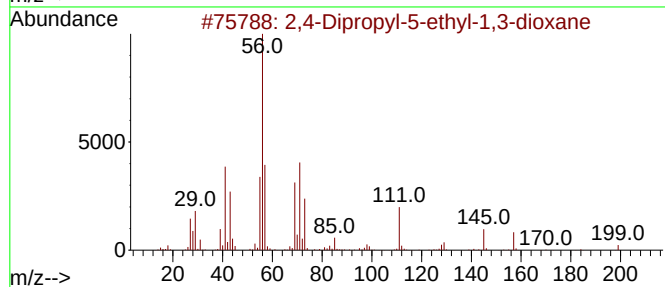
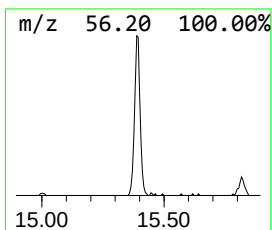
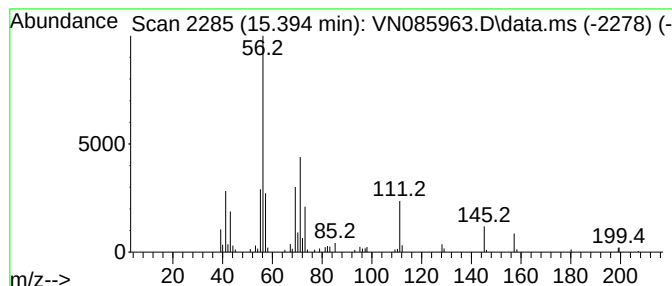
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.394	8.05 ug/l	121531	1,4-Dichlorobenzene-d4	13.788

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	83
2		Cyanoic acid, ethyl ester	71	C3H5NO	000627-48-5	49
3		2-Pyrrolidinone, 1-ethenyl-	111	C6H9NO	000088-12-0	38
4		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38
5		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27



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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
Ethanol	3.789	19.9	ug/l	207358	1	8.224	521217	50.0
1-Hexanol, 2-et...	13.870	33.7	ug/l	509246	4	13.788	754642	50.0
2,4-Dipropyl-5-...	15.394	8.1	ug/l	121531	4	13.788	754642	50.0