

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041224\
 Data File : VN081729.D
 Acq On : 12 Apr 2024 19:43
 Operator : JC\MD
 Sample : P2076-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 240410075-02-VOA

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\82N031824W.M
 Title : SW846 8260

Signal : TIC: VN081729.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.148	29	33	39	rVB2	18922	31102	1.79%	0.364%
2	2.301	55	59	67	rVB4	10603	23466	1.35%	0.275%
3	2.489	84	91	95	rBV4	18275	35574	2.05%	0.417%
4	2.812	139	146	152	rBV2	23459	46336	2.67%	0.543%
5	3.965	329	342	349	rVB4	11927	31466	1.81%	0.369%
6	5.506	593	604	605	rBV3	22710	42168	2.43%	0.494%
7	7.430	918	931	940	rBV2	65096	181274	10.44%	2.124%
8	7.841	990	1001	1015	rBV2	93660	234591	13.50%	2.748%
9	8.165	1044	1056	1061	rBV2	94958	222628	12.82%	2.608%
10	8.224	1061	1066	1080	rVB	185209	418139	24.07%	4.899%
11	8.577	1117	1126	1137	rBV	106330	239730	13.80%	2.808%
12	8.682	1137	1144	1145	rBV	18321	31781	1.83%	0.372%
13	9.100	1207	1215	1229	rBV	292731	597533	34.40%	7.000%
14	10.571	1457	1465	1473	rBV	380621	697865	40.17%	8.176%
15	11.171	1559	1567	1573	rBV	25407	48940	2.82%	0.573%
16	11.312	1583	1591	1600	rBV3	14812	34695	2.00%	0.406%
17	11.871	1675	1686	1695	rBV	888242	1717808	98.89%	20.124%
18	12.071	1712	1720	1731	rVB2	68026	147115	8.47%	1.723%
19	12.400	1770	1776	1782	rBV	65451	114852	6.61%	1.346%
20	12.700	1821	1827	1831	rVB3	16103	25223	1.45%	0.295%
21	12.853	1846	1853	1861	rVB	574945	963489	55.47%	11.287%
22	13.129	1896	1900	1904	rVV5	15555	27037	1.56%	0.317%
23	13.170	1904	1907	1918	rVB3	13448	24400	1.40%	0.286%
24	13.335	1928	1935	1940	rBV3	16759	30046	1.73%	0.352%
25	13.482	1950	1960	1967	rBV3	47496	91470	5.27%	1.072%
26	13.612	1976	1982	1988	rBV6	27588	53620	3.09%	0.628%
27	13.729	1995	2002	2006	rVB5	18043	28757	1.66%	0.337%
28	13.794	2006	2013	2023	rBV2	897087	1737101	100.00%	20.350%
29	13.953	2035	2040	2043	rBV4	12530	18449	1.06%	0.216%
30	14.000	2043	2048	2061	rVB3	39086	90716	5.22%	1.063%
31	14.112	2061	2067	2073	rBV8	15714	28877	1.66%	0.338%
32	14.182	2073	2079	2085	rBV8	9905	21160	1.22%	0.248%
33	14.335	2099	2105	2111	rVB3	17734	30610	1.76%	0.359%
34	14.447	2114	2124	2131	rVV7	21930	50717	2.92%	0.594%
35	14.676	2152	2163	2177	rBV3	65235	170990	9.84%	2.003%
36	15.029	2217	2223	2232	rBV9	22454	55737	3.21%	0.653%

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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

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37	15.206	2249	2253	2258	rVB7	12286	21113	1.22%	0.247%
38	15.282	2260	2266	2275	rBV10	18048	49981	2.88%	0.586%
39	15.641	2321	2327	2336	rVB	60862	119368	6.87%	1.398%

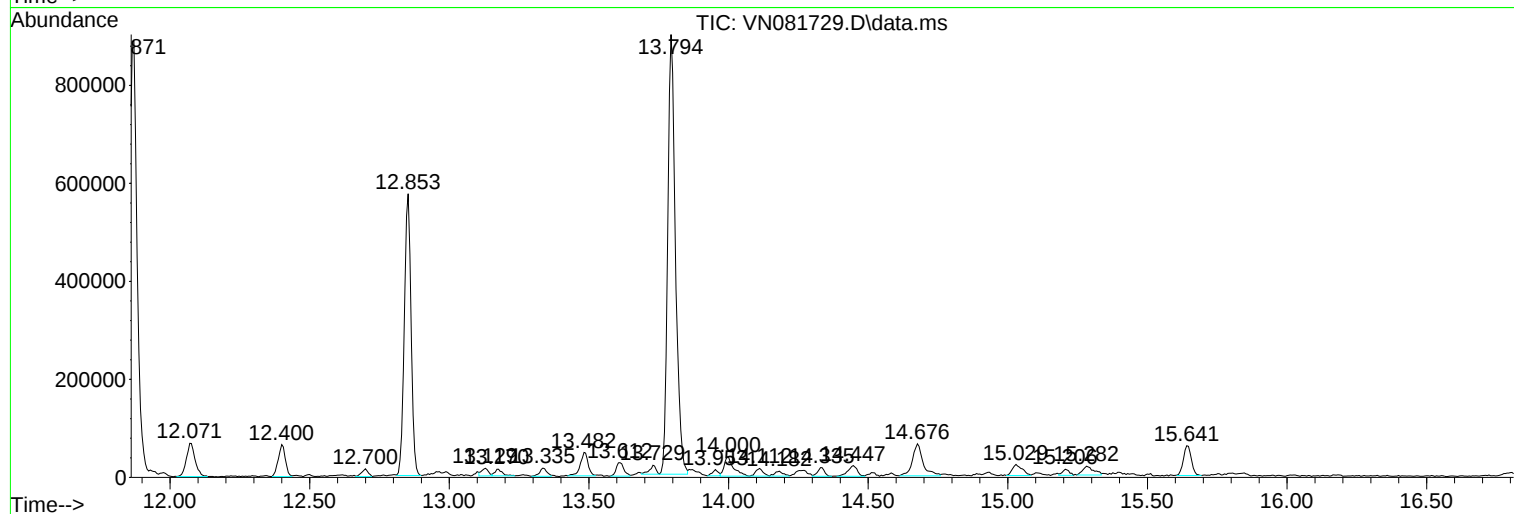
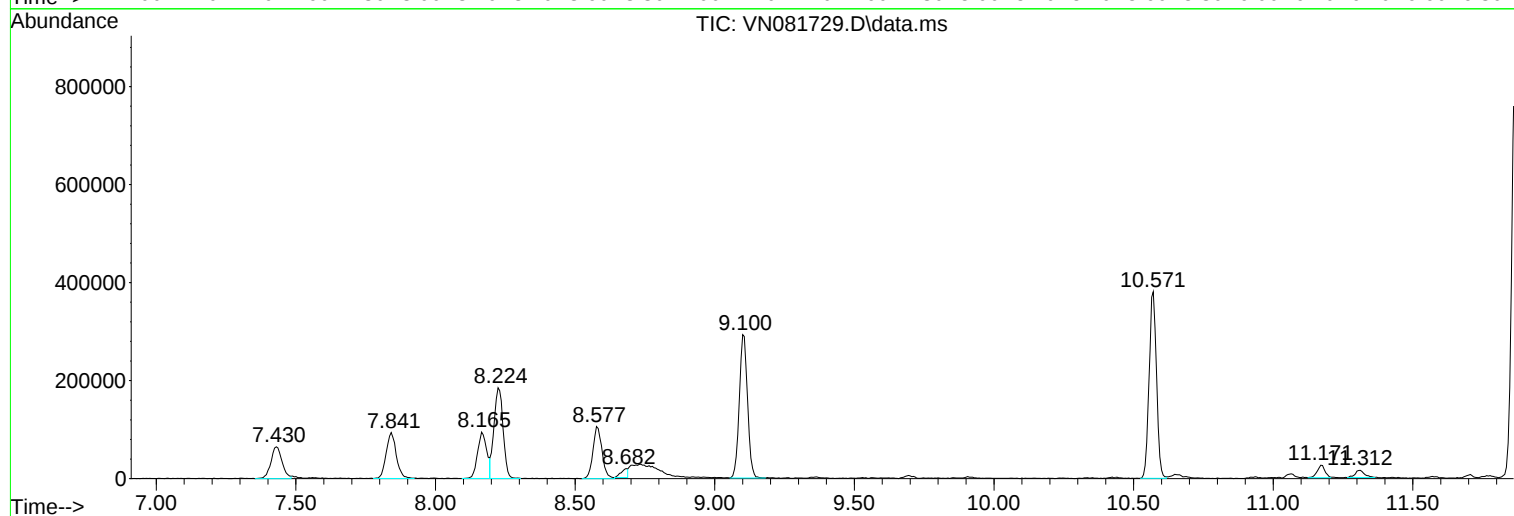
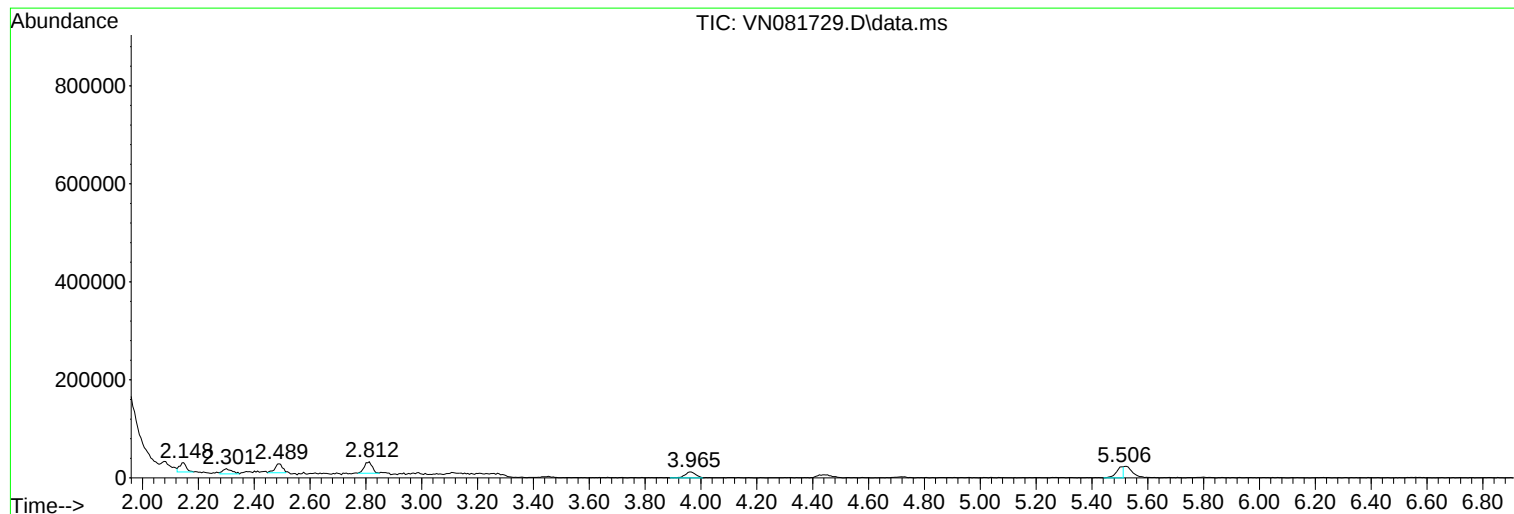
Sum of corrected areas: 8535924

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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



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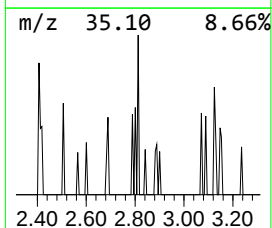
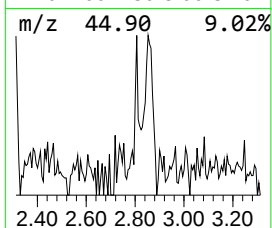
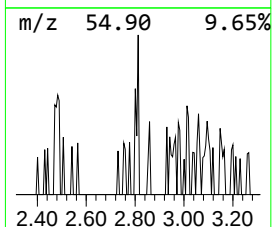
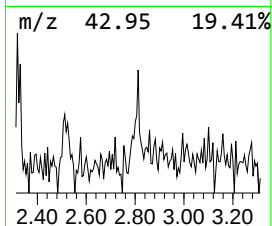
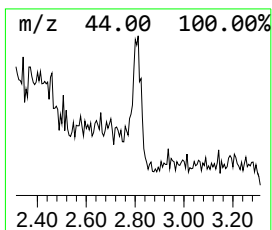
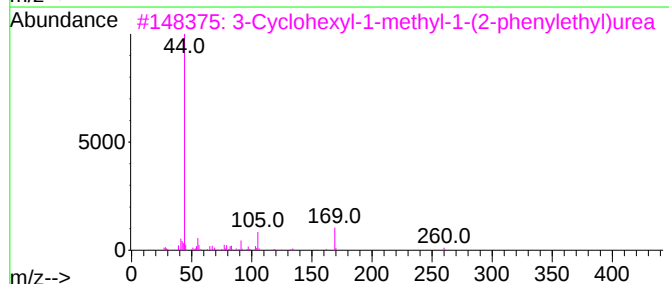
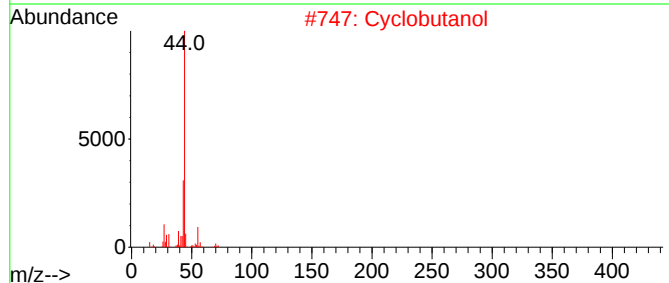
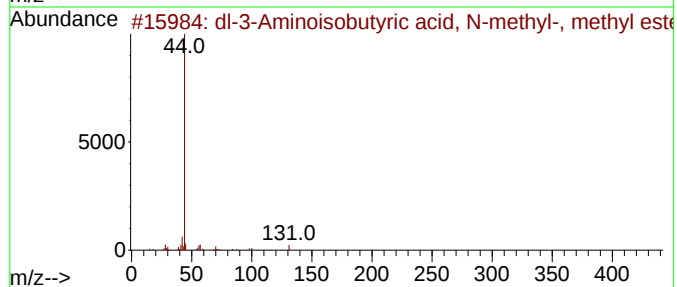
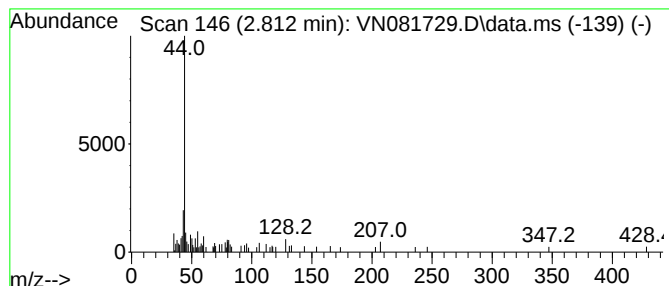
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Peak Number 1 unknown2.812 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.812	5.54 ug/l	46336	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			dl-3-Aminoisobutyric acid, N-met...	131	C6H13NO2	1000332-87-9	42
2			Cyclobutanol	72	C4H8O	002919-23-5	42
3			3-Cyclohexyl-1-methyl-1-(2-pheny...	260	C16H24N2O	1024470-80-1	42
4			Imidazole, 2-amino-5-[(2-carboxy...	153	C6H7N3O2	1000116-74-7	38
5			1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	36



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.812	2.812	5.5	ug/l	46336	1	8.230	418139	50.0