

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081023\
 Data File : VX036915.D
 Acq On : 10 Aug 2023 16:06
 Operator : JC/MD
 Sample : 03955-22
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TW-1

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\82X072123W.M
 Title : SW846 8260

Signal : TIC: VX036915.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.575	70	80	82	rBV4	2927	7870	1.16%	0.196%
2	2.782	270	278	290	rVB	20140	42761	6.30%	1.067%
3	4.215	500	513	524	rVB3	4845	14247	2.10%	0.356%
4	5.391	694	706	721	rBV	77844	230252	33.90%	5.748%
5	5.550	721	732	757	rVB	124185	386387	56.89%	9.645%
6	5.958	789	799	815	rBV	84110	224191	33.01%	5.596%
7	6.245	835	846	858	rBV2	44630	132963	19.58%	3.319%
8	6.763	921	931	944	rBV	209861	493368	72.65%	12.316%
9	7.604	1062	1069	1075	rVB2	3663	7872	1.16%	0.197%
10	7.982	1124	1131	1139	rVB	28405	55271	8.14%	1.380%
11	8.104	1143	1151	1161	rVV	23659	47851	7.05%	1.194%
12	8.647	1227	1240	1257	rBV	424252	679144	100.00%	16.953%
13	9.525	1378	1384	1395	rBV2	5251	8337	1.23%	0.208%
14	10.055	1465	1471	1492	rBV	444508	611670	90.06%	15.269%
15	11.079	1634	1639	1653	rBV	370089	470344	69.26%	11.741%
16	12.024	1788	1794	1806	rBV	441148	575637	84.76%	14.369%
17	12.244	1822	1830	1834	rBV	14106	17895	2.63%	0.447%

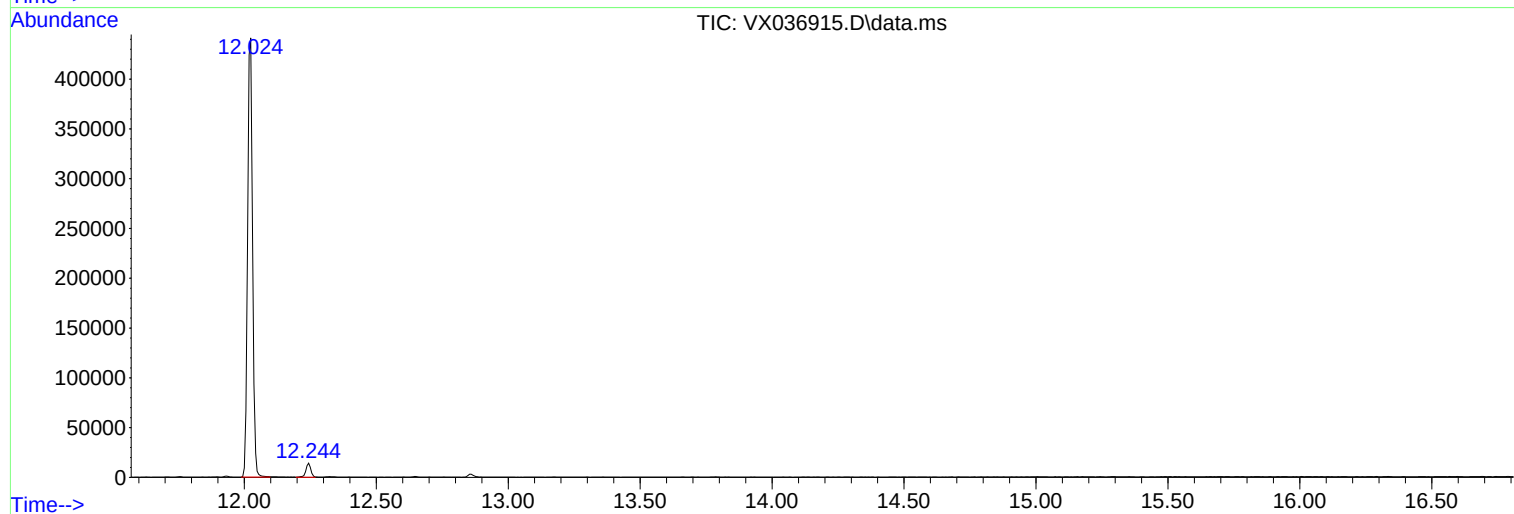
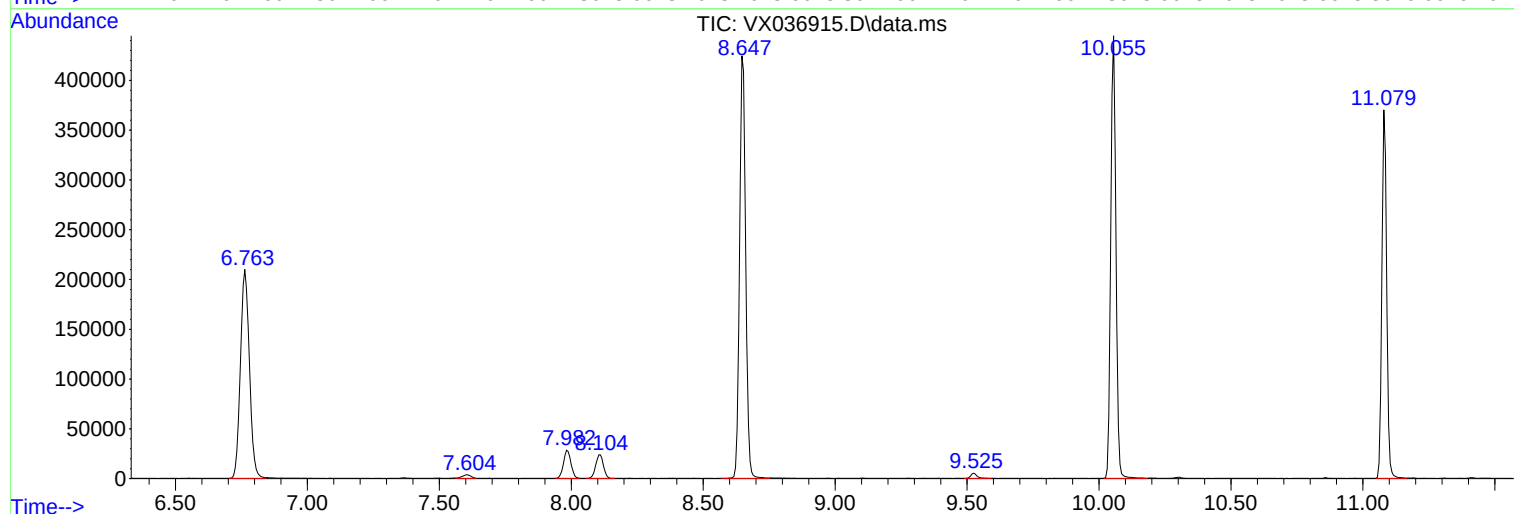
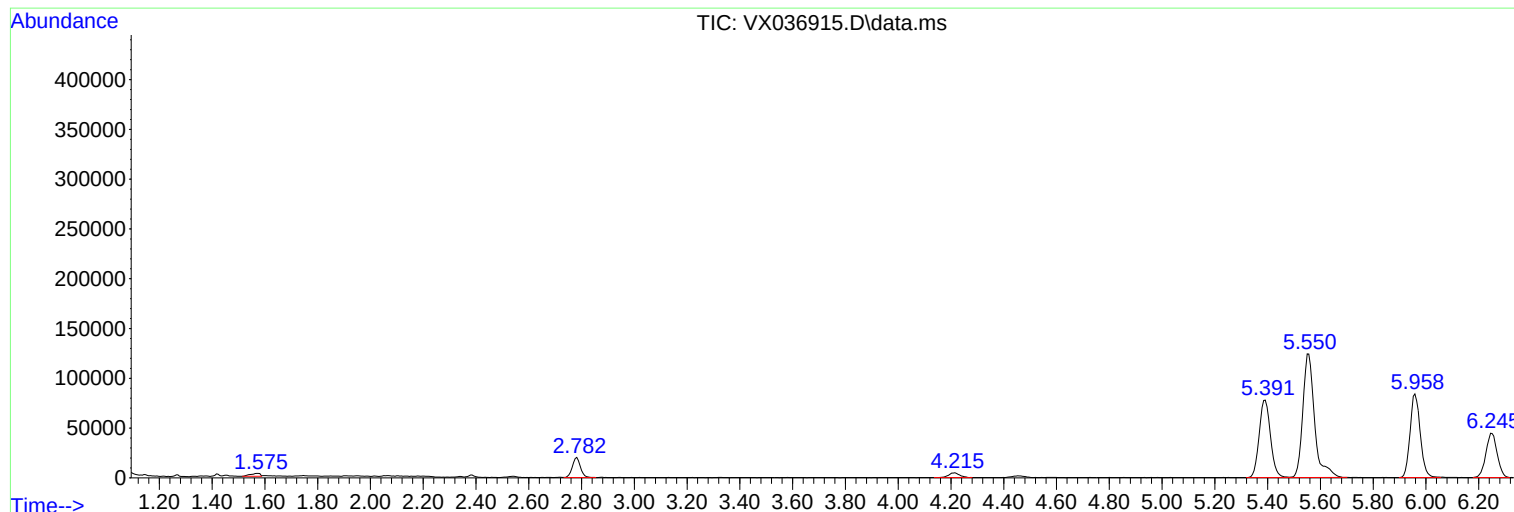
Sum of corrected areas: 4006060

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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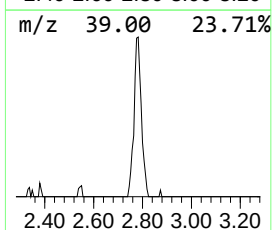
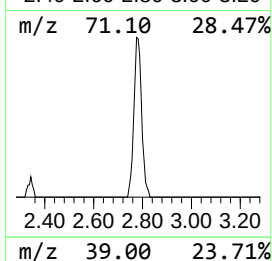
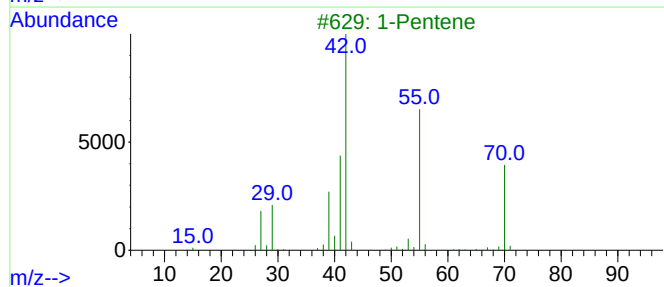
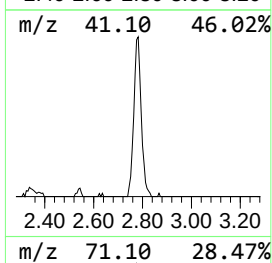
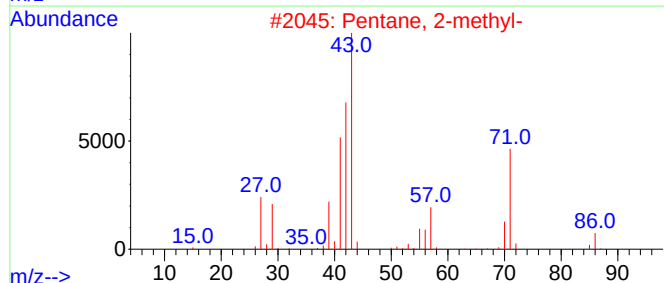
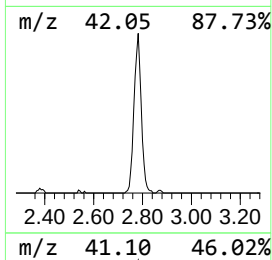
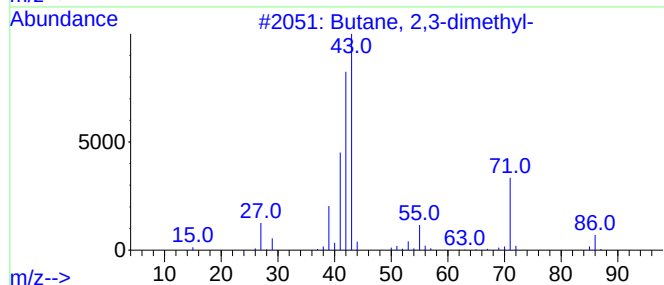
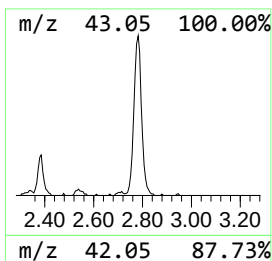
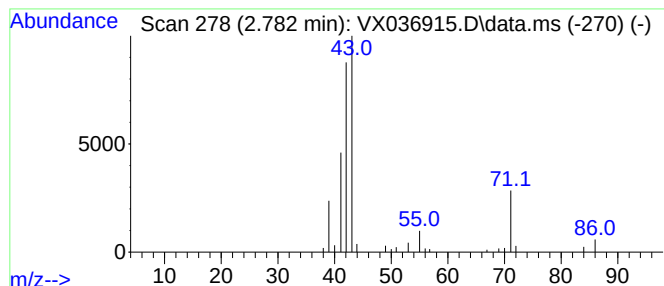
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	5.53 ug/l	42761	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	64
3		1-Pentene	70	C5H10	000109-67-1	28
4		Pyrrolidine	71	C4H9N	000123-75-1	16
5		C2H5C(CH3)2COCH3	114	C7H14O	020669-04-9	12



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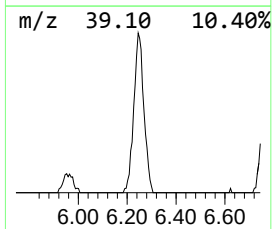
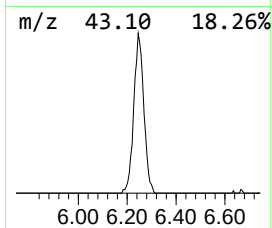
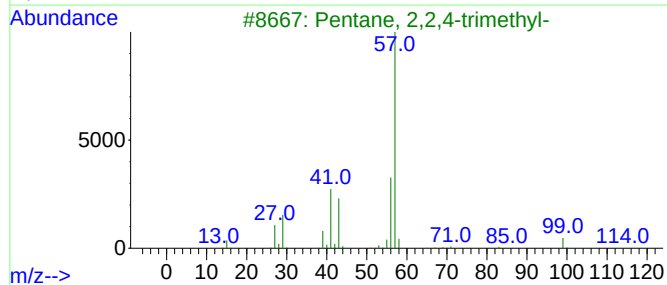
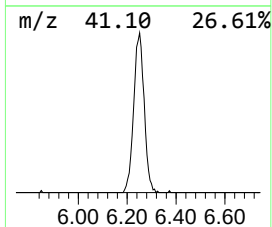
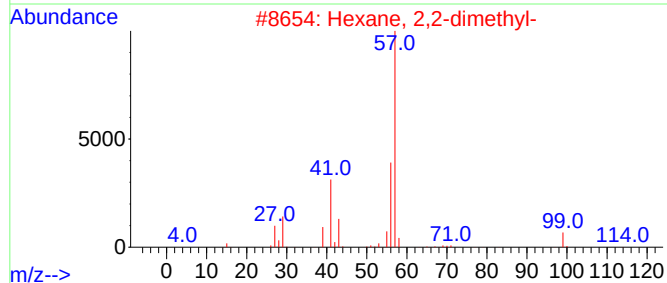
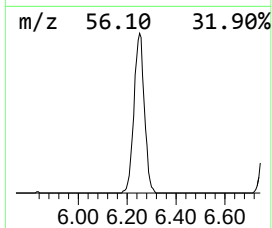
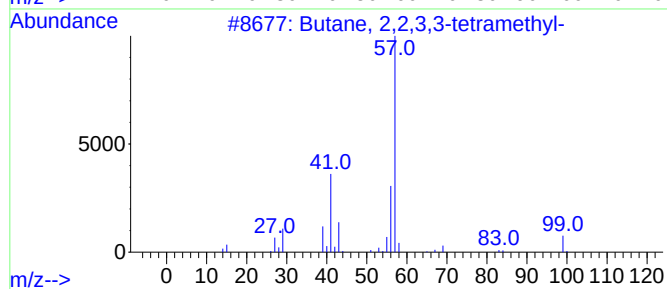
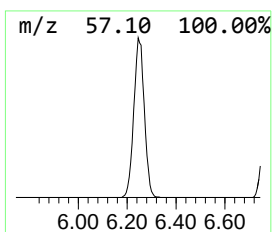
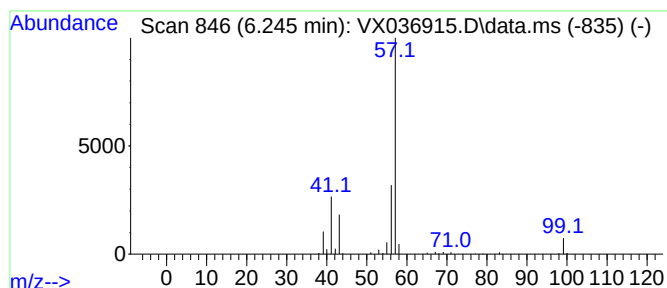
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	13.48 ug/l	132963	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	50



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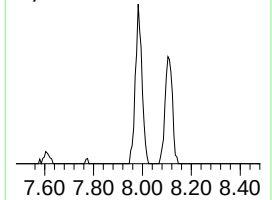
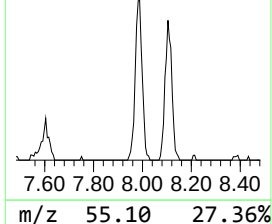
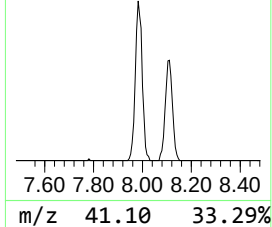
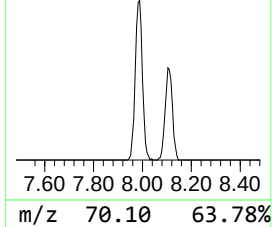
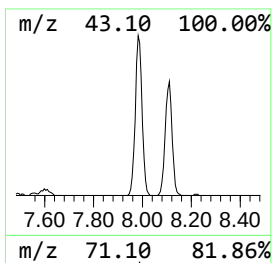
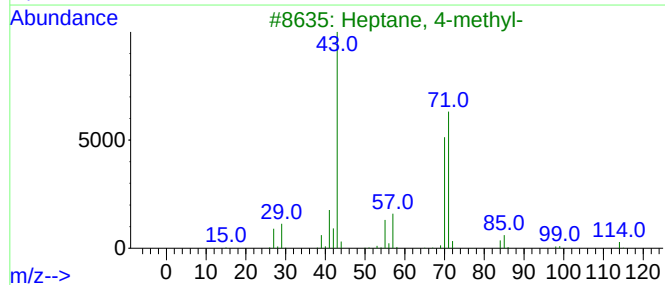
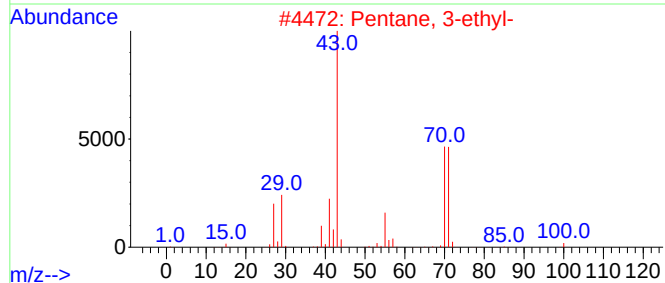
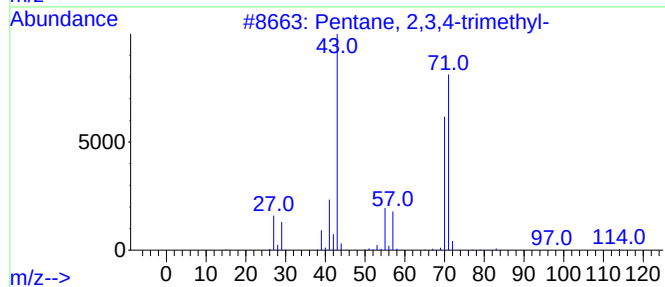
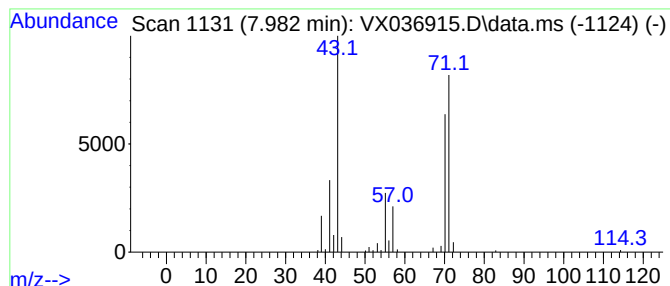
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Peak Number 3 Pentane, 2,3,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.982	5.60 ug/l	55271	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4			3,3-Dimethyl-2-pentanol	116	C7H16O	019781-24-9	78
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	78



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MSVOA_X
ClientSampleId :
TW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
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
Butane, 2,3-dim...	2.782	5.5	ug/l	42761	1	5.556	386387	50.0
Butane, 2,2,3,3...	6.245	13.5	ug/l	132963	2	6.763	493368	50.0
Pentane, 2,3,4-...	7.982	5.6	ug/l	55271	2	6.763	493368	50.0