

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY062723\
 Data File : VY014455.D
 Acq On : 27 Jun 2023 14:02
 Operator : KP/MD
 Sample : 03402-07
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 TP4-0623RE

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_Y\methods\82Y062323S.M

Title : SW846 8260

Signal : TIC: VY014455.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.661	137	138	144	rVB3	898	1062	1.50%	0.219%
2	3.948	345	349	351	rBV4	835	1081	1.53%	0.223%
3	4.210	382	392	399	rBV4	1632	5405	7.65%	1.113%
4	4.716	468	475	483	rBV5	2044	5498	7.78%	1.132%
5	5.752	640	645	646	rBV2	653	720	1.02%	0.148%
6	6.984	837	847	861	rBV2	12868	38933	55.09%	8.019%
7	7.722	959	968	974	rBV3	10997	26458	37.44%	5.450%
8	7.795	974	980	987	rVB2	21114	46166	65.33%	9.509%
9	8.142	1028	1037	1047	rVB2	11768	27572	39.02%	5.679%
10	8.691	1119	1127	1136	rVV	27227	53866	76.23%	11.095%
11	10.185	1364	1372	1379	rBV	39370	70666	100.00%	14.555%
12	10.581	1431	1437	1444	rBV2	4364	7864	11.13%	1.620%
13	10.947	1493	1497	1503	rBV2	3718	6337	8.97%	1.305%
14	11.318	1554	1558	1564	rVB2	2870	4460	6.31%	0.919%
15	11.489	1580	1586	1598	rBV	35113	59814	84.64%	12.320%
16	12.489	1744	1750	1760	rVB3	33918	59098	83.63%	12.173%
17	12.824	1798	1805	1810	rBV4	1466	2435	3.45%	0.502%
18	13.184	1859	1864	1870	rVV4	942	1783	2.52%	0.367%
19	13.428	1897	1904	1912	rBV	31467	49006	69.35%	10.094%
20	13.964	1987	1992	1998	rBV3	1659	2434	3.44%	0.501%
21	14.269	2041	2042	2050	rVB2	605	798	1.13%	0.164%
22	14.489	2074	2078	2082	rVB5	755	1204	1.70%	0.248%
23	14.836	2130	2135	2140	rVB4	370	838	1.19%	0.173%
24	14.940	2149	2152	2156	rVB4	656	789	1.12%	0.163%
25	15.080	2172	2175	2180	rBV3	481	832	1.18%	0.171%
26	15.318	2208	2214	2220	rBV2	4809	7086	10.03%	1.460%
27	15.787	2286	2291	2293	rVB3	534	927	1.31%	0.191%
28	15.976	2319	2322	2325	rBV4	545	804	1.14%	0.166%
29	16.208	2358	2360	2365	rVB3	675	778	1.10%	0.160%
30	16.604	2421	2425	2428	rVV4	526	788	1.12%	0.162%

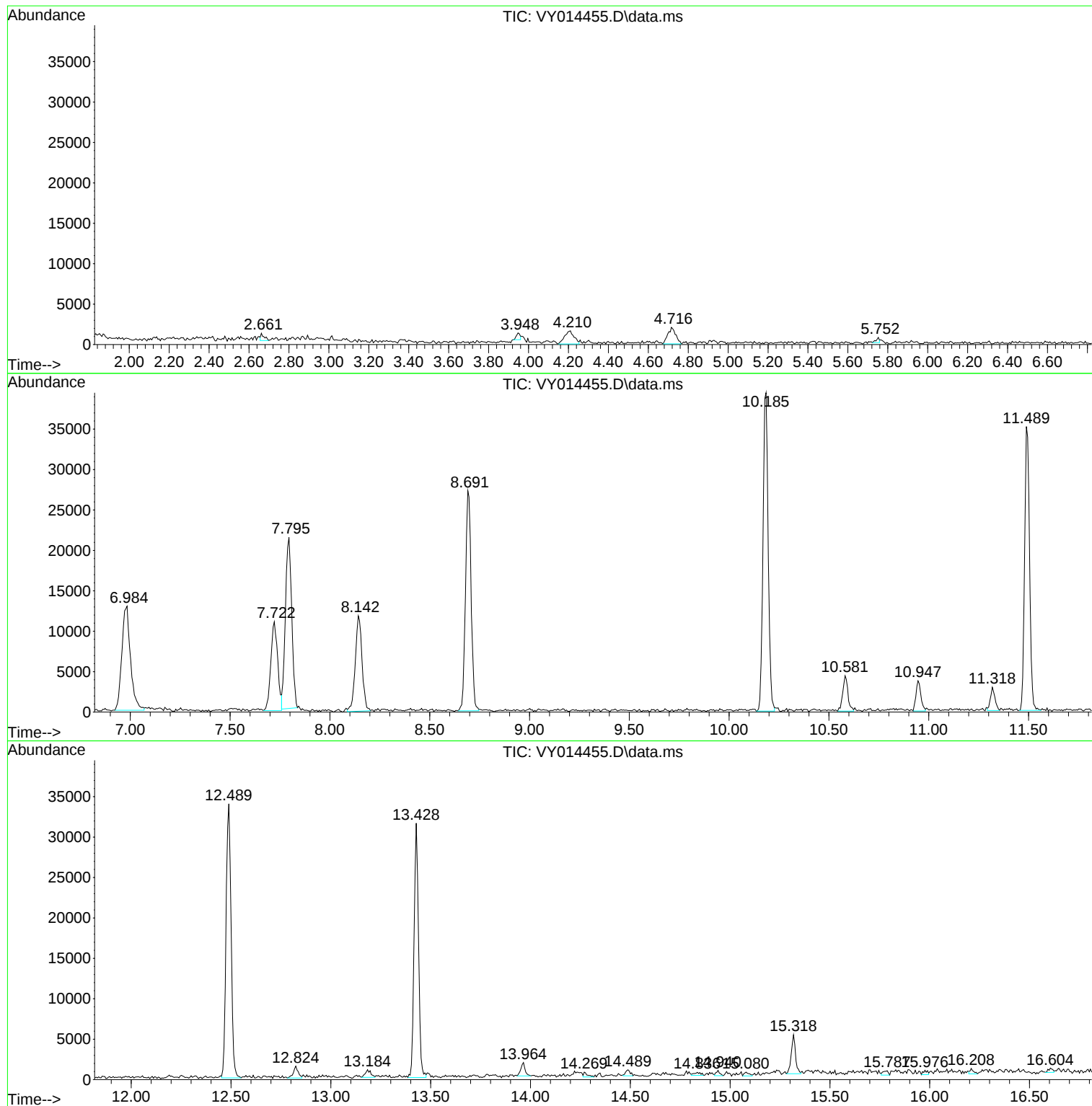
Sum of corrected areas: 485502

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y062323S.M
Quant Title : SW846 8260

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



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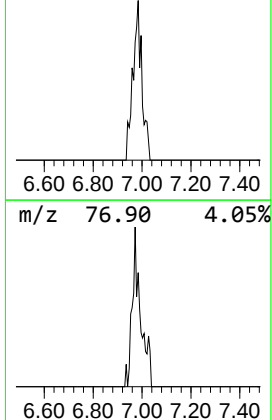
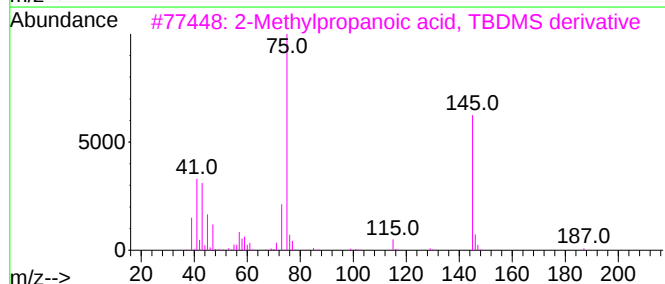
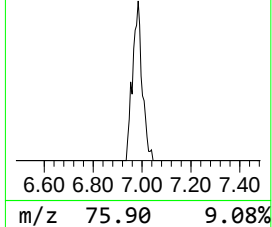
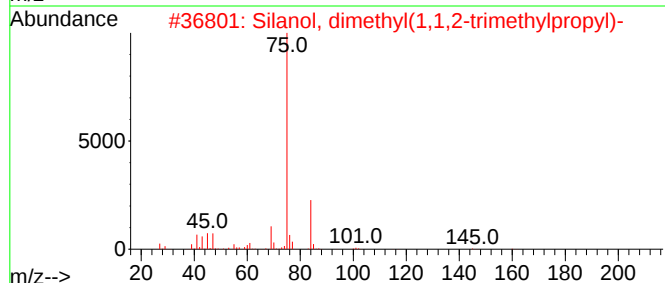
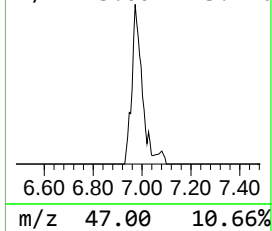
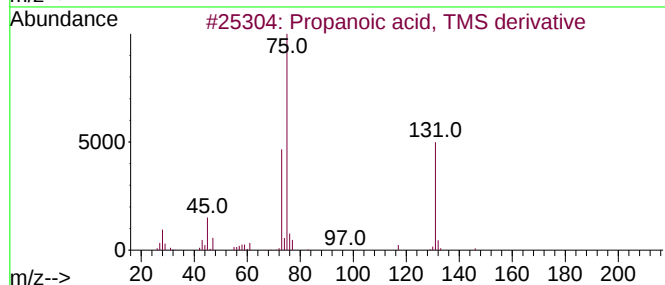
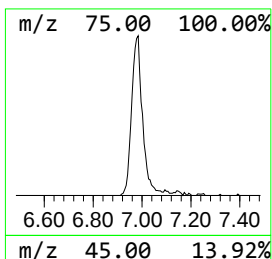
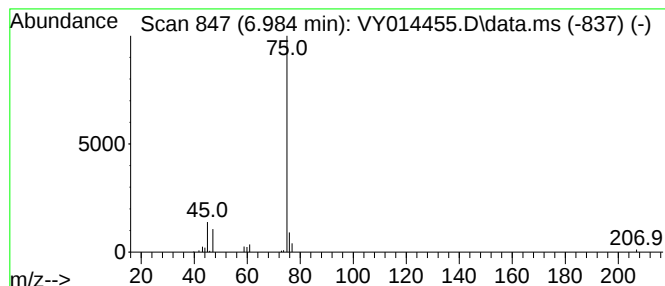
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, TMS derivative Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.984	42.17 ug/l	38933	Pentafluorobenzene	7.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, TMS derivative	146	C6H14O2Si	016844-98-7	83
2			Silanol, dimethyl(1,1,2-trimethylpropyl)-	160	C8H20OSi	055644-10-5	83
3			2-Methylpropanoic acid, TBDMS derivative	202	C10H22O2Si	111864-21-2	74
4			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	64
5			Ethylene glycol, TMS derivative	134	C5H14O2Si	004403-13-8	64



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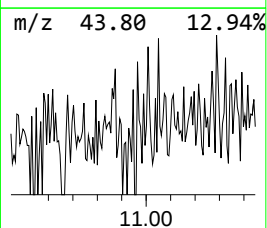
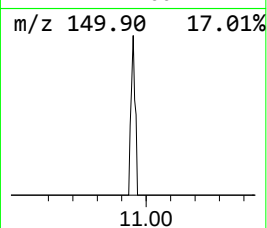
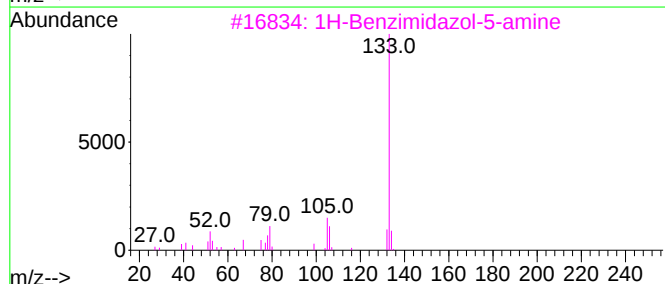
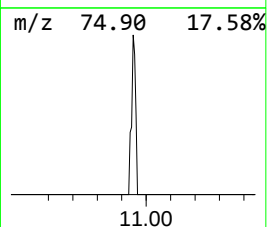
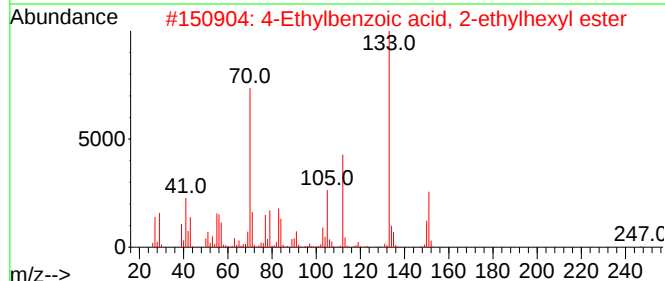
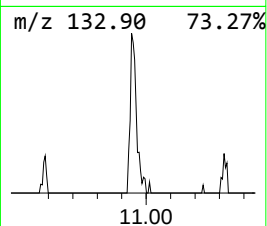
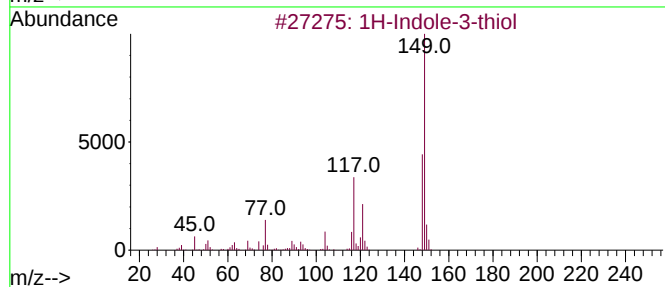
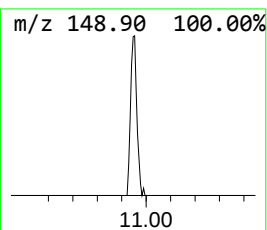
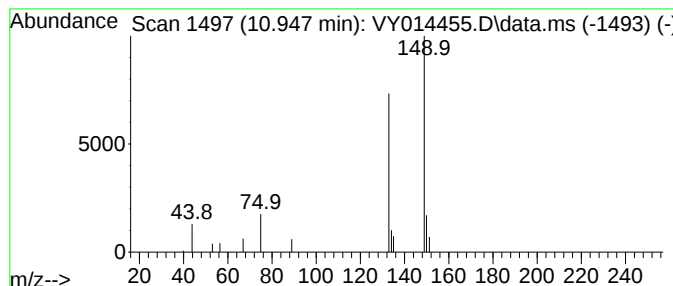
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Peak Number 5 unknown10.947 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	5.30 ug/l	6337	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indole-3-thiol	149	C8H7NS	000480-94-4	25
2			4-Ethylbenzoic acid, 2-ethylhexy...	262	C17H26O2	1000293-49-9	23
3			1H-Benzimidazol-5-amine	133	C7H7N3	000934-22-5	9
4			Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	9
5			Carbamic acid, acetylthio-, O-me...	133	C4H7NO2S	016696-87-0	9



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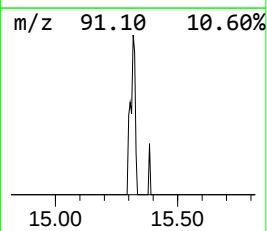
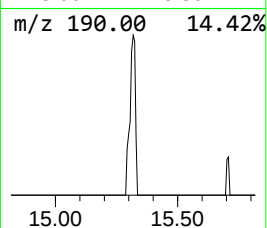
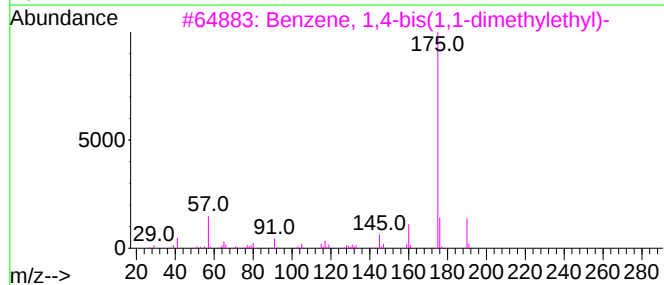
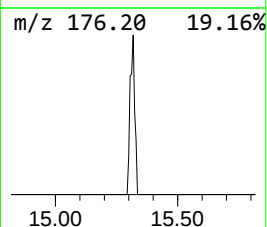
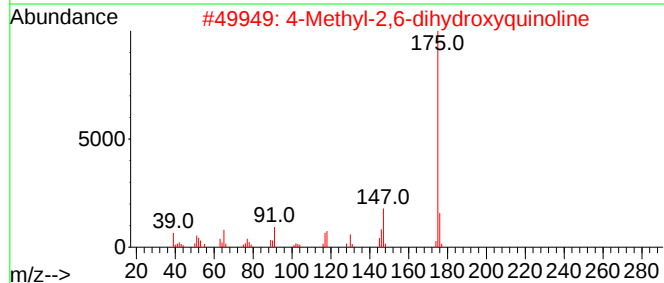
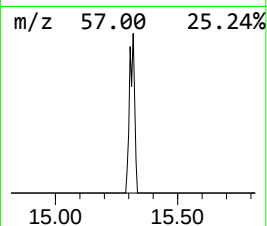
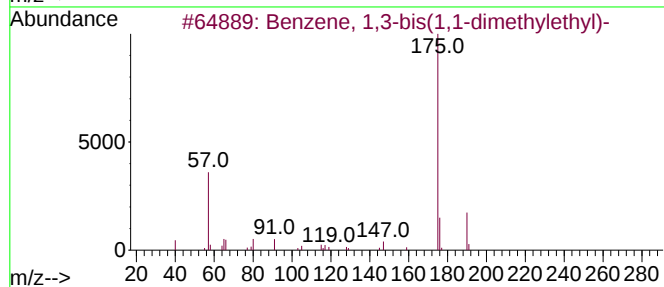
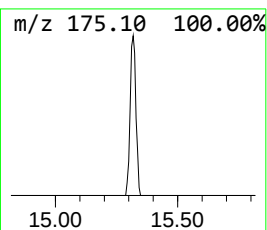
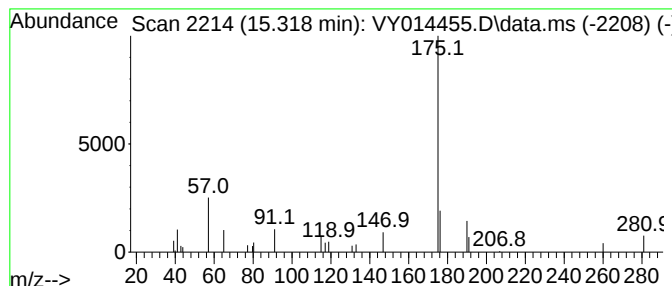
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Peak Number 6 Benzene, 1,3-bis(1,1-dimeth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.318	7.23 ug/l	7086	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-bis(1,1-dimethyleth...	190	C14H22	001014-60-4	80
2			4-Methyl-2,6-dihydroxyquinoline	175	C10H9NO2	034982-01-9	64
3			Benzene, 1,4-bis(1,1-dimethyleth...	190	C14H22	001012-72-2	64
4			Benzenepropanal, 4-(1,1-dimethyl...	190	C13H18O	018127-01-0	50
5			Precocene I	190	C12H14O2	017598-02-6	45



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	6.984	42.2	ug/l	38933	1	7.795	46166	50.0
unknown10.947	10.947	5.3	ug/l	6337	3	11.489	59814	50.0
Benzene, 1,3-bi...	15.318	7.2	ug/l	7086	4	13.428	49006	50.0