

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
 Data File : VN069911.D
 Acq On : 9 Dec 2021 15:04
 Operator : JC/MD
 Sample : M4940-05
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-11

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\82N120221W.M
 Title : SW846 8260

Signal : TIC: VN069911.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.239	82	93	100	rBV2	154504	314710	3.62%	0.601%
2	3.143	419	430	450	rVB3	176390	390989	4.50%	0.746%
3	4.259	824	846	877	rBV7	47197	209114	2.41%	0.399%
4	5.082	1125	1153	1185	rBV3	201380	813548	9.36%	1.553%
5	5.618	1325	1353	1382	rBV3	159160	552346	6.36%	1.054%
6	7.053	1864	1888	1905	rBV4	40172	125447	1.44%	0.239%
7	8.024	2226	2250	2261	rBV2	977058	2369501	27.28%	4.522%
8	8.088	2261	2274	2293	rVV	1682827	3908594	44.99%	7.459%
9	8.174	2295	2306	2331	rVB4	124817	325590	3.75%	0.621%
10	8.440	2385	2405	2429	rBV3	1165270	2979943	34.30%	5.687%
11	8.547	2431	2445	2447	rBV4	62885	113842	1.31%	0.217%
12	8.619	2462	2472	2494	rVB2	230705	612455	7.05%	1.169%
13	8.968	2583	2602	2634	rBV	2818659	5836885	67.19%	11.139%
14	9.424	2753	2772	2780	rBV5	49979	114150	1.31%	0.218%
15	9.883	2924	2943	2962	rBV3	176459	361183	4.16%	0.689%
16	9.974	2962	2977	2982	rBV2	122101	221896	2.55%	0.423%
17	10.014	2983	2992	3016	rVB2	271140	558507	6.43%	1.066%
18	10.202	3046	3062	3068	rBV5	91892	185327	2.13%	0.354%
19	10.440	3134	3151	3171	rBV	4411873	8380363	96.47%	15.993%
20	10.553	3183	3193	3209	rVB3	99394	182054	2.10%	0.347%
21	10.636	3219	3224	3240	rVB8	52188	89773	1.03%	0.171%
22	10.859	3295	3307	3327	rVV6	60235	154771	1.78%	0.295%
23	11.744	3619	3637	3665	rBV	4731603	8687413	100.00%	16.579%
24	12.278	3813	3836	3853	rBV8	36772	93364	1.07%	0.178%
25	12.731	3989	4005	4028	rBV	3572768	6333973	72.91%	12.088%
26	13.369	4231	4243	4258	rVB2	62298	106836	1.23%	0.204%
27	13.675	4341	4357	4385	rBV	3897599	6869880	79.08%	13.111%
28	13.839	4407	4418	4423	rBV3	148759	237685	2.74%	0.454%
29	13.876	4424	4432	4442	rVV	411520	710095	8.17%	1.355%
30	13.919	4443	4448	4468	rVB4	92723	153899	1.77%	0.294%
31	14.327	4590	4600	4612	rVB2	120216	203399	2.34%	0.388%
32	15.196	4911	4924	4936	rBV9	41417	93150	1.07%	0.178%
33	15.504	5029	5039	5053	rVB	58525	108901	1.25%	0.208%

Sum of corrected areas: 52399583

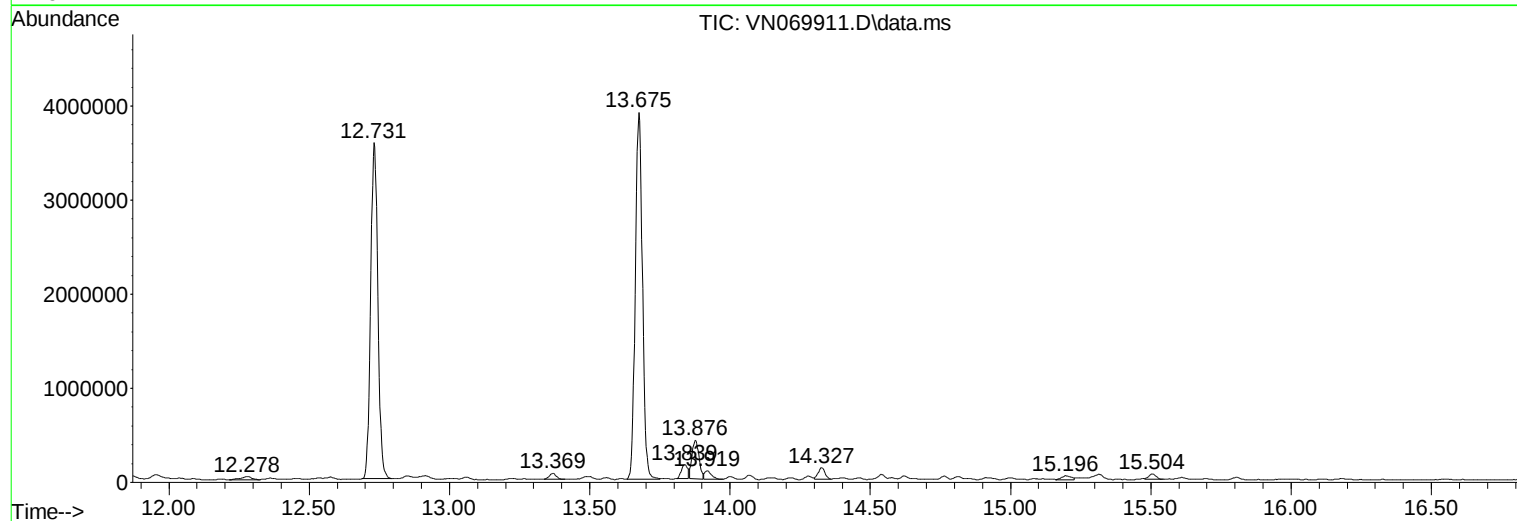
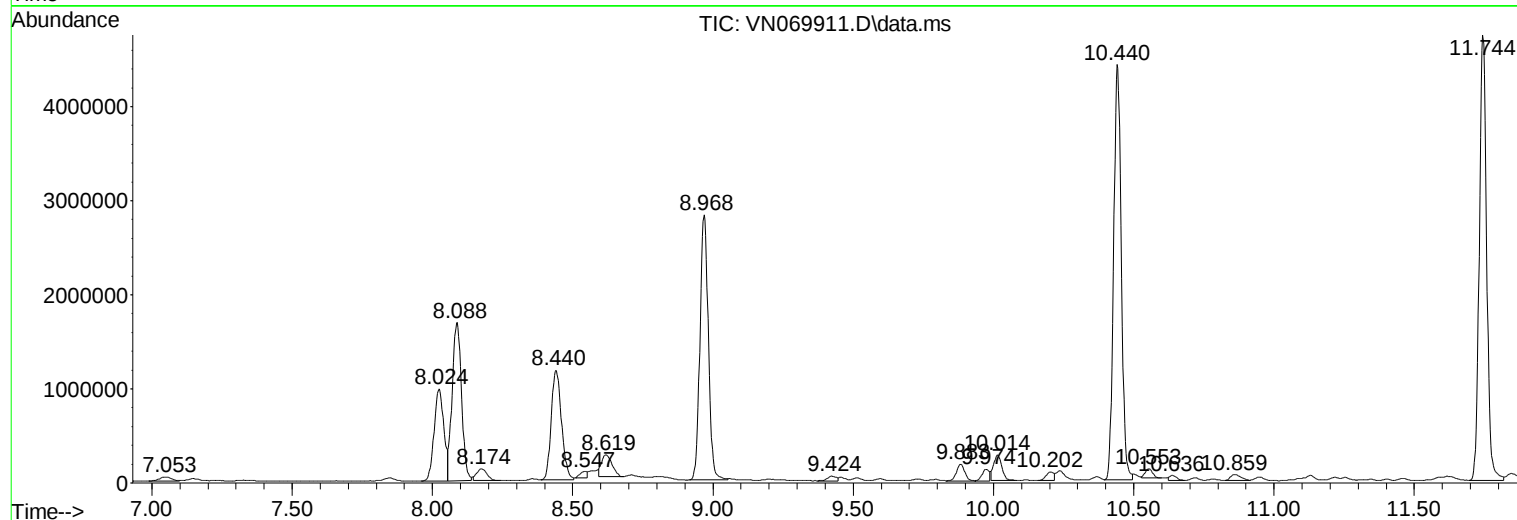
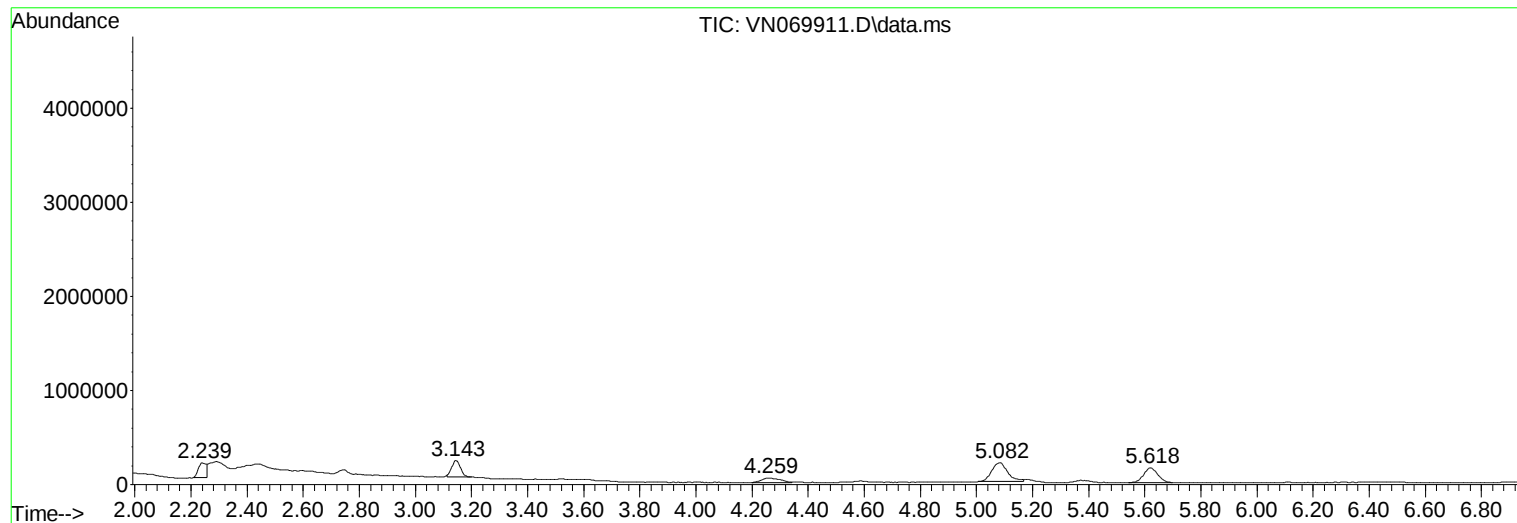
Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



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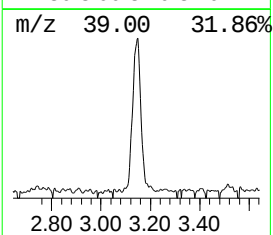
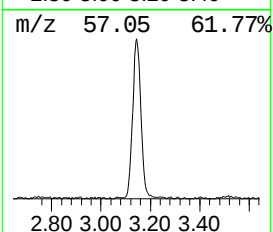
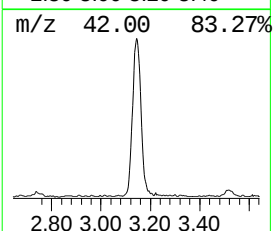
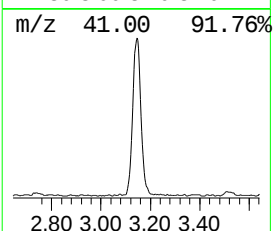
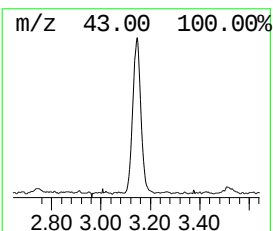
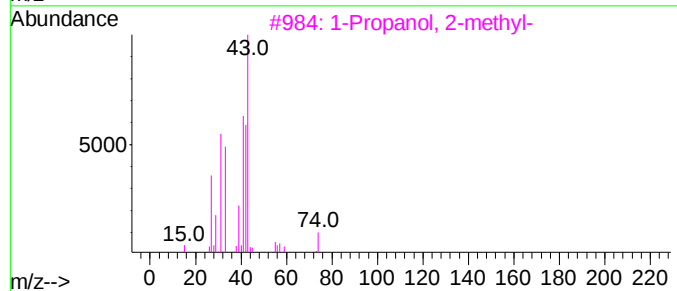
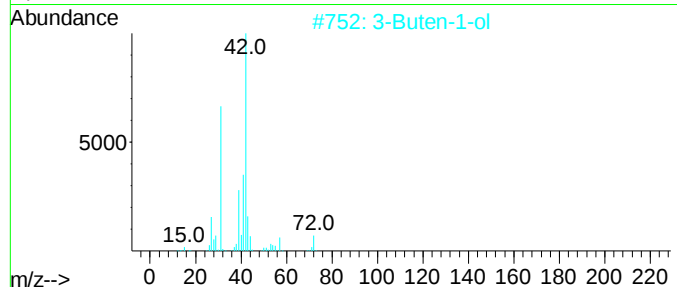
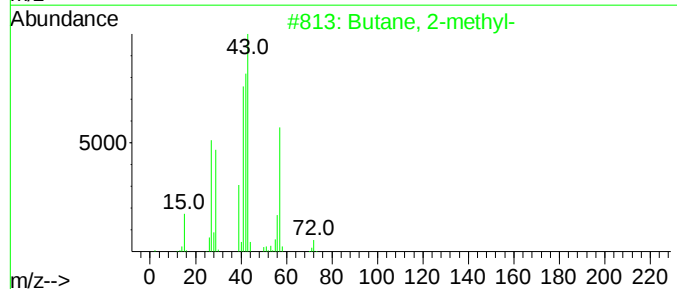
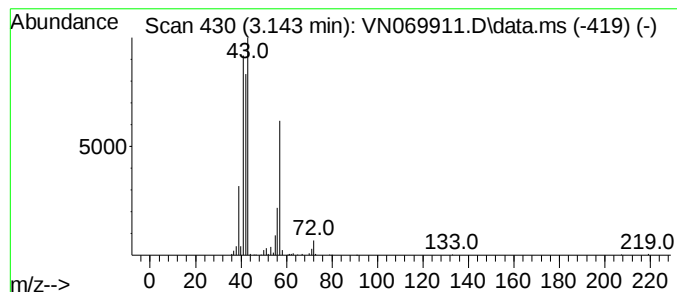
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.143	5.00 ug/l	390989	Pentafluorobenzene	8.088

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	86
2		3-Buten-1-ol	72	C4H8O	000627-27-0	47
3		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	38
4		Cyclobutane, methyl-	70	C5H10	000598-61-8	37
5		Pentane	72	C5H12	000109-66-0	33



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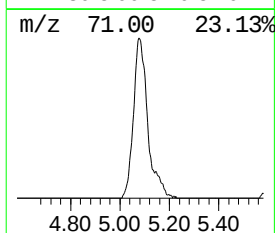
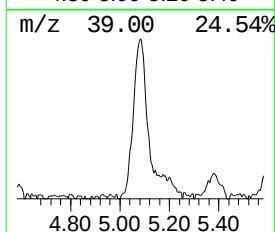
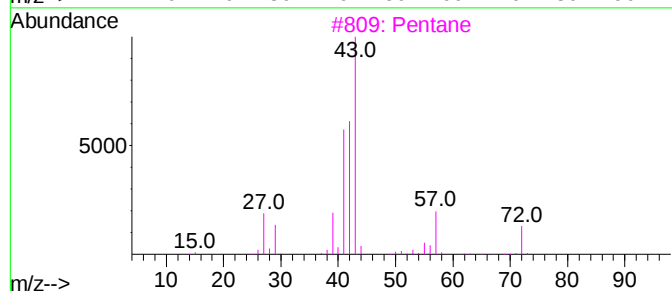
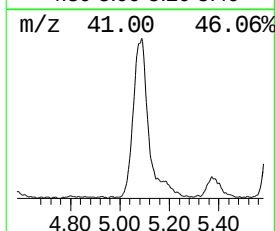
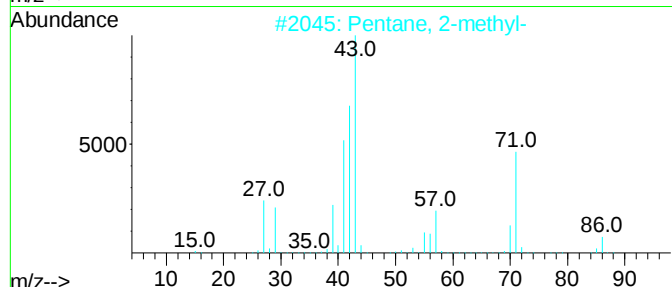
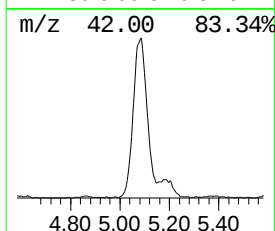
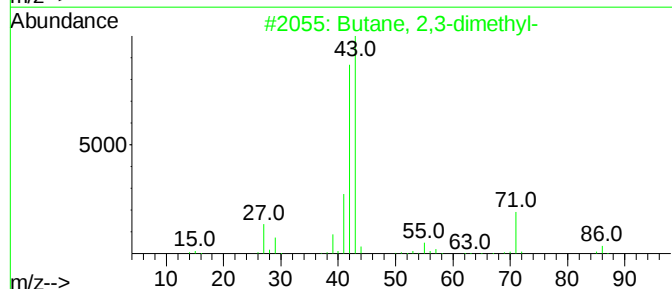
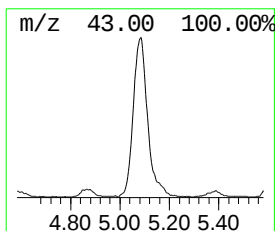
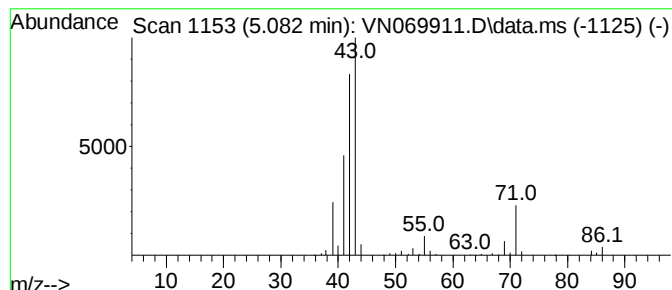
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.082	10.41 ug/l	813548	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	72
3			Pentane	72	C5H12	000109-66-0	36
4			1-Pentene	70	C5H10	000109-67-1	28
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	12



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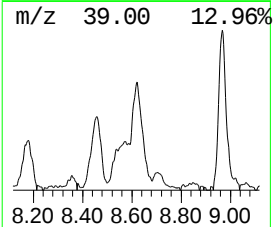
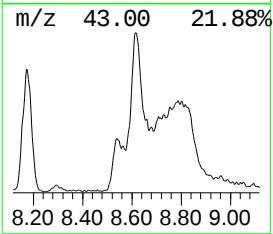
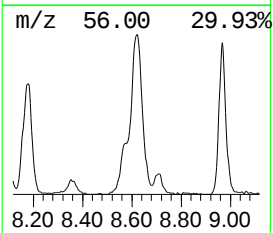
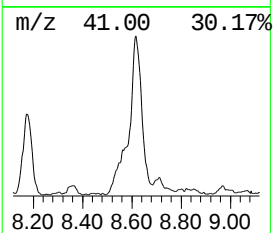
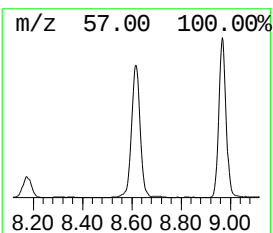
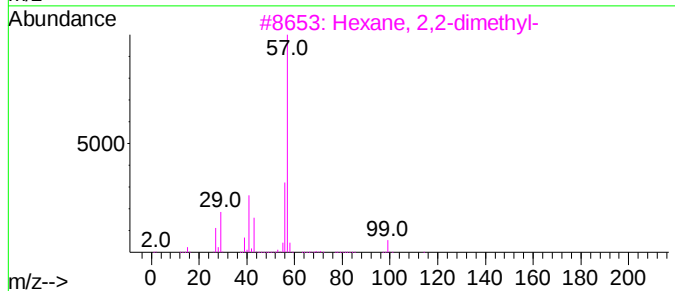
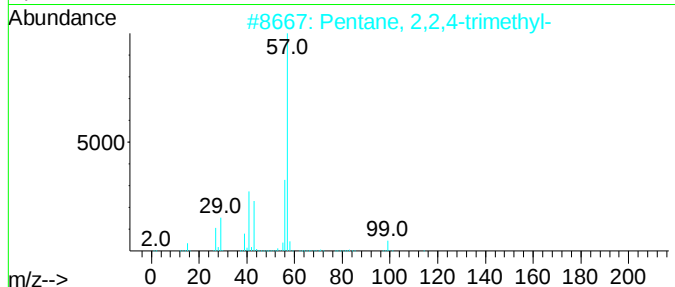
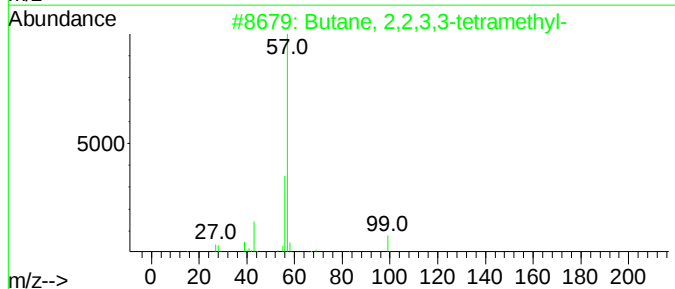
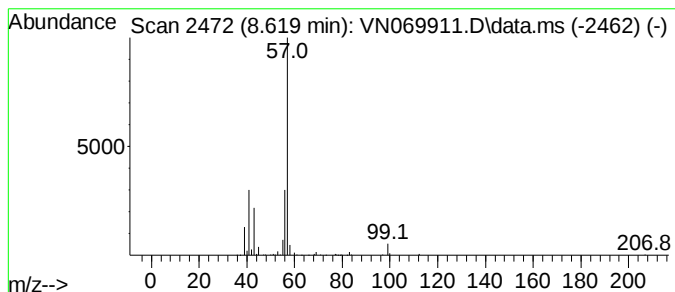
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Peak Number 3 Butane, 2,2,3,3-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	5.25 ug/l	612455	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	59
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	59
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
4	Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	53
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	42



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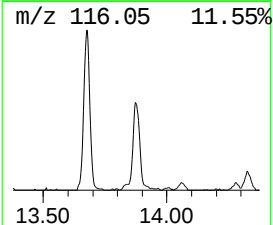
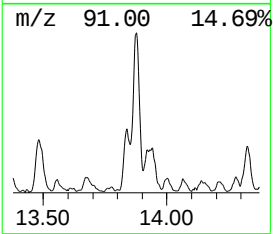
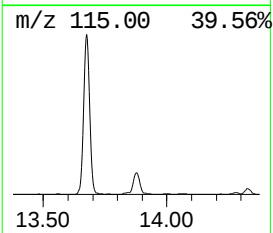
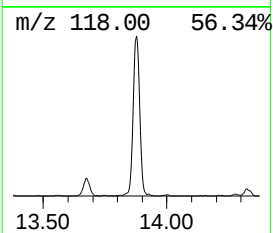
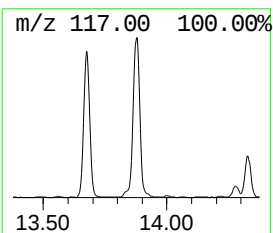
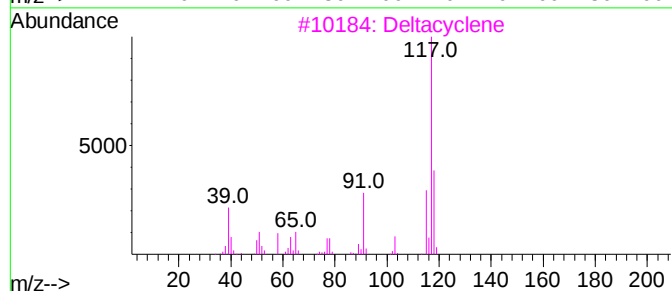
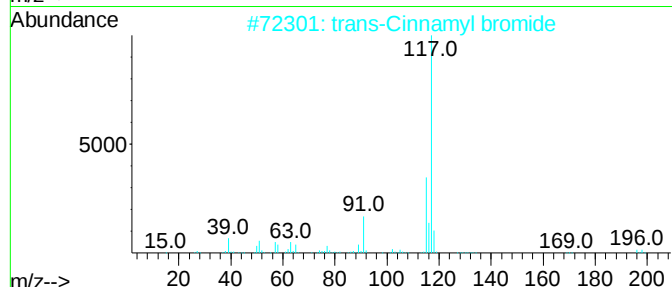
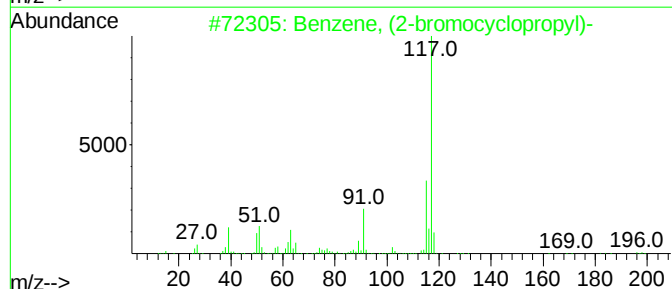
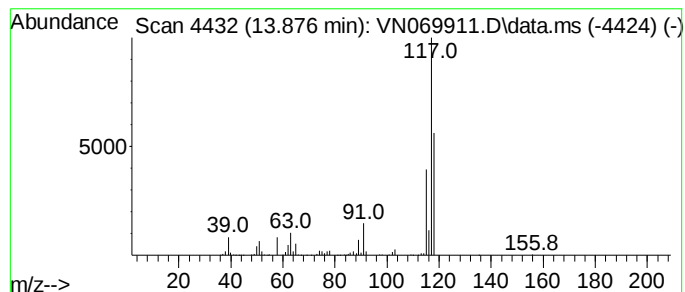
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Peak Number 4 Benzene, (2-bromocyclopropyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	5.17 ug/l	710095	1,4-Dichlorobenzene-d4	13.675

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	59
2		trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
3		Deltacyclene	118	C9H10	007785-10-6	47
4		Indolizine	117	C8H7N	000274-40-8	47
5		Indole	117	C8H7N	000120-72-9	46



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Butane, 2-methyl-	3.143	5.0	ug/l	390989	1	8.088	3908590	50.0
Butane, 2,3-dim...	5.082	10.4	ug/l	813548	1	8.088	3908590	50.0
Butane, 2,2,3,3...	8.619	5.3	ug/l	612455	2	8.968	5836890	50.0
Benzene, (2-bro...	13.876	5.2	ug/l	710095	4	13.675	6869880	50.0