

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
 Data File : VN070636.D
 Acq On : 14 Jan 2022 20:45
 Operator : JC/MD
 Sample : N1148-09
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-49

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\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070636.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.079	1118	1152	1175	rBV6	59635	271111	1.54%	0.470%
2	5.382	1229	1265	1301	rBV2	1009409	3645809	20.74%	6.315%
3	5.618	1321	1353	1398	rBV	4951303	17579590	100.00%	30.448%
4	8.021	2226	2249	2260	rBV2	670655	1599945	9.10%	2.771%
5	8.086	2261	2273	2295	rVV	1109598	2577302	14.66%	4.464%
6	8.442	2383	2406	2426	rBV3	948604	2571596	14.63%	4.454%
7	8.536	2426	2441	2459	rVV	771093	1706873	9.71%	2.956%
8	8.968	2581	2602	2631	rBV	1763111	3711803	21.11%	6.429%
9	9.883	2927	2943	2959	rBV2	98086	192813	1.10%	0.334%
10	10.014	2966	2992	3010	rBV3	172354	386573	2.20%	0.670%
11	10.204	3045	3063	3065	rBV2	264737	393152	2.24%	0.681%
12	10.237	3067	3075	3100	rVB	569686	1117623	6.36%	1.936%
13	10.440	3134	3151	3172	rBV	2915568	5480287	31.17%	9.492%
14	10.550	3179	3192	3217	rVB	656956	1222553	6.95%	2.118%
15	11.089	3375	3393	3421	rBV3	161957	364862	2.08%	0.632%
16	11.621	3572	3591	3618	rVB5	232855	610426	3.47%	1.057%
17	11.744	3619	3637	3664	rBV	2883845	5489882	31.23%	9.509%
18	11.846	3664	3675	3697	rVV	159493	355810	2.02%	0.616%
19	11.958	3701	3717	3743	rVB2	232343	522347	2.97%	0.905%
20	12.731	3988	4005	4030	rBV	2121425	3815264	21.70%	6.608%
21	12.843	4034	4047	4058	rBV3	113069	212481	1.21%	0.368%
22	13.366	4233	4242	4258	rVB	131154	224383	1.28%	0.389%
23	13.675	4341	4357	4383	rBV	1721098	3110918	17.70%	5.388%
24	15.507	5018	5040	5059	rBV	285453	572140	3.25%	0.991%

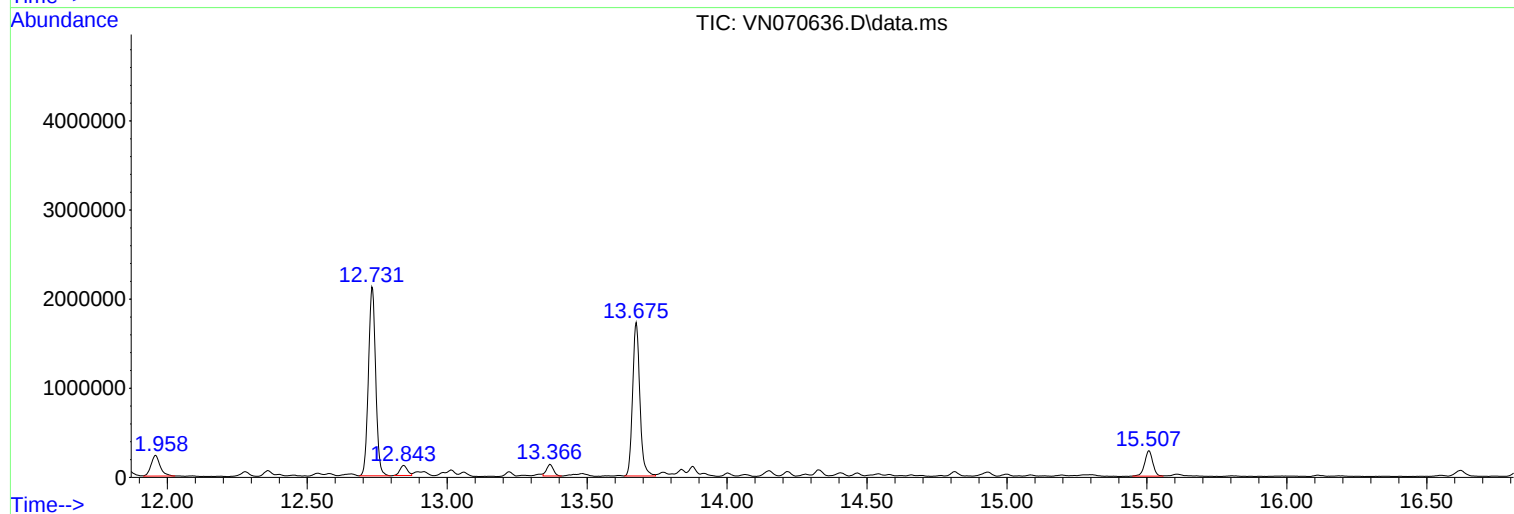
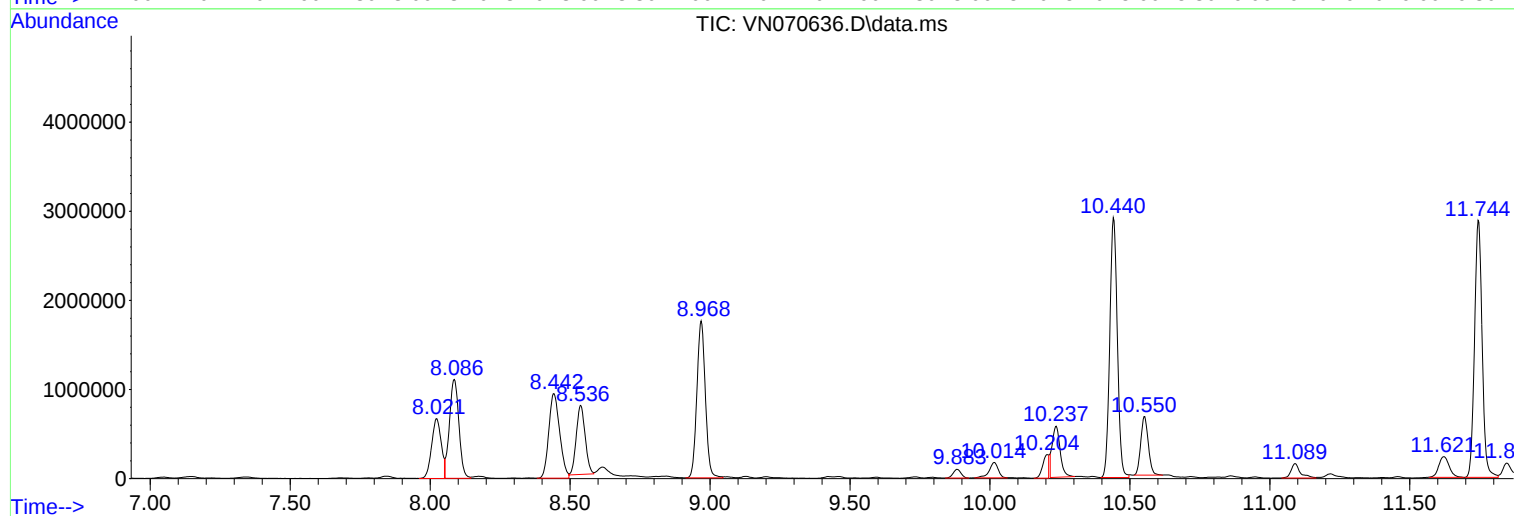
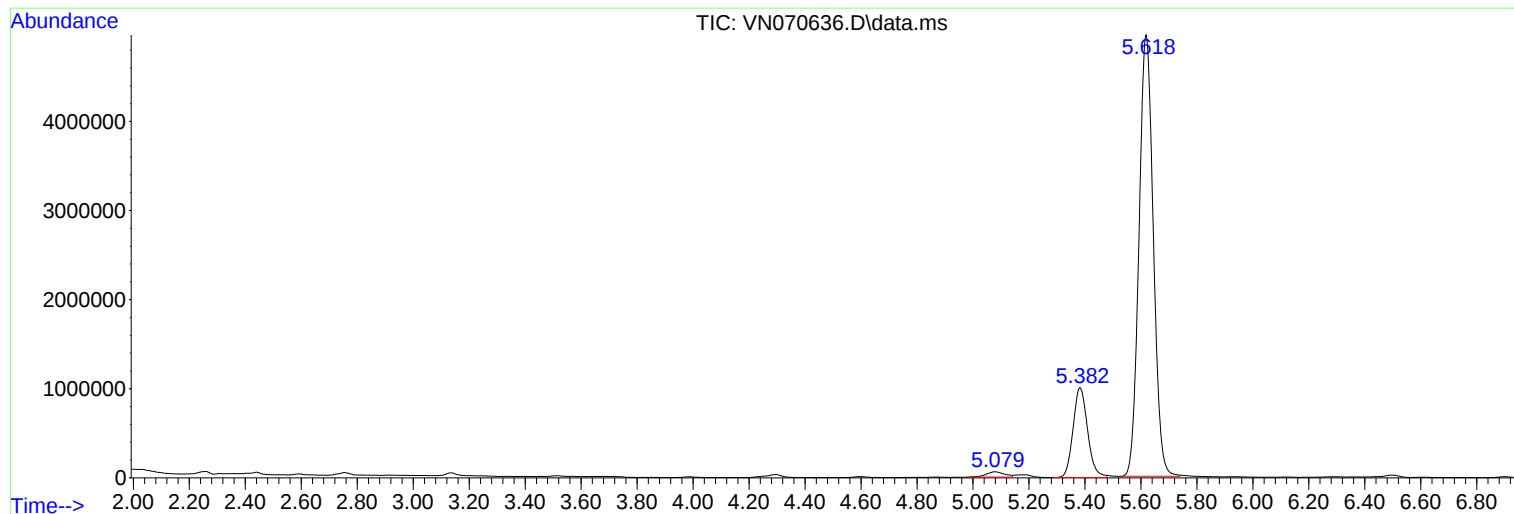
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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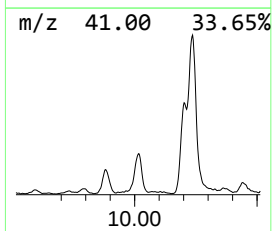
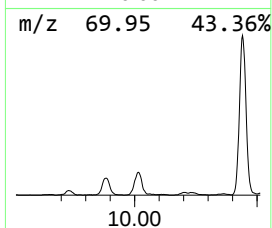
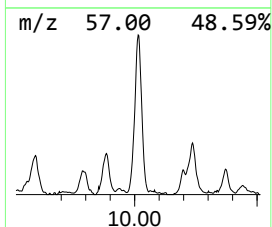
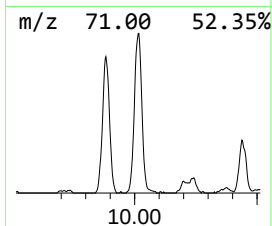
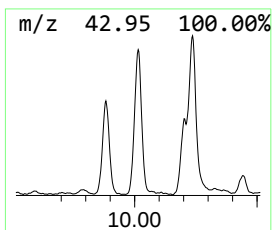
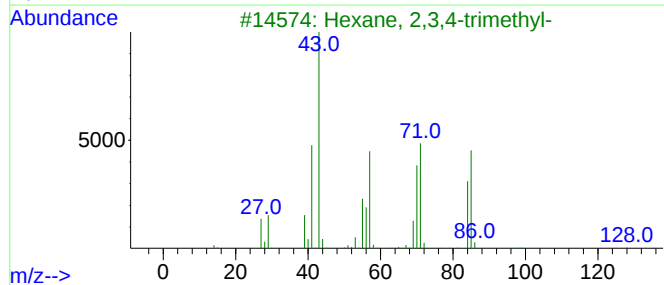
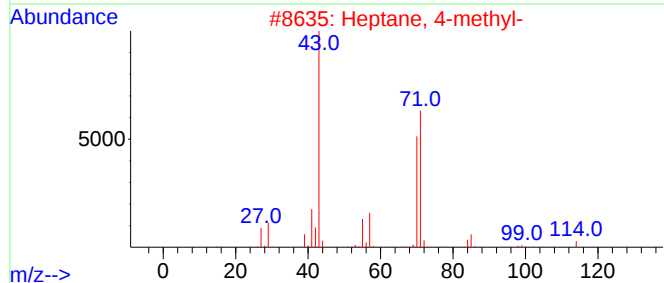
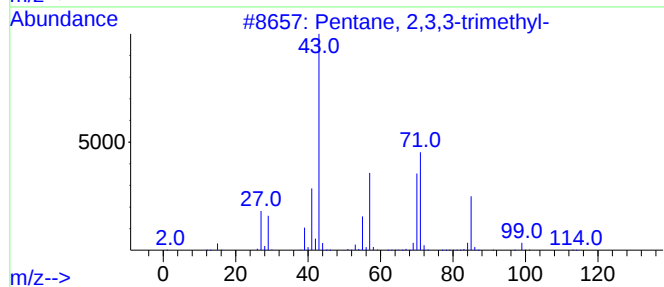
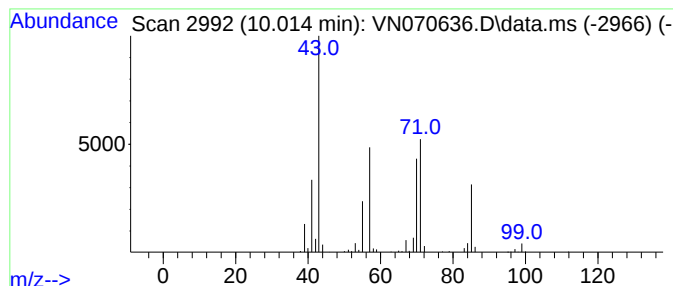
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,3,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	5.21 ug/l	386573	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
4			Propanoic acid, 2-methyl-, 2-eth...	200	C12H24O2	035061-61-1	59
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59



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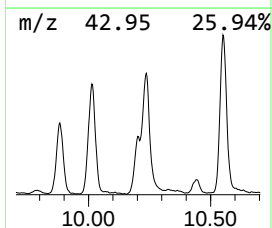
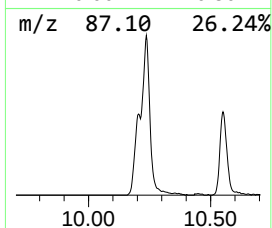
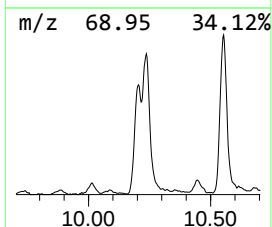
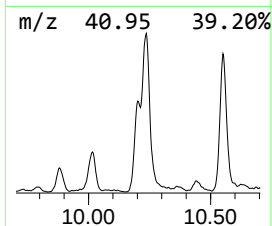
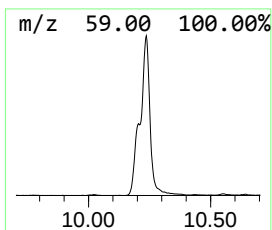
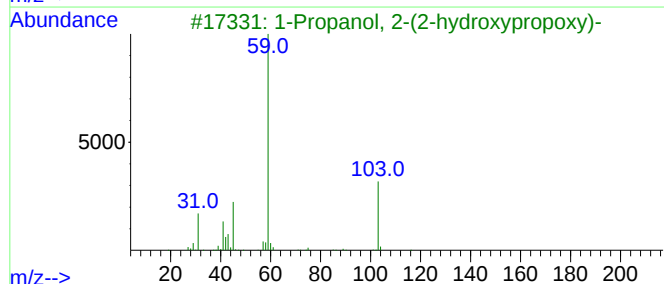
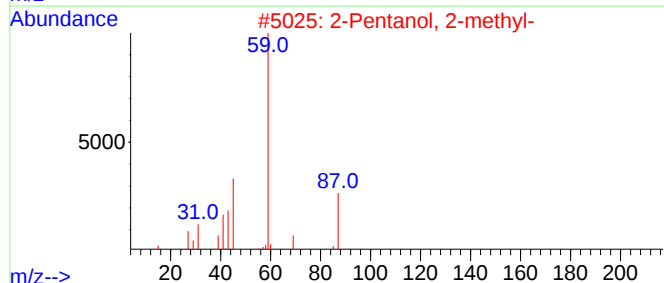
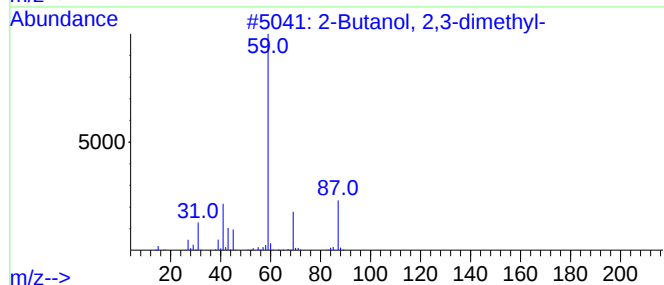
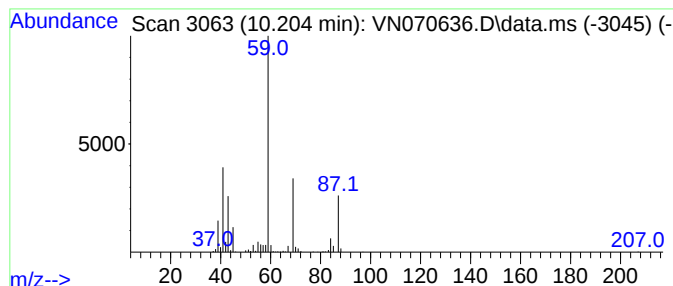
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Butanol, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.204	5.30 ug/l	393152	1,4-Difluorobenzene	8.968

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	56
3		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	50
4		HEX-5-EN-3-OL	100	C6H12O	000688-99-3	47
5		Pentane, 2-methoxy-	102	C6H14O	006795-88-6	45



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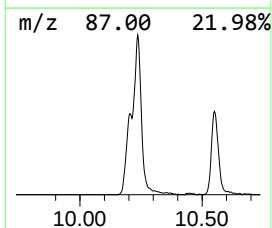
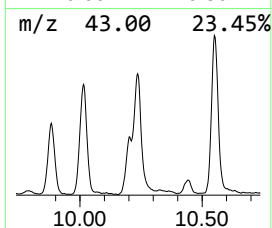
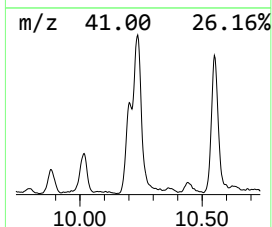
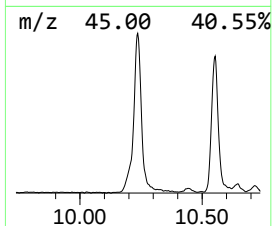
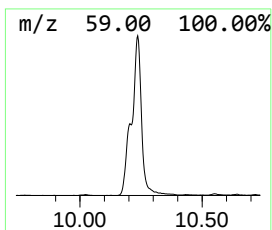
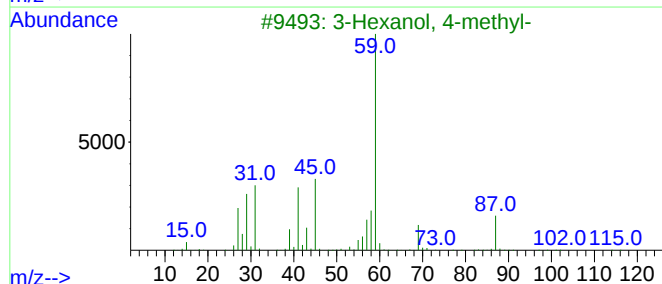
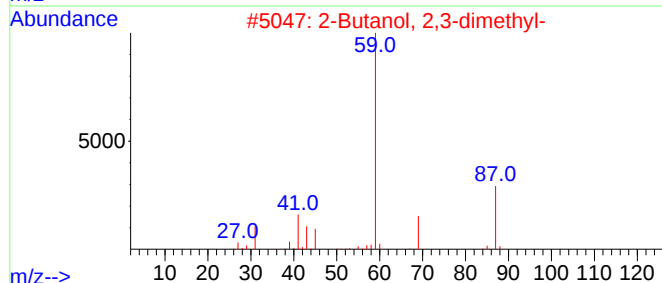
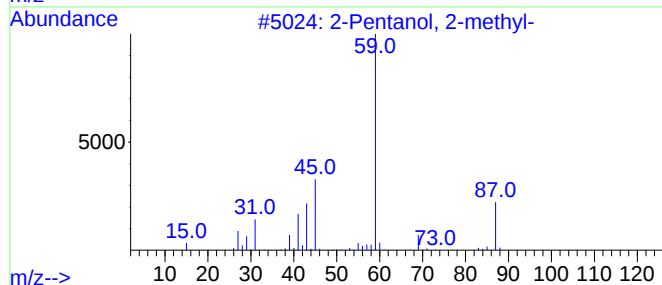
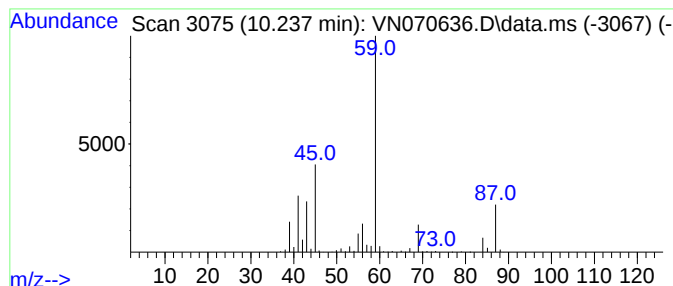
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Peak Number 3 2-Pentanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.237	15.06 ug/l	1117620	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
2			2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	53
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	50
4			3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	45
5			2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	28



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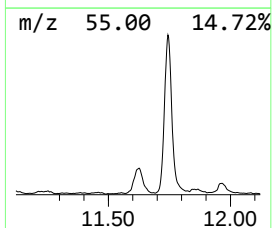
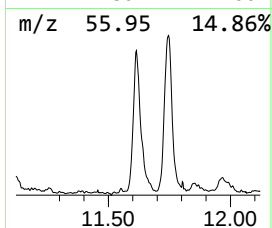
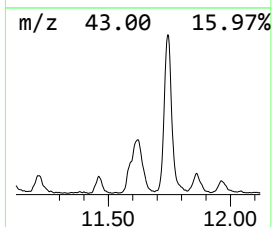
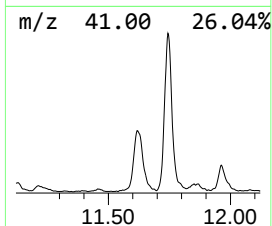
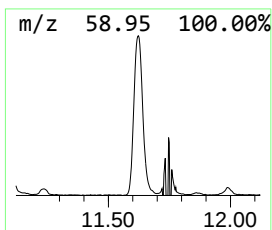
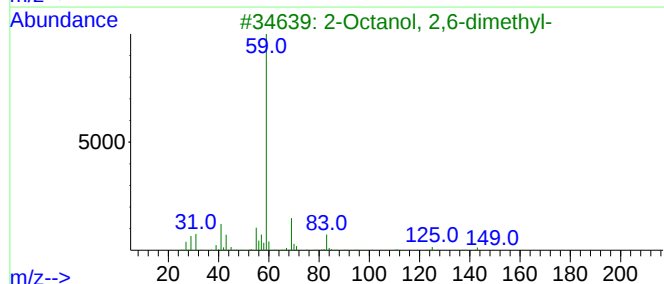
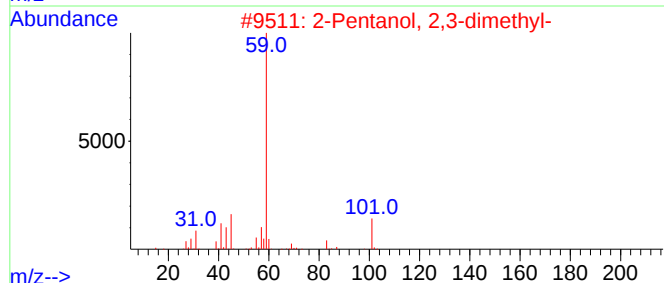
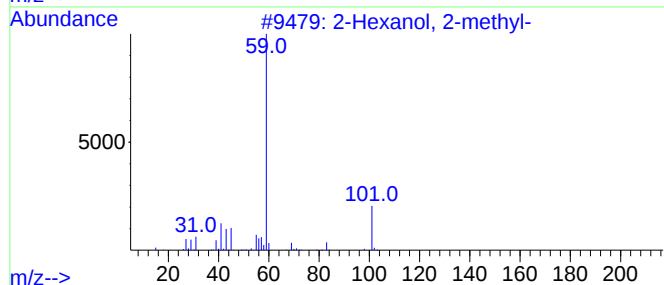
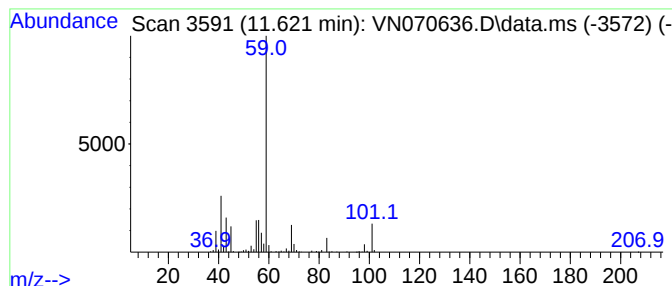
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Peak Number 4 2-Hexanol, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.621	5.56 ug/l	610426	Chlorobenzene-d5	11.744	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	72
2	2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	64
3	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	59
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	50
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,3,3-...	10.014	5.2	ug/l	386573	2	8.968	3711800	50.0
2-Butanol, 2,3-...	10.204	5.3	ug/l	393152	2	8.968	3711800	50.0
2-Pentanol, 2-m...	10.237	15.1	ug/l	1117620	2	8.968	3711800	50.0
2-Hexanol, 2-me...	11.621	5.6	ug/l	610426	3	11.744	5489880	50.0