

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101918\
 Data File : VX005455.D
 Acq On : 19 Oct 2018 13:53
 Operator : JC/MD
 Sample : J5538-03
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WWT1-6

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.282	18	21	25	rVB3	10859	12055	1.05%	0.128%
2	1.635	65	79	83	rBV8	10021	27476	2.40%	0.291%
3	2.446	206	212	220	rBV	36901	60457	5.27%	0.641%
4	2.714	250	256	262	rBV	17378	32369	2.82%	0.343%
5	2.775	262	266	272	rVV	8005	15534	1.35%	0.165%
6	2.855	272	279	292	rVV	153068	287076	25.03%	3.045%
7	4.708	574	583	589	rBV	5430	15303	1.33%	0.162%
8	5.500	701	713	727	rBV2	142481	410186	35.76%	4.351%
9	5.665	729	740	757	rBV2	249780	710120	61.90%	7.533%
10	6.073	796	807	819	rBV	158355	410477	35.78%	4.354%
11	6.238	825	834	849	rVB3	15868	44801	3.91%	0.475%
12	6.458	861	870	884	rBV2	111711	280671	24.47%	2.977%
13	6.860	926	936	958	rBV	351635	884418	77.10%	9.382%
14	7.884	1097	1104	1124	rBV	163585	287363	25.05%	3.048%
15	8.646	1227	1229	1234	rVV3	7165	12154	1.06%	0.129%
16	8.719	1234	1241	1249	rVV	693106	1147116	100.00%	12.168%
17	8.786	1249	1252	1257	rVV	20904	39324	3.43%	0.417%
18	8.835	1257	1260	1270	rVB	14960	25891	2.26%	0.275%
19	9.103	1298	1304	1312	rBV	11999	19534	1.70%	0.207%
20	9.408	1350	1354	1367	rVB	16809	27588	2.40%	0.293%
21	9.548	1371	1377	1382	rBV	73098	101979	8.89%	1.082%
22	9.640	1388	1392	1402	rVB	24695	35388	3.08%	0.375%
23	9.975	1439	1447	1457	rBV	68662	95778	8.35%	1.016%
24	10.115	1463	1470	1488	rBV	716605	998757	87.07%	10.595%
25	10.359	1505	1510	1516	rVB	19492	27921	2.43%	0.296%
26	10.701	1560	1566	1574	rBV4	10559	16836	1.47%	0.179%
27	11.140	1632	1638	1655	rBV	593470	763413	66.55%	8.098%
28	11.810	1743	1748	1754	rBV	17996	24596	2.14%	0.261%
29	12.078	1786	1792	1799	rVV	791957	956225	83.36%	10.143%
30	12.139	1799	1802	1806	rVV	8663	12975	1.13%	0.138%
31	12.182	1806	1809	1816	rVB	13205	17479	1.52%	0.185%
32	12.298	1825	1828	1836	rVB2	13562	21470	1.87%	0.228%
33	12.469	1848	1856	1862	rBV	54418	72043	6.28%	0.764%
34	13.023	1943	1947	1951	rBV2	13210	18676	1.63%	0.198%

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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

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Peak separation: 5

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35	13.347	1995	2000	2005	rVV3	16726	24117	2.10%	0.256%
36	13.401	2005	2009	2016	rVV3	10736	14836	1.29%	0.157%
37	13.481	2017	2022	2028	rVB	22148	30303	2.64%	0.321%
38	13.834	2070	2080	2087	rBV	741429	906823	79.05%	9.619%
39	13.926	2087	2095	2102	rVV	21405	42752	3.73%	0.453%
40	14.285	2147	2154	2162	rVB3	11495	23288	2.03%	0.247%
41	14.700	2212	2222	2232	rVB	108263	152846	13.32%	1.621%
42	14.840	2240	2245	2253	rBV	94251	121999	10.64%	1.294%
43	15.273	2307	2316	2321	rBV	14957	28917	2.52%	0.307%
44	15.547	2356	2361	2366	rBV	14975	25946	2.26%	0.275%
45	15.688	2377	2384	2388	rBV	24745	42615	3.71%	0.452%
46	15.724	2388	2390	2396	rVB3	11740	17504	1.53%	0.186%
47	15.919	2414	2422	2428	rVB3	7867	20158	1.76%	0.214%
48	16.175	2459	2464	2472	rVB	14355	25196	2.20%	0.267%
49	16.419	2497	2504	2513	rVB2	18724	36376	3.17%	0.386%

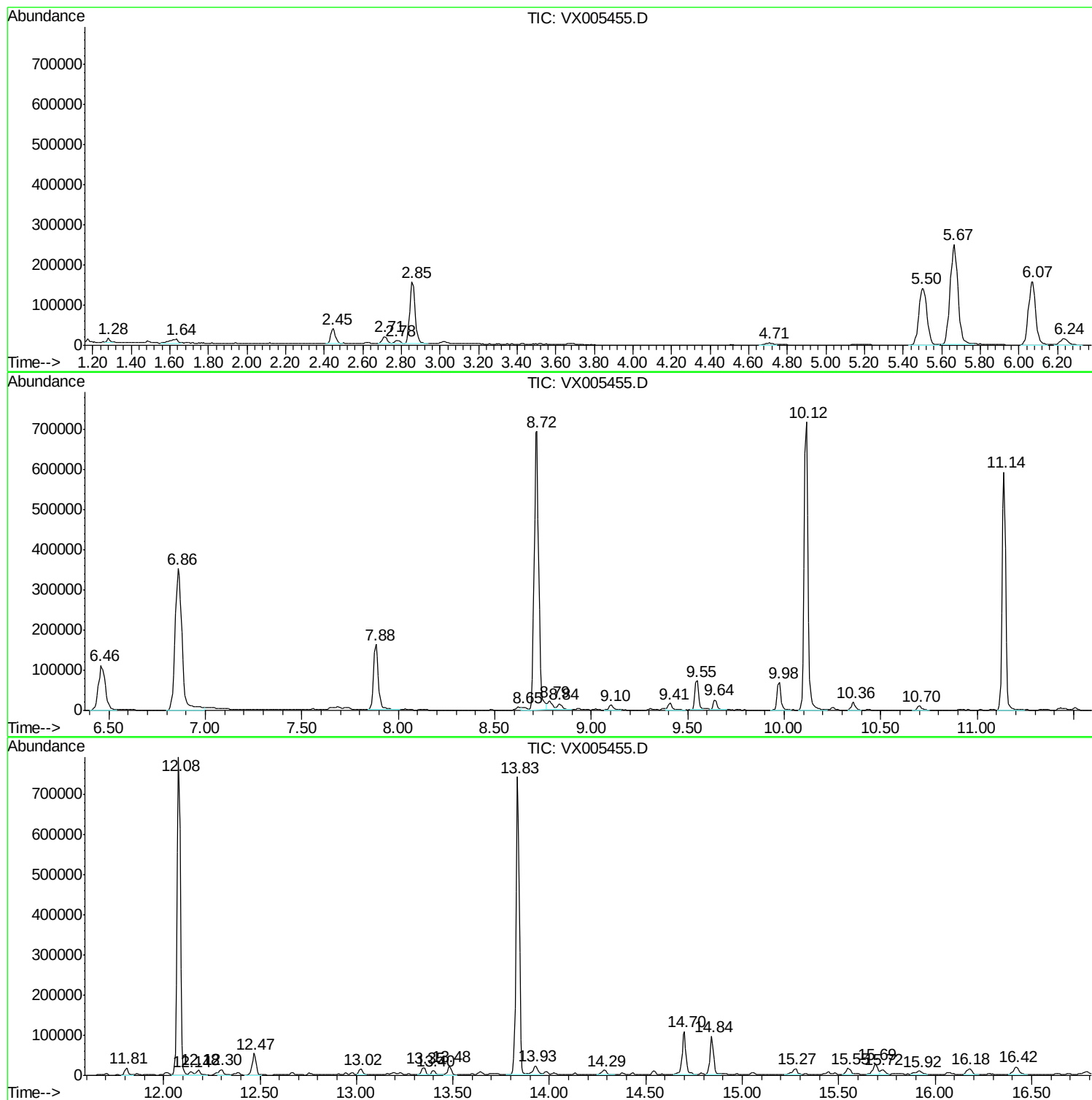
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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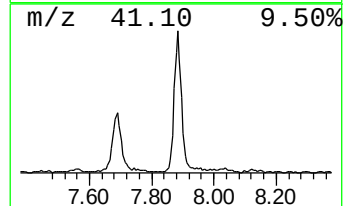
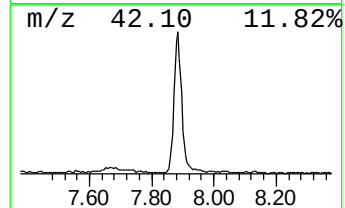
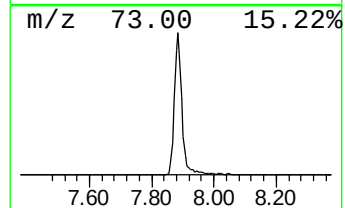
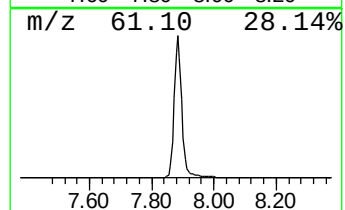
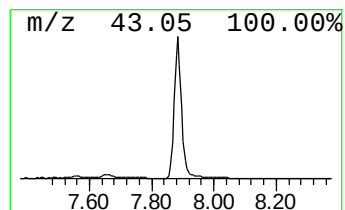
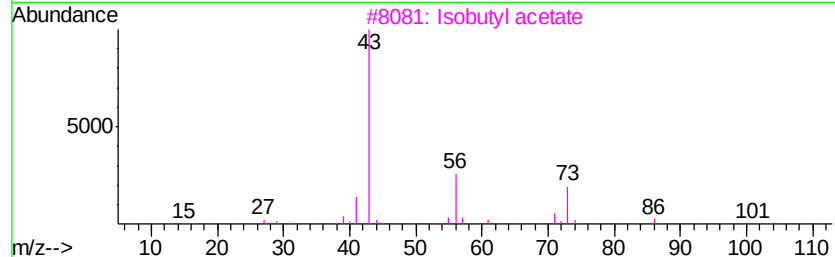
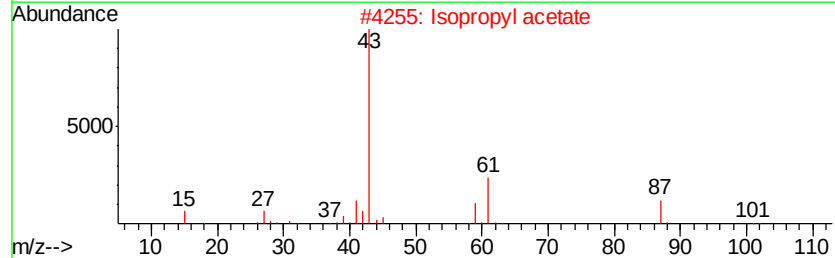
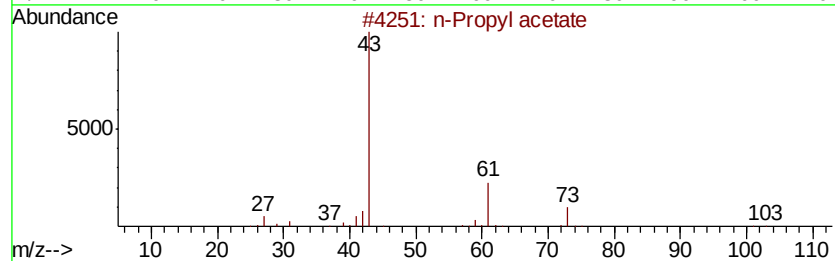
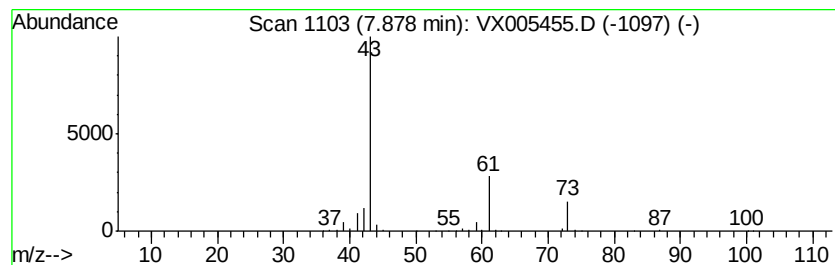
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
7.88	16.25 ug/l	287363	1,4-Difluorobenzene	6.86		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate		102	C5H10O2	000109-60-4	83
2	Isopropyl acetate		102	C5H10O2	000108-21-4	36
3	Isobutyl acetate		116	C6H12O2	000110-19-0	9
4	Isobutylamine		73	C4H11N	000078-81-9	7
5	1-Butanamine		73	C4H11N	000109-73-9	5



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Instrument :
MSVOA_X
ClientSampled :
WWT1-6

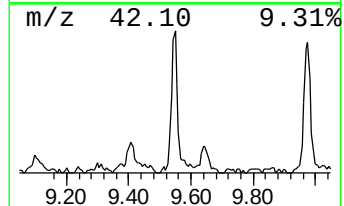
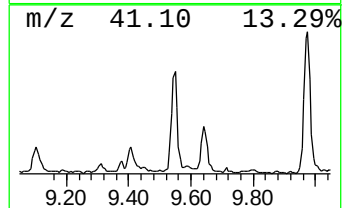
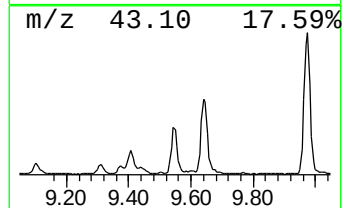
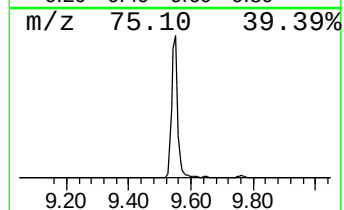
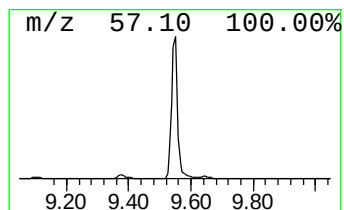
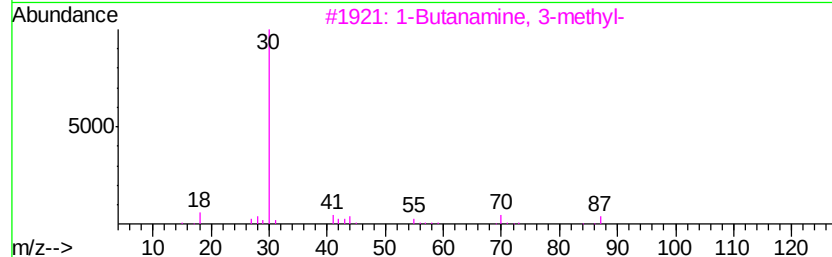
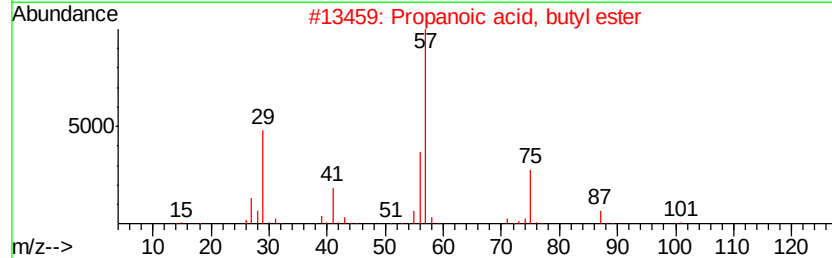
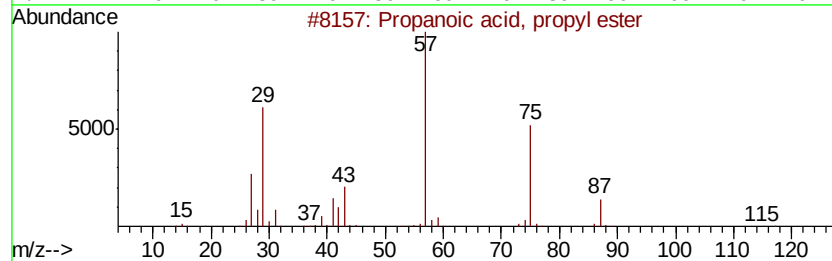
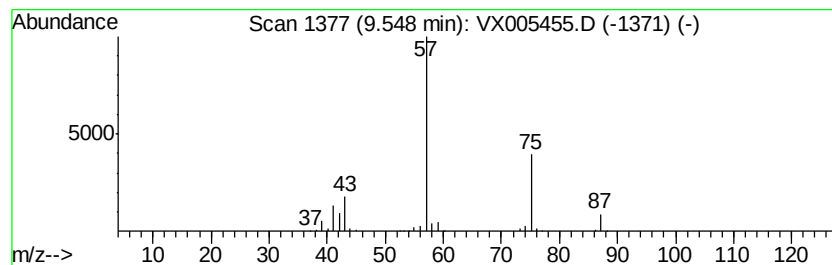
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Peak Number 2 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	5.11 ug/l	101979	Chlorobenzene-d5	10.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	45
3			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9
4			Oxalic acid, bis(isobutyl) ester	202	C10H18O4	1000309-36-8	9
5			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9



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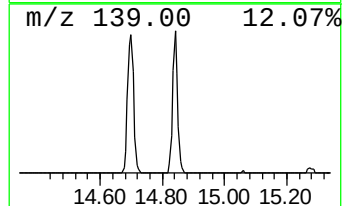
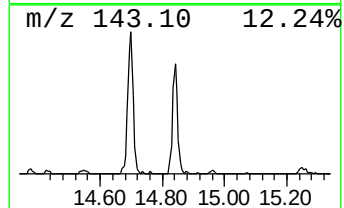
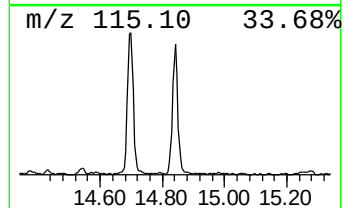
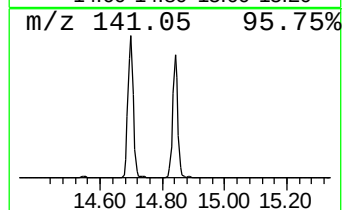
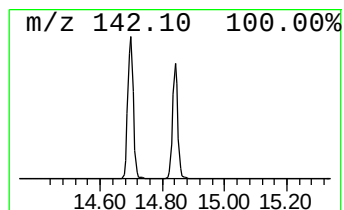
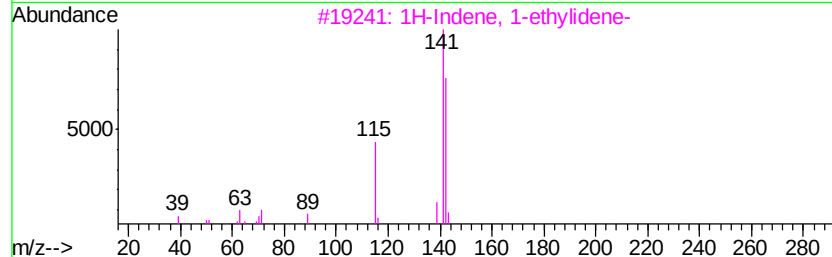
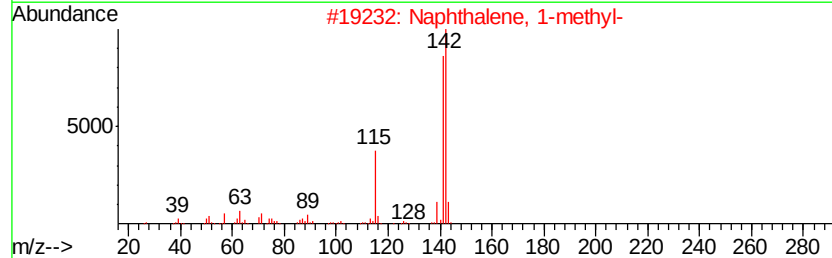
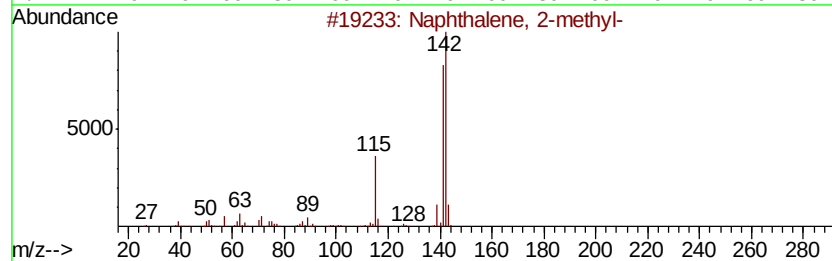
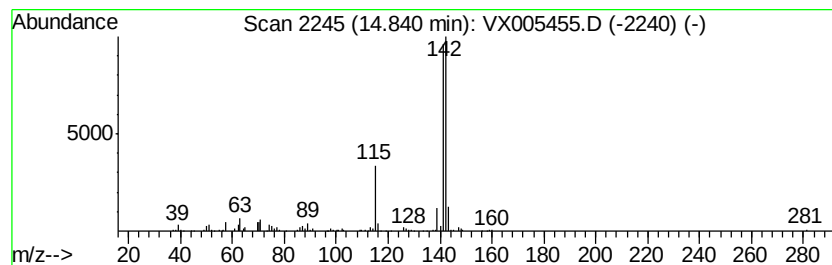
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Peak Number 4 Naphthalene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.84	6.38 ug/l	121999	1,4-Dichlorobenzene-d4	12.08		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91
4		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.88	16.3	ug/l	287363	2	6.86	884418	50.0
Propanoic acid, p...	9.55	5.1	ug/l	101979	3	10.12	998757	50.0
Naphthalene, 2-me...	14.84	6.4	ug/l	121999	4	12.08	956225	50.0