

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN051319\
 Data File : VN055576.D
 Acq On : 13 May 2019 14:17
 Operator : JC/SP
 Sample : K2718-16
 Misc : 5.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 P026-SS007-0002-01

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_N\METHODS\82N050819W.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	2.011	61	74	86	rBV2	73371	173132	3.63%	0.536%
2	2.490	196	223	224	rBV5	79748	201525	4.23%	0.624%
3	2.754	289	305	328	rVB2	312012	690324	14.48%	2.139%
4	4.516	831	853	854	rBV2	28833	58143	1.22%	0.180%
5	4.571	855	870	901	rVB4	124065	443761	9.31%	1.375%
6	5.030	994	1013	1042	rVB2	57683	205005	4.30%	0.635%
7	5.548	1156	1174	1194	rBV6	16540	52939	1.11%	0.164%
8	6.615	1486	1506	1533	rVB2	181644	575278	12.07%	1.783%
9	7.587	1787	1808	1818	rBV2	541959	1369272	28.72%	4.243%
10	7.657	1819	1830	1847	rVB	1031501	2523830	52.94%	7.820%
11	7.869	1883	1896	1907	rBV4	39106	87011	1.83%	0.270%
12	8.024	1928	1944	1964	rBV	622215	1447274	30.36%	4.484%
13	8.149	1971	1983	1995	rBV3	78333	178701	3.75%	0.554%
14	8.230	1996	2008	2017	rVV2	72196	164752	3.46%	0.510%
15	8.294	2018	2028	2043	rVB3	107819	259013	5.43%	0.803%
16	8.429	2064	2070	2083	rVB4	47813	89139	1.87%	0.276%
17	8.583	2102	2118	2153	rBV	1427736	3138166	65.82%	9.724%
18	9.075	2251	2271	2288	rBV2	596848	1320513	27.70%	4.092%
19	9.265	2321	2330	2341	rVB3	49344	97818	2.05%	0.303%
20	9.361	2350	2360	2370	rBV2	44277	87308	1.83%	0.271%
21	9.506	2399	2405	2420	rVB4	46392	87685	1.84%	0.272%
22	9.721	2467	2472	2488	rVB3	48765	83220	1.75%	0.258%
23	10.088	2573	2586	2619	rBV	2317472	4767662	100.00%	14.773%
24	11.406	2985	2996	3017	rBV	1954385	3495119	73.31%	10.830%
25	11.615	3052	3061	3071	rBV	401522	782902	16.42%	2.426%
26	12.400	3295	3305	3313	rBV	1730145	3313054	69.49%	10.266%
27	13.040	3497	3504	3514	rVB	268230	419021	8.79%	1.298%
28	13.342	3590	3598	3616	rVB	1925585	3639511	76.34%	11.277%
29	14.599	3976	3989	4012	rBV4	362067	1347190	28.26%	4.174%
30	15.133	4147	4155	4175	rVB3	305636	684524	14.36%	2.121%
31	16.159	4467	4474	4487	rVB2	113790	202051	4.24%	0.626%
32	16.348	4527	4533	4546	rVB	150008	287968	6.04%	0.892%

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Integration Parameters: RTEINT.P

Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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

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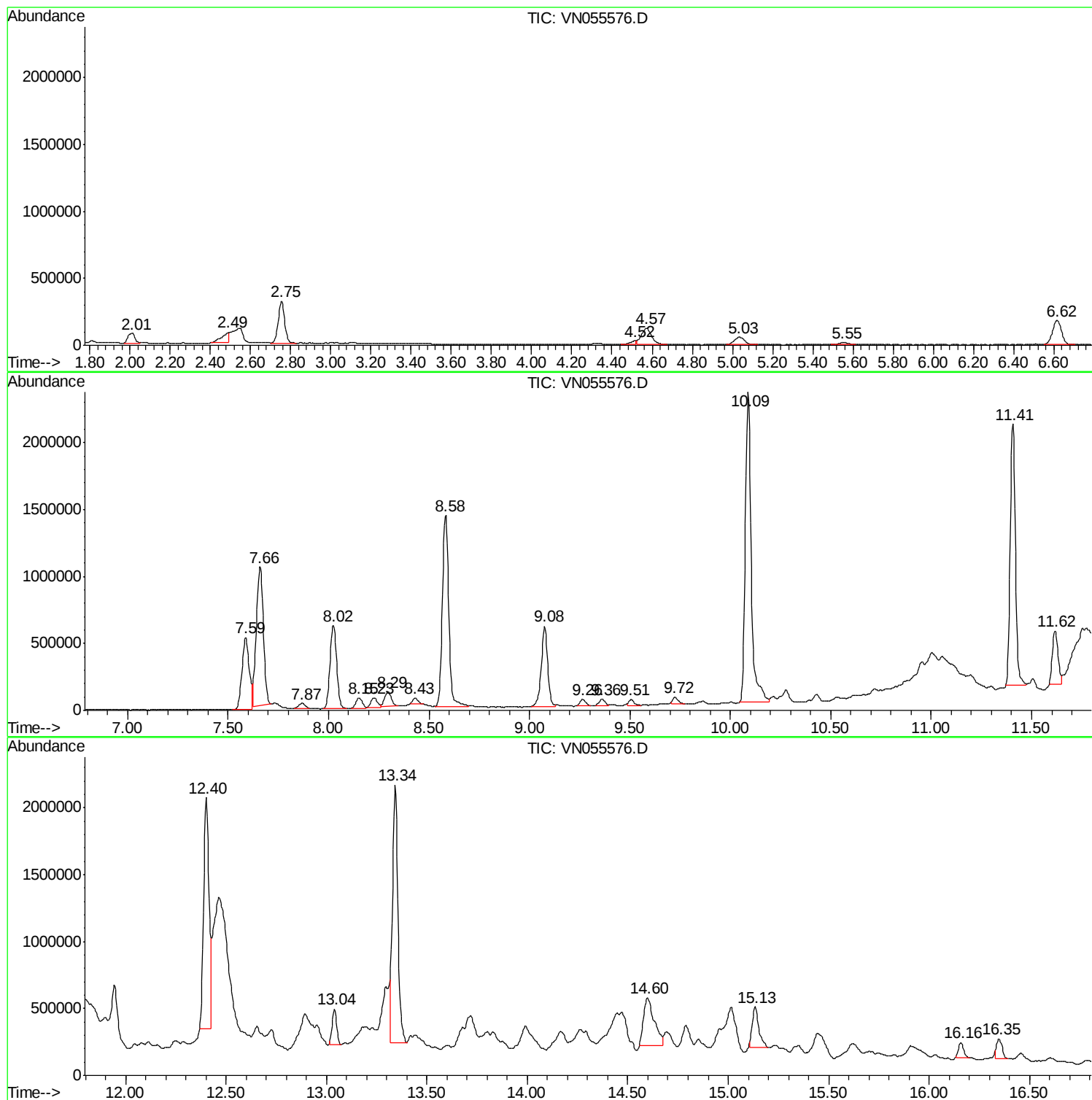
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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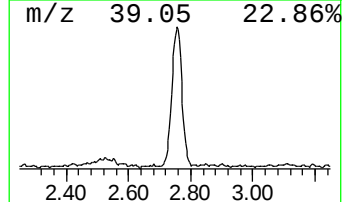
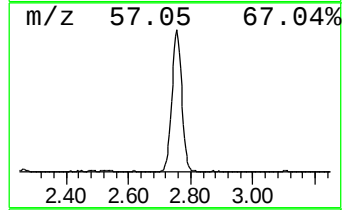
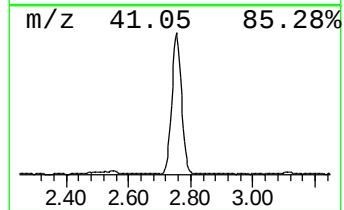
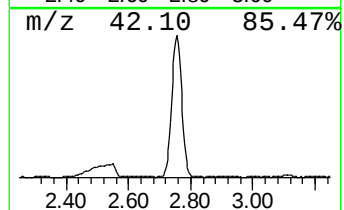
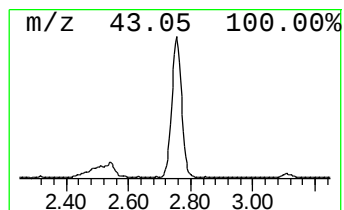
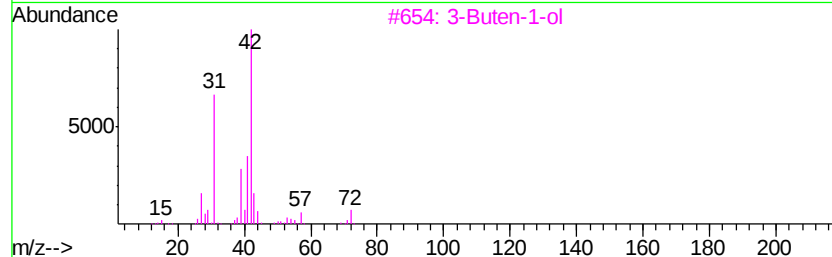
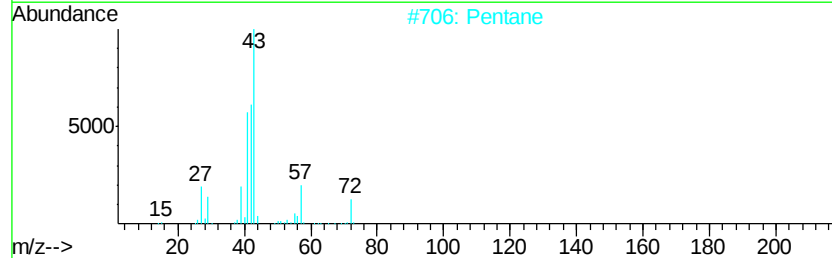
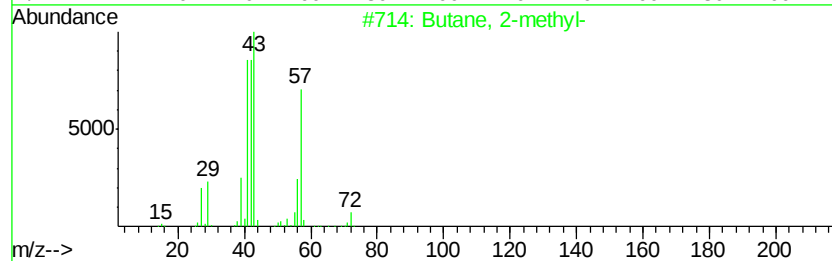
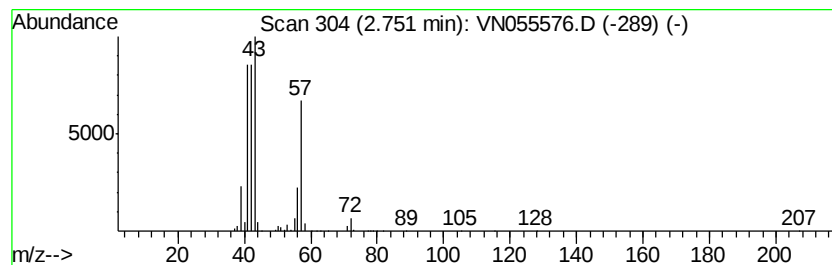
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N050819W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.75	13.68 ug/l	690324	Pentafluorobenzene	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2		Pentane	72	C5H12	000109-66-0	56
3		3-Buten-1-ol	72	C4H8O	000627-27-0	49
4		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	17
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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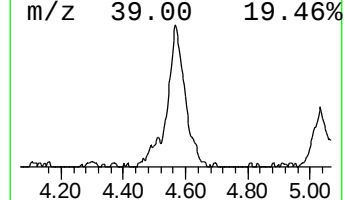
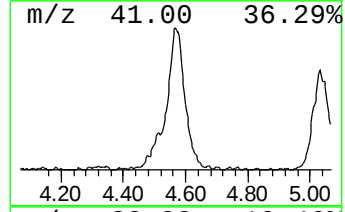
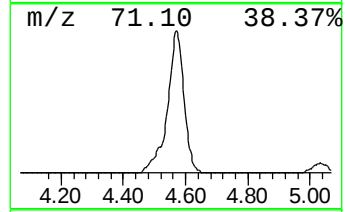
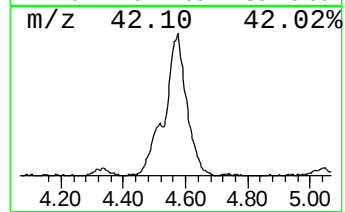
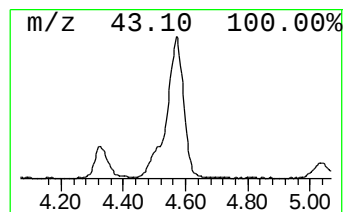
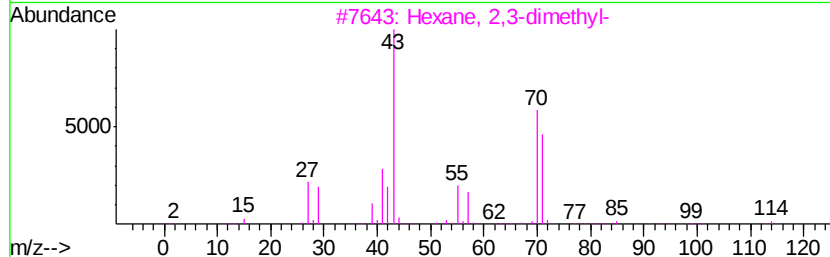
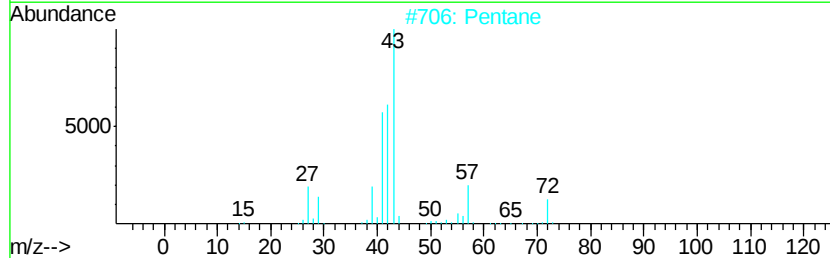
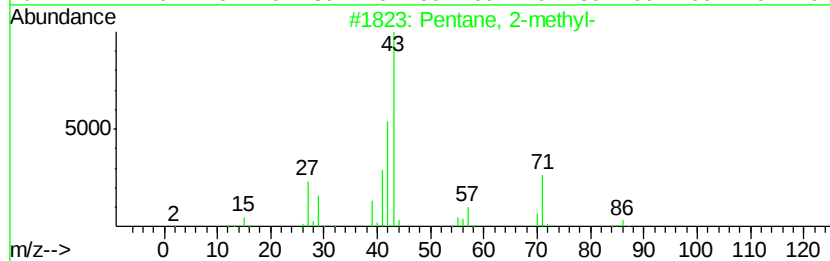
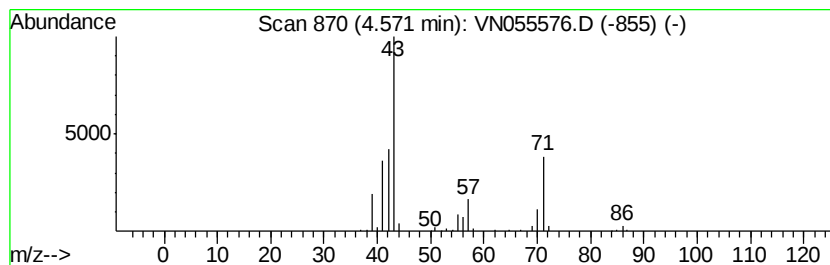
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	8.79 ug/l	443761	Pentafluorobenzene	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2		Pentane	72	C5H12	000109-66-0	38
3		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	33
4		Pentanal, 2-methyl-	100	C6H12O	000123-15-9	25
5		Butane, 2-methyl-	72	C5H12	000078-78-4	17



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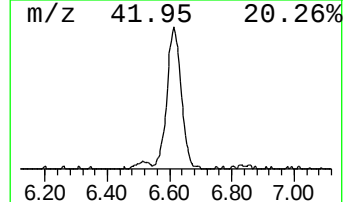
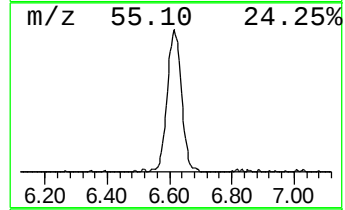
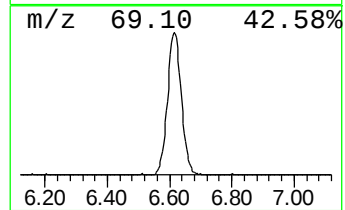
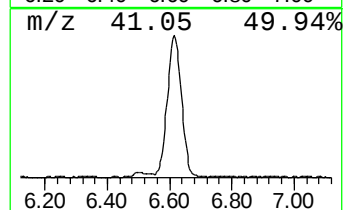
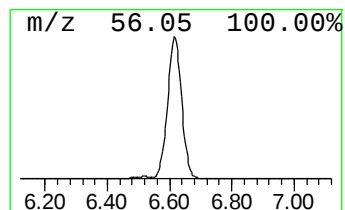
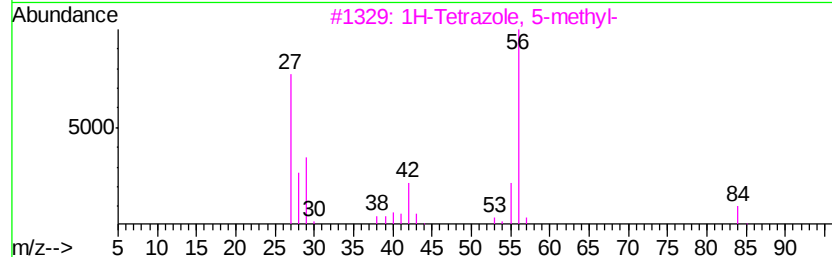
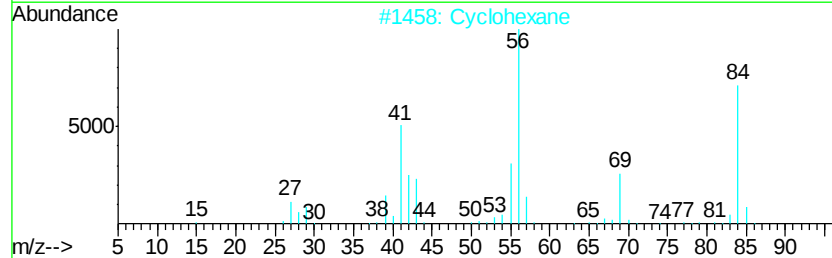
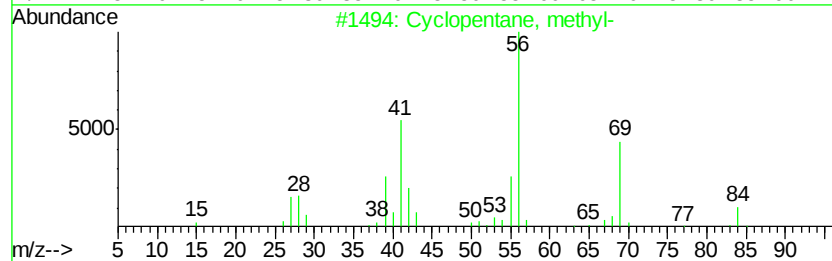
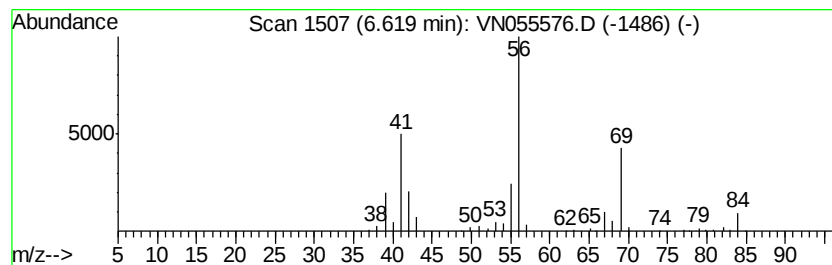
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	11.40 ug/l	575278	Pentafluorobenzene	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		Cyclohexane	84	C6H12	000110-82-7	78
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43



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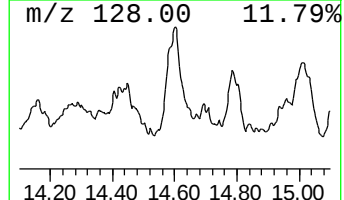
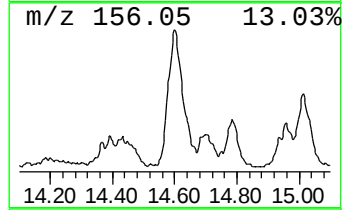
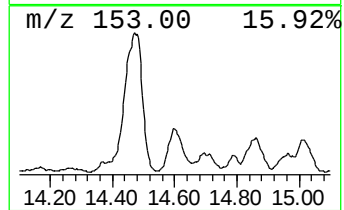
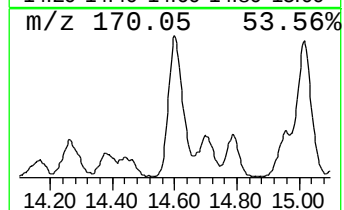
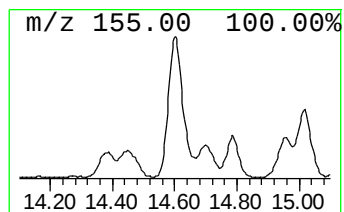
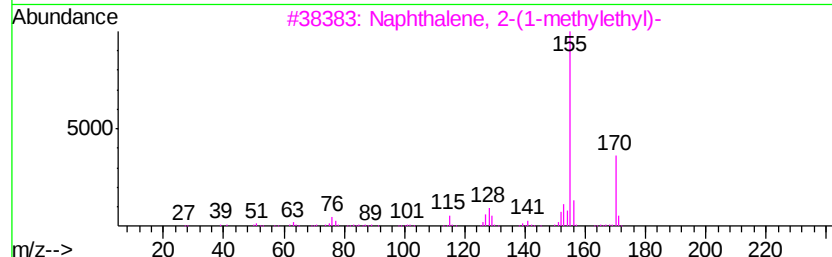
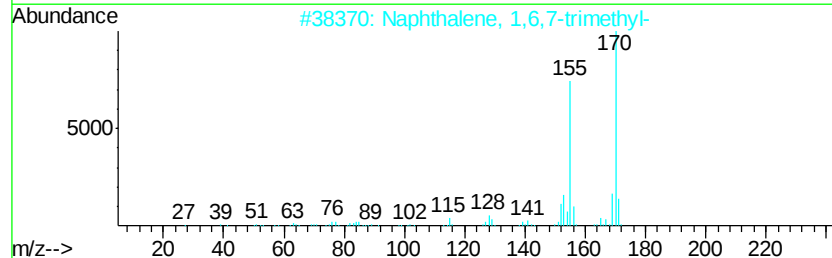
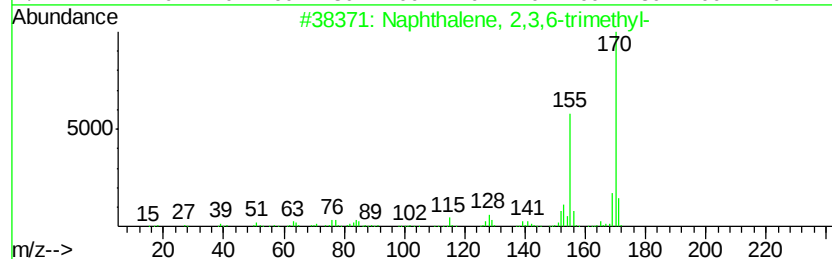
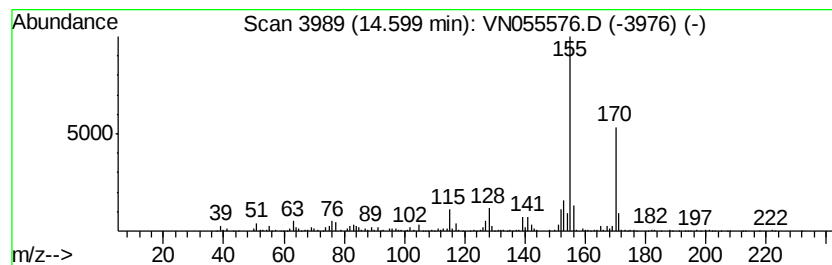
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Peak Number 4 Naphthalene, 2,3,6-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	18.51 ug/l	1347190	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, 2,3,6-trimethyl-	170 C13H14	000829-26-5 94
2		Naphthalene, 1,6,7-trimethyl-	170 C13H14	002245-38-7 91
3		Naphthalene, 2-(1-methylethyl)-	170 C13H14	002027-17-0 91
4		4,6,8-Trimethylazulene	170 C13H14	000941-81-1 76
5		2-Naphthyl methyl ketone	170 C12H10O	000093-08-3 72



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	2.75	13.7	ug/l	690324	1	7.66	2523830	50.0
Pentane, 2-methyl-	4.57	8.8	ug/l	443761	1	7.66	2523830	50.0
Cyclopentane, met...	6.62	11.4	ug/l	575278	1	7.66	2523830	50.0
Naphthalene, 2,3,...	14.60	18.5	ug/l	1347190	4	13.34	3639510	50.0