

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA G\DATA\BG121417\
 Data File : BG031570.D
 Acq On : 14 Dec 2017 22:18
 Operator : SJ/JU
 Sample : I6884-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FB-20171211

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:\HPCHEM1\BNA_G\METHODS\8270-BG121117.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.560	211	216	228	rBV	133909	226855	3.57%	1.001%
2	5.177	311	321	334	rBV	1876486	2951383	46.45%	13.021%
3	5.665	398	404	422	rBV2	119981	239523	3.77%	1.057%
4	7.275	672	678	689	rBV	88945	185863	2.93%	0.820%
5	7.633	732	739	749	rBV	316815	621936	9.79%	2.744%
6	8.097	812	818	829	rBV	229462	411517	6.48%	1.816%
7	8.421	864	873	883	rBV	878017	1594530	25.10%	7.035%
8	8.755	923	930	944	rBV2	31125	71101	1.12%	0.314%
9	9.267	1008	1017	1037	rBV	554463	1104426	17.38%	4.873%
10	10.912	1290	1297	1305	rBV	260658	549536	8.65%	2.424%
11	13.344	1704	1711	1732	rBV	2040144	3280165	51.62%	14.472%
12	14.725	1937	1946	1963	rBV3	472133	829811	13.06%	3.661%
13	16.229	2197	2202	2212	rBV2	57077	118737	1.87%	0.524%
14	17.469	2406	2413	2427	rBV2	666867	1161842	18.29%	5.126%
15	20.060	2848	2854	2865	rBV	4643548	6353841	100.00%	28.032%
16	21.734	3133	3139	3153	rBV2	880980	1583668	24.92%	6.987%
17	25.019	3685	3698	3716	rBV2	435768	1381336	21.74%	6.094%

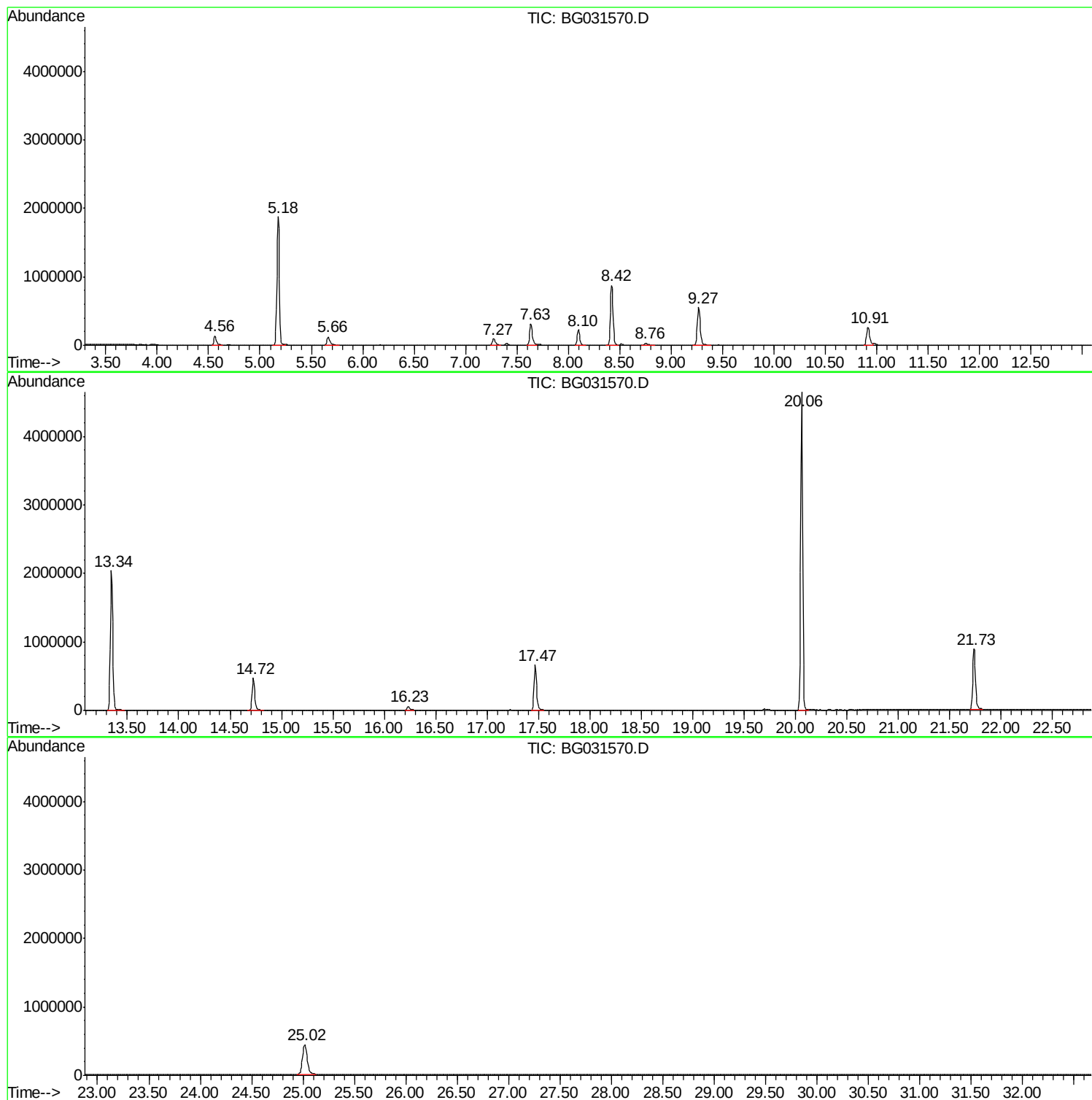
Sum of corrected areas: 22666070

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



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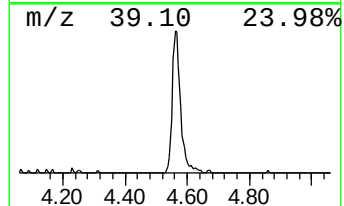
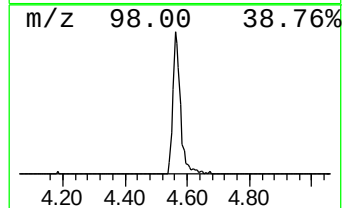
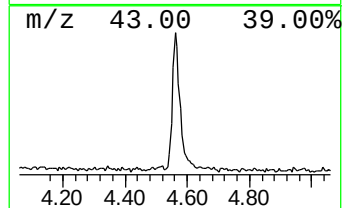
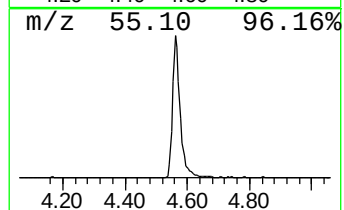
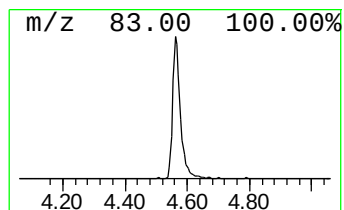
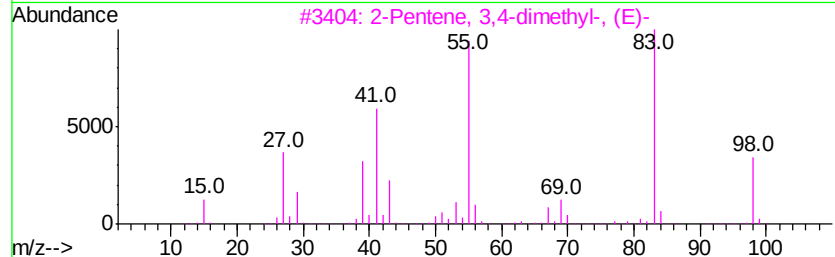
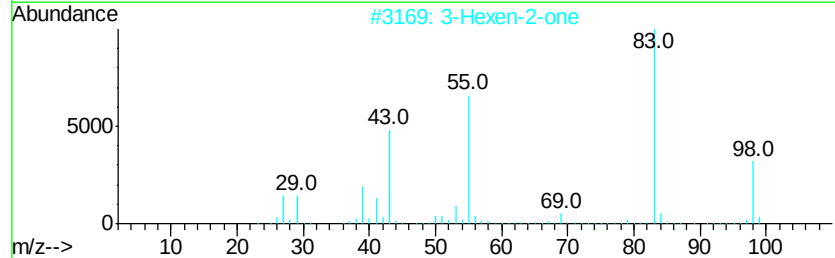
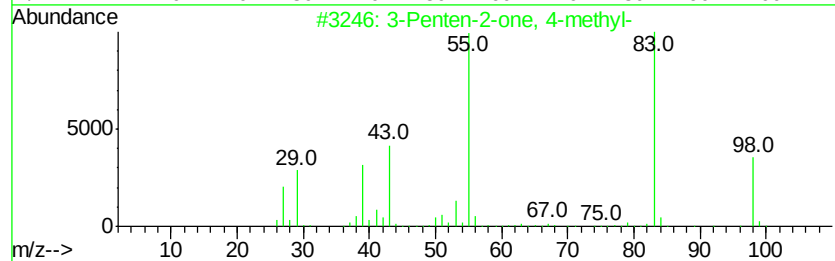
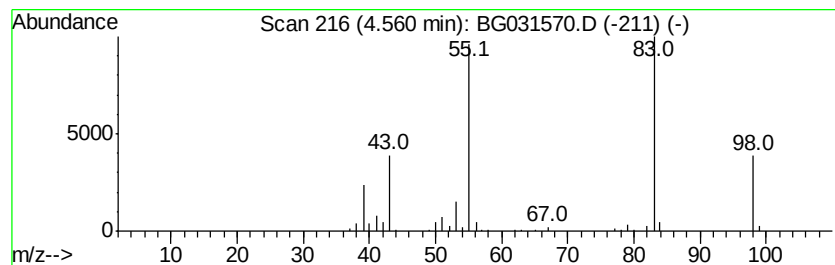
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	11.03 ng	226855	1,4-Dichlorobenzene-d4	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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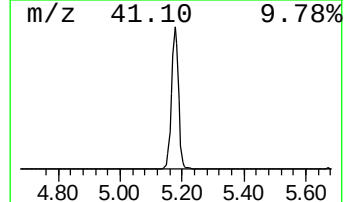
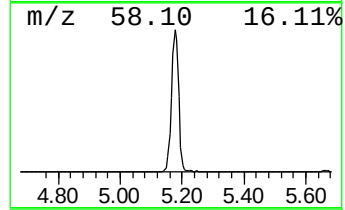
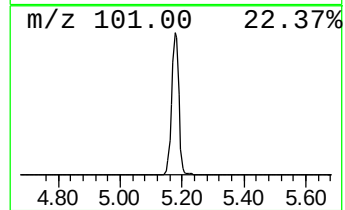
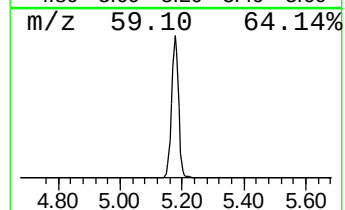
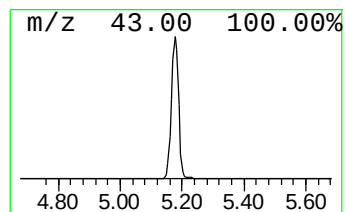
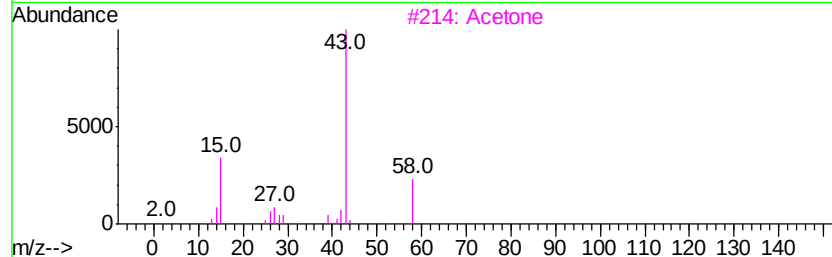
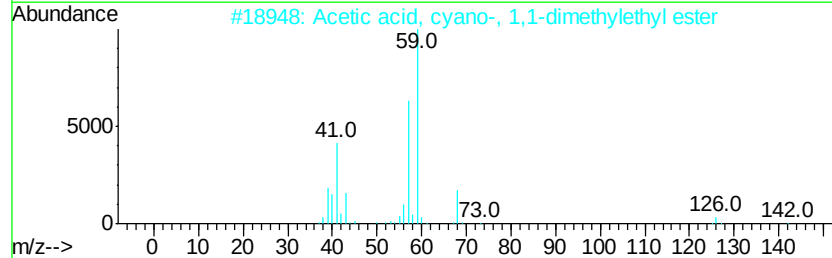
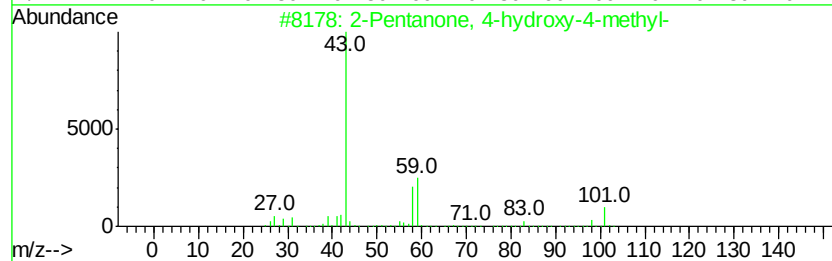
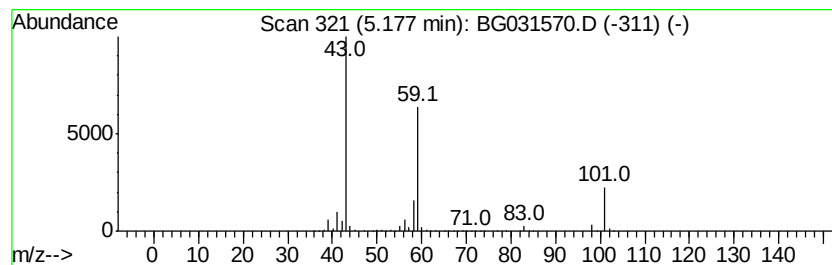
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	143.44 ng	2951380	1,4-Dichlorobenzene-d4	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Acetone	58	C3H6O	000067-64-1	10
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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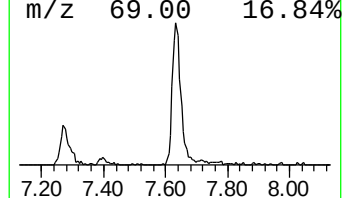
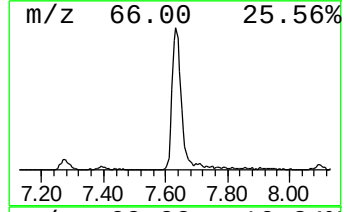
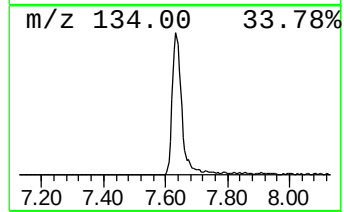
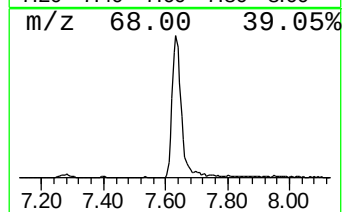
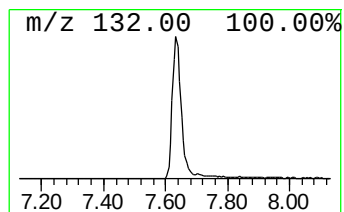
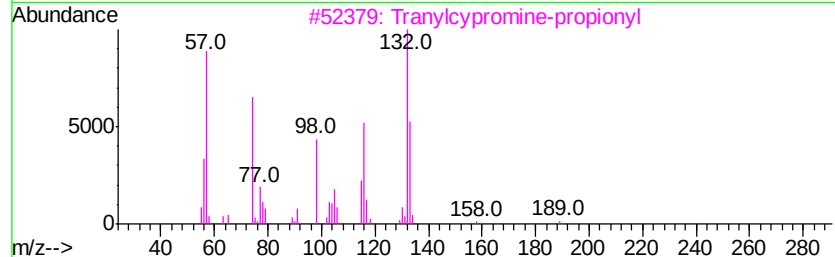
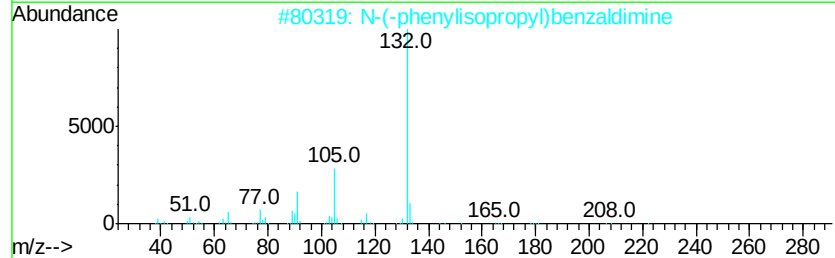
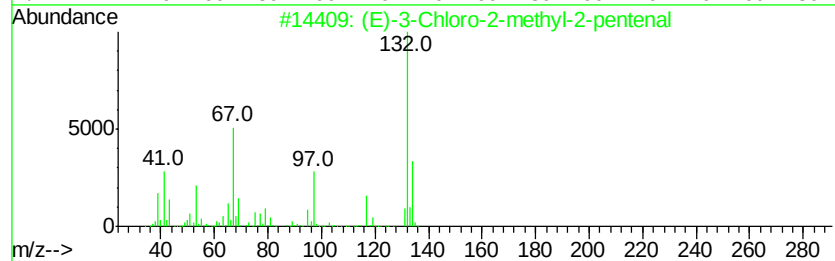
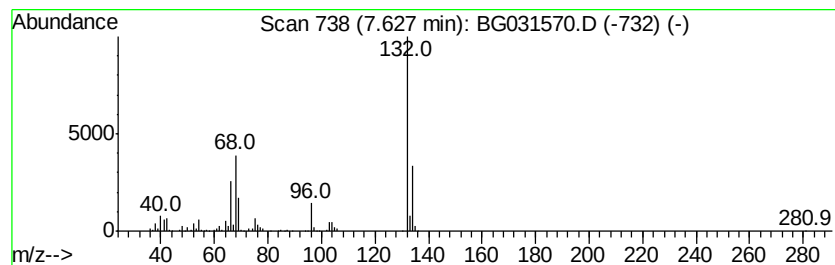
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Peak Number 3 unknown7.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	30.23 ng	621936	1,4-Dichlorobenzene-d4	8.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35	
2	N-(-phenylisopropyl)benzalimine	223	C16H17N	1000379-01-3	12	
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12	
4	4-Ethylphenyl isocyanate	147	C9H9NO	023138-50-3	10	
5	3H-Benzo[4,5]imidazo[1,2-c]oxazo...	218	C12H14N2O2	1000316-99-9	10	



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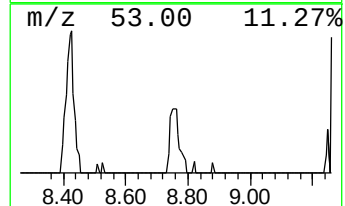
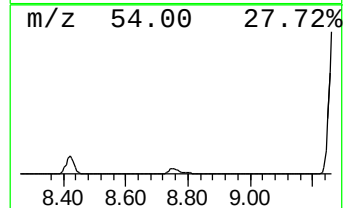
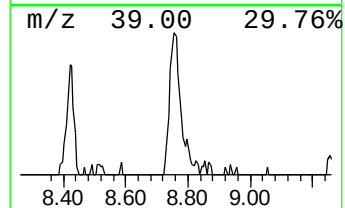
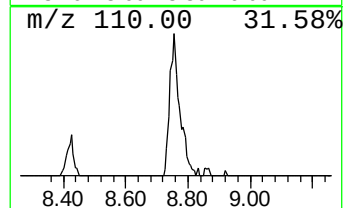
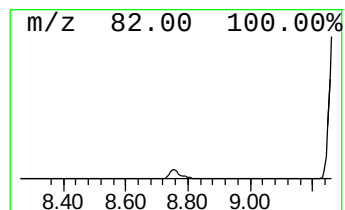
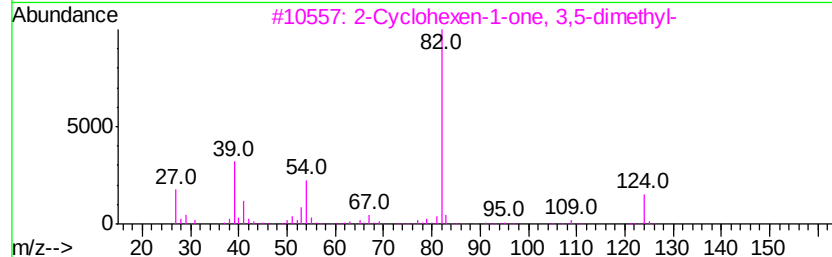
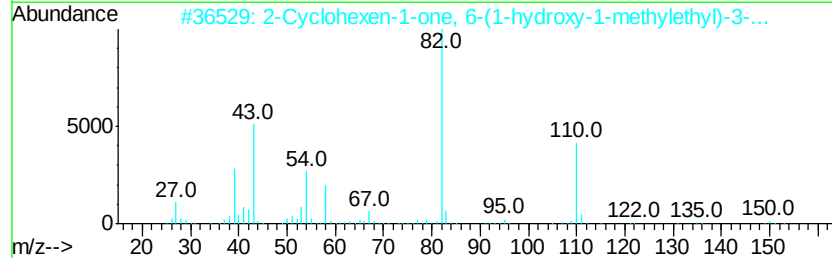
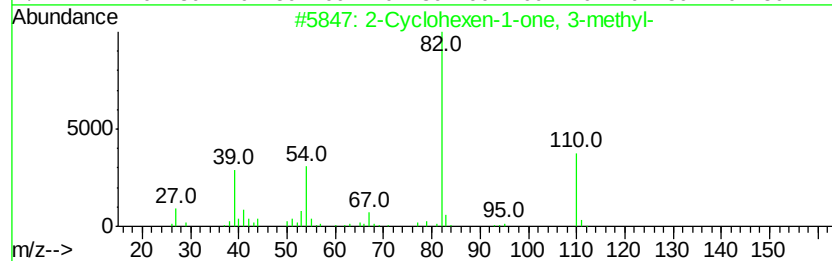
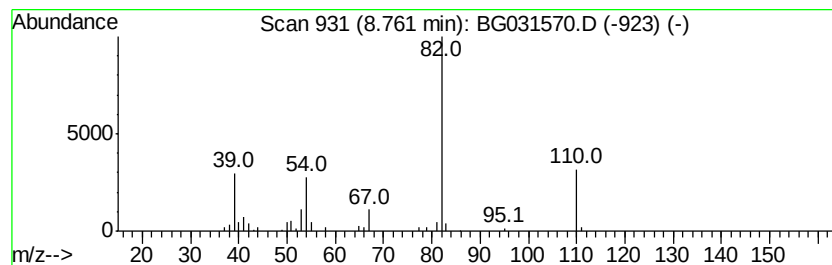
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Peak Number 5 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.76	3.46 ng	71101	1,4-Dichlorobenzene-d4	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2		2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	74
3		2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	59
4		Furan, 3-methyl-	82	C5H6O	000930-27-8	47
5		1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.56	11.0	ng	226855	1	8.10	411517	20.0
2-Pentanone, 4-hy...	5.18	143.4	ng	2951380	1	8.10	411517	20.0
unknown7.63	7.63	30.2	ng	621936	1	8.10	411517	20.0
2-Cyclohexen-1-on...	8.76	3.5	ng	71101	1	8.10	411517	20.0