

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG121517\
 Data File : BG031595.D
 Acq On : 15 Dec 2017 19:36
 Operator : SJ/JU
 Sample : PB105059BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB105059BL

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	3.941	105	111	116	rBV	44533	69543	1.21%	0.294%
2	4.558	211	216	224	rBV	61349	100834	1.76%	0.426%
3	5.169	312	320	332	rBV	218254	346191	6.03%	1.463%
4	5.656	396	403	423	rBV	900153	1558316	27.16%	6.587%
5	7.266	670	677	700	rVB	902059	1643033	28.64%	6.945%
6	7.631	732	739	754	rBV	943561	1659943	28.93%	7.017%
7	8.095	811	818	829	rBV	187826	330777	5.77%	1.398%
8	8.424	865	874	886	rBV	710221	1310329	22.84%	5.539%
9	9.264	1010	1017	1036	rBV	478629	978572	17.06%	4.137%
10	10.915	1290	1298	1316	rBV	219353	482467	8.41%	2.039%
11	13.347	1704	1712	1732	rBV	1683782	2801216	48.83%	11.841%
12	14.229	1856	1862	1869	rBV	49907	94702	1.65%	0.400%
13	14.722	1940	1946	1960	rBV2	395987	737152	12.85%	3.116%
14	16.209	2193	2199	2216	rBV	1283192	2204674	38.43%	9.319%
15	17.466	2407	2413	2430	rBV2	657520	1093838	19.07%	4.624%
16	20.063	2848	2855	2867	rBV	4084394	5737043	100.00%	24.251%
17	21.738	3133	3140	3155	rBV2	824912	1479019	25.78%	6.252%
18	25.028	3688	3700	3716	rBV	325929	1028957	17.94%	4.350%

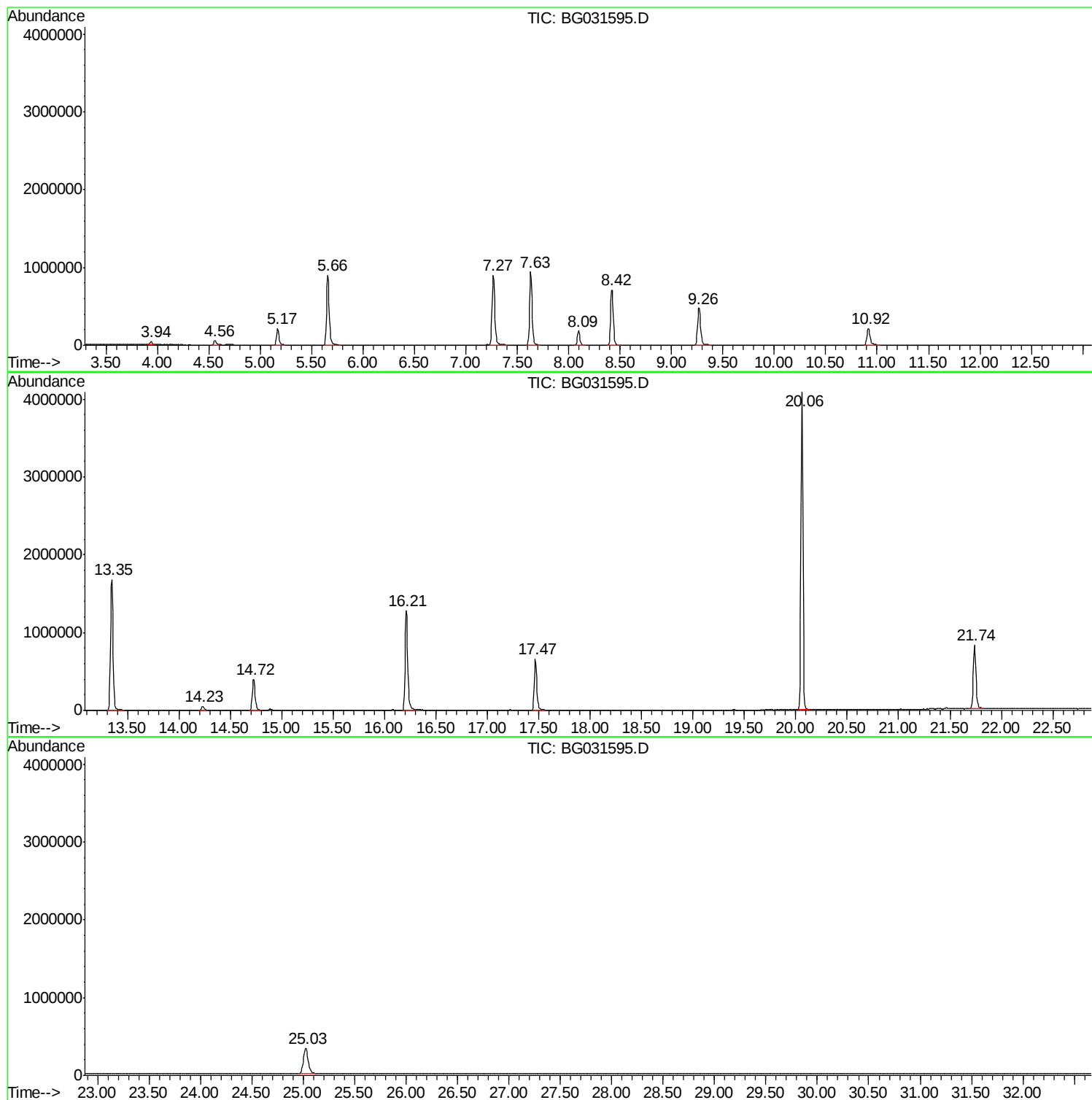
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG121117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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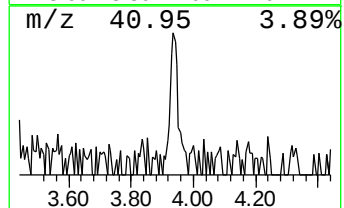
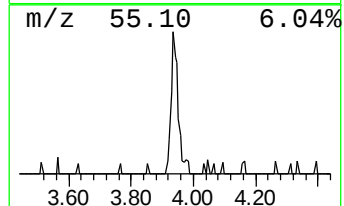
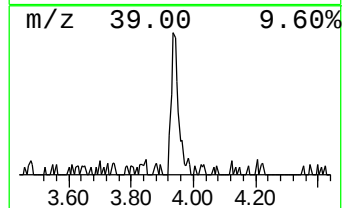
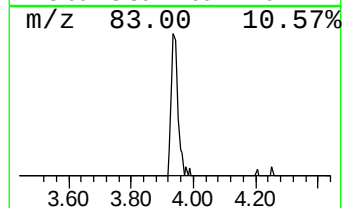
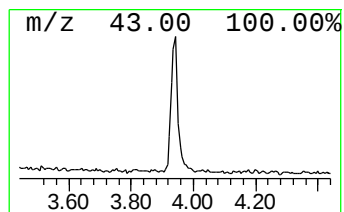
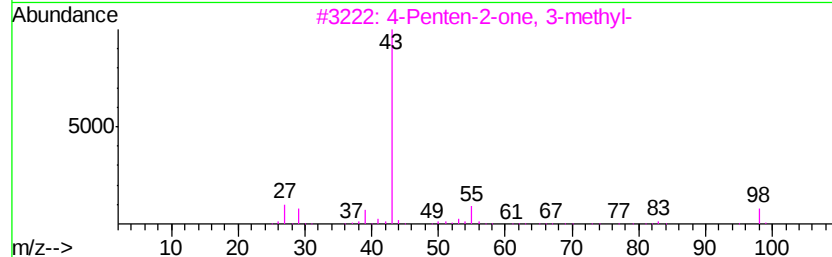
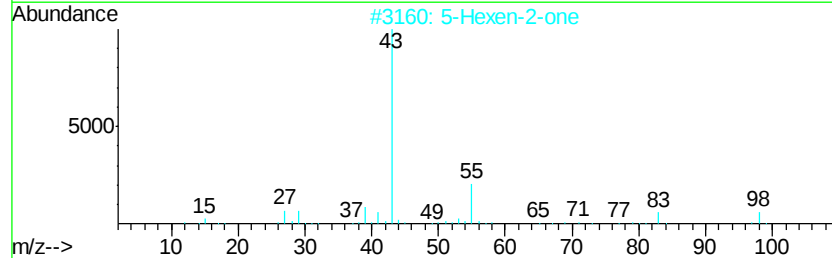
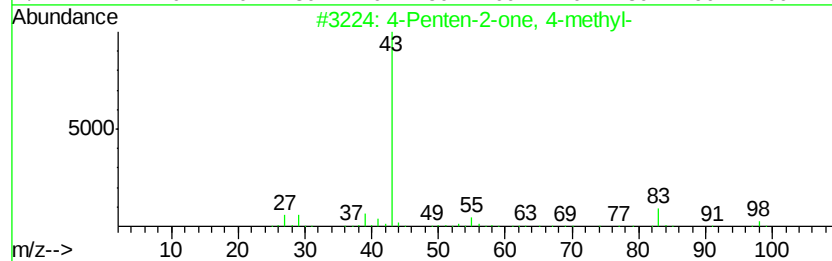
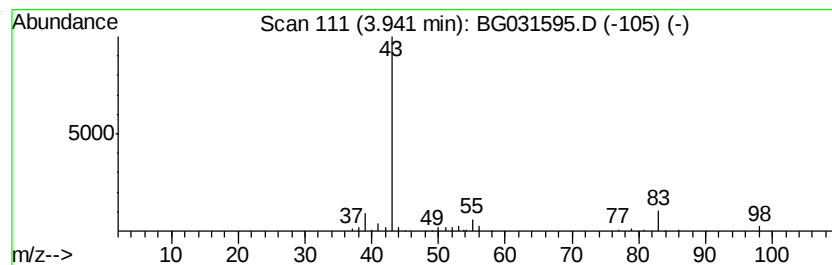
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG121117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.94	4.20 ng	69543	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2		5-Hexen-2-one	98	C6H10O	000109-49-9	38
3		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	37
4		3,5-Hexadien-2-ol	98	C6H10O	003280-51-1	9
5		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9



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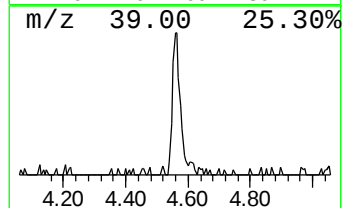
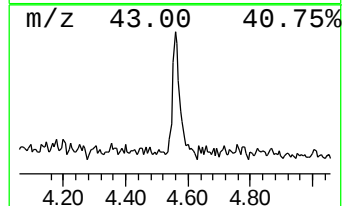
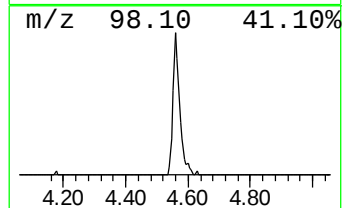
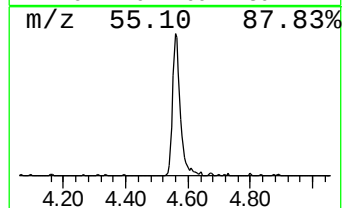
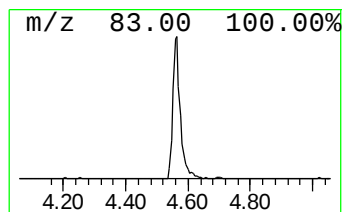
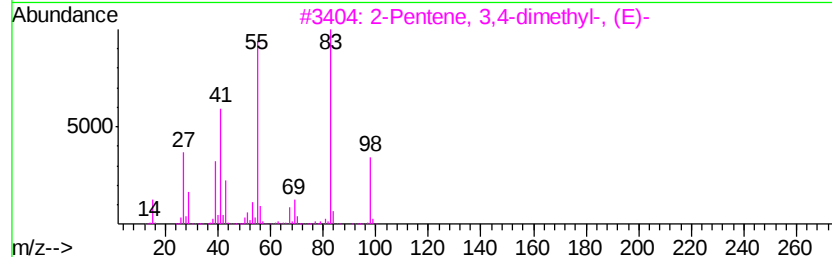
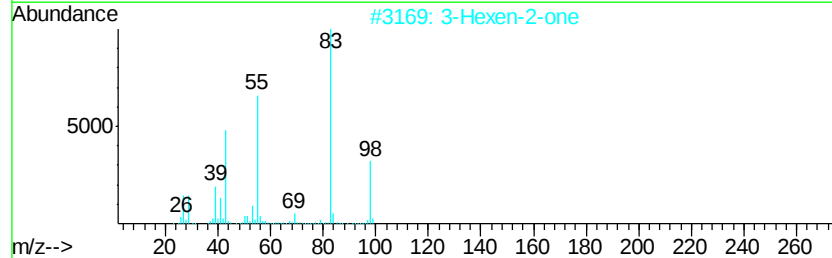
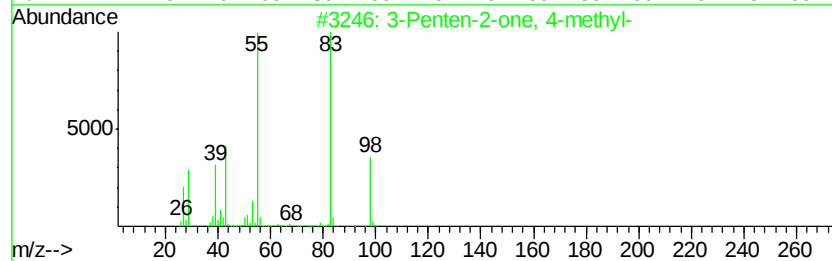
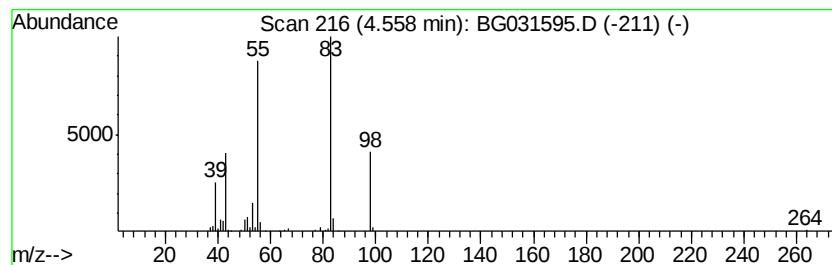
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	6.10 ng	100834	1,4-Dichlorobenzene-d4	8.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
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, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	83



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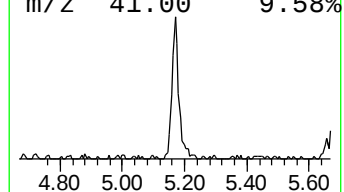
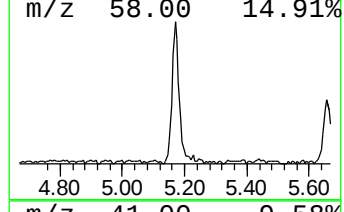
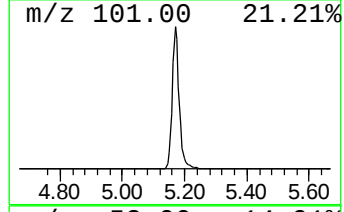
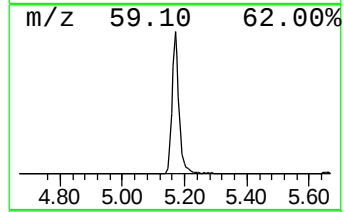
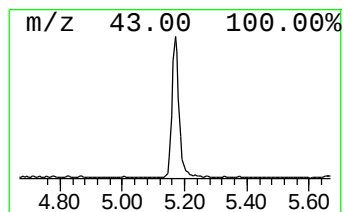
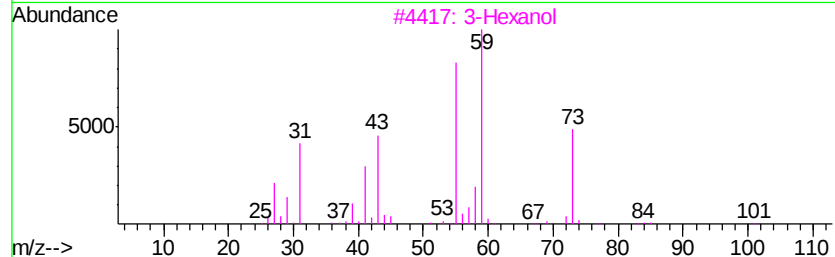
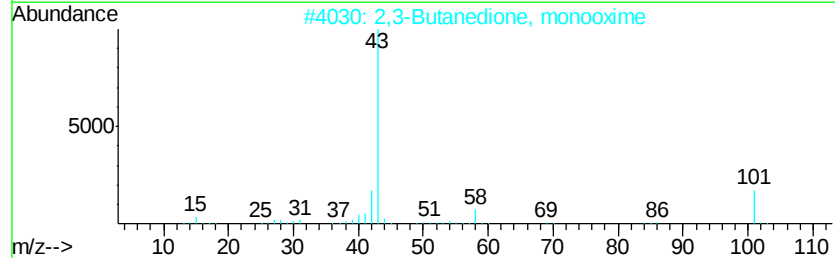
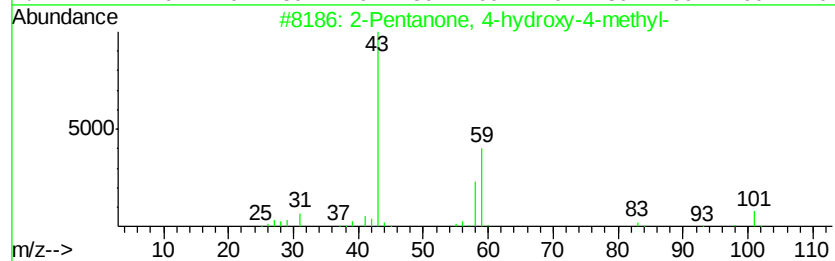
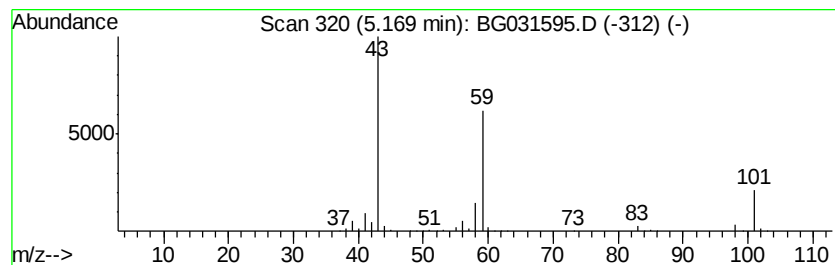
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	20.93 ng	346191	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		3-Hexanol	102	C6H14O	000623-37-0	28
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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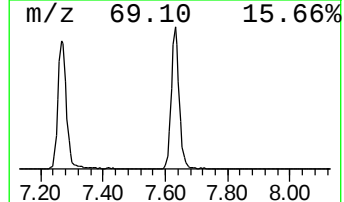
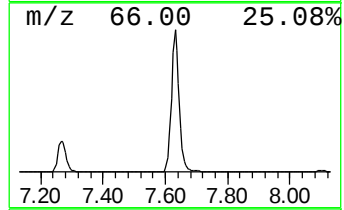
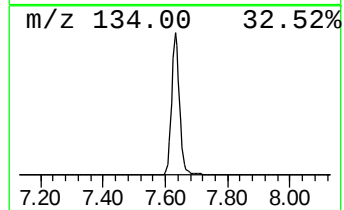
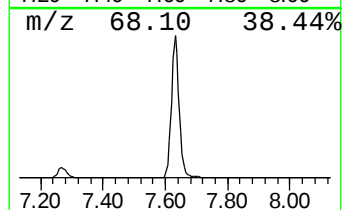
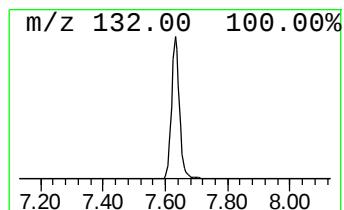
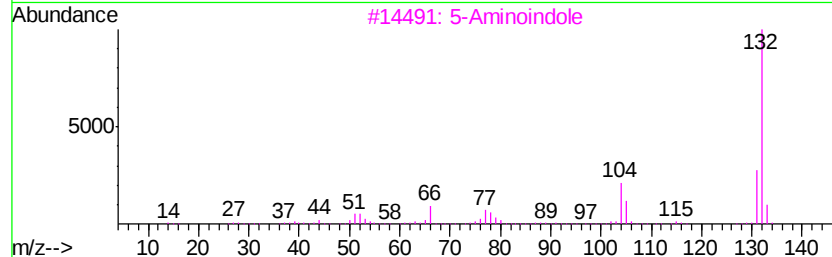
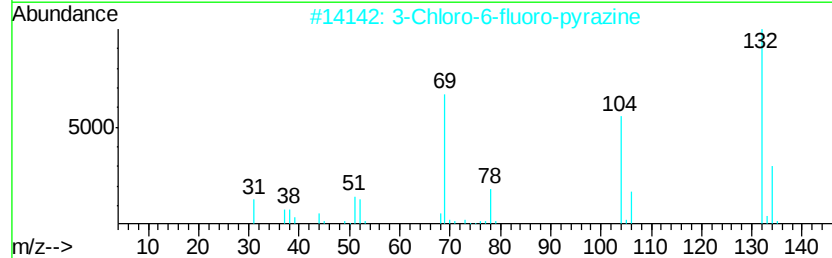
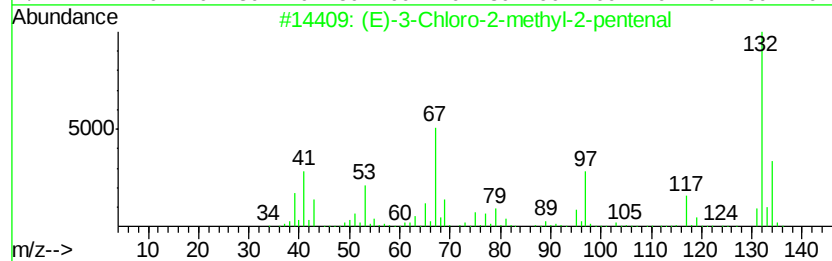
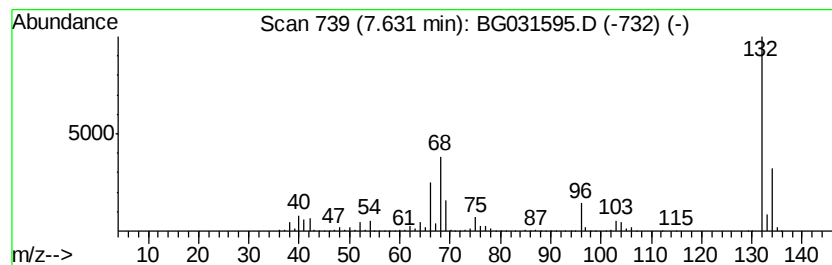
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Peak Number 4 unknown7.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	100.37 ng	1659940	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		N-(-phenylisopropyl)benzalimine	223	C16H17N	1000379-01-3	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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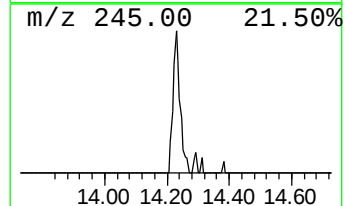
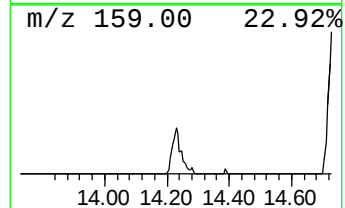
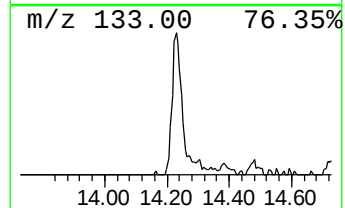
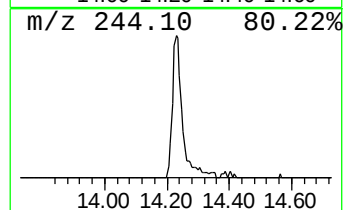
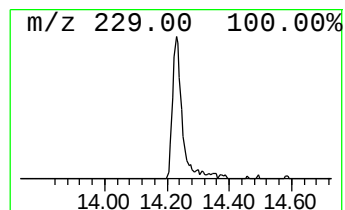
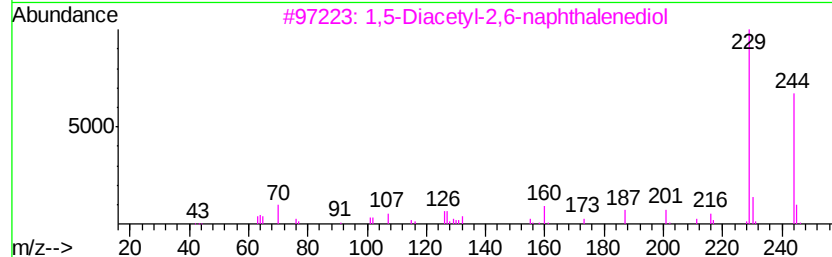
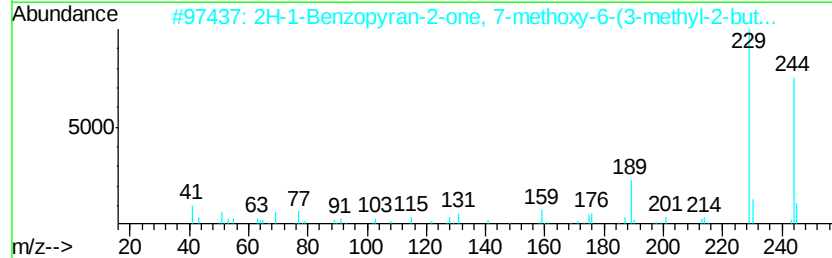
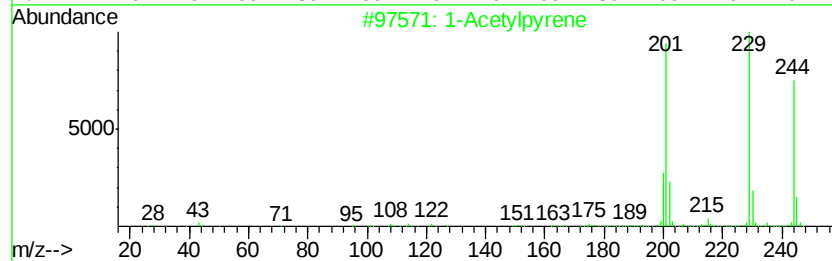
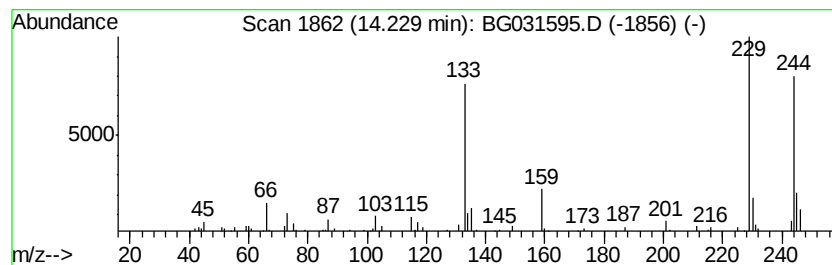
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown14.23 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.23	2.57 ng	94702	Acenaphthene-d10		14.72
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Acetylpyrene	244	C18H12O	003264-21-9	47
2	2H-1-Benzopyran-2-one, 7-methoxy...	244	C15H16O3	000581-31-7	46
3	1,5-Diacetyl-2,6-naphthalenediol	244	C14H12O4	038790-70-4	43
4	Isoquinoline-1-carbonitrile, 3,4...	244	C14H16N2O2	1000277-26-5	43
5	Silane, diethylpropoxy(trans-4-m...	258	C14H30O2Si	1000363-56-3	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one, 4...	3.94	4.2	ng	69543	1	8.09	330777	20.0
3-Penten-2-one, 4...	4.56	6.1	ng	100834	1	8.09	330777	20.0
2-Pentanone, 4-hy...	5.17	20.9	ng	346191	1	8.09	330777	20.0
unknown7.63	7.63	100.4	ng	1659940	1	8.09	330777	20.0
unknown14.23	14.23	2.6	ng	94702	3	14.72	737152	20.0