

Data Path : Z:\HPCHEM1\BNA N\DATA\BN040918\
 Data File : BN000719.D
 Acq On : 09 Apr 2018 20:52
 Operator : JU/SJ
 Sample : J2268-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MH-33

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:\HPCHEM1\BNA_N\METHODS\8270-BN040918.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	4.811	305	310	317	rBV	98431	134216	1.99%	0.350%
2	5.263	380	387	396	rVB	1011328	1440571	21.37%	3.760%
3	5.552	430	436	442	rBV	119330	167129	2.48%	0.436%
4	5.711	457	463	468	rBV	332135	481796	7.15%	1.257%
5	6.058	516	522	533	rBV2	43494	79963	1.19%	0.209%
6	6.810	641	650	660	rBV	584530	910793	13.51%	2.377%
7	7.175	704	712	720	rBV	1860620	2877704	42.69%	7.511%
8	7.634	783	790	797	rBV	596277	909732	13.50%	2.374%
9	7.875	826	831	837	rBV	111904	197823	2.93%	0.516%
10	7.952	837	844	852	rVB	2581511	4050631	60.09%	10.572%
11	8.781	977	985	997	rVB	2073509	3305833	49.04%	8.628%
12	10.399	1253	1260	1267	rBV	755594	1245774	18.48%	3.251%
13	12.887	1676	1683	1694	rVB	4529227	6740550	100.00%	17.592%
14	13.728	1822	1826	1831	rBV	51679	68487	1.02%	0.179%
15	14.263	1911	1917	1924	rVV2	958185	1446373	21.46%	3.775%
16	14.328	1924	1928	1936	rVB	54765	75450	1.12%	0.197%
17	15.757	2164	2171	2180	rBV	1906243	2681080	39.78%	6.997%
18	17.010	2378	2384	2389	rBV2	1080055	1515370	22.48%	3.955%
19	17.051	2389	2391	2397	rVB	134288	156423	2.32%	0.408%
20	17.933	2537	2541	2546	rBV	68336	103231	1.53%	0.269%
21	19.075	2731	2735	2740	rBV	60854	78204	1.16%	0.204%
22	19.663	2829	2835	2844	rBV	5360989	6615908	98.15%	17.267%
23	20.969	3053	3057	3065	rBV2	61366	119292	1.77%	0.311%
24	21.216	3093	3099	3104	rBV	1172705	1482445	21.99%	3.869%
25	23.404	3464	3471	3484	rVB2	772113	1430632	21.22%	3.734%

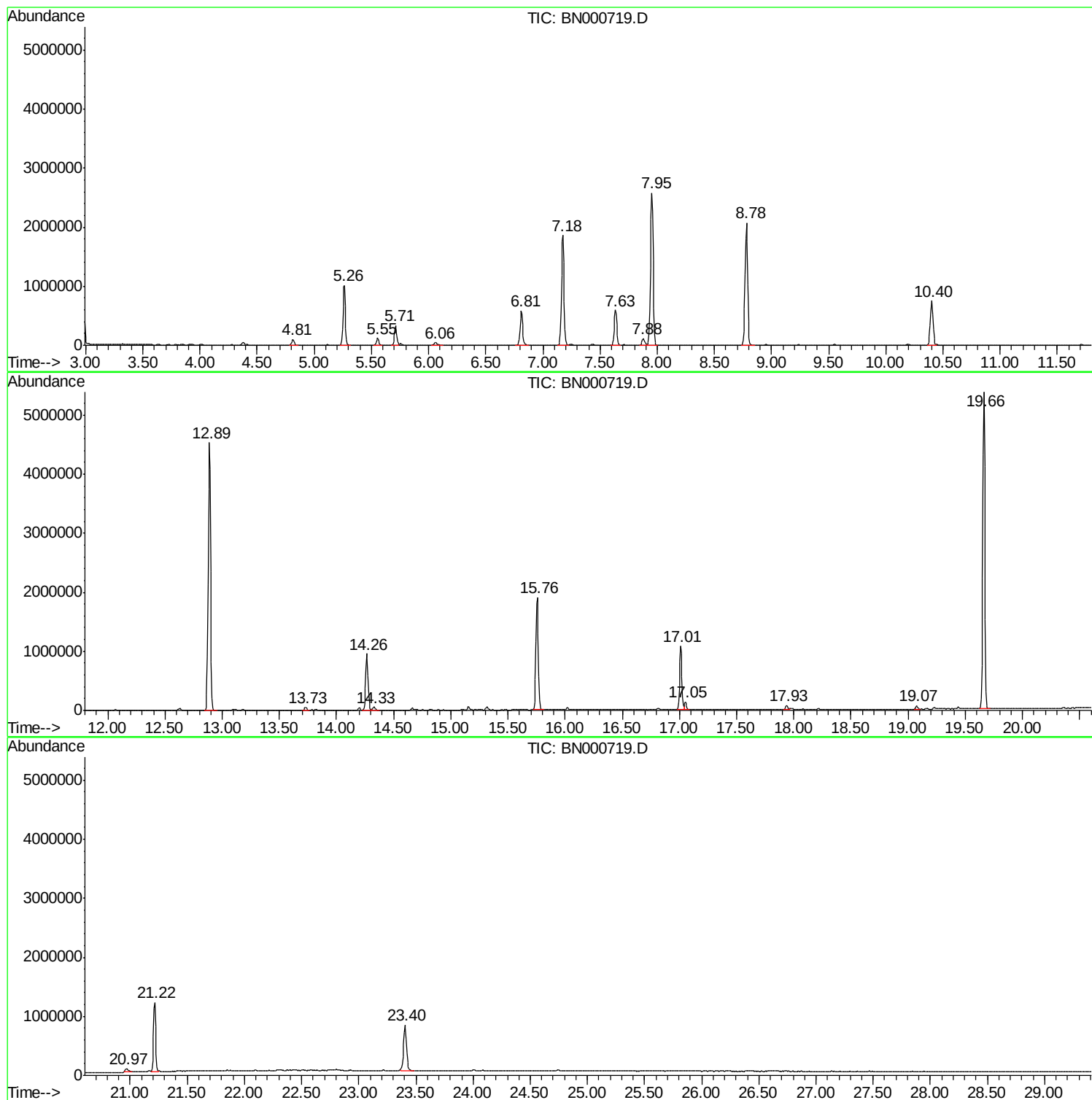
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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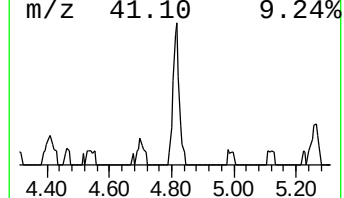
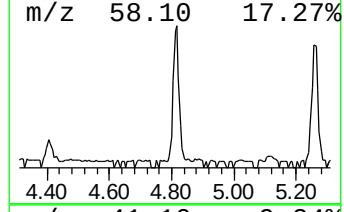
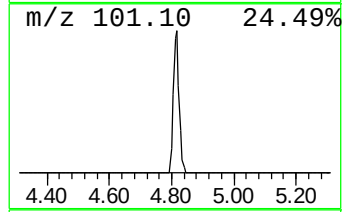
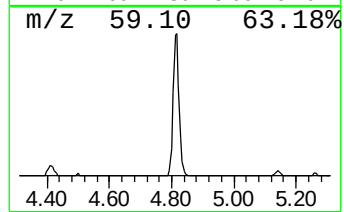
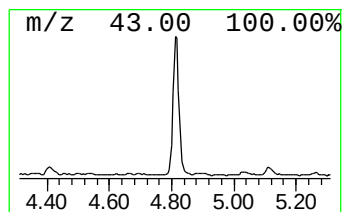
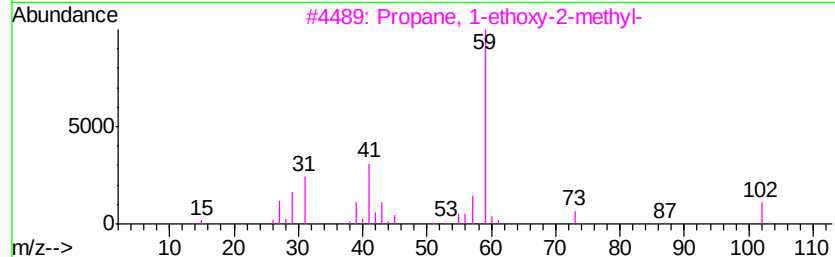
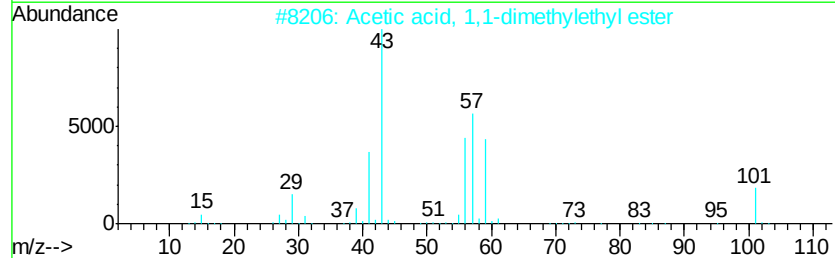
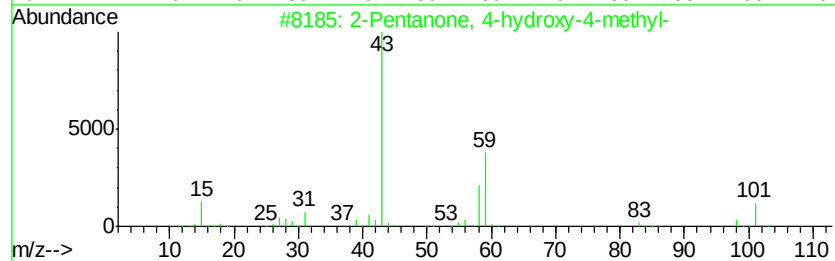
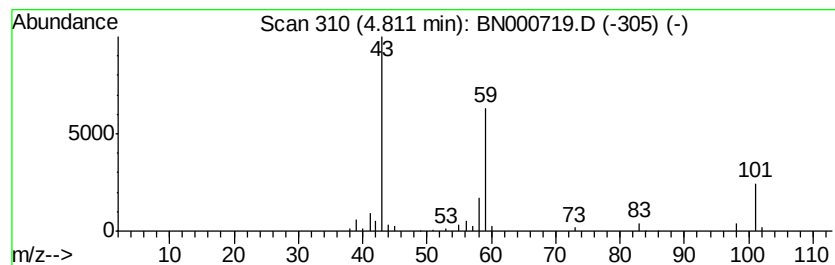
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	2.95 ng	134216	1,4-Dichlorobenzene-d4	7.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
4			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25



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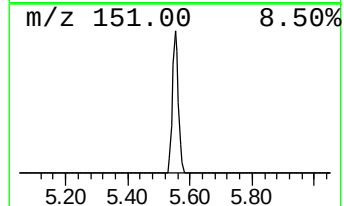
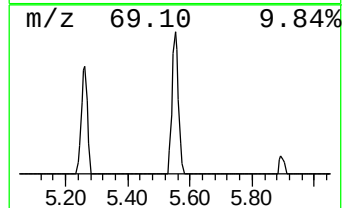
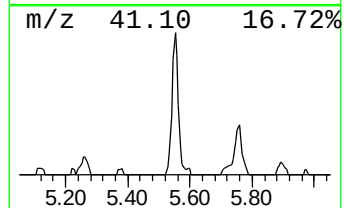
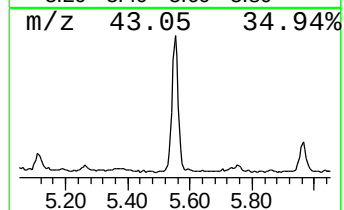
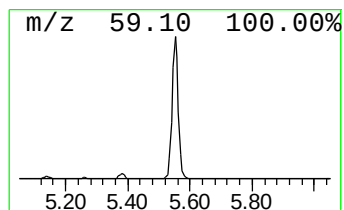
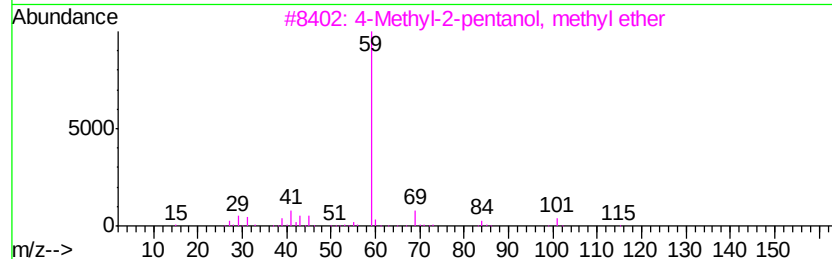
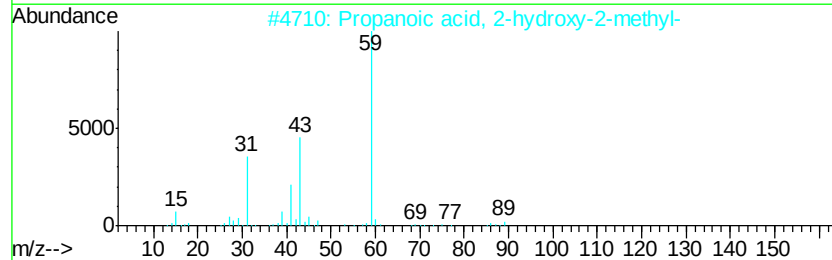
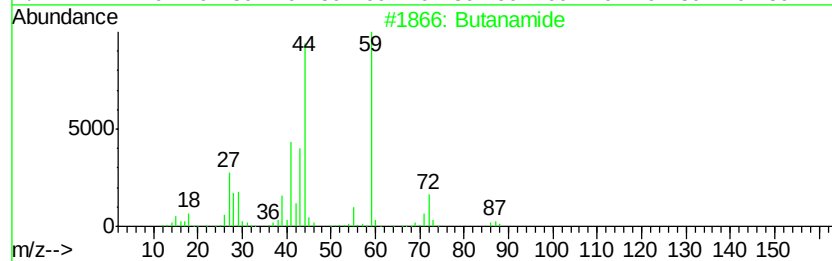
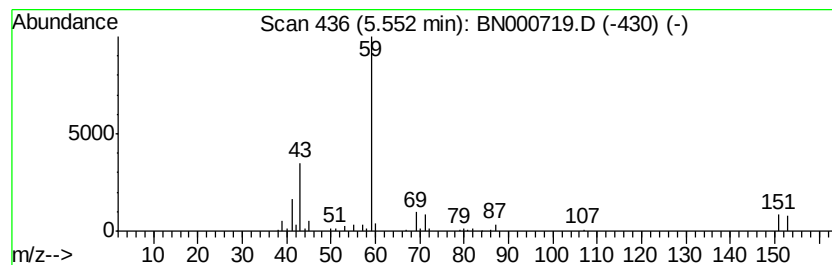
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Peak Number 2 Butanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.55	3.67 ng	167129	1,4-Dichlorobenzene-d4	7.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanamide		87	C4H9NO	000541-35-5	64
2	Propanoic acid, 2-hydroxy-2-methyl-		104	C4H8O3	000594-61-6	53
3	4-Methyl-2-pentanol, methyl ether		116	C7H16O	1000333-93-5	50
4	2-Hexanone, 3-hydroxy-3,5-dimethyl-		144	C8H16O2	006321-14-8	50
5	2-Methyl-3-bromo-2-butanol		166	C5H11BrO	002588-77-4	47



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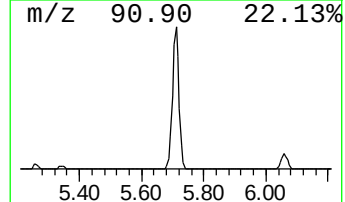
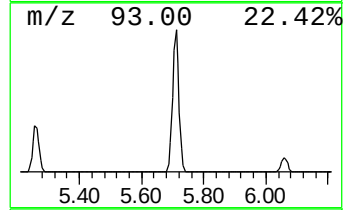
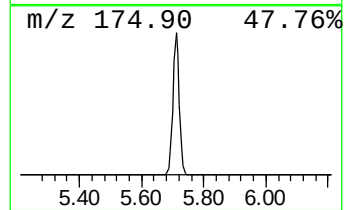
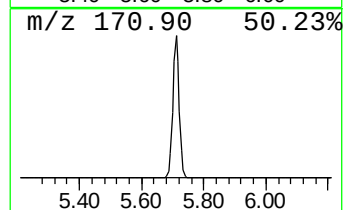
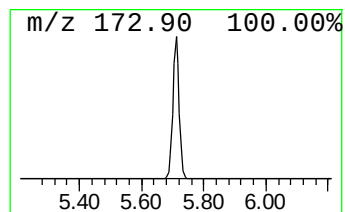
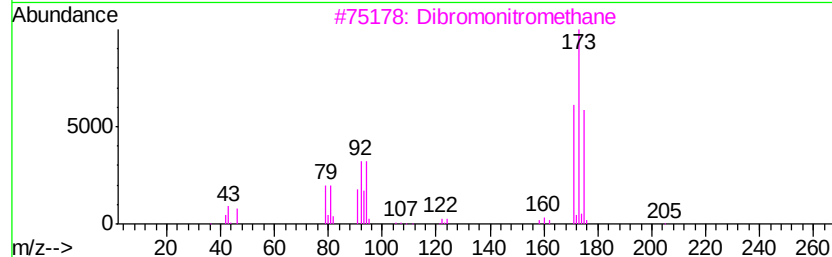
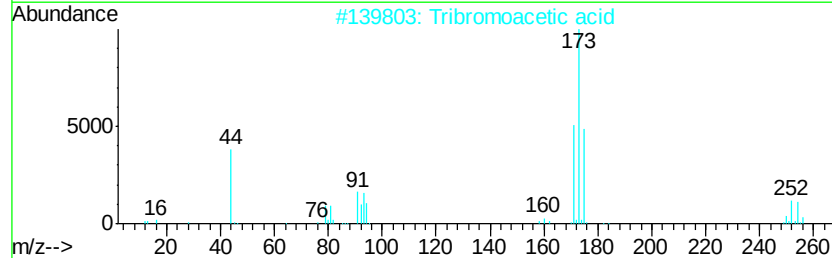
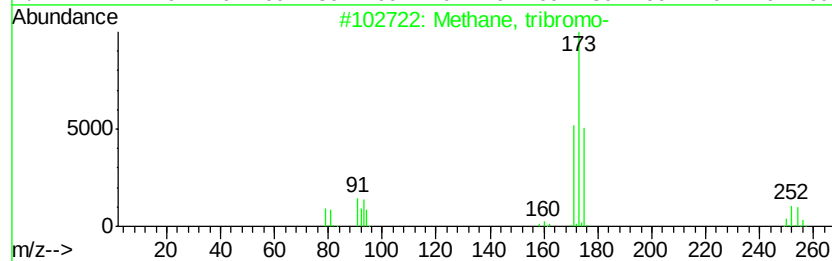
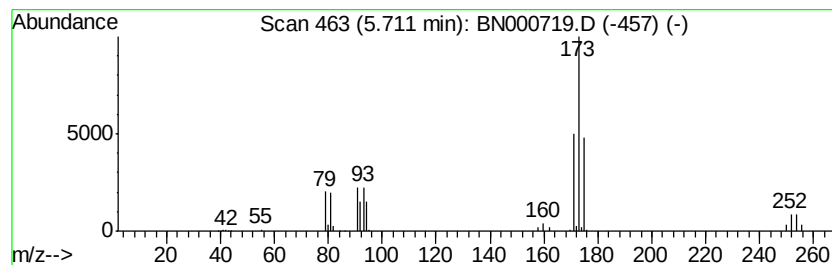
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Peak Number 3 Methane, tribromo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.71	10.59 ng	481796	1,4-Dichlorobenzene-d4	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methane, tribromo-	250	CHBr3	000075-25-2	97
2		Tribromoacetic acid	294	C2HBr3O2	000075-96-7	86
3		Dibromonitromethane	217	CHBr2NO2	000598-91-4	40
4		5-Chloro-6-hydroxynicotinic acid	173	C6H4ClNO3	054127-63-8	25
5		Chromone, 2-methyl-3-bromomethyl-	252	C11H9BrO2	117970-61-3	12



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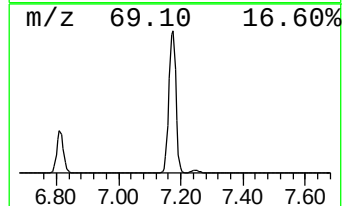
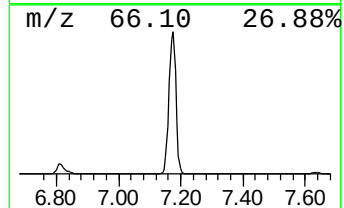
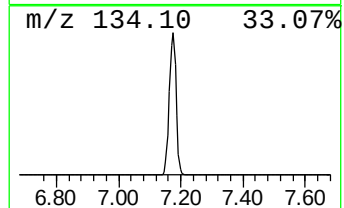
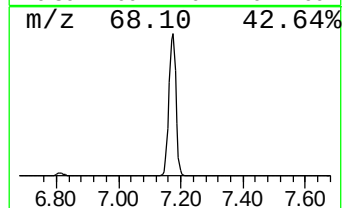
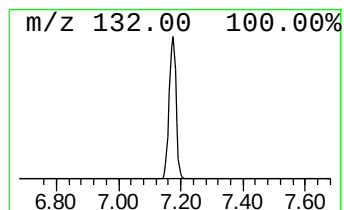
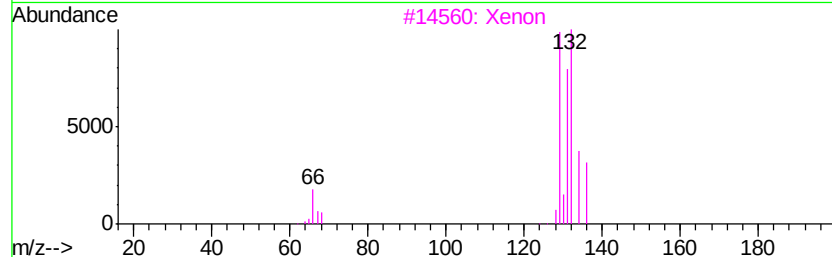
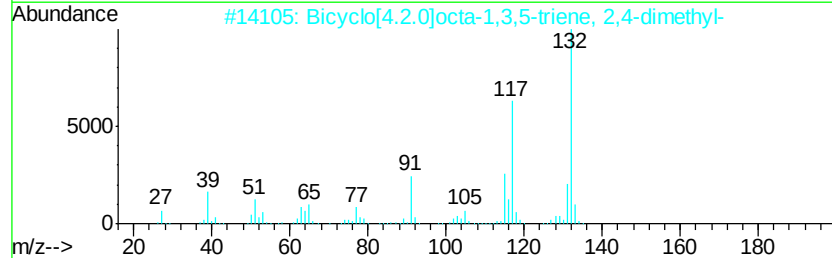
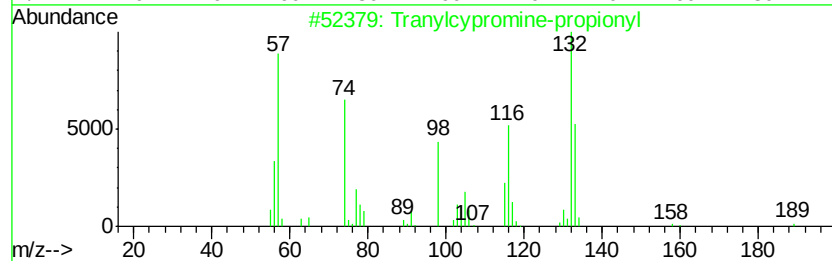
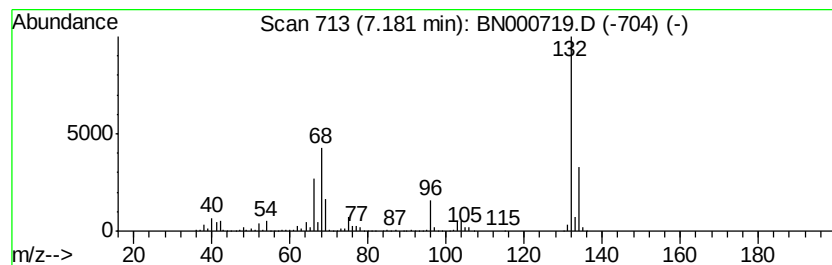
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Peak Number 4 unknown7.18 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.18	63.26 ng	2877700	1,4-Dichlorobenzene-d4	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		Xenon	132	Xe	007440-63-3	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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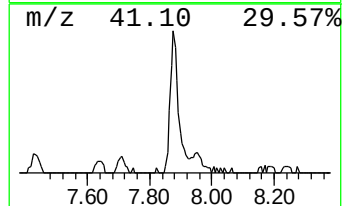
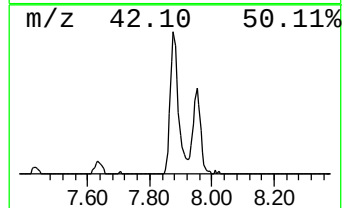
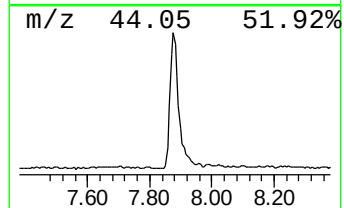
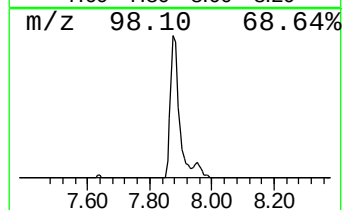
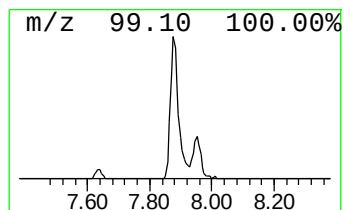
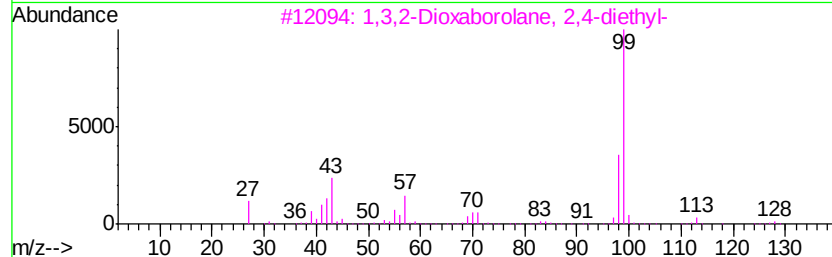
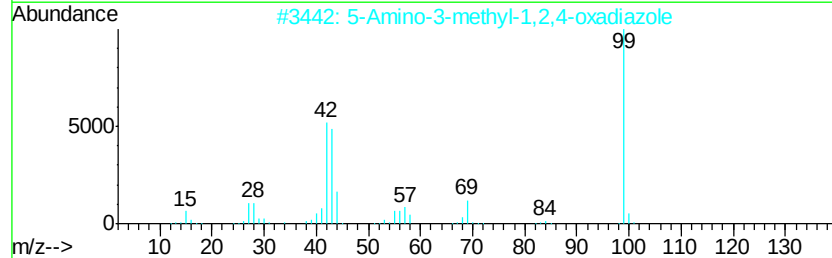
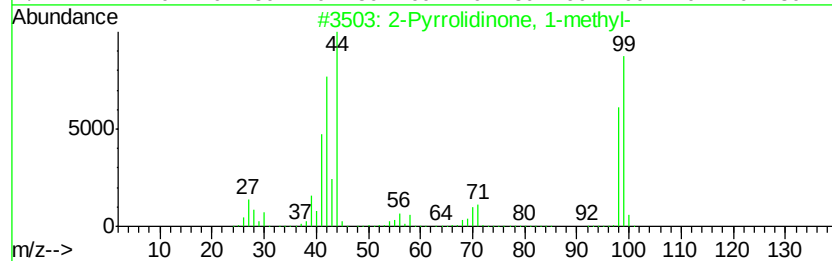
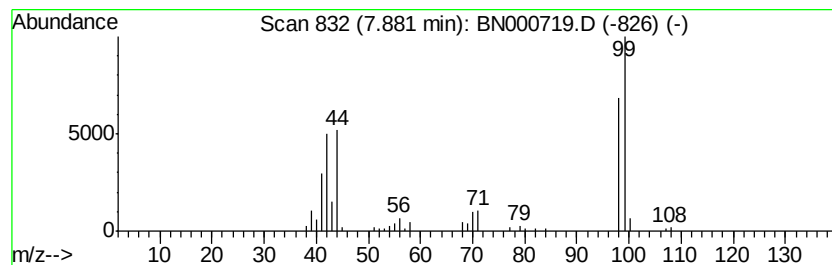
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Peak Number 5 2-Pyrrolidinone, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.88	4.35 ng	197823	1,4-Dichlorobenzene-d4	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	91
2		5-Amino-3-methyl-1,2,4-oxadiazole	99	C3H5N3O	003663-39-6	47
3		1,3,2-Dioxaborolane, 2,4-diethyl-	128	C6H13BO2	057633-63-3	38
4		Imidosulfurous difluoride, methyl-	99	CH3F2NS	000758-20-3	37
5		4-Piperidone	99	C5H9NO	041661-47-6	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.81	3.0	ng	134216	1	7.63	909732	20.0
Butanamide	5.55	3.7	ng	167129	1	7.63	909732	20.0
Methane, tribromo-	5.71	10.6	ng	481796	1	7.63	909732	20.0
unknown7.18	7.18	63.3	ng	2877700	1	7.63	909732	20.0
2-Pyrrolidinone, ...	7.88	4.3	ng	197823	1	7.63	909732	20.0