

Data Path : Z:\HPCHEM1\BNA N\DATA\BN021918\
 Data File : BN000116.D
 Acq On : 19 Feb 2018 18:46
 Operator : JU/SJ
 Sample : J1573-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW-4

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_N\METHODS\8270-BN020718.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	3.234	37	42	51	rBV	313889	604865	1.90%	0.392%
2	3.316	51	56	77	rVB	2859544	4862695	15.30%	3.148%
3	5.440	411	417	428	rVB2	238016	399856	1.26%	0.259%
4	5.934	493	501	512	rBV	3324481	5368311	16.89%	3.475%
5	6.046	514	520	528	rVB	244522	414007	1.30%	0.268%
6	7.581	768	781	792	rBV	2259785	3797445	11.95%	2.458%
7	7.975	840	848	857	rBV	6667839	11214666	35.28%	7.260%
8	8.457	922	930	943	rBV	1526411	2570683	8.09%	1.664%
9	8.787	978	986	998	rVB	6010535	10361149	32.59%	6.708%
10	9.640	1120	1131	1139	rBV	5286979	8993881	28.29%	5.822%
11	11.298	1406	1413	1420	rBV	2488957	4226504	13.30%	2.736%
12	13.698	1813	1821	1832	rBV	15137589	22612209	71.13%	14.639%
13	15.069	2047	2054	2062	rBV2	3820298	5886610	18.52%	3.811%
14	16.533	2297	2303	2324	rBV	10365776	15761645	49.58%	10.204%
15	17.786	2509	2516	2522	rBV2	5034342	7315773	23.01%	4.736%
16	18.621	2654	2658	2667	rBV2	296082	455212	1.43%	0.295%
17	20.345	2945	2951	2960	rBV	24777436	31788101	100.00%	20.579%
18	21.898	3209	3215	3221	rBV2	6515398	8997002	28.30%	5.824%
19	24.380	3629	3637	3649	rVB2	4156010	8839936	27.81%	5.723%

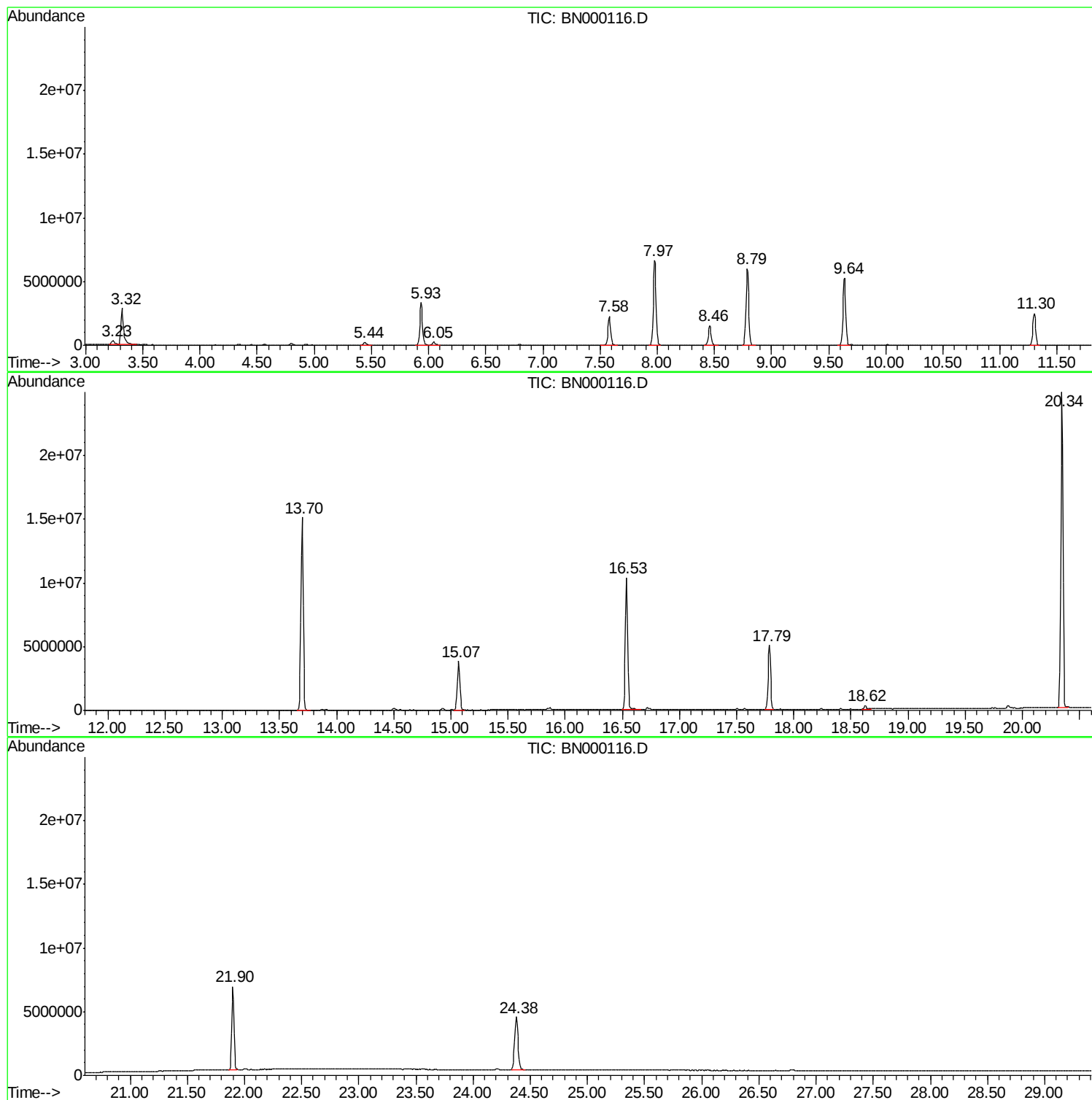
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Quant Method : Z:\HPCHEM1\BNA N\METHODS\8270-BN020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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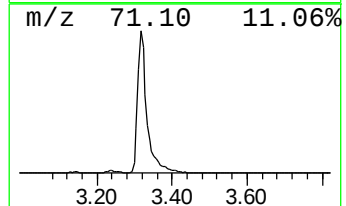
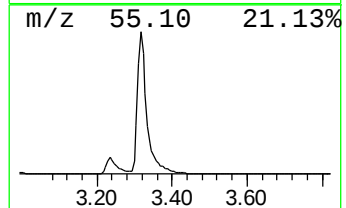
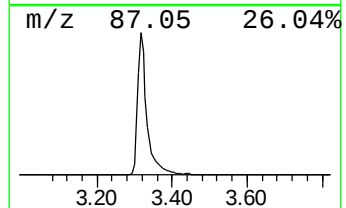
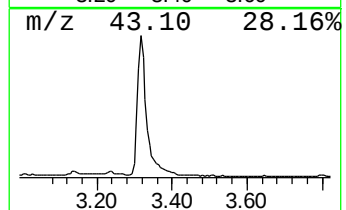
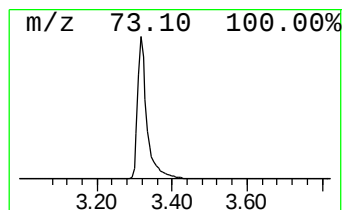
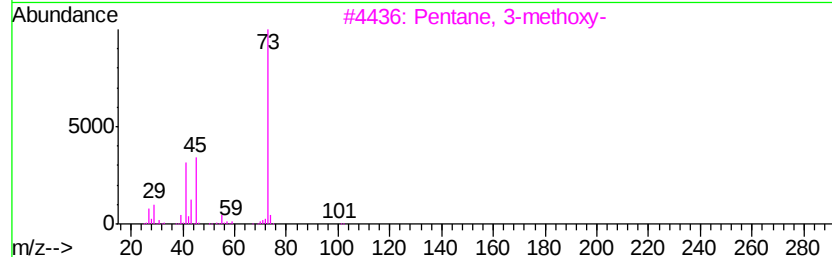
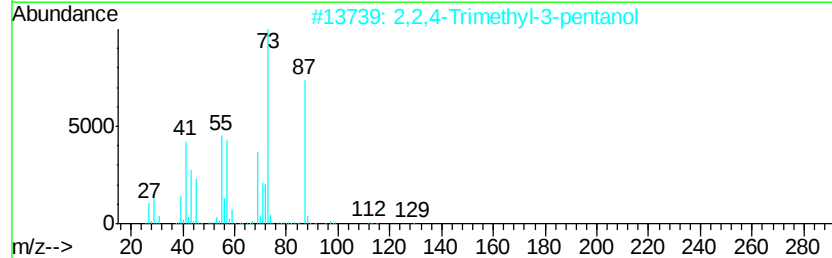
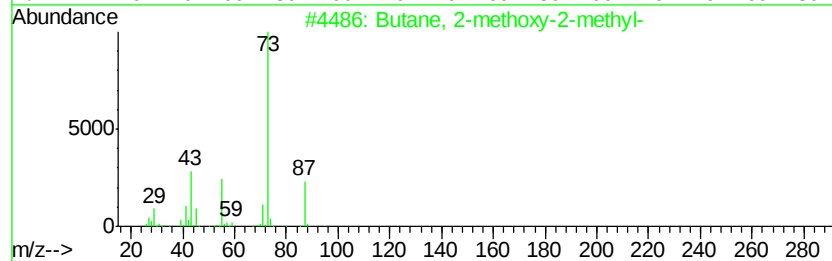
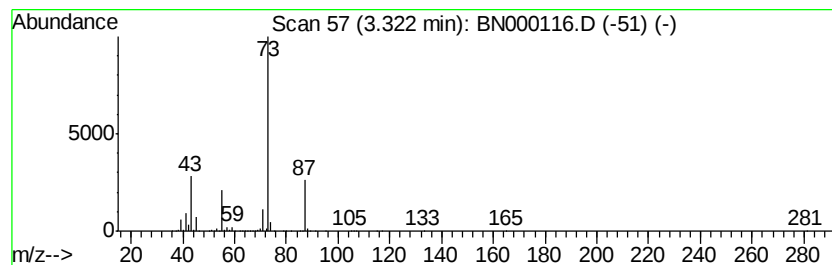
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.32	37.83 ng	4862700	1,4-Dichlorobenzene-d4	8.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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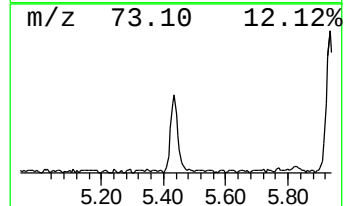
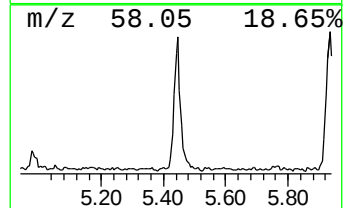
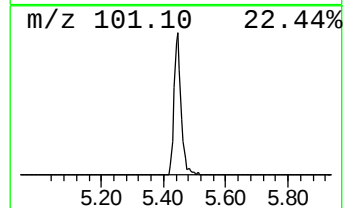
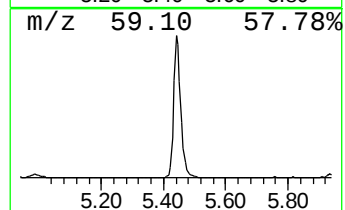
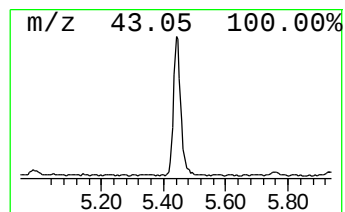
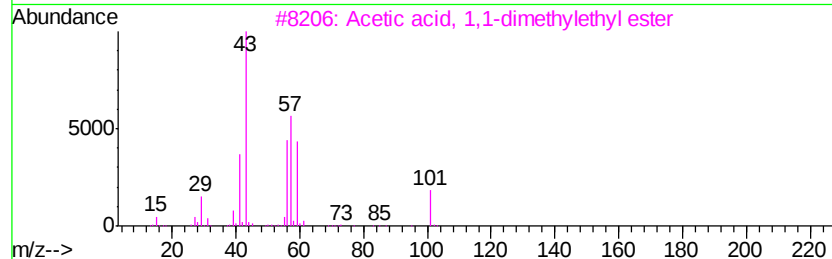
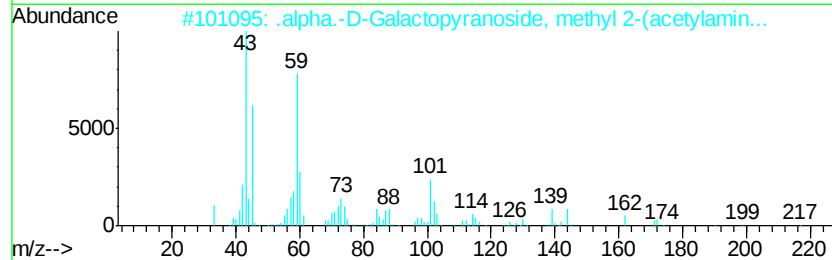
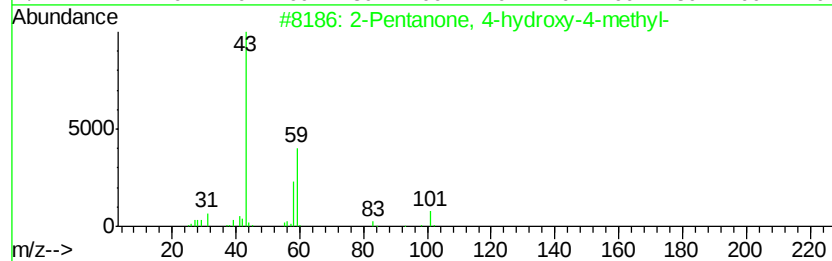
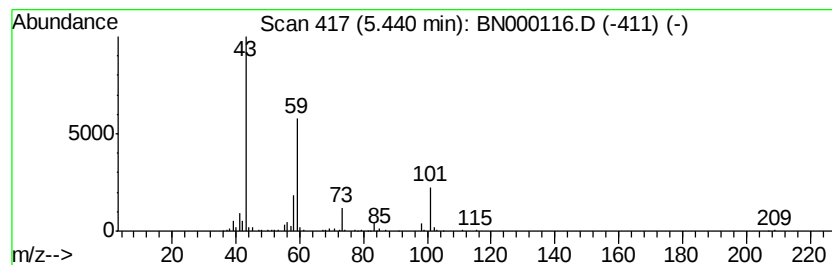
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Peak Number 3 unknown5.44 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.44	3.11 ng	399856	1,4-Dichlorobenzene-d4	8.46

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	39
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
4			Dimethadione	129	C5H7NO3	000695-53-4	28
5			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25



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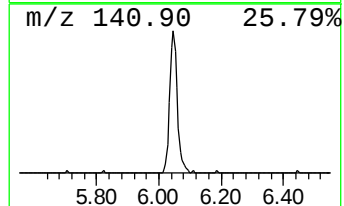
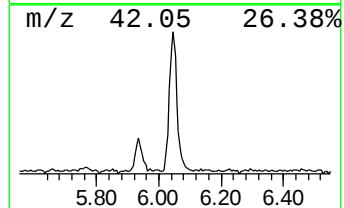
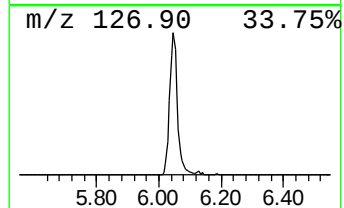
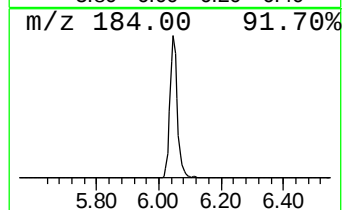
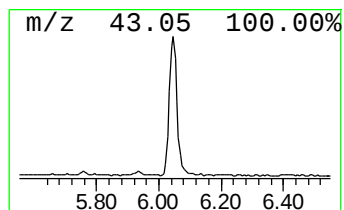
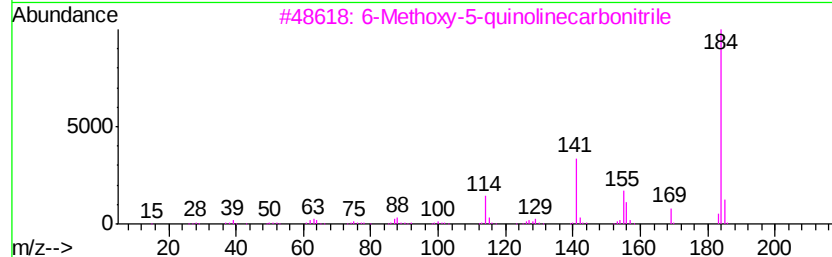
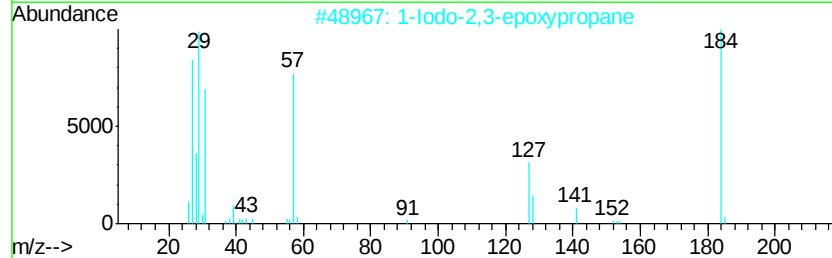
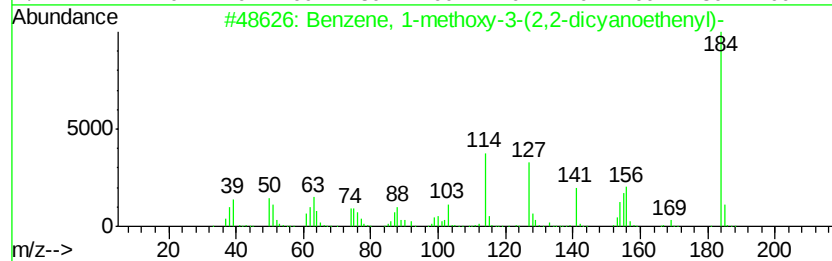
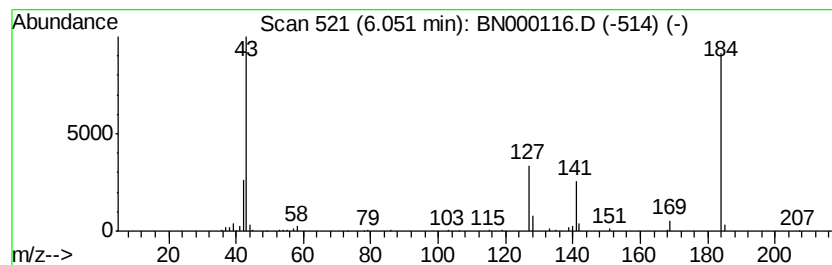
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Peak Number 4 Benzene, 1-methoxy-3-(2,2-d... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.05	3.22 ng	414007	1,4-Dichlorobenzene-d4	8.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methoxy-3-(2,2-dicyanoethenyl)-	184	C11H8N2O	002972-72-7	53
2		1-Iodo-2,3-epoxypropane	184	C3H5IO	000624-57-7	28
3		6-Methoxy-5-quinolinecarbonitrile	184	C11H8N2O	087299-97-6	28
4		1,1'-Biphenyl, 4-methoxy-	184	C13H12O	000613-37-6	9
5		Isobutane	58	C4H10	000075-28-5	9



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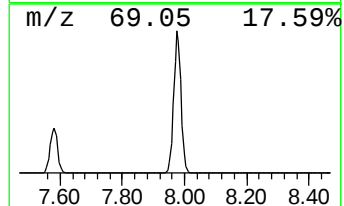
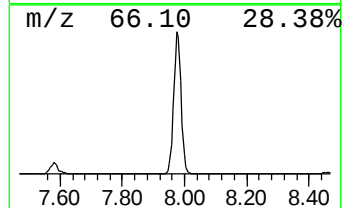
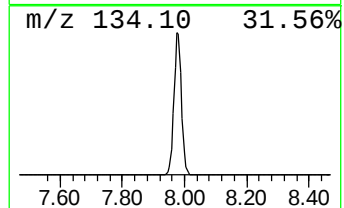
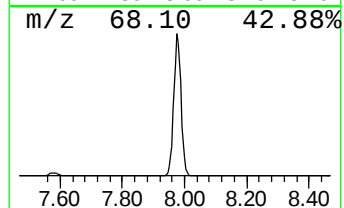
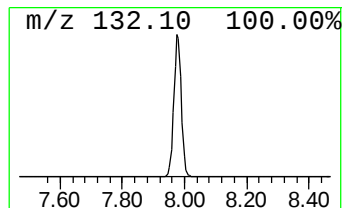
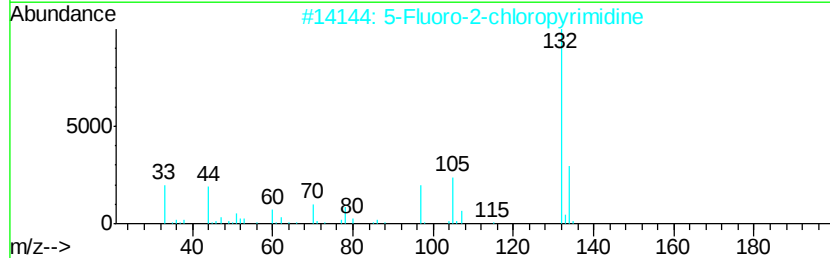
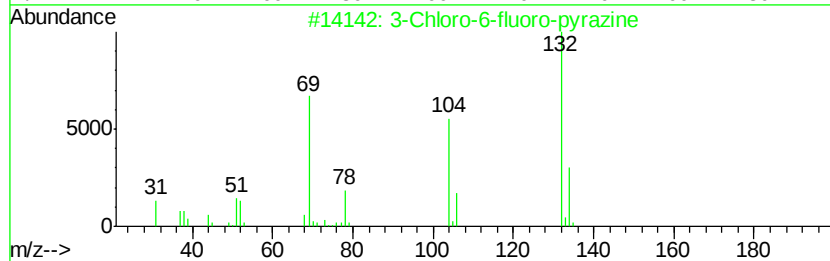
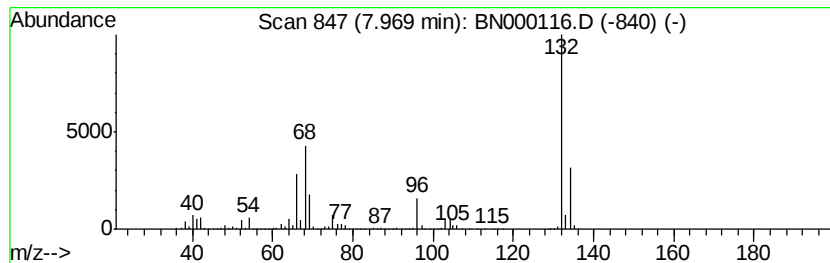
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Peak Number 5 unknown7.97 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.97	87.25 ng	11214700	1,4-Dichlorobenzene-d4	8.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.32	37.8	ng	4862700	1	8.46	2570680	20.0
unknown5.44	5.44	3.1	ng	399856	1	8.46	2570680	20.0
Benzene, 1-methox...	6.05	3.2	ng	414007	1	8.46	2570680	20.0
unknown7.97	7.97	87.3	ng	11214700	1	8.46	2570680	20.0