

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040318\
 Data File : BG033549.D
 Acq On : 4 Apr 2018 7:36
 Operator : SJ/JU
 Sample : J2177-06
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 032818-DBRI-F-U-S

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-BG031918.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	3.481	26	33	43	rBV2	144017	288037	7.24%	1.930%
2	3.569	43	48	57	rVB	116796	190278	4.78%	1.275%
3	5.773	418	423	433	rVB2	27285	48389	1.22%	0.324%
4	6.296	506	512	525	rBV	120586	280088	7.04%	1.877%
5	7.982	793	799	820	rBV	73964	234201	5.89%	1.569%
6	8.375	860	866	881	rBV	289875	659382	16.57%	4.418%
7	8.869	942	950	967	rBV	75218	194464	4.89%	1.303%
8	9.198	997	1006	1019	rBV	473845	961210	24.16%	6.440%
9	10.062	1145	1153	1165	rBV	375891	847706	21.31%	5.680%
10	11.748	1431	1440	1461	rBV	126399	312557	7.86%	2.094%
11	14.110	1834	1842	1862	rBV	1359572	2364334	59.43%	15.842%
12	14.903	1970	1977	1987	rBV	43444	76869	1.93%	0.515%
13	15.479	2069	2075	2087	rVB2	310414	540276	13.58%	3.620%
14	16.695	2278	2282	2287	rVB	42679	54099	1.36%	0.362%
15	16.954	2318	2326	2340	rBV	826684	1400898	35.21%	9.387%
16	17.101	2347	2351	2360	rVB	25466	46367	1.17%	0.311%
17	18.211	2534	2540	2554	rBV	428690	766130	19.26%	5.133%
18	19.010	2672	2676	2683	rBV4	24010	40293	1.01%	0.270%
19	20.732	2963	2969	2984	rBV	2885059	3978627	100.00%	26.658%
20	22.559	3273	3280	3295	rBV2	426310	864264	21.72%	5.791%
21	26.331	3911	3922	3941	rBV2	212560	776079	19.51%	5.200%

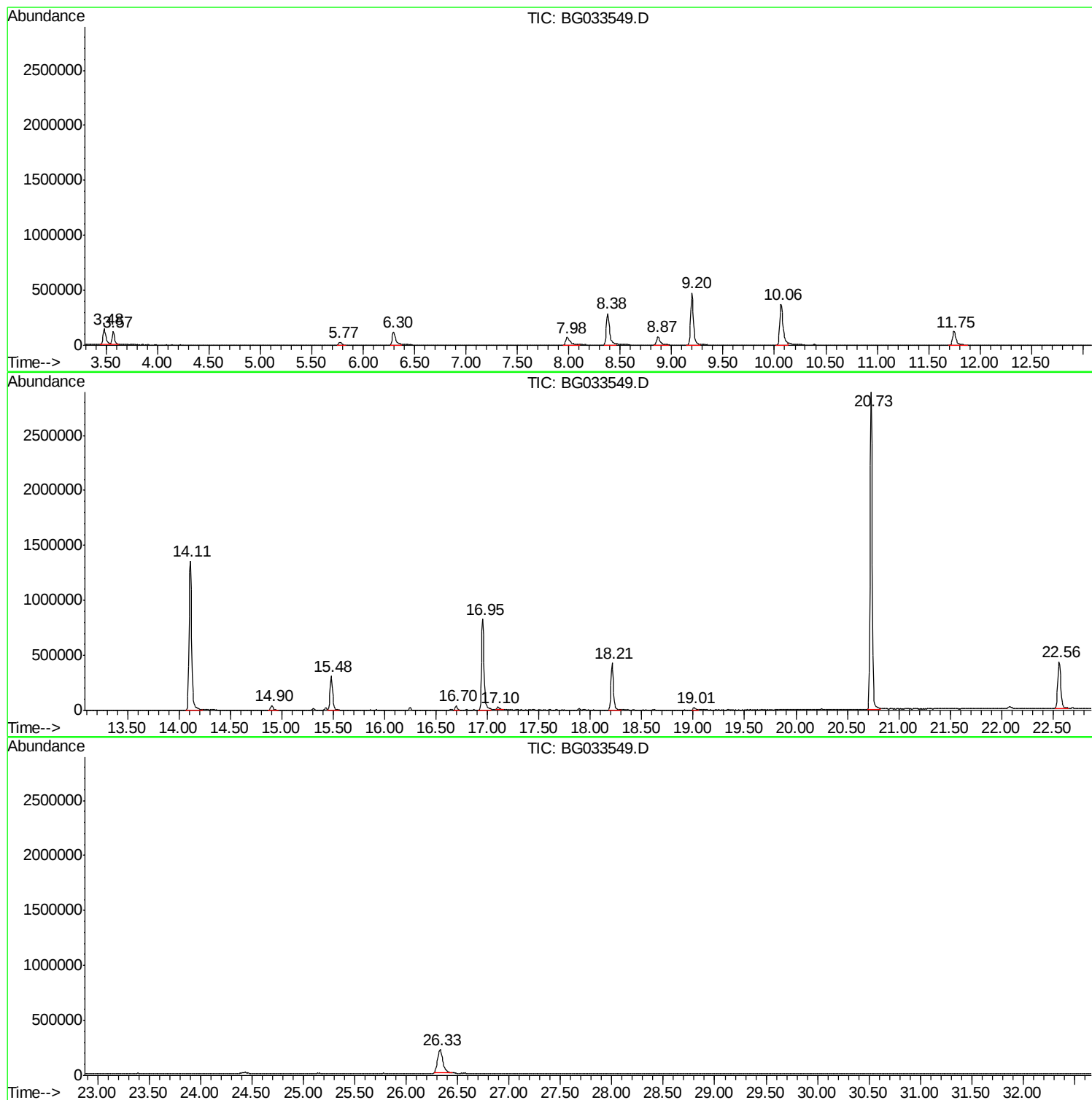
Sum of corrected areas: 14924548

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.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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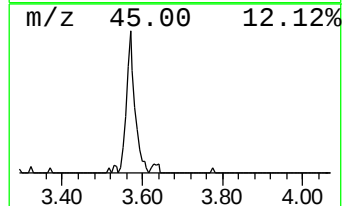
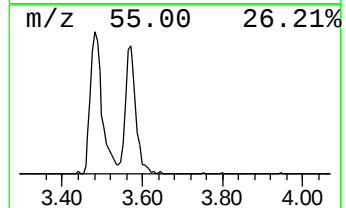
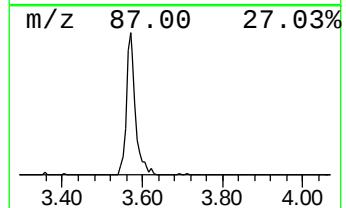
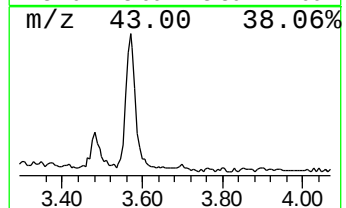
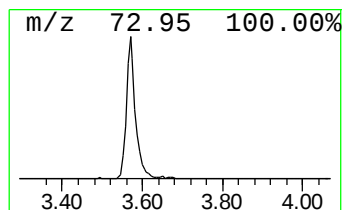
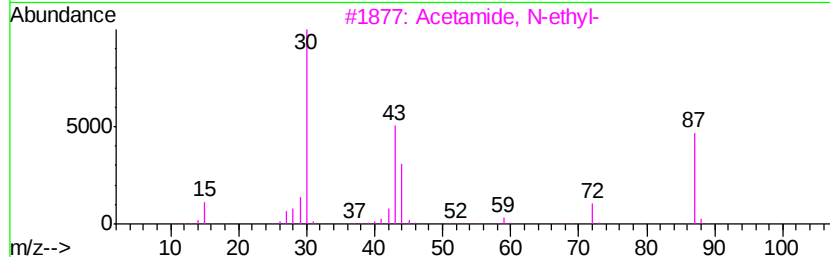
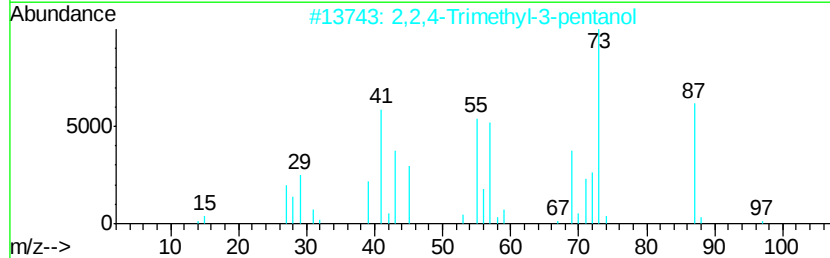
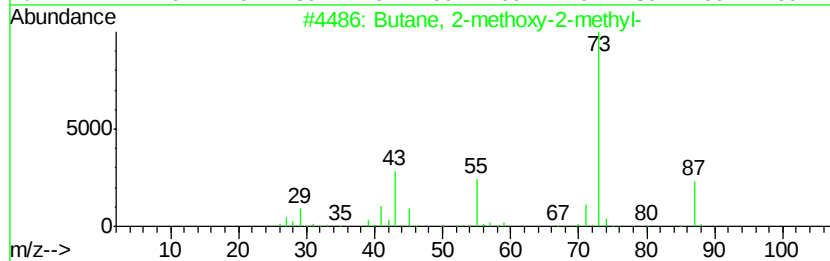
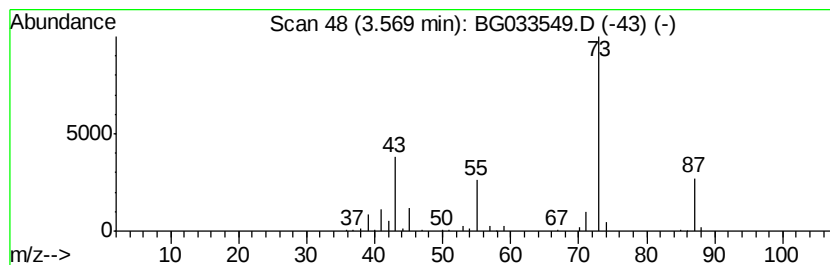
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	19.57 ng	190278	1,4-Dichlorobenzene-d4	8.87

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	50
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
4		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	12
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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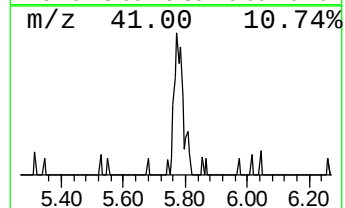
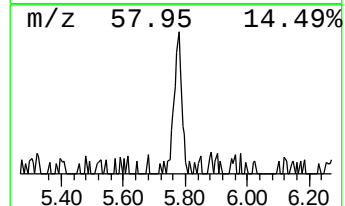
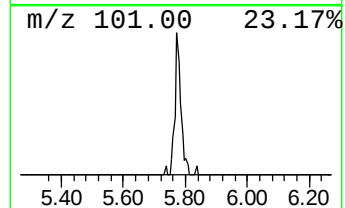
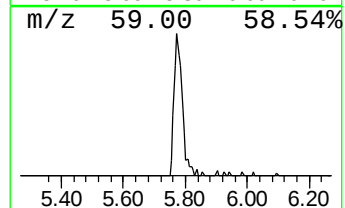
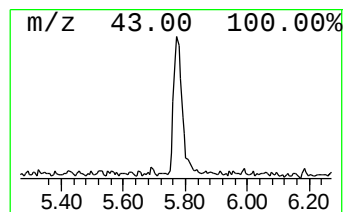
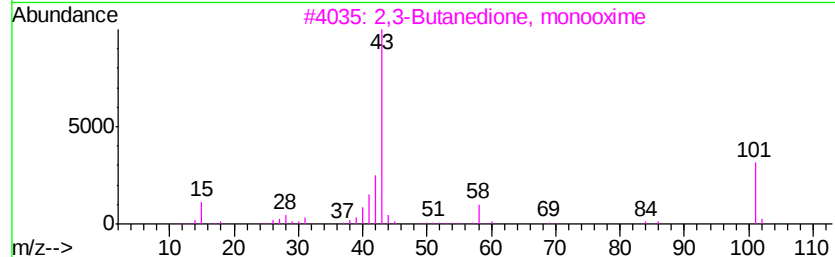
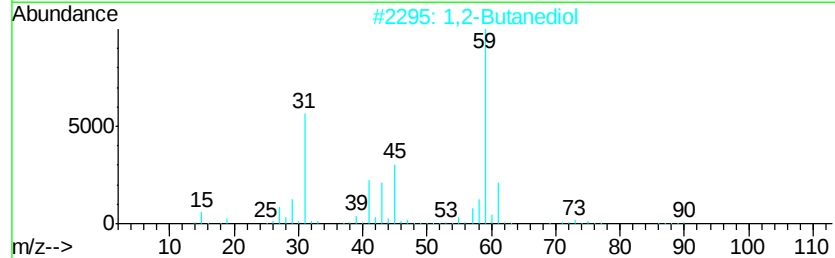
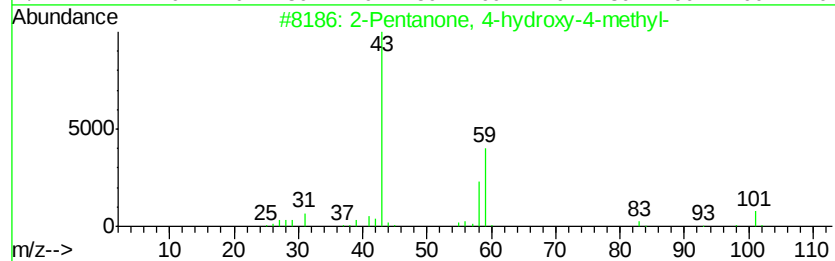
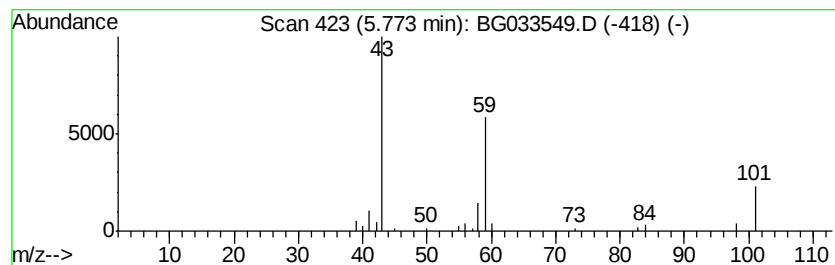
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Peak Number 3 unknown5.77 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	4.98 ng	48389	1,4-Dichlorobenzene-d4	8.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2			1,2-Butanediol	90	C4H10O2	000584-03-2	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9



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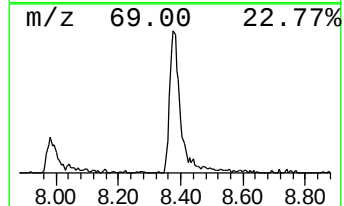
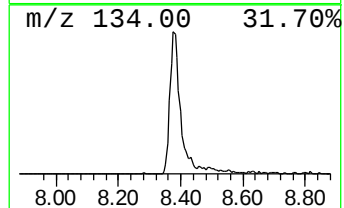
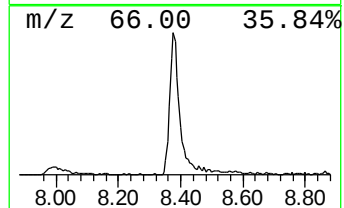
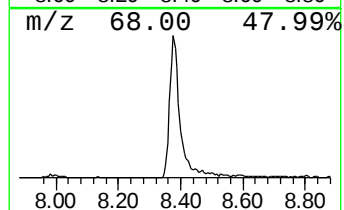
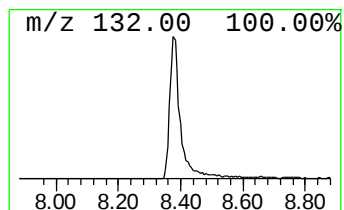
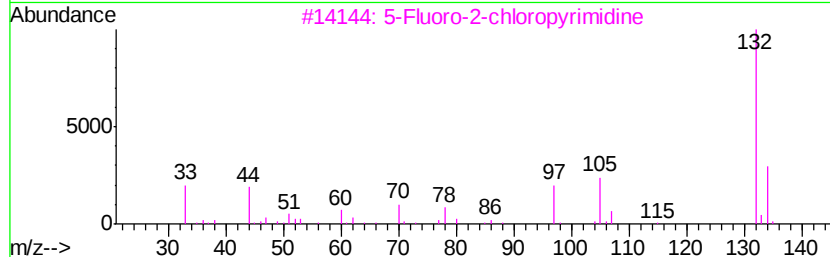
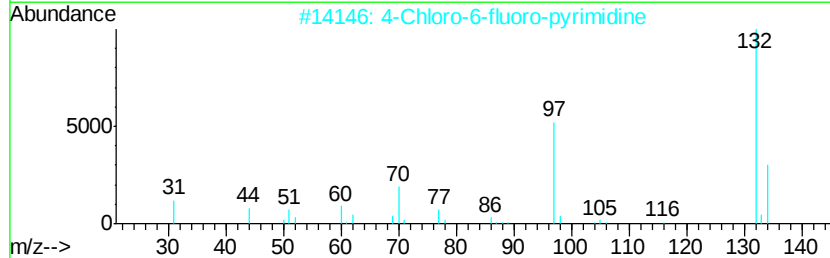
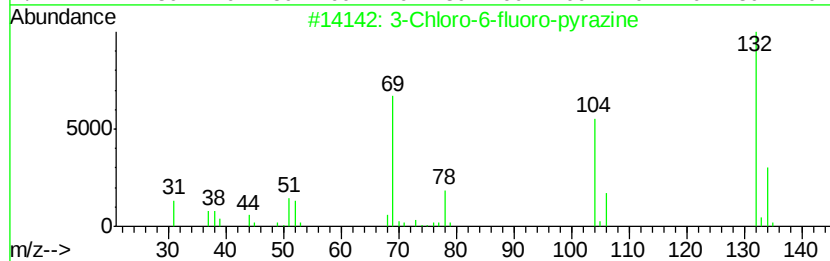
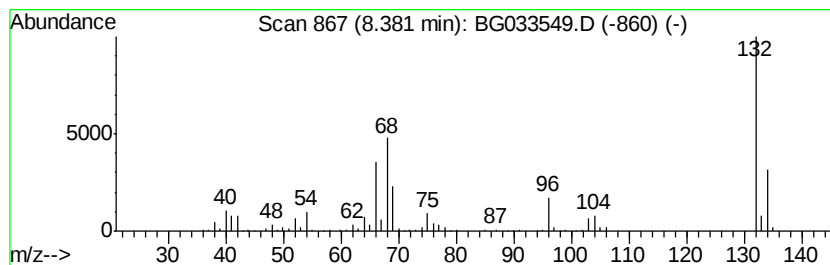
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Peak Number 4 unknown8.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	67.82 ng	659382	1,4-Dichlorobenzene-d4	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22



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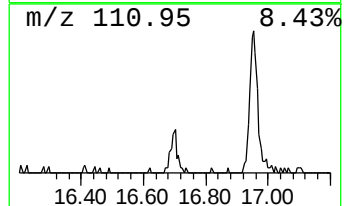
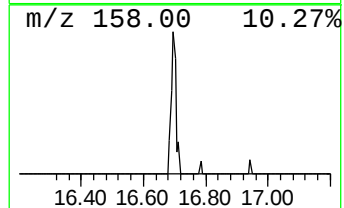
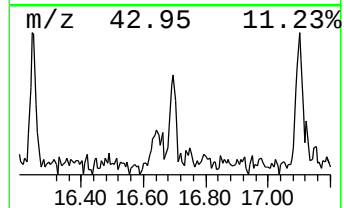
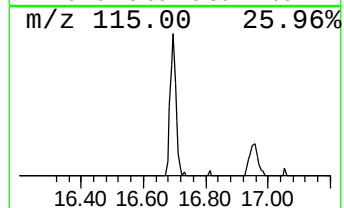
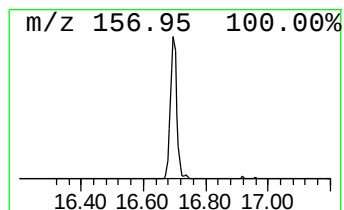
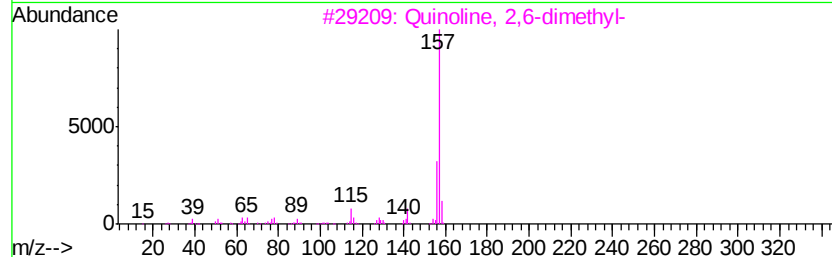
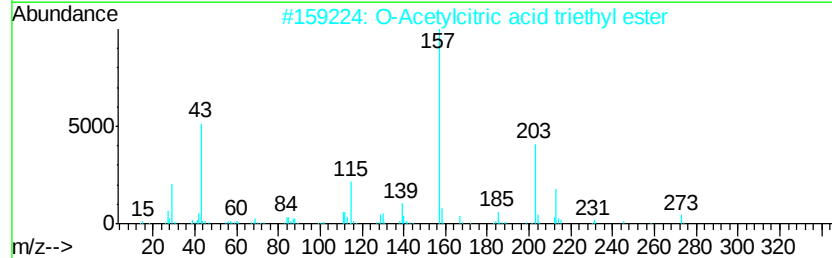
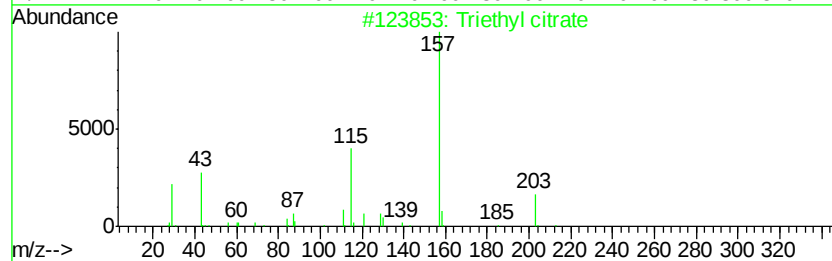
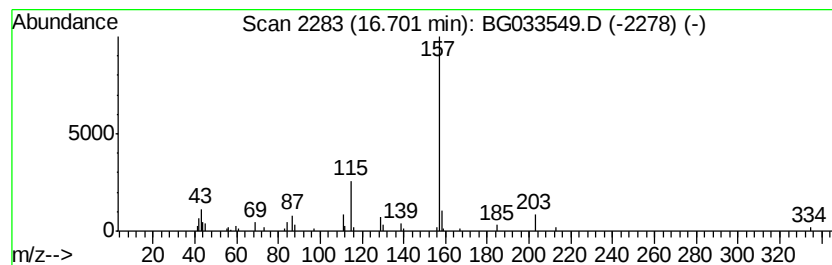
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Peak Number 6 Triethyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.70	2.00 ng	54099	Acenaphthene-d10	15.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triethyl citrate	276	C12H20O7	000077-93-0	83
2		O-Acetylcitric acid triethyl ester	318	C14H22O8	000077-89-4	56
3		Quinoline, 2,6-dimethyl-	157	C11H11N	000877-43-0	50
4		Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-79-9	42
5		Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.57	19.6	ng	190278	1	8.87	194464	20.0
unknown5.77	5.77	5.0	ng	48389	1	8.87	194464	20.0
unknown8.38	8.38	67.8	ng	659382	1	8.87	194464	20.0
Triethyl citrate	16.70	2.0	ng	54099	3	15.48	540276	20.0