

Data Path : Z:\HPCHEM1\BNA G\DATA\BG013118\
 Data File : BG032486.D
 Acq On : 1 Feb 2018 9:31
 Operator : SJ/JU
 Sample : J1377-01
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 STONE

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-BG012918.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	3.370	9	14	25	rVB5	11606	31263	1.22%	0.248%
2	3.464	25	30	40	rVB3	27138	53868	2.10%	0.427%
3	5.650	396	402	410	rBV4	17304	31709	1.24%	0.252%
4	6.167	483	490	509	rBV	354398	712744	27.81%	5.654%
5	7.848	768	776	795	rBV	346160	761709	29.72%	6.042%
6	8.241	835	843	856	rBV	415748	833968	32.54%	6.615%
7	8.723	918	925	938	rBV	95455	190409	7.43%	1.510%
8	9.058	973	982	998	rBV	381237	739101	28.84%	5.863%
9	9.922	1121	1129	1150	rBV	241876	497966	19.43%	3.950%
10	11.602	1407	1415	1425	rBV	128421	265132	10.34%	2.103%
11	13.976	1812	1819	1828	rBV	964707	1609719	62.81%	12.769%
12	14.775	1951	1955	1962	rBV	67224	114047	4.45%	0.905%
13	15.145	2014	2018	2020	rBV5	36969	59527	2.32%	0.472%
14	15.339	2046	2051	2059	rVB2	451942	852102	33.25%	6.759%
15	16.126	2182	2185	2190	rVB4	127568	194988	7.61%	1.547%
16	16.831	2300	2305	2311	rBV	767223	1234578	48.17%	9.793%
17	18.088	2516	2519	2525	rVB	292537	428363	16.71%	3.398%
18	20.621	2946	2950	2957	rVB	1856306	2562933	100.00%	20.330%
19	22.413	3250	3255	3266	rVB2	382445	714620	27.88%	5.668%
20	26.091	3870	3881	3892	rVB	220684	718176	28.02%	5.697%

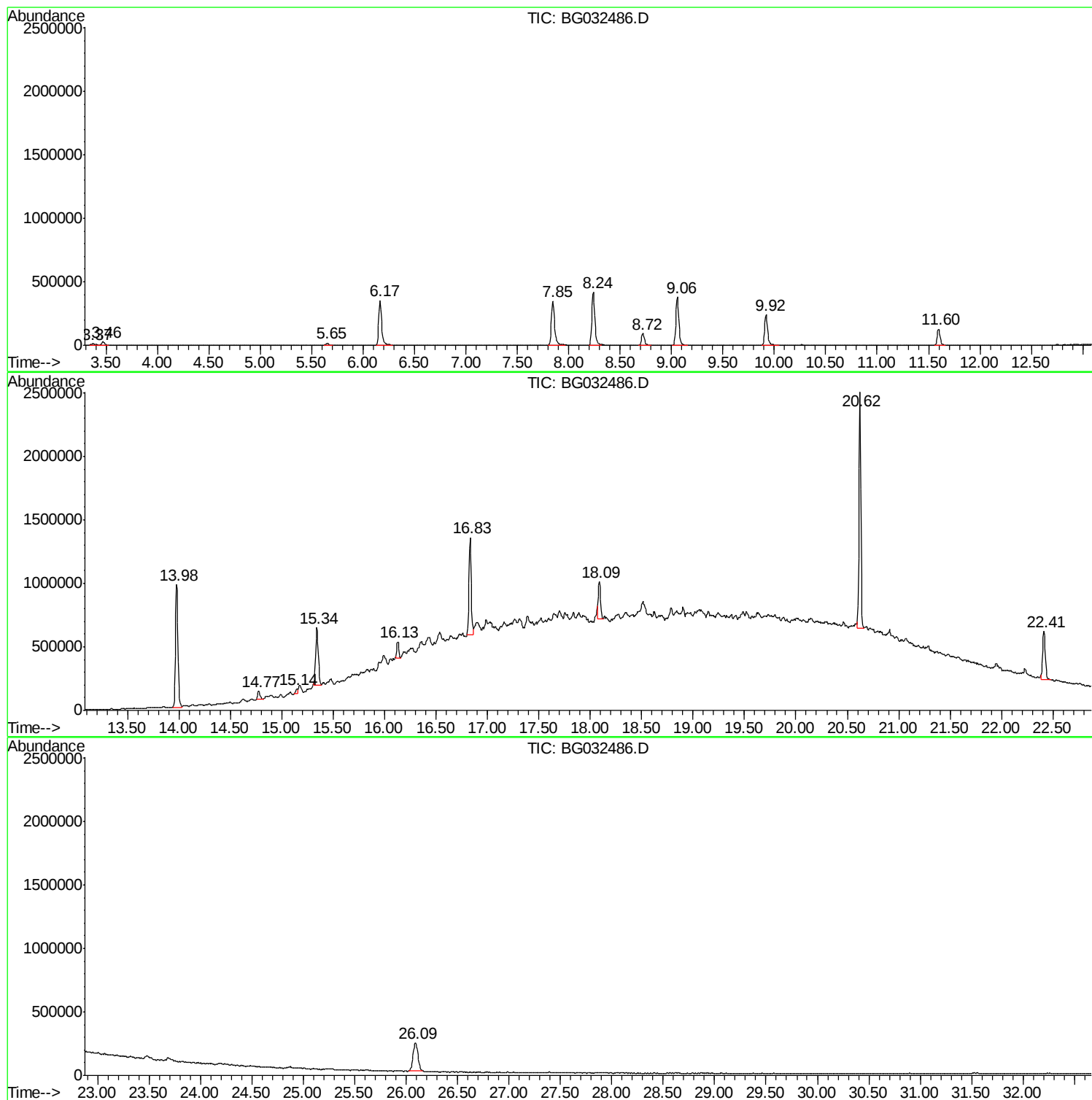
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG012918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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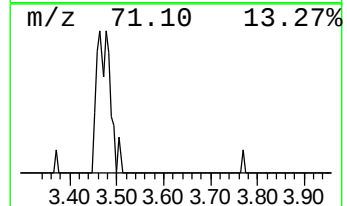
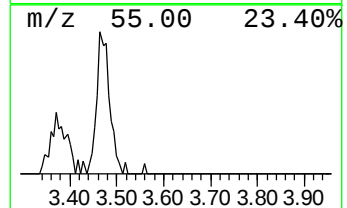
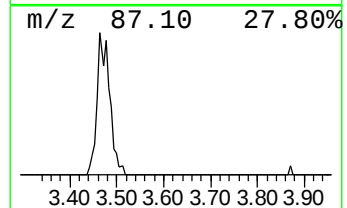
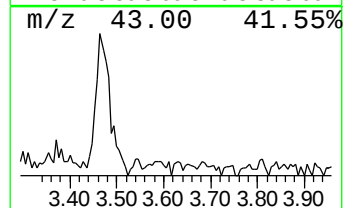
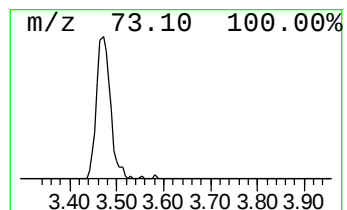
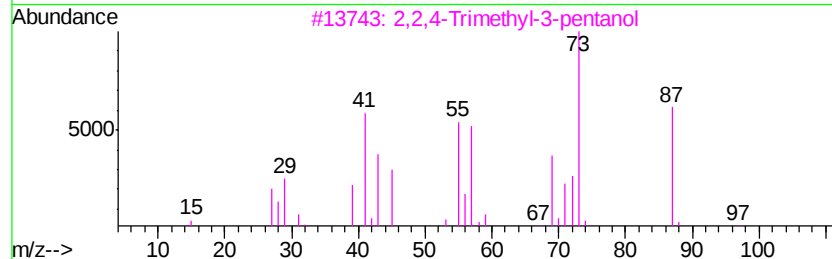
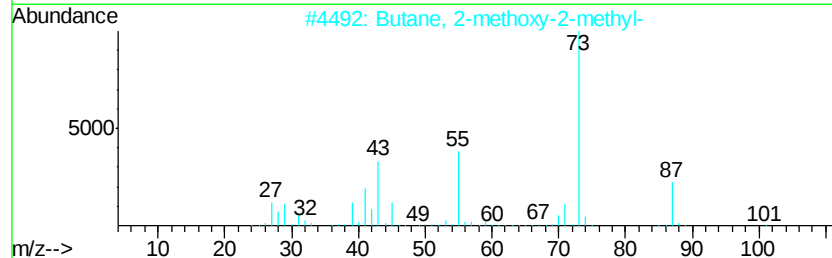
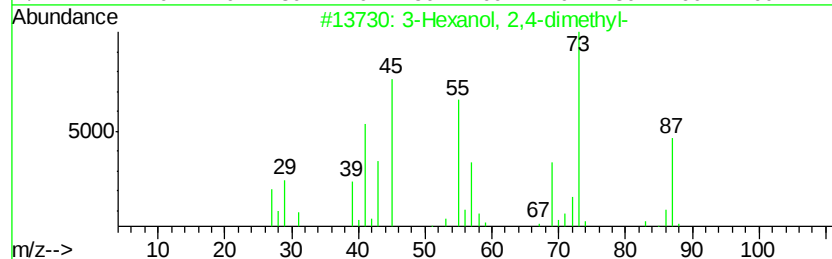
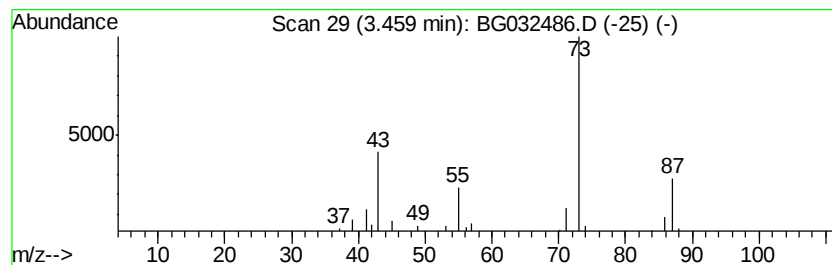
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Hexanol, 2,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.46	5.66 ng	53868	1,4-Dichlorobenzene-d4	8.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	53
2			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	42
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
4			3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	36
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	12



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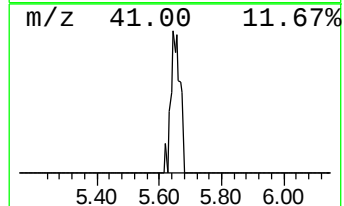
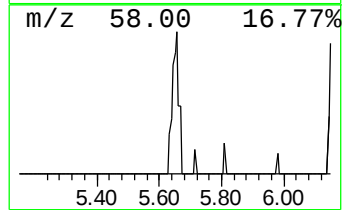
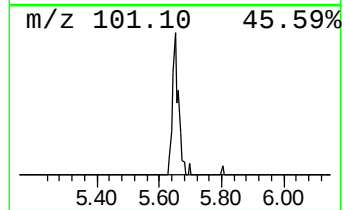
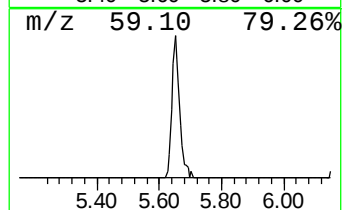
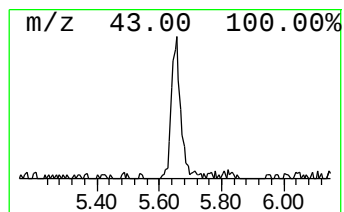
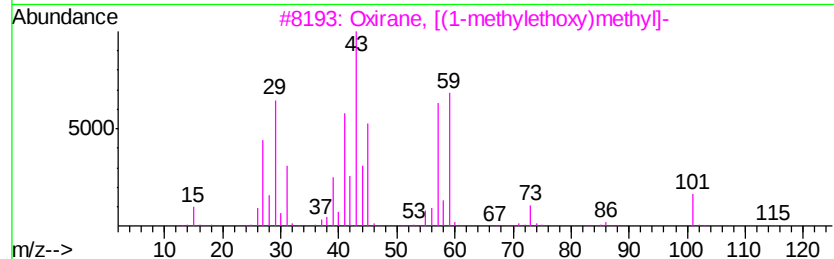
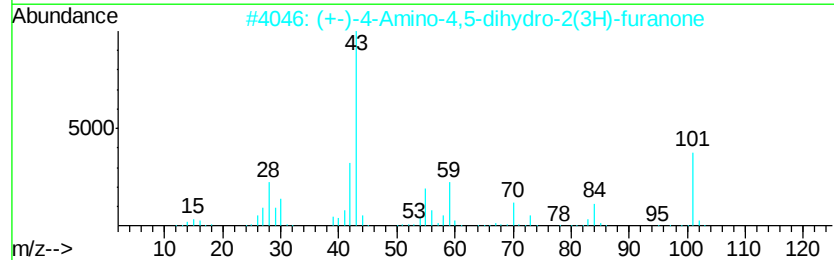
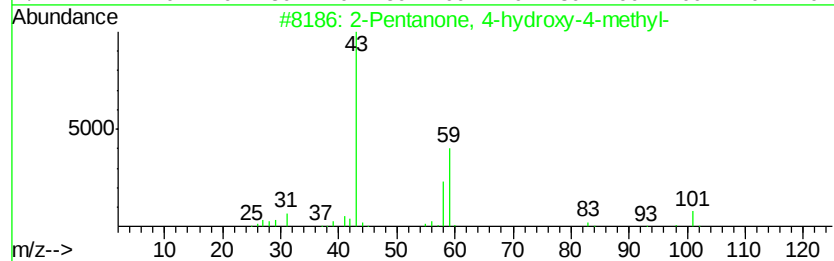
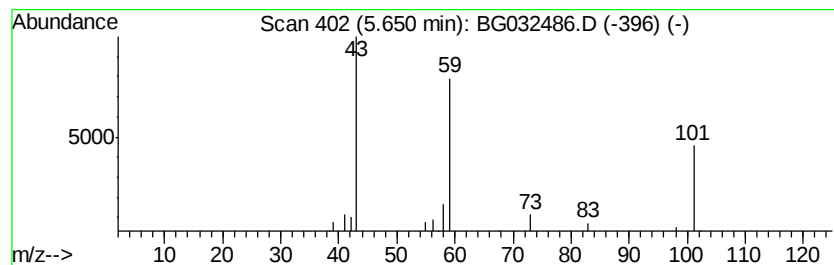
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.65	3.33 ng	31709	1,4-Dichlorobenzene-d4	8.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	43
3		Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	36
4		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	10



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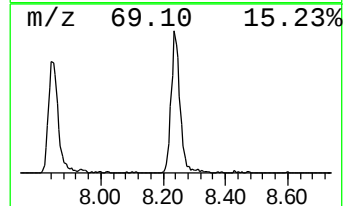
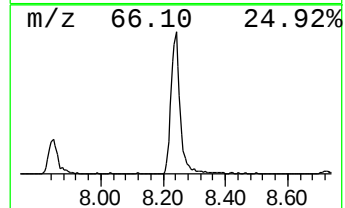
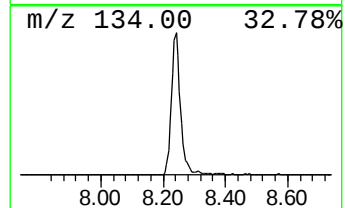
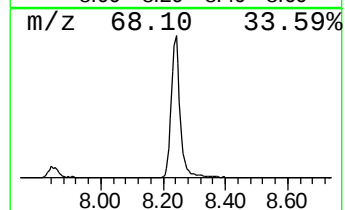
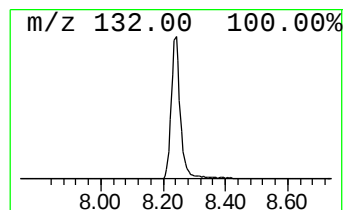
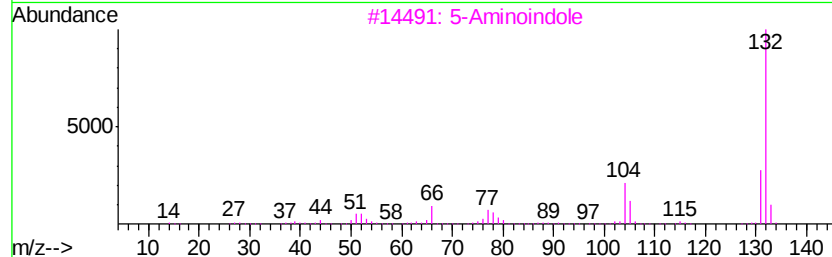
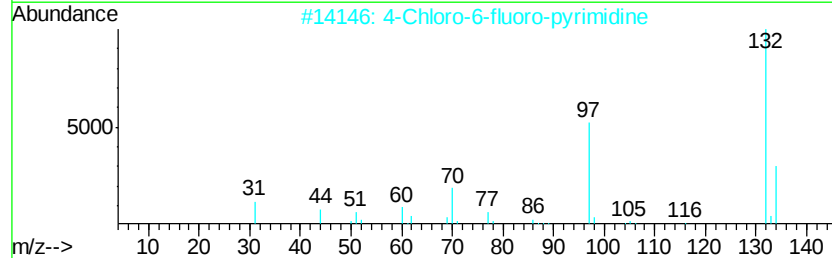
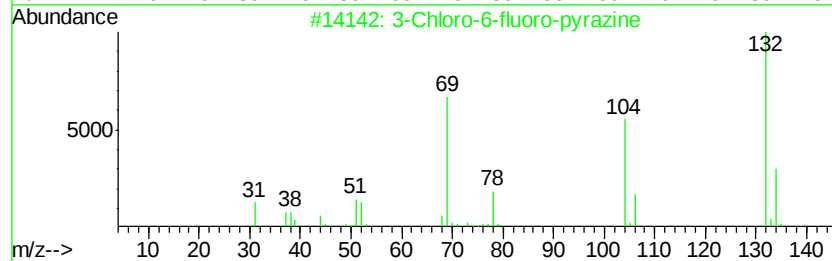
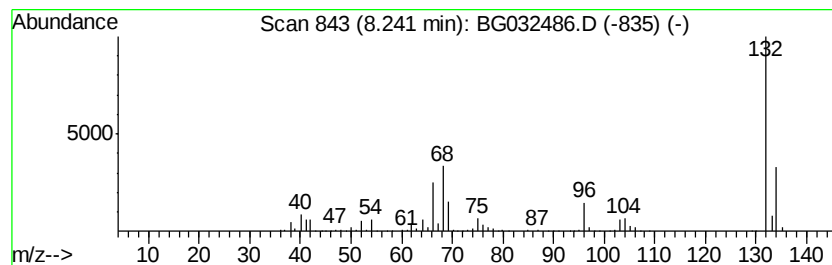
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Peak Number 4 unknown8.24 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.24	87.60 ng	833968	1,4-Dichlorobenzene-d4	8.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	35
3		5-Aminoindole	132	C8H8N2	005192-03-0	27
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17



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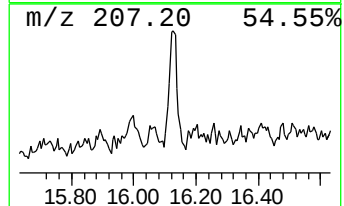
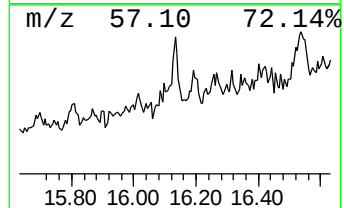
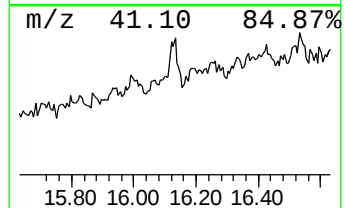
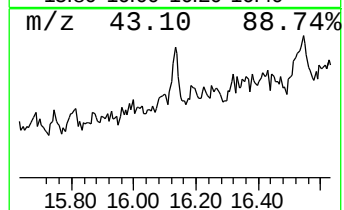
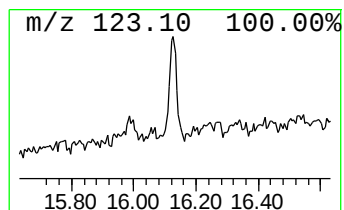
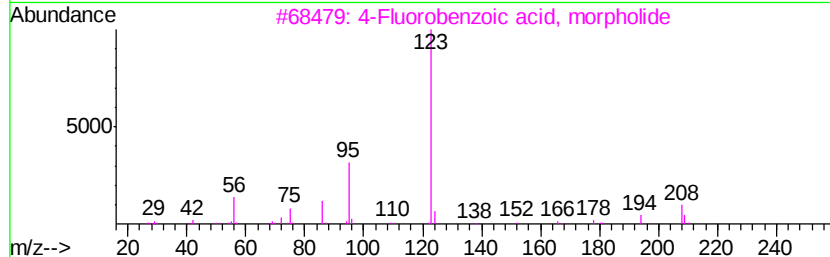
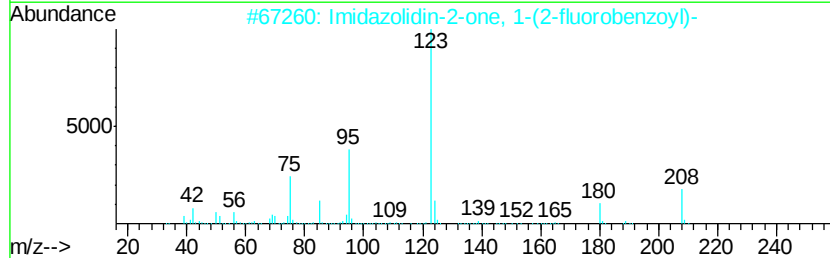
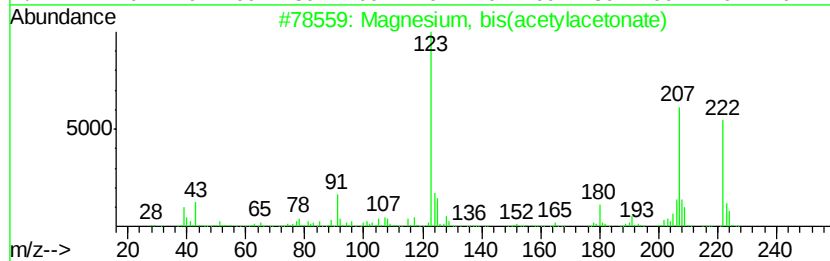
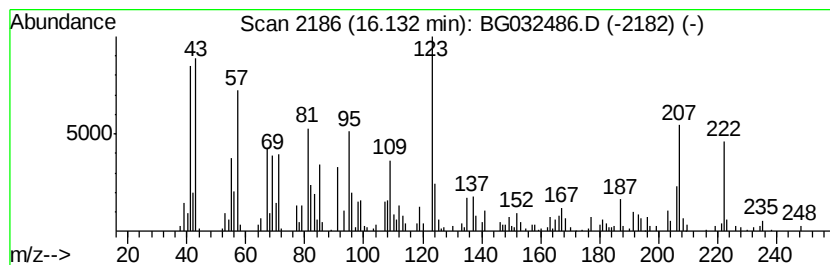
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Peak Number 6 unknown16.13 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.13	4.58 ng	194988	Acenaphthene-d10	15.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Magnesium, bis(acetylacetonate)	222	C10H14MqO4	068488-07-3	47
2	Imidazolidin-2-one, 1-(2-fluorobenzoyl)-	208	C10H9FN2O2	1000310-62-2	38
3	4-Fluorobenzoic acid, morpholide	209	C11H12FN02	1000307-09-9	35
4	2-Fluorobenzoic acid, 2-fluorophenyl	234	C13H8F2O2	1000325-75-1	30
5	1-Butanone, 4-chloro-1-(4-fluorophenyl)-	200	C10H10ClFO	003874-54-2	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexanol, 2,4-di...	3.46	5.7	ng	53868	1	8.72	190409	20.0
2-Pentanone, 4-hy...	5.65	3.3	ng	31709	1	8.72	190409	20.0
unknown8.24	8.24	87.6	ng	833968	1	8.72	190409	20.0
unknown16.13	16.13	4.6	ng	194988	3	15.35	852102	20.0