

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
 Data File : BG043548.D
 Acq On : 7 Nov 2019 20:47
 Operator : JU
 Sample : K5723-11
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 9-D

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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	3.178	9	15	26	rVB	100008	195402	13.09%	2.009%
2	5.111	339	344	351	rBV	76798	120967	8.11%	1.243%
3	5.610	422	429	441	rBV	367850	646935	43.35%	6.650%
4	7.214	694	702	717	rBV	383646	750332	50.28%	7.713%
5	7.555	752	760	774	rBV	410078	744903	49.91%	7.657%
6	8.007	829	837	845	rBV	106206	193397	12.96%	1.988%
7	8.330	884	892	907	rBV	307367	545732	36.57%	5.610%
8	9.171	1027	1035	1047	rBV	204082	422953	28.34%	4.348%
9	10.816	1307	1315	1324	rBV	119649	243901	16.34%	2.507%
10	13.260	1724	1731	1742	rBV	575409	942168	63.13%	9.685%
11	14.088	1866	1872	1883	rBV	55474	99454	6.66%	1.022%
12	14.541	1943	1949	1956	rBV3	30058	48462	3.25%	0.498%
13	14.635	1956	1965	1980	rBV2	220345	387232	25.95%	3.980%
14	15.023	2024	2031	2036	rBV3	22006	34433	2.31%	0.354%
15	16.127	2213	2219	2232	rBV	526600	934777	62.64%	9.609%
16	16.680	2308	2313	2318	rBV3	10335	14991	1.00%	0.154%
17	17.385	2426	2433	2448	rBV	288474	488479	32.73%	5.021%
18	17.502	2448	2453	2458	rVB7	18275	31588	2.12%	0.325%
19	17.567	2460	2464	2468	rVB7	14668	20682	1.39%	0.213%
20	18.278	2581	2585	2589	rBV4	16687	21861	1.46%	0.225%
21	19.188	2737	2740	2743	rBV5	12996	17601	1.18%	0.181%
22	19.993	2872	2877	2887	rBV	1092834	1492398	100.00%	15.340%
23	20.745	3001	3005	3008	rBV	138531	164779	11.04%	1.694%
24	21.650	3154	3159	3169	rBV	299332	544964	36.52%	5.602%
25	24.841	3696	3702	3716	rVB2	207477	620171	41.56%	6.375%

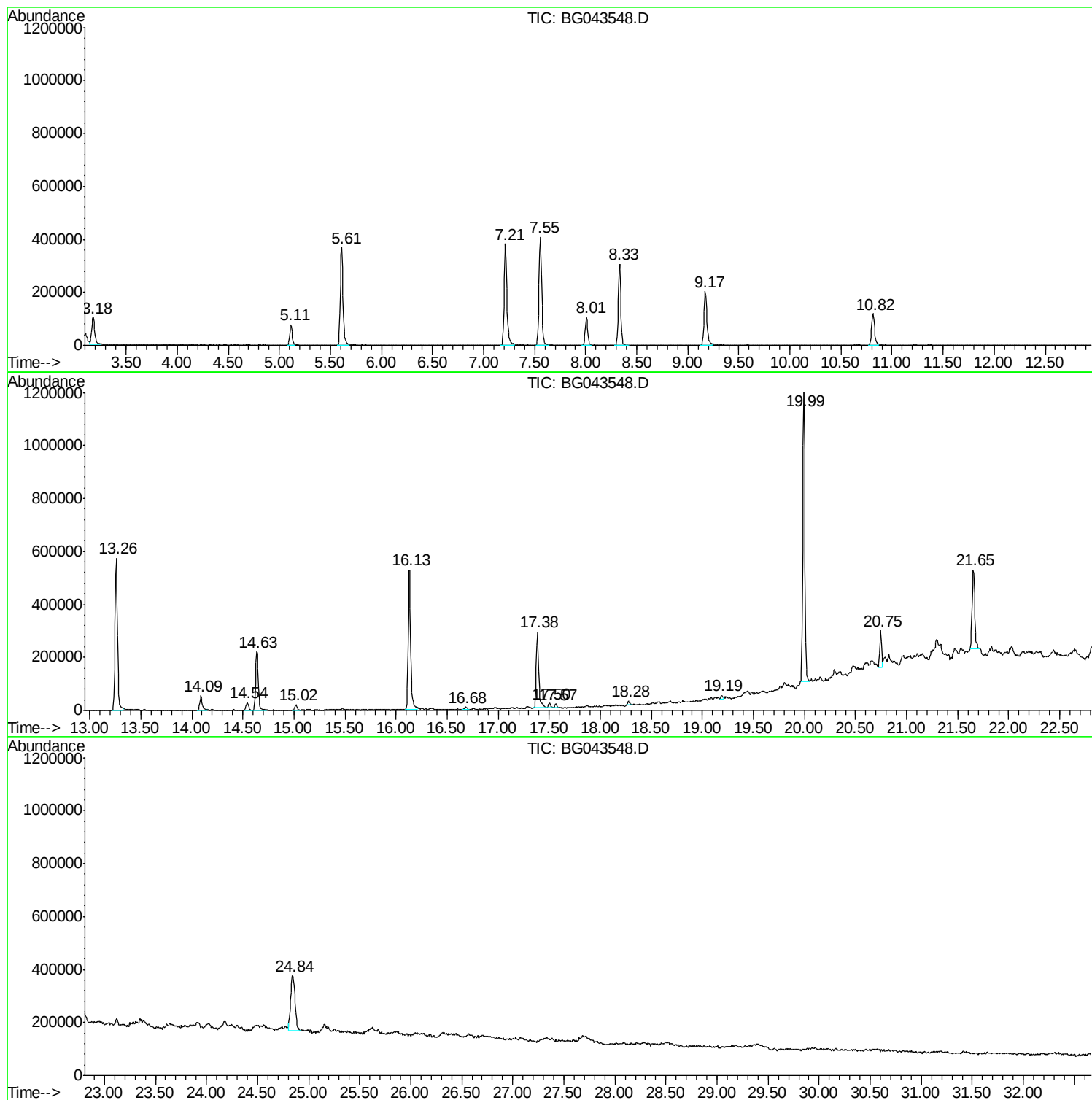
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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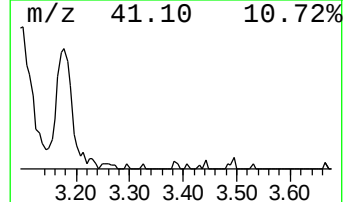
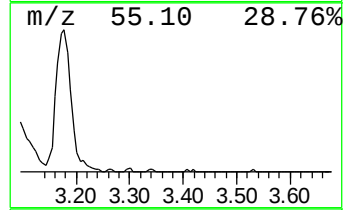
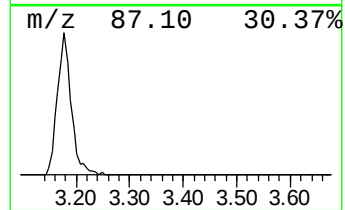
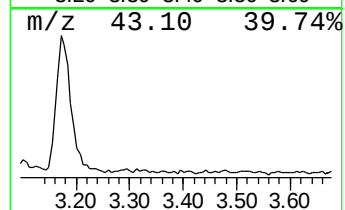
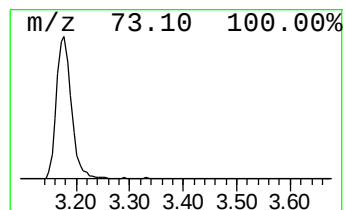
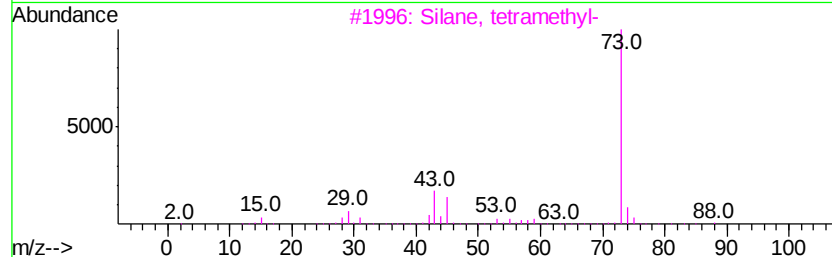
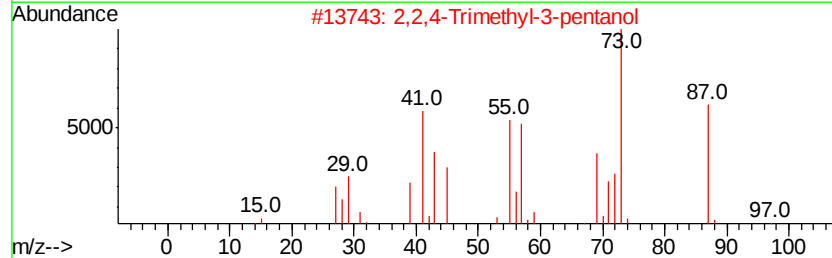
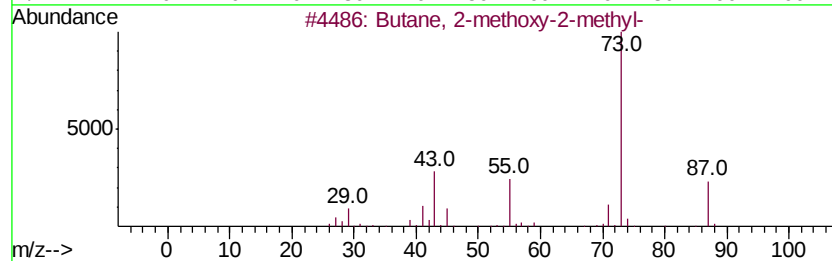
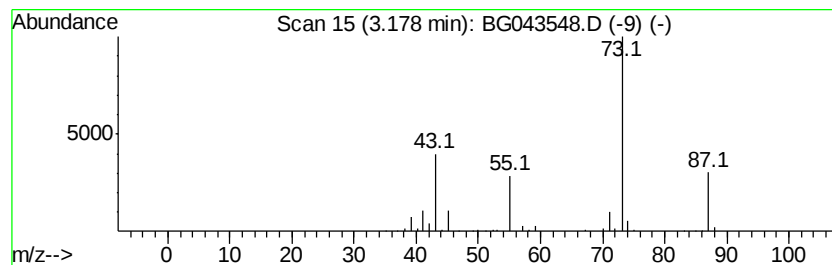
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	20.21 ng	195402	1,4-Dichlorobenzene-d4	8.01

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		Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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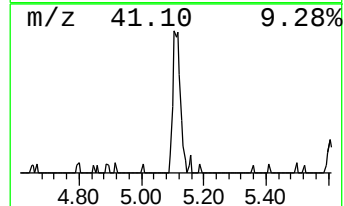
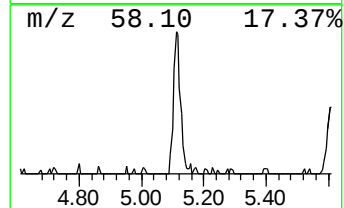
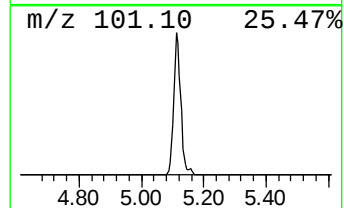
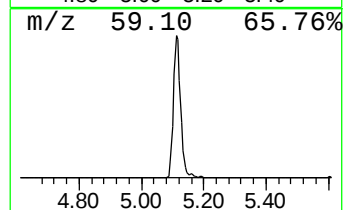
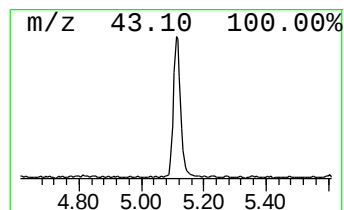
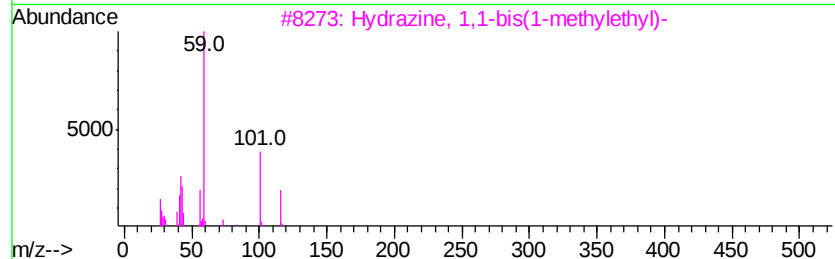
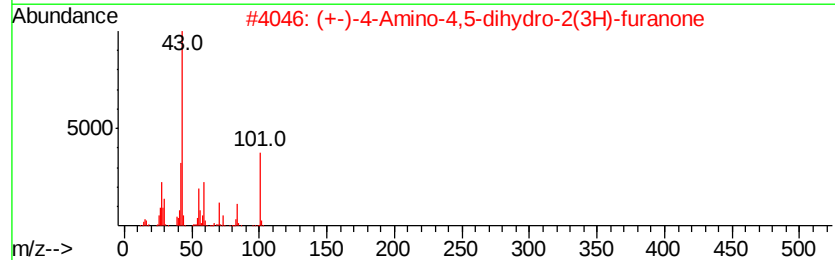
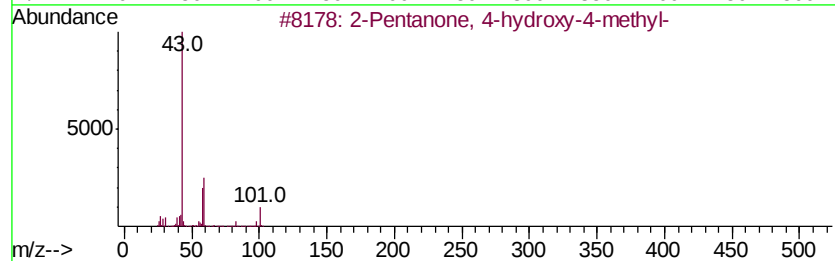
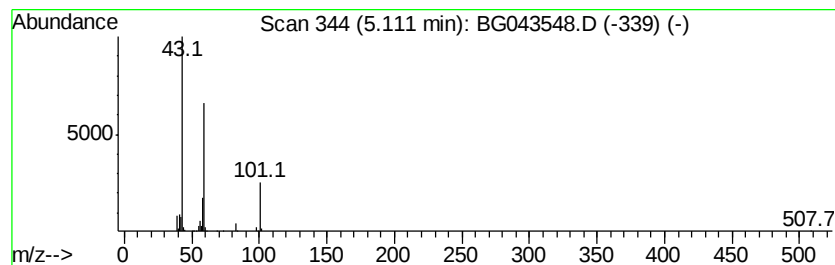
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	12.51 ng	120967	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	47
3		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
4		4-Ethyl-3-octanol	158	C10H22O	019781-26-1	23
5		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17



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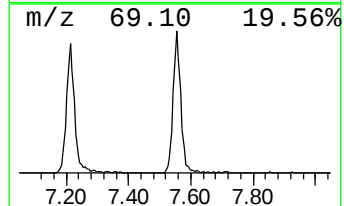
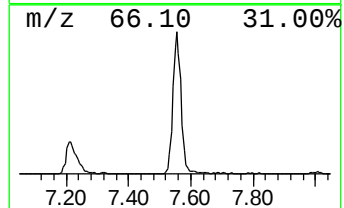
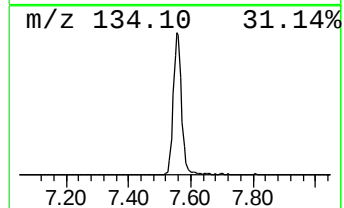
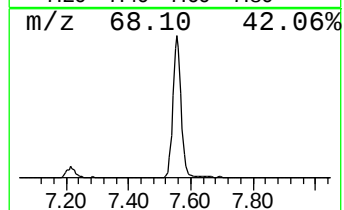
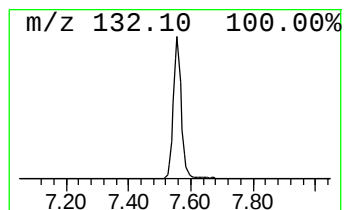
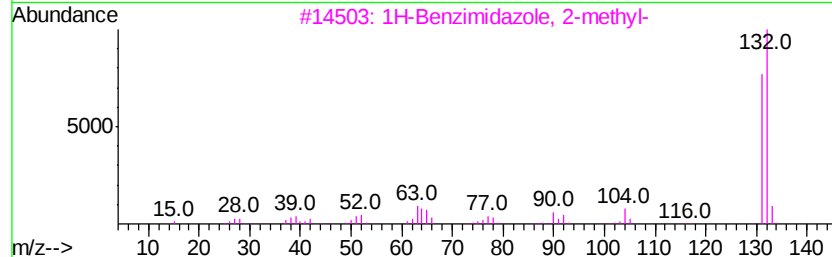
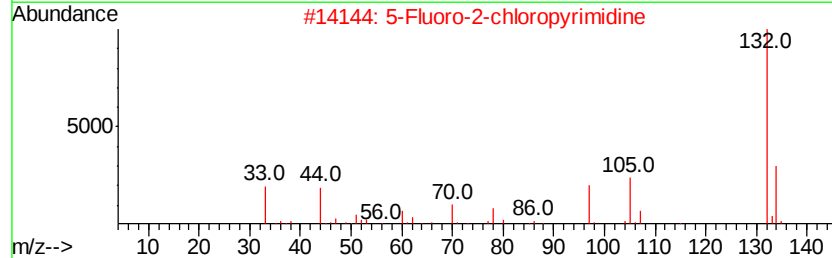
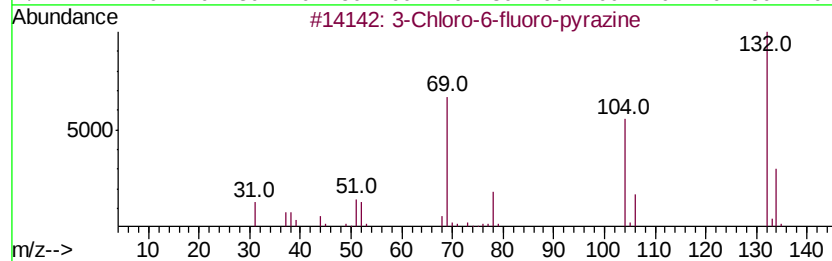
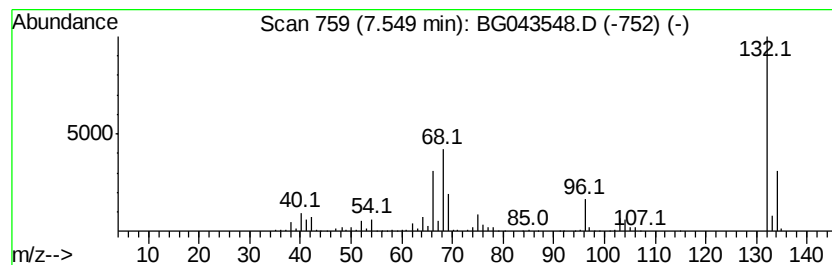
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Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	77.03 ng	744903	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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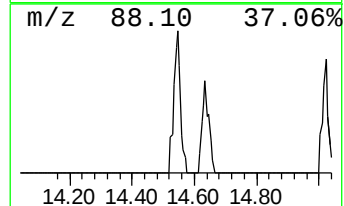
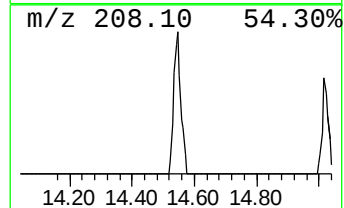
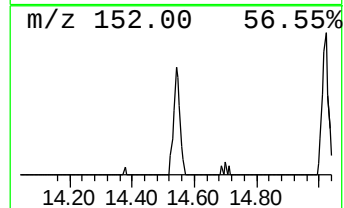
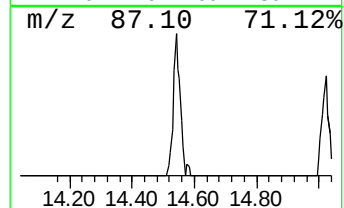
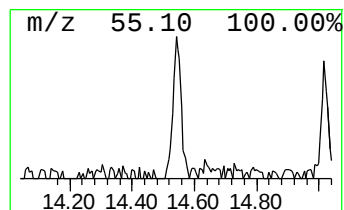
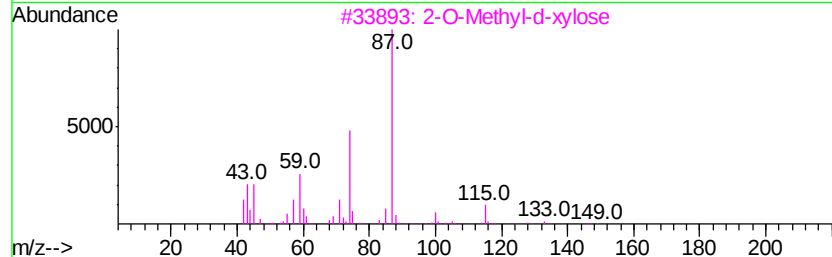
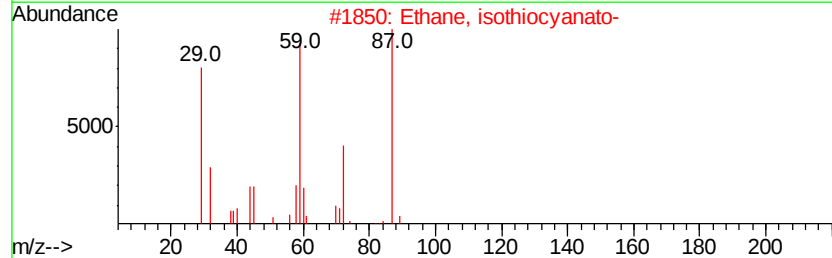
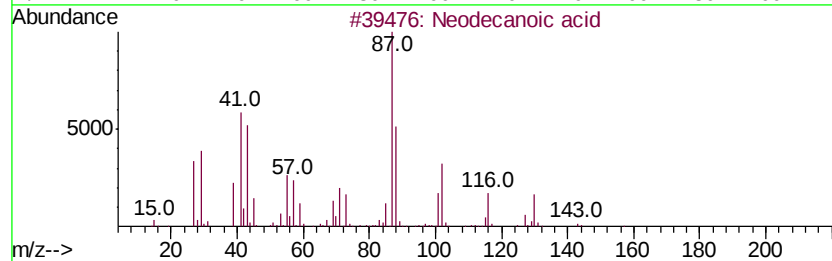
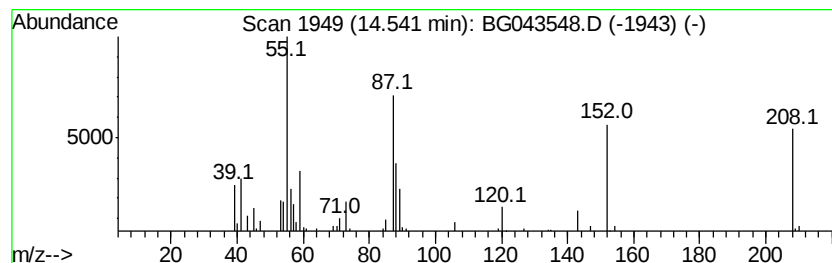
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Peak Number 5 unknown14.54 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.54	2.50 ng	48462	Acenaphthene-d10		14.63
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neodecanoic acid	172	C10H20O2	026896-20-8	22
2	Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	14
3	2-O-Methyl-d-xvlose	164	C6H12O5	1000130-01-3	14
4	Benzofuran, 7-chloro-	152	C8H5ClO	024410-55-7	14
5	Benzene, 1,2,3-trimethoxy-5-(2-p...	208	C12H16O3	000487-11-6	12



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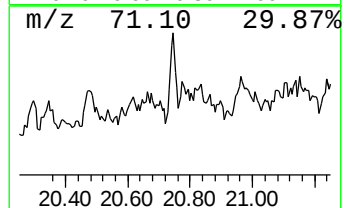
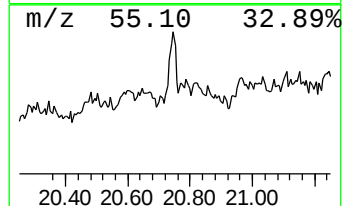
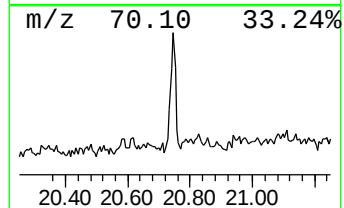
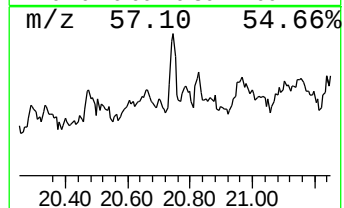
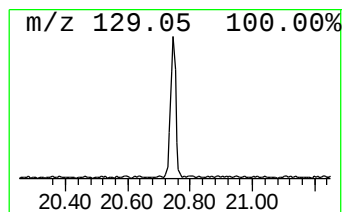
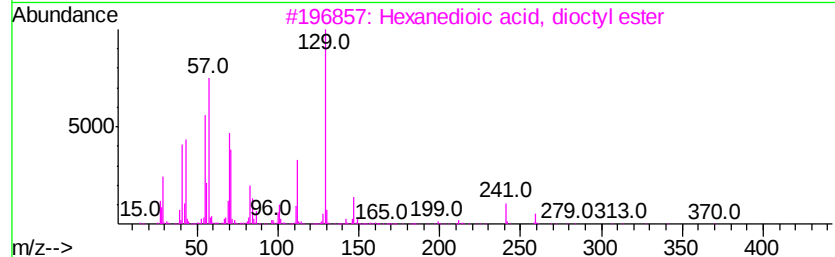
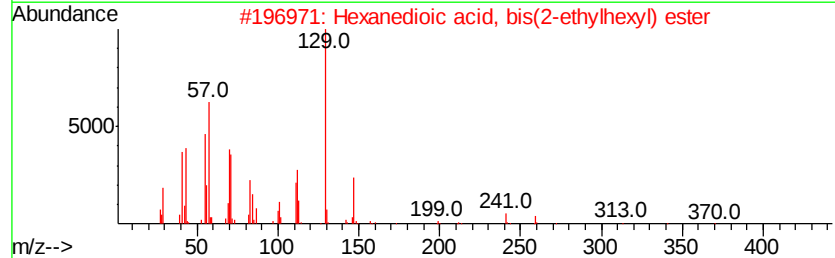
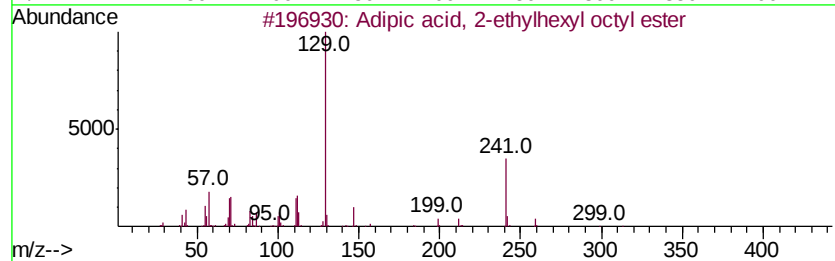
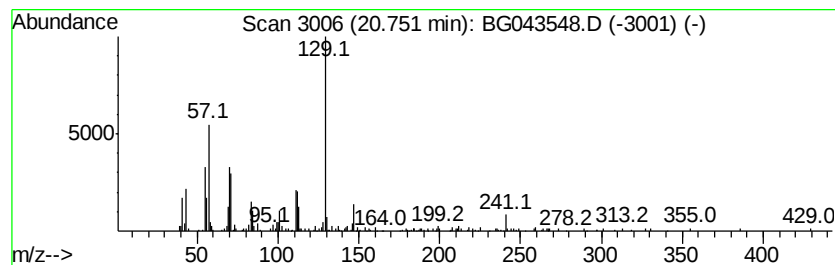
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Peak Number 6 Adipic acid, 2-ethylhexyl o... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
20.75	6.05 ng	164779	Chrysene-d12	21.65		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	78	
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	70	
3	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	55	
4	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	53	
5	Diisooctyl adipate	370	C22H42O4	001330-86-5	50	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.18	20.2	ng	195402	1	8.01	193397	20.0
2-Pentanone, 4-hy...	5.11	12.5	ng	120967	1	8.01	193397	20.0
unknown7.55	7.55	77.0	ng	744903	1	8.01	193397	20.0
unknown14.54	14.54	2.5	ng	48462	3	14.63	387232	20.0
Adipic acid, 2-et...	20.75	6.0	ng	164779	5	21.65	544964	20.0