

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
 Data File : BG043405.D
 Acq On : 30 Oct 2019 17:58
 Operator : JU
 Sample : K5543-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 R-1

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	3.190	12	17	29	rVB	126800	197887	6.36%	1.292%
2	5.123	340	346	354	rBV	93839	155057	4.98%	1.012%
3	5.610	421	429	440	rBV	461038	819701	26.35%	5.352%
4	7.208	692	701	720	rBV	479511	963005	30.96%	6.288%
5	7.561	753	761	771	rBV	514349	935491	30.07%	6.108%
6	8.019	832	839	848	rBV	135247	244861	7.87%	1.599%
7	8.348	885	895	908	rBV	394262	733803	23.59%	4.791%
8	9.183	1029	1037	1055	rBV	251382	550151	17.69%	3.592%
9	10.828	1309	1317	1327	rBV	142519	306040	9.84%	1.998%
10	13.272	1726	1733	1759	rBV	883645	1526975	49.09%	9.971%
11	14.100	1867	1874	1886	rBV	90379	183798	5.91%	1.200%
12	14.647	1958	1967	1982	rBV2	317609	525476	16.89%	3.431%
13	16.139	2214	2221	2238	rBV	804407	1401997	45.07%	9.155%
14	17.396	2428	2435	2449	rBV2	383397	702574	22.59%	4.588%
15	17.514	2451	2455	2464	rVB4	24792	43104	1.39%	0.281%
16	18.284	2582	2586	2596	rBV2	29966	63767	2.05%	0.416%
17	19.999	2872	2878	2895	rBV	2198422	3110546	100.00%	20.311%
18	21.263	3086	3093	3095	rBV2	31326	63919	2.05%	0.417%
19	21.315	3095	3102	3108	rVV2	83471	233971	7.52%	1.528%
20	21.380	3108	3113	3123	rVB	131694	240499	7.73%	1.570%
21	21.656	3153	3160	3174	rBV	497044	948380	30.49%	6.193%
22	22.449	3289	3295	3299	rBV2	21512	35240	1.13%	0.230%
23	23.137	3405	3412	3417	rBV4	30656	61543	1.98%	0.402%
24	23.319	3438	3443	3452	rVB2	36299	69787	2.24%	0.456%
25	23.930	3541	3547	3556	rVB3	33696	76647	2.46%	0.500%
26	24.852	3690	3704	3718	rBV2	342663	1070002	34.40%	6.987%
27	25.981	3890	3896	3903	rVB4	19330	50479	1.62%	0.330%

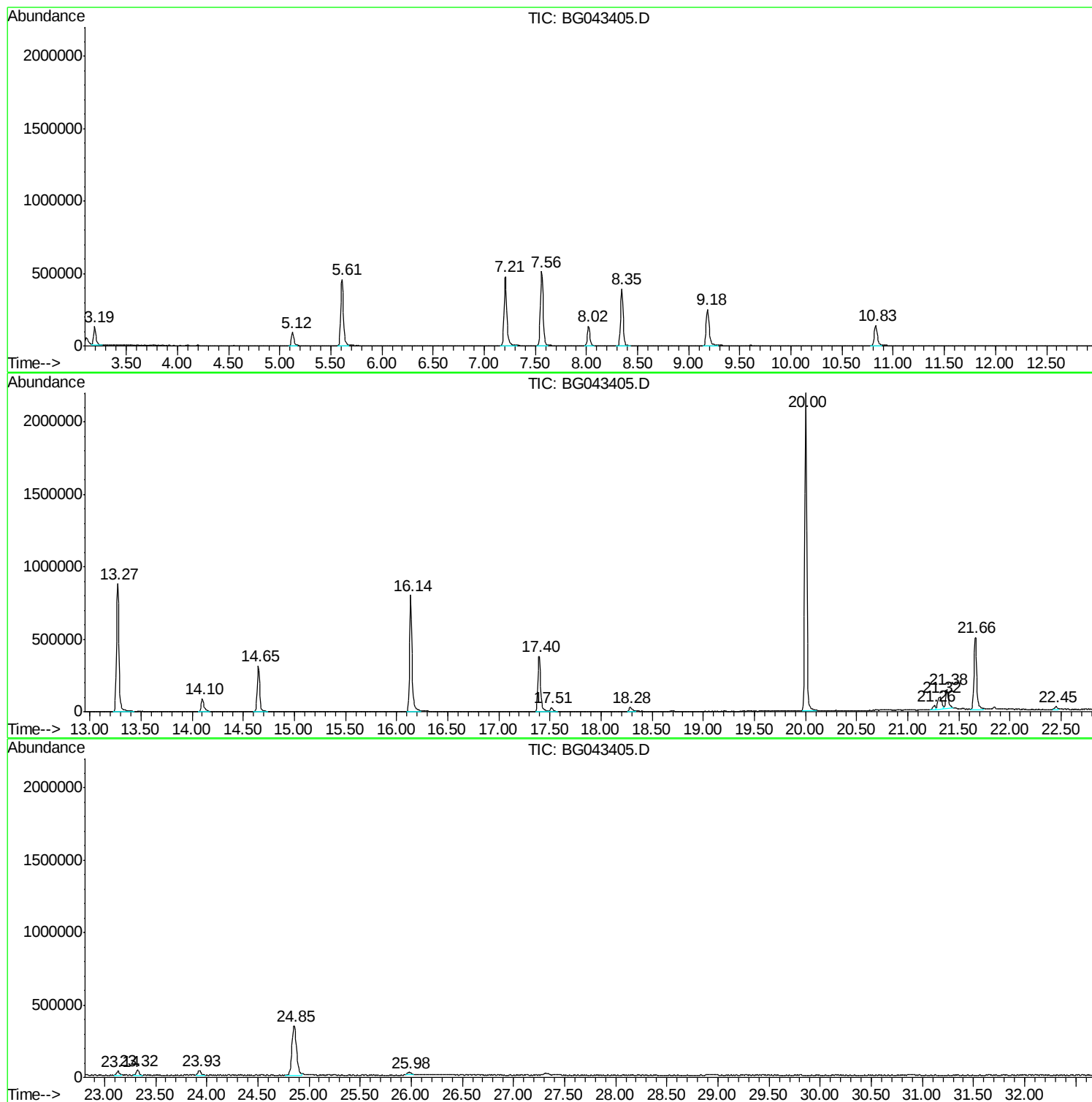
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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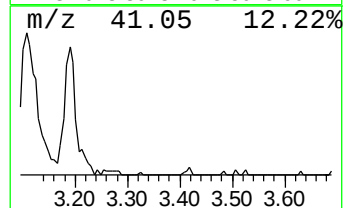
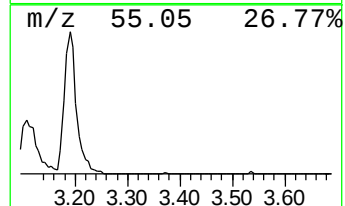
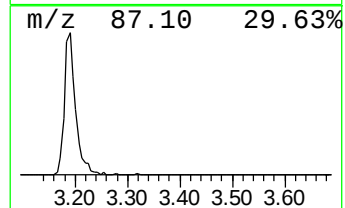
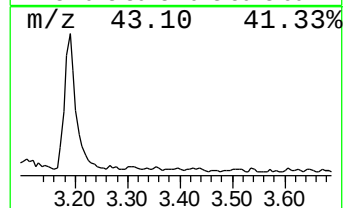
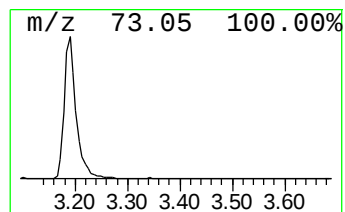
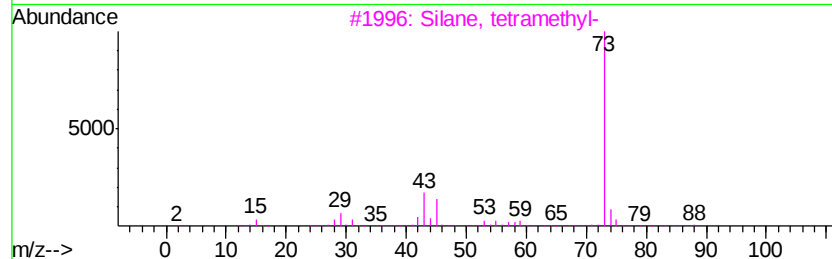
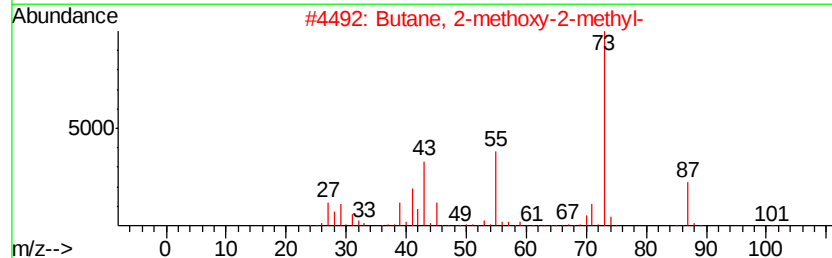
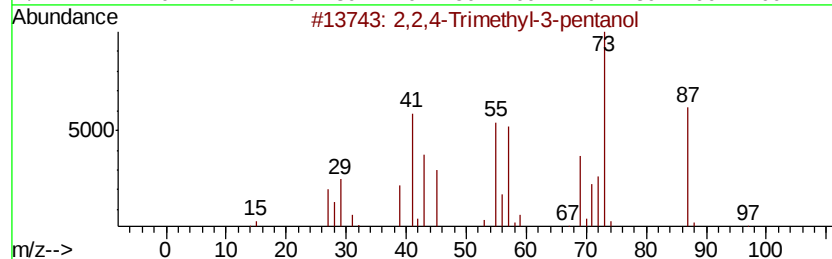
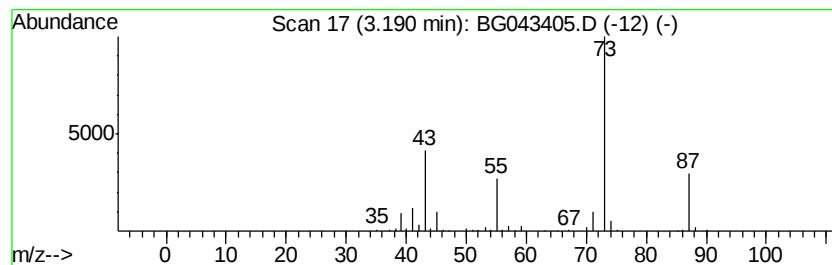
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,2,4-Trimethyl-3-pentanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	16.16 ng	197887	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	64
2		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		1-Propene-1-thiol	74	C3H6S	000925-89-3	9



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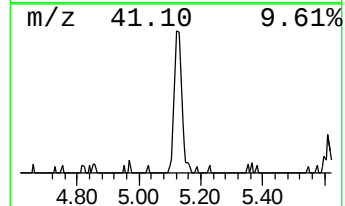
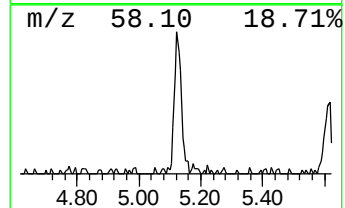
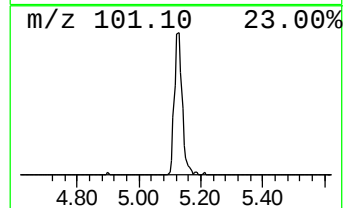
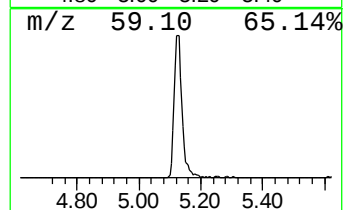
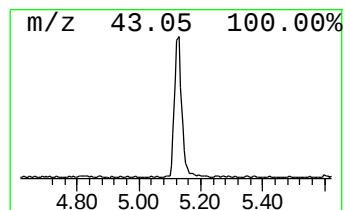
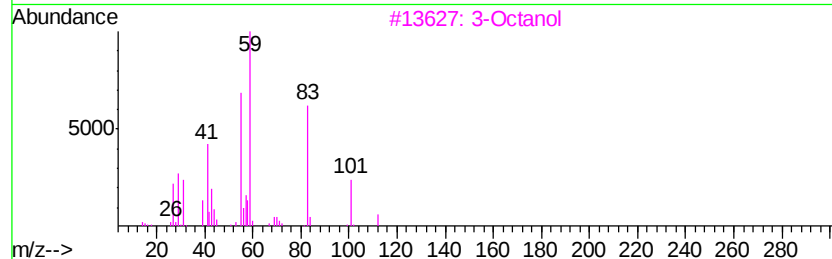
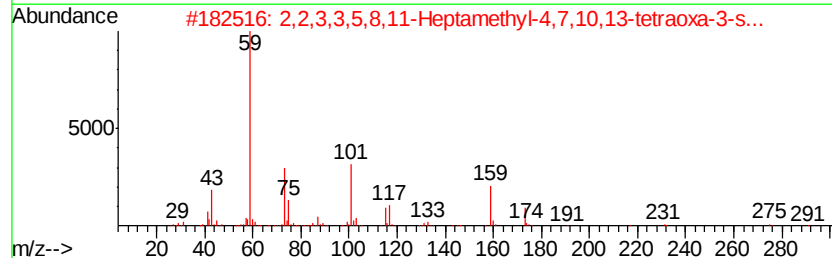
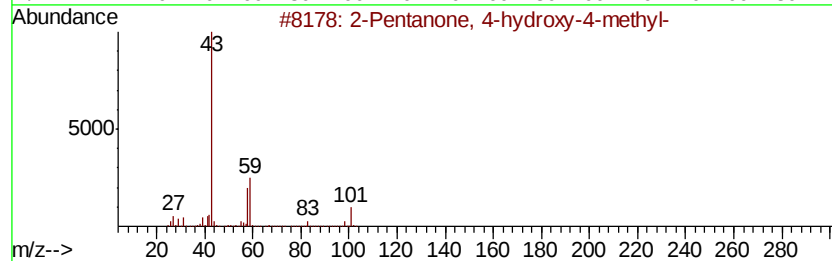
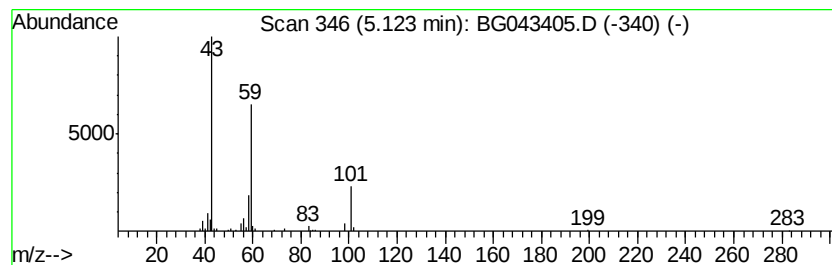
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	12.66 ng	155057	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,2,3,3,5,8,11-Heptamethyl-4,7,1...	348	C18H40O4Si	1000367-07-2	38
3		3-Octanol	130	C8H18O	000589-98-0	36
4		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
5		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28



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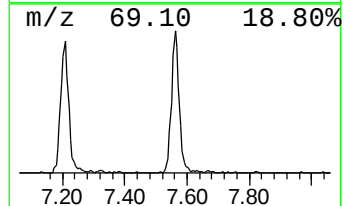
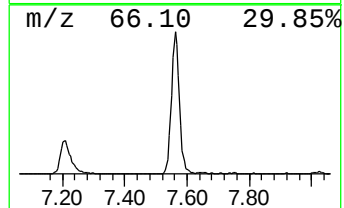
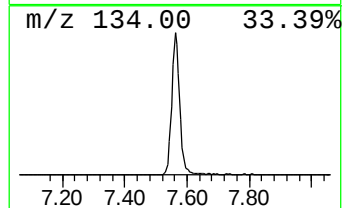
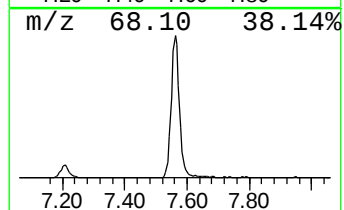
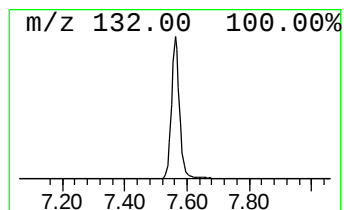
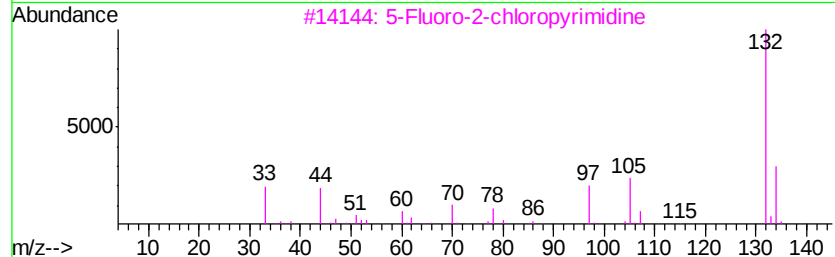
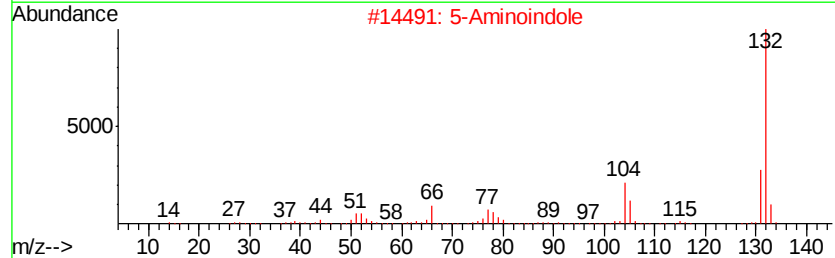
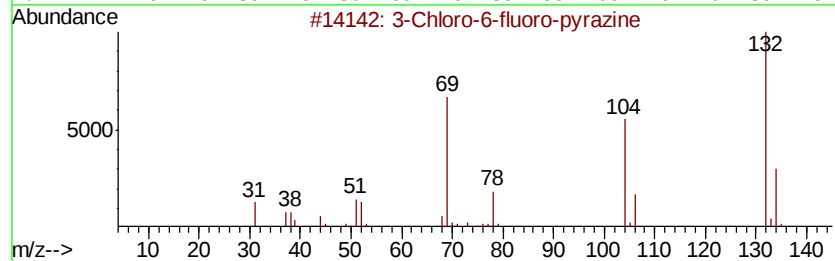
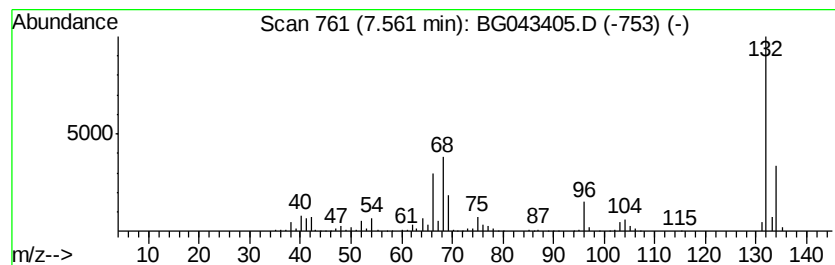
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Peak Number 3 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	76.41 ng	935491	1,4-Dichlorobenzene-d4	8.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	22
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4			Amphetaminil	250	C17H18N2	017590-01-1	10
5			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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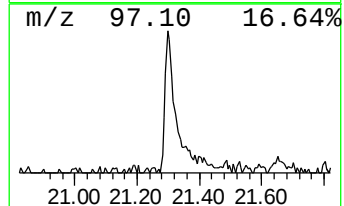
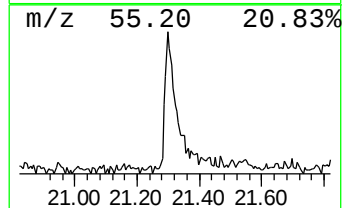
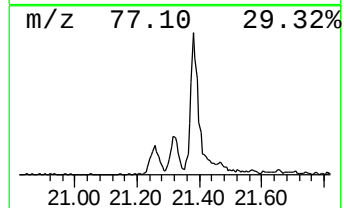
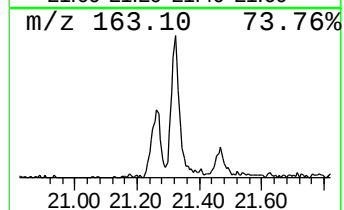
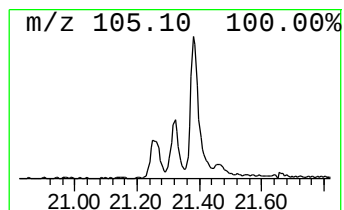
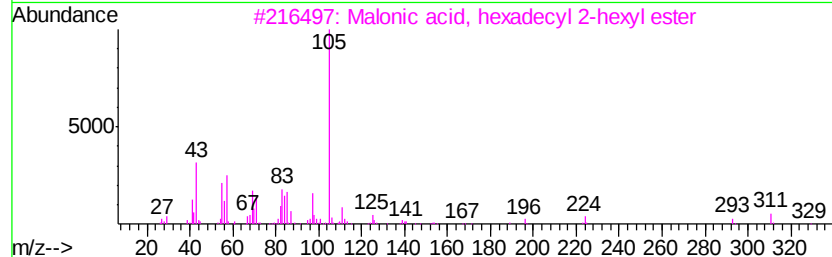
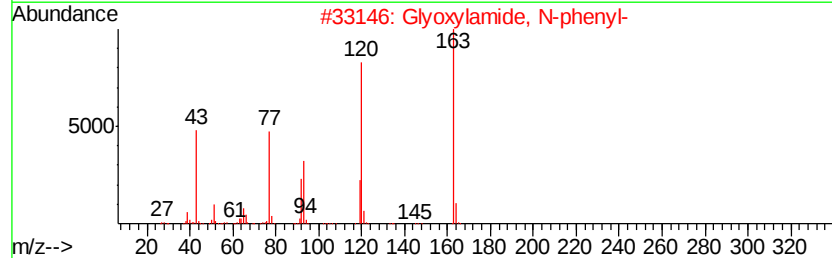
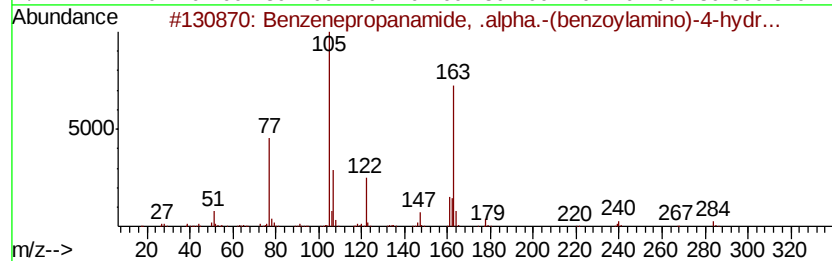
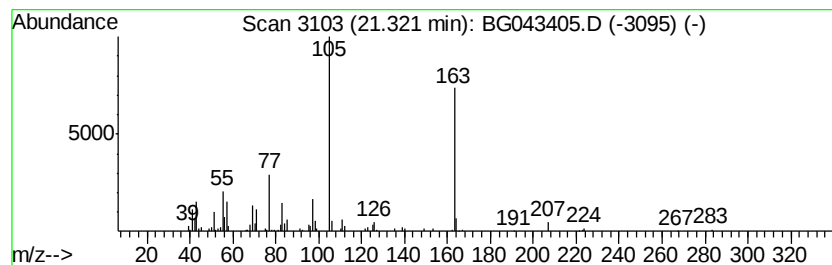
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Peak Number 5 Benzenepropanamide, .alpha.... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	4.93 ng	233971	Chrysene-d12	21.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	50
2		Glyoxylamide, N-phenyl-	163	C9H9N2O2	032331-52-5	38
3		Malonic acid, hexadecyl 2-hexyl ...	412	C25H48O4	1000349-32-9	25
4		1,3-Dimethyl-5-n-hexyladamantane	248	C18H32	052873-50-4	22
5		Malonic acid, 2-hexyl tetradecyl...	384	C23H44O4	1000349-32-7	18



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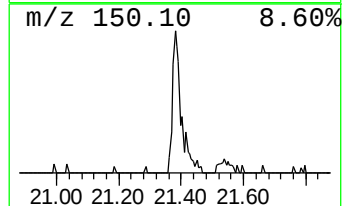
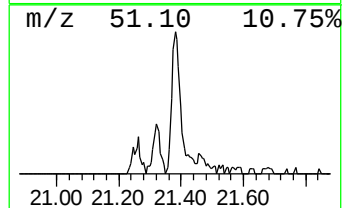
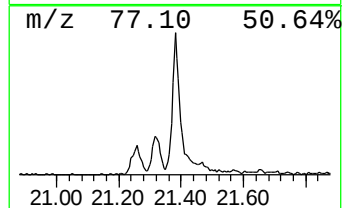
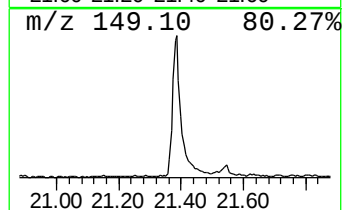
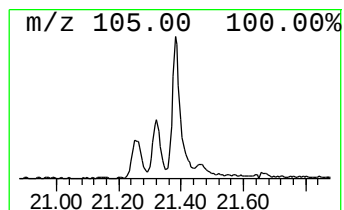
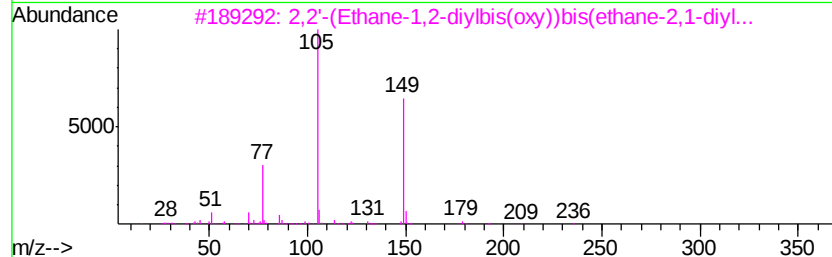
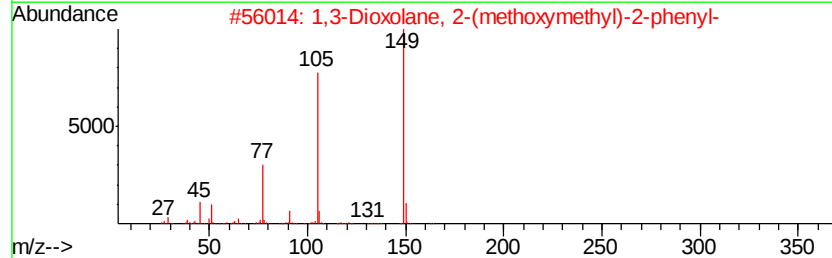
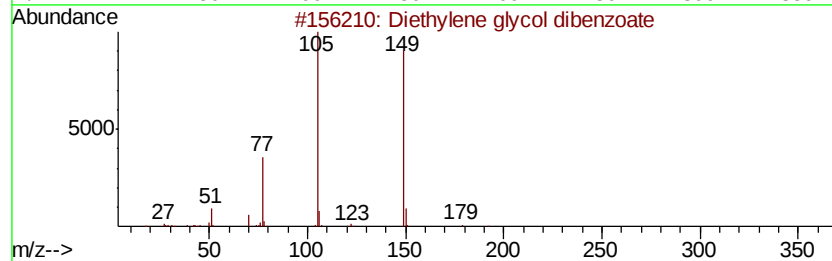
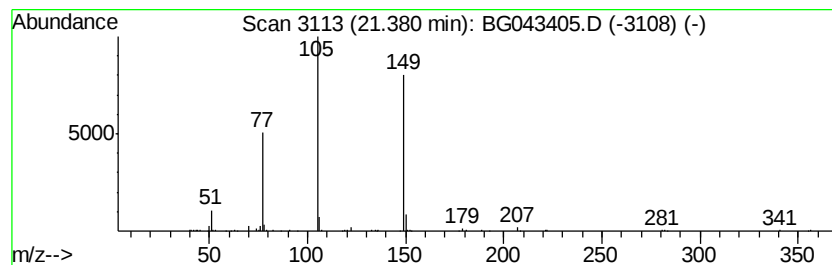
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Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	5.07 ng	240499	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
2		1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
3		2,2'-(Ethane-1,2-diylbis(oxv))bi...	358	C20H22O6	1000366-99-4	56
4		2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52
5		2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,2,4-Trimethyl-3...	3.19	16.2	ng	197887	1	8.02	244861	20.0
2-Pentanone, 4-hy...	5.12	12.7	ng	155057	1	8.02	244861	20.0
unknown7.56	7.56	76.4	ng	935491	1	8.02	244861	20.0
Benzenepropanamid...	21.32	4.9	ng	233971	5	21.66	948380	20.0
Diethylene glycol...	21.38	5.1	ng	240499	5	21.66	948380	20.0