

Data Path : Z:\HPCHEM1\BNA G\DATA\BG091817\
 Data File : BG028803.D
 Acq On : 18 Sep 2017 20:19
 Operator : SJ/JU
 Sample : I5259-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20170601-COMP-B

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-BG091217.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	5.391	303	307	316	rVB	26047	40759	1.18%	0.294%
2	5.856	380	386	399	rBV	300204	514429	14.90%	3.707%
3	7.442	648	656	667	rBV	214995	411898	11.93%	2.968%
4	7.824	713	721	731	rBV	511495	920461	26.65%	6.632%
5	8.288	793	800	807	rBV	113848	201779	5.84%	1.454%
6	8.617	846	856	864	rBV	432948	786002	22.76%	5.663%
7	9.457	992	999	1010	rBV	371956	700910	20.30%	5.050%
8	11.108	1272	1280	1290	rBV	152563	287388	8.32%	2.071%
9	13.529	1684	1692	1700	rBV	1159590	1862244	53.93%	13.418%
10	14.352	1826	1832	1838	rBV	27016	43221	1.25%	0.311%
11	14.904	1920	1926	1939	rVB2	265312	453956	13.15%	3.271%
12	16.396	2173	2180	2190	rBV	1107052	1782029	51.60%	12.840%
13	17.659	2388	2395	2404	rBV	428576	668192	19.35%	4.815%
14	18.300	2496	2504	2510	rBV2	34674	52313	1.51%	0.377%
15	19.904	2771	2777	2783	rBV	68011	83769	2.43%	0.604%
16	20.245	2828	2835	2848	rBV	2491272	3453390	100.00%	24.883%
17	21.984	3123	3131	3142	rBV2	419352	787377	22.80%	5.673%
18	23.182	3329	3335	3342	rVB3	42835	82376	2.39%	0.594%
19	25.444	3709	3720	3734	rBV2	235317	745952	21.60%	5.375%

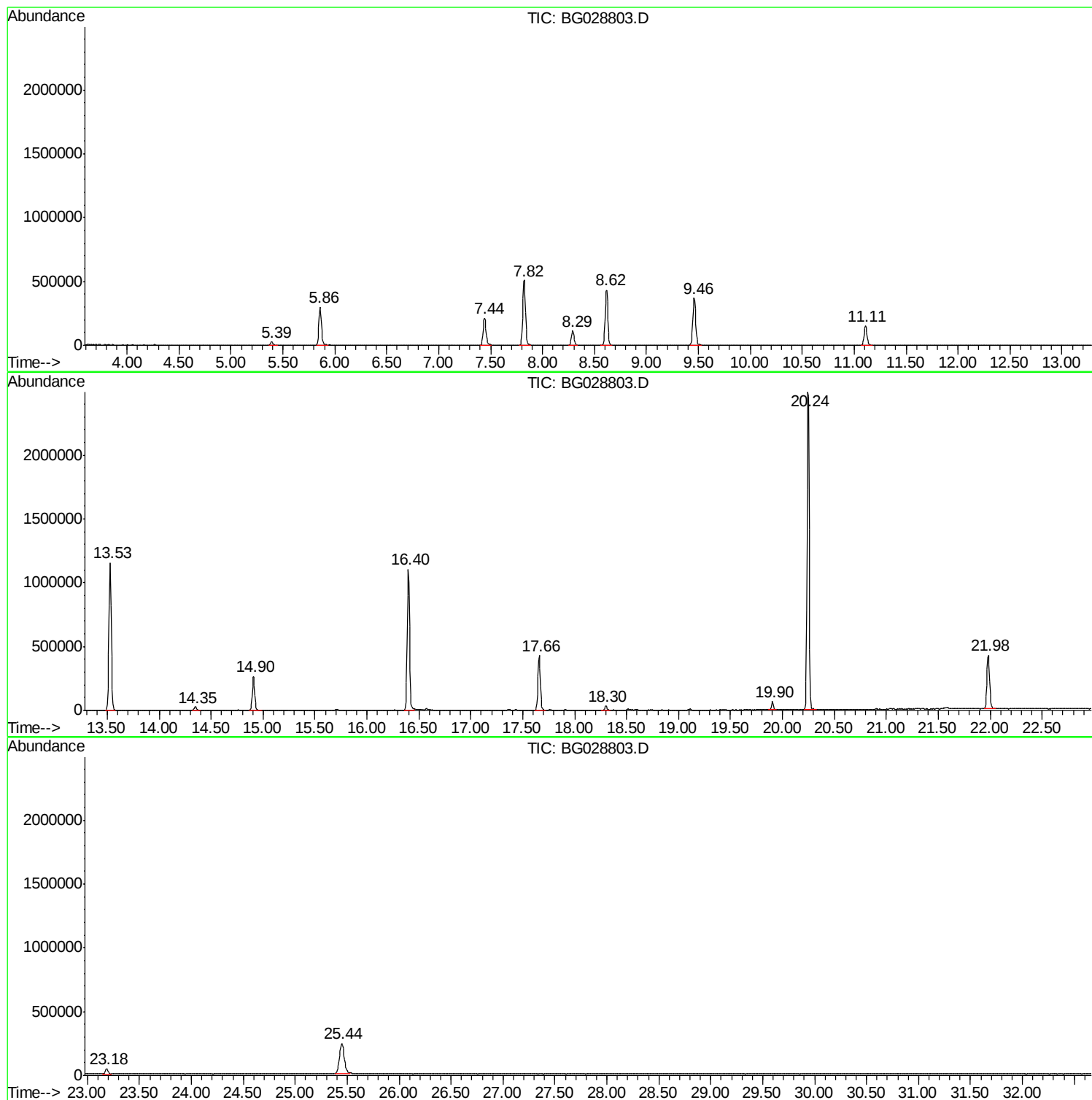
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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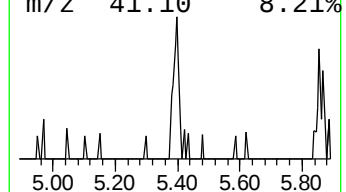
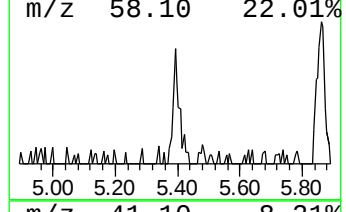
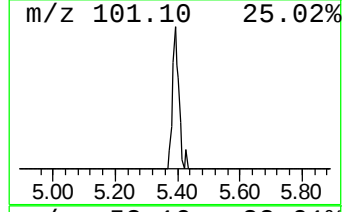
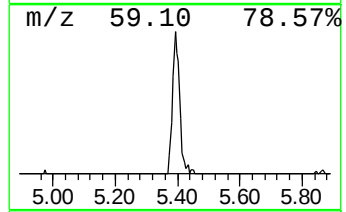
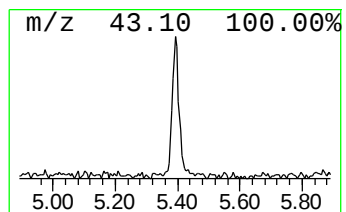
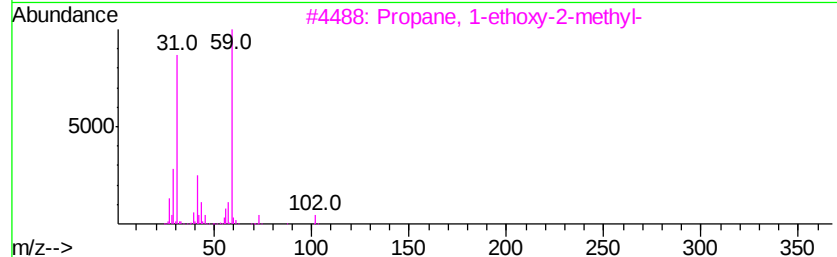
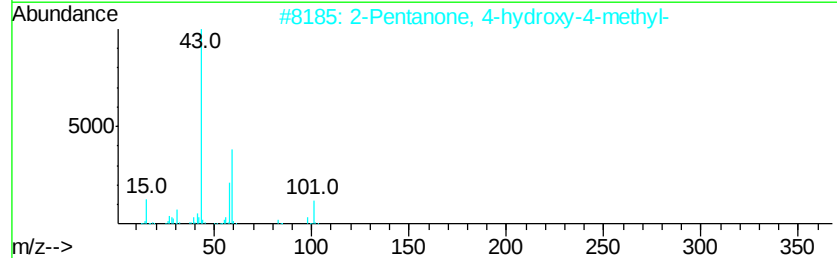
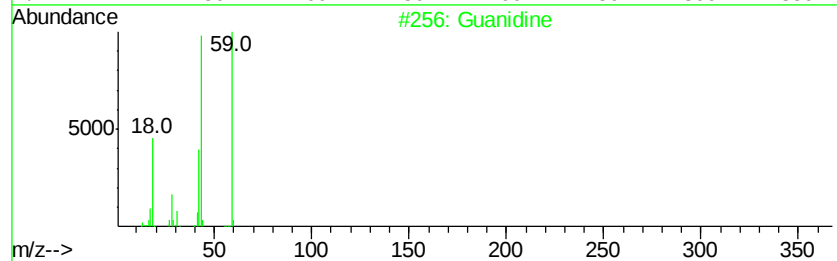
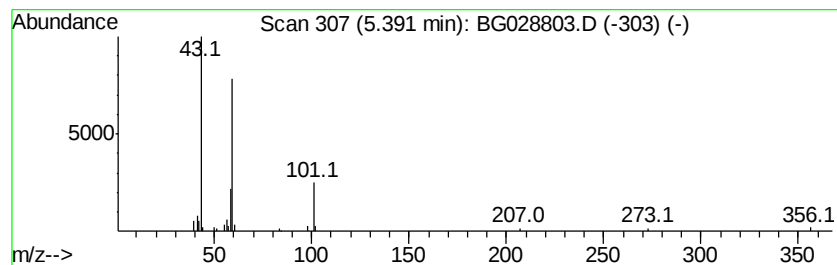
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Guanidine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.39	4.04 ng	40759	1,4-Dichlorobenzene-d4	8.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Guanidine	59	CH5N3	000113-00-8	50
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	43
4		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	42
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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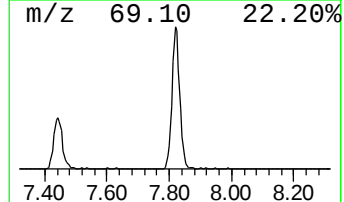
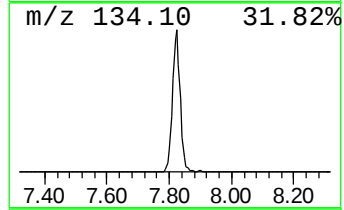
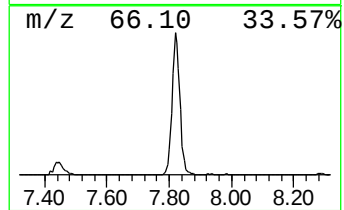
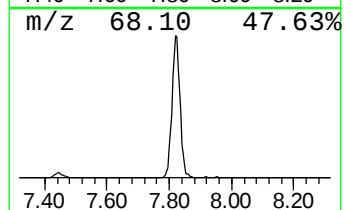
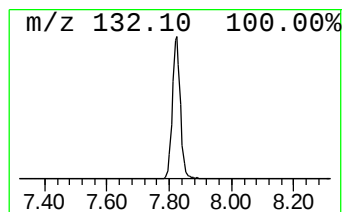
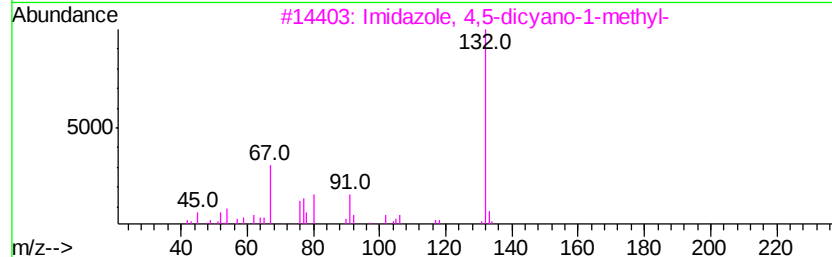
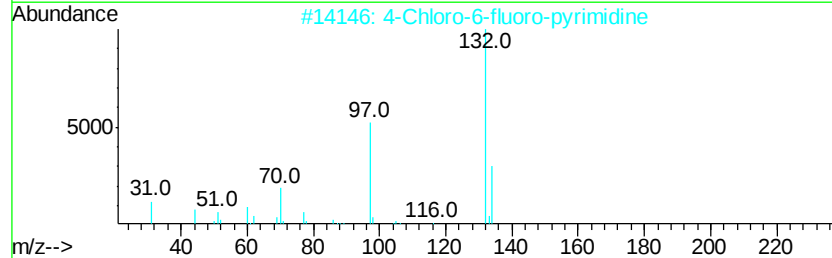
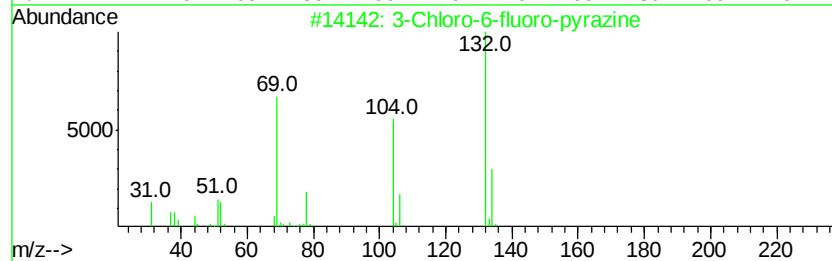
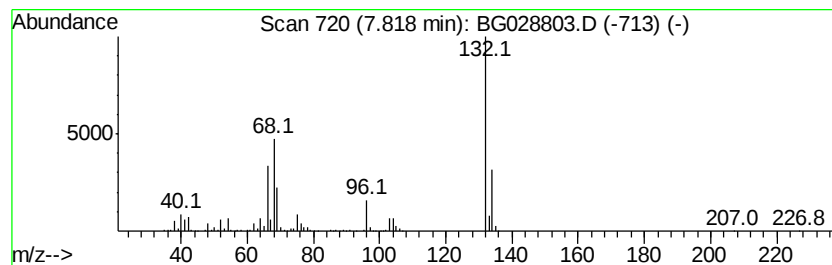
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Peak Number 2 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	91.23 ng	920461	1,4-Dichlorobenzene-d4	8.29

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		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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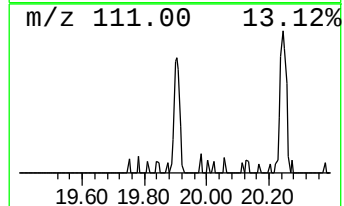
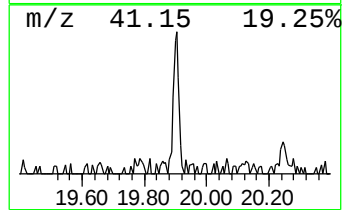
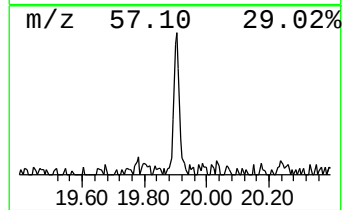
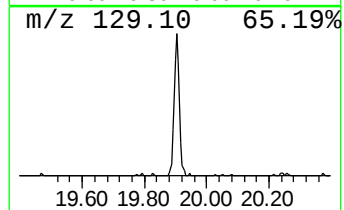
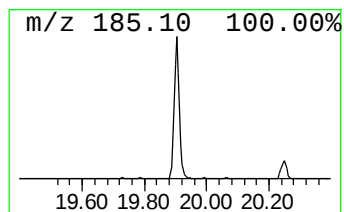
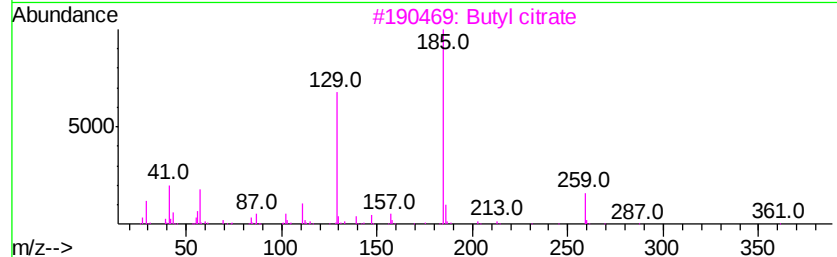
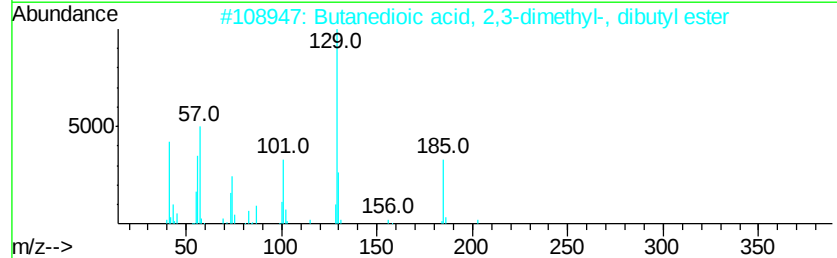
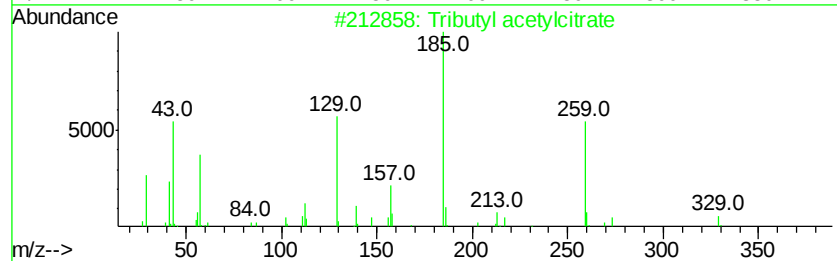
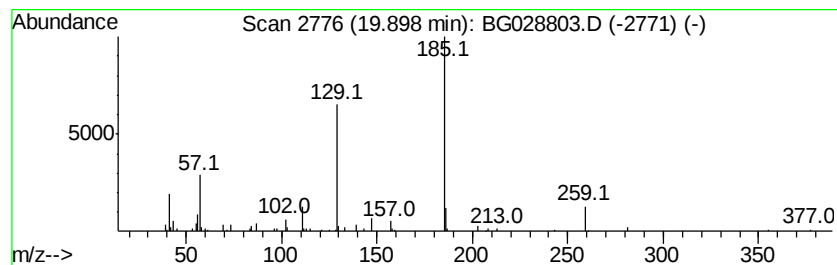
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Peak Number 4 Tributyl acetylcitrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.90	2.13 ng	83769	Chrysene-d12		21.98	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tributyl acetylcitrate	402	C20H34O8	000077-90-7	64
2		Butanedioic acid, 2,3-dimethyl-,...	258	C14H26O4	056051-57-1	59
3		Butyl citrate	360	C18H32O7	000077-94-1	58
4		Adipic acid, 2-heptyl isobutyl e...	300	C17H32O4	1000353-64-3	50
5		Adipic acid, 2,4-dimethylpent-3-...	300	C17H32O4	1000349-77-6	50



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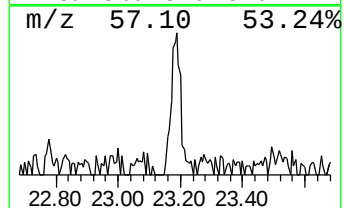
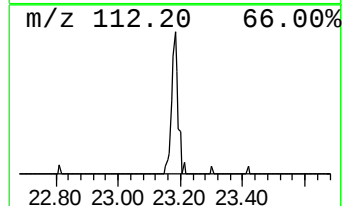
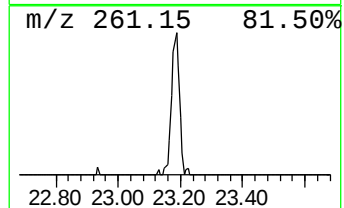
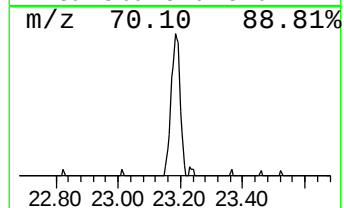
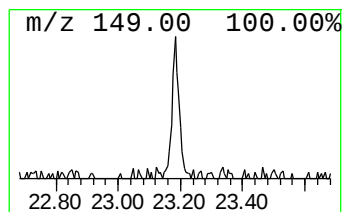
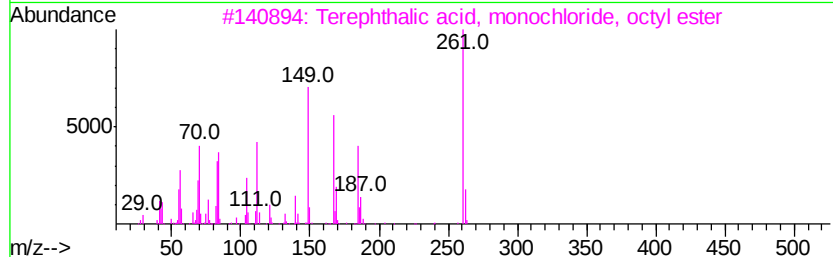
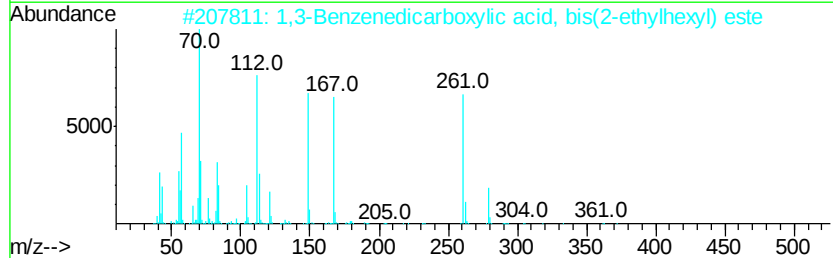
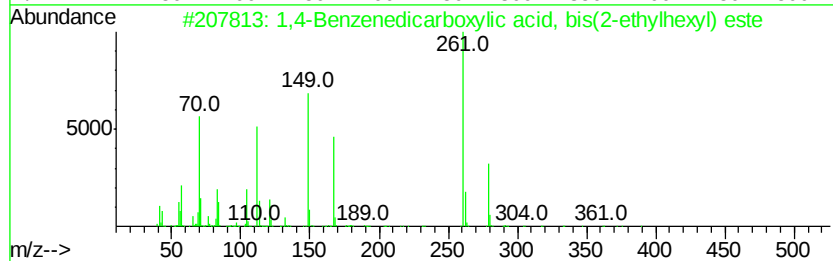
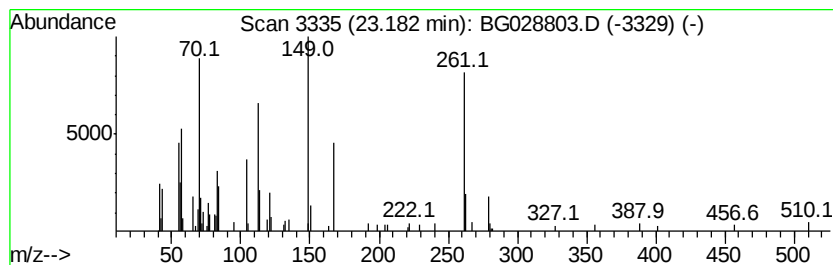
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Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	2.09 ng	82376	Chrysene-d12	21.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	90
2		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	53
3		Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43
4		Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	43
5		Terephthalic acid, phenyl octyl ...	354	C22H26O4	1000324-06-6	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Guanidine	5.39	4.0	ng	40759	1	8.29	201779	20.0
unknown7.82	7.82	91.2	ng	920461	1	8.29	201779	20.0
Tributyl acetylci...	19.90	2.1	ng	83769	5	21.98	787377	20.0
1,4-Benzenedicarb...	23.18	2.1	ng	82376	5	21.98	787377	20.0