

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
 Data File : BG035364.D
 Acq On : 23 Jun 2018 12:15
 Operator : JU/SJ
 Sample : J3623-03
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 061918-DBRI-F-D-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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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	5.173	316	321	328	rBV	36036	60325	1.25%	0.316%
2	5.631	391	399	408	rBV	327607	532182	11.02%	2.791%
3	7.211	661	668	678	rBV	216662	400317	8.29%	2.099%
4	7.587	723	732	742	rBV	574492	1007881	20.87%	5.286%
5	8.057	803	812	824	rBV	192873	334624	6.93%	1.755%
6	8.380	857	867	877	rVB	854779	1516691	31.41%	7.954%
7	9.215	1000	1009	1019	rBV	714327	1278110	26.47%	6.703%
8	10.859	1280	1289	1297	rBV	229629	420845	8.71%	2.207%
9	13.303	1695	1705	1712	rBV	1986237	3149045	65.21%	16.514%
10	14.120	1837	1844	1850	rBV	48301	80406	1.67%	0.422%
11	14.678	1932	1939	1947	rBV2	375122	629883	13.04%	3.303%
12	15.964	2152	2158	2164	rVB	226399	302645	6.27%	1.587%
13	16.158	2184	2191	2204	rBV	1060351	1614588	33.43%	8.467%
14	17.415	2398	2405	2413	rBV2	533367	822180	17.03%	4.312%
15	18.296	2551	2555	2560	rBV2	59854	82878	1.72%	0.435%
16	20.024	2843	2849	2857	rBV	3574525	4829095	100.00%	25.325%
17	21.328	3067	3071	3078	rBV9	39203	80122	1.66%	0.420%
18	21.686	3125	3132	3141	rVB	564598	959422	19.87%	5.031%
19	23.372	3413	3419	3423	rVB2	38270	67494	1.40%	0.354%
20	24.899	3669	3679	3693	rBV2	301599	899909	18.64%	4.719%

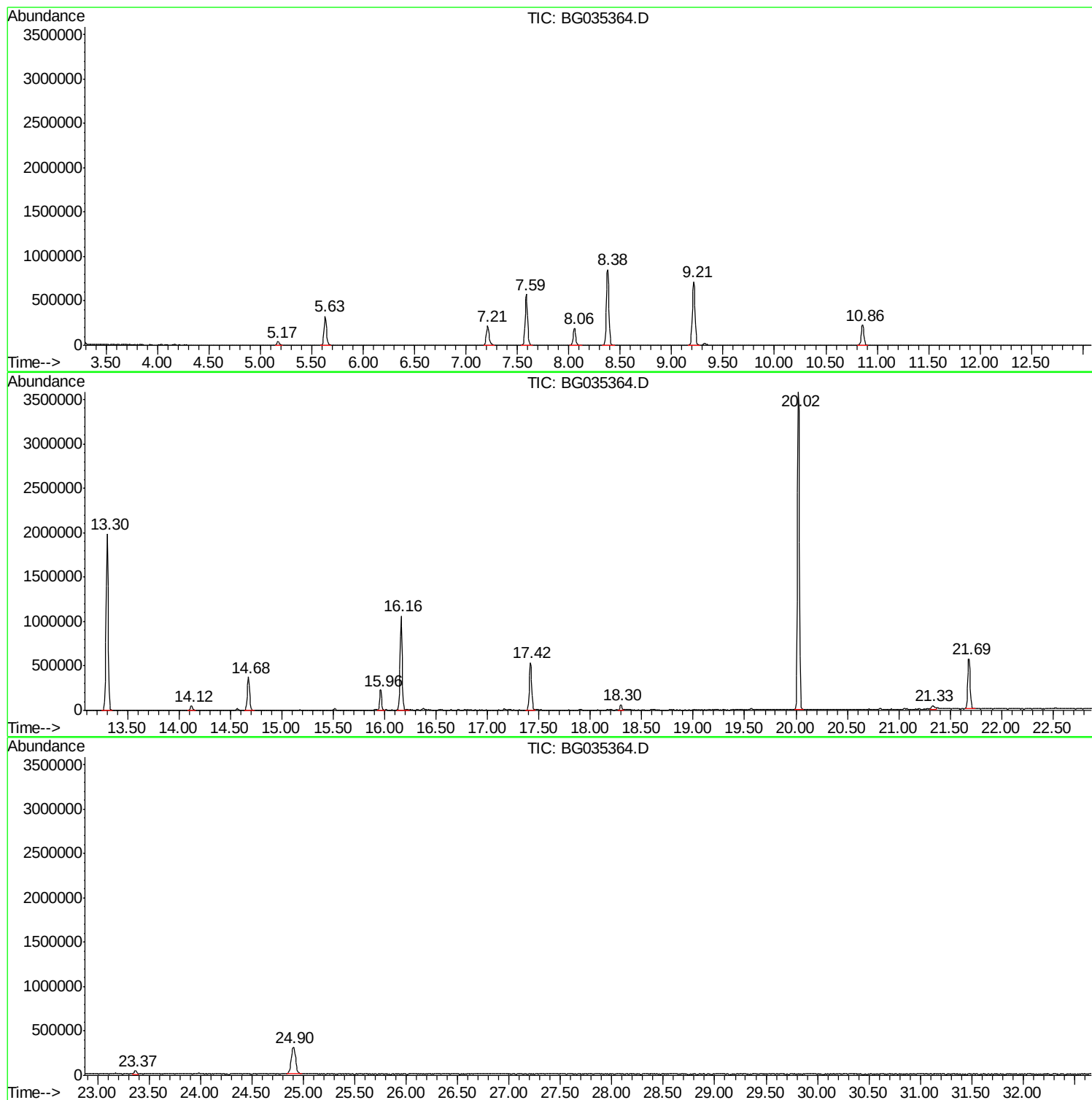
Sum of corrected areas: 19068642

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.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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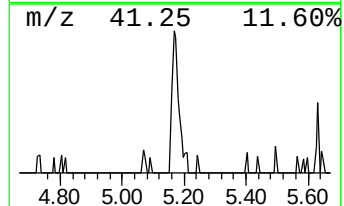
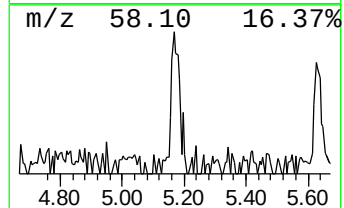
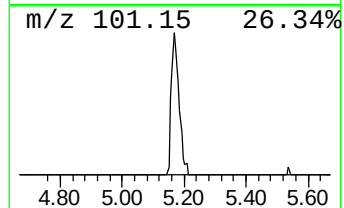
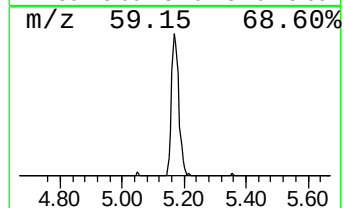
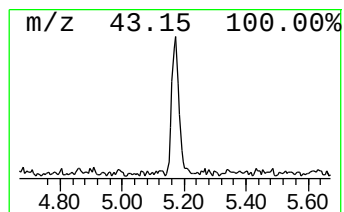
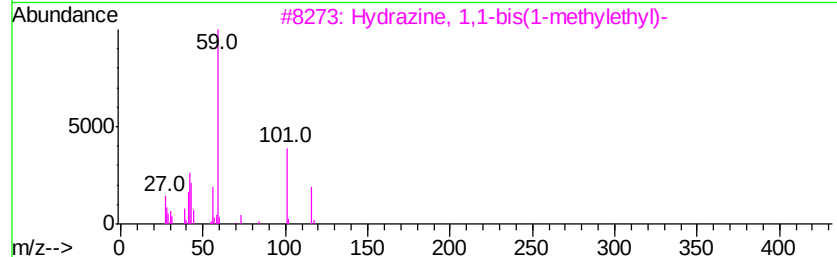
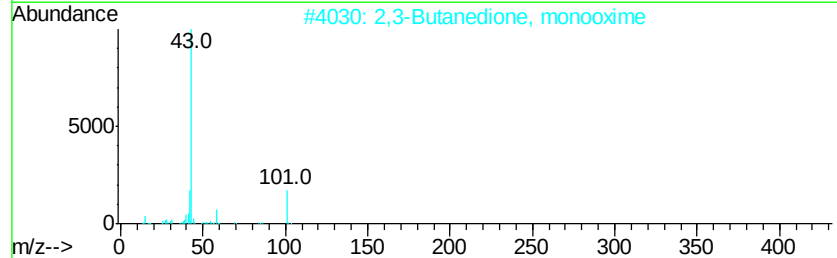
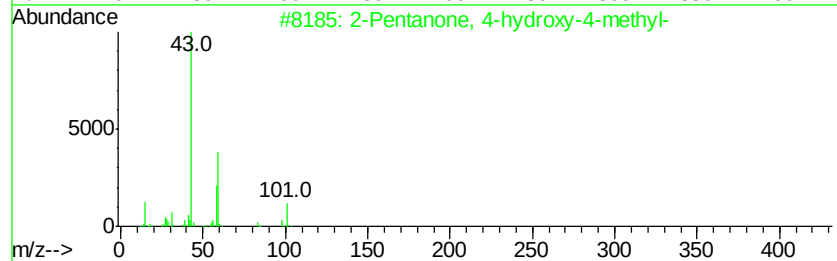
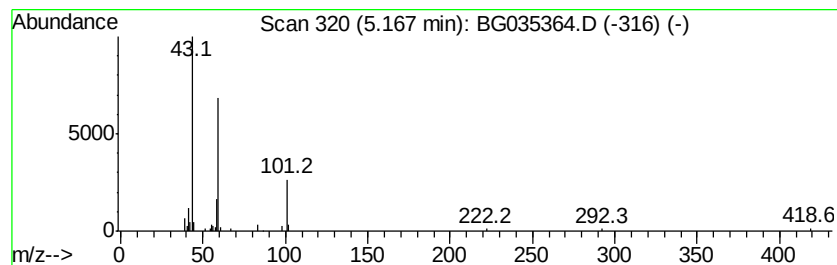
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	3.61 ng	60325	1,4-Dichlorobenzene-d4	8.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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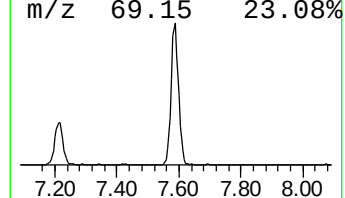
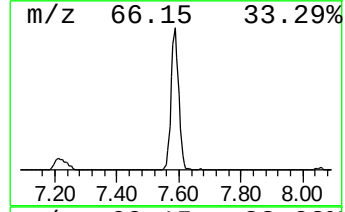
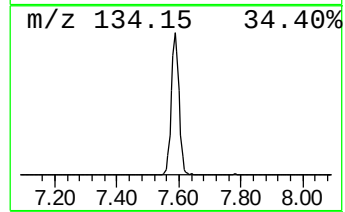
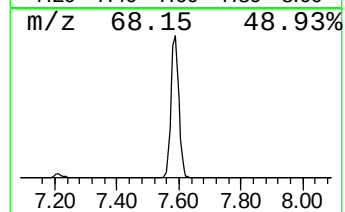
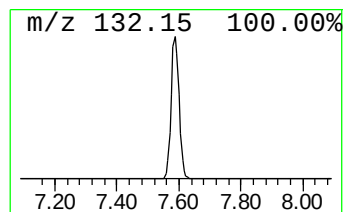
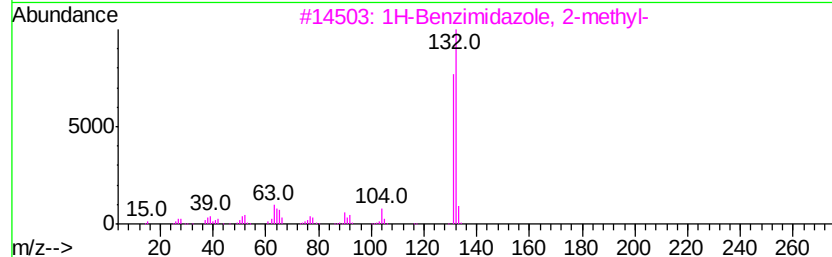
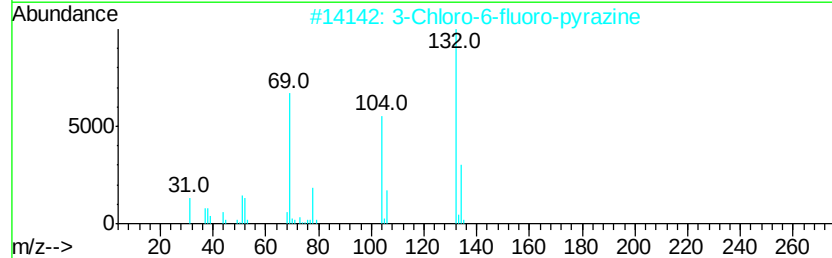
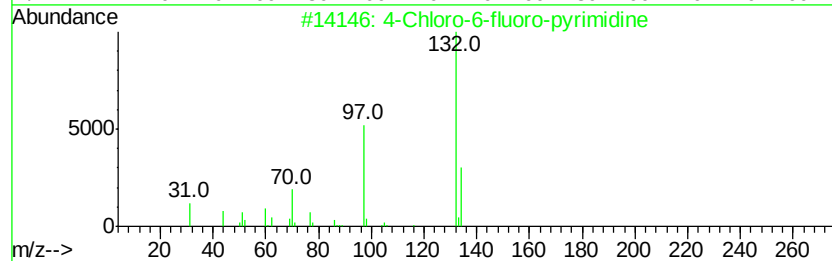
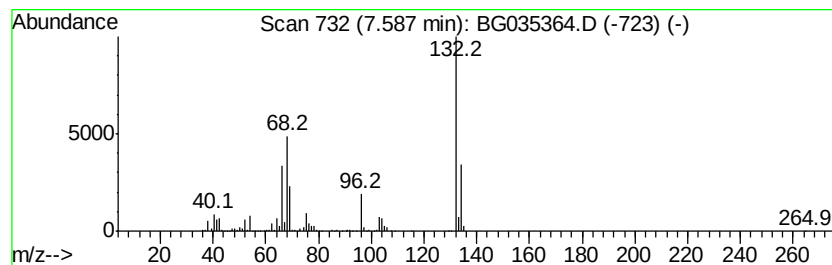
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Peak Number 2 unknown7.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	60.24 ng	1007880	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	18
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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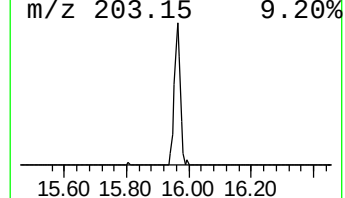
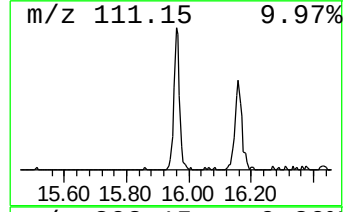
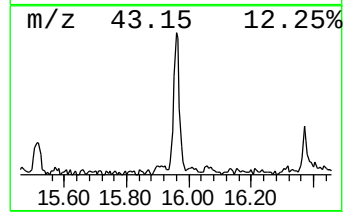
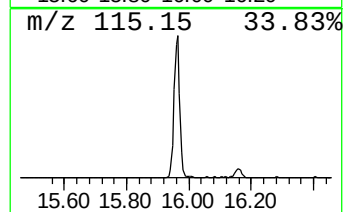
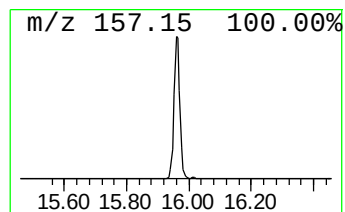
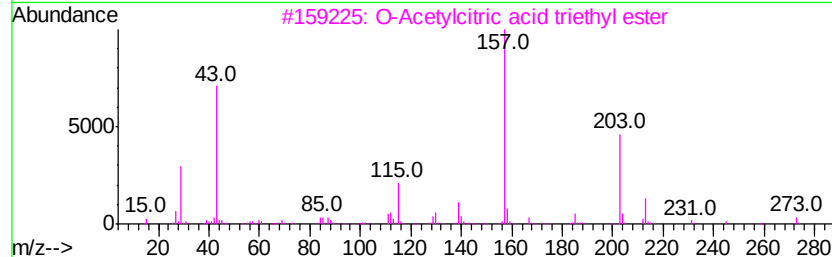
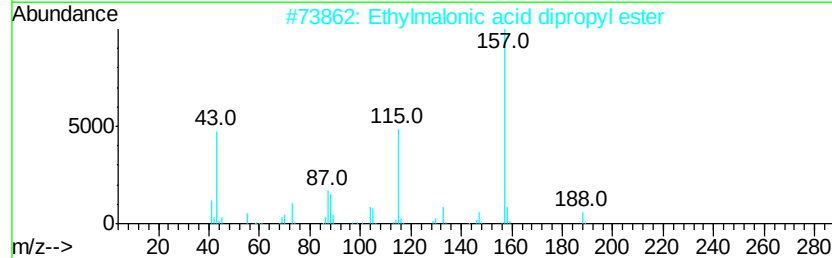
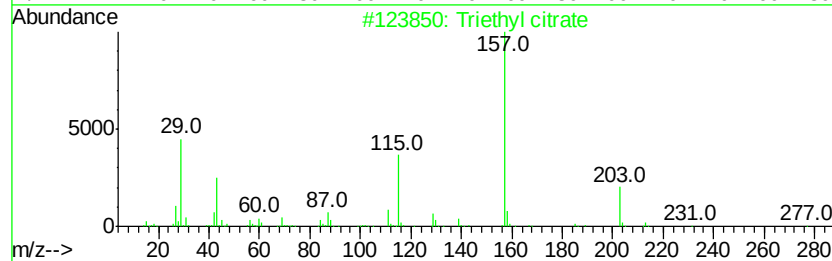
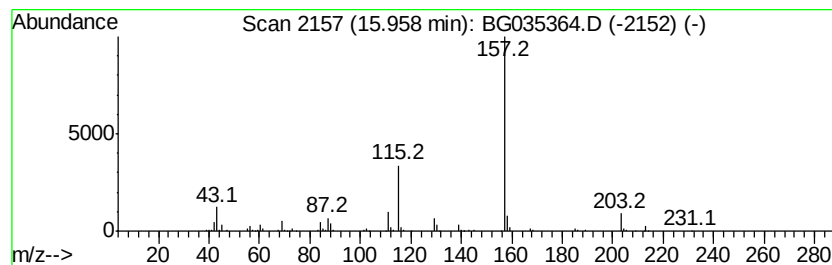
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Peak Number 4 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.96	9.61 ng	302645	Acenaphthene-d10	14.67	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	78
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	O-Acetylcitric acid triethyl ester	318	C14H22O8	000077-89-4	56
4	Adipic acid, isobutyl 3-(2-metho...	358	C20H38O5	1000324-28-7	36
5	3-Chloro2-fluorobenzoic acid, 4-...	384	C22H34ClFO2	1000338-65-1	33



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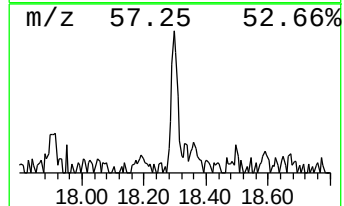
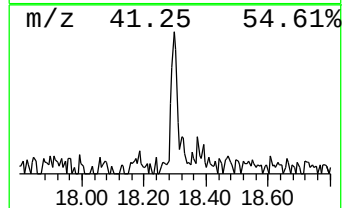
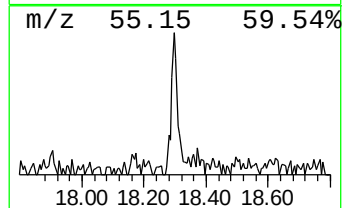
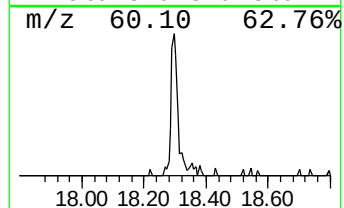
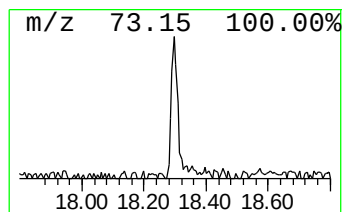
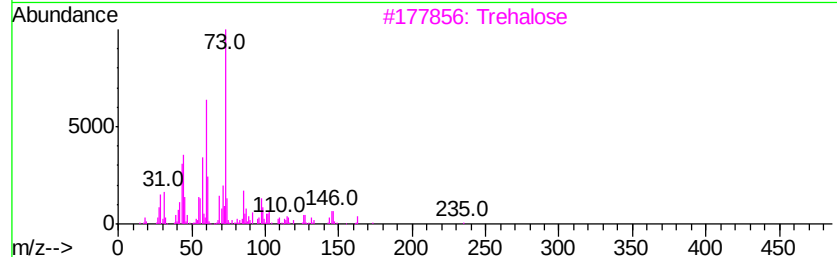
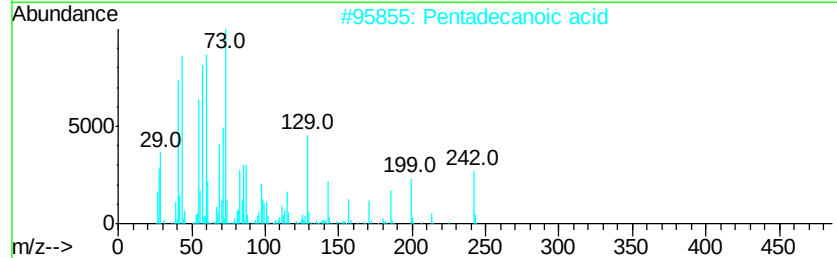
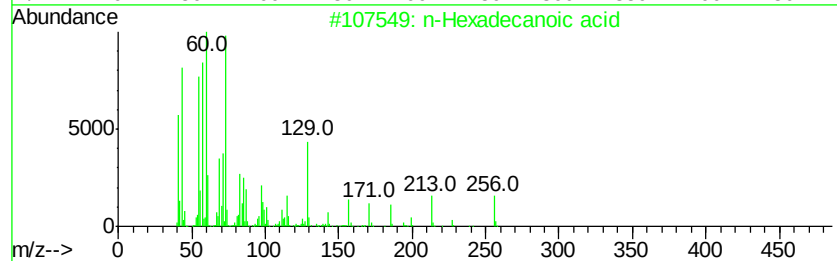
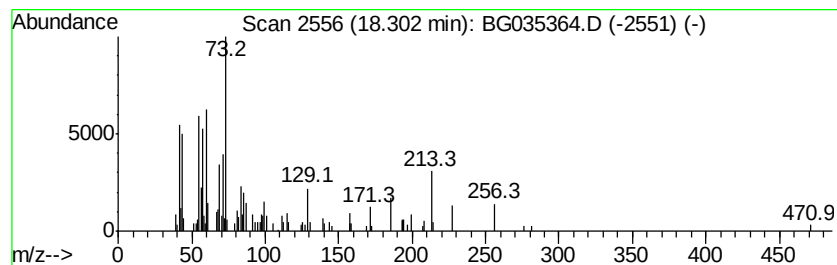
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	2.02 ng	82878	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
3	Trehalose	342	C12H22O11	000099-20-7	47
4	Tridecanoic acid	214	C13H26O2	000638-53-9	43
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	3.6	ng	60325	1	8.05	334624	20.0
unknown7.59	7.59	60.2	ng	1007880	1	8.05	334624	20.0
Triethyl citrate	15.96	9.6	ng	302645	3	14.67	629883	20.0
n-Hexadecanoic acid	18.30	2.0	ng	82878	4	17.42	822180	20.0