

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
 Data File : BG036795.D
 Acq On : 18 Sep 2018 21:06
 Operator : JU/SJ
 Sample : J4922-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PZ-3

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-BG082318.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	5.617	389	396	405	rBV	417810	651930	18.73%	3.569%
2	7.204	657	666	675	rBV	262666	473924	13.62%	2.595%
3	7.580	722	730	738	rBV	710867	1203830	34.59%	6.591%
4	8.050	803	810	819	rBV	190601	320336	9.20%	1.754%
5	8.373	858	865	874	rVB	619647	1074973	30.88%	5.885%
6	9.207	1000	1007	1020	rBV	572340	1008910	28.99%	5.524%
7	10.852	1280	1287	1296	rVB	249943	465719	13.38%	2.550%
8	13.297	1696	1703	1710	rBV	1479964	2302566	66.15%	12.606%
9	14.119	1835	1843	1852	rVB	145102	216615	6.22%	1.186%
10	14.672	1929	1937	1942	rBV2	407144	676680	19.44%	3.705%
11	14.736	1942	1948	1966	rVB	475081	948611	27.25%	5.194%
12	14.907	1972	1977	1983	rBV2	50333	71143	2.04%	0.389%
13	15.670	2098	2107	2111	rBV4	18607	37952	1.09%	0.208%
14	16.158	2183	2190	2205	rBV	1198163	1872857	53.81%	10.254%
15	17.415	2398	2404	2412	rBV	559987	866082	24.88%	4.742%
16	18.185	2531	2535	2539	rBV3	32057	56065	1.61%	0.307%
17	18.303	2550	2555	2563	rBV	106981	169234	4.86%	0.927%
18	18.514	2587	2591	2602	rBV	113069	195772	5.62%	1.072%
19	19.572	2767	2771	2775	rBV4	42224	64443	1.85%	0.353%
20	20.024	2842	2848	2856	rBV	2612293	3480612	100.00%	19.056%
21	21.375	3073	3078	3082	rBV8	25694	62905	1.81%	0.344%
22	21.681	3124	3130	3139	rVB	585926	970823	27.89%	5.315%
23	23.967	3516	3519	3527	rVB6	22400	48331	1.39%	0.265%
24	24.889	3666	3676	3692	rVB	346721	1024991	29.45%	5.612%

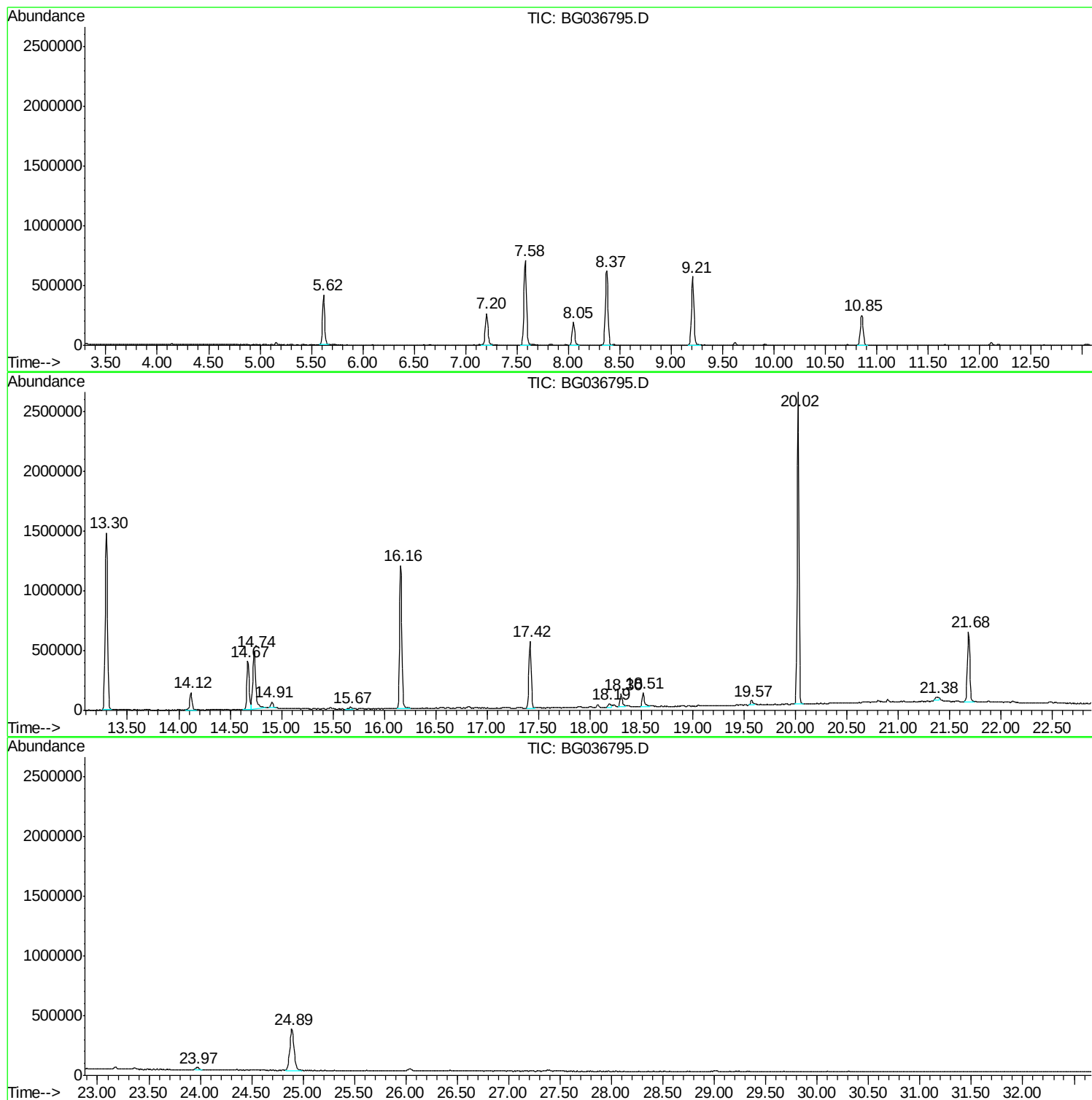
Sum of corrected areas: 18265304

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.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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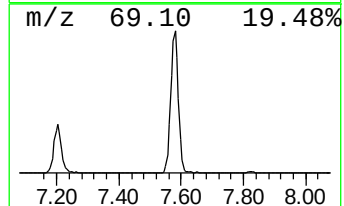
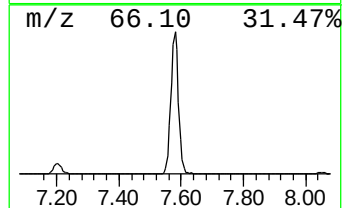
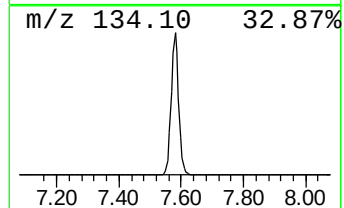
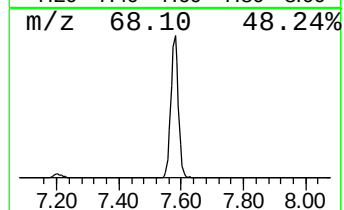
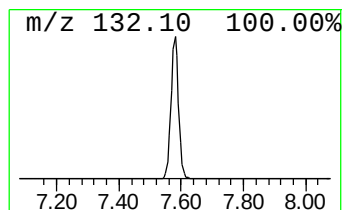
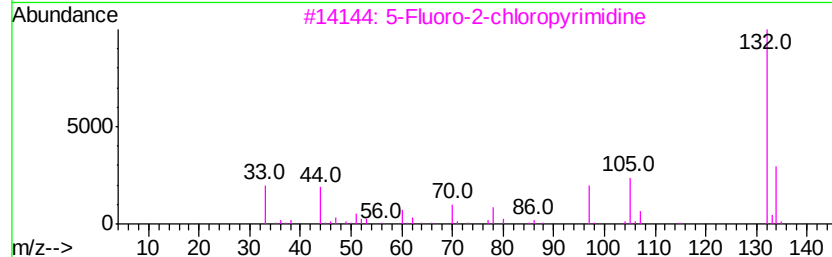
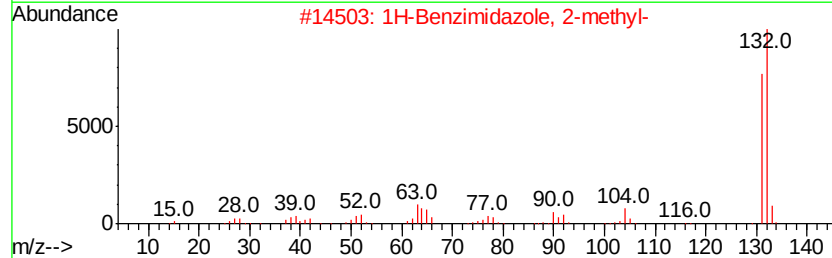
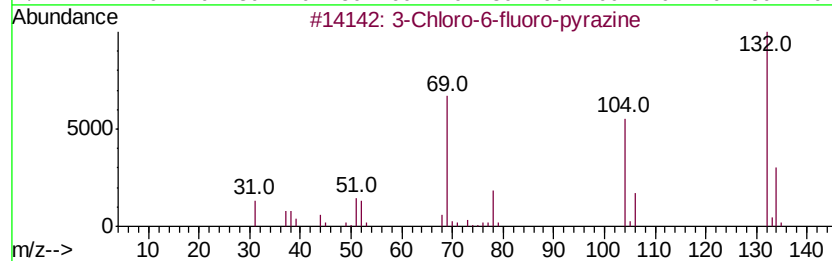
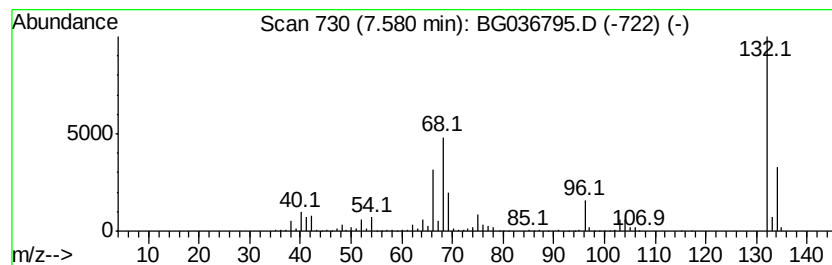
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	75.16 ng	1203830	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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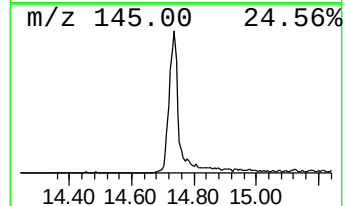
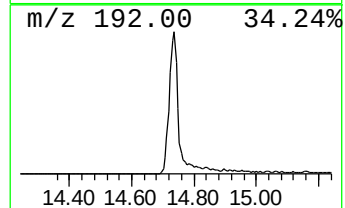
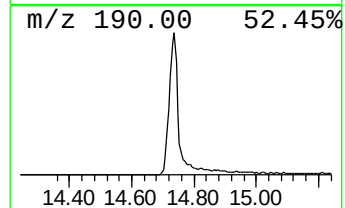
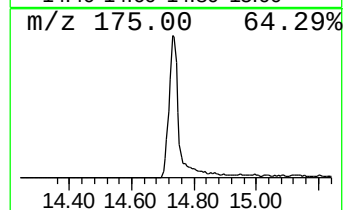
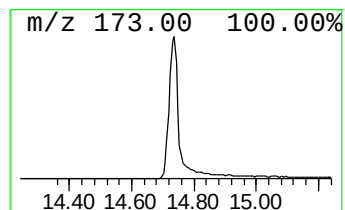
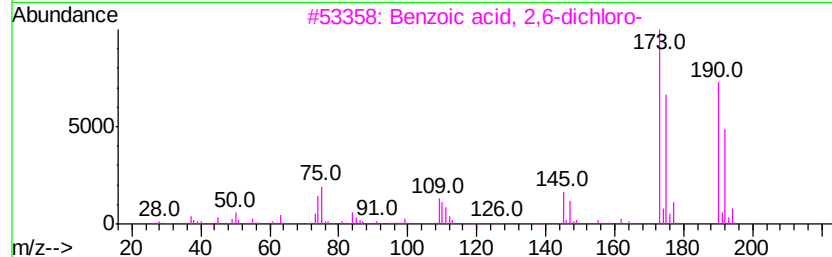
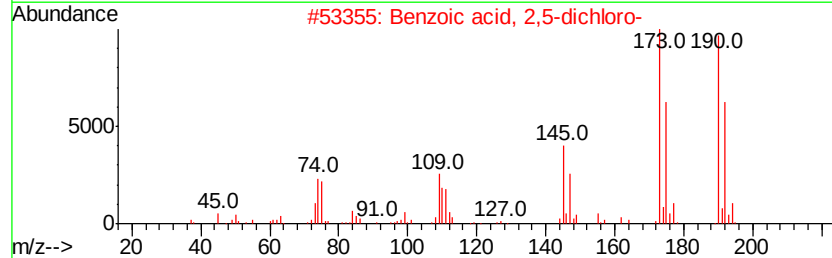
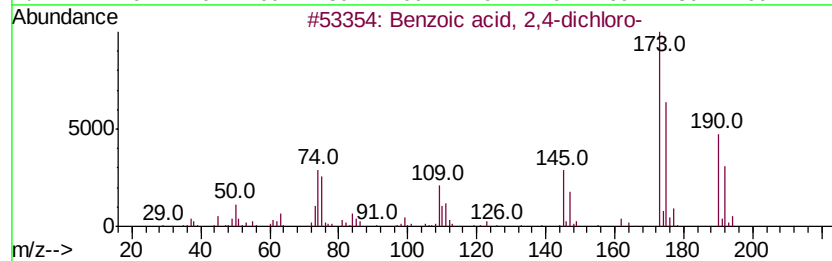
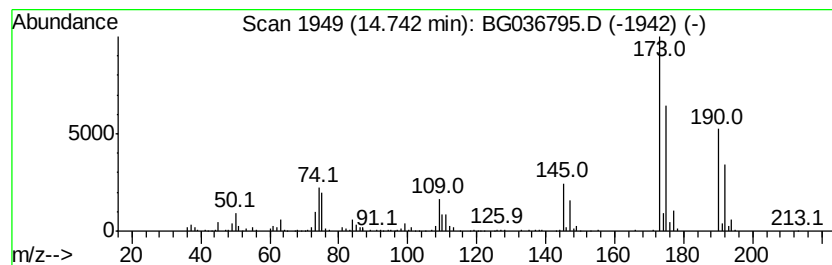
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzoic acid, 2,4-dichloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	28.04 ng	948611	Acenaphthene-d10	14.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzoic acid, 2,4-dichloro-	190 C7H4Cl2O2	000050-84-0 99
2		Benzoic acid, 2,5-dichloro-	190 C7H4Cl2O2	000050-79-3 96
3		Benzoic acid, 2,6-dichloro-	190 C7H4Cl2O2	000050-30-6 96
4		Benzoic acid, 3,4-dichloro-	190 C7H4Cl2O2	000051-44-5 95
5		Butyl 2,4-dichlorobenzoate	246 C11H12Cl2O2	1000373-00-8 86



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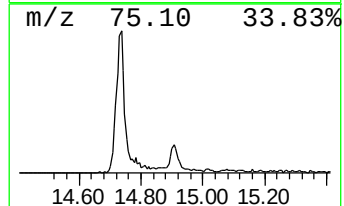
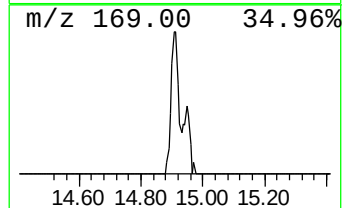
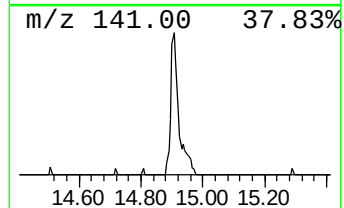
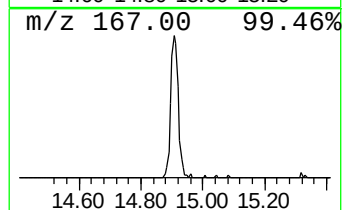
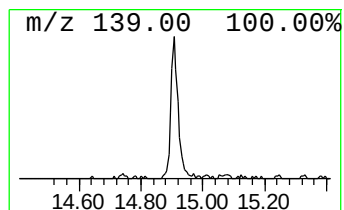
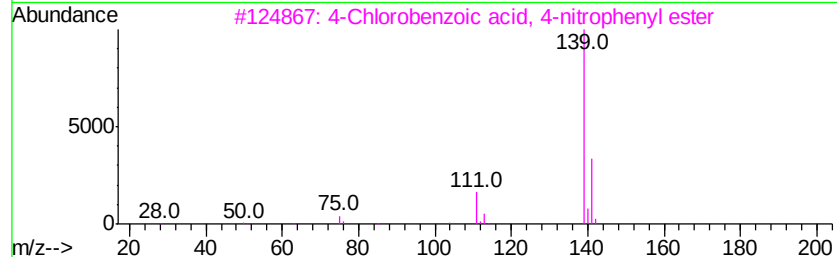
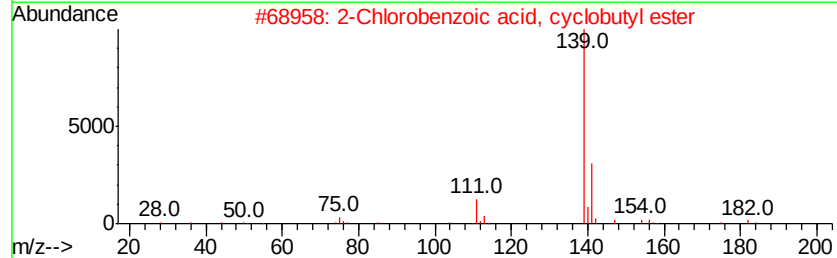
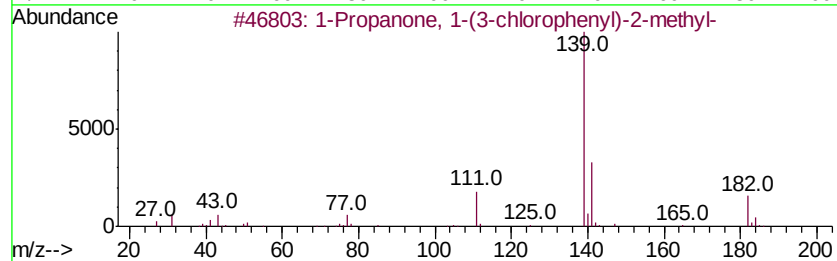
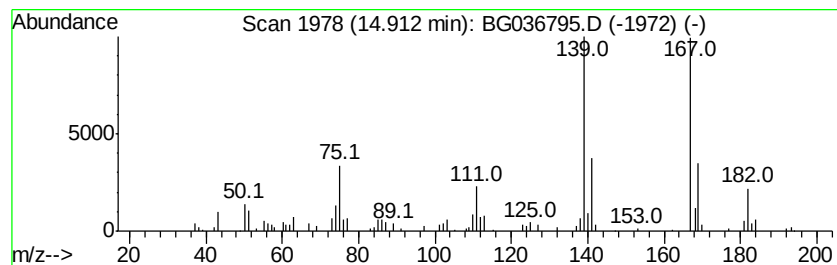
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Peak Number 4 1-Propanone, 1-(3-chlorophe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	2.10 ng	71143	Acenaphthene-d10	14.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanone, 1-(3-chlorophenyl)-...	182	C10H11ClO	055649-98-4	50
2		2-Chlorobenzoic acid, cyclobutyl...	210	C11H11ClO2	1000292-27-5	49
3		4-Chlorobenzoic acid, 4-nitrophe...	277	C13H8ClN04	1000307-76-2	46
4		4-Chlorobenzoic acid, 2-formyl-4...	328	C14H7Cl3O3	1000331-01-2	46
5		2-Chlorobenzoic acid, 4-nitrophe...	277	C13H8ClN04	1000307-82-0	46



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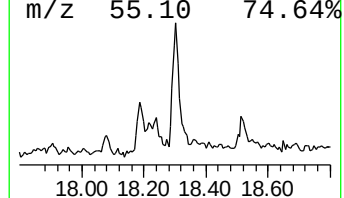
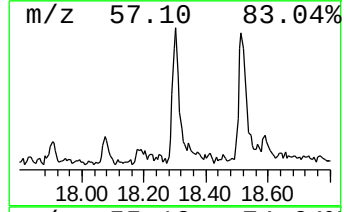
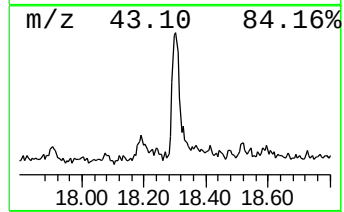
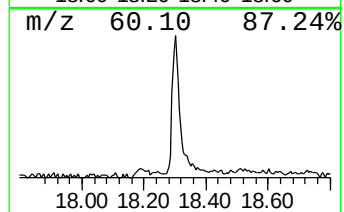
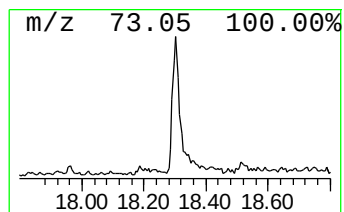
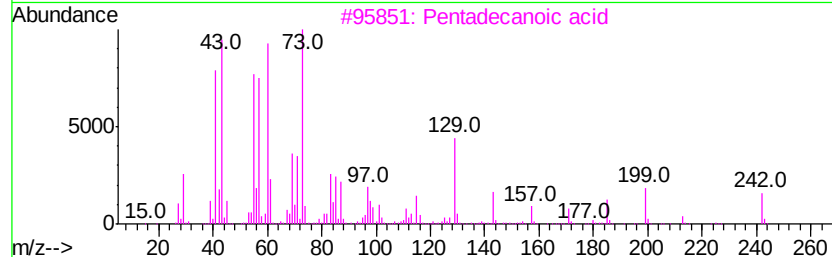
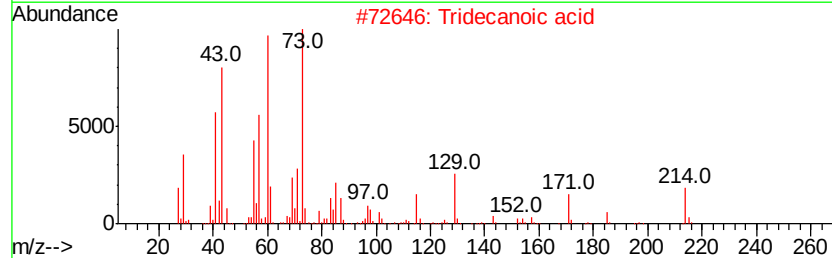
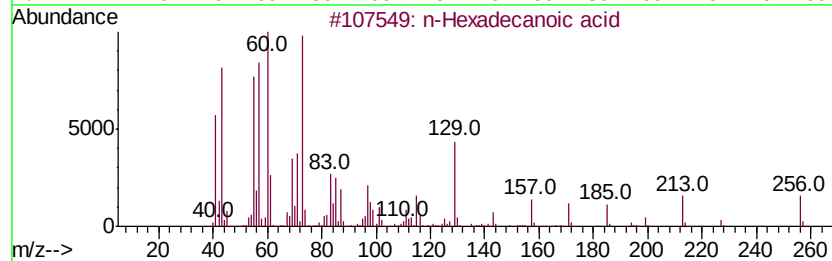
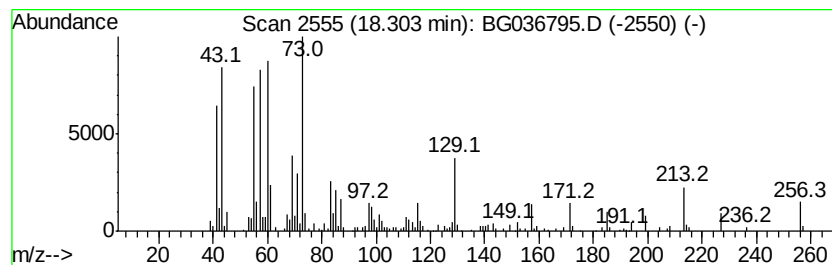
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.91 ng	169234	Phenanthrene-d10	17.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	81
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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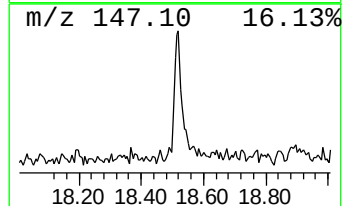
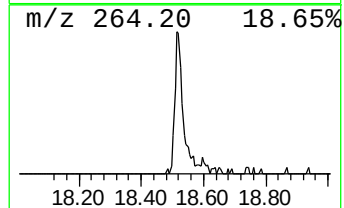
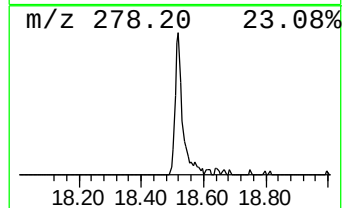
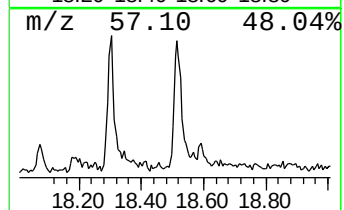
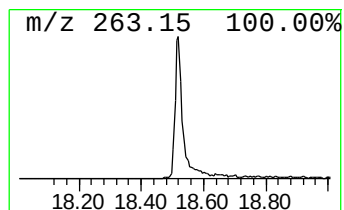
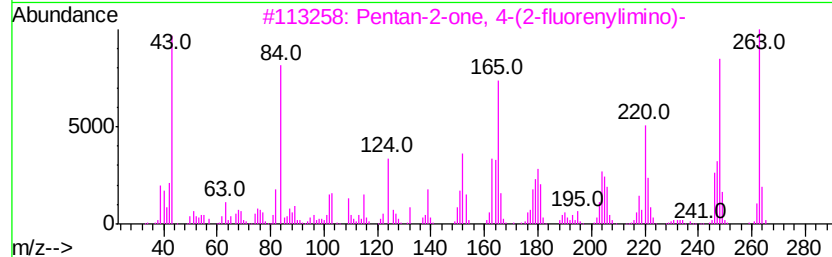
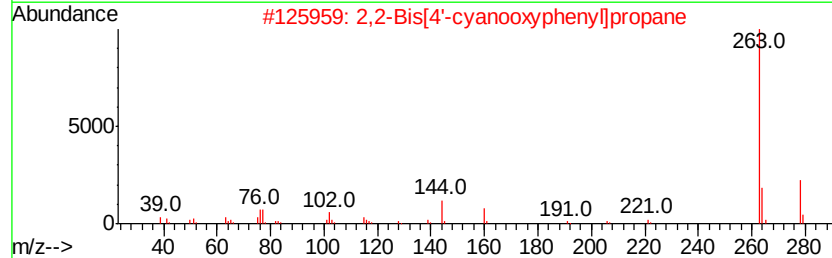
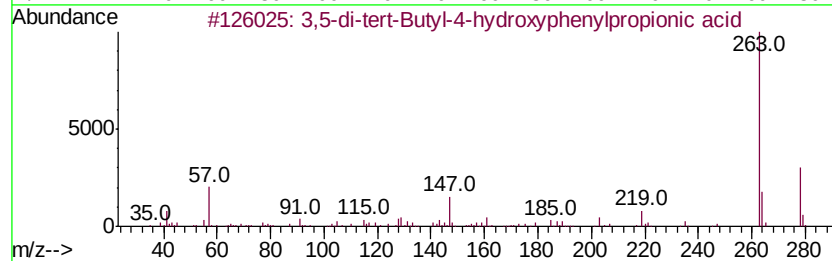
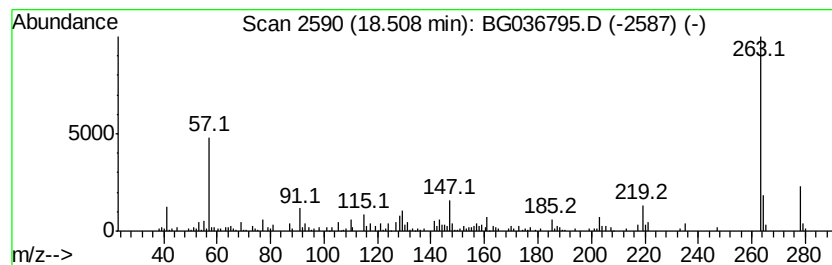
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Peak Number 6 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.51	4.52 ng	195772	Phenanthrene-d10	17.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxyphenyl...	278	C17H26O3	020170-32-5	94
2	2,2-Bis[4'-cyanooxyphenyl]propane	278	C17H14N2O2	1000322-13-3	72
3	Pentan-2-one, 4-(2-fluorenylimino)-	263	C18H17NO	050651-58-6	53
4	Perhydro-3-(4,5,α-trimethoxy...	309	C14H15NO7	093005-00-6	50
5	1H-Pyrazole-4-carbonitrile, 3-(4...	263	C12H10ClN3S	068364-67-0	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.58	7.58	75.2	ng	1203830	1	8.05	320336	20.0
Benzoic acid, 2,4...	14.74	28.0	ng	948611	3	14.67	676680	20.0
1-Propanone, 1-(3...	14.91	2.1	ng	71143	3	14.67	676680	20.0
n-Hexadecanoic acid	18.30	3.9	ng	169234	4	17.42	866082	20.0
3,5-di-tert-Butyl...	18.51	4.5	ng	195772	4	17.42	866082	20.0