

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
 Data File : BG028882.D
 Acq On : 22 Sep 2017 20:00
 Operator : SJ/JU
 Sample : I5301-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20170606-COMP-C

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	5.380	299	305	311	rBV2	28819	50132	1.37%	0.365%
2	5.844	377	384	395	rBV	284330	488512	13.30%	3.555%
3	7.430	647	654	665	rBV	200758	381896	10.40%	2.779%
4	7.812	709	719	729	rBV	455934	826682	22.51%	6.016%
5	8.277	790	798	811	rBV	83683	159337	4.34%	1.160%
6	8.600	845	853	866	rVB	388954	730558	19.89%	5.317%
7	9.446	990	997	1009	rBV	330791	626978	17.07%	4.563%
8	11.097	1270	1278	1286	rBV	109721	204636	5.57%	1.489%
9	13.512	1681	1689	1699	rBV	1065781	1658753	45.17%	12.072%
10	14.334	1824	1829	1836	rBV	24784	37723	1.03%	0.275%
11	14.892	1918	1924	1935	rBV3	213924	358961	9.77%	2.612%
12	16.385	2171	2178	2194	rBV	1227845	1845813	50.26%	13.433%
13	17.642	2385	2392	2404	rVB2	371615	595878	16.22%	4.337%
14	18.282	2494	2501	2507	rBV3	95794	136285	3.71%	0.992%
15	19.886	2770	2774	2781	rBV	397808	449222	12.23%	3.269%
16	20.227	2826	2832	2844	rBV	2722161	3672629	100.00%	26.728%
17	21.960	3119	3127	3137	rBV2	412937	752767	20.50%	5.478%
18	23.153	3324	3330	3337	rBV5	31235	60958	1.66%	0.444%
19	25.409	3704	3714	3726	rVB2	230313	703229	19.15%	5.118%

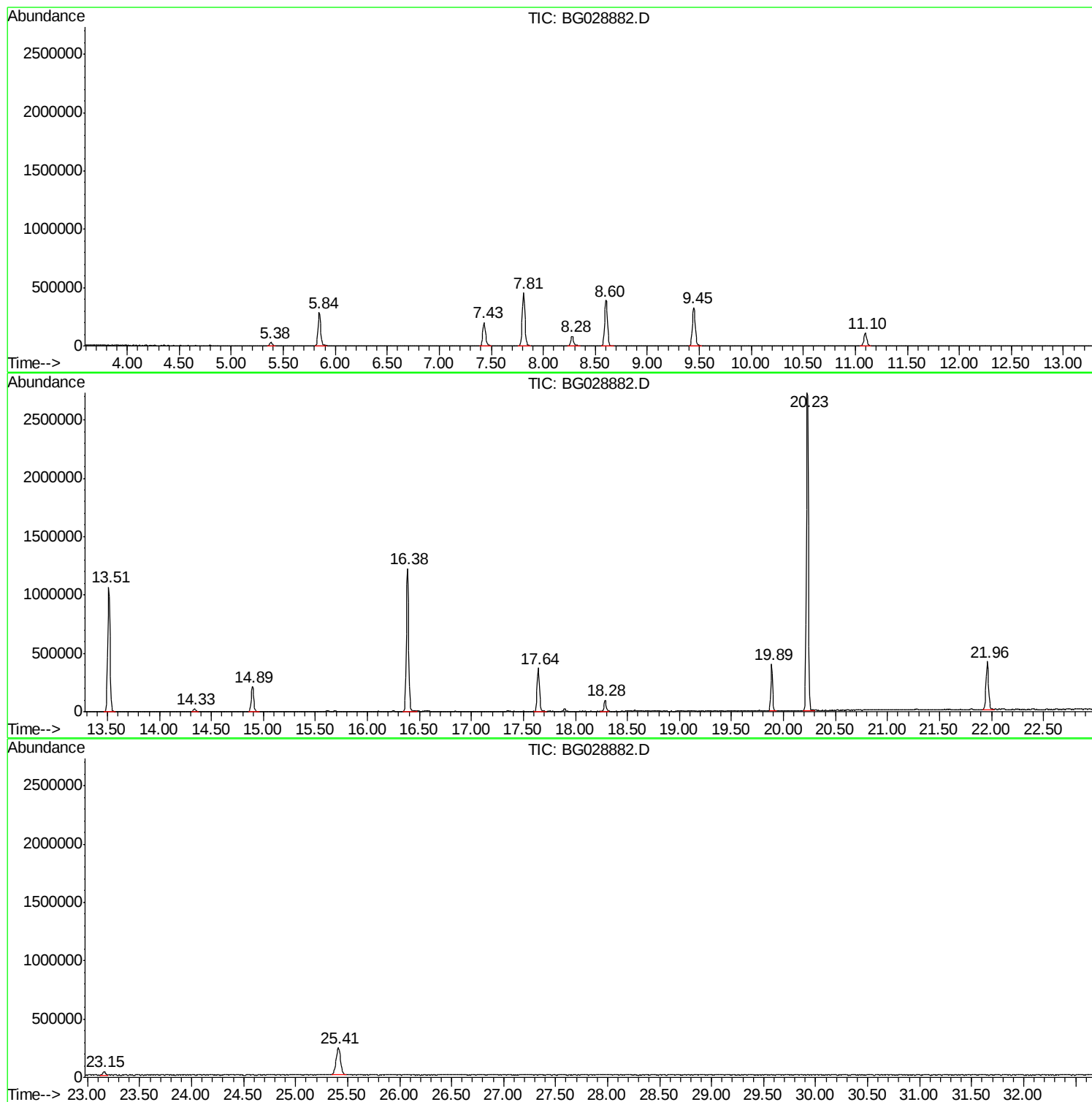
Sum of corrected areas: 13740949

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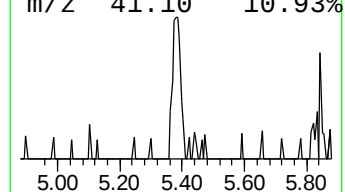
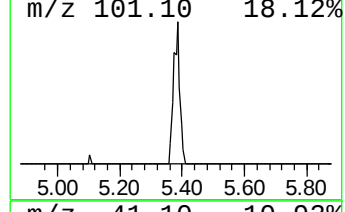
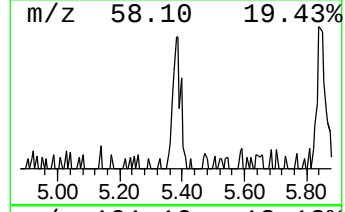
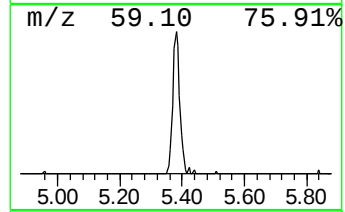
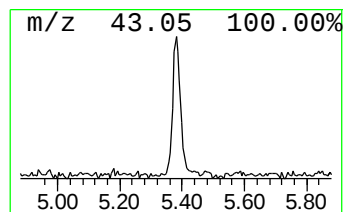
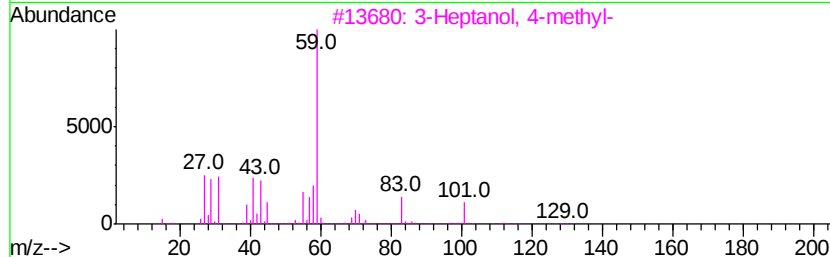
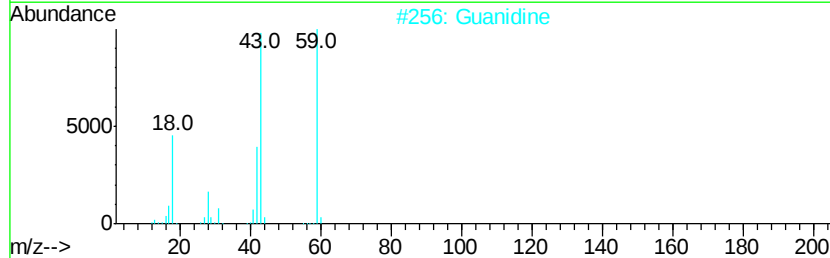
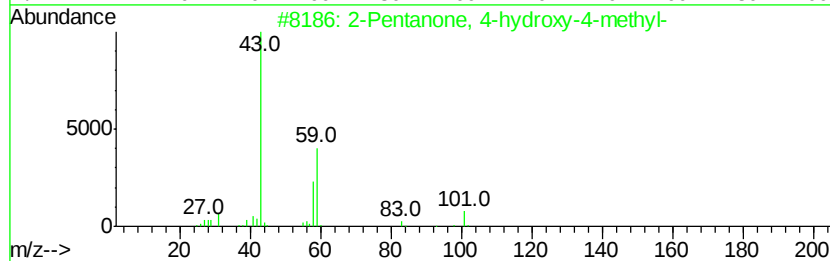
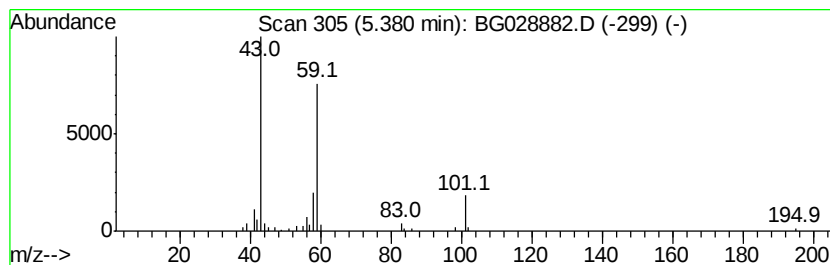
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.38	6.29 ng	50132	1,4-Dichlorobenzene-d4	8.28

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Guanidine	59	CH5N3	000113-00-8	50
3		3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	50
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
5		Dimethadione	129	C5H7NO3	000695-53-4	39



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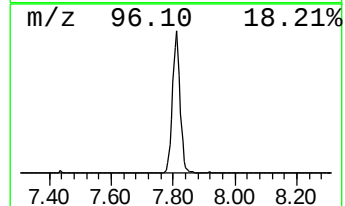
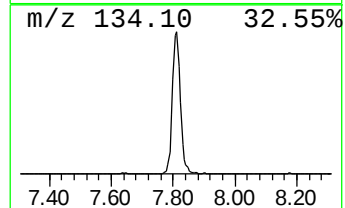
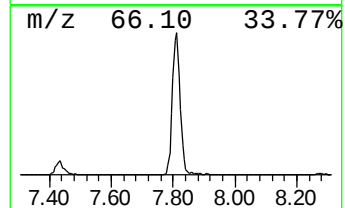
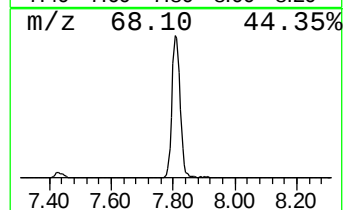
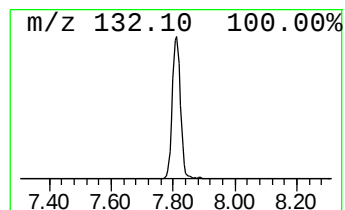
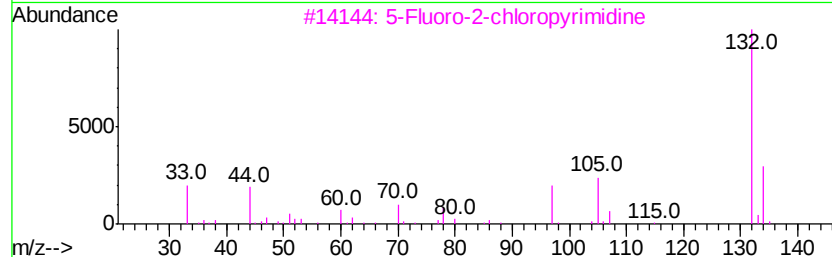
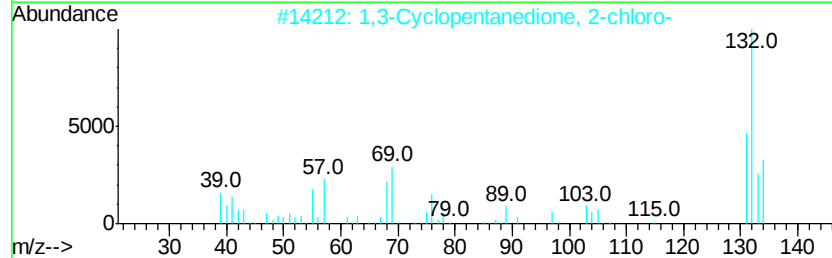
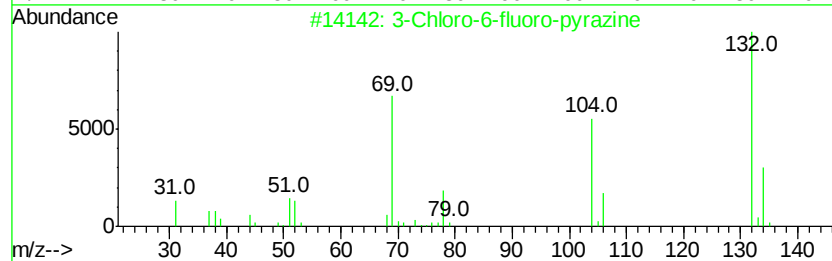
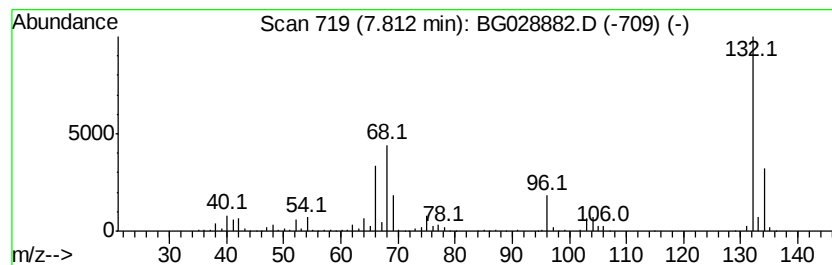
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Peak Number 2 unknown7.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	103.77 ng	826682	1,4-Dichlorobenzene-d4	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10



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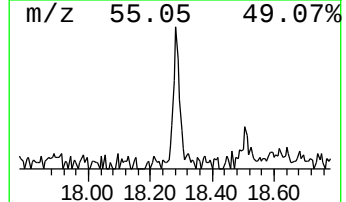
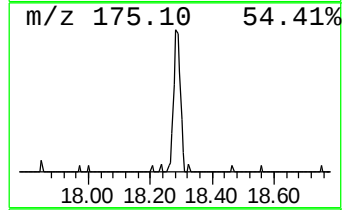
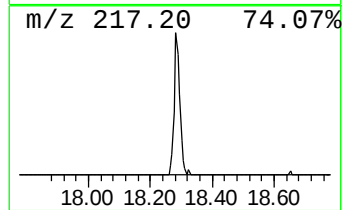
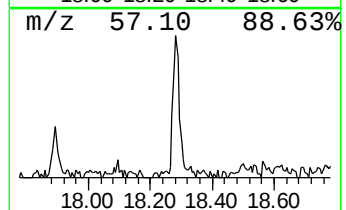
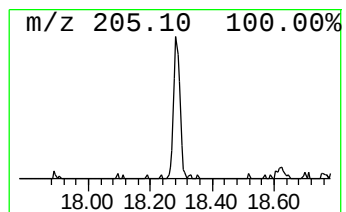
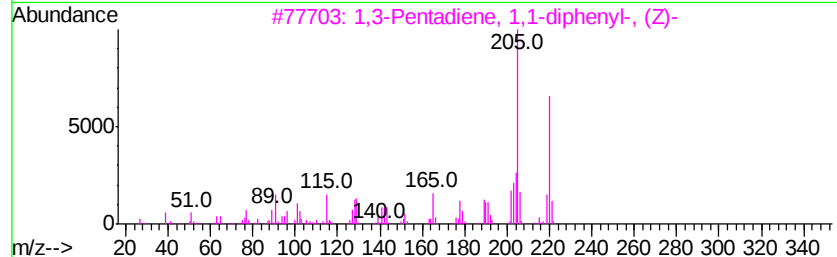
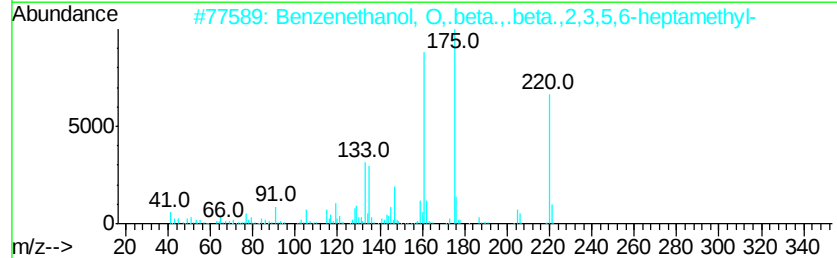
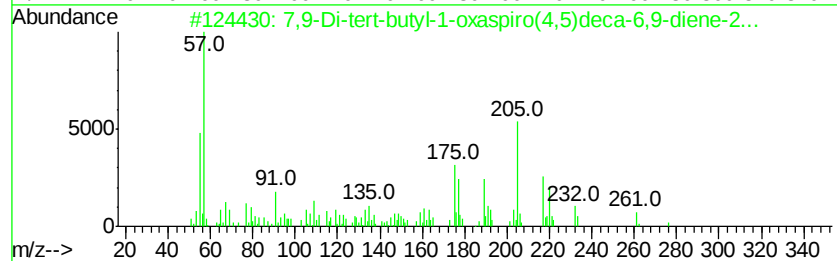
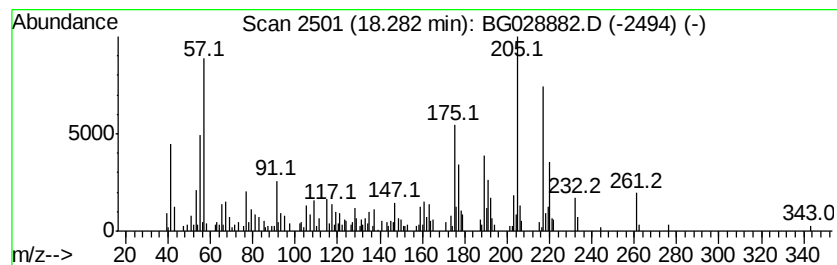
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Peak Number 4 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.28	4.57 ng	136285	Phenanthrene-d10	17.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	94
2	Benzenethanol, O,.beta.,.beta.,2...	220	C15H24O	1000128-94-8	55
3	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	38
4	2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	25
5	2-Methyl-4,5-dimethoxycrotonophe...	220	C13H16O3	207233-94-1	25



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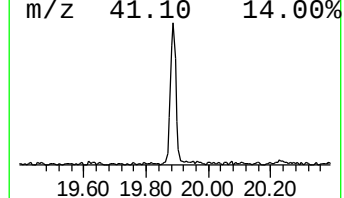
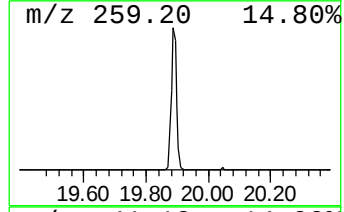
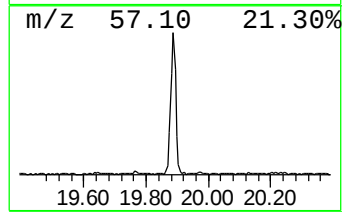
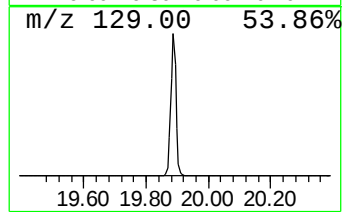
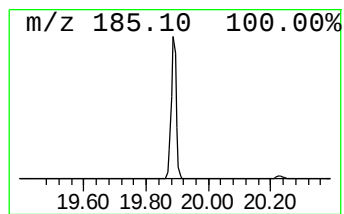
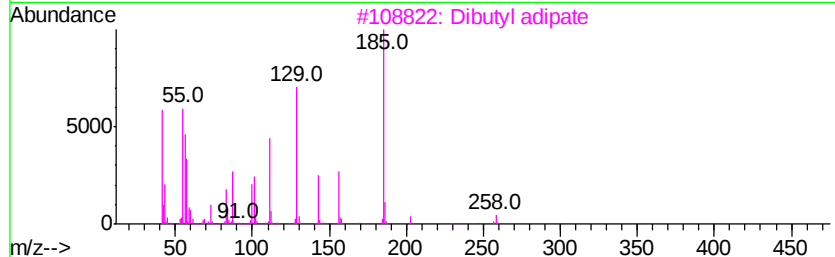
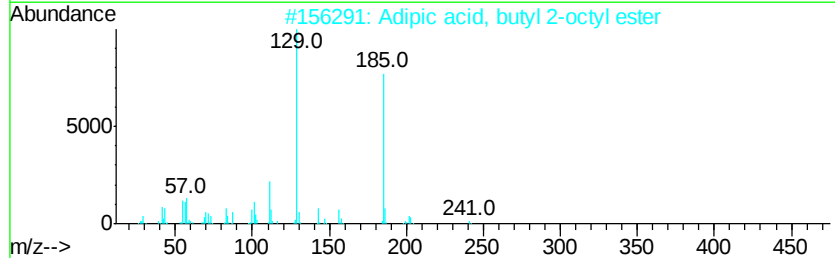
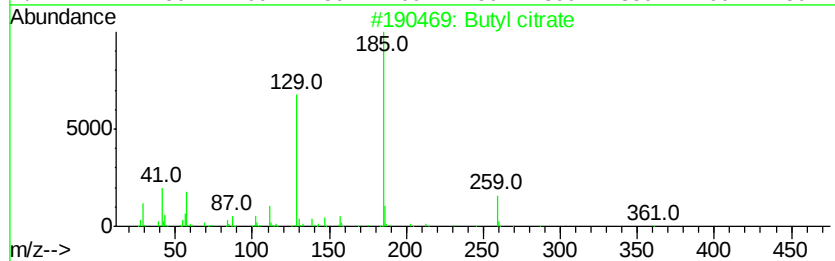
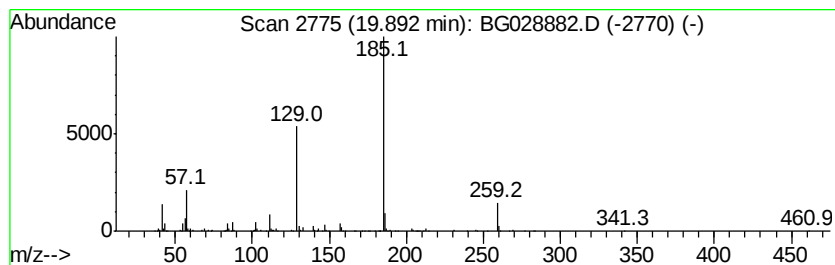
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Peak Number 5 Butyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	11.94 ng	449222	Chrysene-d12	21.96
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Butyl citrate	360 C18H32O7	000077-94-1 91
2		Adipic acid, butyl 2-octyl ester	314 C18H34O4	1000324-44-6 72
3		Dibutyl adipate	258 C14H26O4	000105-99-7 56
4		Hexanedioic acid, bis(2-methylpr...	258 C14H26O4	000141-04-8 56
5		Adipic acid, 3-hexyl isobutyl ester	286 C16H30O4	1000353-62-2 56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.38	6.3	ng	50132	1	8.28	159337	20.0
unknown7.81	7.81	103.8	ng	826682	1	8.28	159337	20.0
7,9-Di-tert-butyl...	18.28	4.6	ng	136285	4	17.64	595878	20.0
Butyl citrate	19.89	11.9	ng	449222	5	21.96	752767	20.0