

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090916\
 Data File : BF090050.D
 Acq On : 9 Sep 2016 17:00
 Operator : UM/SJ
 Sample : H4736-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 090816-DRDC-E-D-M

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:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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	1.724	10	12	63	rVB	4681639	13802675	100.00%	29.709%
2	4.684	269	271	277	rBV	197151	296574	2.15%	0.638%
3	5.153	309	312	319	rBV	1031000	1185040	8.59%	2.551%
4	6.227	403	406	414	rBV	770383	906422	6.57%	1.951%
5	6.353	414	417	419	rBV	1886954	2389960	17.32%	5.144%
6	6.582	435	437	440	rBV	982020	1000931	7.25%	2.154%
7	6.742	448	451	453	rBV	3510658	3287862	23.82%	7.077%
8	7.153	484	487	490	rBV	2291137	2571606	18.63%	5.535%
9	7.873	547	550	552	rBV	1466112	1395037	10.11%	3.003%
10	8.250	578	583	587	rBV	75049	157383	1.14%	0.339%
11	8.959	642	645	647	rBV	4871883	5496599	39.82%	11.831%
12	9.348	677	679	682	rBV	182439	223782	1.62%	0.482%
13	9.622	700	703	705	rBV	1739265	1667573	12.08%	3.589%
14	10.319	759	764	766	rBV	428045	381073	2.76%	0.820%
15	10.399	769	771	774	rBV2	1809543	2279330	16.51%	4.906%
16	11.096	829	832	834	rBV	1350854	1644345	11.91%	3.539%
17	12.674	967	970	973	rBV	3558477	5276735	38.23%	11.358%
18	13.588	1046	1050	1058	rBV	157571	270742	1.96%	0.583%
19	13.702	1058	1060	1071	rVB	1027785	1263996	9.16%	2.721%
20	15.051	1175	1178	1182	rBV	607937	961579	6.97%	2.070%

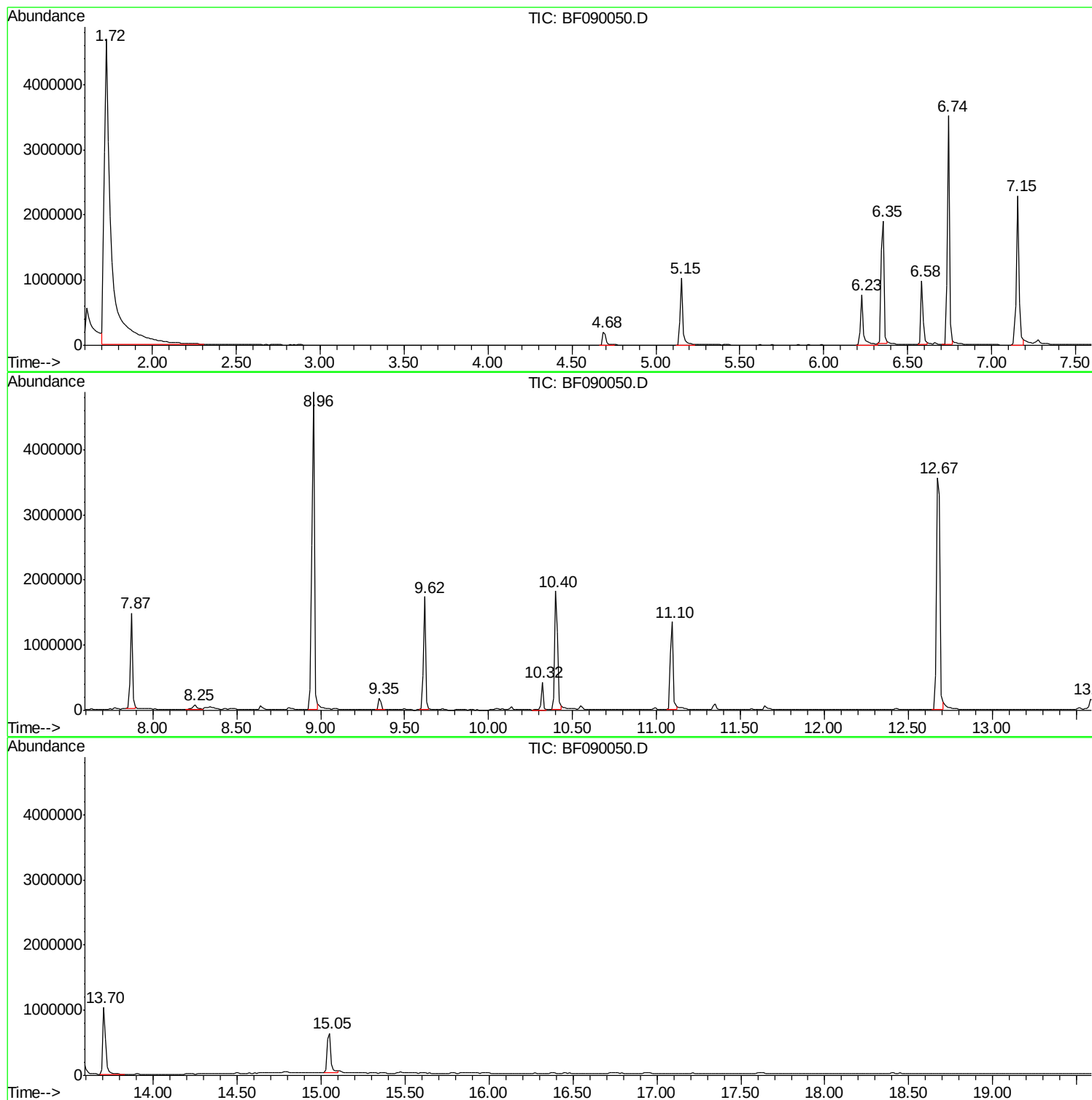
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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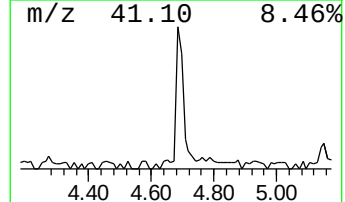
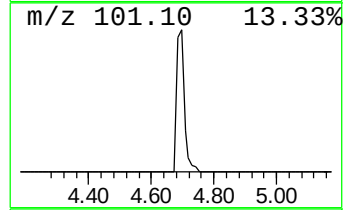
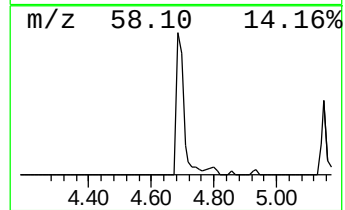
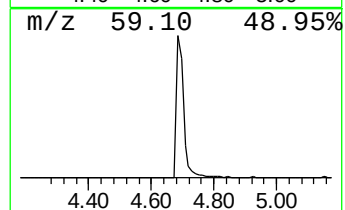
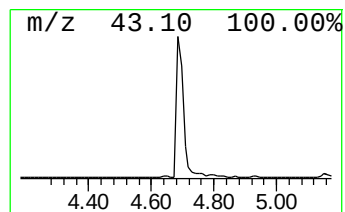
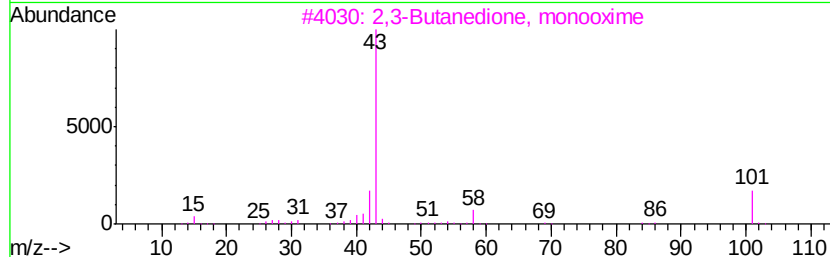
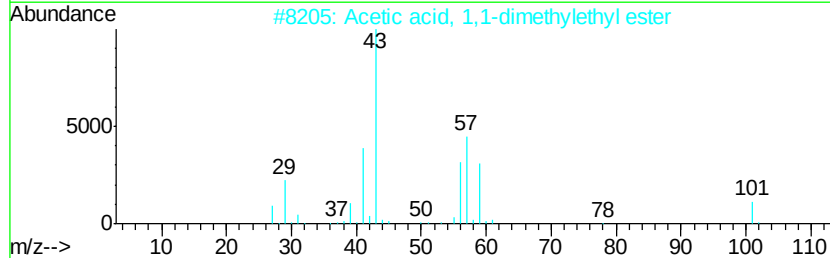
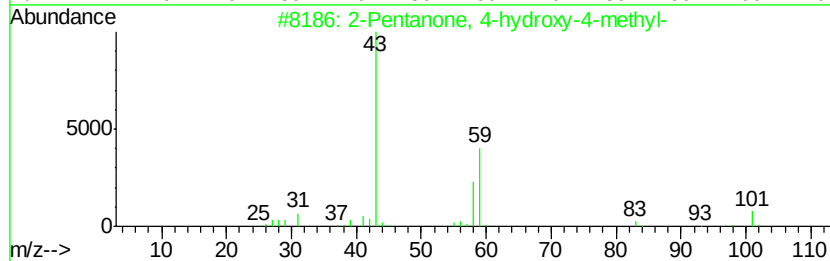
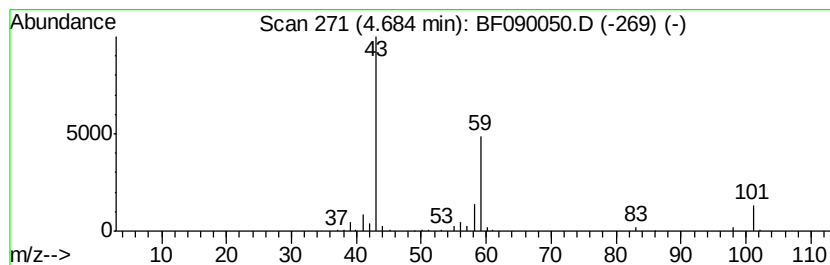
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	5.93 ng	296574	1,4-Dichlorobenzene-d4	6.58
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116 C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116 C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime	101 C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100 C5H8O2	000108-22-5	10
5	2-Propanone, 1-(1-methylethoxy)-	116 C6H12O2	042781-12-4	9



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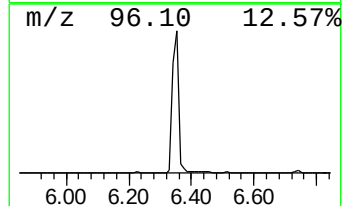
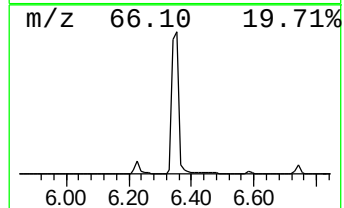
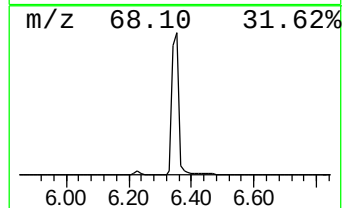
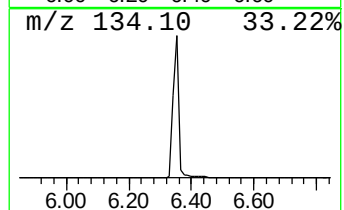
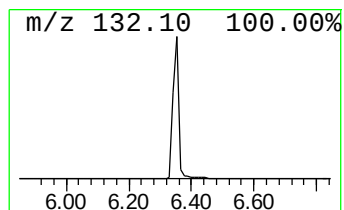
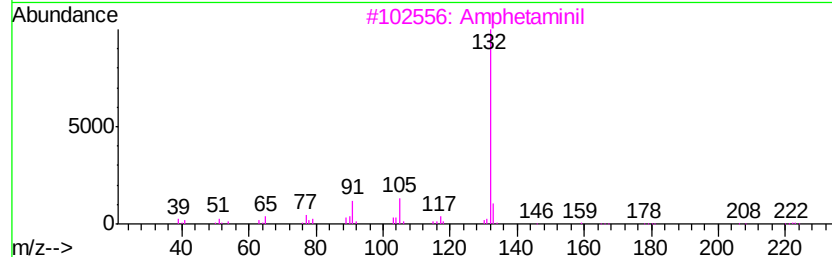
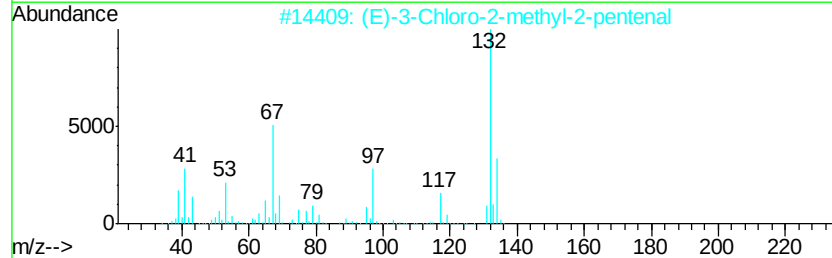
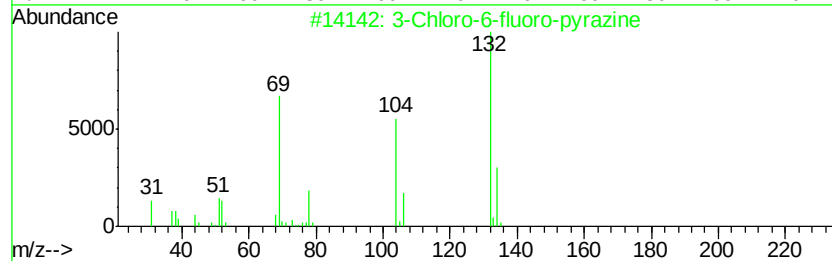
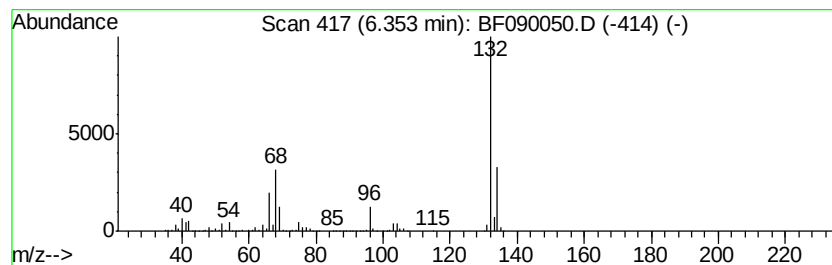
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Peak Number 3 unknown6.35 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	47.75 ng	2389960	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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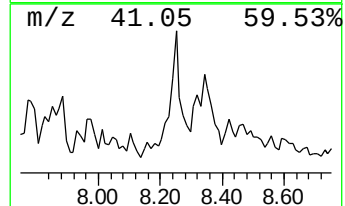
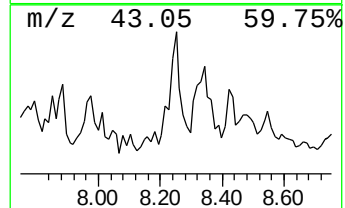
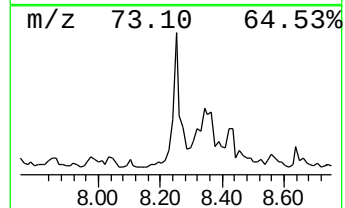
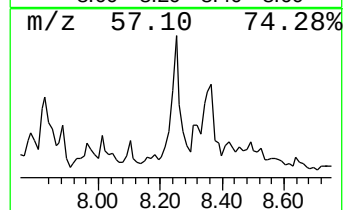
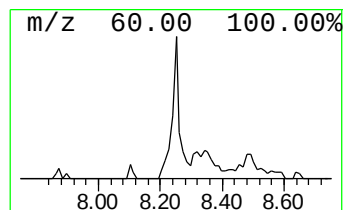
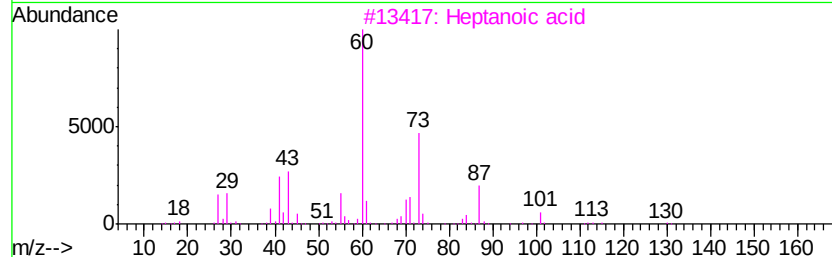
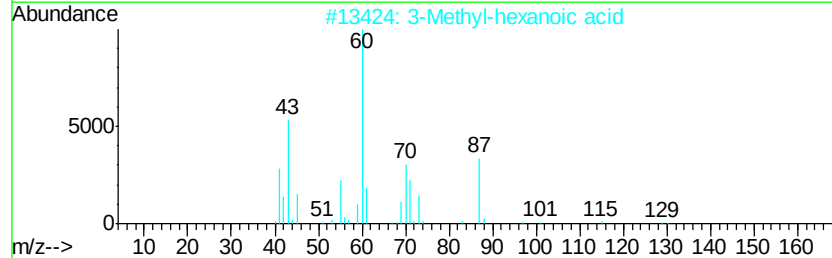
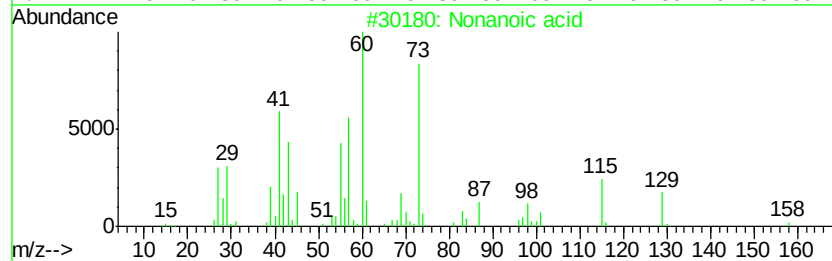
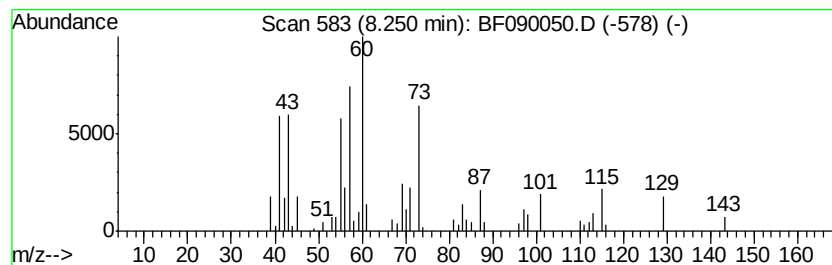
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Peak Number 5 Nonanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.25	2.26 ng	157383	Napthalene-d8	7.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid		158	C9H18O2	000112-05-0	59
2	3-Methyl-hexanoic acid		130	C7H14O2	1000365-65-4	53
3	Heptanoic acid		130	C7H14O2	000111-14-8	50
4	Pentanoic acid, 3-methyl-		116	C6H12O2	000105-43-1	43
5	Hexanoic acid		116	C6H12O2	000142-62-1	38



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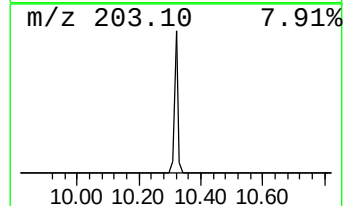
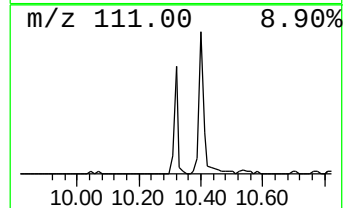
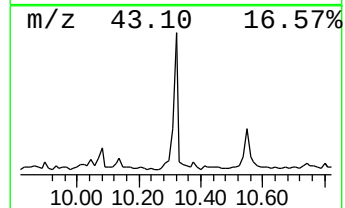
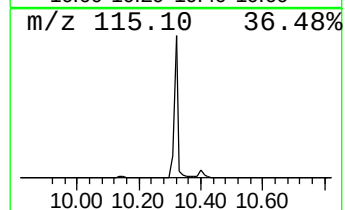
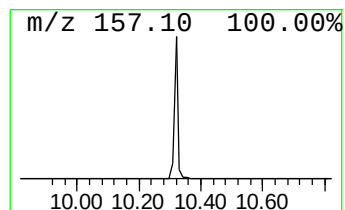
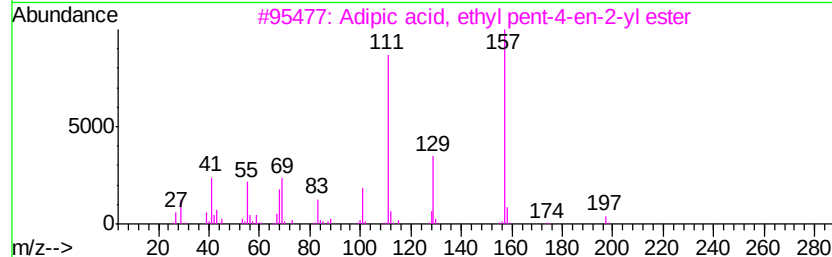
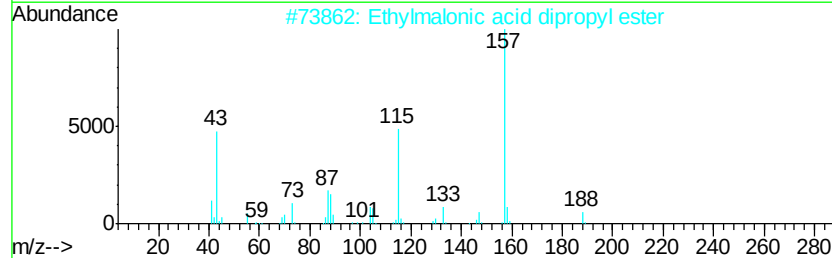
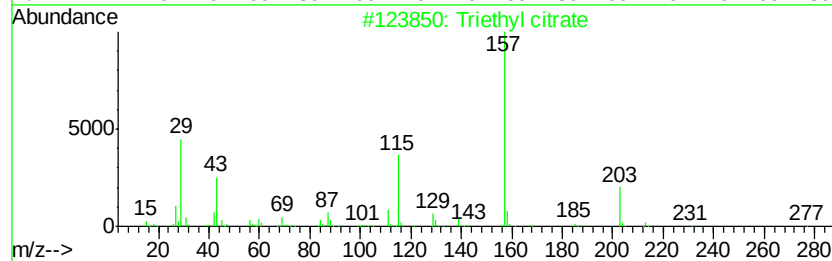
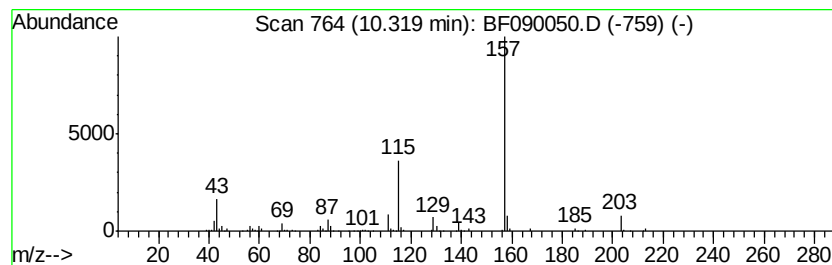
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Peak Number 6 Triethyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.32	4.57 ng	381073	Acenaphthene-d10	9.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	91
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	50
3	Adipic acid, ethyl pent-4-en-2-yl...	242	C13H22O4	1000354-11-7	40
4	1,4-Dioxaspiro[4.4]nonane, 7,8-b...	188	C9H16O4	1000155-54-9	36
5	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	36



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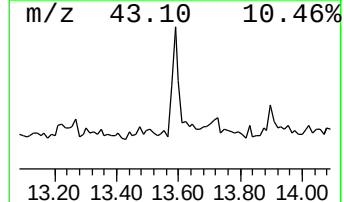
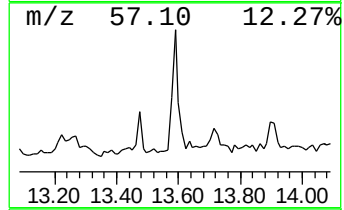
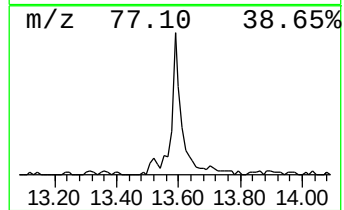
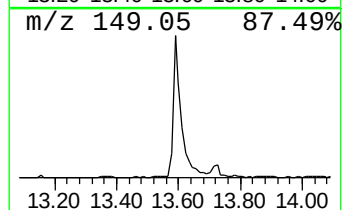
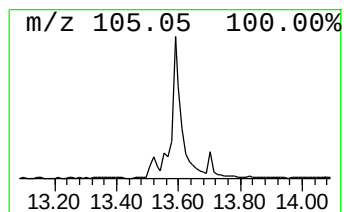
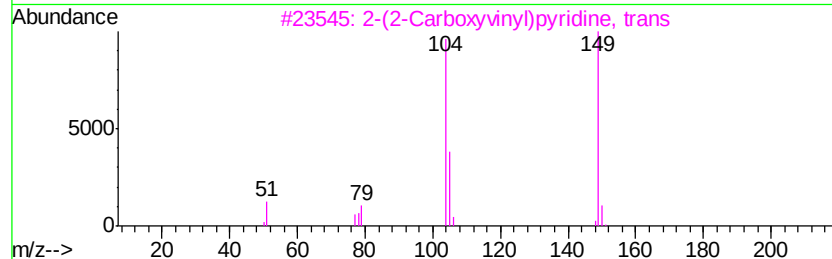
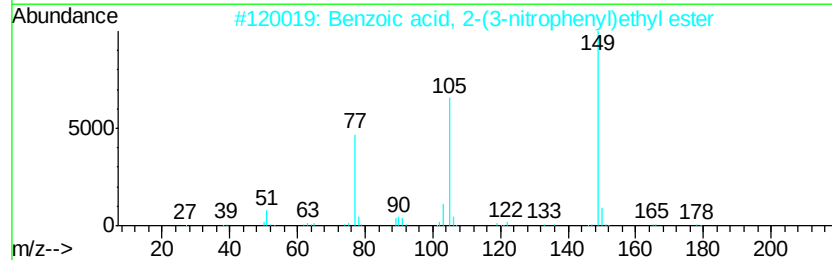
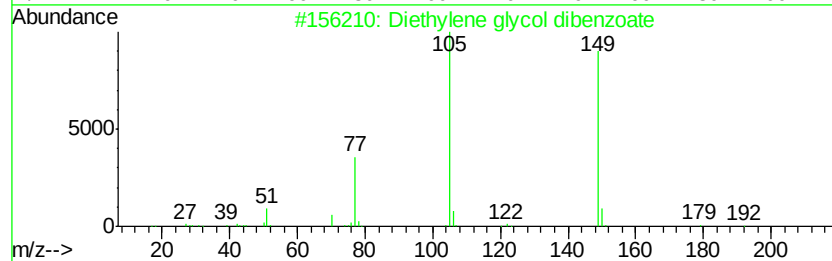
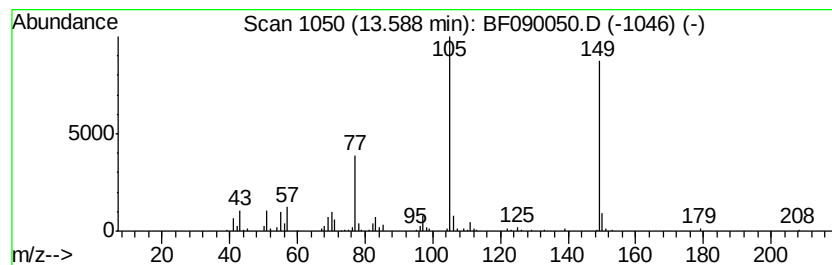
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Peak Number 7 Diethylene glycol dibenzoate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	4.28 ng	270742	Chrysene-d12	13.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	86
2			Benzoic acid, 2-(3-nitrophenyl)ethyl ester	271	C15H13NO4	1000368-22-4	64
3			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	46
4			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	38
5			Phthalic acid, cyclobutyl tetrad...	416	C26H40O4	1000314-90-9	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.68	5.9	ng	296574	1	6.58	1000930	20.0
unknown6.35	6.35	47.8	ng	2389960	1	6.58	1000930	20.0
Nonanoic acid	8.25	2.3	ng	157383	2	7.87	1395040	20.0
Triethyl citrate	10.32	4.6	ng	381073	3	9.62	1667570	20.0
Diethylene glycol...	13.59	4.3	ng	270742	5	13.70	1264000	20.0