

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072921\
 Data File : BF124860.D
 Acq On : 29 Jul 2021 20:00
 Operator : JU/CG
 Sample : M3210-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-1(1.0-1.5)

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_F\METHODS\8270-BF072221.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124860.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	8	13	16	rBB	7367	8416	2.49%	0.526%
2	5.104	510	513	518	rBB	3519	4356	1.29%	0.272%
3	5.492	574	579	582	rBB	181601	182149	53.95%	11.381%
4	6.504	745	751	754	rBB	184275	187767	55.61%	11.732%
5	6.869	811	813	816	rBB	44749	33489	9.92%	2.092%
6	7.439	905	910	912	rBV	120194	124066	36.74%	7.752%
7	8.051	1012	1014	1020	rBB	15062	11713	3.47%	0.732%
8	8.151	1028	1031	1035	rBB	56248	46817	13.87%	2.925%
9	9.233	1210	1215	1217	rBV	285690	250964	74.33%	15.681%
10	9.339	1231	1233	1236	rBB	5614	4597	1.36%	0.287%
11	9.910	1327	1330	1333	rBV	71921	55987	16.58%	3.498%
12	10.704	1460	1465	1468	rBV	188371	167554	49.62%	10.469%
13	11.398	1579	1583	1586	rBV	82882	64101	18.98%	4.005%
14	12.486	1766	1768	1771	rBB	12160	9285	2.75%	0.580%
15	12.992	1848	1854	1856	rBV	341119	337649	100.00%	21.097%
16	13.880	2002	2005	2012	rBV3	7446	11506	3.41%	0.719%
17	14.039	2028	2032	2035	rBB	63421	56307	16.68%	3.518%
18	15.515	2278	2283	2288	rBB	36819	43736	12.95%	2.733%

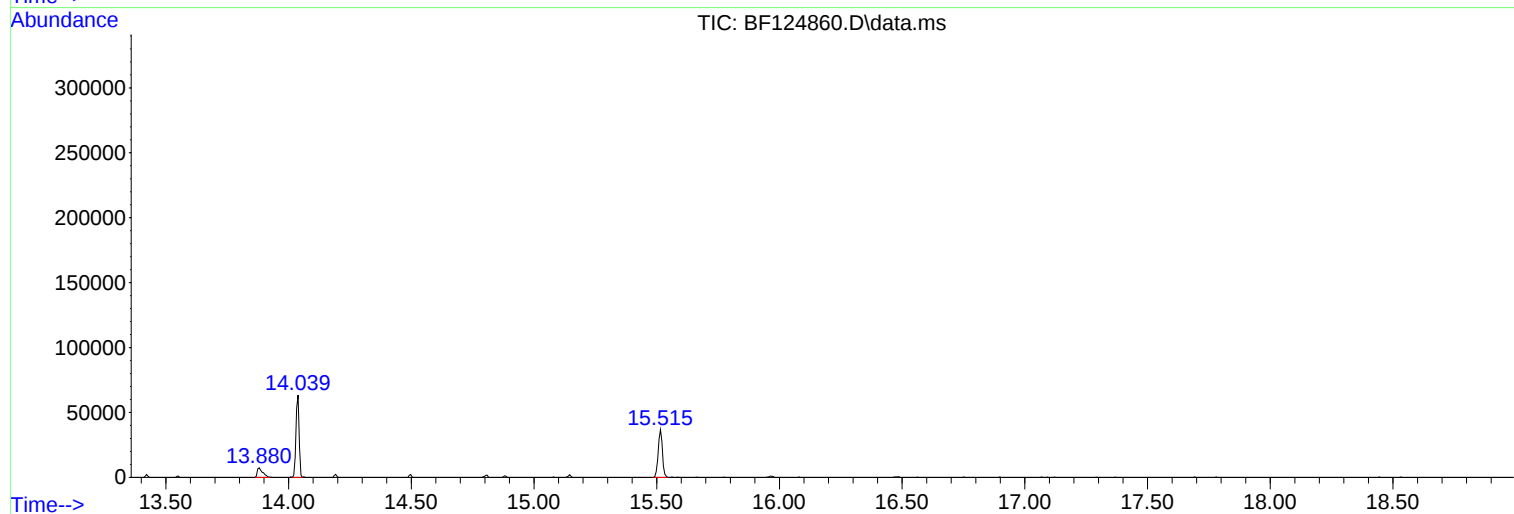
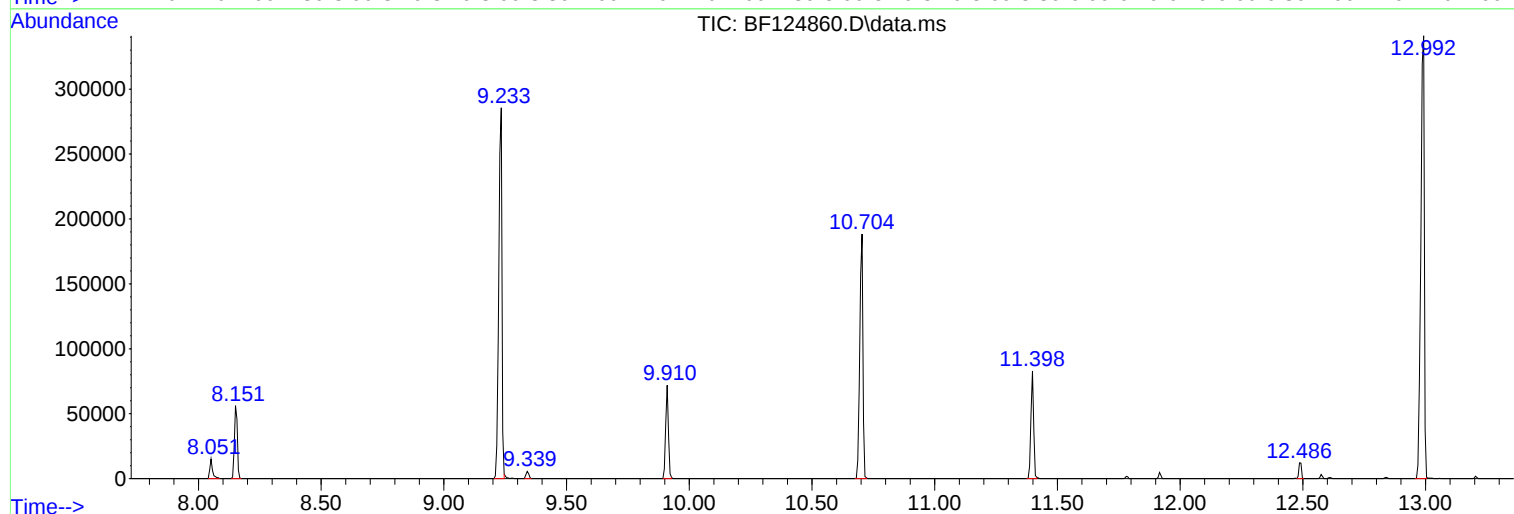
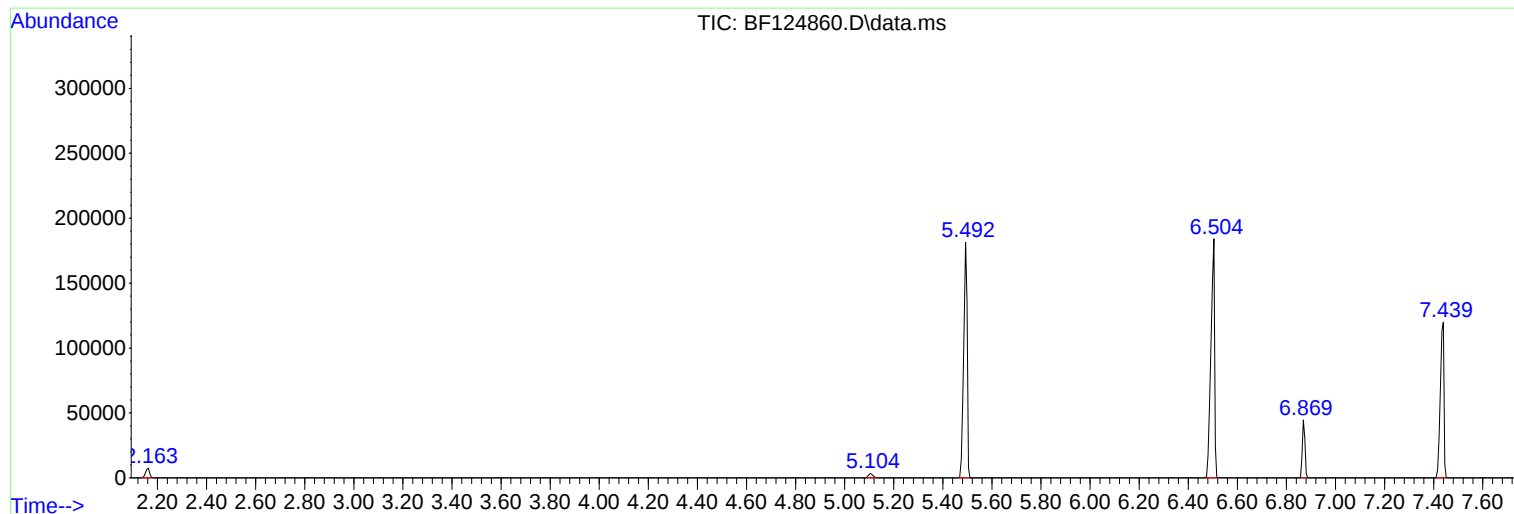
Sum of corrected areas: 1600459

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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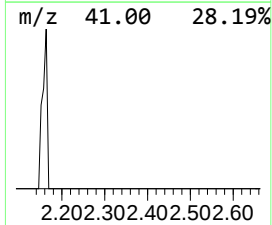
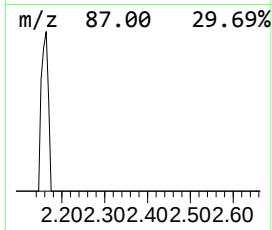
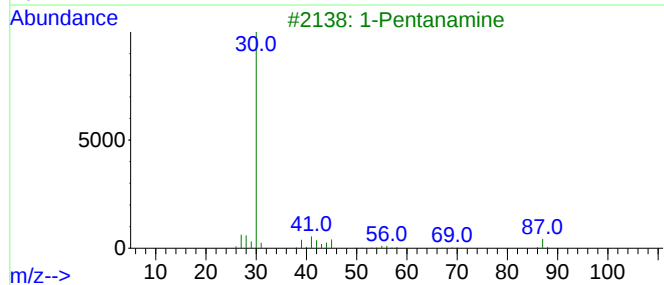
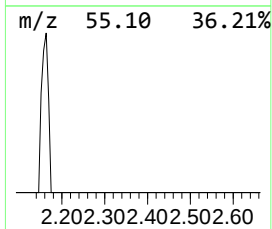
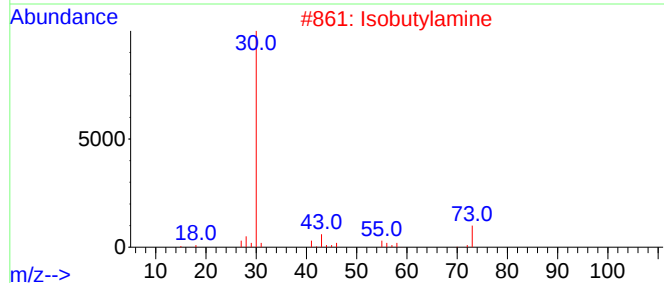
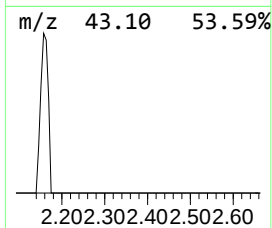
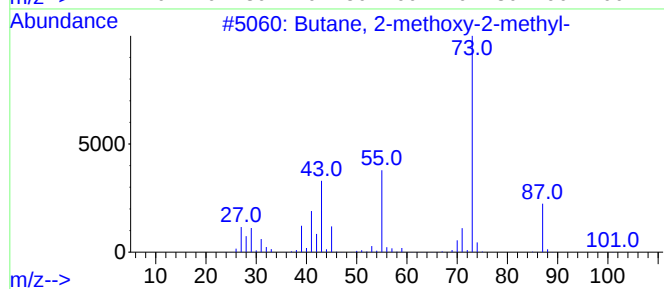
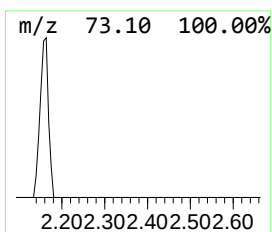
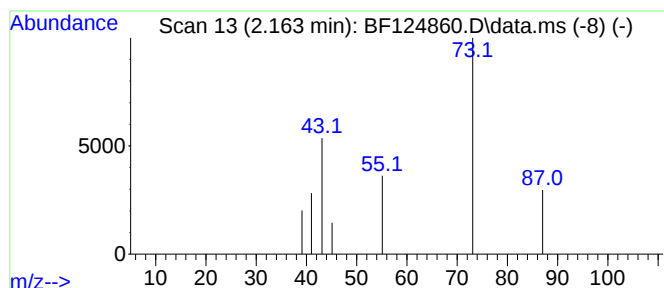
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.163 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	5.03 ng	8416	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
2			Isobutylamine	73	C4H11N	000078-81-9	7
3			1-Pentanamine	87	C5H13N	000110-58-7	4
4			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4
5			S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	4



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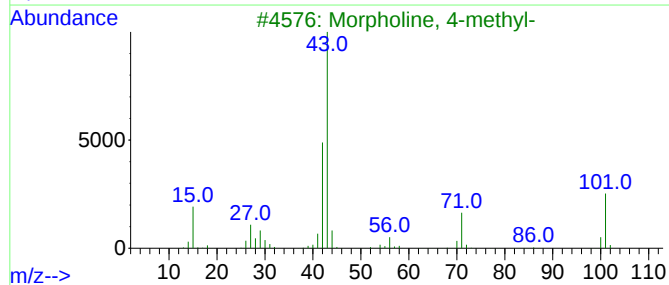
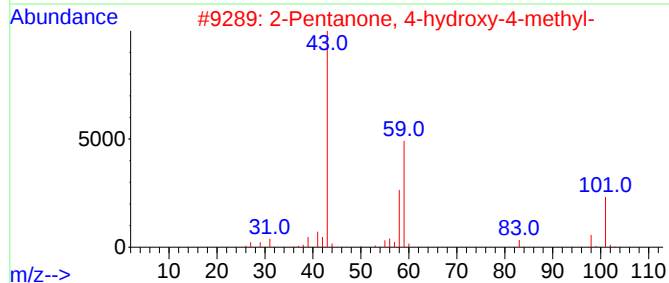
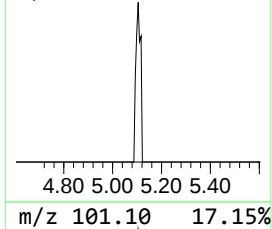
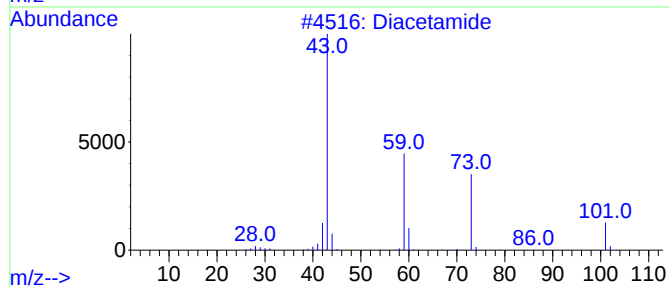
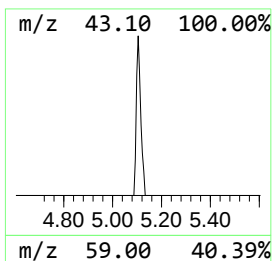
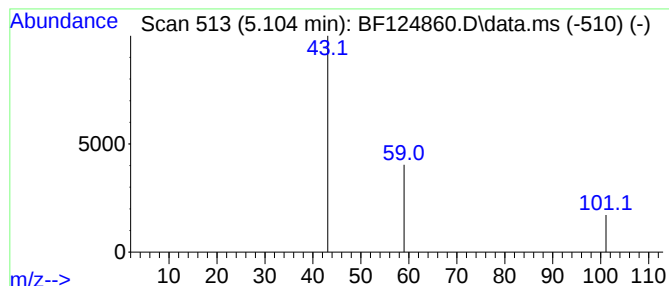
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.104 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	2.60 ng	4356	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diacetamide	101	C4H7NO2	000625-77-4	7
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	4
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	4
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	3
5			2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	2



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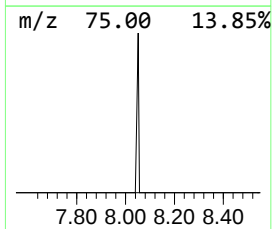
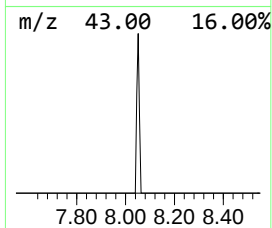
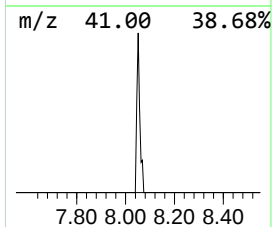
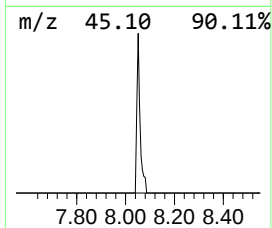
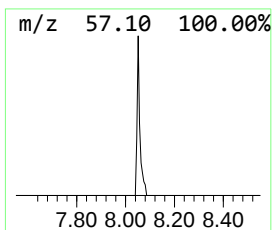
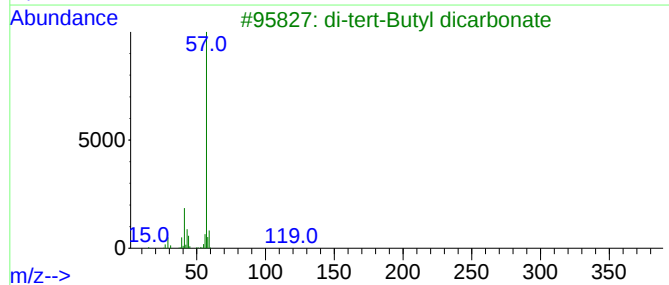
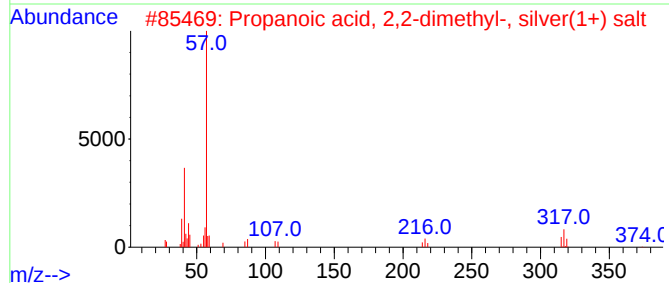
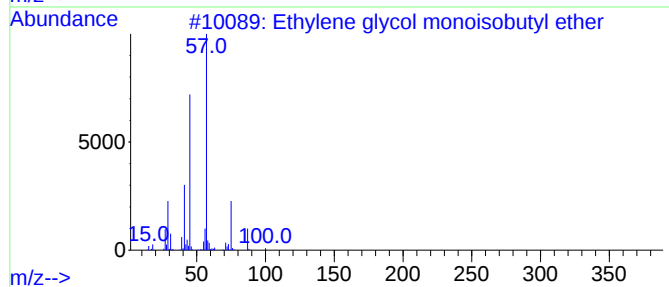
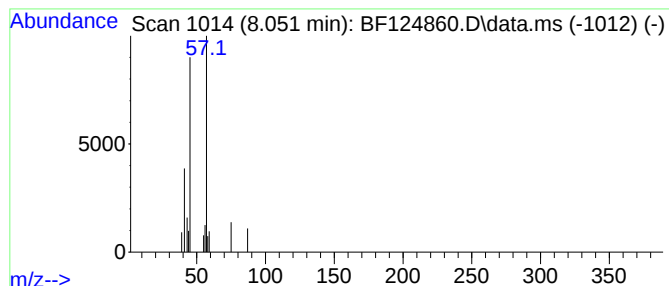
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Peak Number 3 Ethylene glycol monoisobuty... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	5.00 ng	11713	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
2			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	16
3			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	10
4			1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	9
5			1-Pentanamine	87	C5H13N	000110-58-7	9



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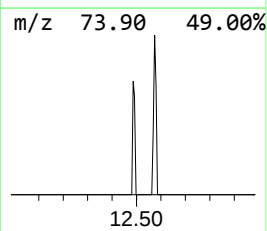
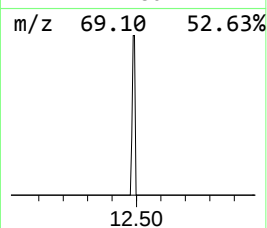
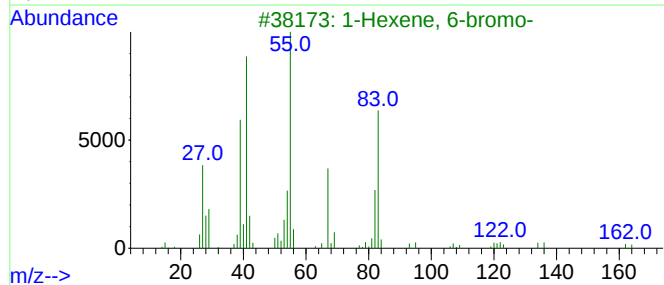
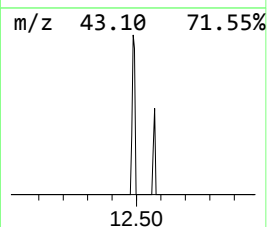
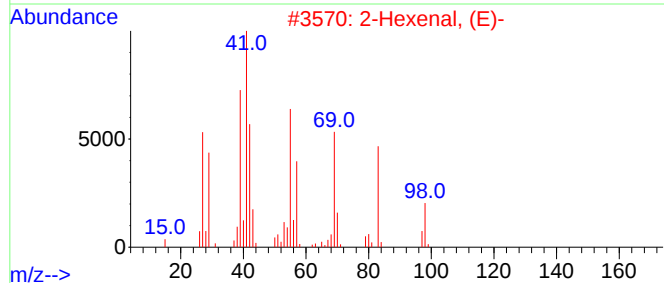
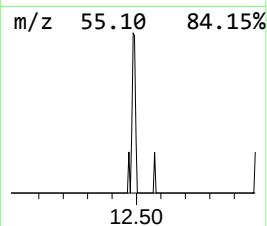
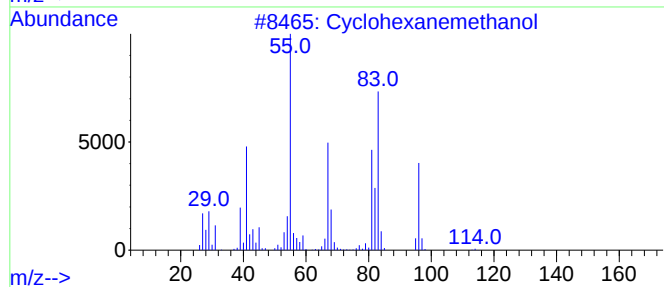
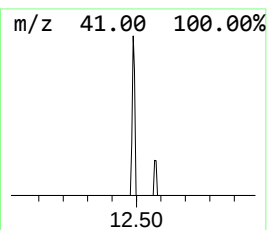
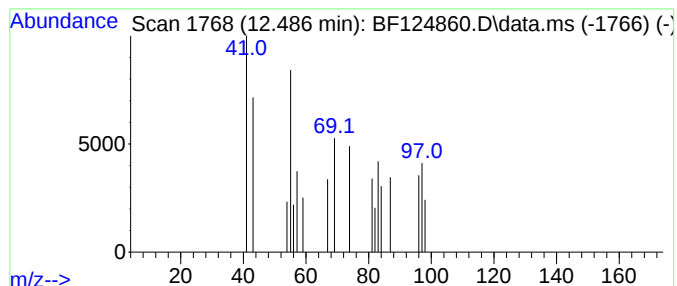
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Peak Number 4 unknown12.486 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.486	2.90 ng	9285	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanemethanol	114	C7H14O	000100-49-2	35
2			2-Hexenal, (E)-	98	C6H10O	006728-26-3	11
3			1-Hexene, 6-bromo-	162	C6H11Br	002695-47-8	10
4			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	9



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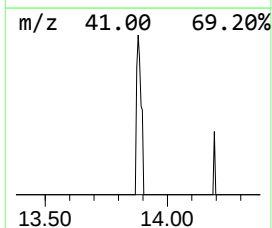
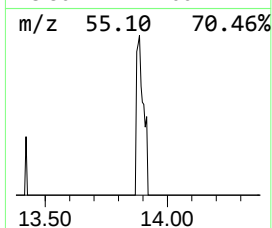
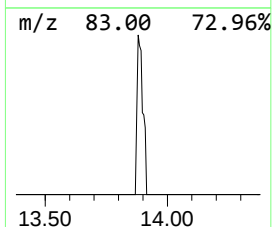
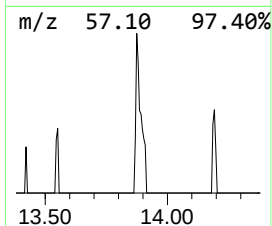
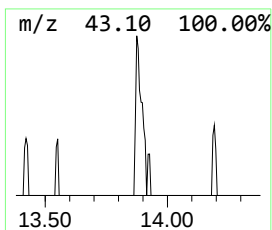
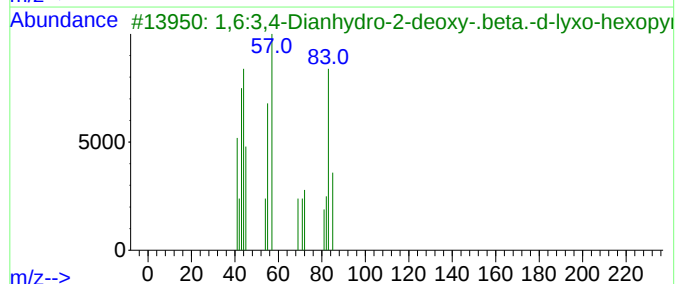
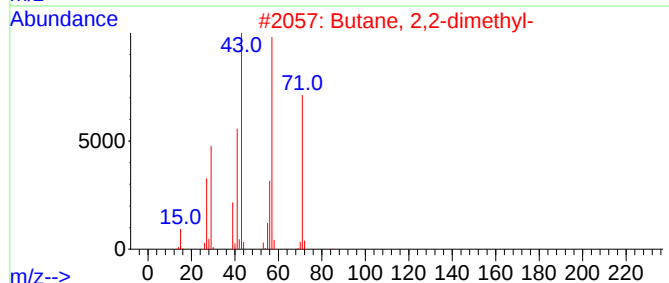
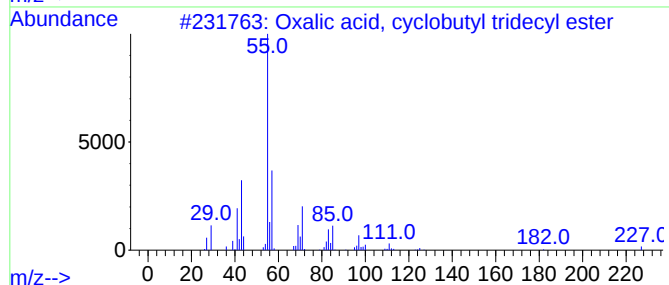
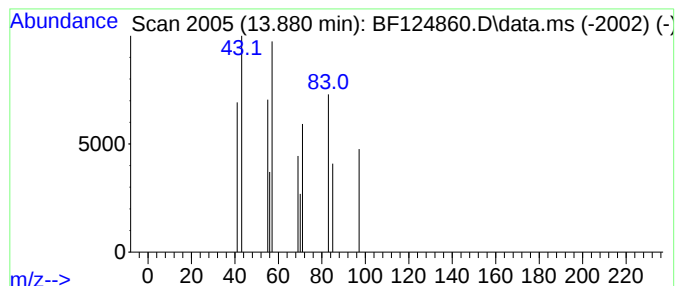
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Peak Number 5 unknown13.880 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	4.09 ng	11506	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl tridecyl...	326	C19H34O4	1000309-70-4	36
2			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	10
3			1,6:3,4-Dianhydro-2-deoxy-.beta....	128	C6H8O3	050767-53-8	9
4			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	9
5			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown5.104	5.104	2.6	ng	4356	1	6.869	33489	20.0
Ethylene glycol...	8.051	5.0	ng	11713	2	8.151	46817	20.0
unknown12.486	12.486	2.9	ng	9285	4	11.398	64101	20.0
unknown13.880	13.880	4.1	ng	11506	5	14.039	56307	20.0