

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
 Data File : BF124804.D
 Acq On : 27 Jul 2021 20:58
 Operator : JU/CG
 Sample : M3118-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20210588-AMENDED-COM-2

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: BF124804.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	8	rVB	8433	7439	5.26%	0.954%
2	5.075	505	508	512	rBB	10001	10374	7.34%	1.330%
3	5.481	573	577	580	rBB	87122	71229	50.37%	9.131%
4	6.492	745	749	752	rBV	96332	83859	59.30%	10.750%
5	6.869	810	813	816	rBB	35958	25096	17.75%	3.217%
6	7.428	905	908	911	rBB	65254	57862	40.92%	7.417%
7	8.051	1011	1014	1020	rBB	25836	19079	13.49%	2.446%
8	8.151	1028	1031	1034	rBB	47489	35313	24.97%	4.527%
9	9.227	1210	1214	1217	rBV	139057	102727	72.65%	13.168%
10	9.910	1327	1330	1333	rBB	53087	42607	30.13%	5.462%
11	10.692	1460	1463	1467	rBB	70354	60377	42.70%	7.740%
12	11.392	1579	1582	1586	rBB	55284	47958	33.92%	6.148%
13	12.980	1848	1852	1855	rBV	175115	141406	100.00%	18.126%
14	13.880	2002	2005	2010	rBB	5581	6856	4.85%	0.879%
15	14.033	2027	2031	2034	rBB	48483	38448	27.19%	4.929%
16	15.504	2277	2281	2288	rBB2	23831	29484	20.85%	3.779%

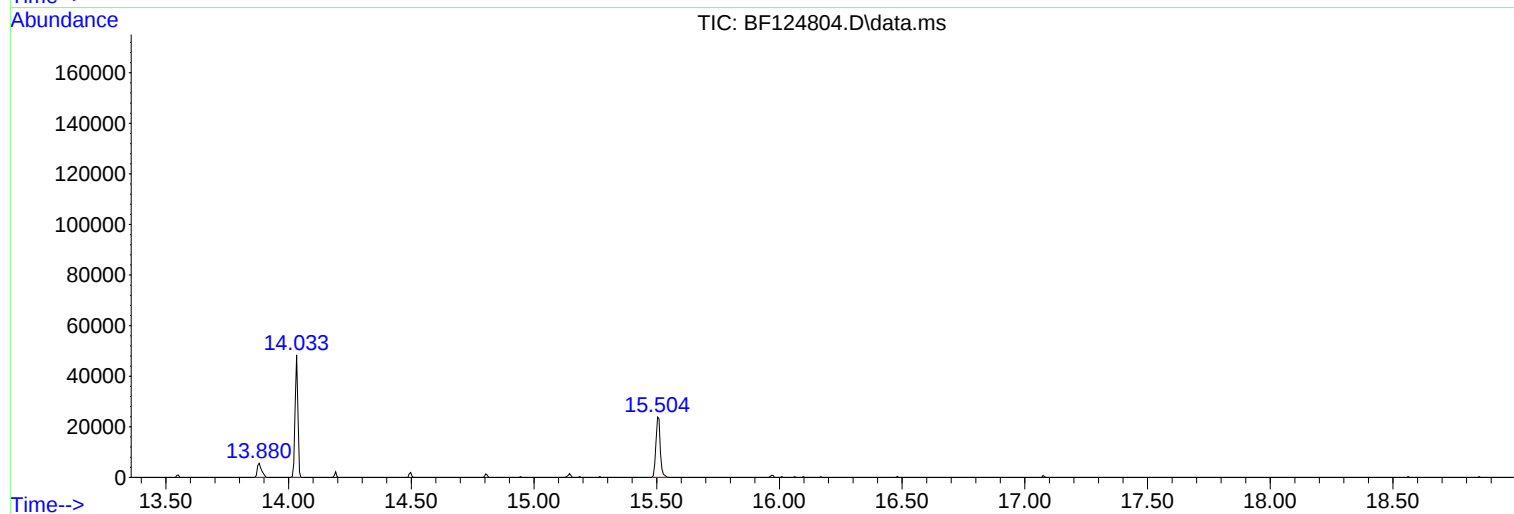
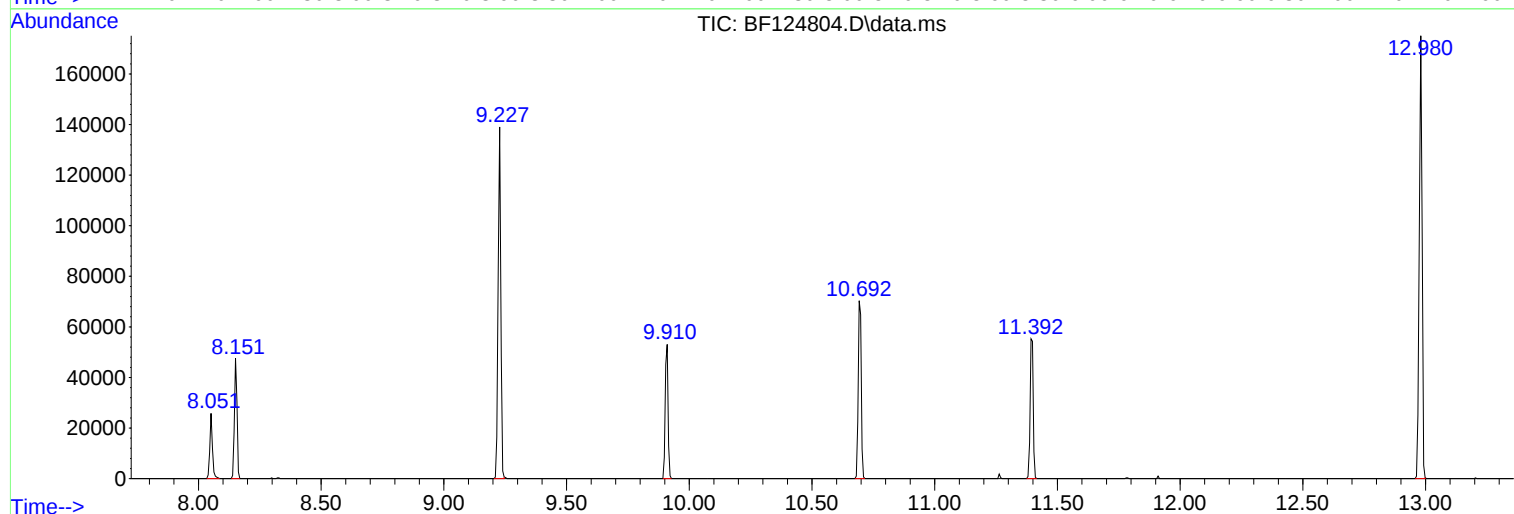
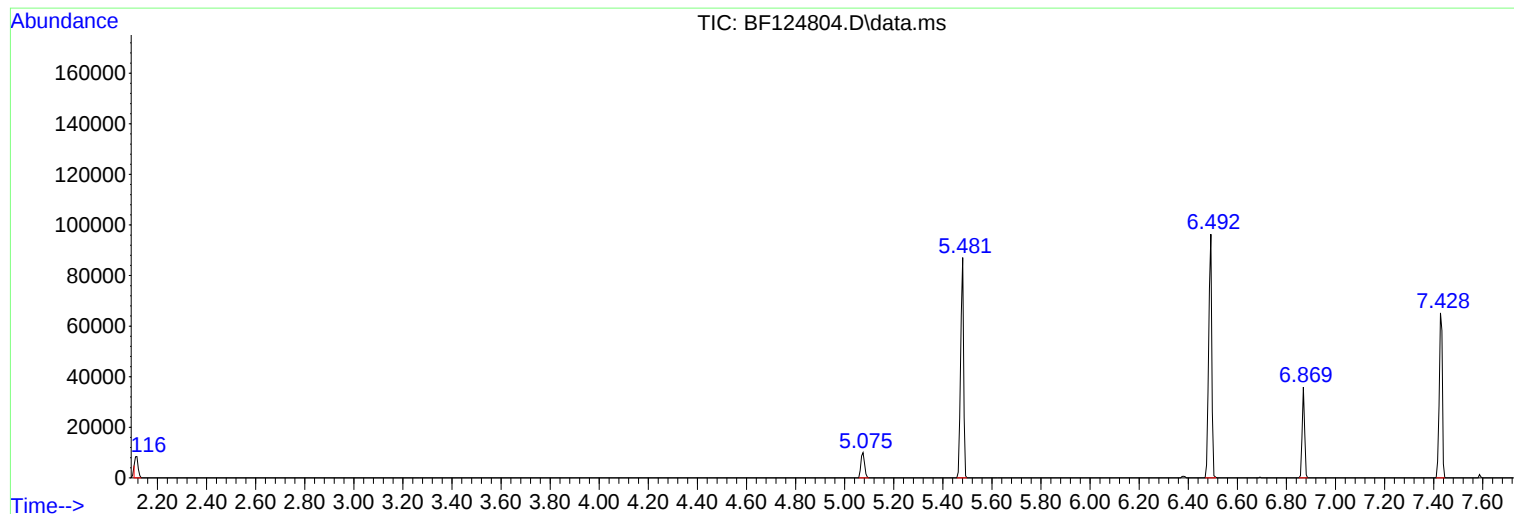
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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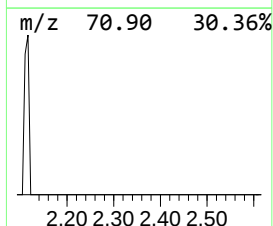
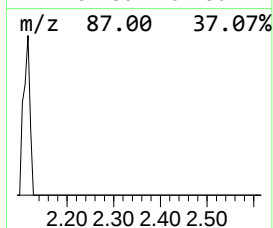
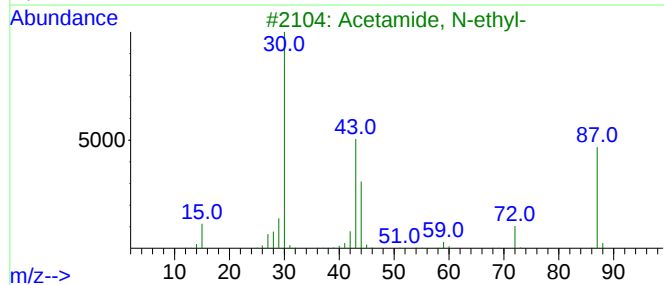
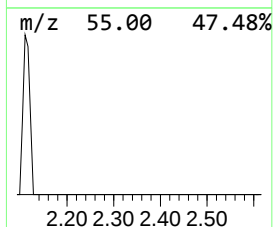
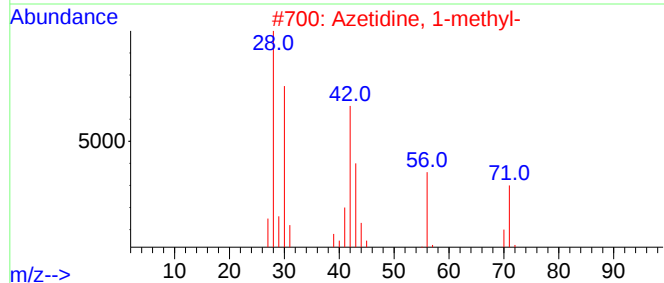
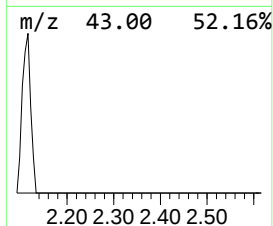
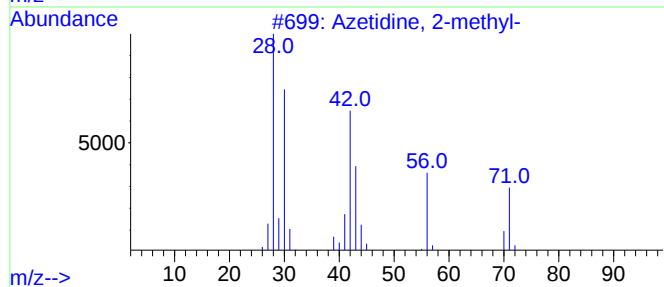
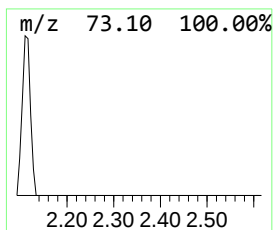
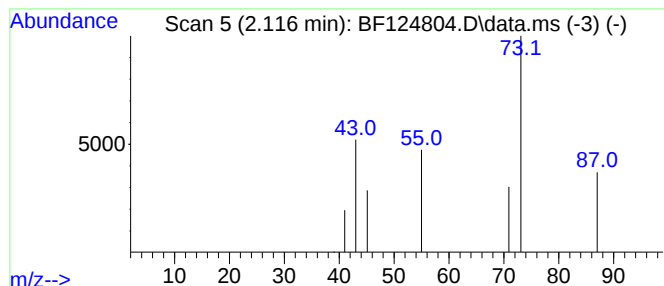
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.116 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	5.93 ng	7439	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
2			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	4
4			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	4
5			2-OXOPROPIONAMIDE	87	C3H5NO2	000631-66-3	4



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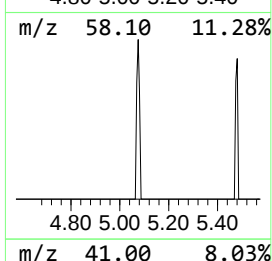
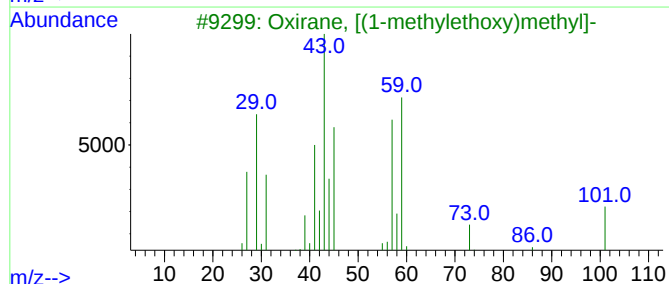
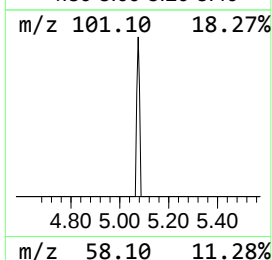
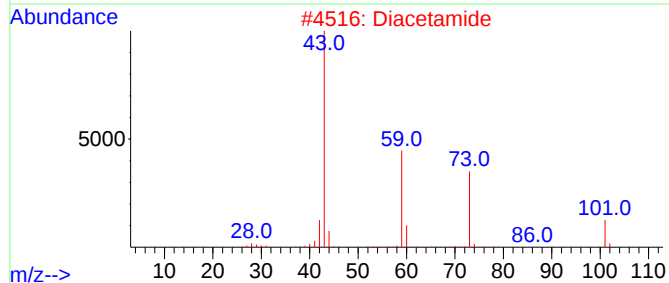
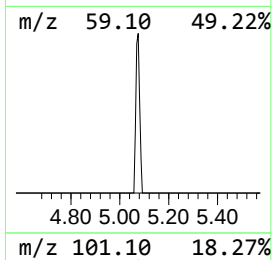
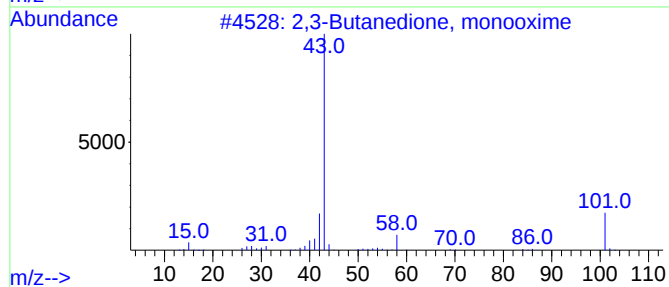
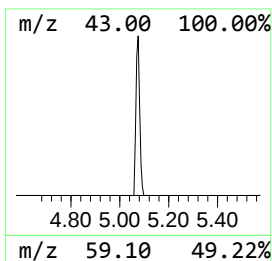
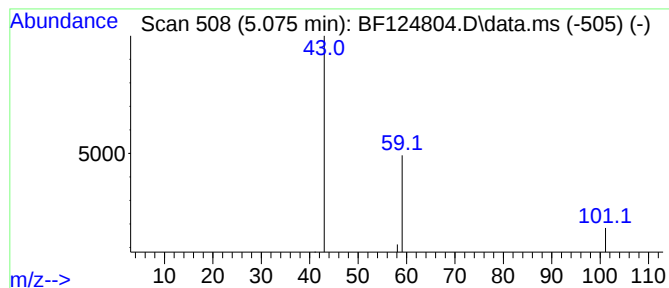
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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Peak Number 2 unknown5.075 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	8.27 ng	10374	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
2			Diacetamide	101	C4H7NO2	000625-77-4	7
3			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	4
4			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	4
5			N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	3



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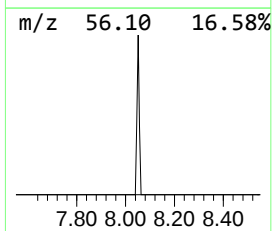
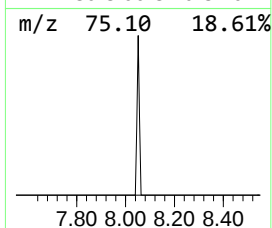
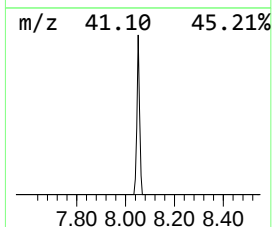
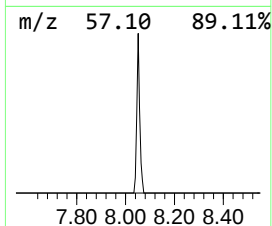
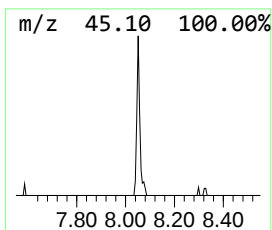
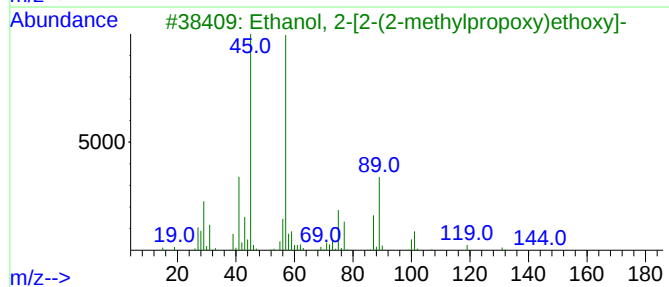
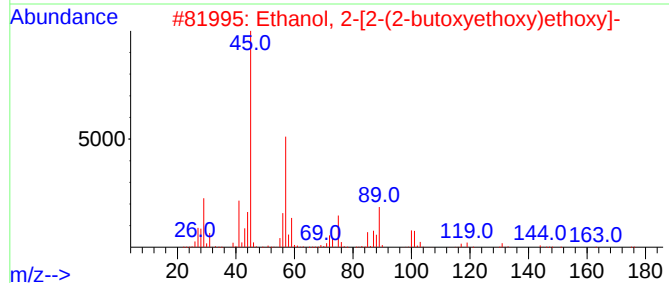
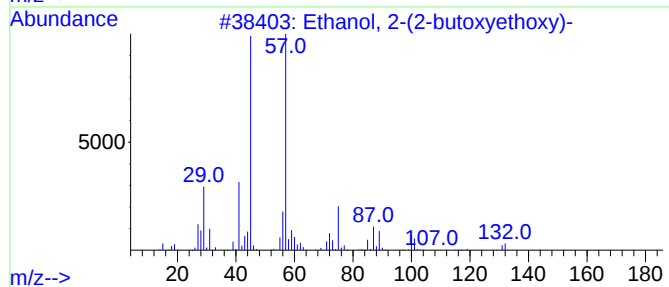
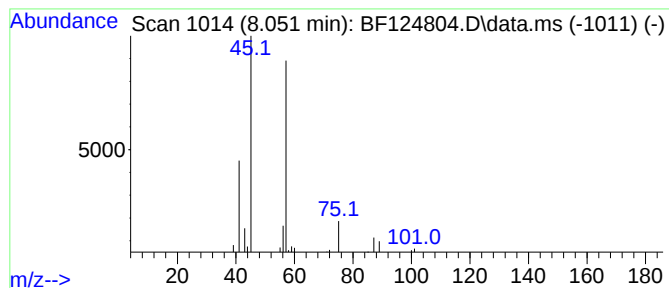
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	10.81 ng	19079	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	40



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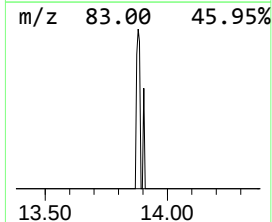
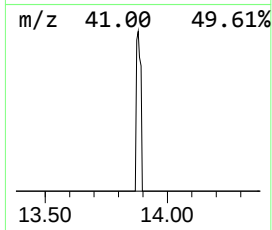
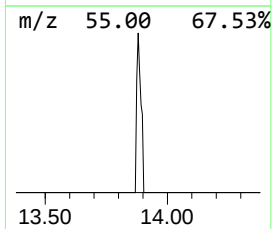
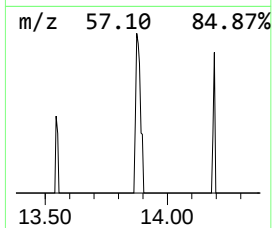
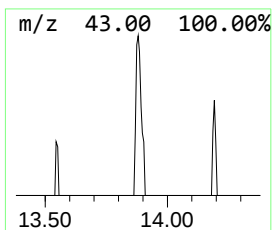
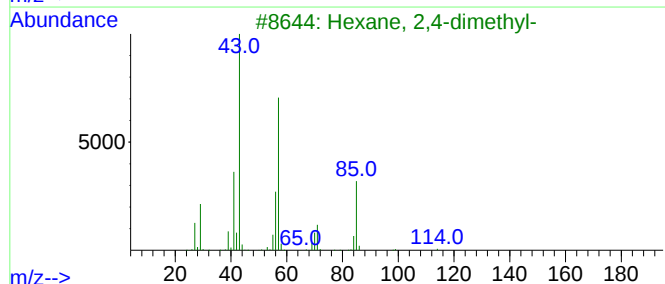
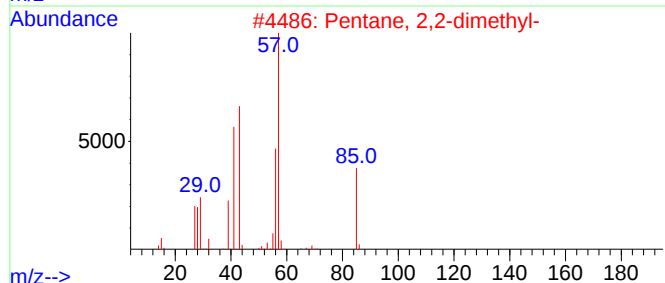
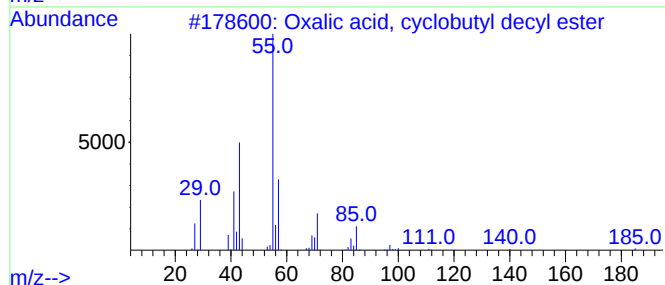
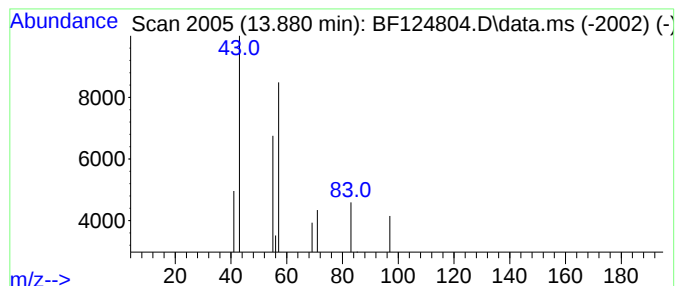
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Peak Number 4 unknown13.880 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	3.57 ng	6856	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl decyl ester	284	C16H28O4	1000309-70-1	9
2			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	9
3			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	9
4			Acetyl valeryl	128	C7H12O2	000096-04-8	9
5			Oxalic acid, cyclobutyl nonyl ester	270	C15H26O4	1000309-70-0	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.116	2.116	5.9	ng	7439	1	6.869	25096	20.0
unknown5.075	5.075	8.3	ng	10374	1	6.869	25096	20.0
Ethanol, 2-(2-b...	8.051	10.8	ng	19079	2	8.151	35313	20.0
unknown13.880	13.880	3.6	ng	6856	5	14.033	38448	20.0