

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
 Data File : BF124766.D
 Acq On : 26 Jul 2021 15:44
 Operator : JU/CG
 Sample : M3117-07
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NJ-CLEAN-7

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: BF124766.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	8	11	15	rBB	9144	9802	8.85%	1.260%
2	5.087	507	510	513	rBB	2212	2213	2.00%	0.284%
3	5.487	574	578	581	rBB	105946	89319	80.64%	11.482%
4	6.492	745	749	752	rBB	106304	92699	83.69%	11.917%
5	6.869	810	813	816	rBB	42159	30405	27.45%	3.909%
6	7.434	905	909	911	rBB	65578	61310	55.35%	7.882%
7	8.051	1012	1014	1019	rBB	24735	19571	17.67%	2.516%
8	8.151	1028	1031	1034	rBB	49419	39779	35.91%	5.114%
9	9.228	1210	1214	1217	rBV	147822	110763	100.00%	14.239%
10	9.910	1326	1330	1333	rBB	52054	44858	40.50%	5.767%
11	10.310	1395	1398	1402	rBB	4060	4209	3.80%	0.541%
12	10.692	1460	1463	1467	rBB	70747	59065	53.33%	7.593%
13	11.392	1579	1582	1585	rBB	52854	40015	36.13%	5.144%
14	11.910	1667	1670	1673	rBB	8455	8086	7.30%	1.039%
15	12.604	1786	1788	1790	rBB	2507	1430	1.29%	0.184%
16	12.698	1802	1804	1806	rBB	4037	2786	2.52%	0.358%
17	12.980	1848	1852	1855	rBB	106915	82930	74.87%	10.661%
18	13.886	2003	2006	2011	rBB3	3102	5141	4.64%	0.661%
19	14.033	2027	2031	2034	rBV	33610	28121	25.39%	3.615%
20	14.762	2152	2155	2159	rBB	1436	2053	1.85%	0.264%
21	14.810	2159	2163	2167	rBB	1496	2340	2.11%	0.301%
22	15.145	2216	2220	2223	rBV	2692	2920	2.64%	0.375%
23	15.504	2276	2281	2288	rBB	27110	30976	27.97%	3.982%
24	15.974	2355	2361	2367	rBB3	2532	4276	3.86%	0.550%
25	16.486	2441	2448	2452	rBB2	1242	2812	2.54%	0.361%

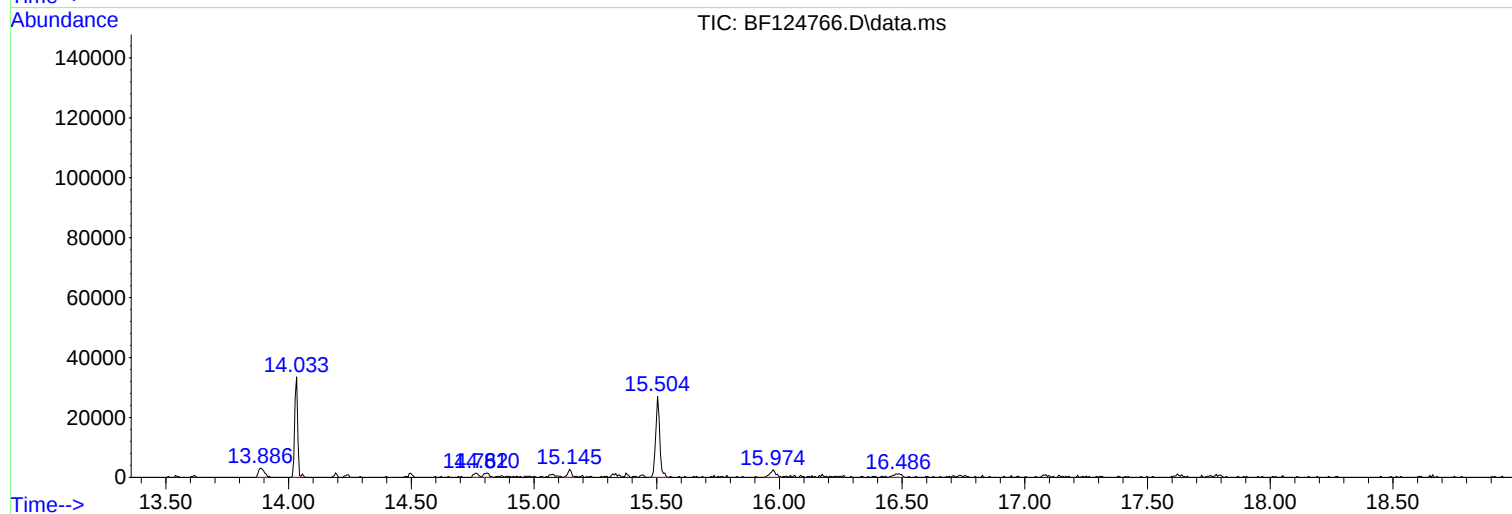
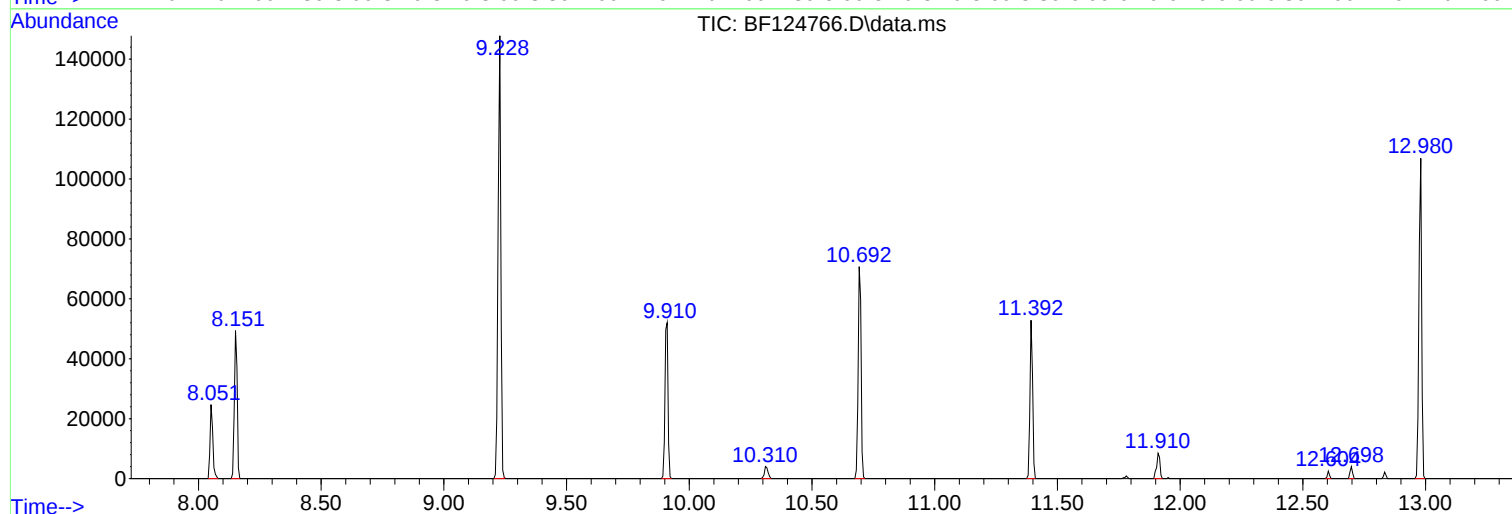
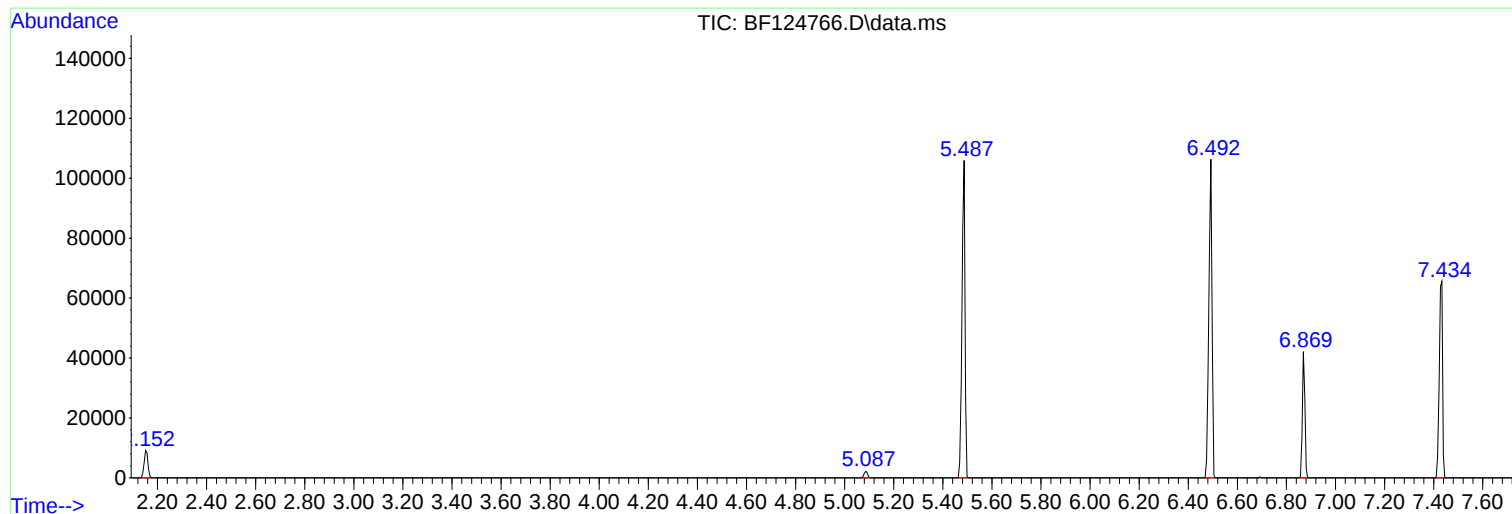
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-7

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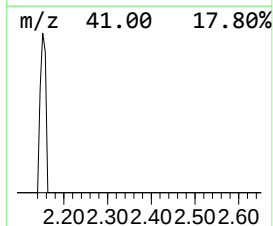
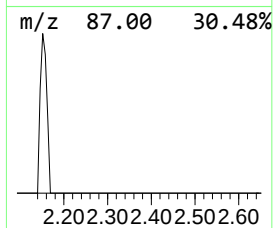
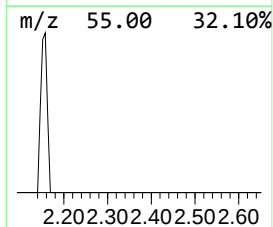
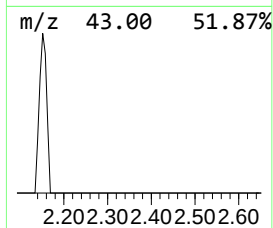
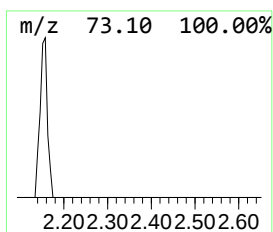
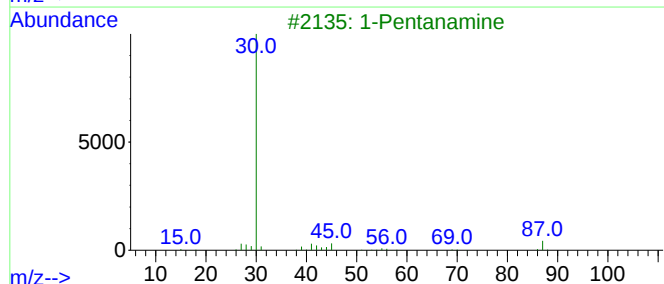
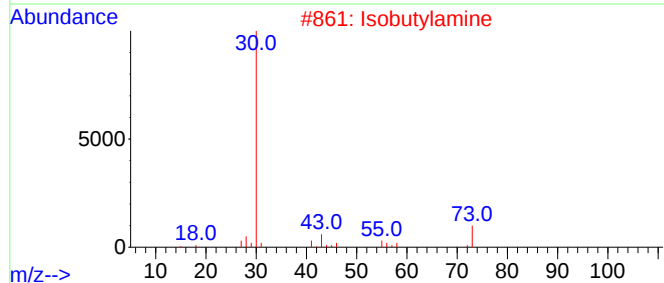
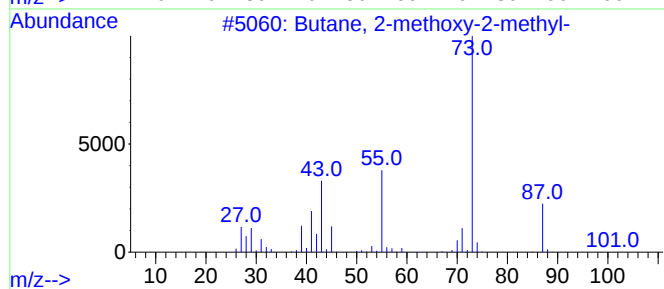
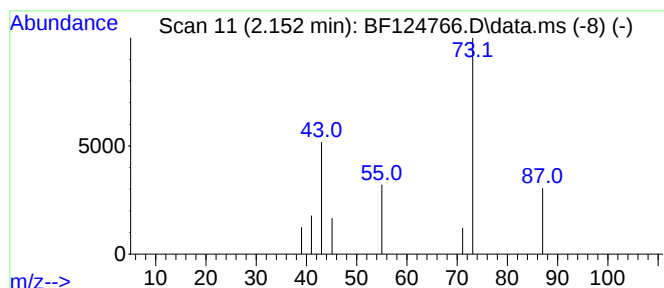
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.152 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	6.45 ng	9802	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	5
3		1-Pentanamine	87	C5H13N	000110-58-7	4
4		2-OXOPROPIONAMIDE	87	C3H5NO2	000631-66-3	4
5		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	4



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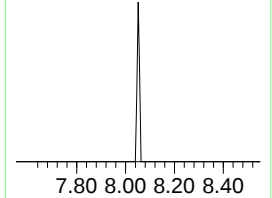
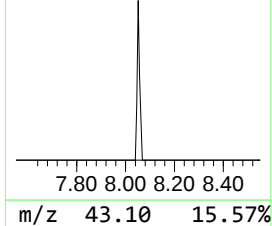
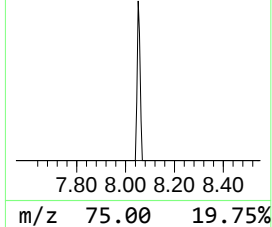
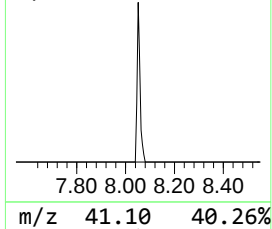
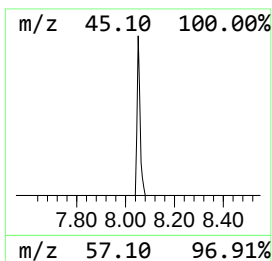
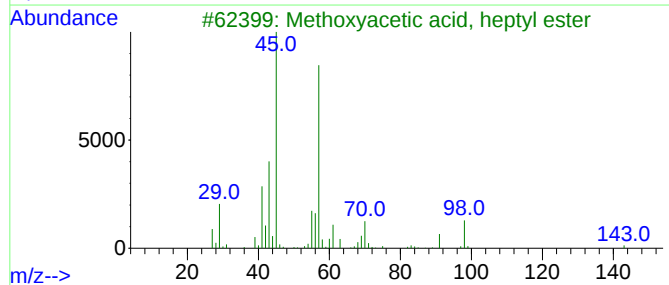
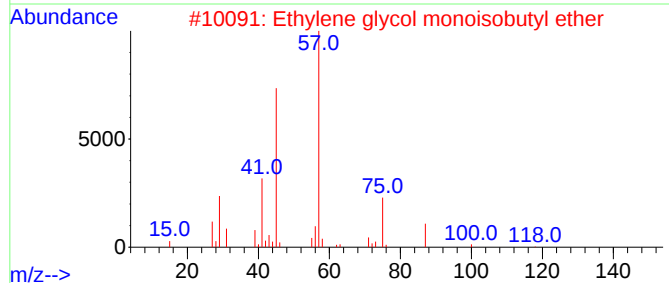
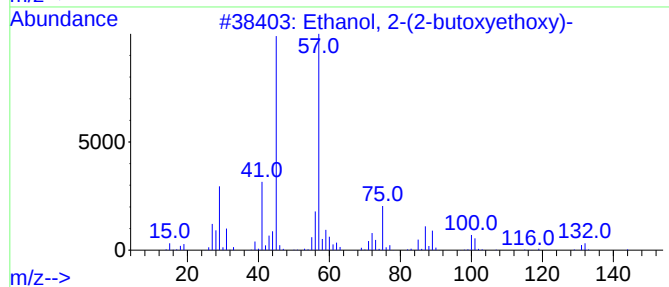
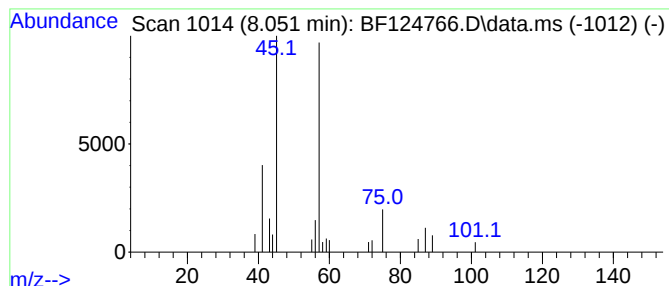
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	9.84 ng	19571	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	64
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
3			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	40
4			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	38
5			Tetraethylene glycol	194	C8H18O5	000112-60-7	33



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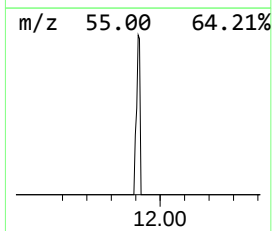
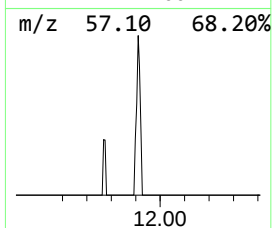
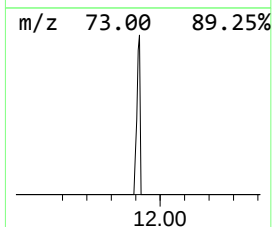
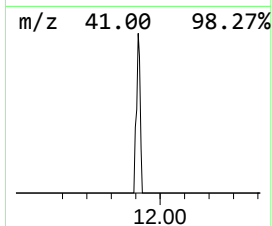
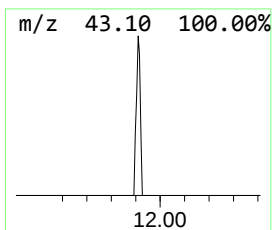
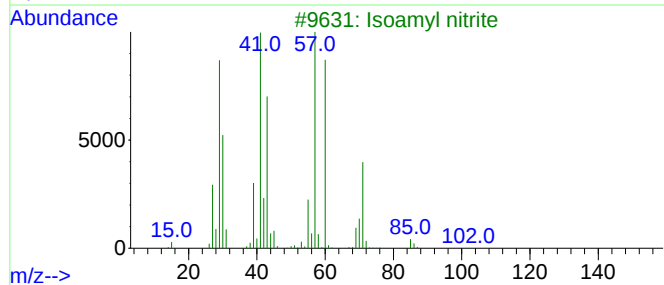
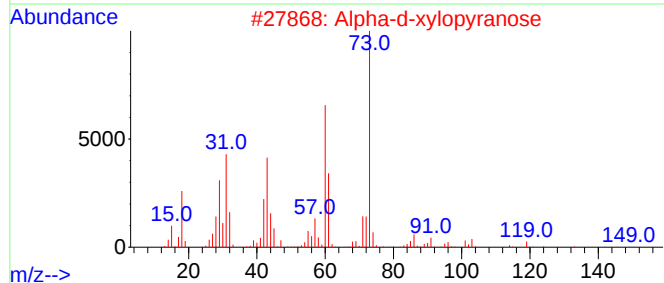
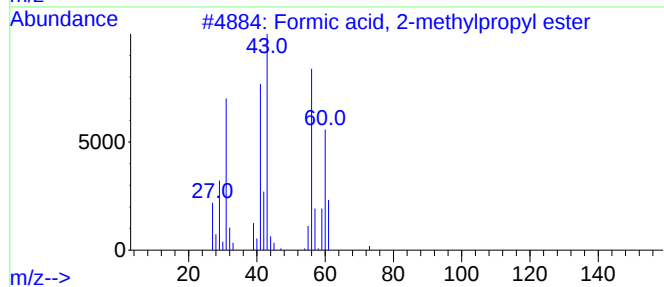
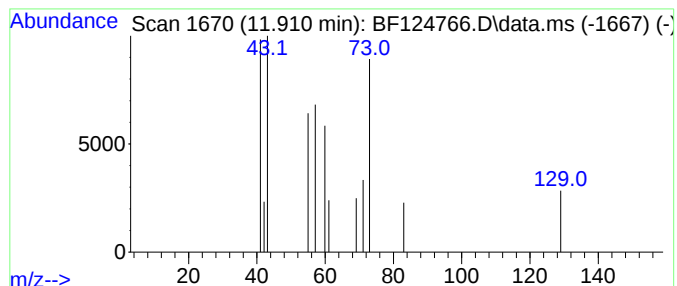
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown11.910 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	4.04 ng	8086	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formic acid, 2-methylpropyl ester	102	C5H10O2	000542-55-2	37
2			Alpha-d-xylopyranose	150	C5H10O5	006763-34-4	36
3			Isoamyl nitrite	117	C5H11NO2	000110-46-3	32
4			Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	28
5			2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	25



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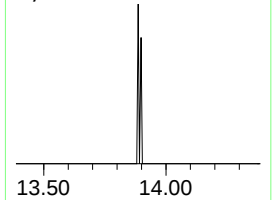
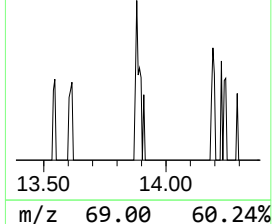
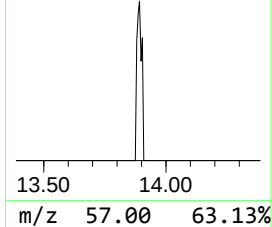
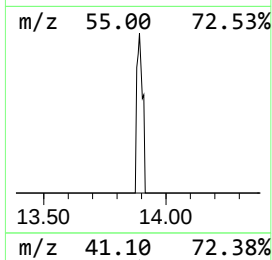
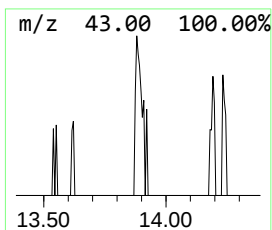
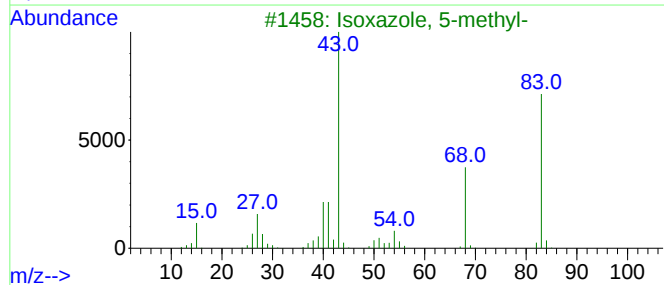
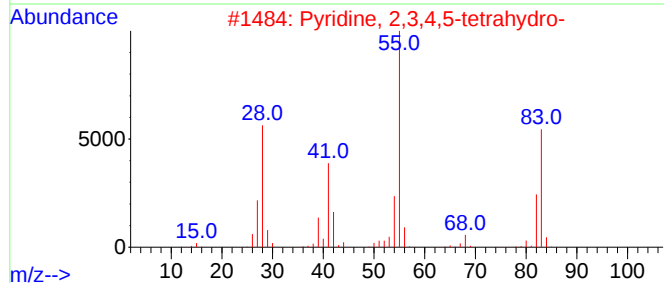
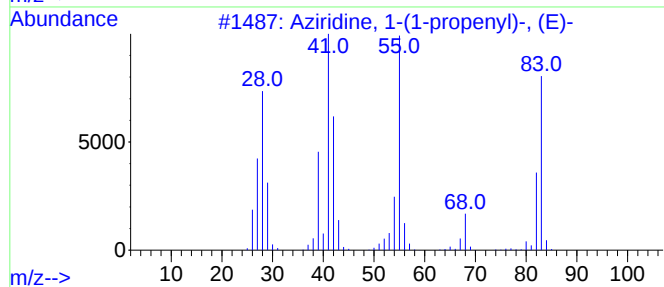
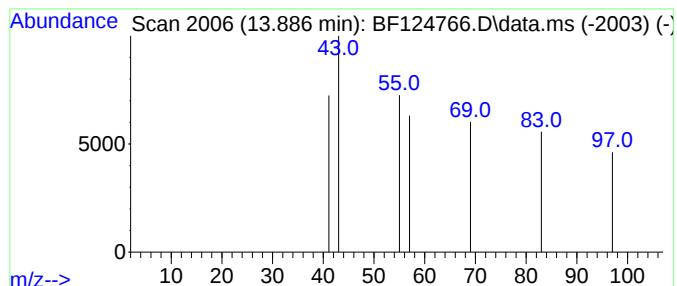
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown13.886 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.66 ng	5141	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	7
2			Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	4
3			Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	4
4			1-Hexene, 6-bromo-	162	C6H11Br	002695-47-8	2
5			3-Hexyn-2-ol, 5-methyl-	112	C7H12O	023293-50-7	2



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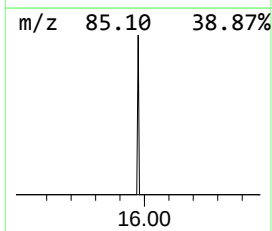
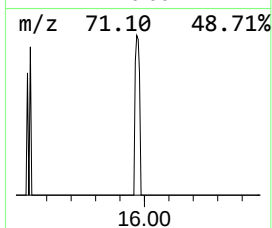
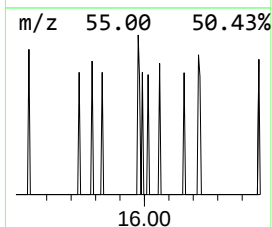
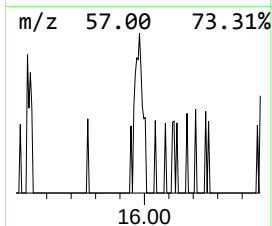
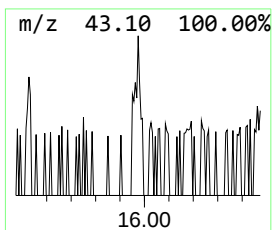
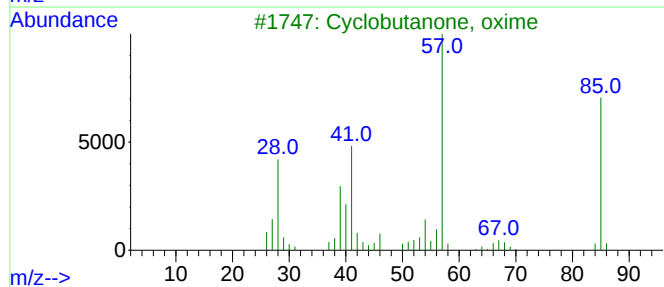
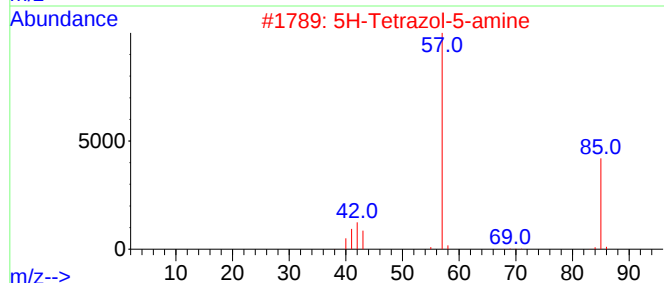
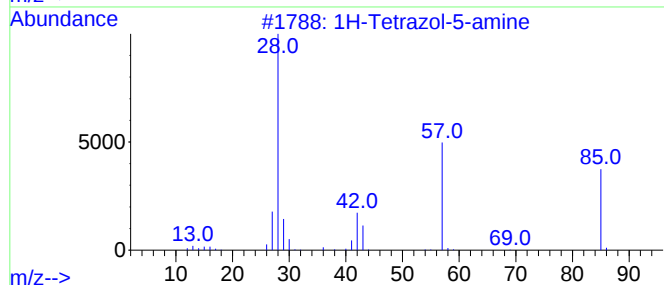
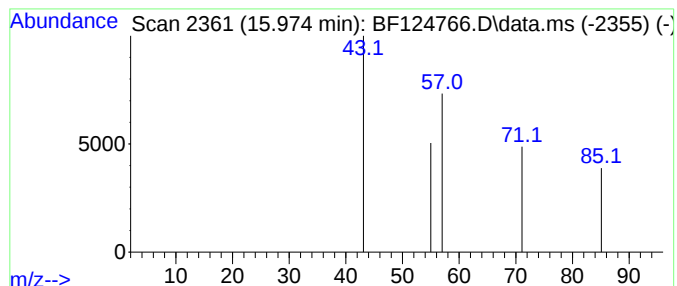
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Peak Number 5 unknown15.974 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	2.76 ng	4276	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
2			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
3			Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
4			Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	4
5			Azetidine, 1,3-dimethyl-	85	C5H11N	055683-38-0	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.152	2.152	6.5	ng	9802	1	6.869	30405	20.0
Ethanol, 2-(2-b...	8.051	9.8	ng	19571	2	8.151	39779	20.0
unknown11.910	11.910	4.0	ng	8086	4	11.392	40015	20.0
unknown13.886	13.886	3.7	ng	5141	5	14.033	28121	20.0
unknown15.974	15.974	2.8	ng	4276	6	15.504	30976	20.0