

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
 Data File : BF124746.D
 Acq On : 24 Jul 2021 14:23
 Operator : JU/CG
 Sample : M3117-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NJ-CLEAN-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: BF124746.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	5	8	12	rBB	7651	8231	8.46%	1.161%
2	5.075	505	508	512	rBB	8591	8352	8.59%	1.178%
3	5.475	572	576	579	rBB	82113	73753	75.82%	10.405%
4	6.486	744	748	751	rBB	94321	77994	80.18%	11.003%
5	6.869	810	813	816	rBB	48331	34036	34.99%	4.802%
6	7.428	904	908	911	rBB	66807	51485	52.93%	7.264%
7	8.051	1011	1014	1017	rBV	29022	20514	21.09%	2.894%
8	8.151	1028	1031	1034	rBB	67981	48530	49.89%	6.847%
9	9.227	1210	1214	1217	rBV	125667	97269	100.00%	13.723%
10	9.904	1326	1329	1332	rBV	67893	51138	52.57%	7.215%
11	10.692	1460	1463	1466	rBB	53730	43071	44.28%	6.076%
12	11.392	1579	1582	1584	rBV	52109	39121	40.22%	5.519%
13	11.780	1646	1648	1650	rBB	2685	1556	1.60%	0.220%
14	11.910	1668	1670	1672	rBB	4642	2548	2.62%	0.359%
15	12.604	1785	1788	1790	rBB	6095	4872	5.01%	0.687%
16	12.827	1824	1826	1829	rBB	5638	4580	4.71%	0.646%
17	12.974	1848	1851	1854	rBB	75791	54283	55.81%	7.658%
18	13.874	2002	2004	2009	rBB	1889	2163	2.22%	0.305%
19	14.027	2026	2030	2033	rBV	34829	28358	29.15%	4.001%
20	14.051	2033	2034	2036	rVB	3587	1873	1.93%	0.264%
21	14.804	2160	2162	2164	rBB	1785	1420	1.46%	0.200%
22	15.062	2202	2206	2210	rBV	3344	4785	4.92%	0.675%
23	15.139	2216	2219	2223	rBB	1647	2366	2.43%	0.334%
24	15.374	2256	2259	2262	rBB	2103	2085	2.14%	0.294%
25	15.433	2266	2269	2273	rBB	2152	2291	2.36%	0.323%
26	15.498	2276	2280	2284	rBV	25393	28595	29.40%	4.034%
27	15.527	2284	2285	2288	rVB	2977	2195	2.26%	0.310%
28	15.968	2356	2360	2364	rBB	3106	4279	4.40%	0.604%
29	16.486	2443	2448	2452	rBB2	2124	3369	3.46%	0.475%
30	17.074	2546	2548	2552	rBB2	1439	1817	1.87%	0.256%
31	17.792	2665	2670	2673	rBB	958	1885	1.94%	0.266%

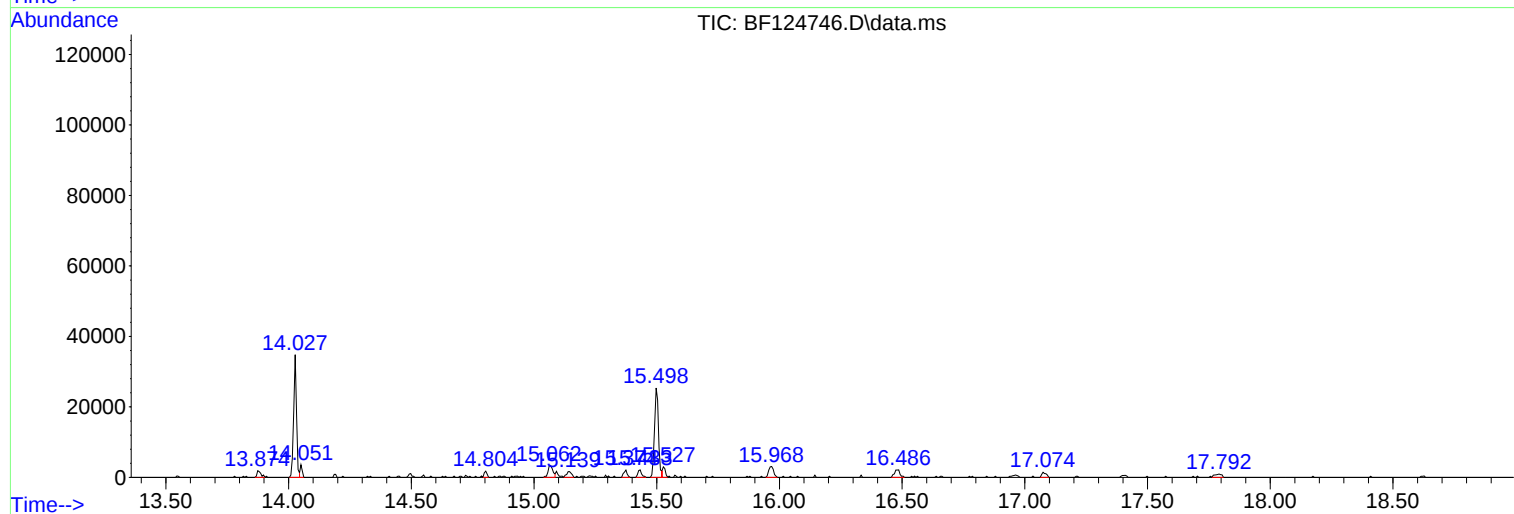
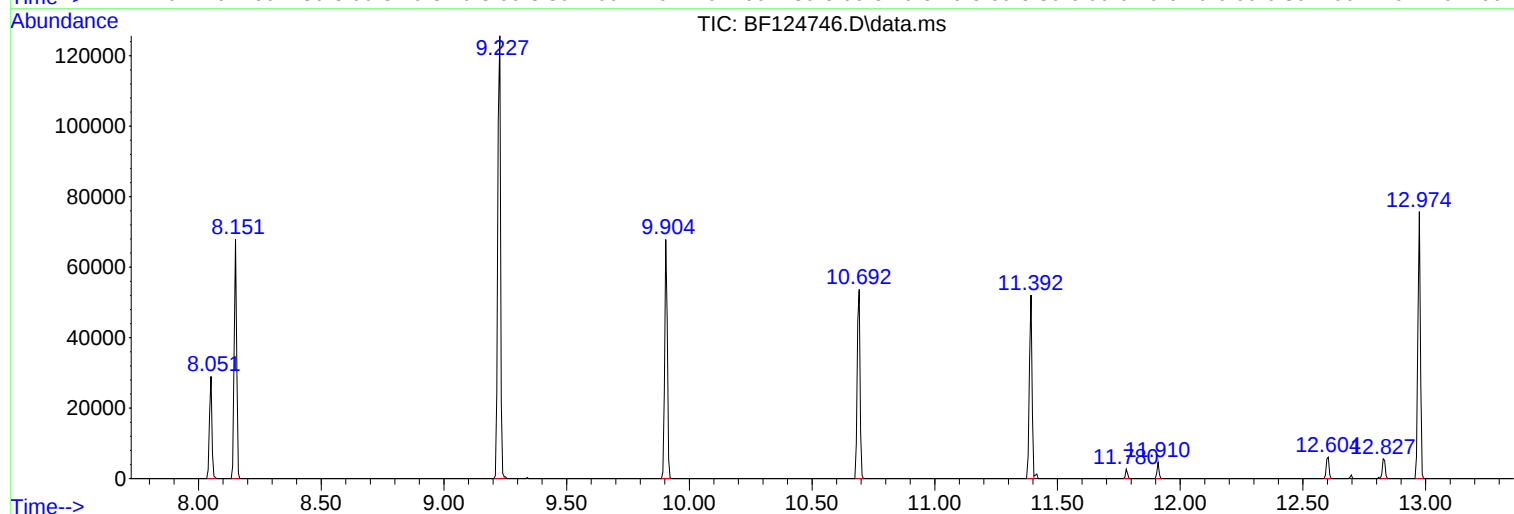
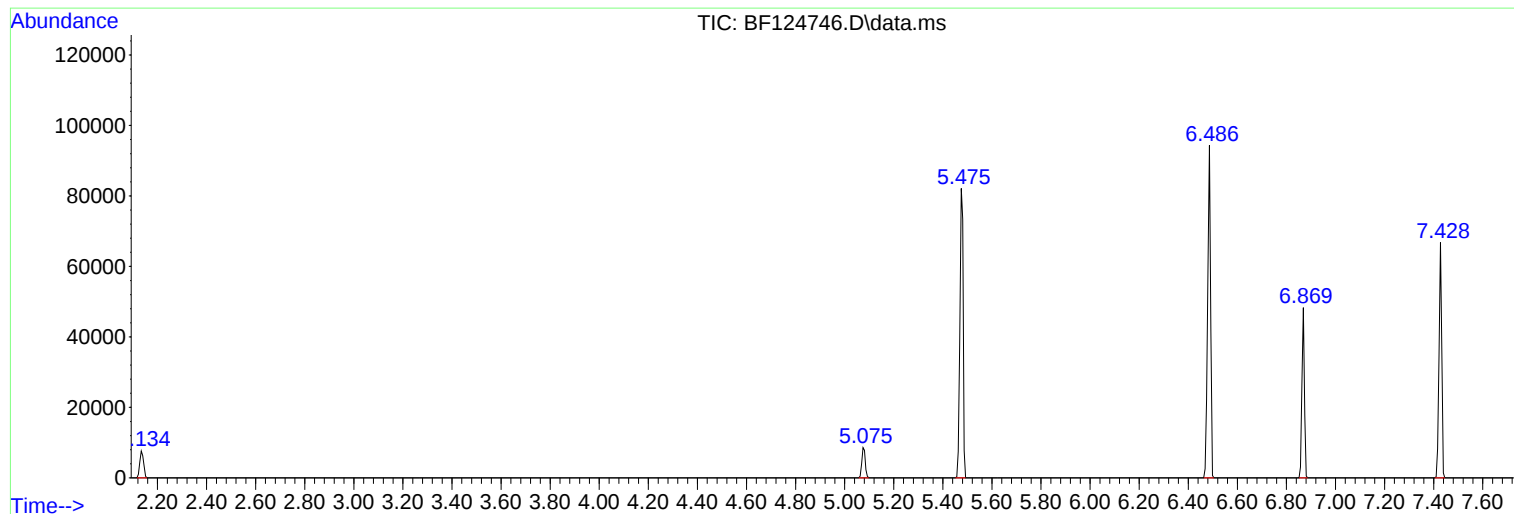
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ClientSampleId :
NJ-CLEAN-2

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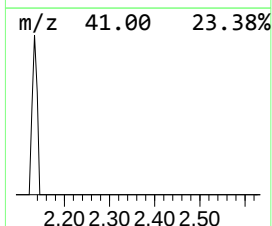
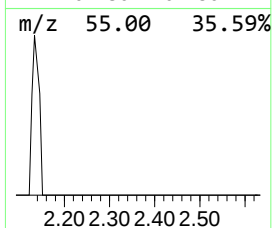
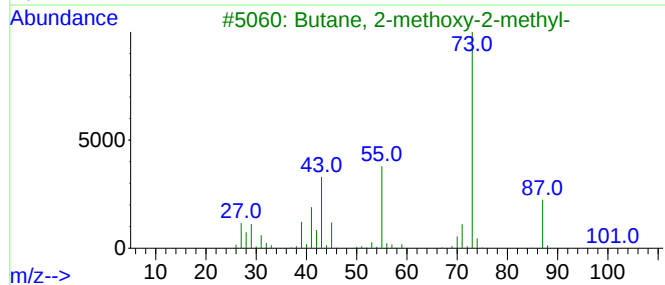
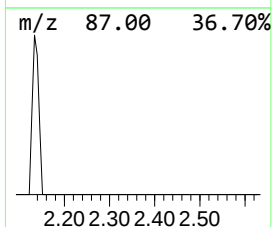
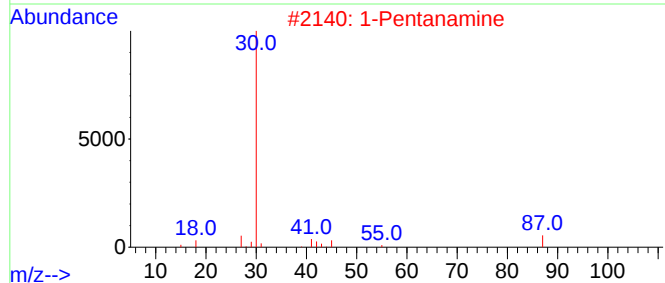
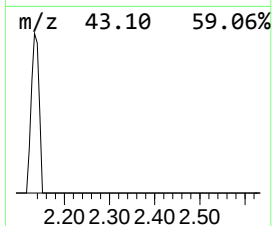
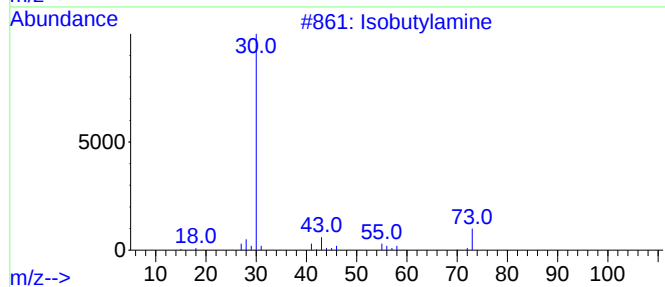
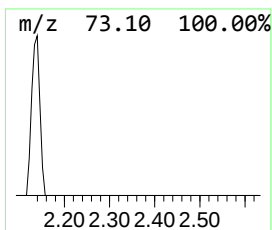
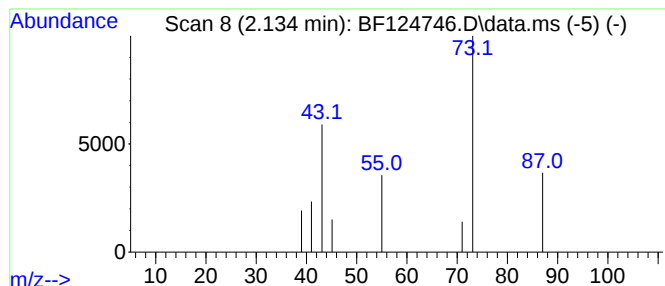
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.134 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	4.84 ng	8231	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutylamine	73	C4H11N	000078-81-9	5
2			1-Pentanamine	87	C5H13N	000110-58-7	4
3			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	4
4			3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	4
5			2-Pentanol, acetate	130	C7H14O2	000626-38-0	4



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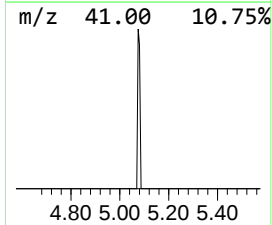
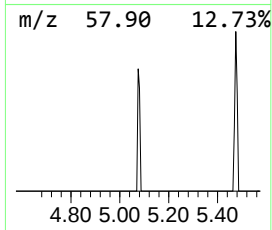
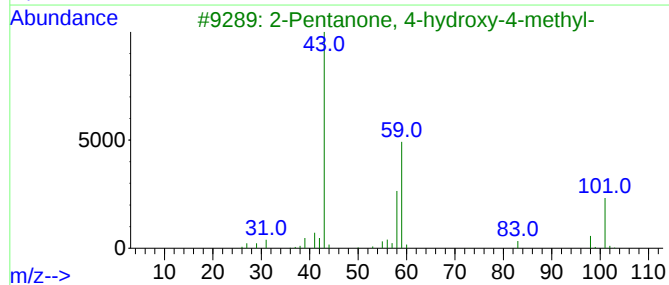
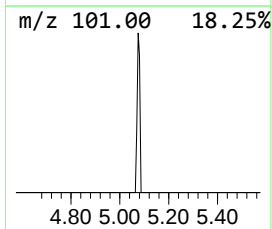
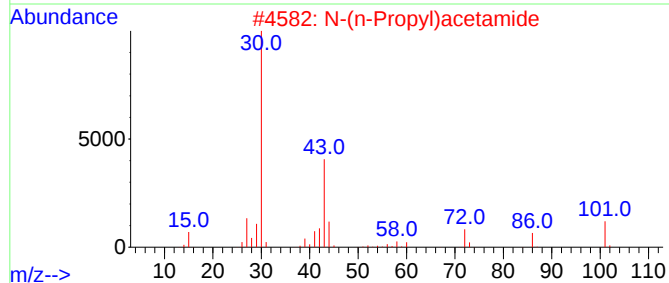
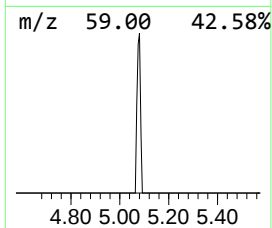
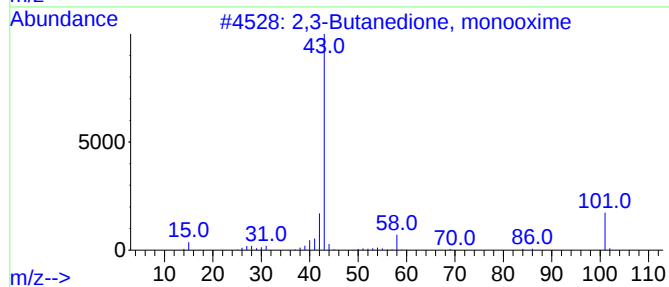
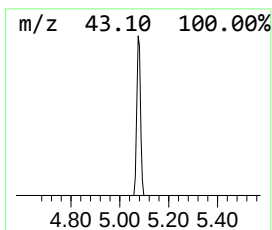
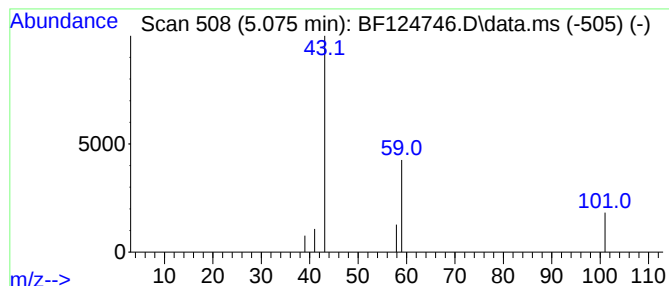
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown5.075 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	4.91 ng	8352	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	N-(n-Propyl)acetamide		101	C5H11NO	005331-48-6	4	
3	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	4	
4	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	4	
5	Oxirane, [(1-methylethoxy)methyl]-		116	C6H12O2	004016-14-2	4	



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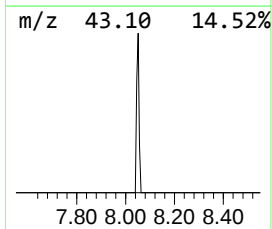
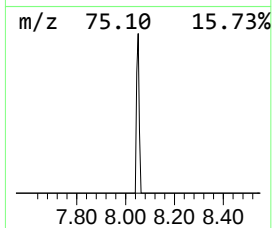
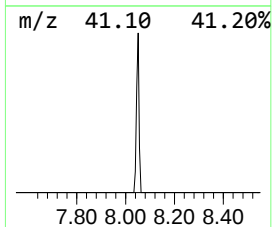
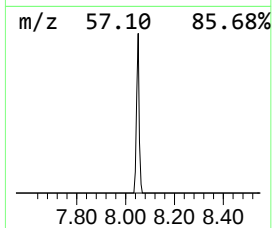
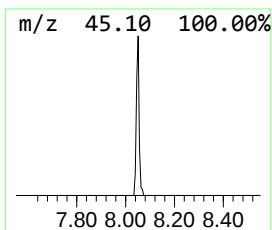
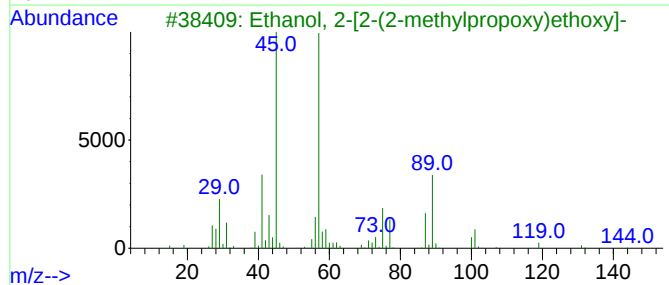
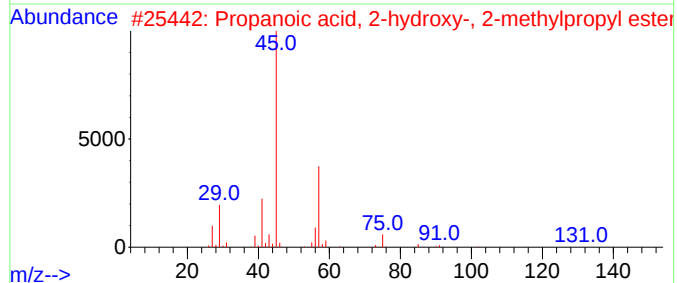
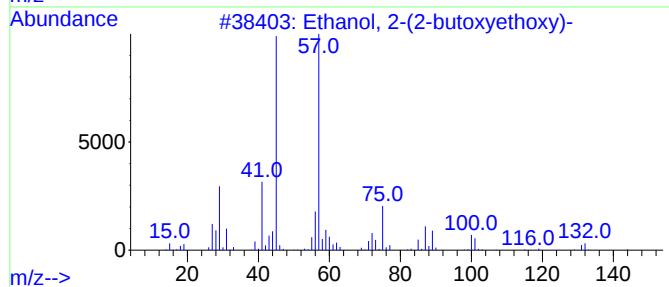
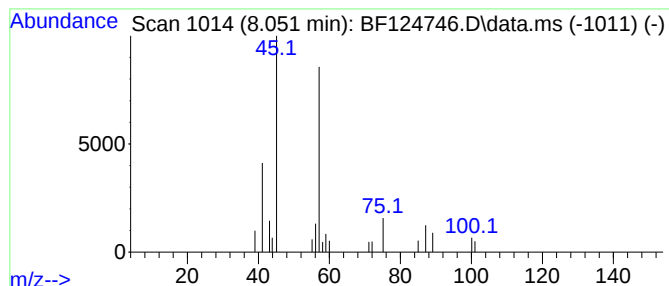
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	8.45 ng	20514	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			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	42
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	39



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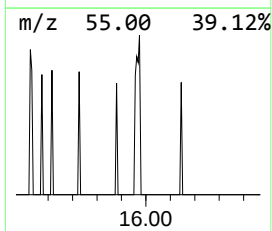
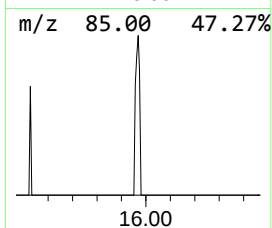
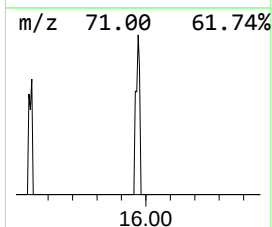
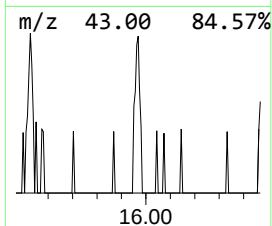
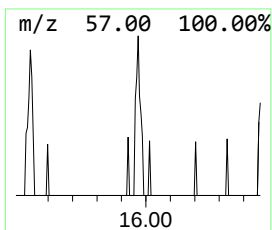
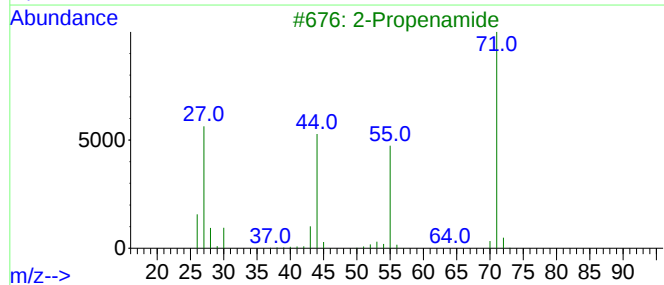
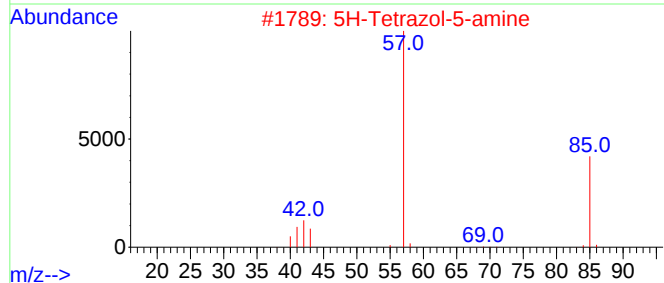
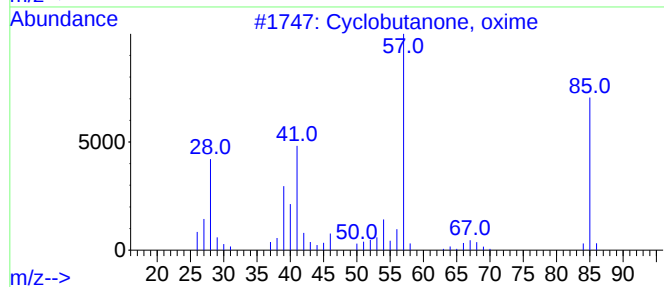
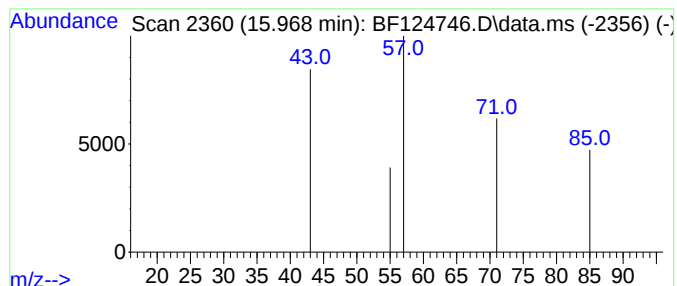
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Peak Number 4 unknown15.968 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.968	2.99 ng	4279	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
2			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
3			2-Propenamide	71	C3H5NO	000079-06-1	4
4			Azetidine, 1,2-dimethyl-	85	C5H11N	051764-32-0	4
5			Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	4



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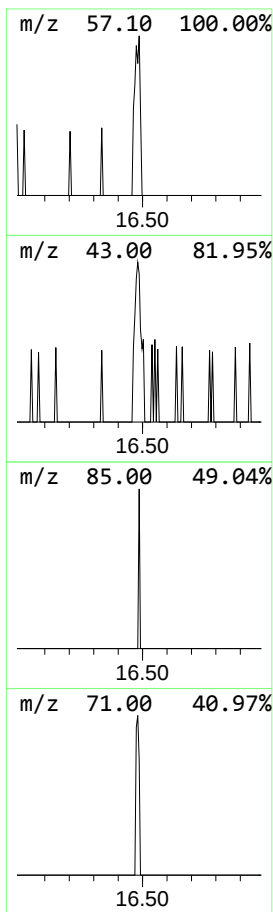
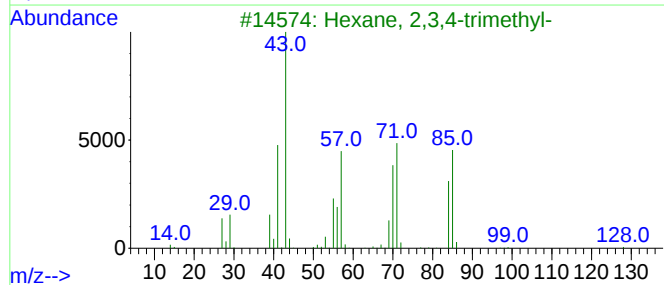
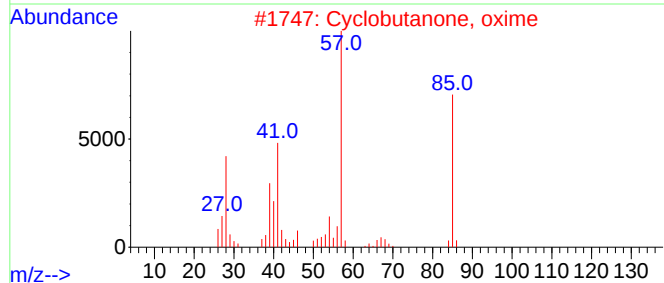
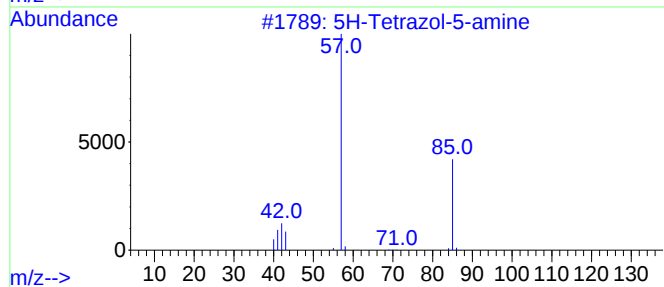
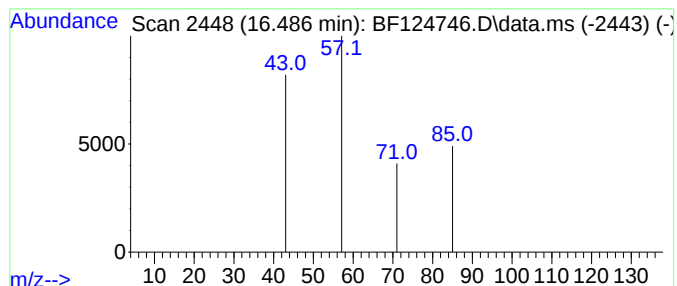
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown16.486 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.486	2.36 ng	3369	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
2			Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
3			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	4
4			Oxirane, 2-methyl-3-propyl-, cis-	100	C6H12O	006124-90-9	4
5			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	3



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.134	2.134	4.8	ng	8231	1	6.869	34036	20.0
unknown5.075	5.075	4.9	ng	8352	1	6.869	34036	20.0
Ethanol, 2-(2-b...	8.051	8.4	ng	20514	2	8.151	48530	20.0
unknown15.968	15.968	3.0	ng	4279	6	15.498	28595	20.0
unknown16.486	16.486	2.4	ng	3369	6	15.498	28595	20.0