

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010615\
 Data File : BF076757.D
 Acq On : 6 Jan 2015 14:23
 Operator : IZ / TP
 Sample : PB81207BL
 Misc : W DOD
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB81207BL

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-BF121714.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	1.144	3	5	8	rVB	14226	21172	1.34%	0.182%
2	1.418	27	29	35	rBV	9431	20660	1.31%	0.178%
3	1.498	35	36	48	rVB2	24486	46815	2.97%	0.403%
4	4.230	272	275	282	rBV	165828	304595	19.32%	2.622%
5	4.904	331	334	337	rBV	715500	1103723	69.99%	9.503%
6	6.322	456	458	461	rBV	1106000	1023754	64.92%	8.814%
7	6.413	464	466	469	rBV	910341	1121601	71.12%	9.656%
8	6.710	490	492	494	rBV	251227	252124	15.99%	2.171%
9	6.893	506	508	511	rBB	904232	842417	53.42%	7.253%
10	7.419	552	554	557	rBV	741241	665000	42.17%	5.725%
11	8.299	628	631	633	rBV	380241	358145	22.71%	3.083%
12	9.648	747	749	752	rBV	1052581	1333016	84.53%	11.477%
13	10.448	817	819	822	rBB	406792	398109	25.25%	3.428%
14	11.419	902	904	907	rBV	821929	892888	56.62%	7.687%
15	12.265	976	978	981	rBV	473930	435346	27.61%	3.748%
16	14.254	1150	1152	1155	rBV	1156084	1576970	100.00%	13.577%
17	15.511	1259	1262	1265	rBV	417590	441499	28.00%	3.801%
18	16.974	1382	1390	1391	rBV4	13563	44355	2.81%	0.382%
19	17.077	1397	1399	1406	rVB6	14609	49235	3.12%	0.424%
20	17.237	1410	1413	1416	rVV	335534	432113	27.40%	3.720%
21	17.294	1416	1418	1424	rVB4	14890	38839	2.46%	0.334%
22	17.580	1436	1443	1446	rBV6	13315	57765	3.66%	0.497%
23	18.083	1483	1487	1490	rBV5	8837	30573	1.94%	0.263%
24	18.414	1512	1516	1517	rBV3	9191	24064	1.53%	0.207%
25	19.637	1617	1623	1626	rBV7	8071	34202	2.17%	0.294%
26	19.729	1630	1631	1640	rVB8	12036	40682	2.58%	0.350%
27	21.066	1743	1748	1749	rBV4	10191	25381	1.61%	0.219%

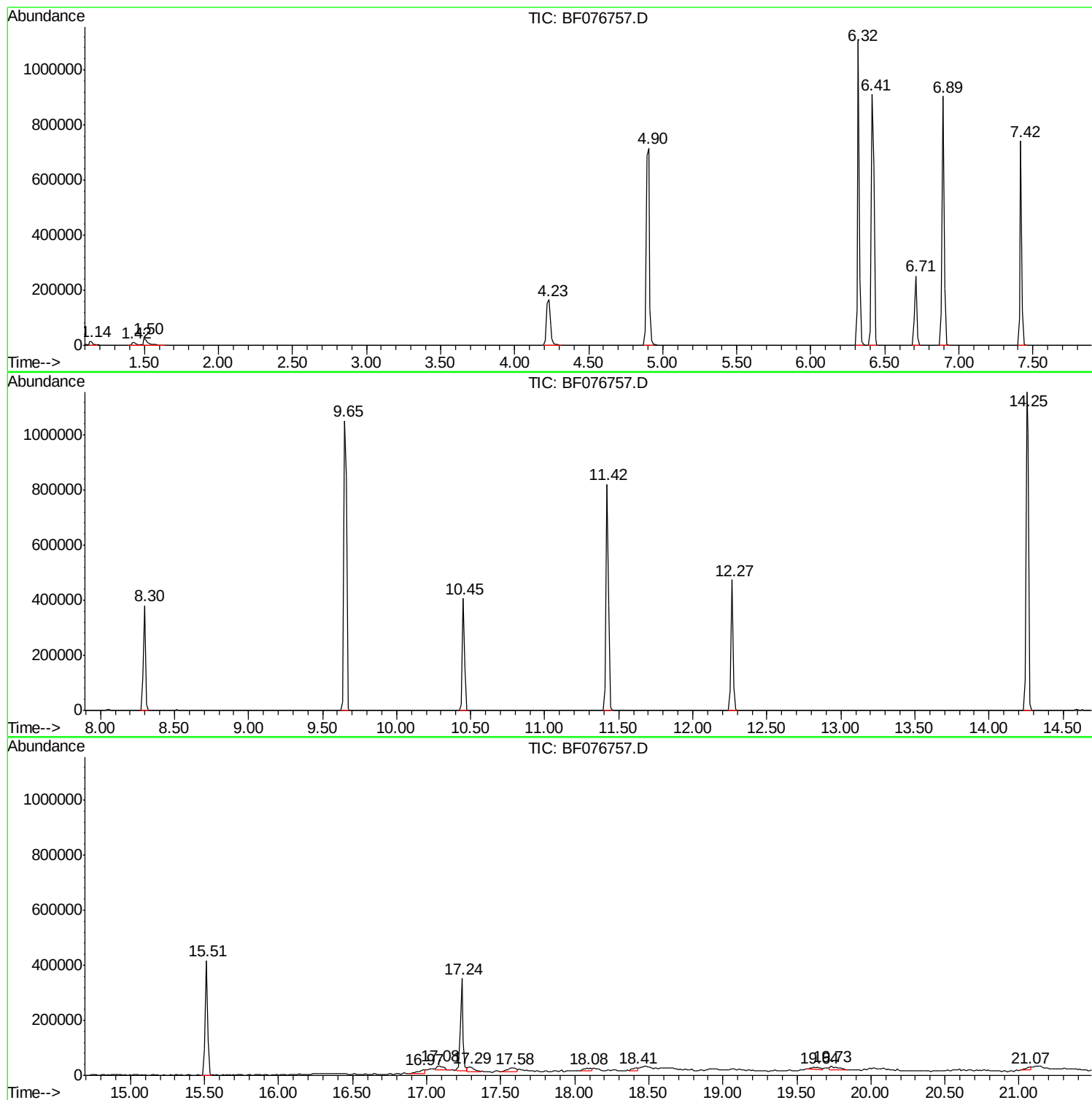
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121714.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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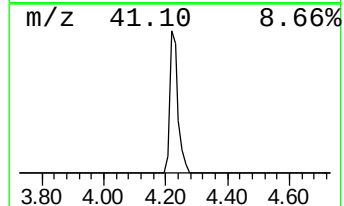
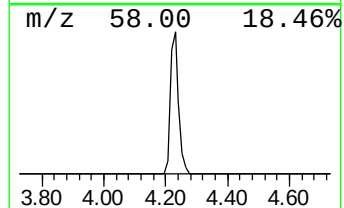
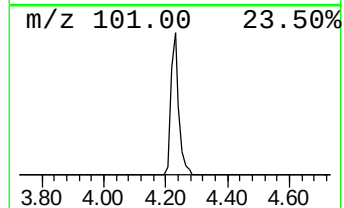
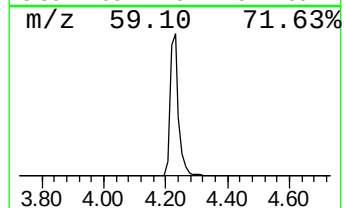
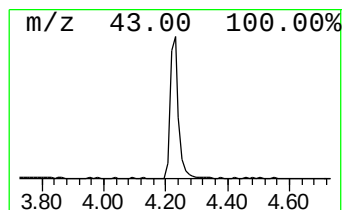
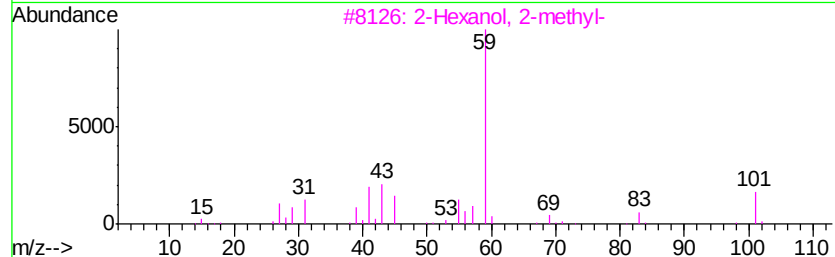
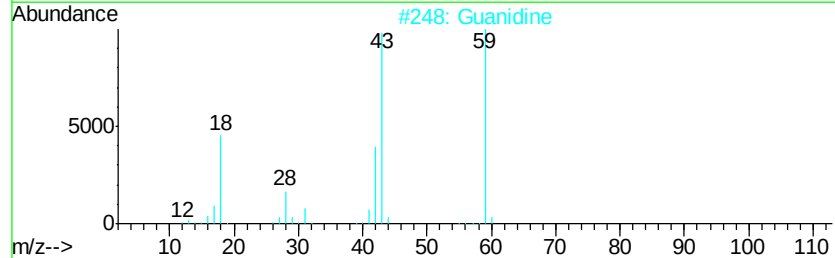
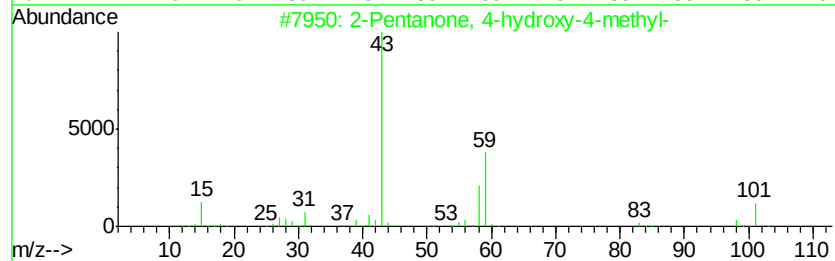
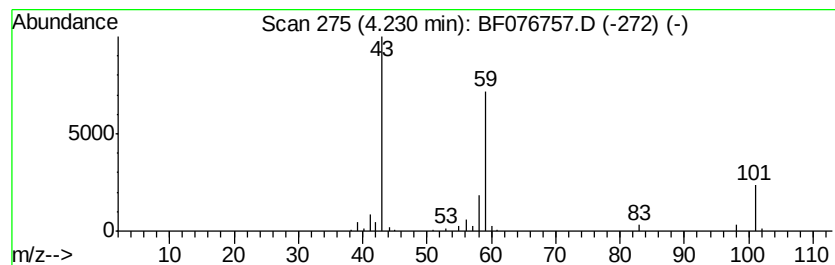
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121714.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.23	24.16 ng	304595	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Guanidine	59	CH5N3	000113-00-8	43
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5		Acetone	58	C3H6O	000067-64-1	9



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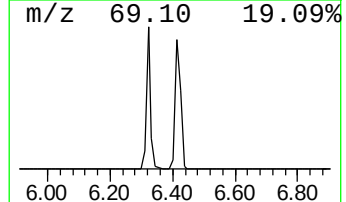
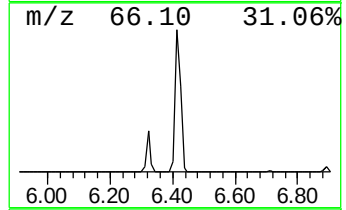
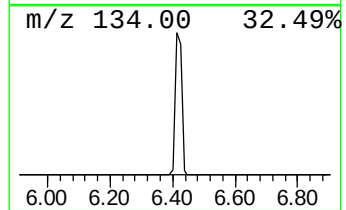
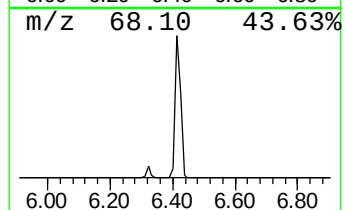
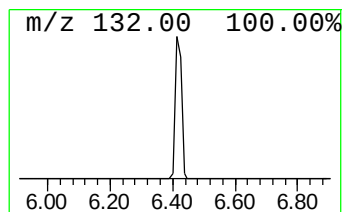
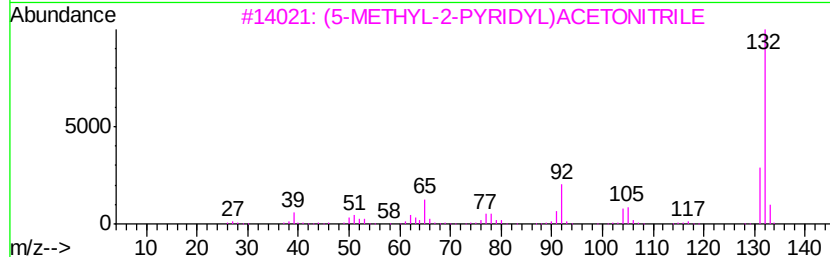
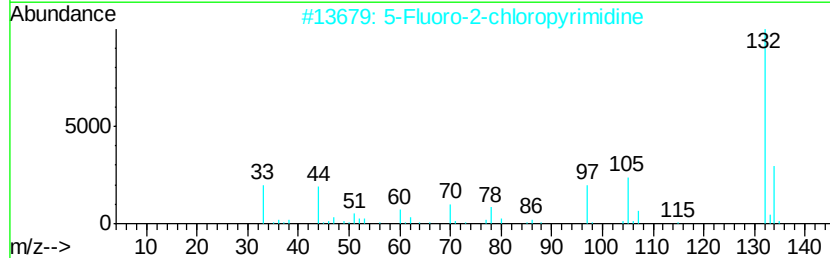
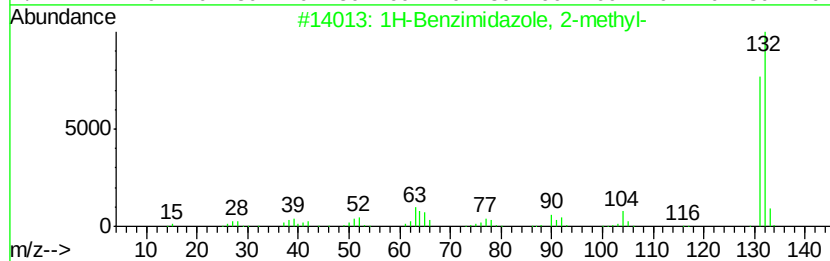
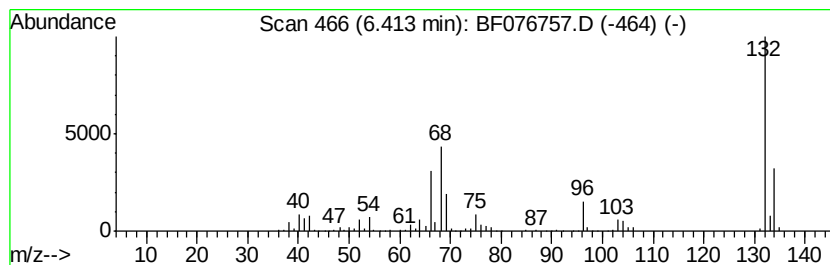
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	88.97 ng	1121600	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Aminoindole	132	C8H8N2	005192-03-0	10



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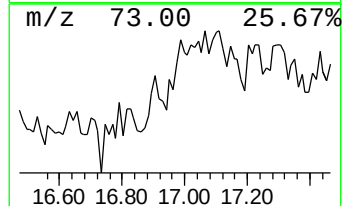
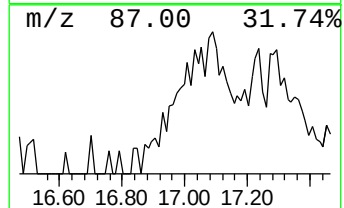
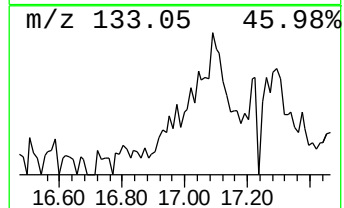
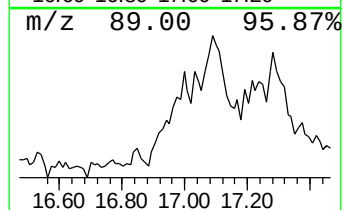
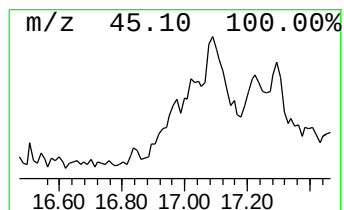
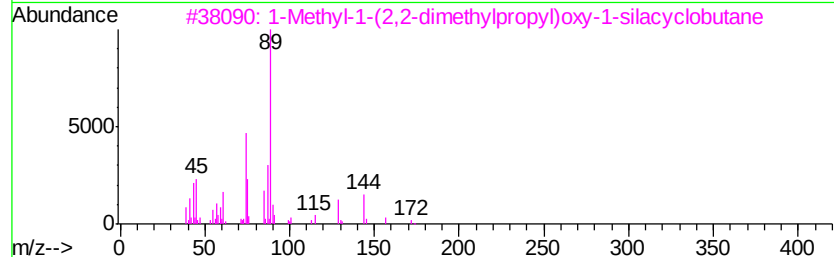
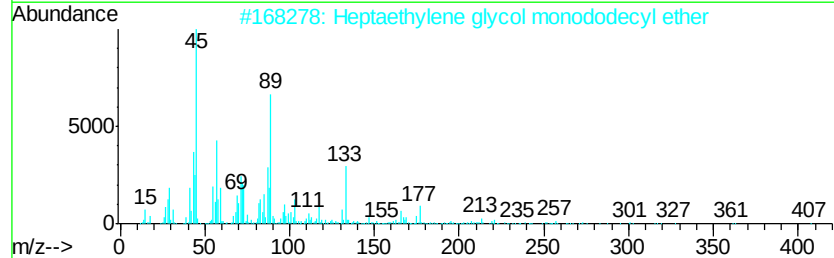
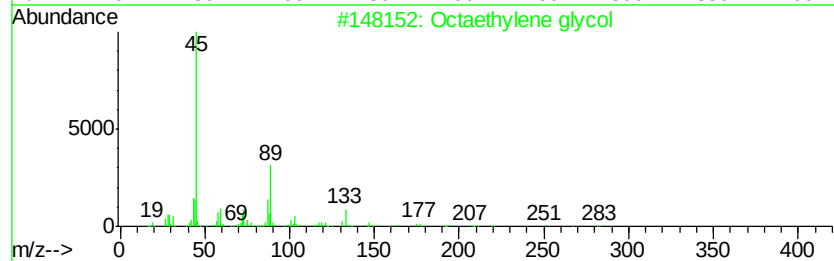
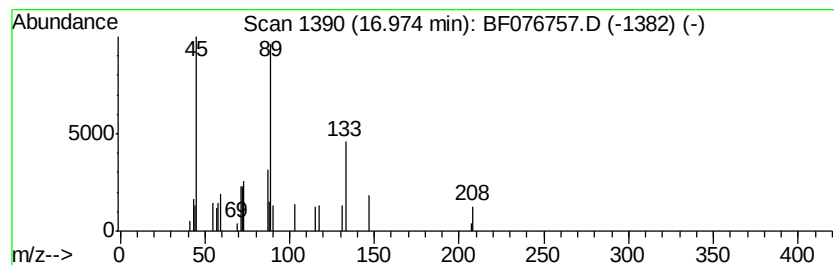
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Peak Number 5 Octaethylene glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	2.05 ng	44355	Perylene-d12	17.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octaethylene glycol	370	C16H34O9	1000289-34-2	72
2		Heptaethylene glycol monododecyl...	494	C26H54O8	003055-97-8	64
3		1-Methyl-1-(2,2-dimethylpropyl)oxy...	172	C9H20OSi	1000216-97-6	64
4		3-(1,3-Dihydroxyisopropyl)-1,5,8...	264	C12H24O6	109773-63-9	64
5		Pentaethylene glycol	238	C10H22O6	004792-15-8	56



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PB81207BL

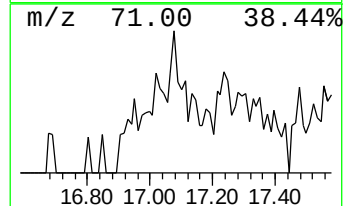
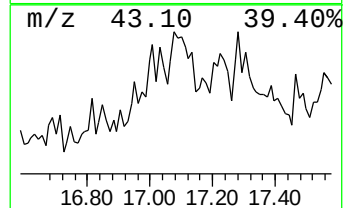
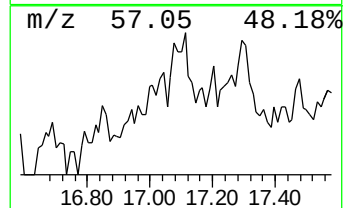
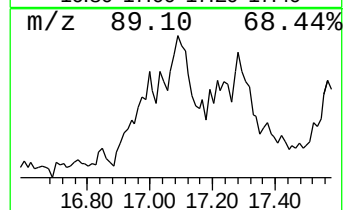
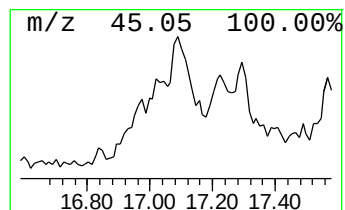
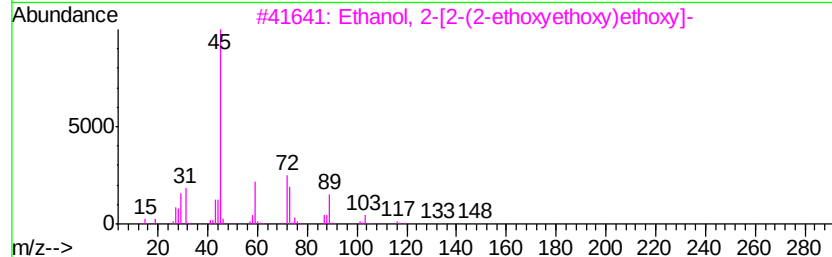
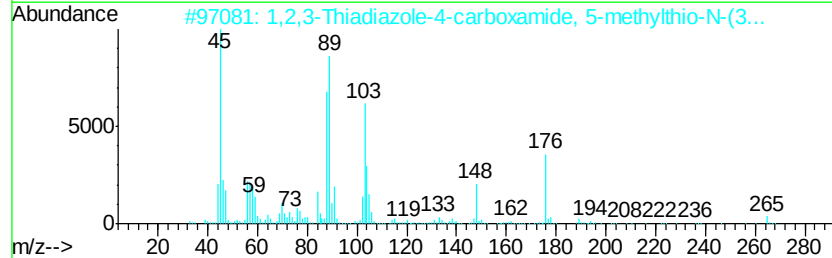
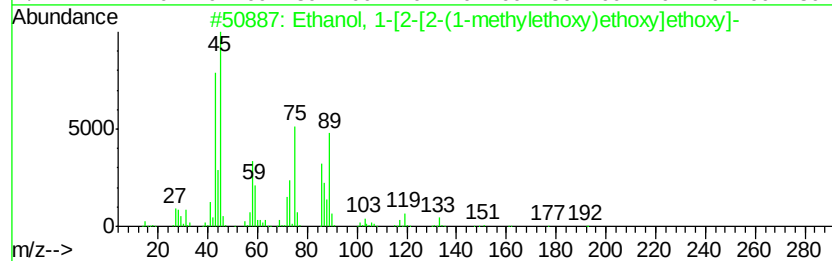
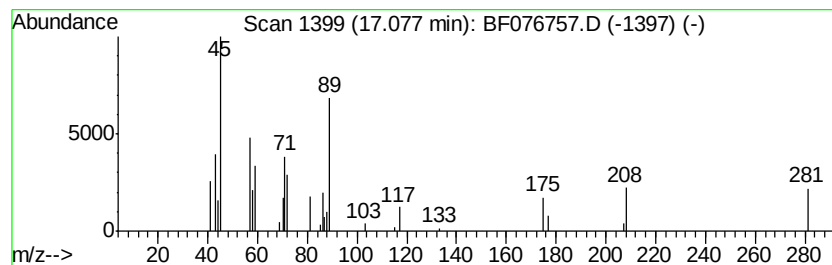
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 unknown17.08 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.08	2.28 ng	49235	Perylene-d12	17.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 1-[2-[2-(1-methylethoxy)ethoxy]ethoxy]-	192	C9H20O4	029681-21-8	17
2		1,2,3-Thiadiazole-4-carboxamide,...	265	C11H11N3OS2	1000294-15-1	17
3		Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	17
4		1,4,7,10,13,16-Hexaoxonadecane...	318	C16H30O6	1000163-64-0	17
5		Ethane, 1,1'-oxybis[2-ethoxy-]	162	C8H18O3	000112-36-7	16



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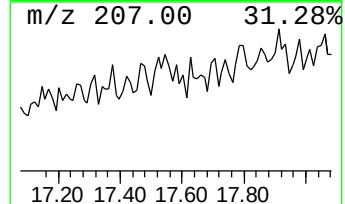
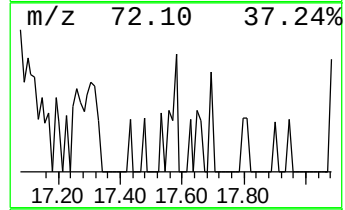
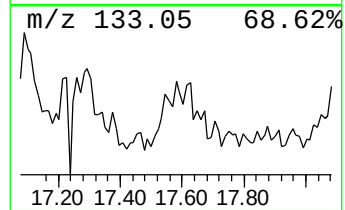
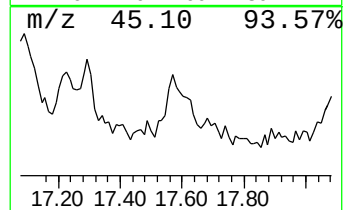
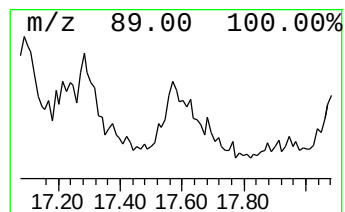
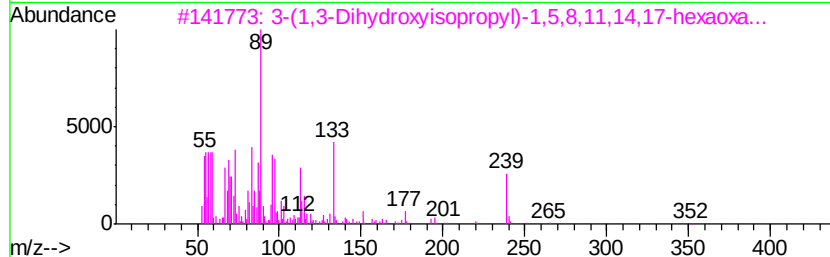
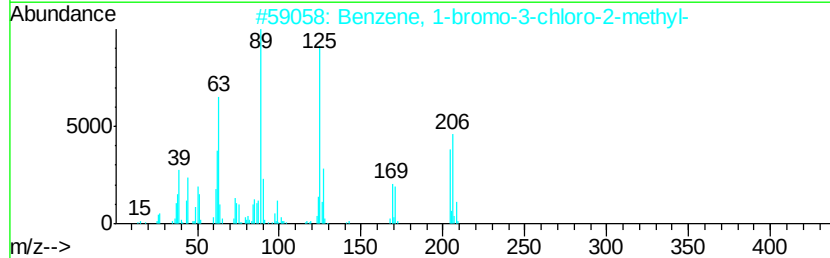
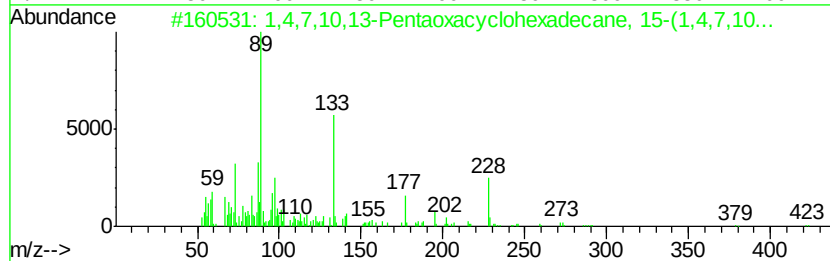
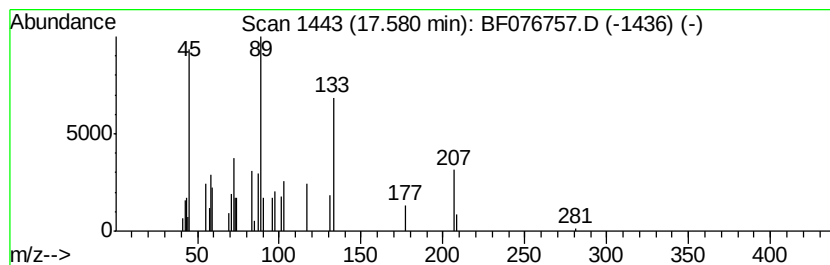
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Peak Number 7 1,4,7,10,13-Pentaoxacyclohe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.58	2.67 ng	57765	Perylene-d12	17.24
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1,4,7,10,13-Pentaoxacyclohexadec...	422 C20H38O9	109773-69-5	50
2	Benzene, 1-bromo-3-chloro-2-methyl-	204 C7H6BrCl	062356-27-8	43
3	3-(1,3-Dihydroxyisopropyl)-1,5,8...	352 C16H32O8	109773-65-1	42
4	15-Crown-5	220 C10H20O5	033100-27-5	39
5	Hexagol	282 C12H26O7	002615-15-8	39



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.23	24.2	ng	304595	1	6.71	252124	20.0
unknown6.41	6.41	89.0	ng	1121600	1	6.71	252124	20.0
Octaethylene glycol	16.97	2.0	ng	44355	6	17.24	432113	20.0
unknown17.08	17.08	2.3	ng	49235	6	17.24	432113	20.0
1,4,7,10,13-Penta...	17.58	2.7	ng	57765	6	17.24	432113	20.0