

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022417\
 Data File : BG025956.D
 Acq On : 25 Feb 2017 6:59
 Operator : SJ/MA
 Sample : I1985-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 INF-170223-01A

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:\HPCHEM1\BNA_G\METHODS\8270-BG021717.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	5.177	307	313	323	rBV	119602	177496	2.01%	0.515%
2	5.647	387	393	401	rBV	323147	503324	5.71%	1.460%
3	7.227	655	662	673	rBV2	253596	491367	5.57%	1.425%
4	7.609	720	727	734	rBV	588492	981189	11.13%	2.846%
5	8.079	799	807	814	rBV	267629	456919	5.18%	1.325%
6	8.402	854	862	876	rVB	944119	1664545	18.88%	4.827%
7	9.231	996	1003	1012	rBV	801980	1432943	16.26%	4.156%
8	10.453	1204	1211	1217	rBV	60638	100084	1.14%	0.290%
9	10.882	1275	1284	1291	rBV	425654	771875	8.76%	2.239%
10	13.314	1690	1698	1704	rBV	2709052	4203290	47.69%	12.190%
11	14.683	1923	1931	1938	rBV2	776678	1262583	14.32%	3.662%
12	16.158	2175	2182	2190	rBV	1252195	1899616	21.55%	5.509%
13	17.204	2356	2360	2368	rVB	119721	170739	1.94%	0.495%
14	17.409	2389	2395	2402	rBV2	1172181	1830051	20.76%	5.307%
15	18.291	2540	2545	2551	rBV	122232	187996	2.13%	0.545%
16	18.367	2552	2558	2570	rVB	6286439	8814332	100.00%	25.562%
17	18.561	2583	2591	2599	rVB7	83264	187516	2.13%	0.544%
18	19.554	2752	2760	2768	rBV2	94243	160919	1.83%	0.467%
19	20.006	2831	2837	2843	rBV	3624754	4793216	54.38%	13.901%
20	20.688	2949	2953	2959	rVB	83064	97312	1.10%	0.282%
21	21.299	3053	3057	3070	rBV6	60025	125340	1.42%	0.363%
22	21.657	3111	3118	3133	rBV	1280610	2109946	23.94%	6.119%
23	24.865	3654	3664	3675	rVB2	718889	2058969	23.36%	5.971%

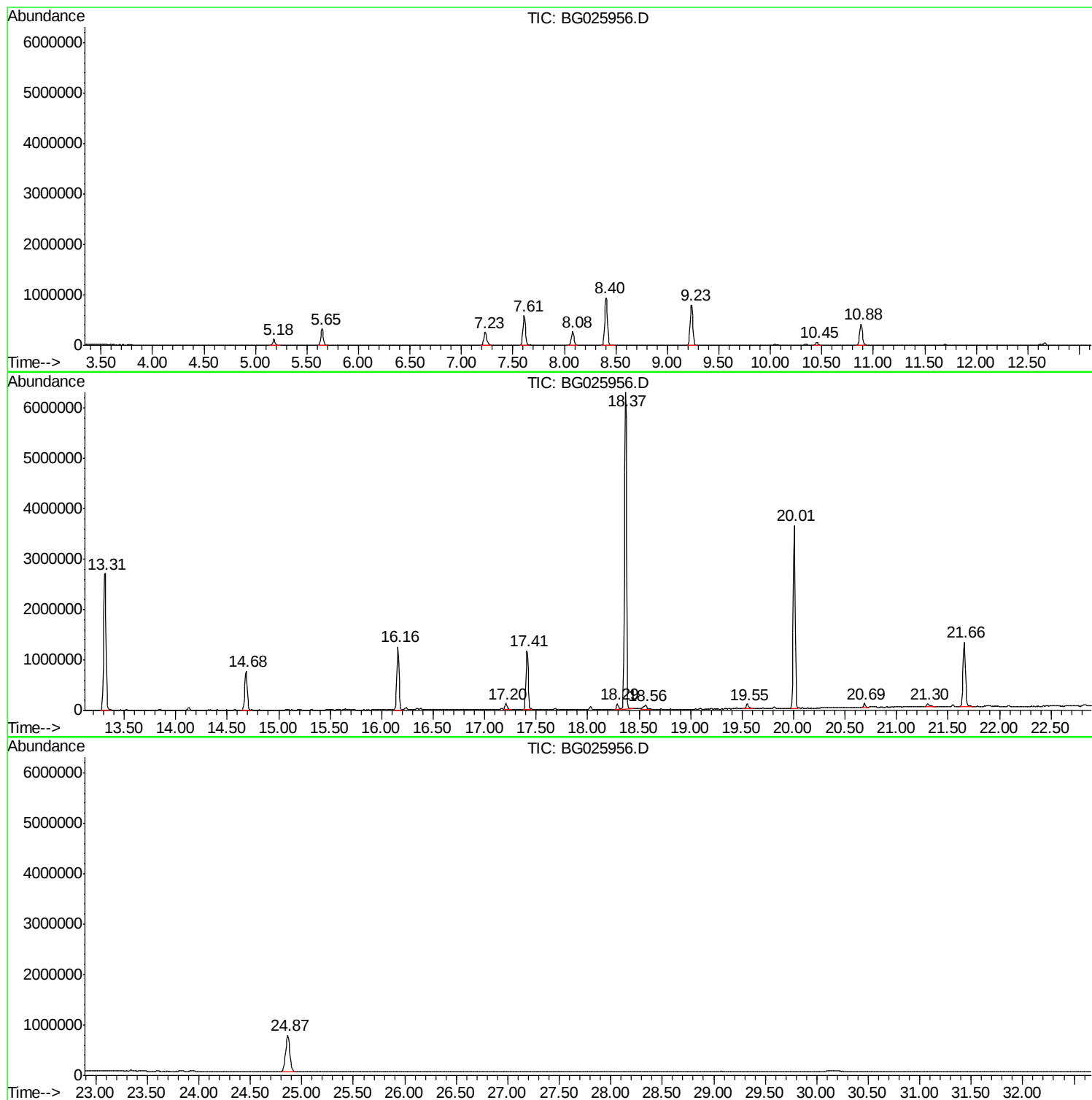
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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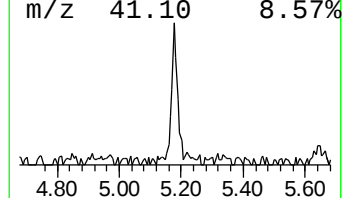
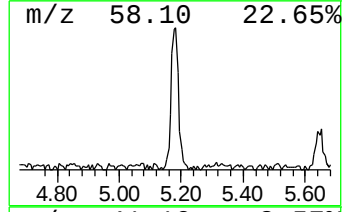
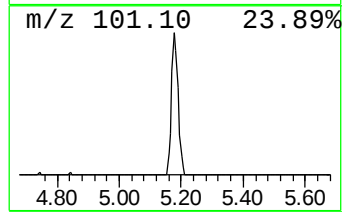
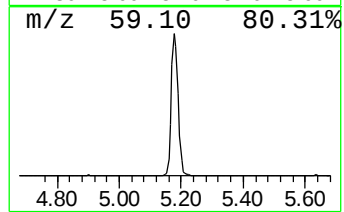
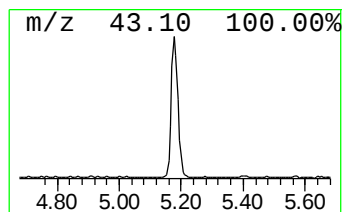
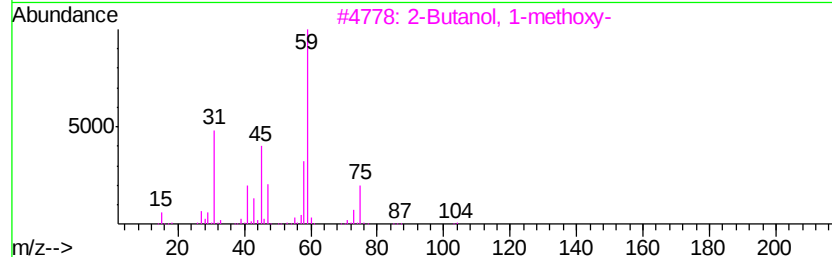
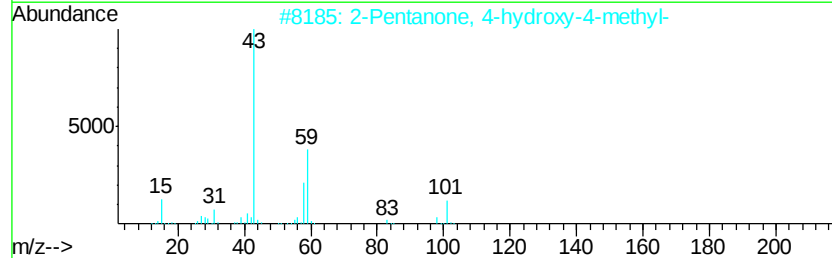
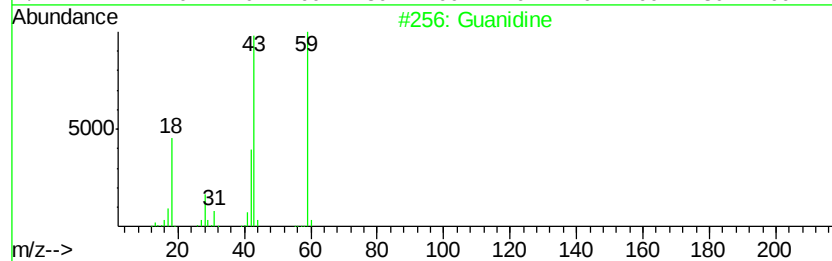
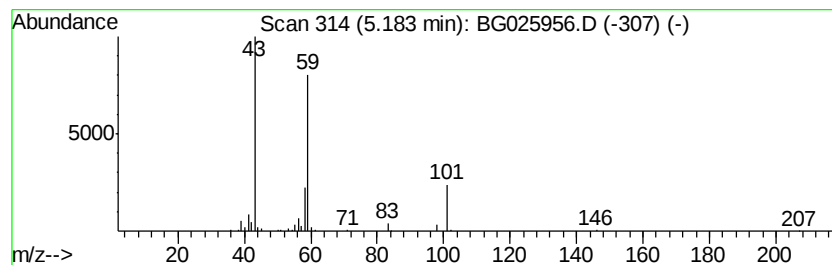
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Guanine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	7.77 ng	177496	1,4-Dichlorobenzene-d4	8.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Guanine	59	CH5N3	000113-00-8	50
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3		2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	33
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	28
5		Acetic acid, chloro-, 1,1-dimeth...	150	C6H11ClO2	000107-59-5	25



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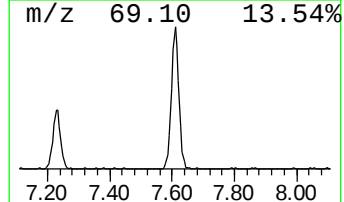
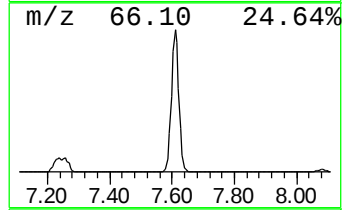
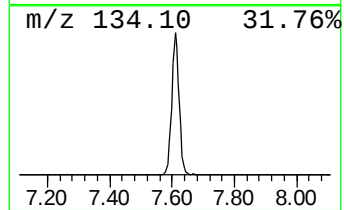
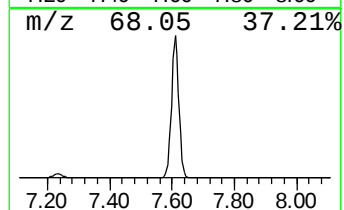
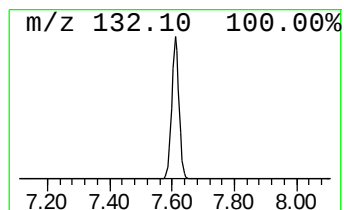
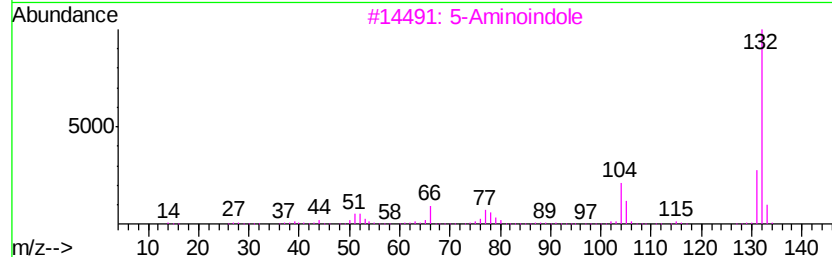
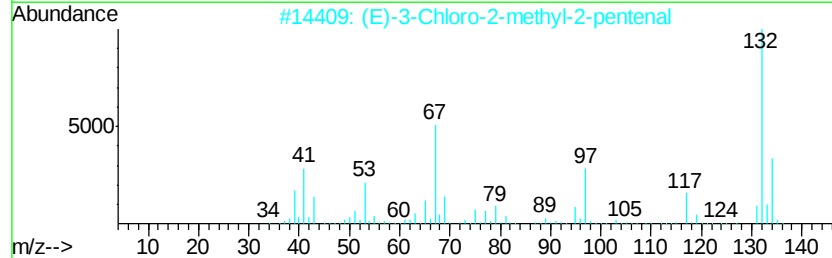
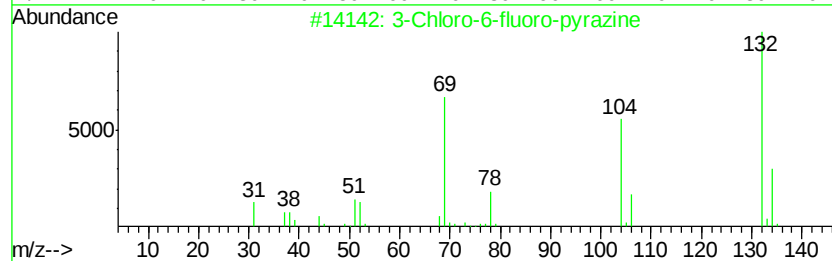
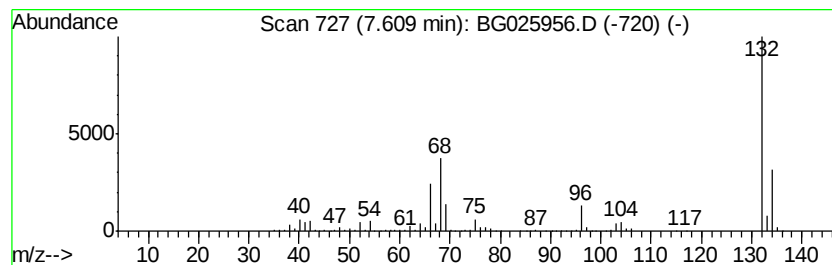
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.61 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	42.95 ng	981189	1,4-Dichlorobenzene-d4	8.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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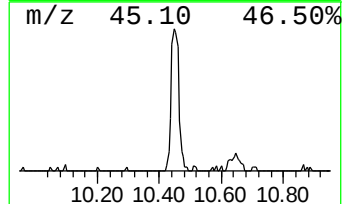
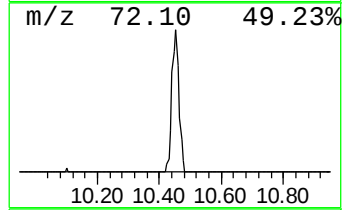
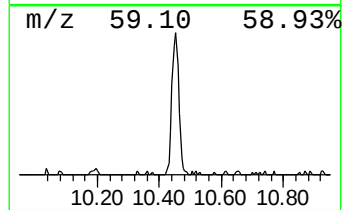
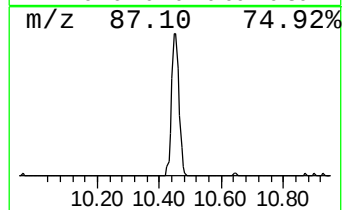
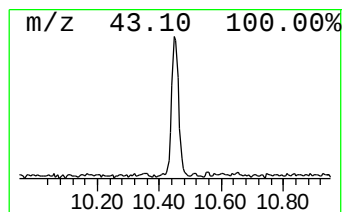
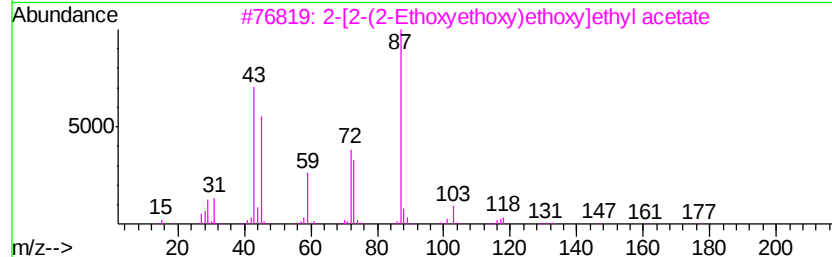
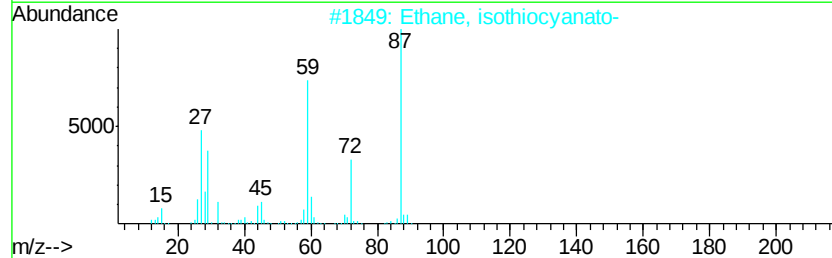
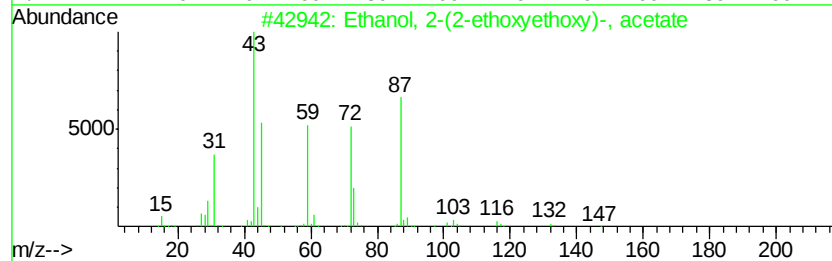
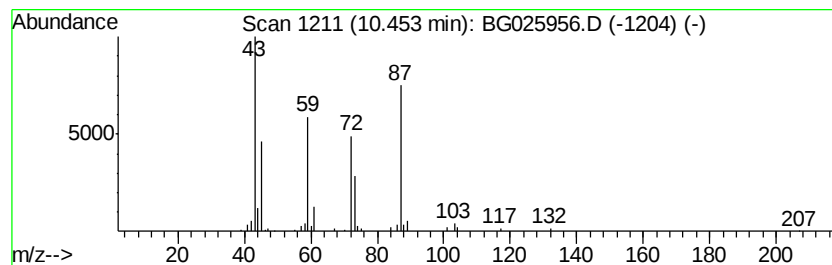
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	2.59 ng	100084	Naphthalene-d8	10.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(2-ethoxyethoxy)-, ac...	176	C8H16O4	000112-15-2	86
2		Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	52
3		2-[2-(2-Ethoxyethoxy)ethoxy]ethy...	220	C10H20O5	1000351-93-2	45
4		2-[2-[2-[2-[2-[2-[2-(2-Acetyl...	498	C22H42O12	1000351-90-5	43
5		Propane, 2,2-diethoxy-	132	C7H16O2	000126-84-1	43



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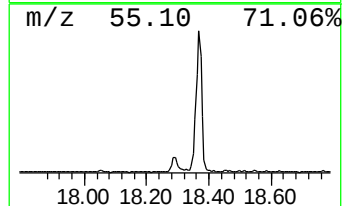
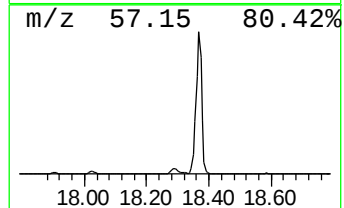
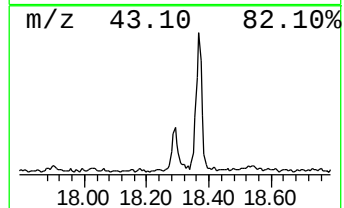
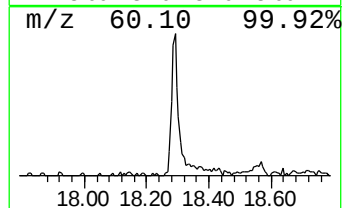
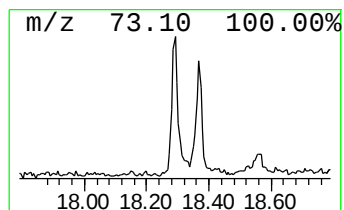
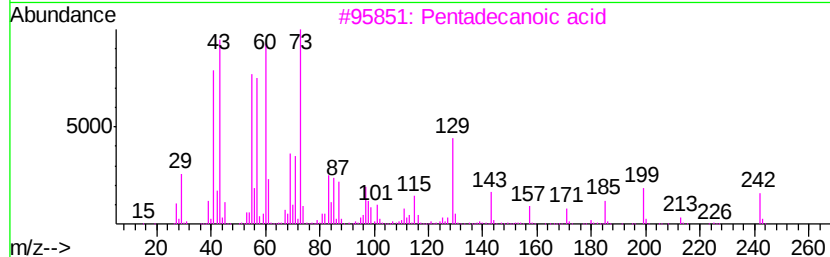
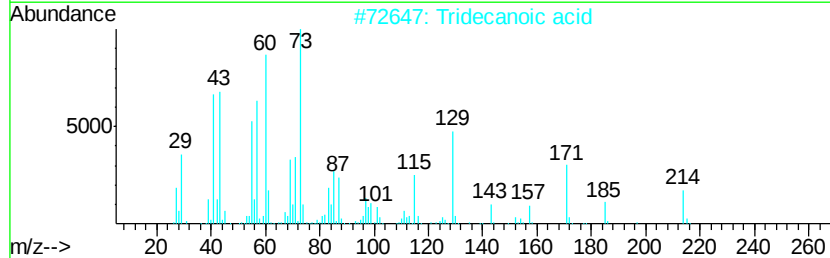
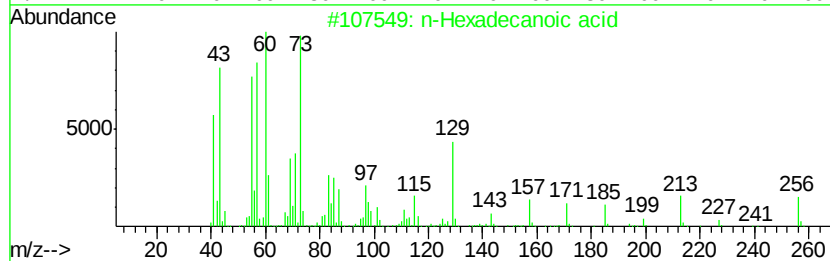
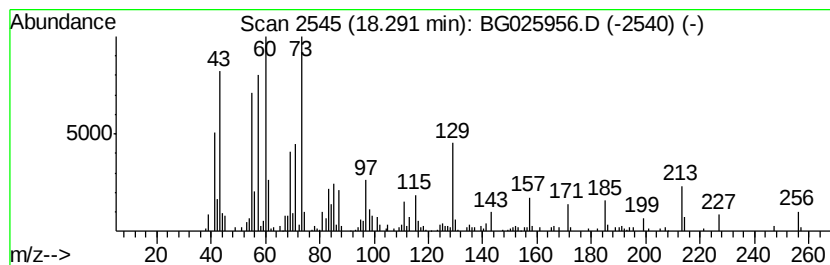
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.29	2.05 ng	187996	Phenanthrene-d10	17.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



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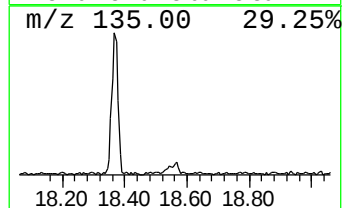
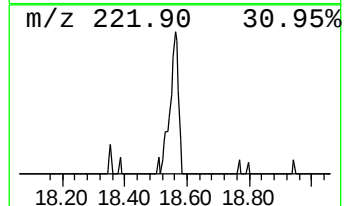
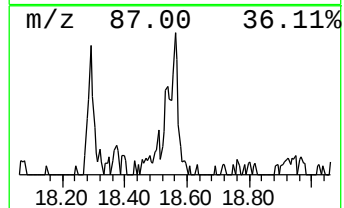
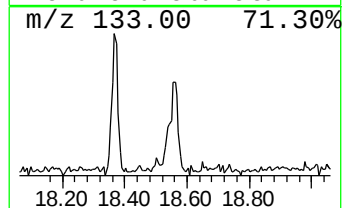
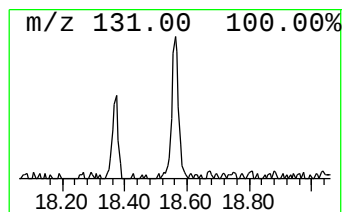
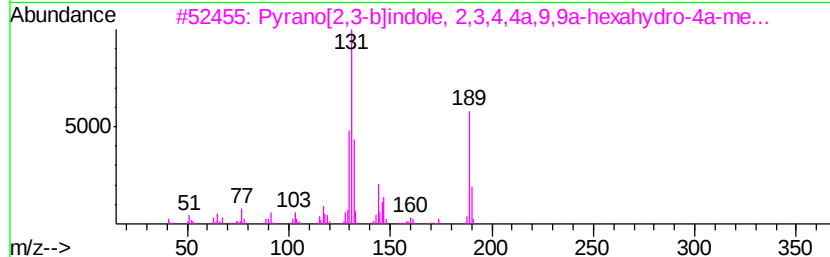
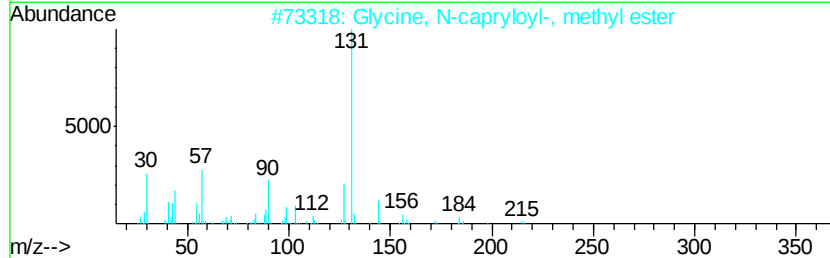
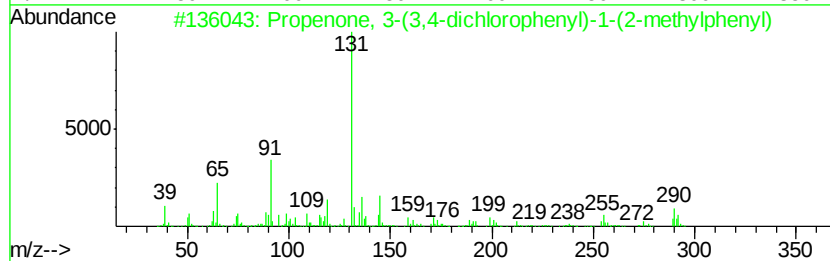
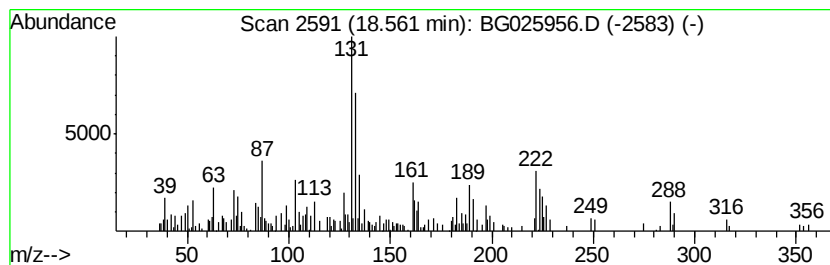
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown18.56 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.56	2.05 ng	187516	Phenanthrene-d10	17.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propenone, 3-(3,4-dichlorophenyl...	290	C16H12Cl2O	312700-11-1	25
2	Glycine, N-capryloyl-, methyl ester	215	C11H21NO3	1000299-72-3	25
3	Pyrano[2,3-b]indole, 2,3,4,4a,9,...	189	C12H15NO	054789-35-4	16
4	2-Propenamide, 3-phenyl-N-propyl-	189	C12H15NO	006329-15-3	16
5	4-Pyrimidinamine, 2,6-difluoro-	131	C4H3F2N3	000675-12-7	14



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Guanidine	5.18	7.8	ng	177496	1	8.08	456919	20.0
unknown7.61	7.61	43.0	ng	981189	1	8.08	456919	20.0
Ethanol, 2-(2-eth...	10.45	2.6	ng	100084	2	10.88	771875	20.0
n-Hexadecanoic acid	18.29	2.0	ng	187996	4	17.41	1830050	20.0
unknown18.56	18.56	2.0	ng	187516	4	17.41	1830050	20.0