

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032717\
 Data File : BF093963.D
 Acq On : 28 Mar 2017 1:04
 Operator : SJ/MA
 Sample : I2409-10
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PZ-6

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-BF032217.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	4.075	368	372	378	rBV	176007	205734	3.95%	0.569%
2	4.463	434	438	442	rBV	2133548	2181988	41.93%	6.030%
3	5.528	614	619	622	rBV	1566376	1490420	28.64%	4.119%
4	5.681	639	645	648	rBV	3450600	3777107	72.58%	10.438%
5	5.934	684	688	692	rBV	975480	956355	18.38%	2.643%
6	6.116	714	719	723	rVB	3080997	3230577	62.08%	8.928%
7	6.587	793	799	802	rBV	2396579	2875075	55.25%	7.945%
8	6.898	845	852	855	rBV2	73296	105332	2.02%	0.291%
9	7.140	890	893	903	rVB	38204	56027	1.08%	0.155%
10	7.357	918	930	937	rBV5	59460	166654	3.20%	0.461%
11	7.439	939	944	948	rBV	1344498	1338445	25.72%	3.699%
12	7.928	1021	1027	1030	rBV3	60814	87200	1.68%	0.241%
13	8.039	1041	1046	1051	rVB6	36129	66266	1.27%	0.183%
14	8.351	1094	1099	1104	rBV4	51349	83095	1.60%	0.230%
15	8.522	1122	1128	1132	rVB5	61763	126320	2.43%	0.349%
16	8.628	1139	1146	1151	rBV9	42375	108904	2.09%	0.301%
17	8.681	1152	1155	1157	rVV2	51450	59813	1.15%	0.165%
18	8.769	1161	1170	1173	rBV	4464472	5204040	100.00%	14.382%
19	8.916	1183	1195	1198	rBV8	52825	144407	2.77%	0.399%
20	9.086	1221	1224	1227	rBV	76937	90827	1.75%	0.251%
21	9.169	1234	1238	1244	rVB5	79882	113189	2.18%	0.313%
22	9.222	1244	1247	1249	rBV4	46524	57330	1.10%	0.158%
23	9.386	1270	1275	1277	rBV4	63086	104571	2.01%	0.289%
24	9.510	1293	1296	1301	rBV5	32706	61001	1.17%	0.169%
25	9.586	1304	1309	1313	rVB2	1439066	1487224	28.58%	4.110%
26	10.051	1384	1388	1391	rVB5	67879	91266	1.75%	0.252%
27	10.133	1399	1402	1406	rVB	86442	99364	1.91%	0.275%
28	10.298	1427	1430	1435	rBV2	66871	91425	1.76%	0.253%
29	10.345	1435	1438	1443	rVV4	33041	54899	1.05%	0.152%
30	10.563	1465	1475	1478	rBV	2560897	3121806	59.99%	8.627%
31	11.257	1589	1593	1597	rVB4	42205	54396	1.05%	0.150%
32	11.410	1615	1619	1623	rVB	1424837	1392336	26.75%	3.848%
33	13.398	1950	1957	1960	rBV	3686502	4639868	89.16%	12.823%
34	14.127	2077	2081	2085	rVB	219335	215465	4.14%	0.595%

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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

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35	14.663	2167	2172	2176	rBV	1223854	1273580	24.47%	3.520%
36	16.298	2445	2450	2459	rVB	797645	972761	18.69%	2.688%

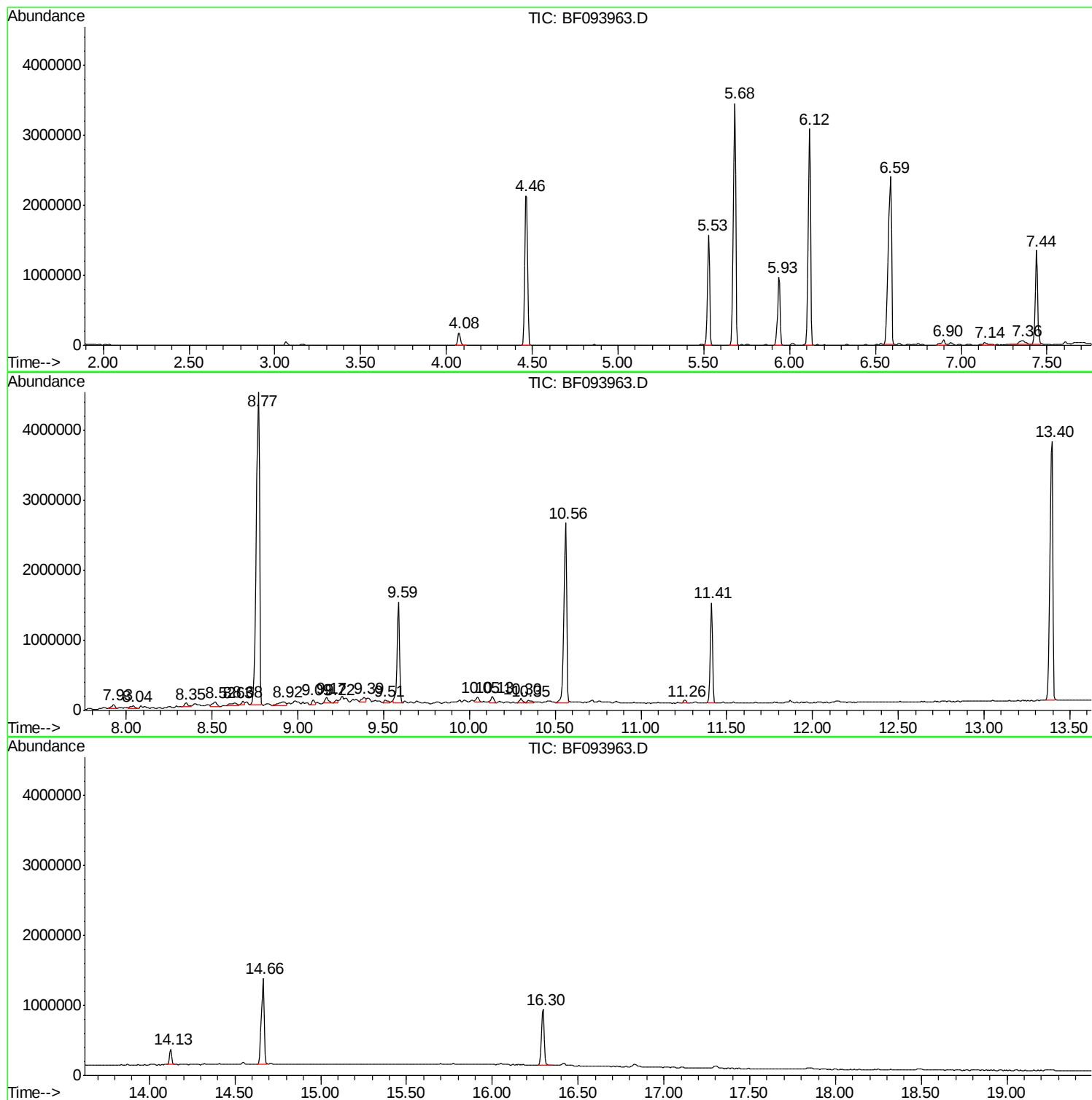
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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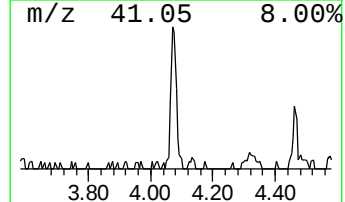
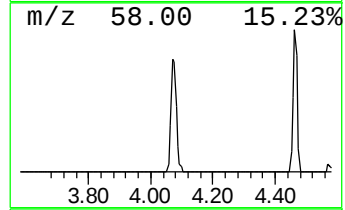
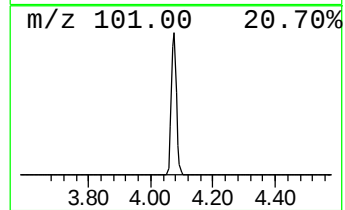
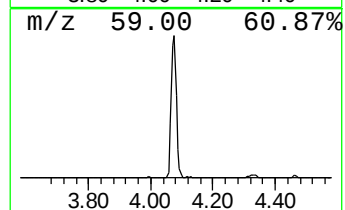
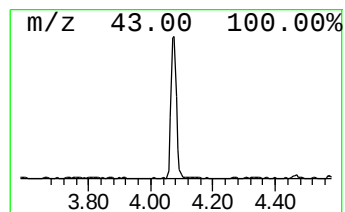
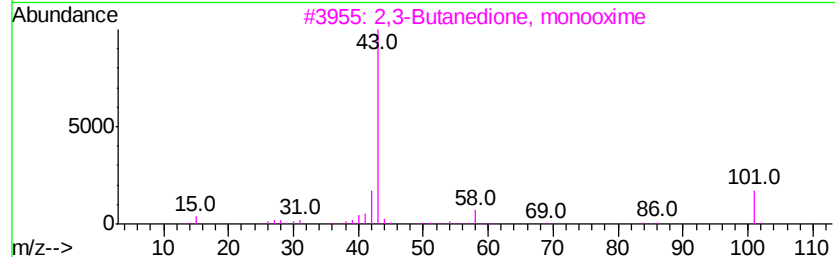
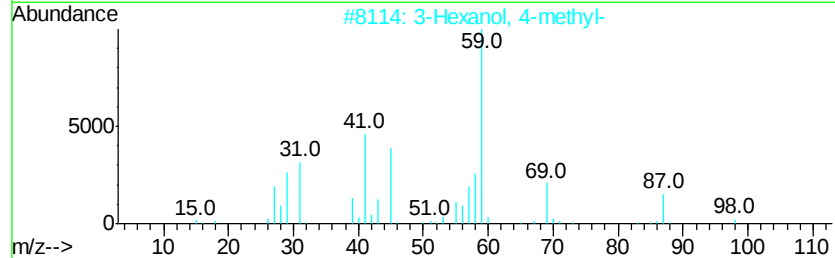
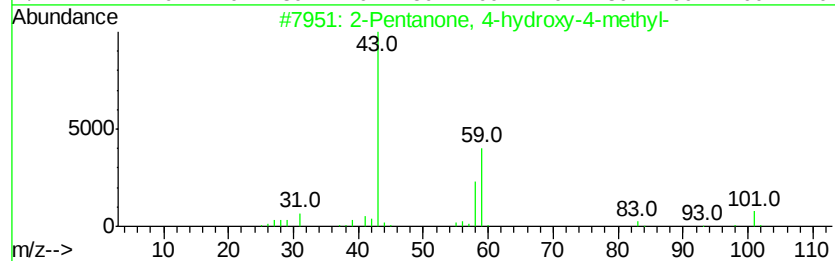
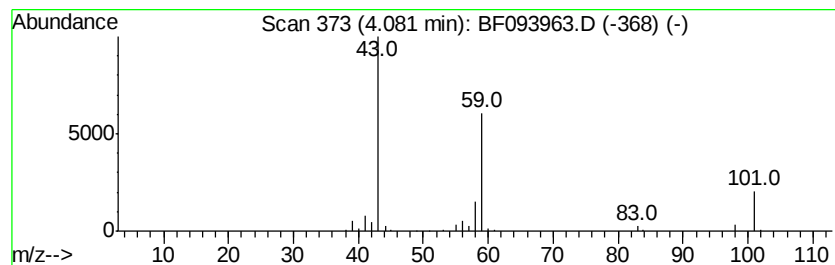
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.08	4.30 ng	205734	1,4-Dichlorobenzene-d4	5.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17



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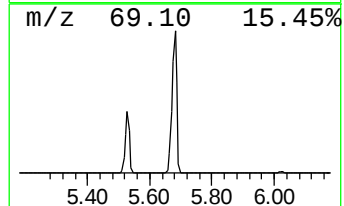
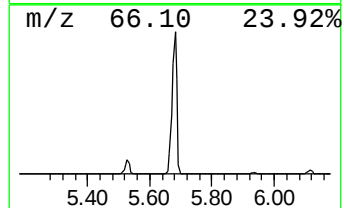
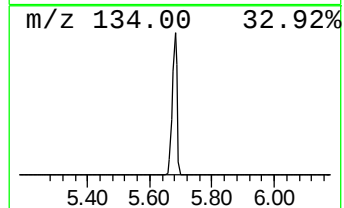
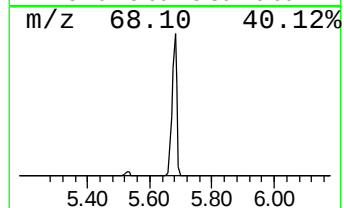
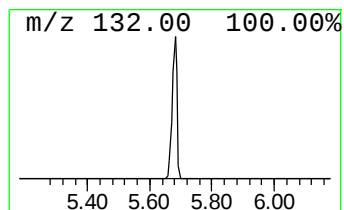
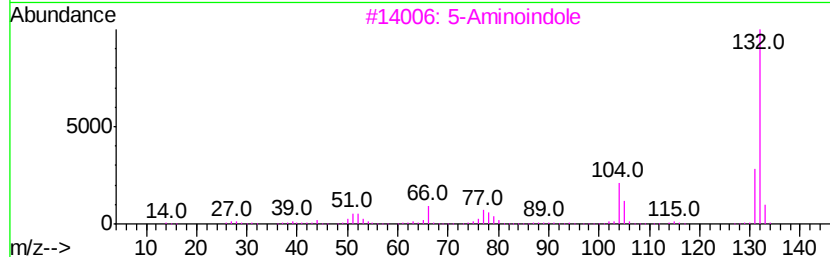
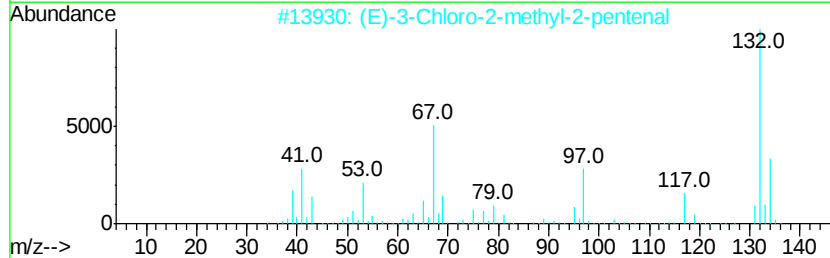
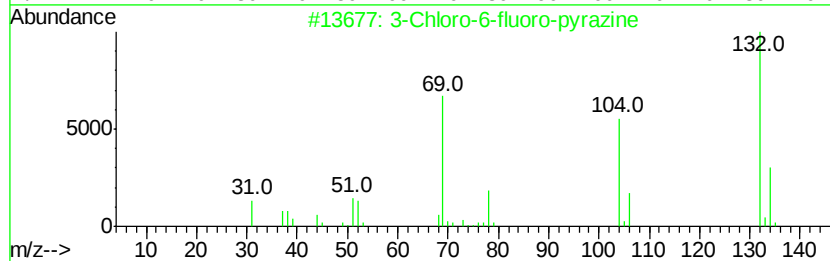
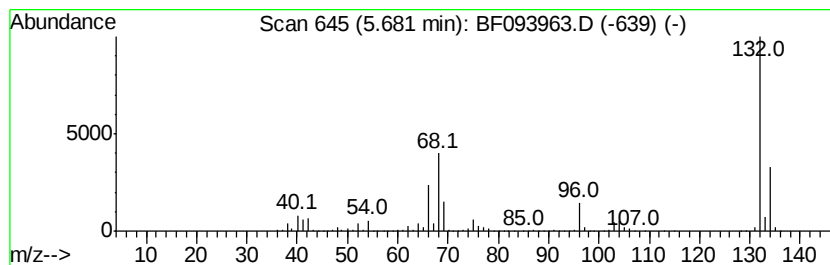
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.68	78.99 ng	3777110	1,4-Dichlorobenzene-d4	5.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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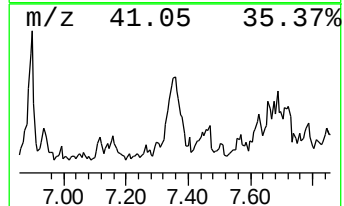
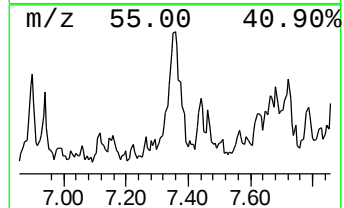
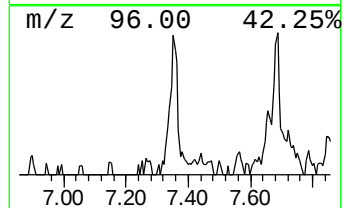
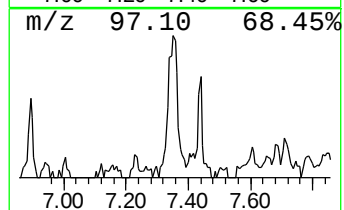
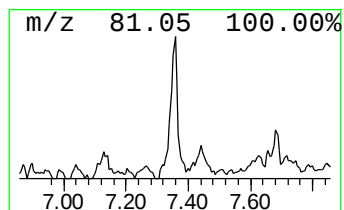
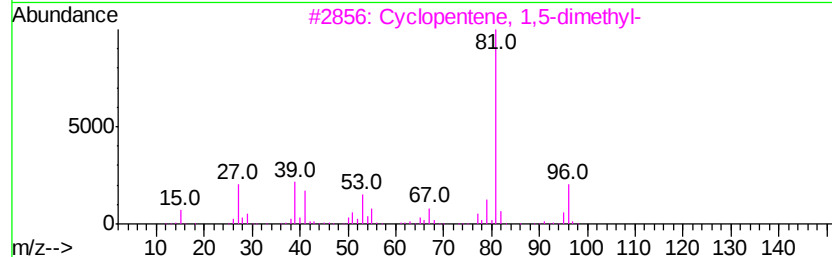
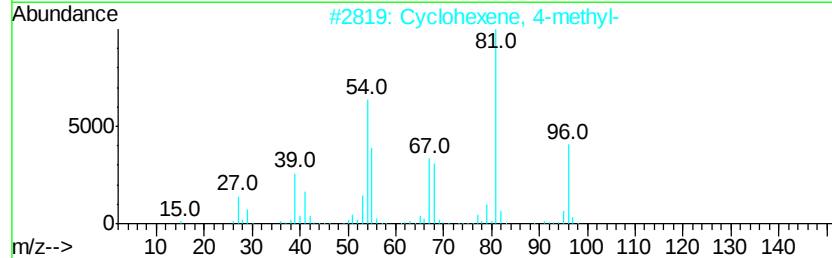
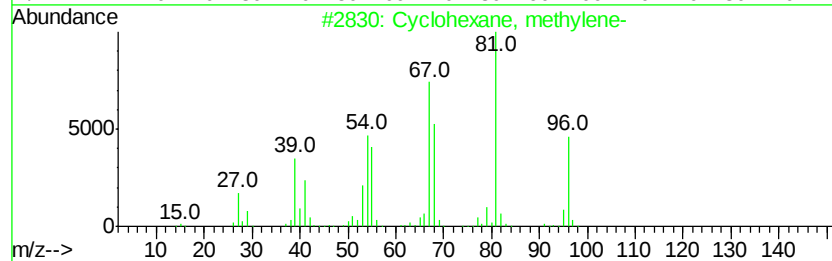
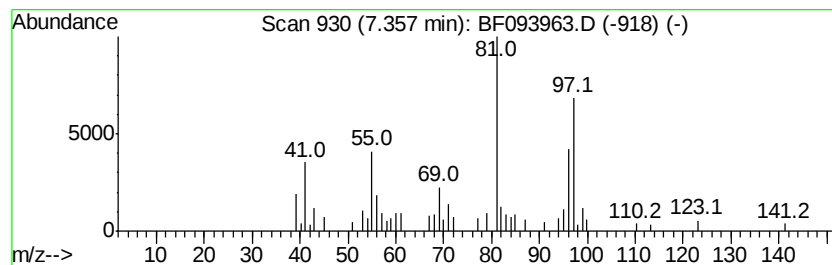
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.36 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	2.49 ng	166654	Naphthalene-d8	7.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, methylene-	96	C7H12	001192-37-6	47
2		Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	47
3		Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	47
4		Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	47
5		1-Octadecyne	250	C18H34	000629-89-0	40



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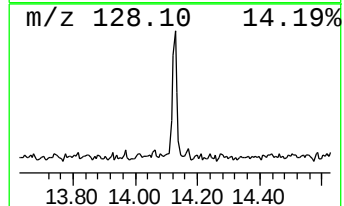
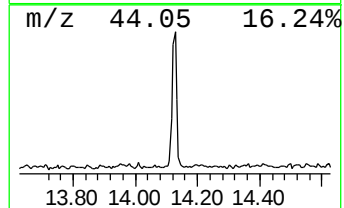
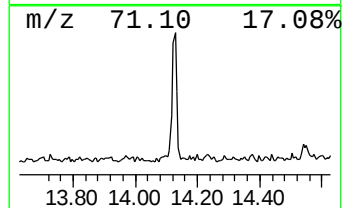
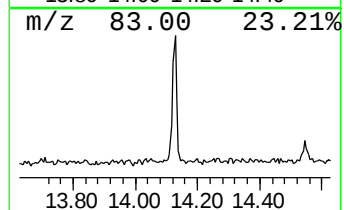
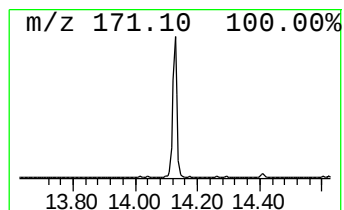
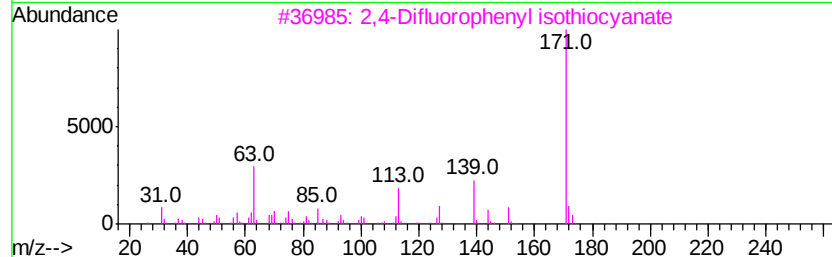
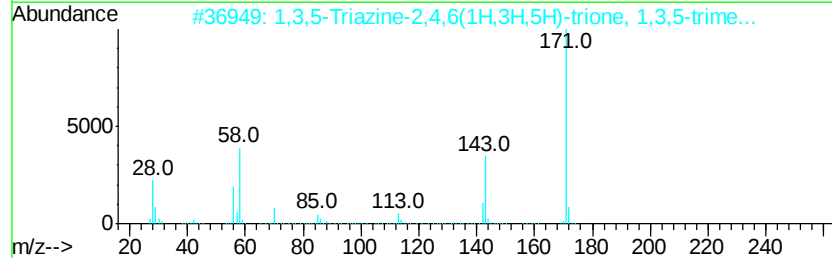
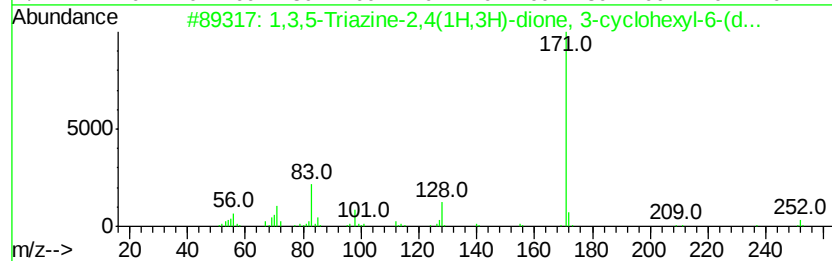
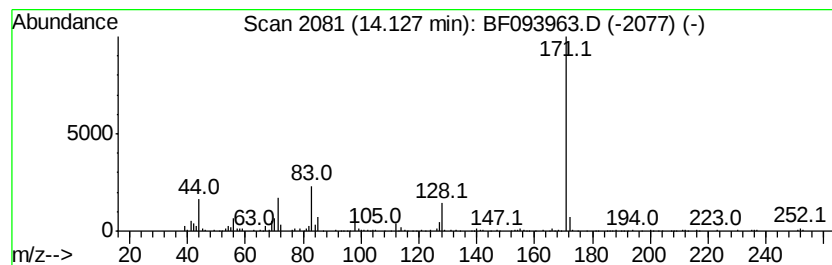
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	3.38 ng	215465	Chrysene-d12	14.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	90
2		1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	171	C6H9N3O3	000827-16-7	47
3		2,4-Difluorophenyl isothiocyanate	171	C7H3F2NS	141106-52-7	40
4		Thiazolo[5,4-d]pyrimidine, 5-chl...	171	C5H2ClN3S	013316-08-0	38
5		4-Pyridinol, 2-phenyl-	171	C11H9NO	1000253-54-5	28



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.08	4.3	ng	205734	1	5.93	956355	20.0
unknown5.68	5.68	79.0	ng	3777110	1	5.93	956355	20.0
unknown7.36	7.36	2.5	ng	166654	2	7.44	1338450	20.0
1,3,5-Triazine-2,...	14.13	3.4	ng	215465	5	14.66	1273580	20.0