

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
 Data File : BF092457.D
 Acq On : 25 Jan 2017 4:14
 Operator : UM/SJ
 Sample : I1397-03
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-11

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-BF012417.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	5.138	265	267	270	rBV	483870	612951	13.68%	1.796%
2	5.550	301	303	306	rBV	1849592	2119066	47.29%	6.210%
3	6.579	390	393	395	rBV	1712171	1423805	31.78%	4.173%
4	6.727	403	406	409	rBV	3381278	3500303	78.12%	10.258%
5	6.967	425	427	429	rBV	1124160	951950	21.25%	2.790%
6	7.127	438	441	443	rVB	3754874	3615062	80.68%	10.594%
7	7.539	473	477	479	rBV	2385928	3266822	72.91%	9.574%
8	8.259	538	540	542	rBV	1467675	1244068	27.77%	3.646%
9	9.345	632	635	638	rBV	4595275	4480611	100.00%	13.131%
10	9.733	667	669	671	rVB	177137	203476	4.54%	0.596%
11	10.030	692	695	697	rBV	1013916	1281203	28.59%	3.755%
12	10.316	716	720	722	rBV	74061	86585	1.93%	0.254%
13	10.442	729	731	734	rVB2	34407	55155	1.23%	0.162%
14	10.545	737	740	741	rBV	50913	57753	1.29%	0.169%
15	10.670	748	751	753	rBV	755724	713716	15.93%	2.092%
16	10.819	761	764	766	rBV	2161948	2644605	59.02%	7.750%
17	10.865	766	768	770	rVV	721959	652811	14.57%	1.913%
18	10.933	772	774	777	rVB	57573	68812	1.54%	0.202%
19	11.379	811	813	819	rVB3	42689	73156	1.63%	0.214%
20	11.516	822	825	827	rBV	1112352	1156011	25.80%	3.388%
21	12.042	869	871	876	rBV3	193426	245002	5.47%	0.718%
22	12.831	938	940	943	rBV	103093	105880	2.36%	0.310%
23	13.105	961	964	967	rBV	3413234	3309288	73.86%	9.698%
24	13.996	1040	1042	1048	rVB	183371	199075	4.44%	0.583%
25	14.145	1053	1055	1058	rVV	651531	827674	18.47%	2.426%
26	15.288	1153	1155	1159	rVB2	31621	50033	1.12%	0.147%
27	15.631	1182	1185	1187	rBV	645536	865630	19.32%	2.537%
28	15.677	1187	1189	1192	rVB	44518	63305	1.41%	0.186%
29	16.122	1225	1228	1230	rBV	37879	63183	1.41%	0.185%
30	16.648	1271	1274	1281	rVB2	37749	86014	1.92%	0.252%
31	17.254	1324	1327	1331	rBV2	25455	52780	1.18%	0.155%
32	17.974	1387	1390	1394	rVB2	20045	47306	1.06%	0.139%

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ALS Vial : 38 Sample Multiplier: 1

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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_F\METHODS\8270-BF012417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

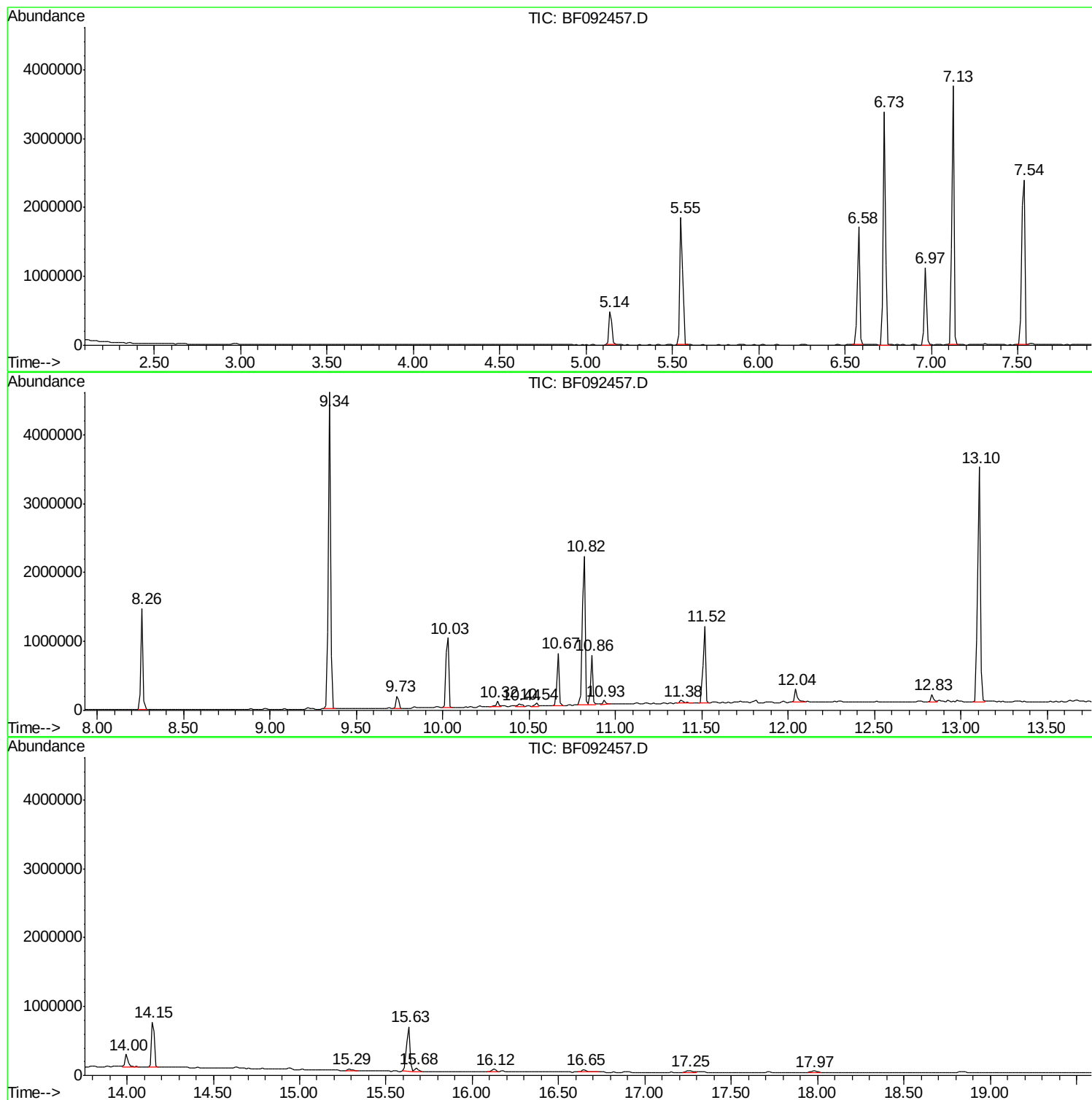
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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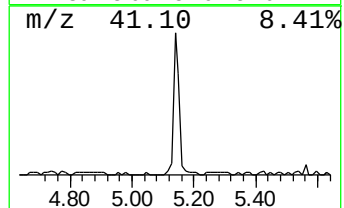
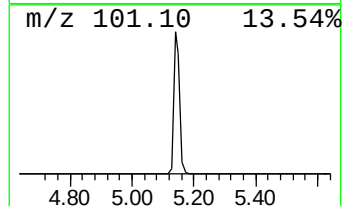
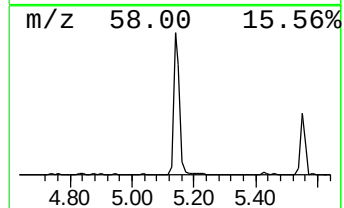
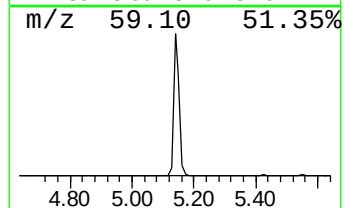
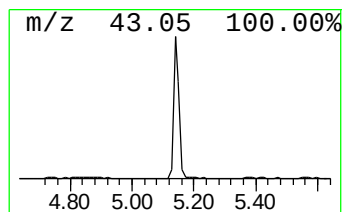
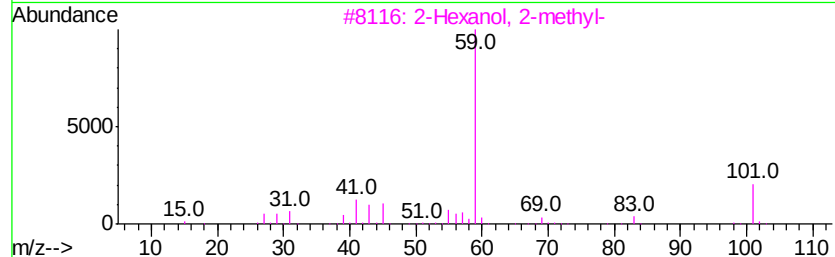
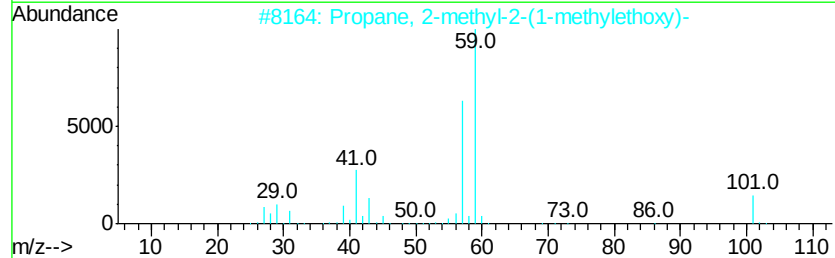
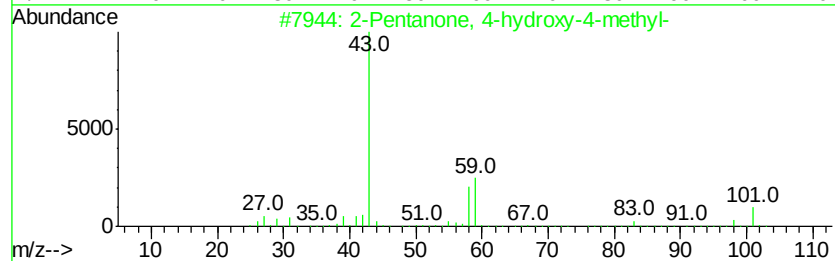
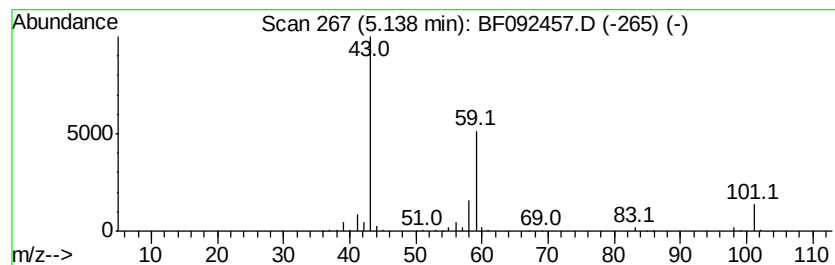
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	12.88 ng	612951	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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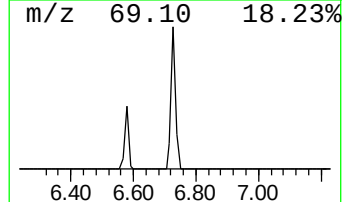
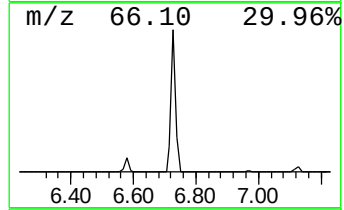
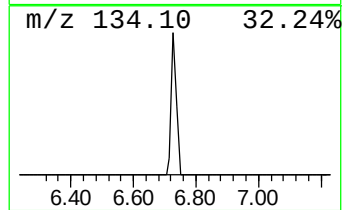
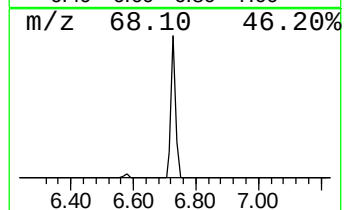
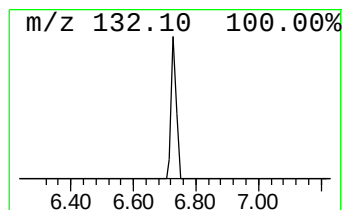
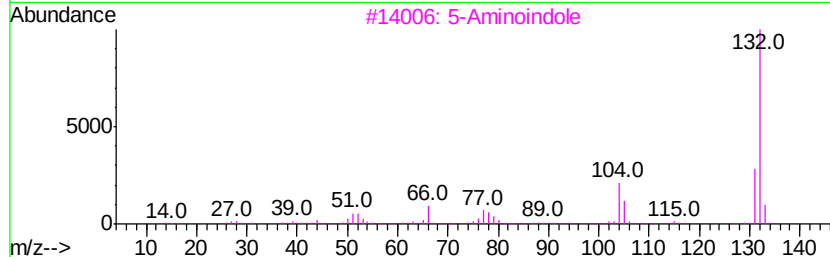
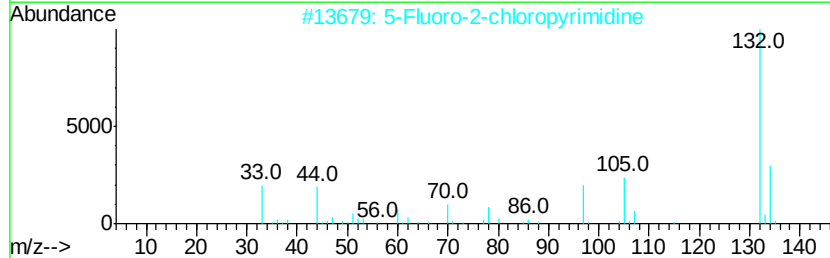
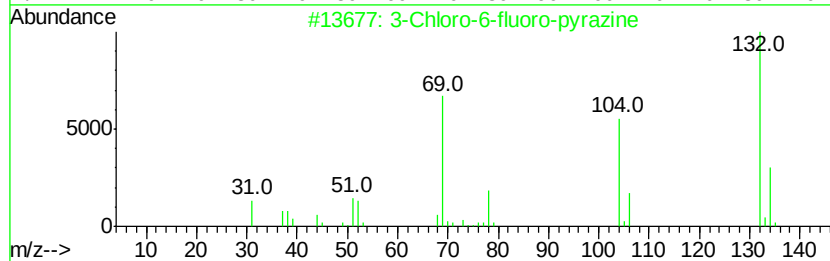
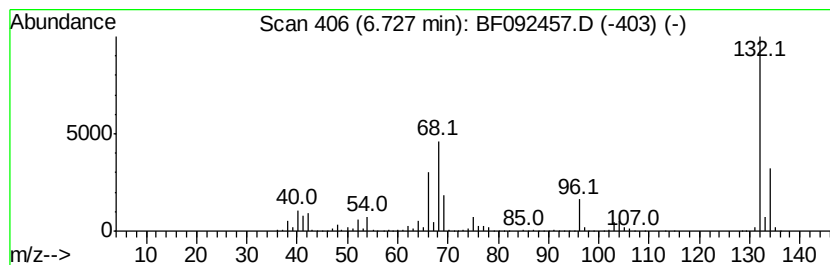
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.73 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	73.54 ng	3500300	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
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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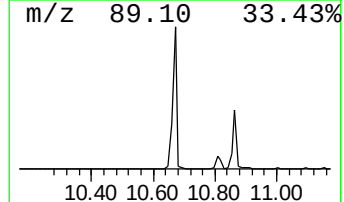
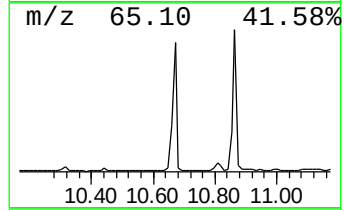
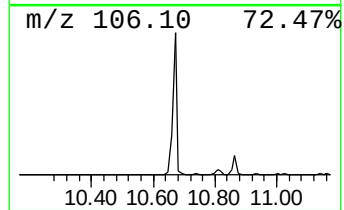
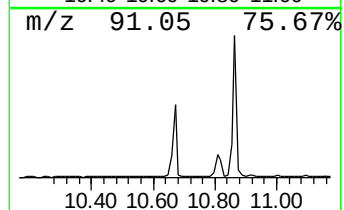
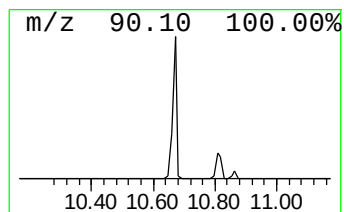
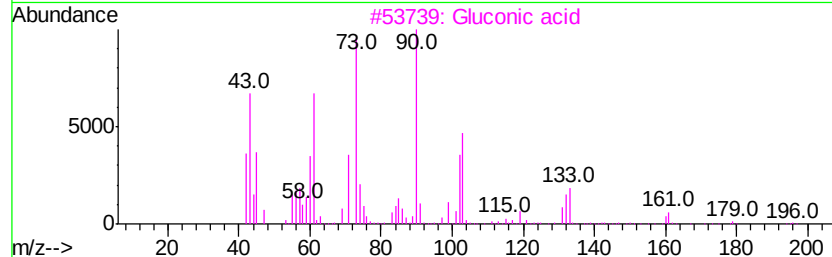
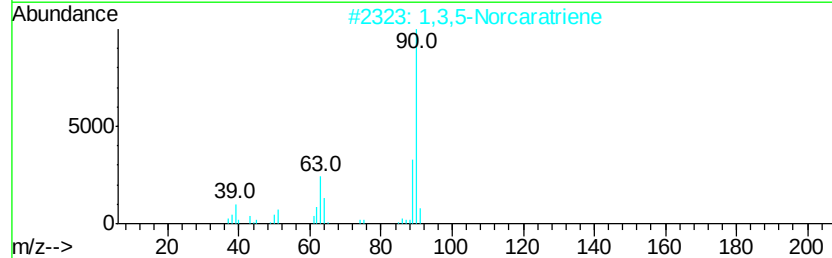
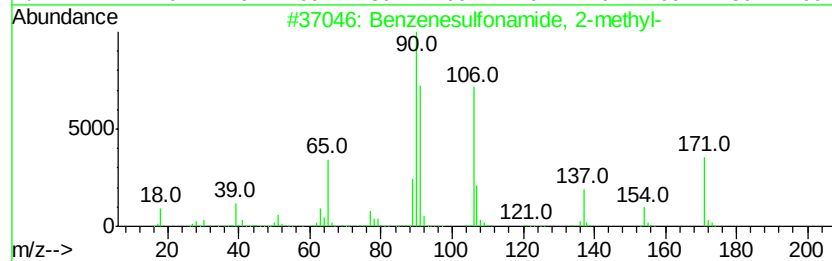
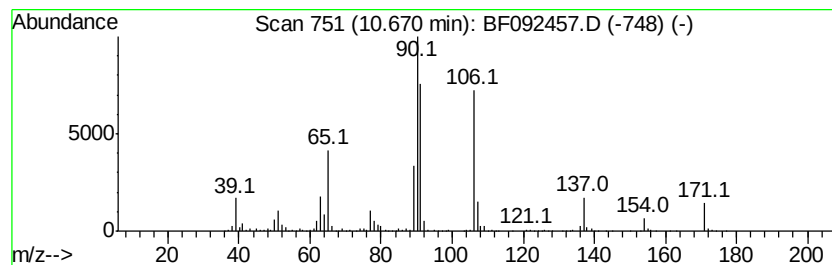
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzenesulfonamide, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.67	11.14 ng	713716	Acenaphthene-d10		10.03
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	96
2	1,3,5-Norcaratriene	90	C7H6	004646-69-9	46
3	Gluconic acid	196	C6H12O7	000526-95-4	38
4	Benzene, 1-methyl-3-nitro-	137	C7H7NO2	000099-08-1	30
5	Benzenemethanesulfonamide	171	C7H9NO2S	004563-33-1	30



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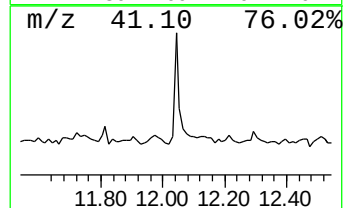
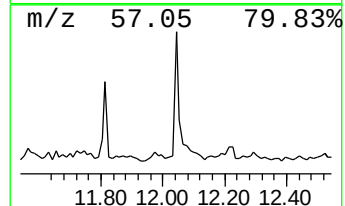
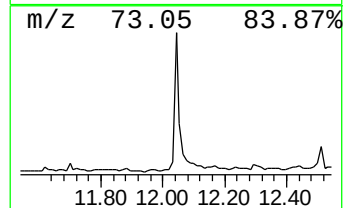
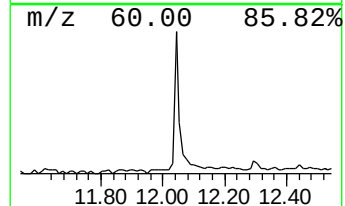
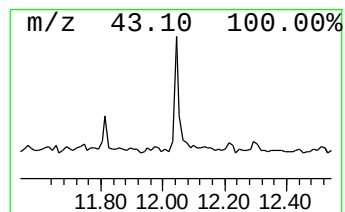
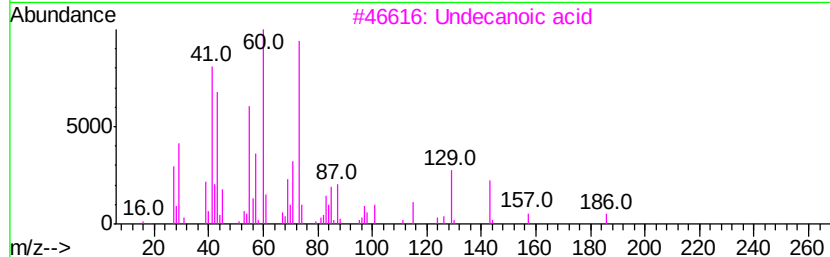
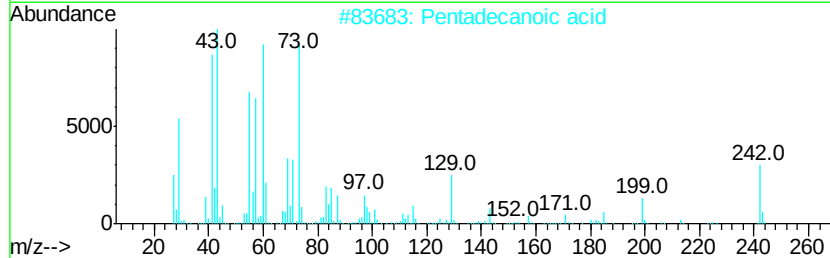
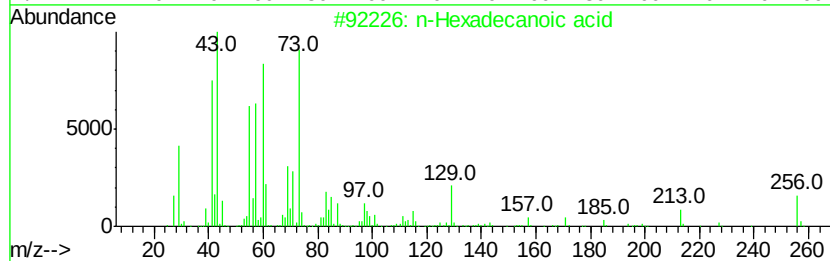
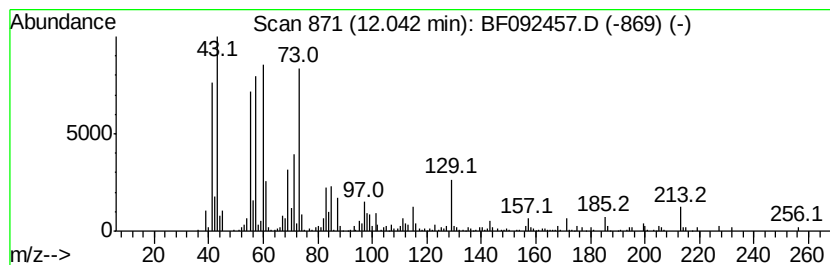
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.04	4.24 ng	245002	Phenanthrene-d10	11.52	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Undecanoic acid	186	C11H22O2	000112-37-8	86
4	Dodecanoic acid	200	C12H24O2	000143-07-7	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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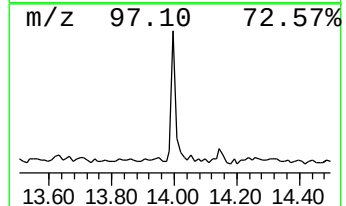
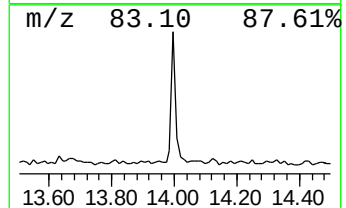
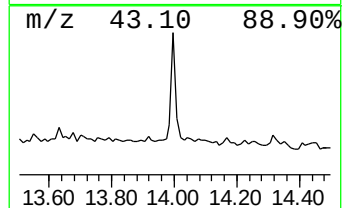
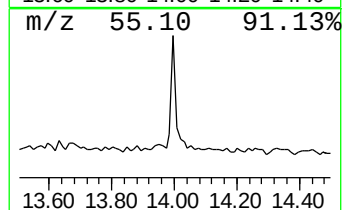
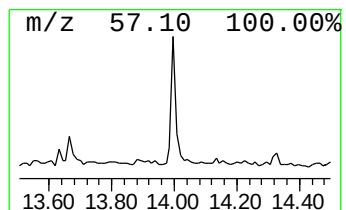
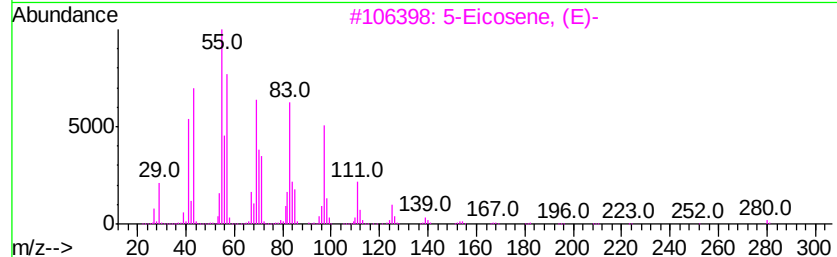
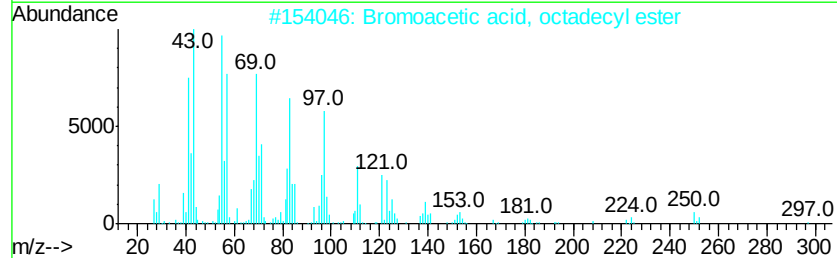
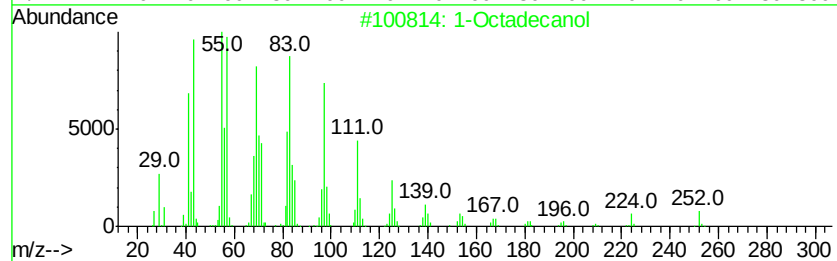
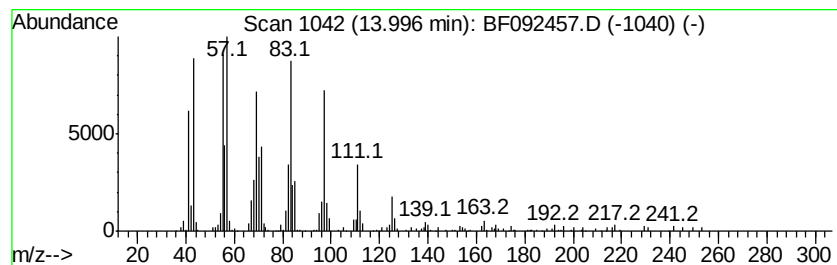
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Octadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	4.81 ng	199075	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	94
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	12.9	ng	612951	1	6.97	951950	20.0
unknown6.73	6.73	73.5	ng	3500300	1	6.97	951950	20.0
Benzenesulfonamid...	10.67	11.1	ng	713716	3	10.03	1281200	20.0
n-Hexadecanoic acid	12.04	4.2	ng	245002	4	11.52	1156010	20.0
1-Octadecanol	14.00	4.8	ng	199075	5	14.15	827674	20.0