

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
 Data File : BF092775.D
 Acq On : 3 Feb 2017 12:58
 Operator : SJ/MA
 Sample : I1378-06
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RVE-7

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-BF013017.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	5.116	263	265	271	rBV	1045725	1538271	40.04%	4.550%
2	5.550	300	303	305	rBV	2335672	3348440	87.15%	9.903%
3	6.579	389	393	395	rBV	2364418	3581867	93.23%	10.594%
4	6.704	401	404	406	rBV	3508999	3367004	87.63%	9.958%
5	6.933	422	424	426	rBV	1009018	860265	22.39%	2.544%
6	7.093	435	438	440	rBV	2472580	2711975	70.59%	8.021%
7	7.493	470	473	476	rBV	1579791	2109950	54.92%	6.240%
8	8.225	534	537	539	rBV	748559	1069968	27.85%	3.164%
9	9.299	628	631	633	rBV	3791953	3842123	100.00%	11.363%
10	9.688	663	665	669	rBV	400066	366436	9.54%	1.084%
11	9.973	688	690	692	rBV	1396062	1204414	31.35%	3.562%
12	10.396	724	727	729	rBV	67223	94191	2.45%	0.279%
13	10.625	744	747	750	rBV	30164	51624	1.34%	0.153%
14	10.762	756	759	762	rBV	1613503	1827180	47.56%	5.404%
15	10.876	764	769	772	rBV	146795	235812	6.14%	0.697%
16	11.071	784	786	790	rBV4	16565	45726	1.19%	0.135%
17	11.322	806	808	809	rBV	121923	108970	2.84%	0.322%
18	11.356	809	811	813	rVB2	30629	45664	1.19%	0.135%
19	11.459	818	820	826	rBV	1344323	1276151	33.21%	3.774%
20	11.745	843	845	848	rBV	77939	77903	2.03%	0.230%
21	12.156	879	881	884	rVB	35866	41264	1.07%	0.122%
22	12.671	924	926	928	rVB	68276	61466	1.60%	0.182%
23	12.865	940	943	944	rBV	125669	127803	3.33%	0.378%
24	12.899	944	946	948	rVV	53332	59185	1.54%	0.175%
25	12.934	948	949	953	rVB3	29415	42295	1.10%	0.125%
26	13.048	956	959	961	rBV	3184297	3270318	85.12%	9.672%
27	13.562	1002	1004	1006	rBV	80627	82035	2.14%	0.243%
28	13.951	1035	1038	1045	rBV2	83831	162323	4.22%	0.480%
29	14.099	1048	1051	1053	rBV	981747	1053835	27.43%	3.117%
30	14.591	1092	1094	1100	rVB4	19142	42714	1.11%	0.126%
31	15.014	1128	1131	1133	rVB2	32755	38564	1.00%	0.114%
32	15.128	1139	1141	1145	rVB	24772	46192	1.20%	0.137%
33	15.254	1149	1152	1158	rBV6	10714	40636	1.06%	0.120%
34	15.562	1176	1179	1185	rBV	556732	866508	22.55%	2.563%

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BNA_F
ClientSampleId :
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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

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35	16.008	1215	1218	1222	rVB	33454	58901	1.53%	0.174%
36	17.174	1317	1320	1323	rVB4	28881	53762	1.40%	0.159%

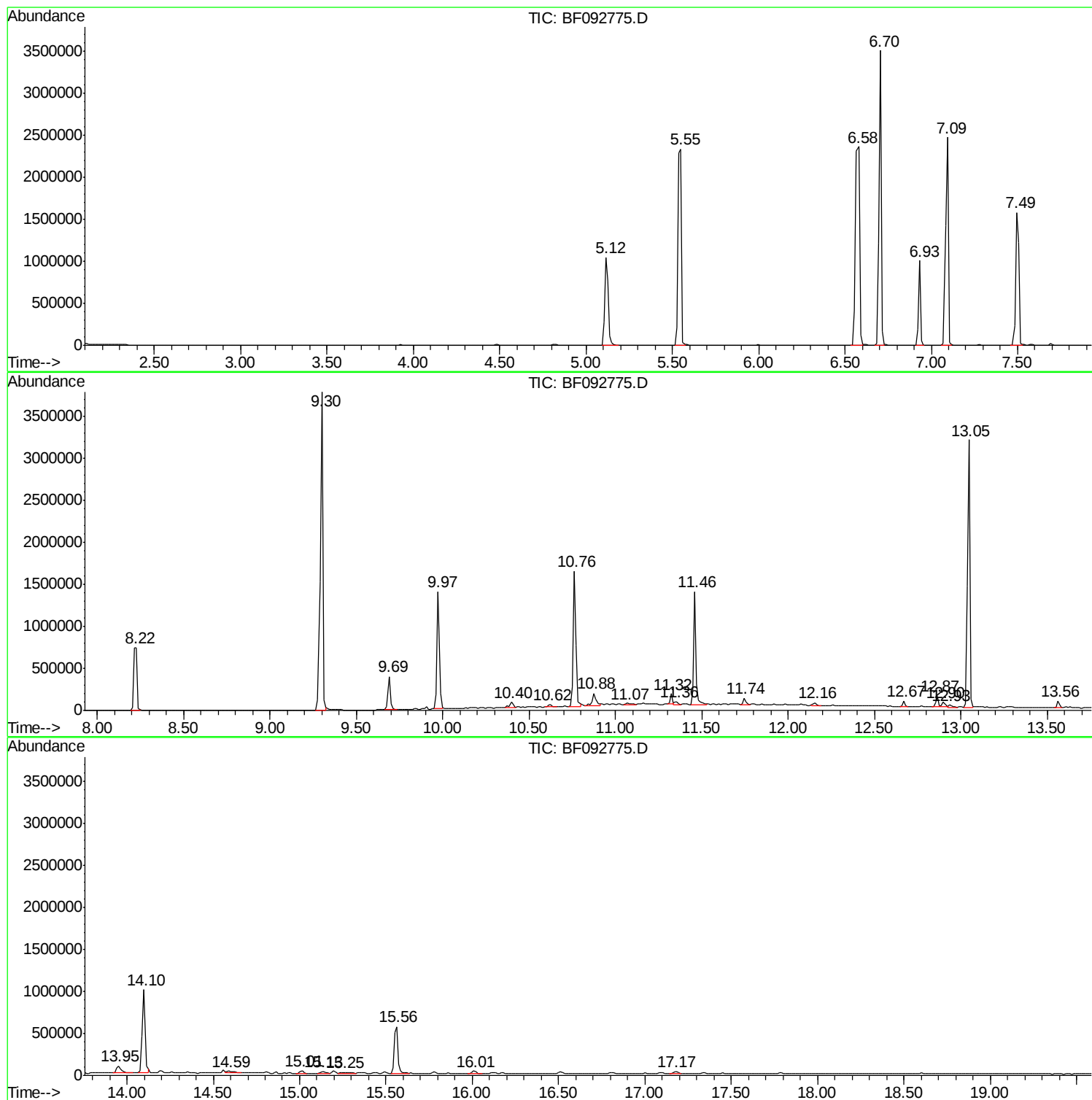
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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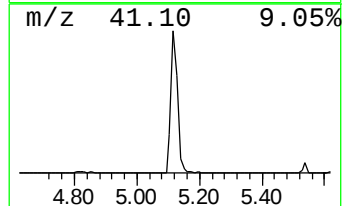
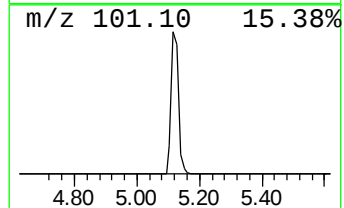
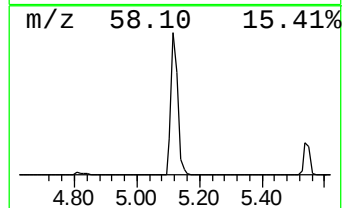
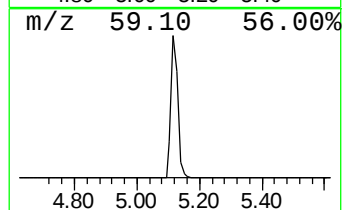
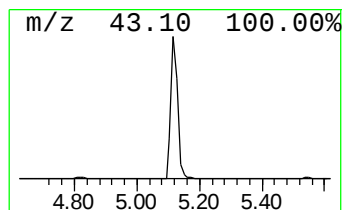
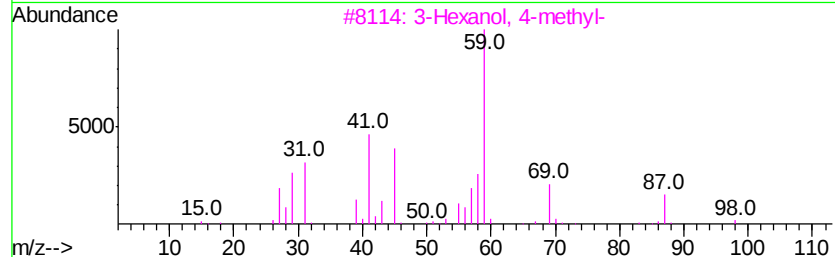
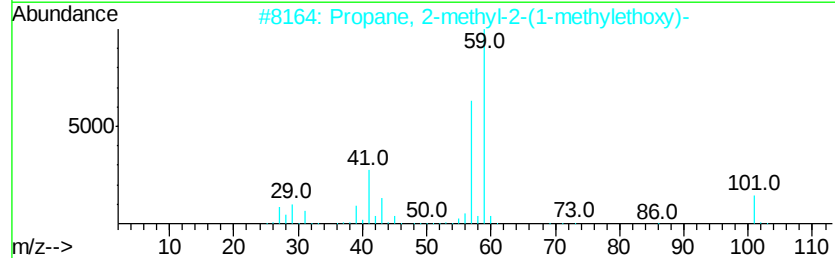
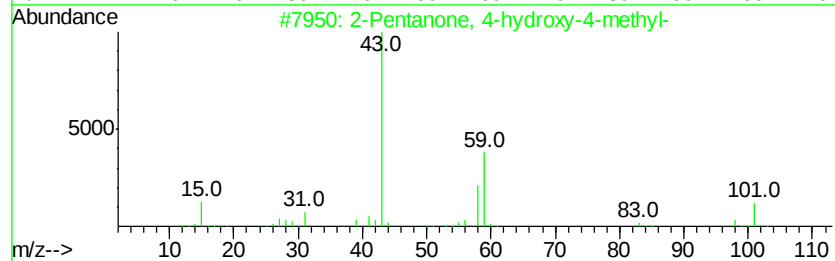
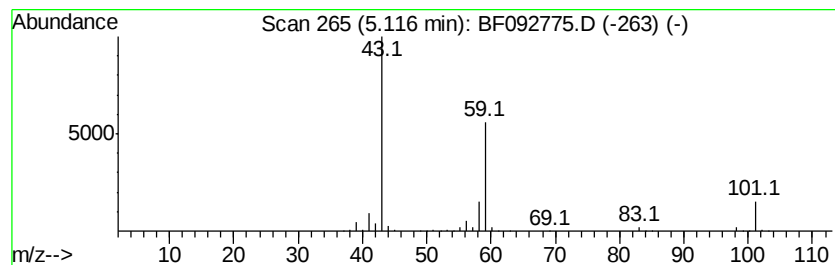
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	35.76 ng	1538270	1,4-Dichlorobenzene-d4	6.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32	



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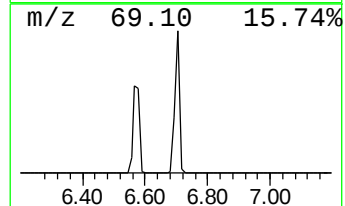
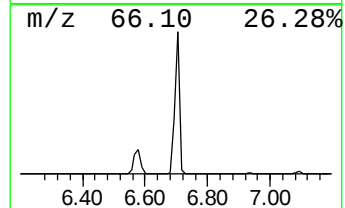
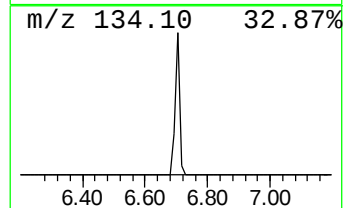
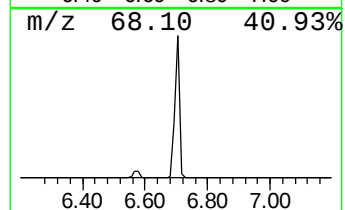
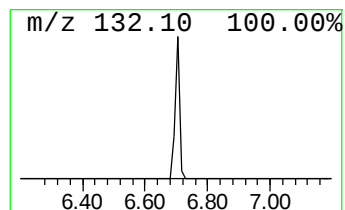
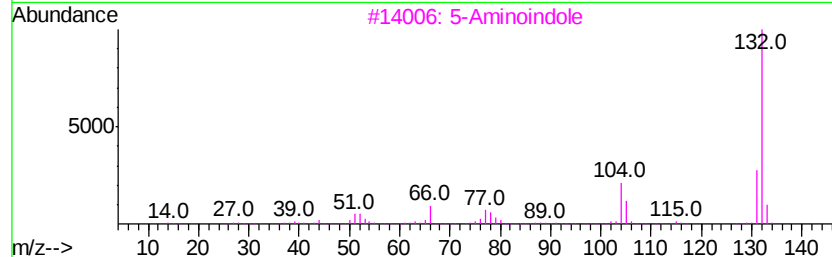
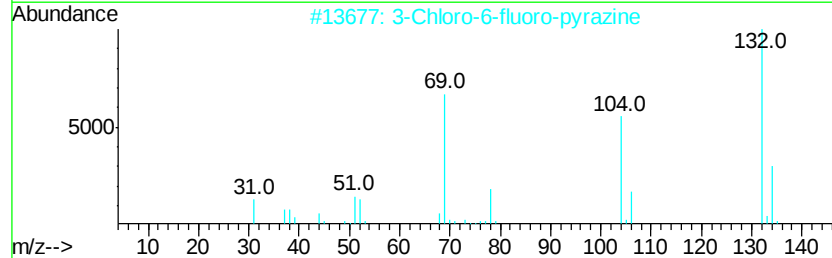
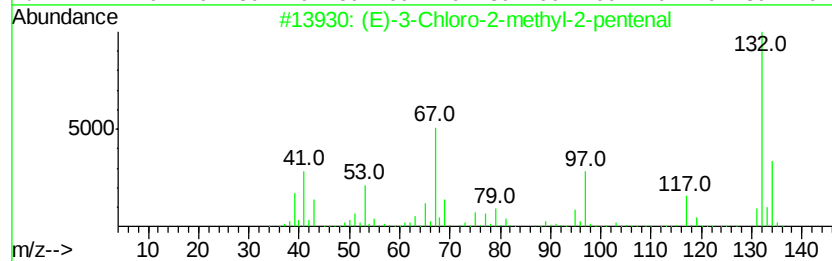
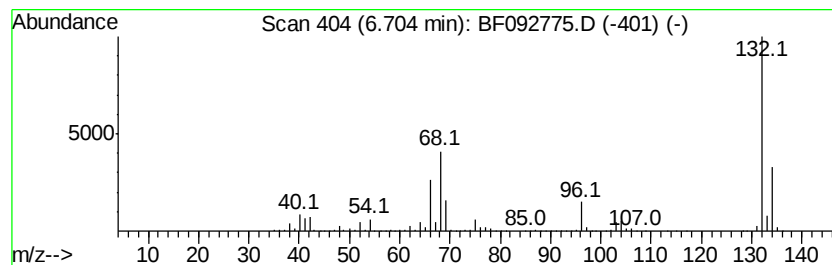
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	78.28 ng	3367000	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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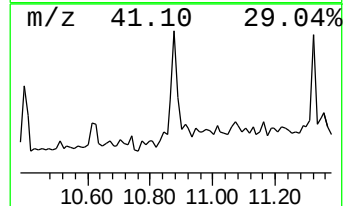
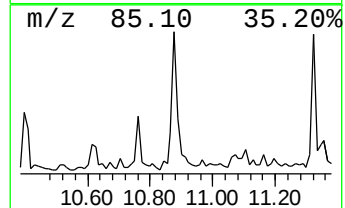
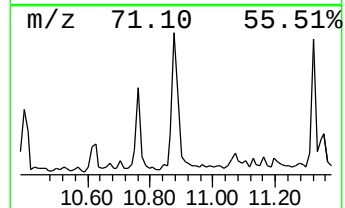
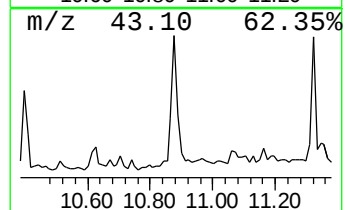
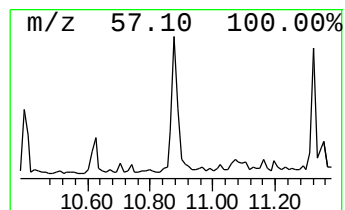
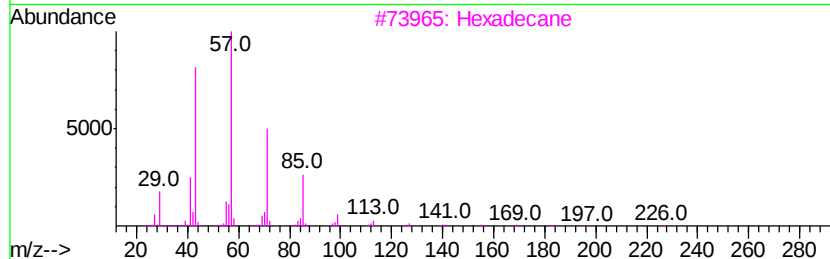
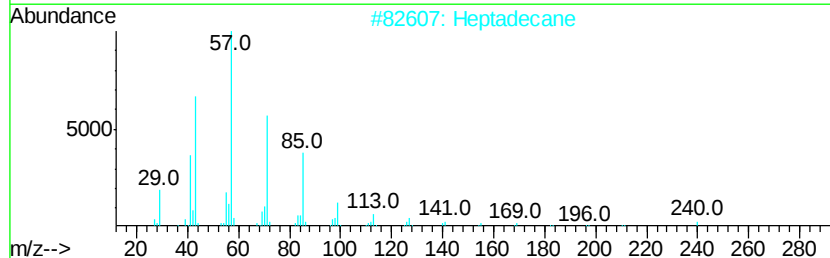
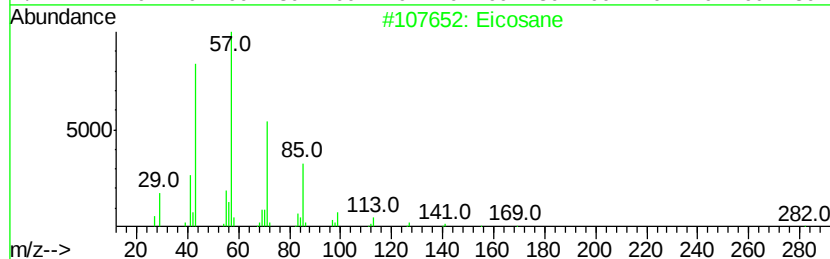
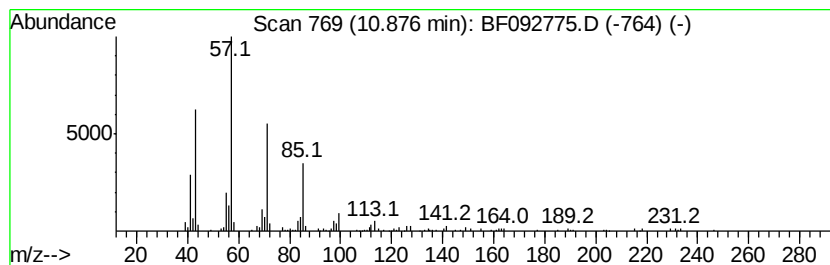
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	3.70 ng	235812	Phenanthrene-d10	11.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	90
2	Heptadecane		240	C17H36	000629-78-7	86
3	Hexadecane		226	C16H34	000544-76-3	86
4	Tetradecane		198	C14H30	000629-59-4	83
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	80



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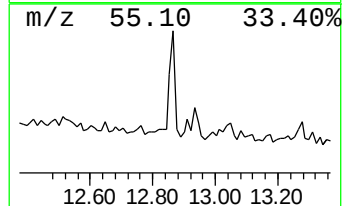
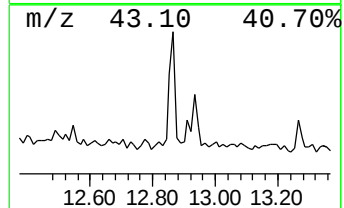
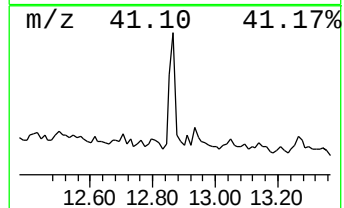
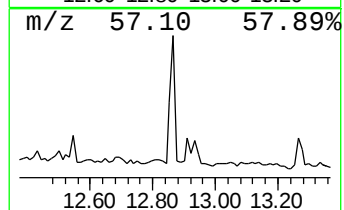
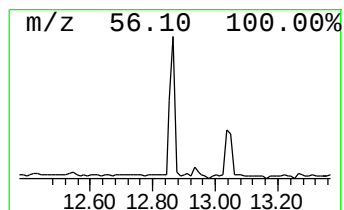
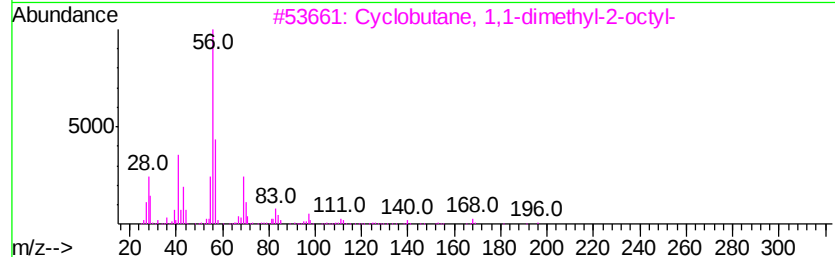
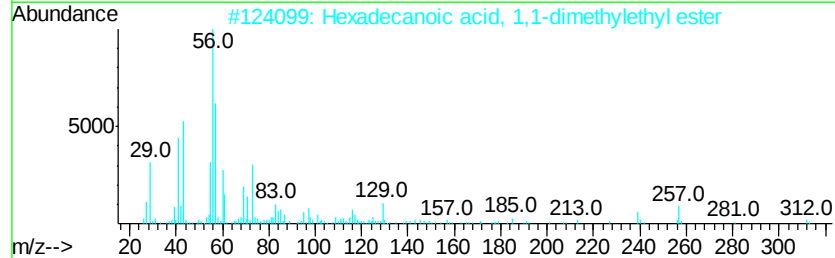
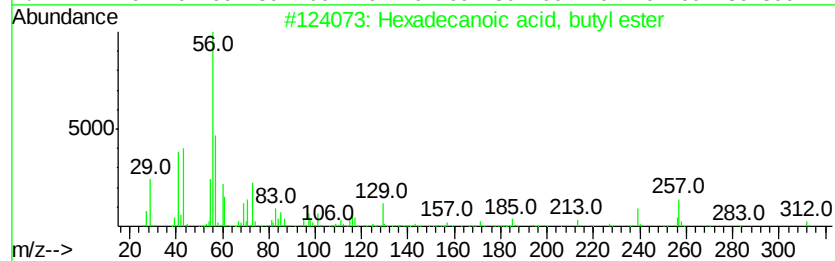
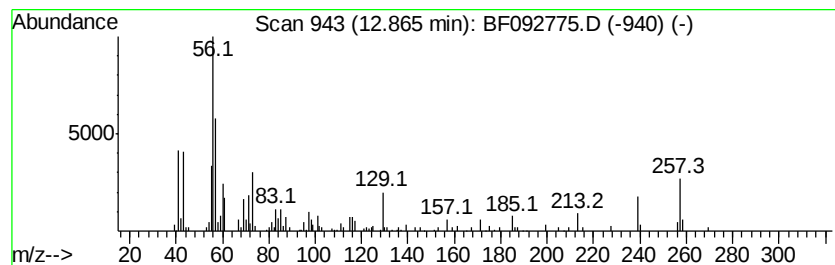
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	2.43 ng	127803	Chrysene-d12	14.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	74
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
4		3-Amino-2,2-dimethyl-1-propanol	103	C5H13NO	026734-09-8	27
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



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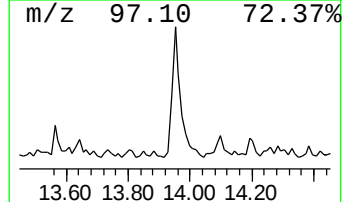
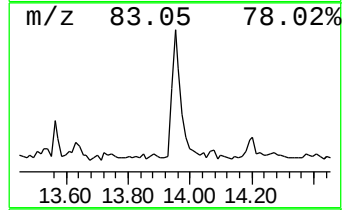
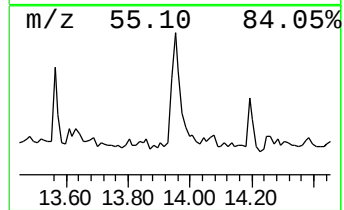
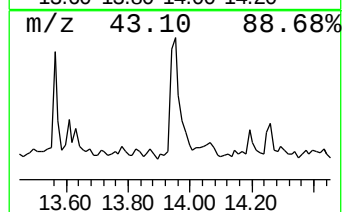
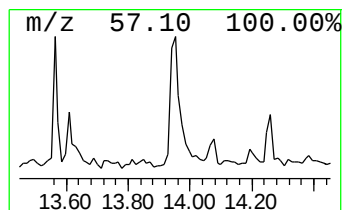
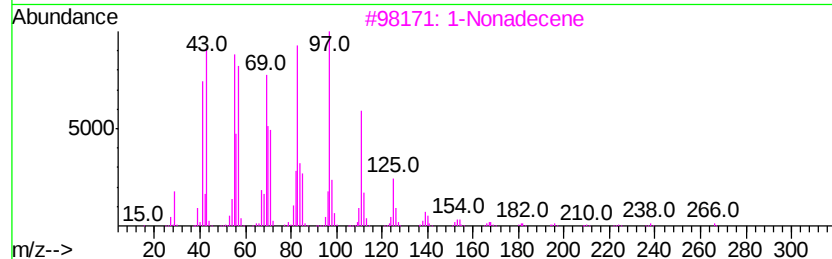
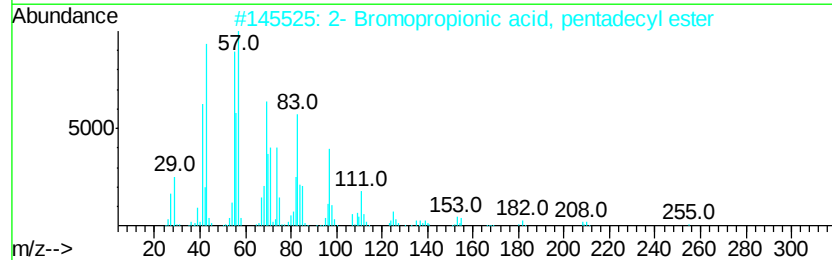
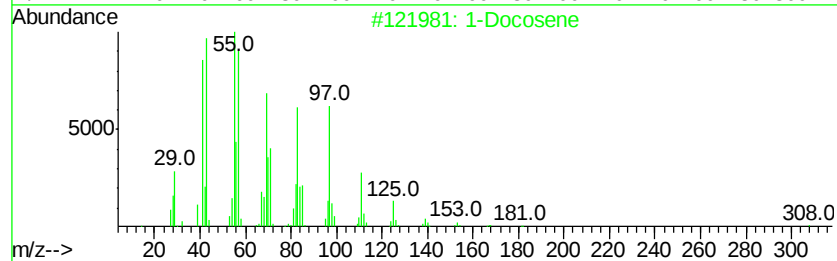
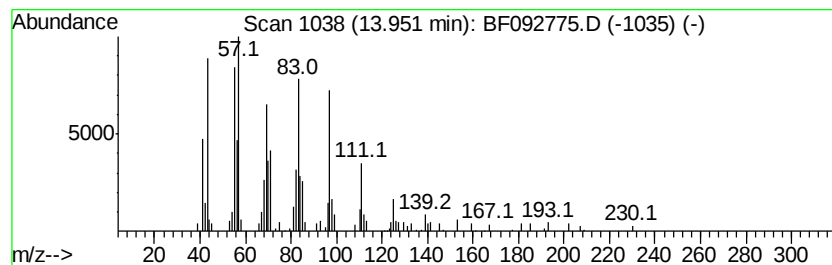
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Peak Number 6 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.08 ng	162323	Chrysene-d12	14.10
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene		308 C22H44	001599-67-3 94
2	2- Bromopropionic acid, pentadec...		362 C18H35BrO2	1000292-44-2 91
3	1-Nonadecene		266 C19H38	018435-45-5 91
4	3-Chloropropionic acid, heptadec...		346 C20H39ClO2	1000283-05-1 91
5	Bromoacetic acid, hexadecyl ester		362 C18H35BrO2	005454-48-8 91



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RVE-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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...	5.12	35.8	ng	1538270	1	6.93	860265	20.0
unknown6.70	6.70	78.3	ng	3367000	1	6.93	860265	20.0
Eicosane	10.88	3.7	ng	235812	4	11.46	1276150	20.0
Hexadecanoic acid...	12.87	2.4	ng	127803	5	14.10	1053840	20.0
1-Docosene	13.95	3.1	ng	162323	5	14.10	1053840	20.0