

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040715\
 Data File : BF078308.D
 Acq On : 7 Apr 2015 20:01
 Operator : TP/IZ
 Sample : G1783-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FD-2

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-BF040115.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	1.092	16	18	21	rBV	691681	823629	53.71%	6.440%
2	1.207	24	28	31	rVB	104168	168857	11.01%	1.320%
3	1.355	39	41	44	rVB	89906	97000	6.33%	0.758%
4	1.664	66	68	79	rBV	47903	82968	5.41%	0.649%
5	4.624	325	327	336	rVB	82465	113234	7.38%	0.885%
6	5.196	375	377	385	rBV	678494	931318	60.73%	7.282%
7	6.533	491	494	496	rBV	657888	974636	63.55%	7.620%
8	6.647	501	504	506	rBV	1006004	1032486	67.33%	8.073%
9	6.933	526	529	531	rBV	166923	192654	12.56%	1.506%
10	7.116	543	545	547	rBV	860011	806390	52.58%	6.305%
11	7.630	587	590	592	rBV	708747	619510	40.40%	4.844%
12	8.510	665	667	669	rBV	253538	269847	17.60%	2.110%
13	9.230	727	730	731	rBV	49497	51350	3.35%	0.401%
14	9.859	783	785	787	rBV	1389674	1255174	81.85%	9.814%
15	10.042	799	801	804	rBV	26236	27662	1.80%	0.216%
16	10.373	827	830	832	rBV	85291	89603	5.84%	0.701%
17	10.671	853	856	859	rVB	335719	317506	20.70%	2.482%
18	10.865	870	873	877	rBV3	8818	21230	1.38%	0.166%
19	11.219	902	904	907	rBB	14222	16232	1.06%	0.127%
20	11.573	933	935	937	rBV	293656	268920	17.54%	2.103%
21	11.642	939	941	944	rVB2	588379	776369	50.62%	6.070%
22	12.065	975	978	980	rBB	12335	15546	1.01%	0.122%
23	12.122	980	983	985	rBV	58250	84245	5.49%	0.659%
24	12.179	985	988	993	rVB	16618	36523	2.38%	0.286%
25	12.499	1013	1016	1018	rBV	362746	357407	23.31%	2.794%
26	12.568	1018	1022	1024	rVB	29585	29207	1.90%	0.228%
27	12.785	1038	1041	1044	rVB	35786	43917	2.86%	0.343%
28	13.254	1079	1082	1086	rBV	32246	50920	3.32%	0.398%
29	14.488	1188	1190	1193	rBV	1076230	1533576	100.00%	11.991%
30	15.277	1254	1259	1261	rBV2	9205	18827	1.23%	0.147%
31	15.688	1292	1295	1300	rBV	211602	325954	21.25%	2.549%
32	15.780	1300	1303	1305	rVB	330215	394450	25.72%	3.084%
33	16.111	1328	1332	1335	rBV	14383	25071	1.63%	0.196%
34	16.534	1366	1369	1377	rBV	85720	148687	9.70%	1.163%

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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-BF040115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.945	1402	1405	1410	rBV4	11969	30194	1.97%	0.236%
36	17.345	1438	1440	1441	rBV	17660	25213	1.64%	0.197%
37	17.563	1456	1459	1462	rBV	319085	380589	24.82%	2.976%
38	17.757	1473	1476	1479	rBV	13338	26426	1.72%	0.207%
39	17.940	1490	1492	1496	rBV3	16108	25566	1.67%	0.200%
40	18.168	1508	1512	1513	rBV2	17478	30565	1.99%	0.239%
41	18.203	1513	1515	1519	rVV2	41659	83577	5.45%	0.653%
42	18.271	1519	1521	1526	rVB3	11762	24341	1.59%	0.190%
43	18.637	1547	1553	1555	rBV2	18362	46132	3.01%	0.361%
44	19.117	1592	1595	1596	rBV2	9092	16553	1.08%	0.129%
45	19.414	1618	1621	1628	rBV7	8696	23939	1.56%	0.187%
46	19.997	1669	1672	1676	rBV3	8117	16787	1.09%	0.131%
47	21.152	1769	1773	1784	rVB6	11630	59045	3.85%	0.462%

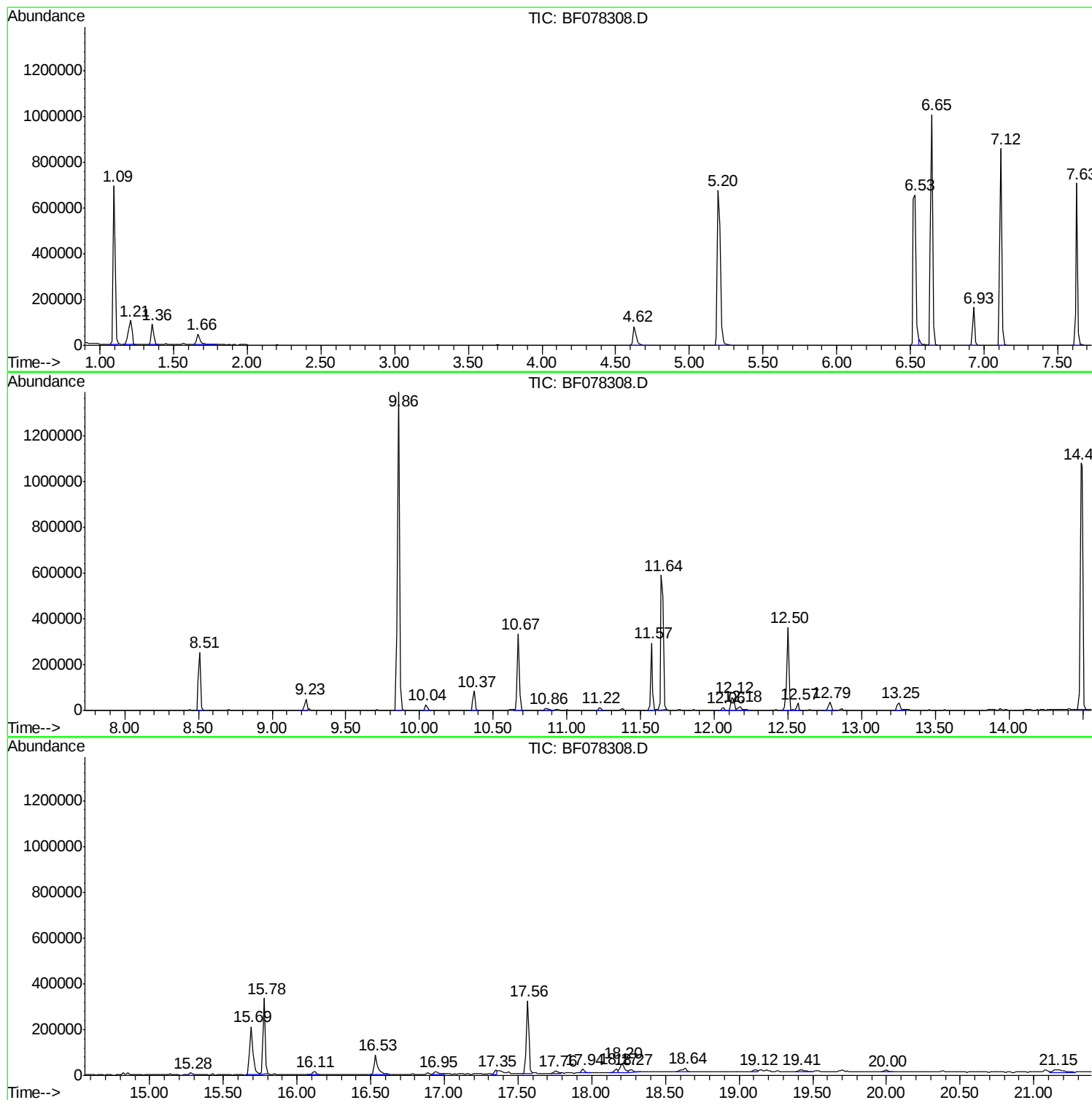
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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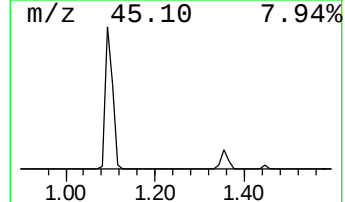
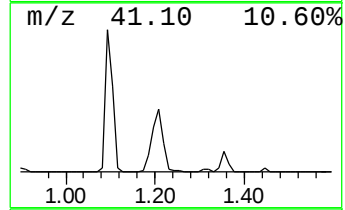
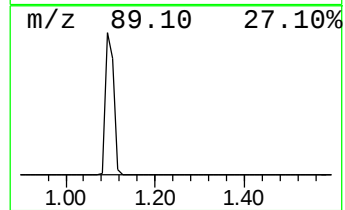
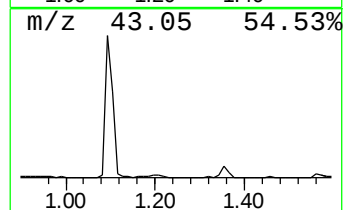
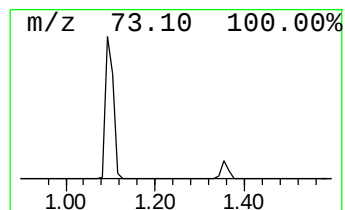
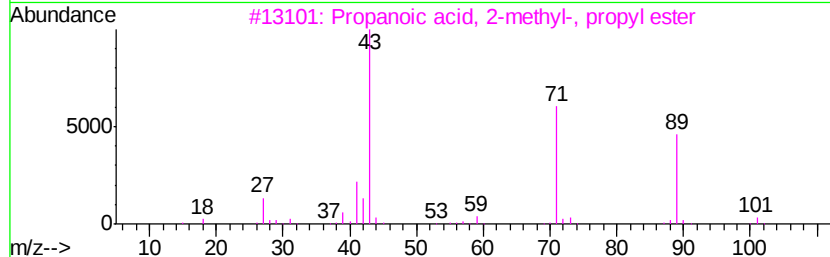
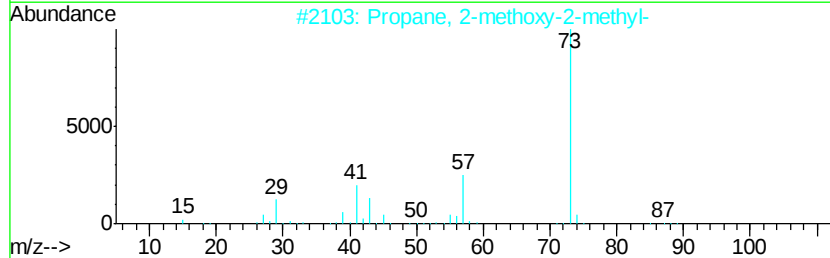
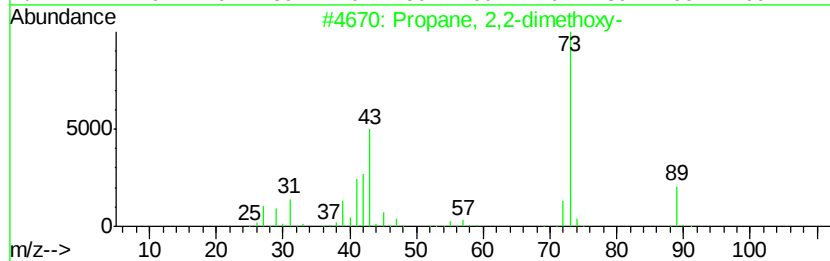
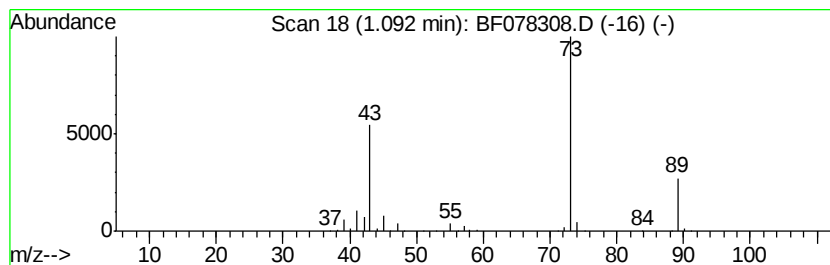
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.09	85.50 ng	823629	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3			Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	9
4			1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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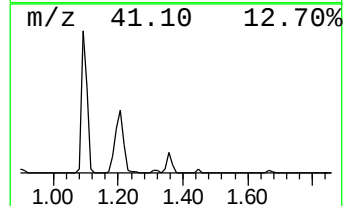
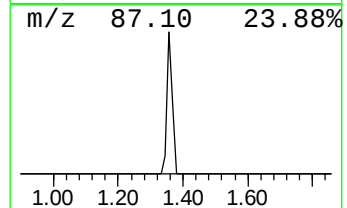
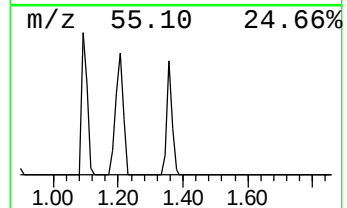
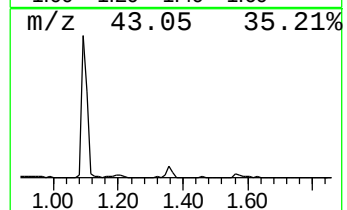
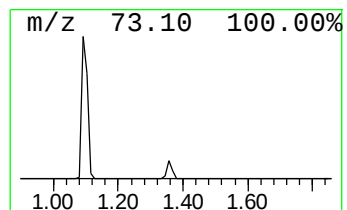
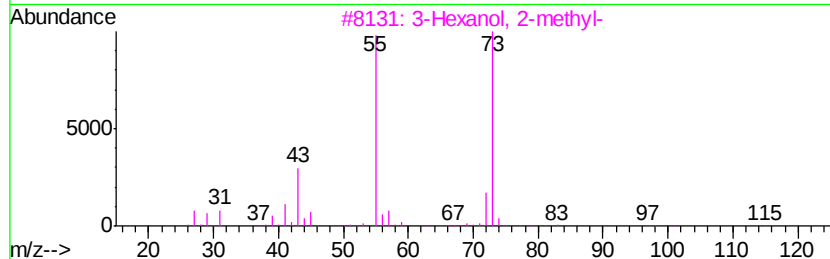
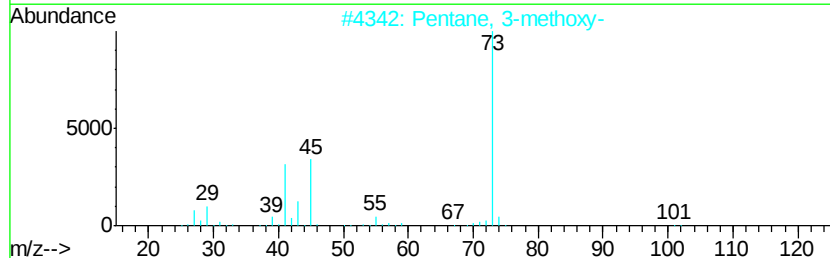
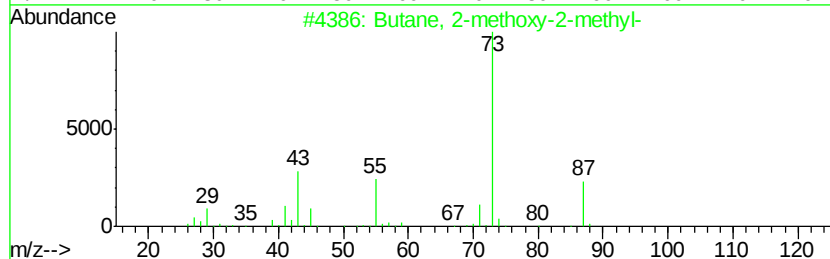
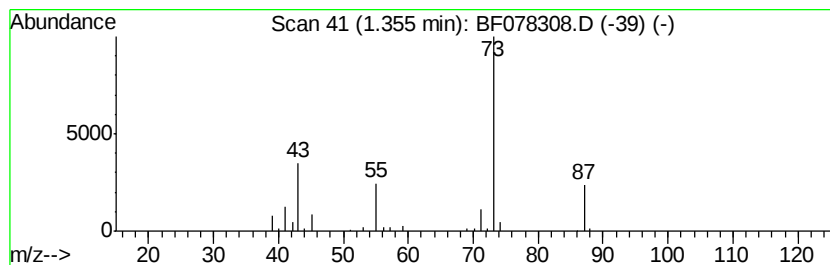
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.36	10.07 ng	97000	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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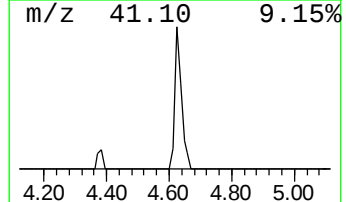
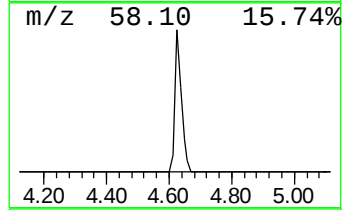
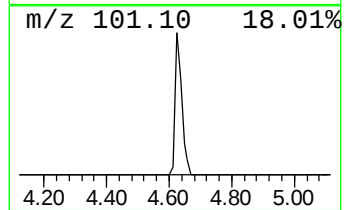
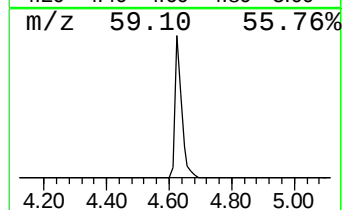
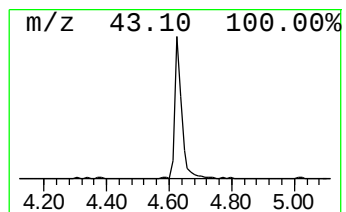
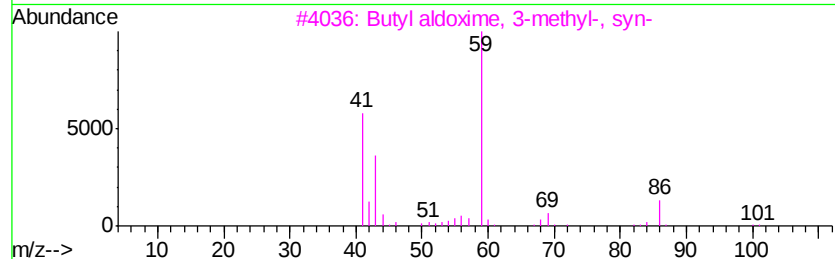
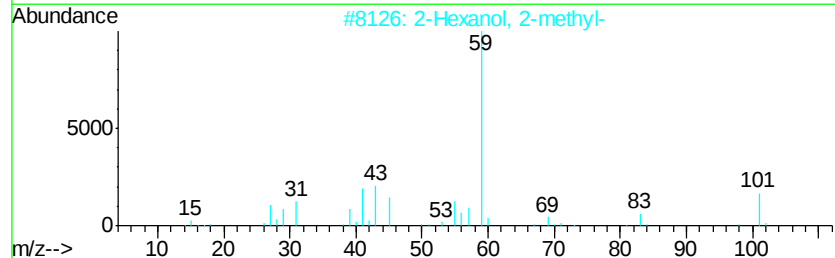
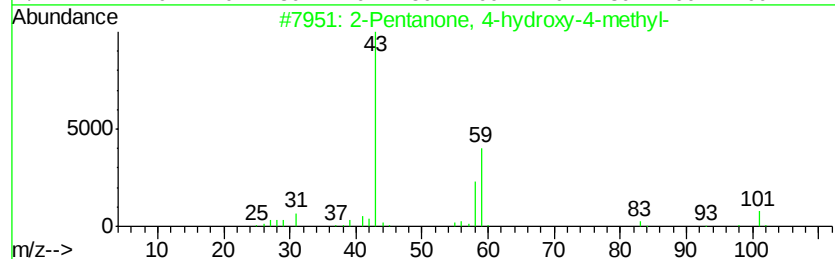
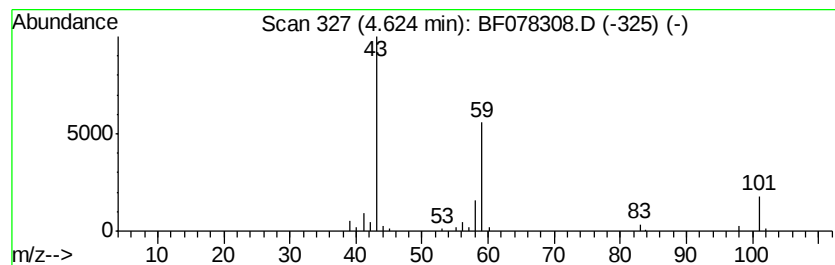
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	11.76 ng	113234	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	45
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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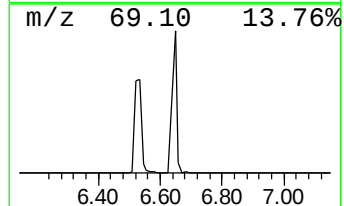
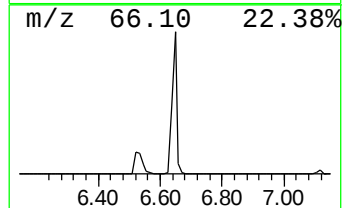
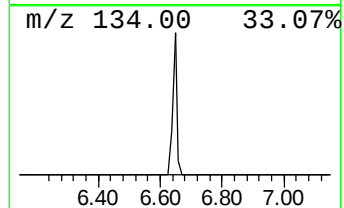
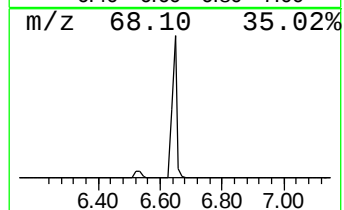
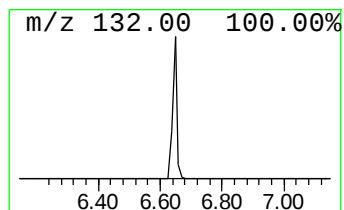
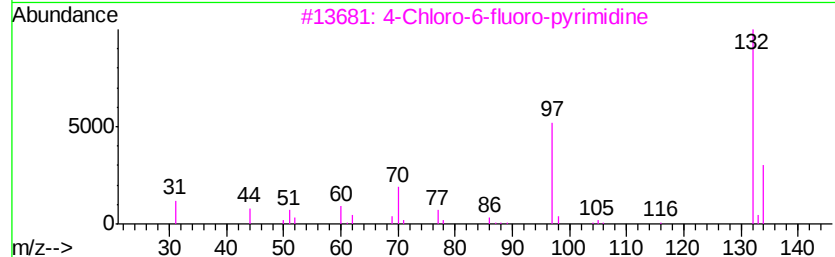
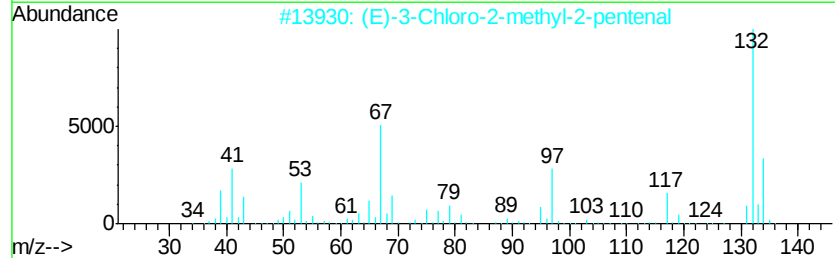
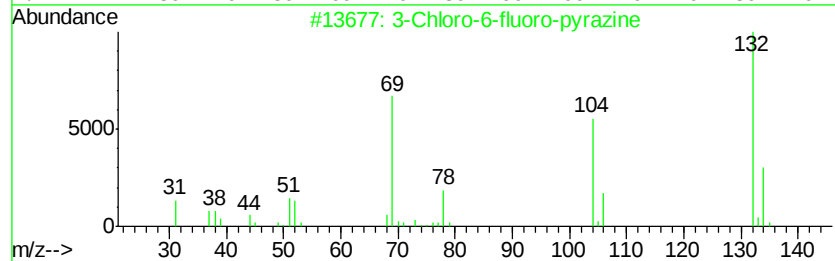
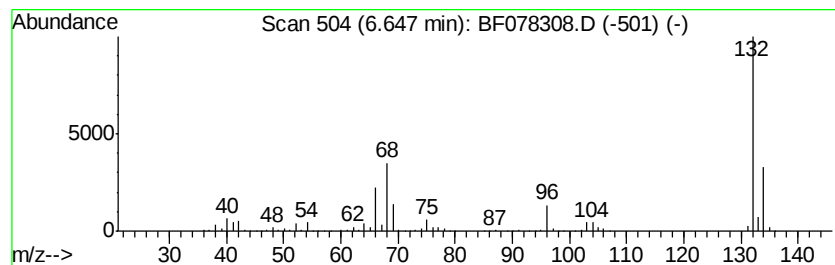
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	107.19 ng	1032490	1,4-Dichlorobenzene-d4	6.93

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	25
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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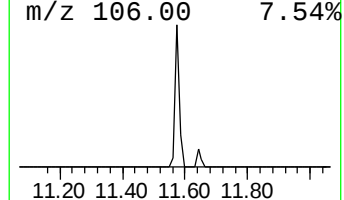
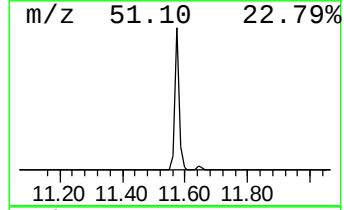
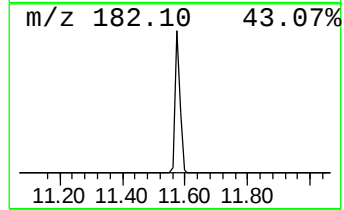
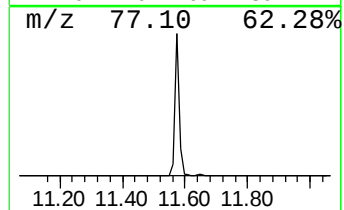
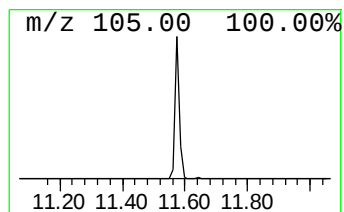
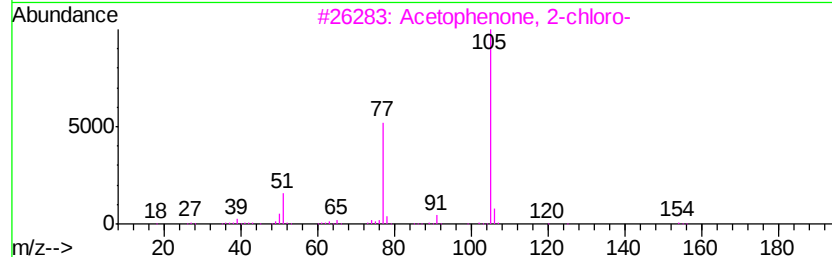
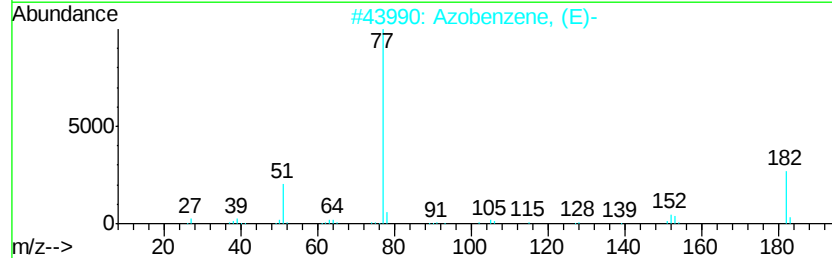
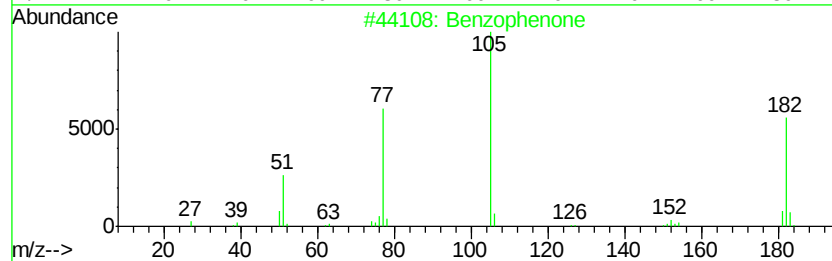
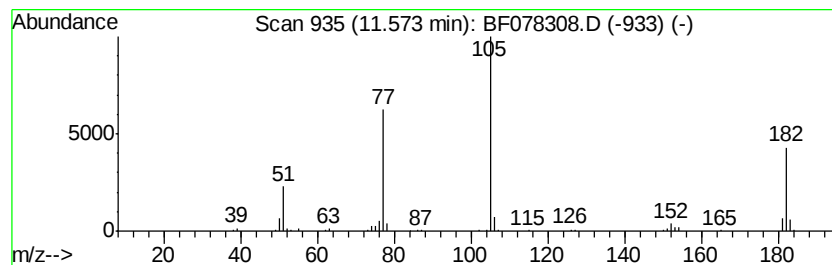
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	16.94 ng	268920	Acenaphthene-d10	10.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	96
2		Azobenzene, (E)-	182	C12H10N2	017082-12-1	50
3		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4		Benzoyl bromide	184	C7H5BrO	000618-32-6	47
5		Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040715\
Data File : BF078308.D
Acq On : 7 Apr 2015 20:01
Operator : TP/IZ
Sample : G1783-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

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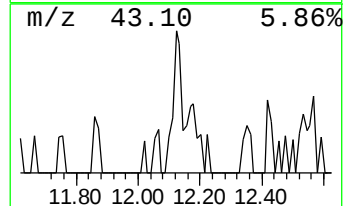
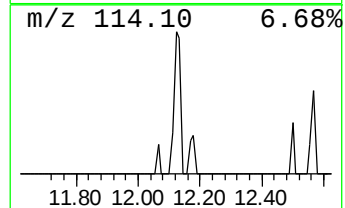
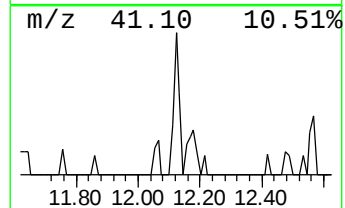
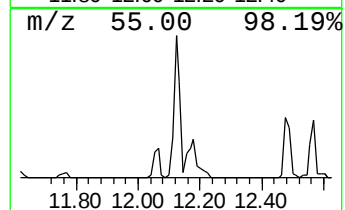
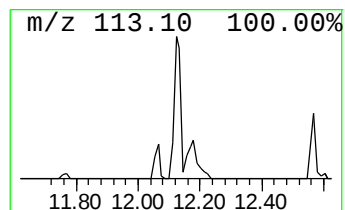
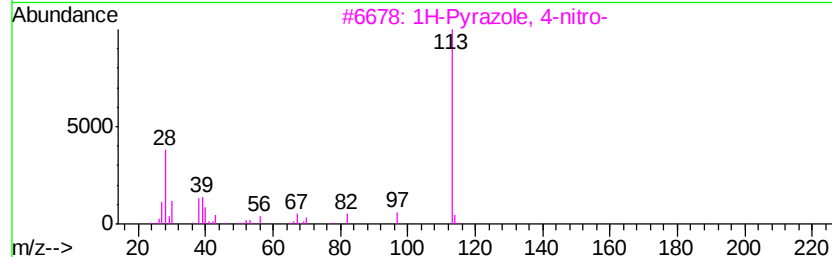
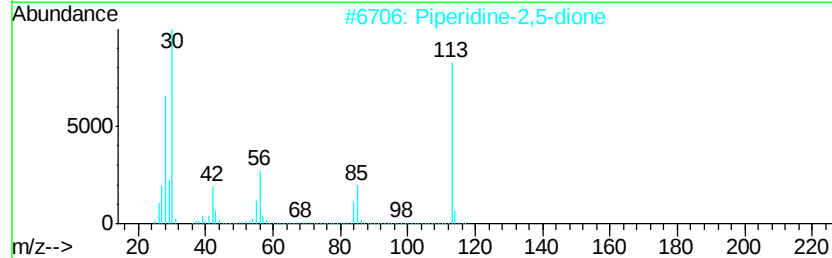
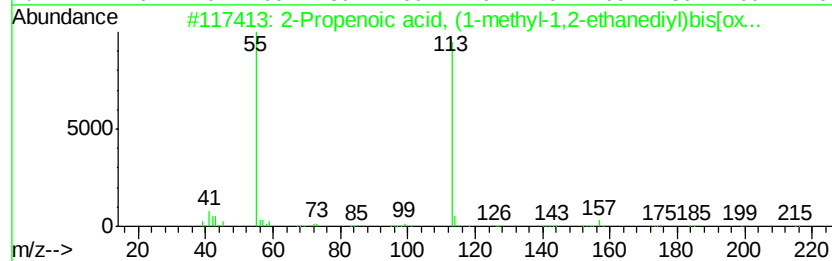
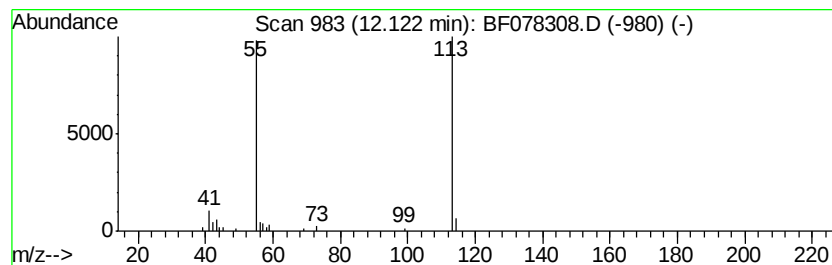
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 2-Propenoic acid, (1-methyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	4.71 ng	84245	Phenanthrene-d10	12.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, (1-methyl-1,2-...	300	C15H24O6		042978-66-5	83
2	Piperidine-2,5-dione	113	C5H7NO2		052065-78-8	9
3	1H-Pyrazole, 4-nitro-	113	C3H3N3O2		002075-46-9	9
4	1-Nitropyrazole	113	C3H3N3O2		007119-95-1	9
5	1H-Imidazole, 4-nitro-	113	C3H3N3O2		003034-38-6	9



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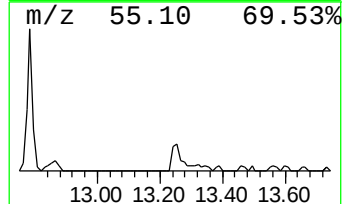
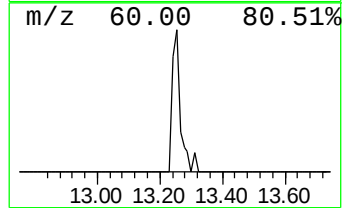
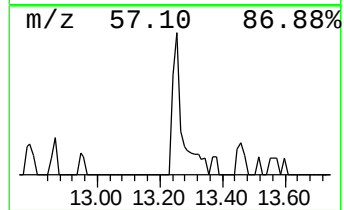
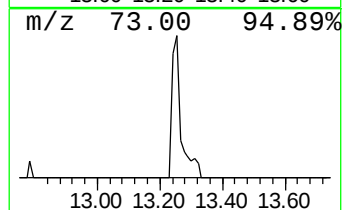
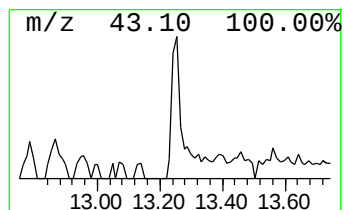
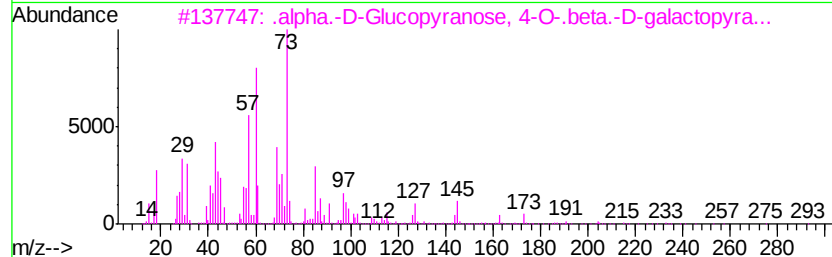
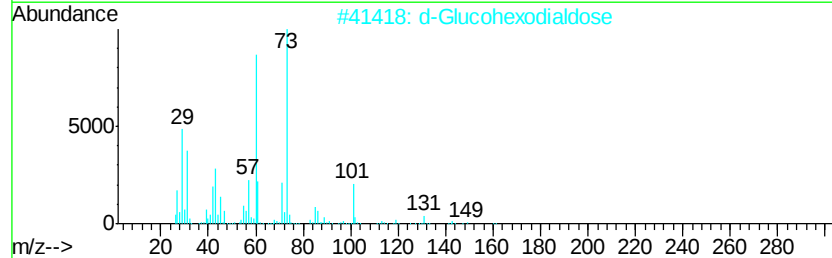
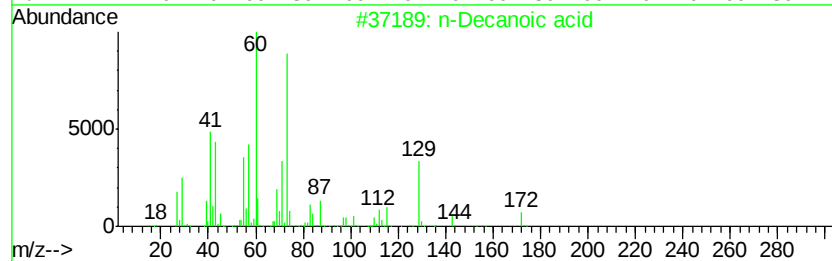
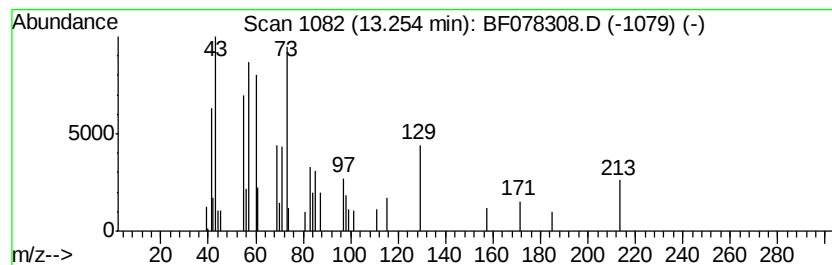
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 n-Decanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.25	2.85 ng	50920	Phenanthrene-d10	12.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Decanoic acid	172	C10H20O2	000334-48-5	53
2		d-Glucohexodialdose	178	C6H10O6	1000149-19-1	35
3		.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	27
4		.alpha.-D-Glucopyranoside, 0-.al...	504	C18H32O16	000597-12-6	27
5		Amyl Nitrite	117	C5H11NO2	000110-46-3	27



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Sample : G1783-03
Misc :
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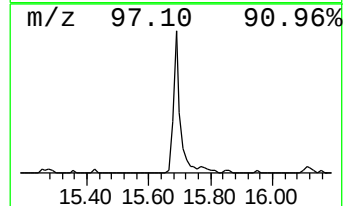
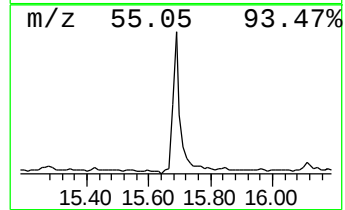
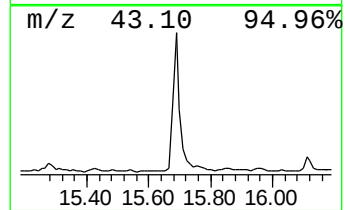
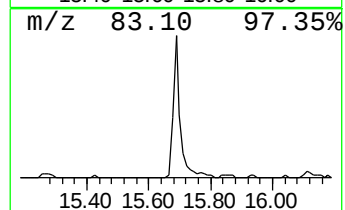
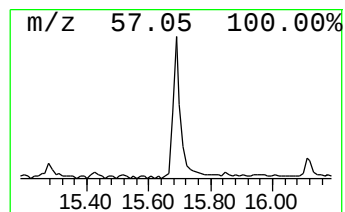
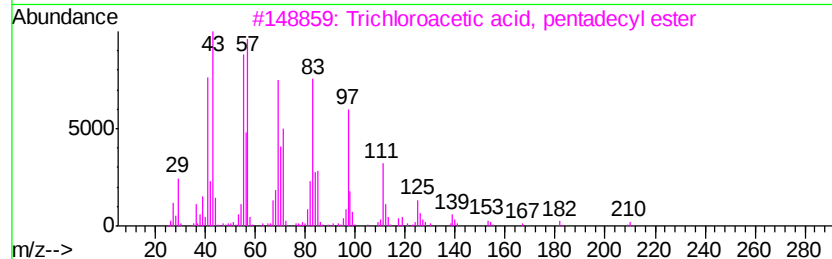
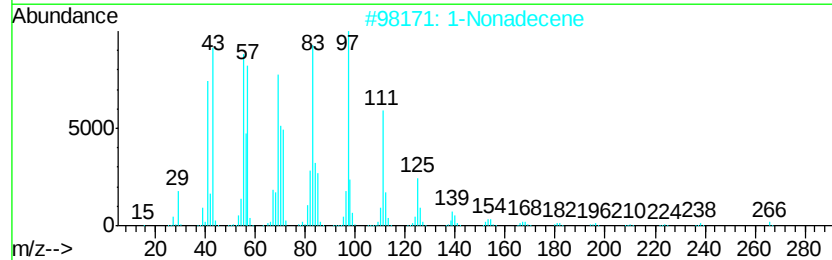
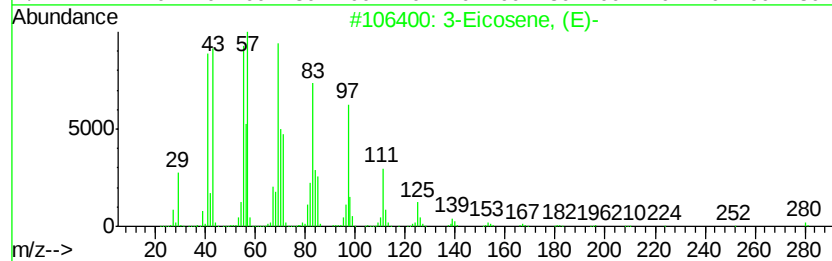
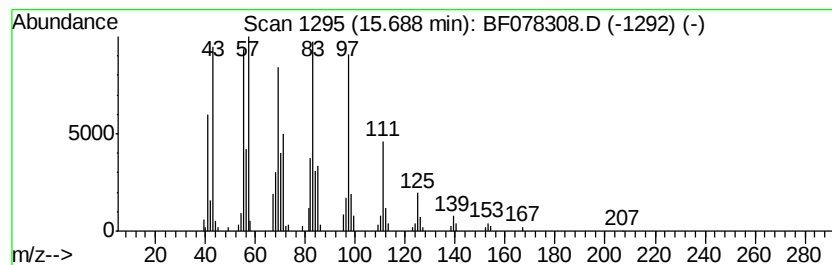
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	16.53 ng	325954	Chrysene-d12	15.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2			1-Nonadecene	266	C19H38	018435-45-5	91
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4			1-Hexadecanol	242	C16H34O	036653-82-4	90
5			9-Eicosene, (E)-	280	C20H40	074685-29-3	90



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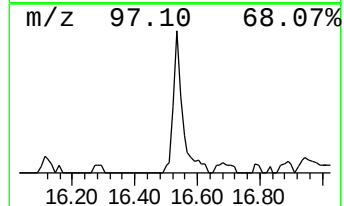
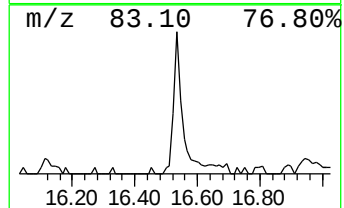
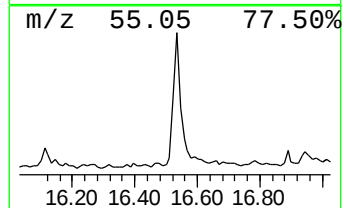
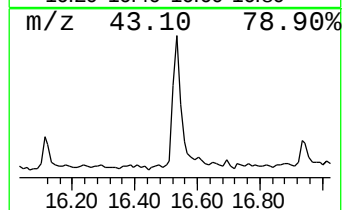
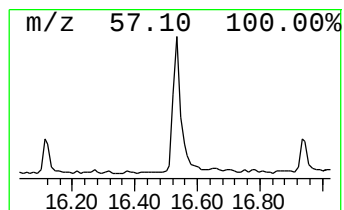
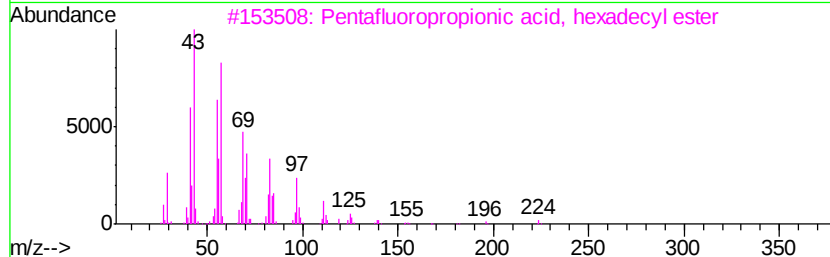
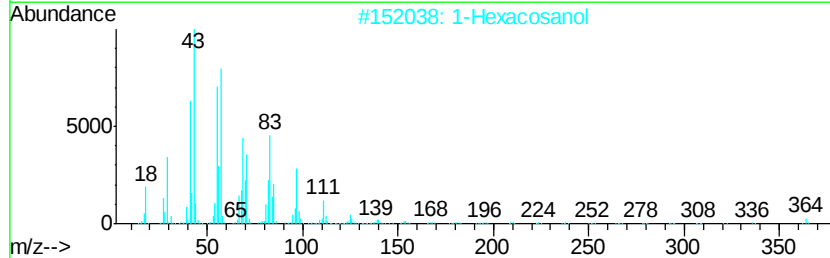
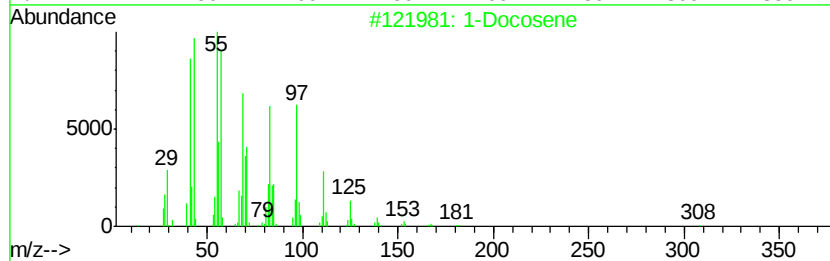
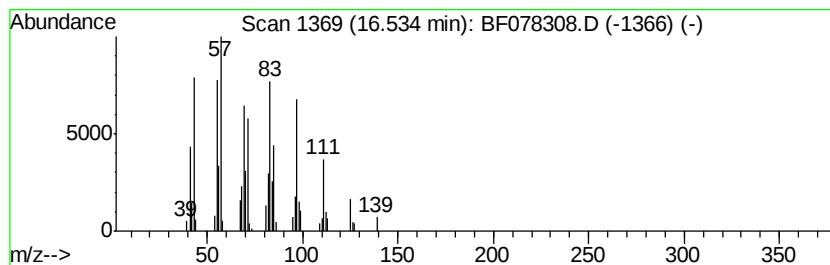
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 1-Docosene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	7.54 ng	148687	Chrysene-d12	15.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	87
2			1-Hexacosanol	382	C26H54O	000506-52-5	87
3			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	86
4			17-Pentatriacontene	491	C35H70	006971-40-0	80
5			1-Tetracosanol	354	C24H50O	000506-51-4	74



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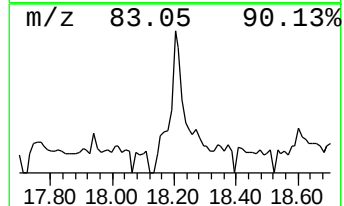
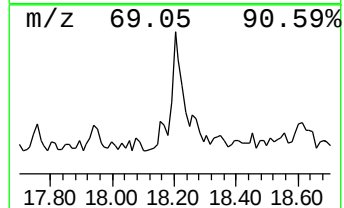
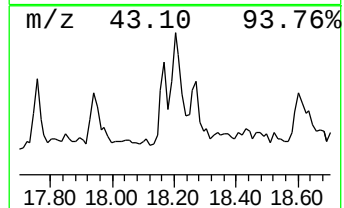
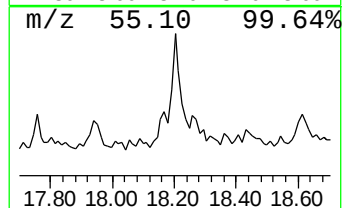
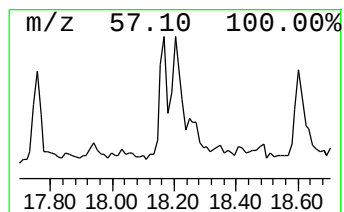
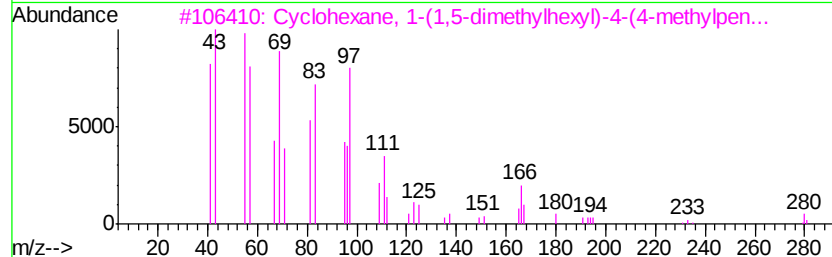
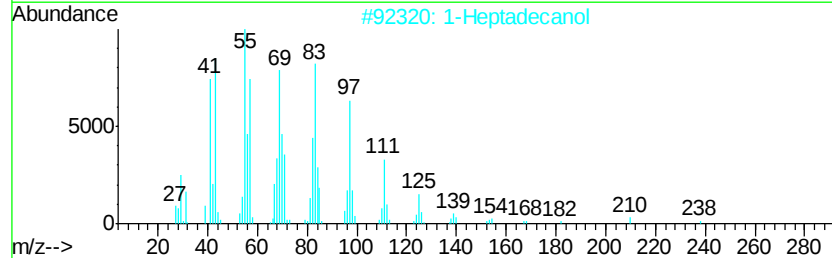
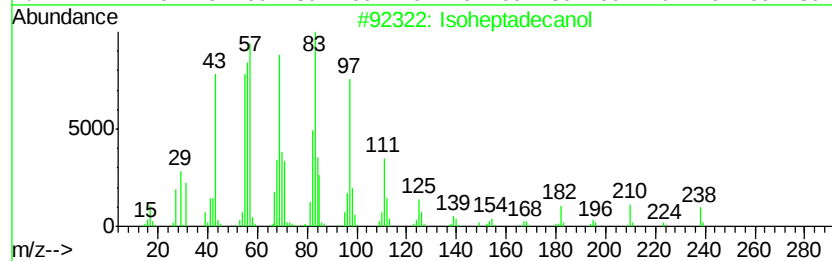
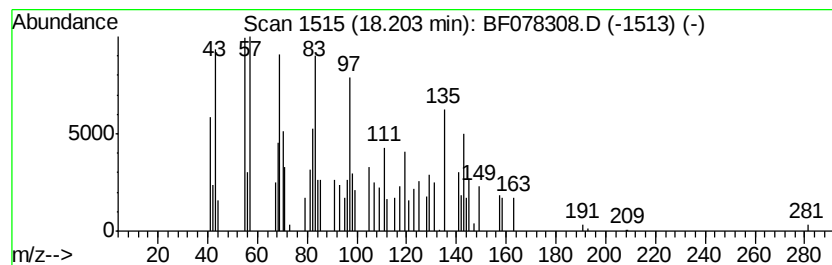
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Isoheptadecanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.20	4.39 ng	83577	Perylene-d12	17.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isoheptadecanol	256	C17H36O	057289-07-3	53
2			1-Heptadecanol	256	C17H36O	001454-85-9	53
3			Cyclohexane, 1-(1,5-dimethylhexyl)-4-(4-methylphenyl)-	280	C20H40	056009-20-2	49
4			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	49
5			1-Hexadecanol	242	C16H34O	036653-82-4	49



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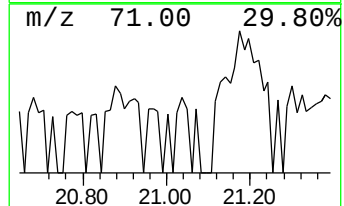
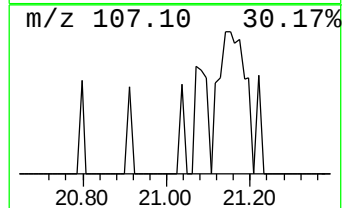
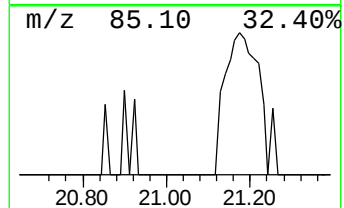
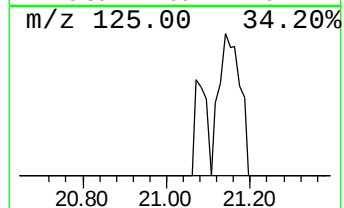
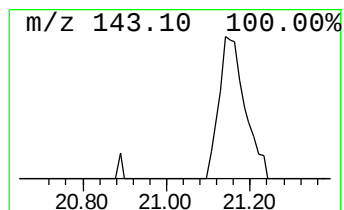
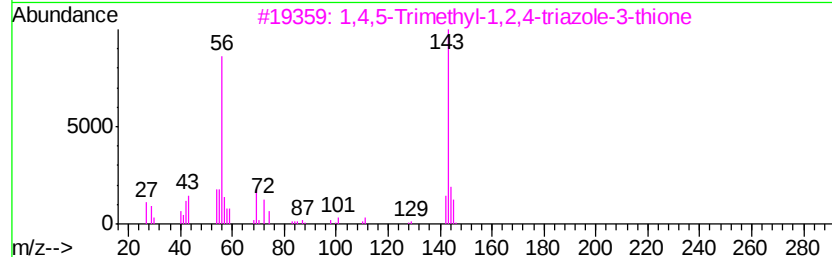
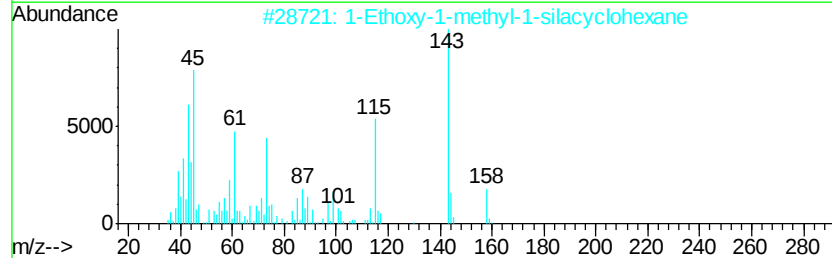
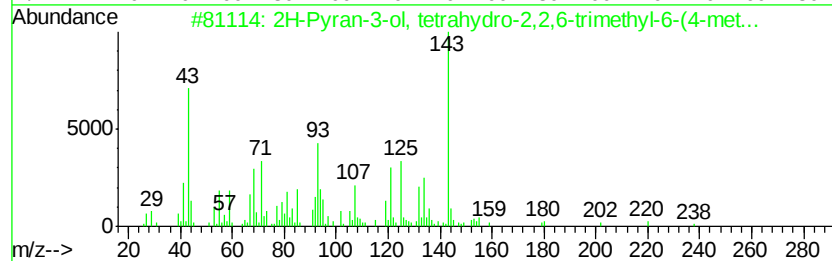
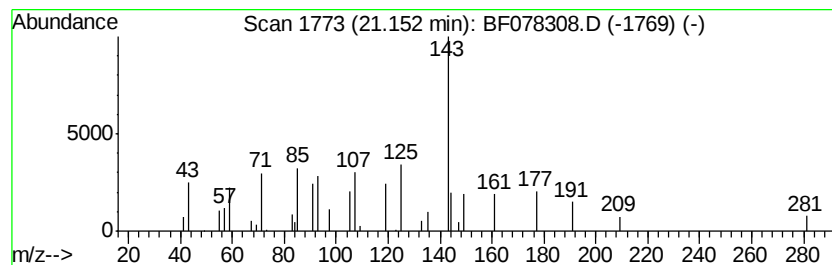
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 unknown21.15 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.15	3.10 ng	59045	Perylene-d12	17.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Pyran-3-ol, tetrahydro-2,2,6-...	238	C15H26O2	022567-36-8	28
2			1-Ethoxy-1-methyl-1-silacyclohexane	158	C8H18OSi	1000245-78-2	23
3			1,4,5-Trimethyl-1,2,4-triazole-3...	143	C5H9N3S	017370-06-8	9
4			2,4-Dimethyl-2-[4-hydroxybutyl]t...	236	C9H20N2OS2	1000255-60-6	9
5			1-Methyl-1-(2-pentadecyl)oxy-1-s...	326	C20H42OSi	1000245-41-8	9



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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
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Butane, 2-methoxy...	1.36	10.1	ng	97000	1	6.93	192654	20.0
2-Pentanone, 4-hy...	4.62	11.8	ng	113234	1	6.93	192654	20.0
unknown6.65	6.65	107.2	ng	1032490	1	6.93	192654	20.0
Benzophenone	11.57	16.9	ng	268920	3	10.67	317506	20.0
2-Propenoic acid,...	12.12	4.7	ng	84245	4	12.50	357407	20.0
n-Decanoic acid	13.25	2.9	ng	50920	4	12.50	357407	20.0
3-Eicosene, (E)-	15.69	16.5	ng	325954	5	15.78	394450	20.0
1-Docosene	16.53	7.5	ng	148687	5	15.78	394450	20.0
Isoheptadecanol	18.20	4.4	ng	83577	6	17.56	380589	20.0
unknown21.15	21.15	3.1	ng	59045	6	17.56	380589	20.0