

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051215\
 Data File : BF079162.D
 Acq On : 12 May 2015 17:21
 Operator : TP/IZ
 Sample : G2155-12
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-42S

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-BF043015.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	1.427	19	21	24	rVB	591456	723102	19.64%	2.918%
2	1.564	30	33	36	rVB	143714	247819	6.73%	1.000%
3	1.724	46	47	56	rVV2	324034	715015	19.42%	2.885%
4	1.850	56	58	100	rVB	1958190	3681797	100.00%	14.855%
5	5.073	339	340	348	rVB	45279	74646	2.03%	0.301%
6	5.587	382	385	387	rBV	1210194	1329248	36.10%	5.363%
7	6.845	493	495	498	rBV	1341683	1306780	35.49%	5.273%
8	6.993	506	508	511	rBV	1504902	1411486	38.34%	5.695%
9	7.279	531	533	535	rBV	408892	398929	10.84%	1.610%
10	7.473	547	550	552	rBV	848757	1089314	29.59%	4.395%
11	7.976	591	594	596	rBV	846401	881205	23.93%	3.556%
12	8.856	669	671	674	rBV	663728	580898	15.78%	2.344%
13	10.205	786	789	791	rBV	1954617	1755680	47.69%	7.084%
14	10.708	831	833	835	rBV	75475	64529	1.75%	0.260%
15	11.028	859	861	864	rBV	561614	648798	17.62%	2.618%
16	12.011	944	947	950	rBV	1131466	1110265	30.16%	4.480%
17	12.879	1020	1023	1024	rBV	676330	689208	18.72%	2.781%
18	12.902	1024	1025	1027	rVB	143242	131195	3.56%	0.529%
19	12.971	1027	1031	1032	rBV	39141	46394	1.26%	0.187%
20	13.588	1083	1085	1087	rBV2	27312	40329	1.10%	0.163%
21	13.634	1087	1089	1091	rBV2	34274	52450	1.42%	0.212%
22	13.908	1109	1113	1114	rBV2	20976	43356	1.18%	0.175%
23	14.194	1136	1138	1140	rBV	25614	38829	1.05%	0.157%
24	14.388	1153	1155	1157	rVB	254242	300122	8.15%	1.211%
25	14.663	1176	1179	1184	rVV	299001	361318	9.81%	1.458%
26	14.868	1195	1197	1200	rBV	1398248	1852901	50.33%	7.476%
27	15.085	1211	1216	1218	rBV2	29940	67609	1.84%	0.273%
28	15.211	1225	1227	1229	rBV	44883	55334	1.50%	0.223%
29	15.508	1250	1253	1256	rBV2	128296	249008	6.76%	1.005%
30	15.714	1268	1271	1274	rVB	34125	62949	1.71%	0.254%
31	15.851	1281	1283	1285	rBV	29033	44082	1.20%	0.178%
32	15.897	1285	1287	1290	rVV2	21563	52199	1.42%	0.211%
33	15.977	1292	1294	1297	rVV	29201	50199	1.36%	0.203%
34	16.046	1297	1300	1305	rVV2	207438	329025	8.94%	1.328%

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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-BF043015.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.171	1307	1311	1313	rVV2	796454	1084227	29.45%	4.375%
36	16.206	1313	1314	1319	rVB2	262567	301551	8.19%	1.217%
37	16.377	1327	1329	1332	rVV3	35129	69847	1.90%	0.282%
38	16.468	1335	1337	1345	rVB4	30721	88561	2.41%	0.357%
39	16.674	1352	1355	1357	rBV	35767	48030	1.30%	0.194%
40	16.868	1370	1372	1376	rVB3	49095	104498	2.84%	0.422%
41	17.268	1404	1407	1408	rBV2	26995	41153	1.12%	0.166%
42	17.337	1411	1413	1415	rBV	188280	222787	6.05%	0.899%
43	17.429	1419	1421	1423	rBV2	33768	46776	1.27%	0.189%
44	17.474	1423	1425	1430	rBV	160252	337736	9.17%	1.363%
45	17.657	1438	1441	1442	rBV	40586	67584	1.84%	0.273%
46	17.794	1451	1453	1456	rBV	91416	126258	3.43%	0.509%
47	17.863	1456	1459	1462	rVB	145932	183360	4.98%	0.740%
48	17.931	1462	1465	1471	rBV	620377	901906	24.50%	3.639%
49	18.503	1512	1515	1517	rBV	37403	67832	1.84%	0.274%
50	18.549	1517	1519	1521	rBV2	41873	74867	2.03%	0.302%
51	18.846	1543	1545	1549	rVB5	29090	60965	1.66%	0.246%
52	19.383	1589	1592	1597	rVB2	69687	154966	4.21%	0.625%
53	19.817	1627	1630	1635	rVB	58829	139162	3.78%	0.561%
54	20.012	1644	1647	1654	rVB5	45232	176086	4.78%	0.710%

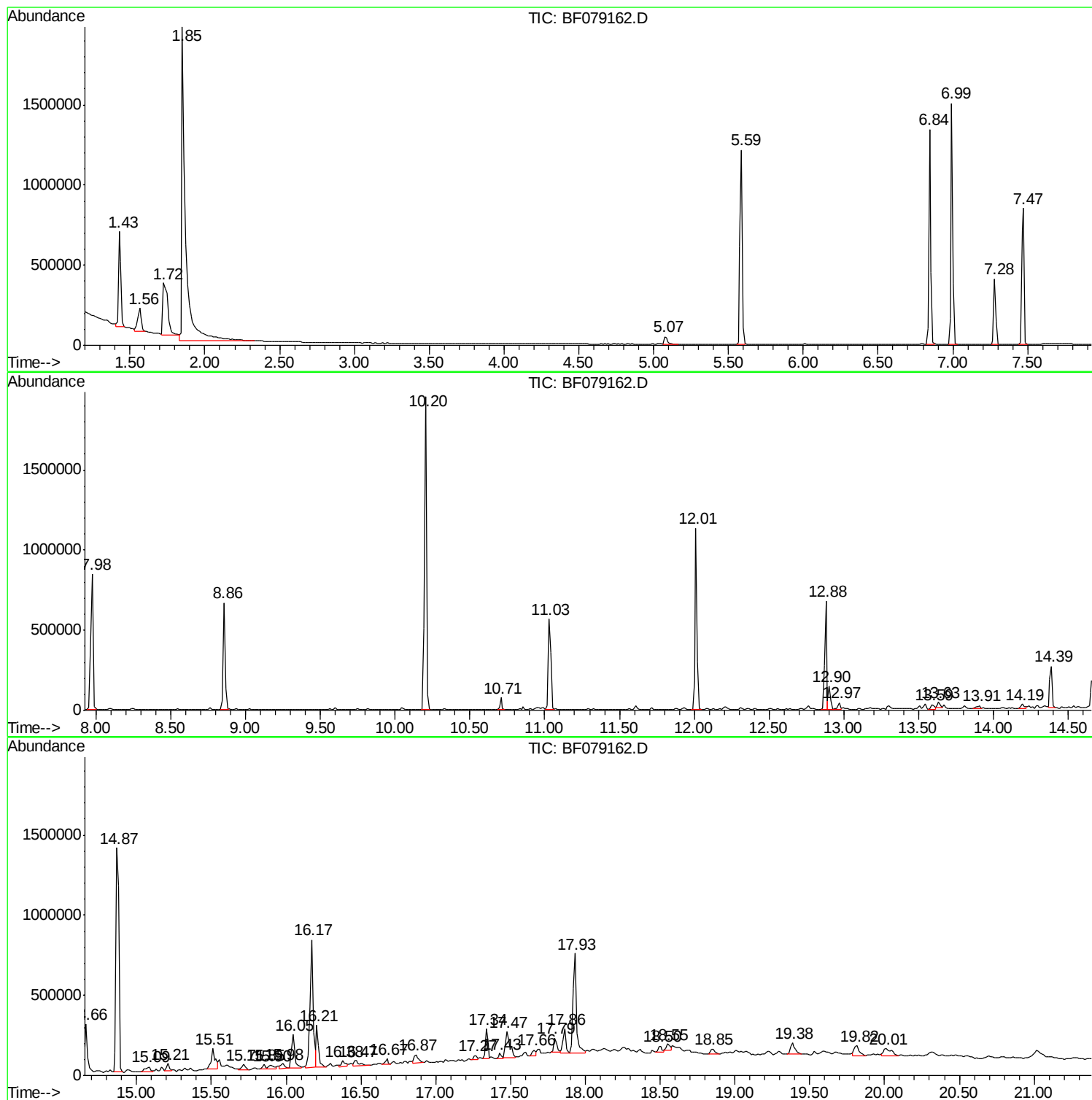
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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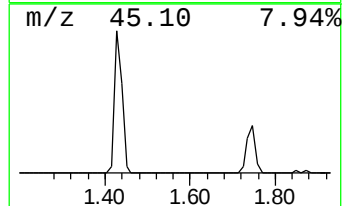
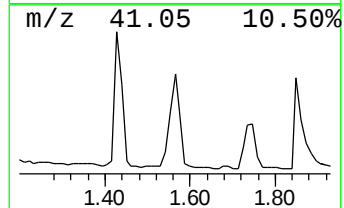
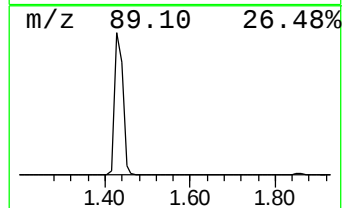
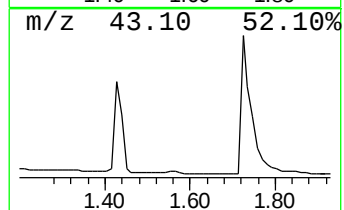
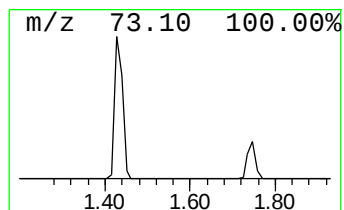
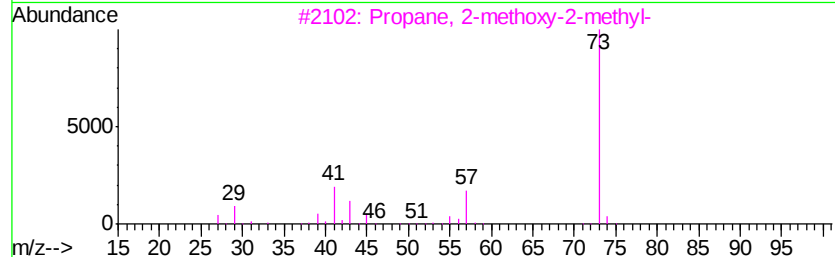
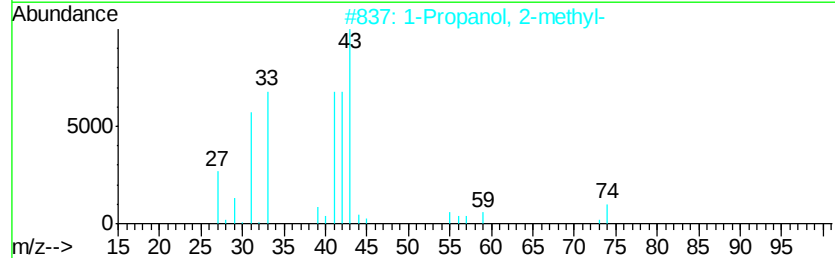
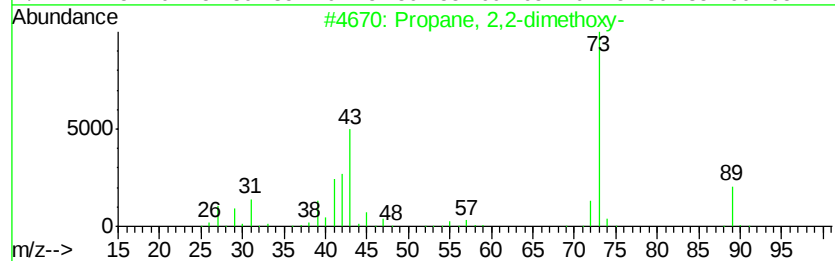
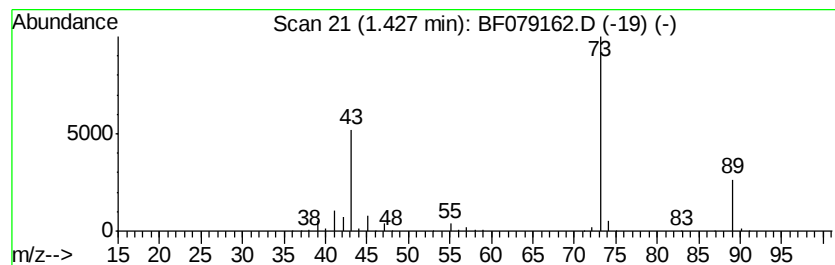
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.43	36.25 ng	723102	1,4-Dichlorobenzene-d4	7.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
5		2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	7



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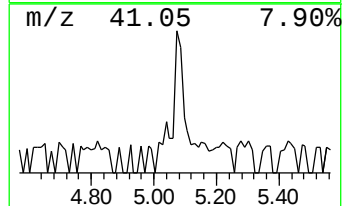
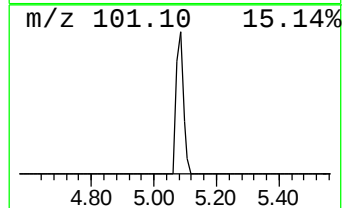
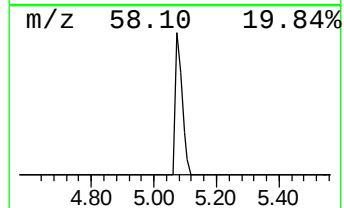
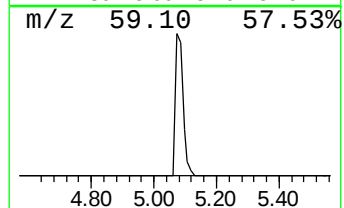
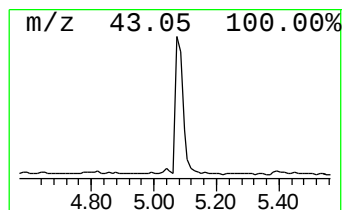
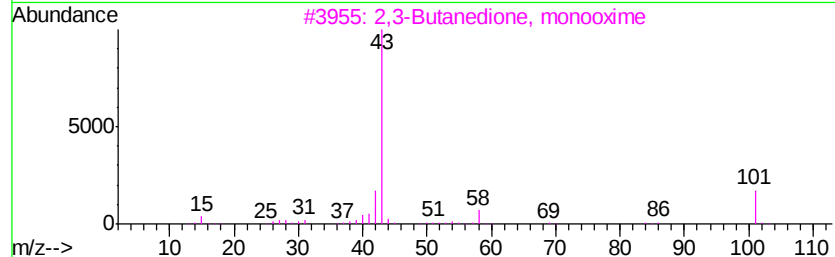
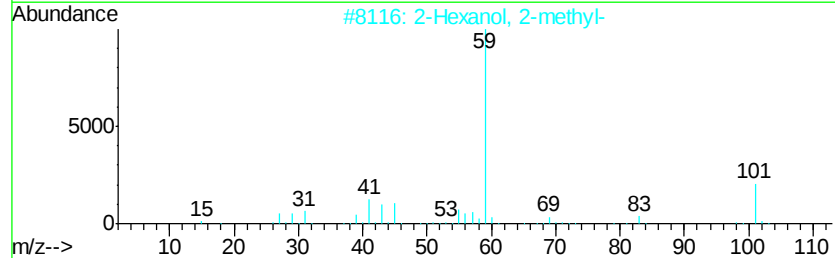
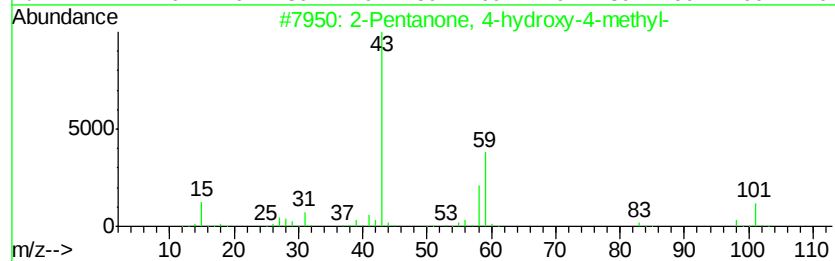
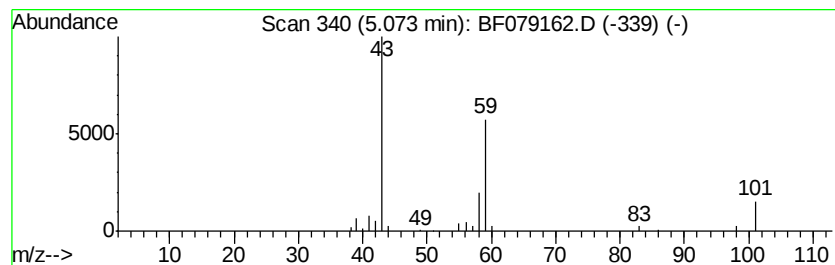
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	3.74 ng	74646	1,4-Dichlorobenzene-d4	7.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12		
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10		
5	Acetone	58	C3H6O	000067-64-1	9		



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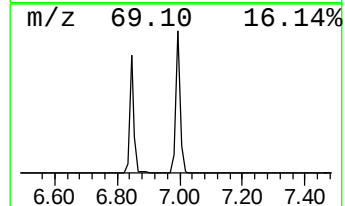
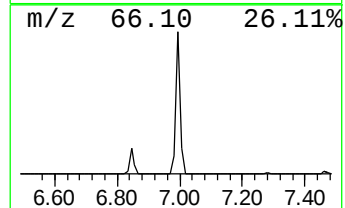
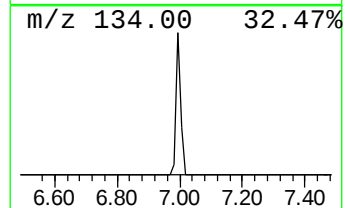
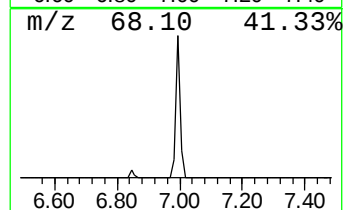
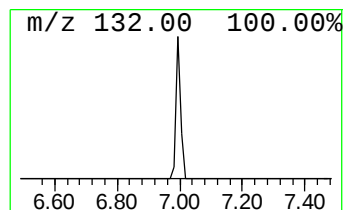
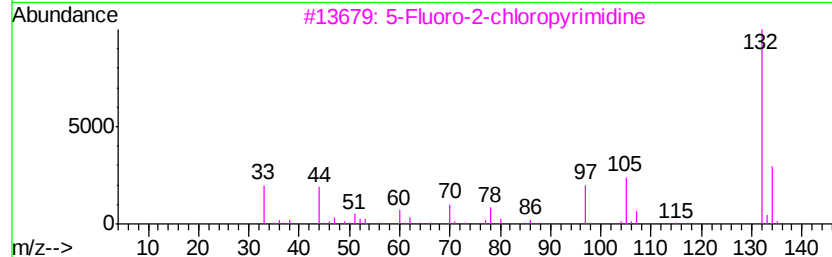
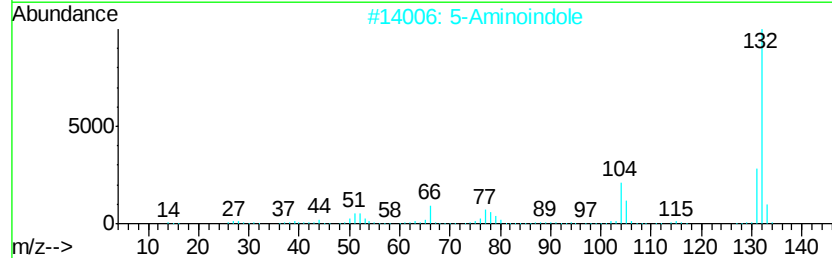
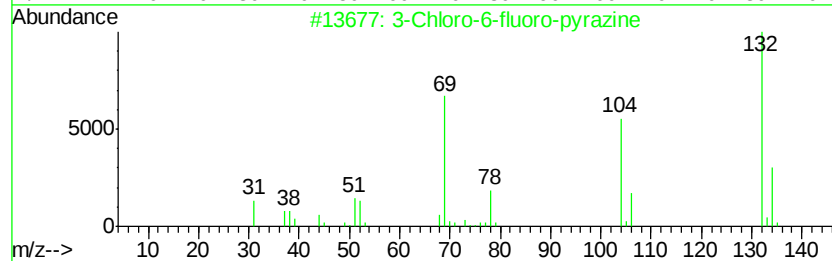
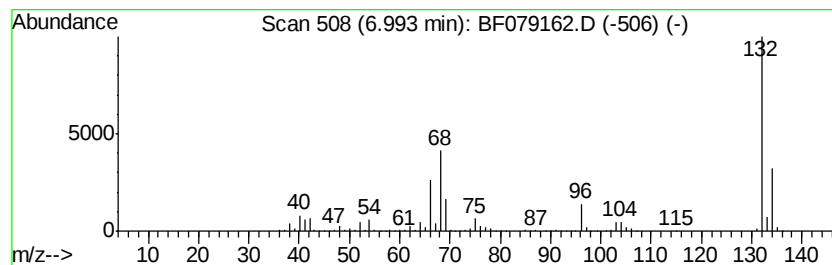
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.99 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.99	70.76 ng	1411490	1,4-Dichlorobenzene-d4	7.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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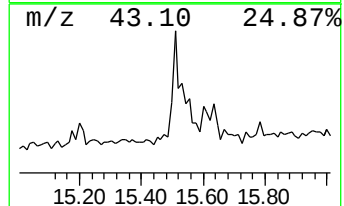
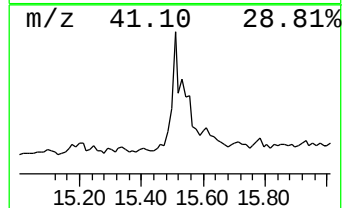
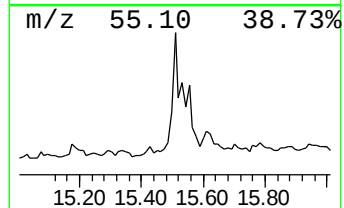
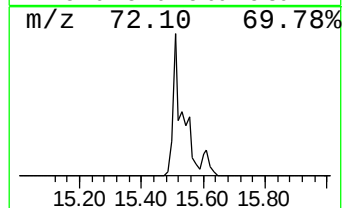
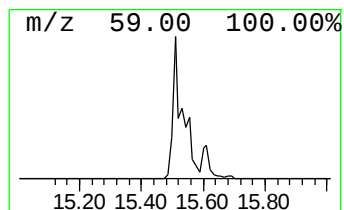
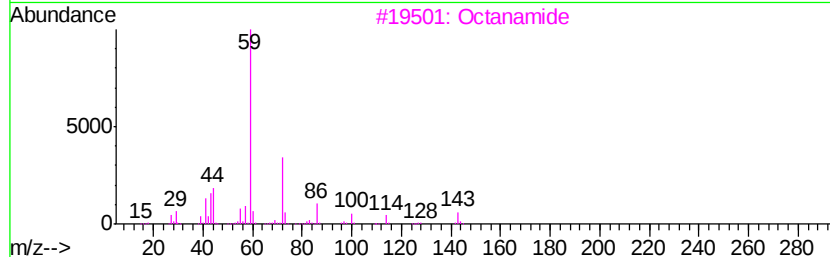
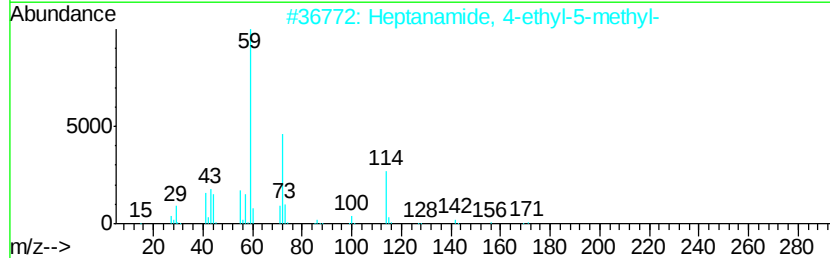
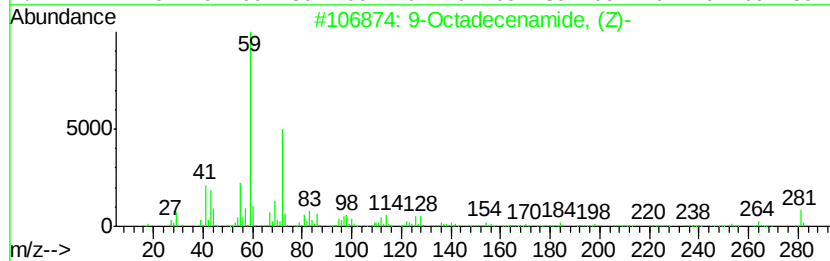
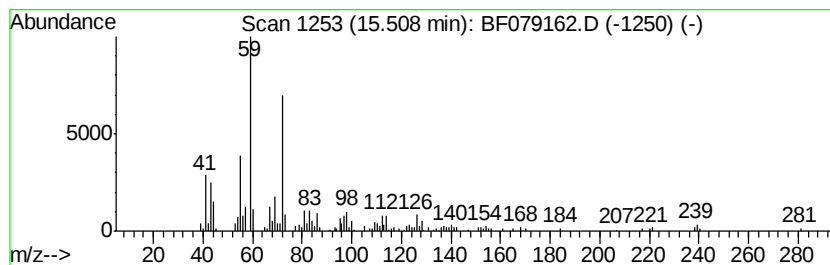
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.51	4.59 ng	249008	Chrysene-d12	16.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
3		Octanamide	143	C8H17NO	000629-01-6	59
4		Nonanamide	157	C9H19NO	001120-07-6	53
5		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50



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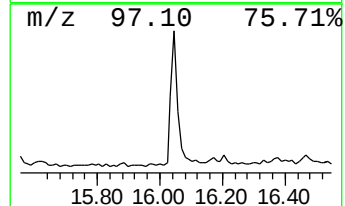
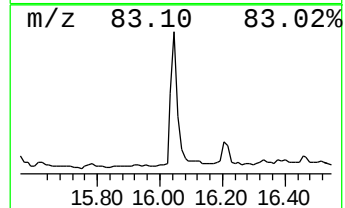
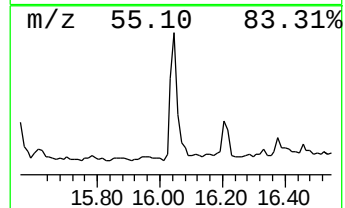
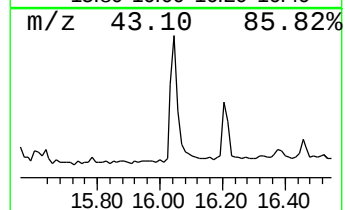
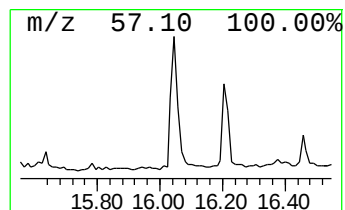
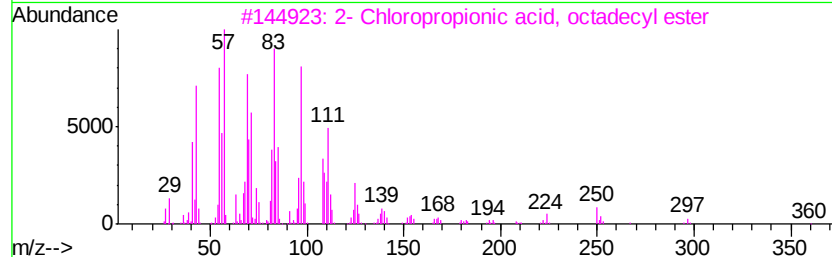
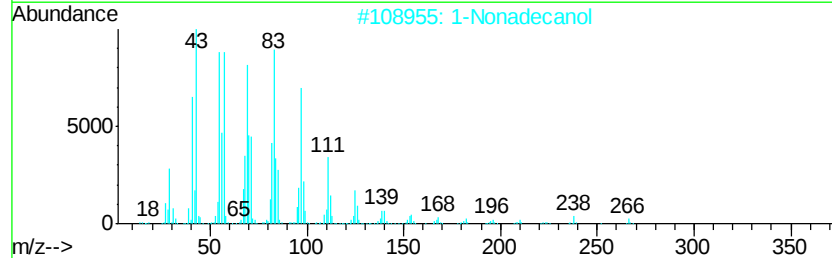
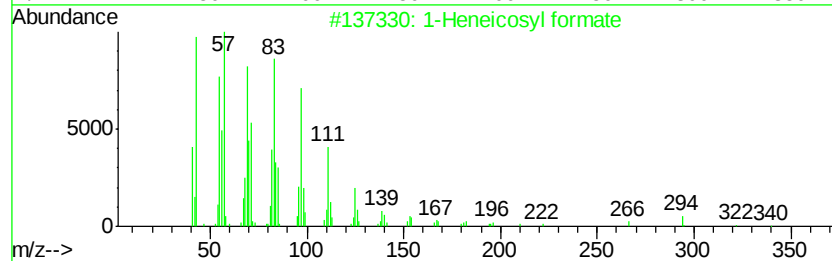
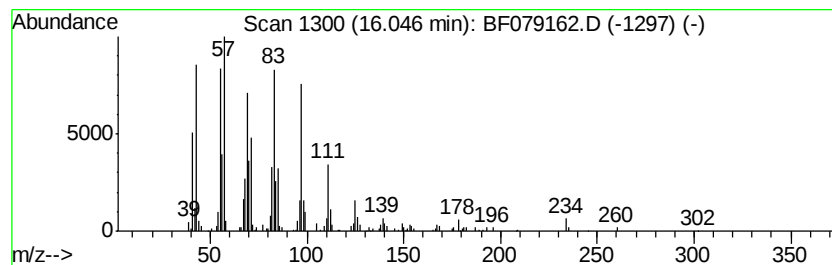
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosyl formate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	6.07 ng	329025	Chrysene-d12	16.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2		1-Nonadecanol	284	C19H40O	001454-84-8	95
3		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051215\
Data File : BF079162.D
Acq On : 12 May 2015 17:21
Operator : TP/IZ
Sample : G2155-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-42S

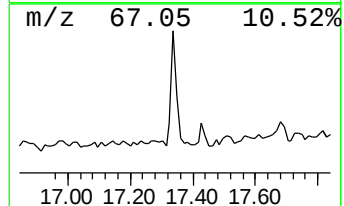
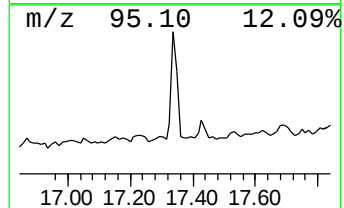
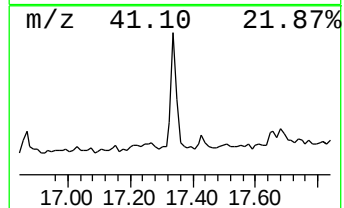
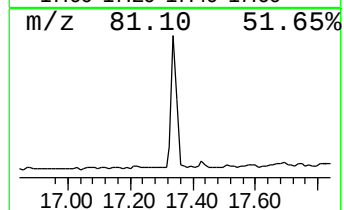
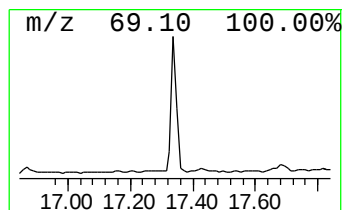
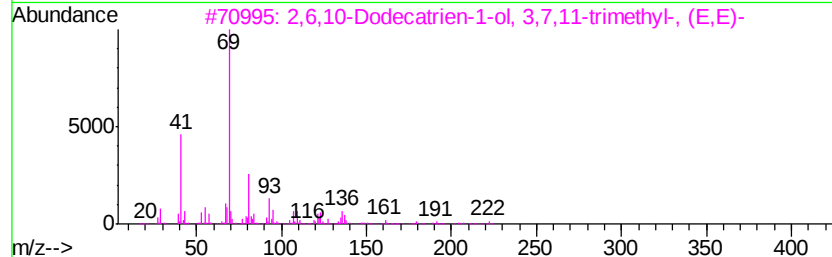
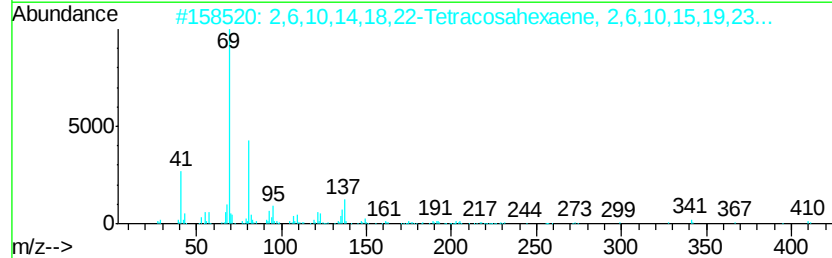
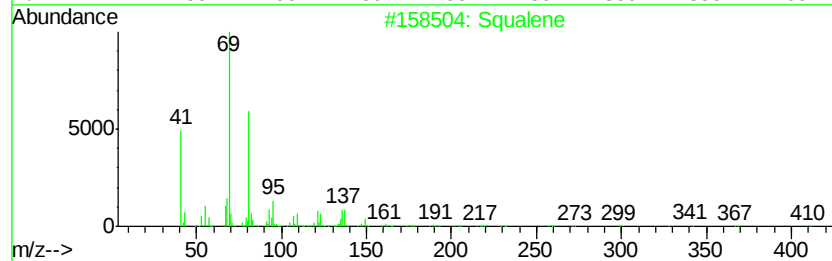
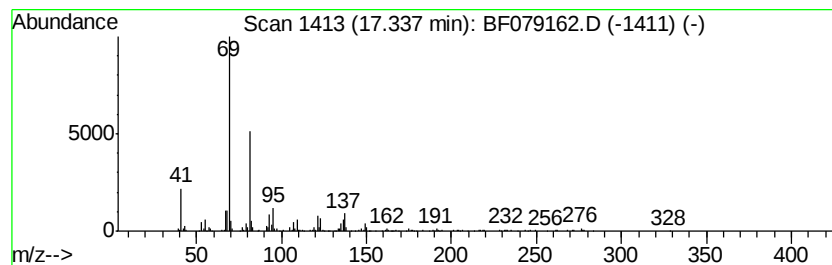
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.34	4.94 ng	222787	Perylene-d12	17.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	72
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5		(E)-all-trans-3,7,11-Trimethyl-2...	235	C15H25NO	1000161-30-7	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051215\
Data File : BF079162.D
Acq On : 12 May 2015 17:21
Operator : TP/IZ
Sample : G2155-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-42S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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
Propane, 2,2-dime...	1.43	36.3	ng	723102	1	7.28	398929	20.0
2-Pentanone, 4-hy...	5.07	3.7	ng	74646	1	7.28	398929	20.0
unknown6.99	6.99	70.8	ng	1411490	1	7.28	398929	20.0
9-Octadecenamamide,...	15.51	4.6	ng	249008	5	16.17	1084230	20.0
1-Heneicosyl formate	16.05	6.1	ng	329025	5	16.17	1084230	20.0
Squalene	17.34	4.9	ng	222787	6	17.93	901906	20.0