

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071516\
 Data File : BF089041.D
 Acq On : 16 Jul 2016 5:03
 Operator : UM/SJ
 Sample : H4048-04
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02-COMP

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-BF063016.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	1.655	4	6	15	rVV	120310	209461	14.09%	1.295%
2	1.770	15	16	24	rVV	993862	1441362	96.95%	8.912%
3	1.873	24	25	41	rVB3	48298	139964	9.41%	0.865%
4	4.261	232	234	236	rBB	18519	20913	1.41%	0.129%
5	4.821	281	283	289	rBB	136335	209263	14.08%	1.294%
6	5.279	320	323	325	rBV	1070117	1469946	98.88%	9.088%
7	6.330	412	415	417	rBV	1351456	1442781	97.05%	8.920%
8	6.444	422	425	428	rBV	1492010	1389314	93.45%	8.590%
9	6.673	443	445	448	rBV	465877	387376	26.06%	2.395%
10	6.833	456	459	461	rVB	1377038	1212823	81.58%	7.499%
11	7.244	492	495	497	rBV	967350	957510	64.41%	5.920%
12	7.359	503	505	508	rVB	16167	19319	1.30%	0.119%
13	7.965	555	558	560	rBV	449658	491349	33.05%	3.038%
14	9.039	649	652	654	rBV	1734121	1486646	100.00%	9.192%
15	9.439	684	687	689	rBV	740895	633434	42.61%	3.916%
16	9.713	708	711	712	rBV	413468	461789	31.06%	2.855%
17	10.159	748	750	751	rVB	25428	24762	1.67%	0.153%
18	10.376	765	769	770	rBV	10778	17746	1.19%	0.110%
19	10.491	777	779	782	rBV	700133	668910	44.99%	4.136%
20	10.628	789	791	794	rBV	33867	42909	2.89%	0.265%
21	11.073	828	830	831	rBV	33175	29731	2.00%	0.184%
22	11.188	837	840	843	rVV	295905	451574	30.38%	2.792%
23	11.256	843	846	848	rVB	41816	36740	2.47%	0.227%
24	11.428	858	861	865	rBV2	8438	19160	1.29%	0.118%
25	11.496	865	867	872	rVB	17451	20238	1.36%	0.125%
26	11.714	884	886	888	rVB	20644	20154	1.36%	0.125%
27	11.794	891	893	896	rBV	31493	44848	3.02%	0.277%
28	12.388	942	945	947	rBV	197078	170485	11.47%	1.054%
29	12.605	962	964	966	rBV	125495	180214	12.12%	1.114%
30	12.765	976	978	981	rVB	1115748	977470	65.75%	6.043%
31	12.936	990	993	996	rBV	18396	30869	2.08%	0.191%
32	13.005	997	999	1001	rVV2	20399	19576	1.32%	0.121%
33	13.039	1001	1002	1006	rVB3	15855	20755	1.40%	0.128%
34	13.257	1018	1021	1026	rBV2	58526	150166	10.10%	0.928%

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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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.325	1026	1027	1034	rVB2	17146	31314	2.11%	0.194%
36	13.439	1034	1037	1042	rBV2	9443	23902	1.61%	0.148%
37	13.599	1048	1051	1054	rBV2	6662	20039	1.35%	0.124%
38	13.679	1054	1058	1064	rVB3	45504	71405	4.80%	0.441%
39	13.805	1066	1069	1070	rBV2	425669	443200	29.81%	2.740%
40	13.908	1075	1078	1079	rBV2	19059	24965	1.68%	0.154%
41	13.931	1079	1080	1084	rVB4	13138	21286	1.43%	0.132%
42	14.285	1108	1111	1112	rBV2	8734	17280	1.16%	0.107%
43	14.319	1112	1114	1117	rVB3	12582	24926	1.68%	0.154%
44	14.514	1127	1131	1133	rBV5	5618	18358	1.23%	0.114%
45	14.651	1141	1143	1145	rVB	19095	21659	1.46%	0.134%
46	14.800	1153	1156	1160	rBV	55839	116927	7.87%	0.723%
47	14.891	1161	1164	1166	rVB	20176	25919	1.74%	0.160%
48	15.062	1176	1179	1181	rVB	28160	41774	2.81%	0.258%
49	15.108	1181	1183	1186	rBV	45610	57600	3.87%	0.356%
50	15.165	1186	1188	1191	rBV	193483	236653	15.92%	1.463%
51	15.600	1223	1226	1228	rBV	11372	21268	1.43%	0.131%
52	16.434	1297	1299	1303	rVB2	16453	28183	1.90%	0.174%
53	16.811	1330	1332	1337	rVB	13810	27797	1.87%	0.172%

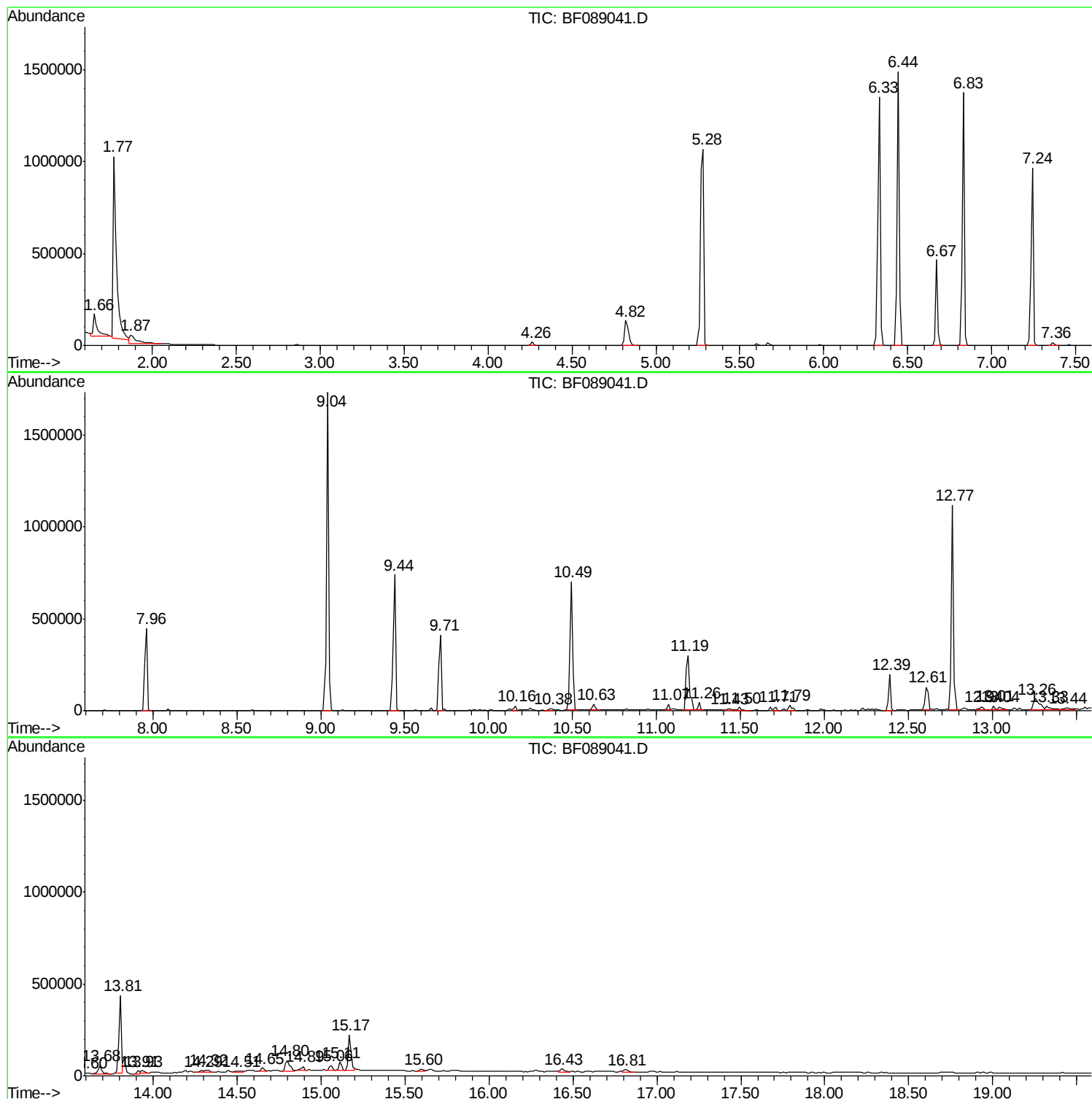
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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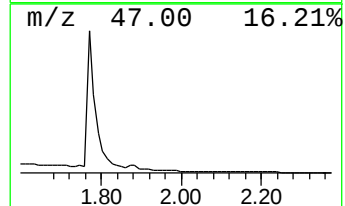
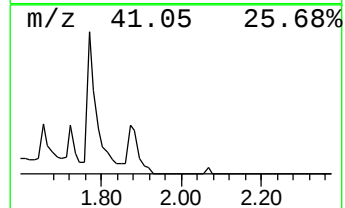
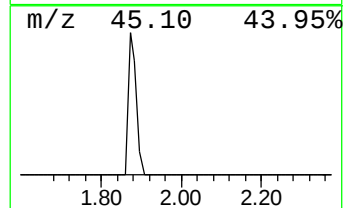
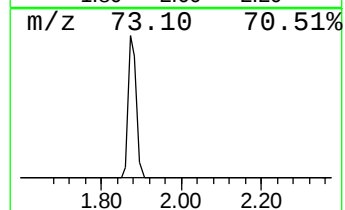
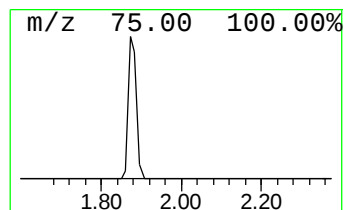
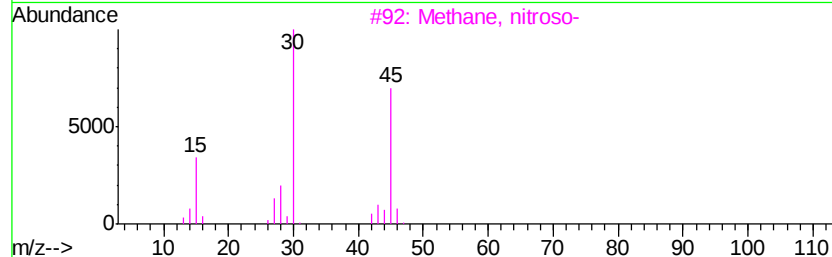
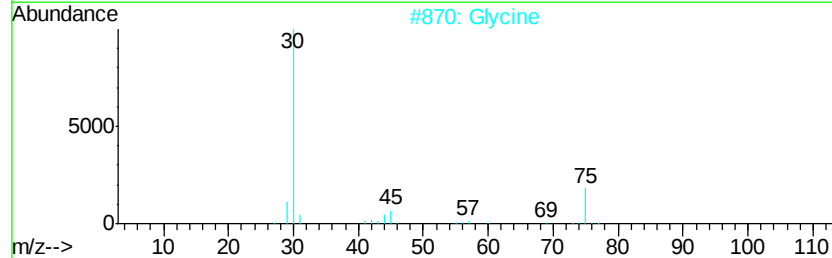
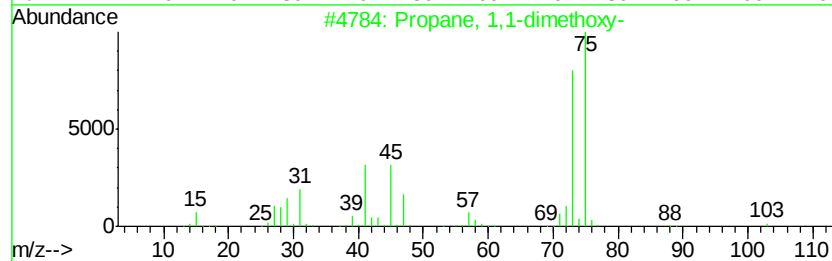
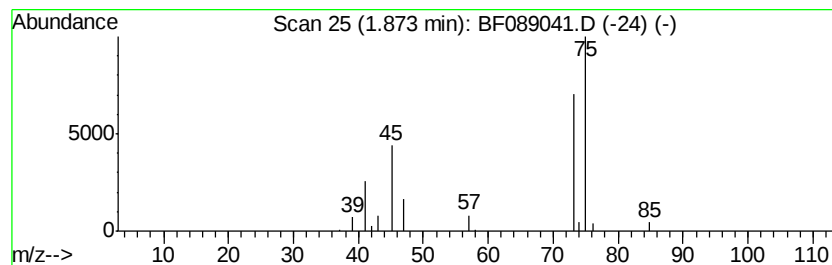
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.87	7.23 ng	139964	1,4-Dichlorobenzene-d4	6.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Glycine	75	C2H5NO2	000056-40-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			2-(3-Bromopropyl)-[1,3]dioxolane	194	C6H11BrO2	062563-07-9	4
5			Formamide, N-methylthio	75	C2H5NS	018952-41-5	4



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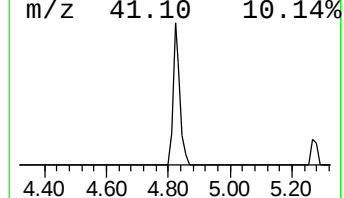
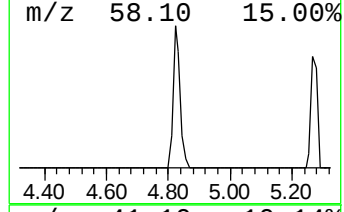
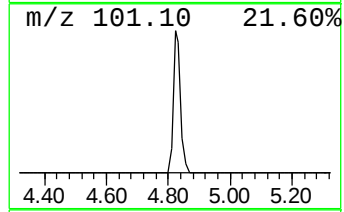
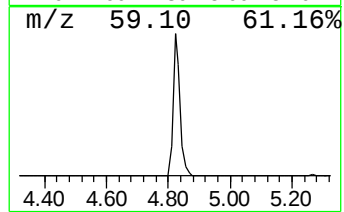
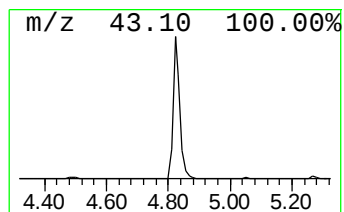
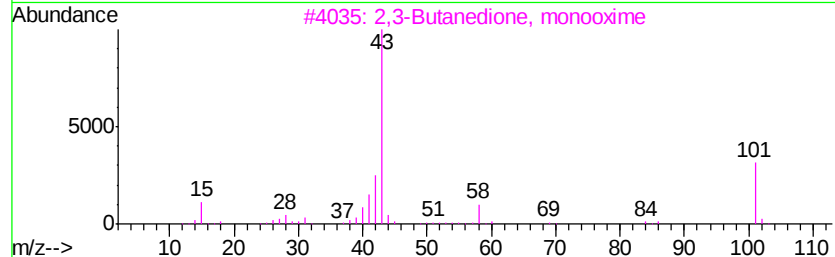
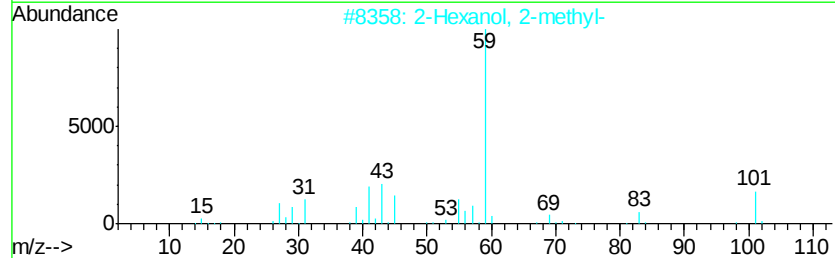
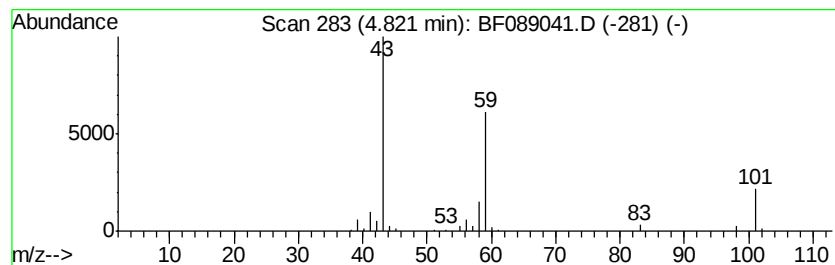
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	10.80 ng	209263	1,4-Dichlorobenzene-d4	6.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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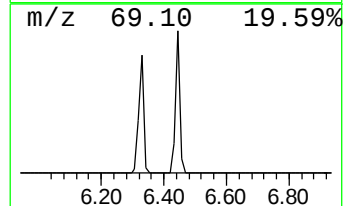
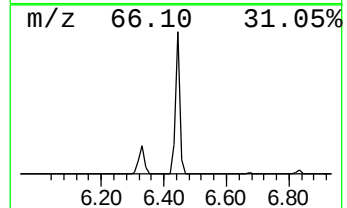
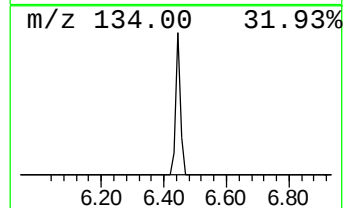
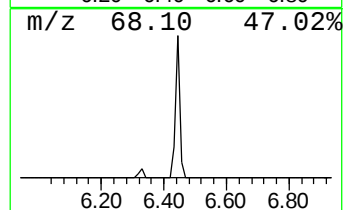
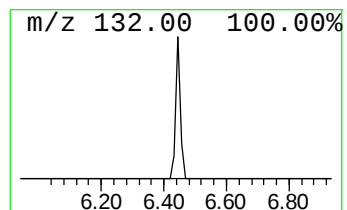
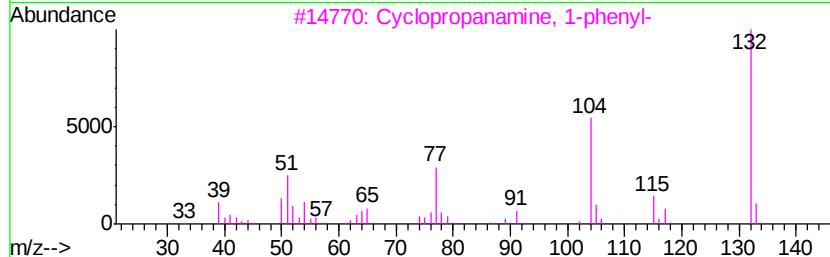
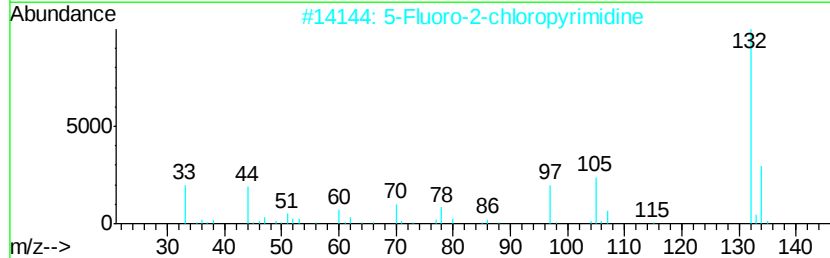
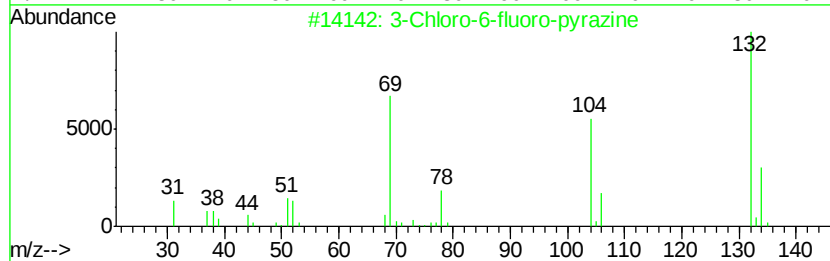
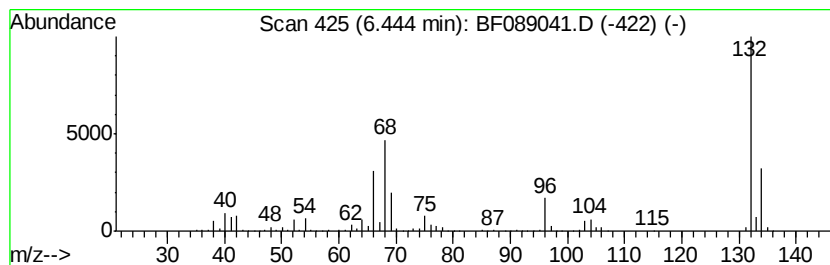
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.44 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	71.73 ng	1389310	1,4-Dichlorobenzene-d4	6.67

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	16
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		N-(-3,4-Methylenedioxyphenyl)isopropylamine	267	C17H17NO2	1000378-96-6	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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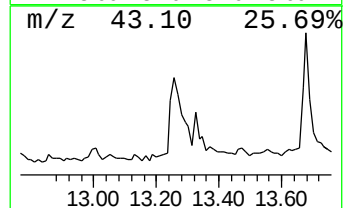
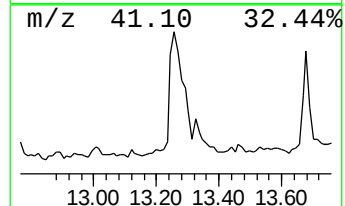
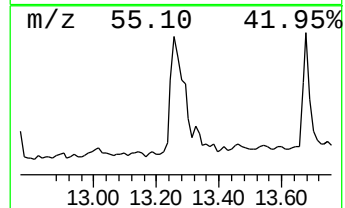
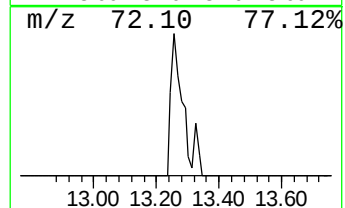
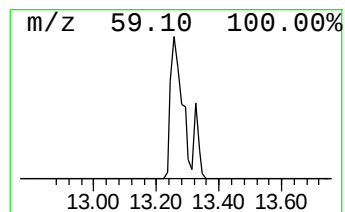
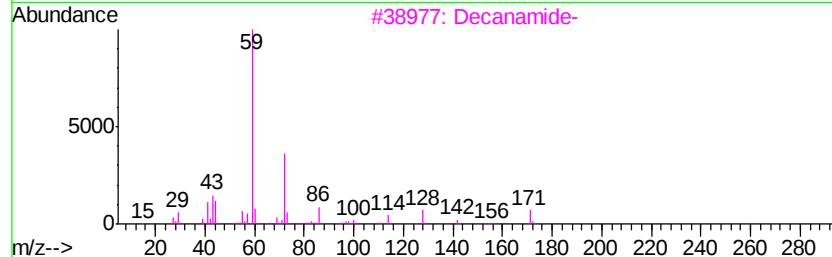
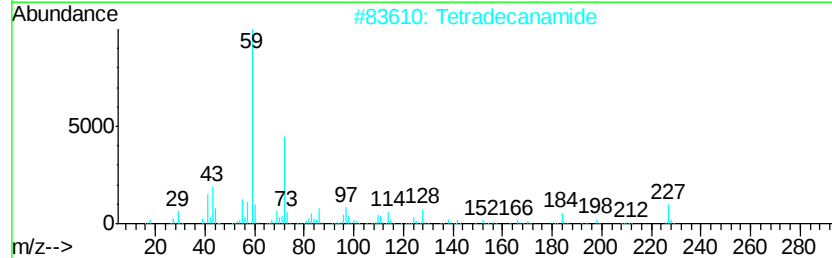
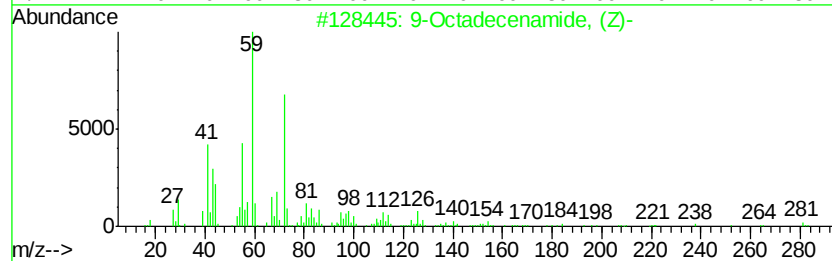
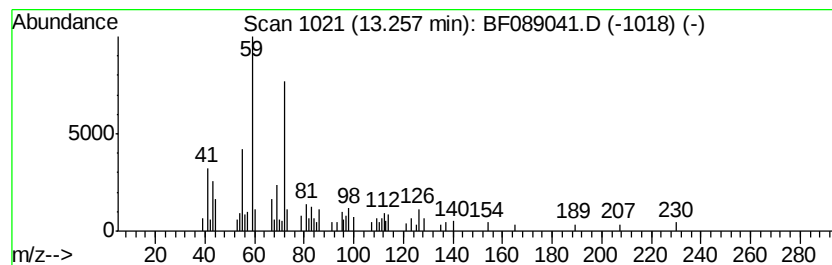
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.26	6.78 ng	150166	Chrysene-d12		13.81
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Tetradecanamide	227	C14H29NO	000638-58-4	50
3	Decanamide-	171	C10H21NO	002319-29-1	45
4	Dodecanamide	199	C12H25NO	001120-16-7	43
5	7-Nonenamide	155	C9H17NO	090949-53-4	42



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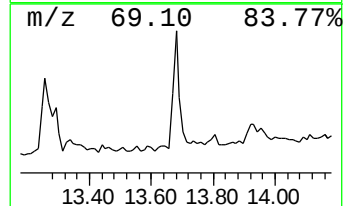
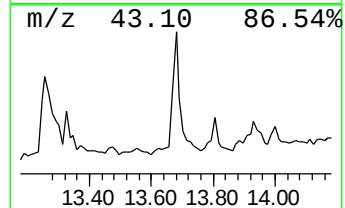
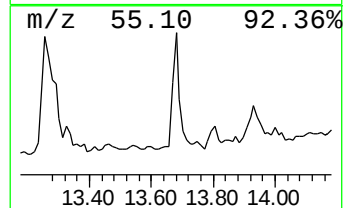
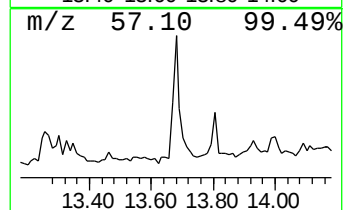
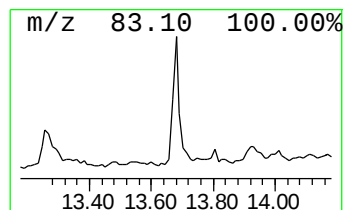
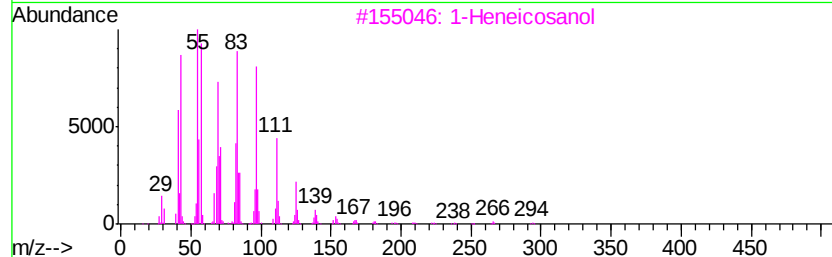
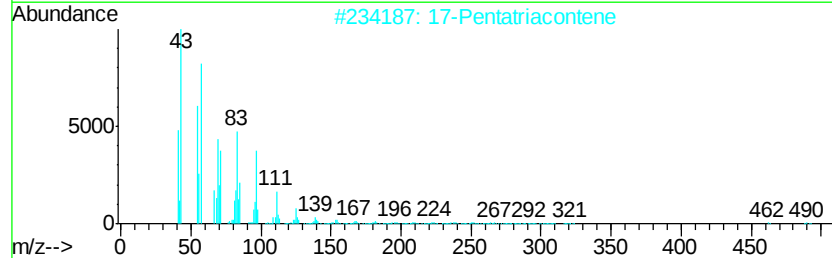
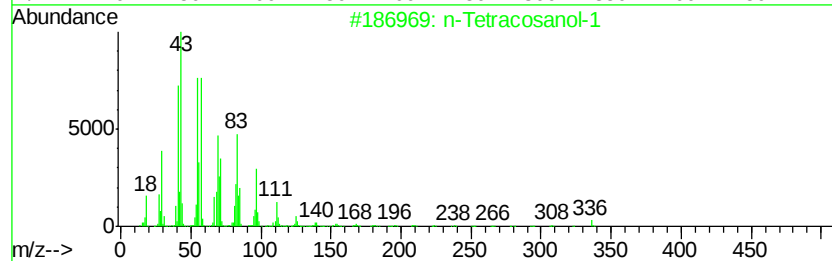
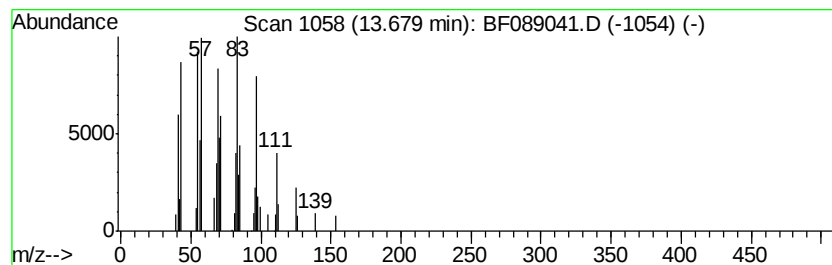
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 n-Tetracosanol-1 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	3.22 ng	71405	Chrysene-d12	13.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2			17-Pentatriacontene	491	C35H70	006971-40-0	91
3			1-Heneicosanol	312	C21H44O	015594-90-8	90
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071516\
Data File : BF089041.D
Acq On : 16 Jul 2016 5:03
Operator : UM/SJ
Sample : H4048-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.87	7.2	ng	139964	1	6.67	387376	20.0
2-Pentanone, 4-hy...	4.82	10.8	ng	209263	1	6.67	387376	20.0
unknown6.44	6.44	71.7	ng	1389310	1	6.67	387376	20.0
9-Octadecenamide, ...	13.26	6.8	ng	150166	5	13.81	443200	20.0
n-Tetracosanol-1	13.68	3.2	ng	71405	5	13.81	443200	20.0