

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080416\
 Data File : BF089608.D
 Acq On : 5 Aug 2016 2:26
 Operator : UM/SJ
 Sample : H4348-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1

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-BF080416.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	4.639	264	267	283	rBV	81767	165404	11.63%	1.645%
2	5.324	325	327	350	rBV	204477	448680	31.54%	4.463%
3	6.970	470	471	479	rBV2	115463	268638	18.88%	2.672%
4	7.085	479	481	503	rVB	678387	1020114	71.71%	10.148%
5	7.439	510	512	530	rBV2	116046	238890	16.79%	2.376%
6	7.679	530	533	549	rBV	639528	927251	65.18%	9.224%
7	8.353	589	592	621	rBV	394926	728500	51.21%	7.247%
8	9.473	687	690	712	rBV	189371	351021	24.68%	3.492%
9	11.245	842	845	848	rBV	870893	1422502	100.00%	14.151%
10	11.942	904	906	915	rBB	36527	52409	3.68%	0.521%
11	12.285	934	936	939	rBV	275480	410305	28.84%	4.082%
12	12.399	944	946	949	rVB	16601	17632	1.24%	0.175%
13	12.879	980	988	998	rBV	248611	687095	48.30%	6.835%
14	13.154	1009	1012	1014	rVB	21034	27323	1.92%	0.272%
15	13.508	1039	1043	1047	rBV	7281	18393	1.29%	0.183%
16	13.577	1047	1049	1058	rBV	555613	826297	58.09%	8.220%
17	13.920	1073	1079	1087	rBV2	24627	51248	3.60%	0.510%
18	14.685	1144	1146	1155	rVB	292409	408972	28.75%	4.068%
19	15.691	1232	1234	1245	rBV	42207	81097	5.70%	0.807%
20	16.800	1328	1331	1340	rBV	14251	31718	2.23%	0.316%
21	17.051	1350	1353	1370	rBV	984566	1204854	84.70%	11.986%
22	18.331	1462	1465	1468	rBV	25569	59145	4.16%	0.588%
23	18.377	1468	1469	1476	rVB	226532	331022	23.27%	3.293%
24	19.543	1568	1571	1573	rBV	21400	29014	2.04%	0.289%
25	20.046	1612	1615	1624	rBV	149211	244927	17.22%	2.436%

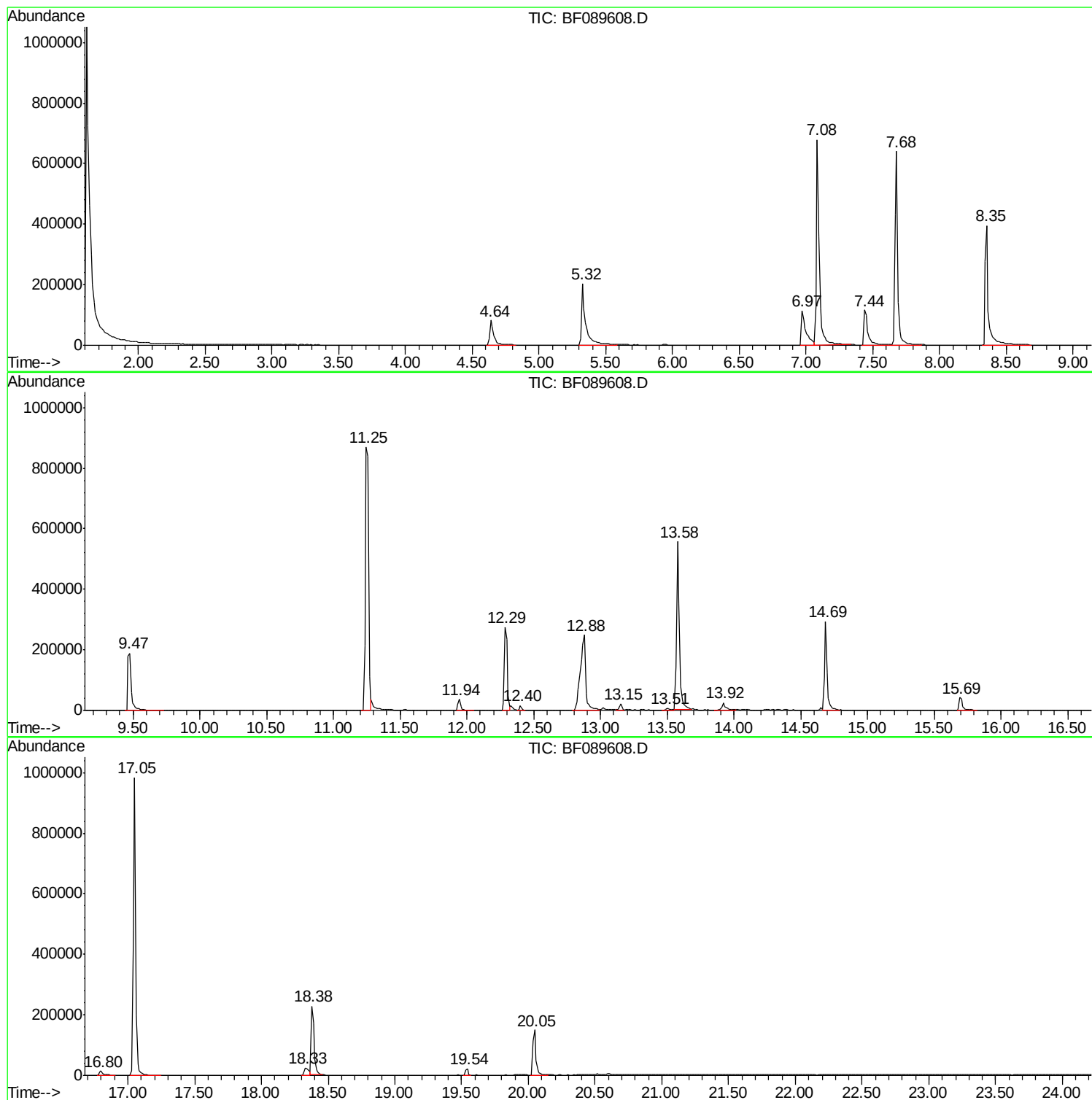
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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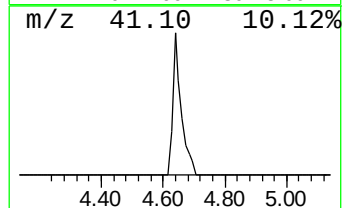
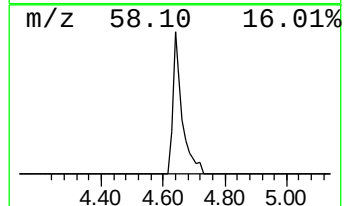
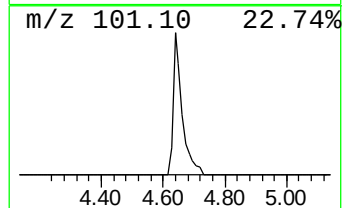
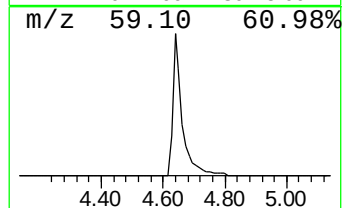
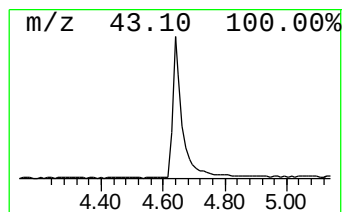
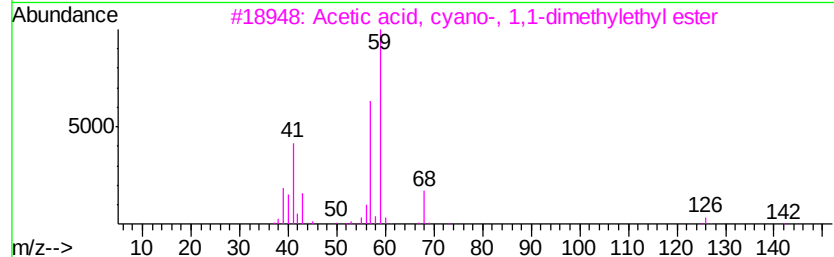
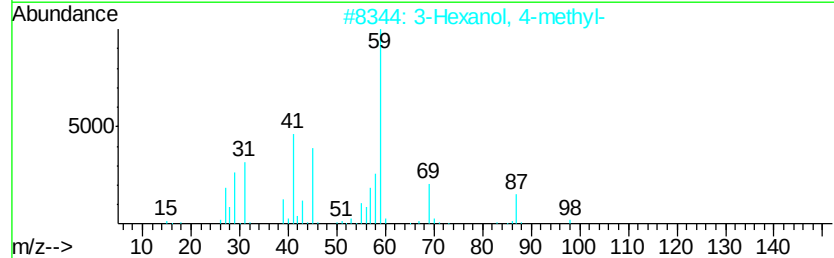
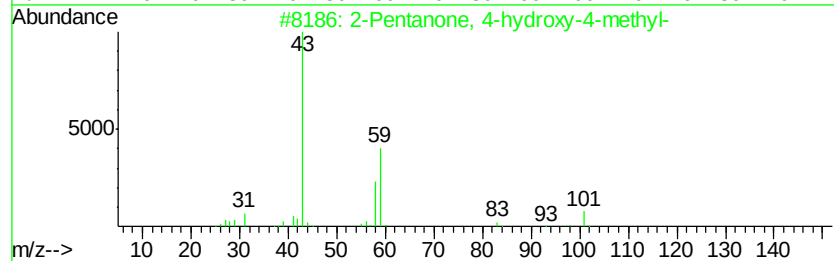
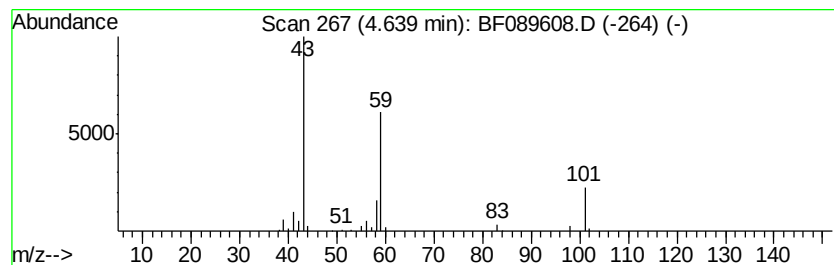
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	13.85 ng	165404	1,4-Dichlorobenzene-d4	7.44

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Acetone	58	C3H6O	000067-64-1	9



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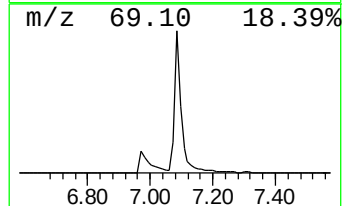
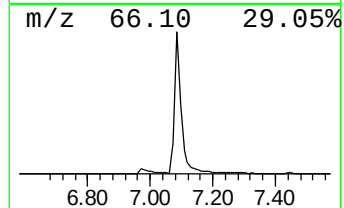
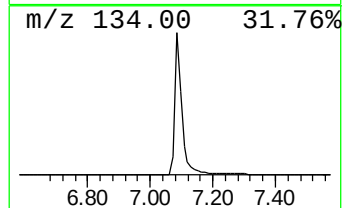
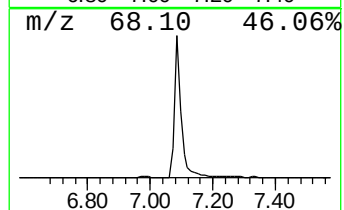
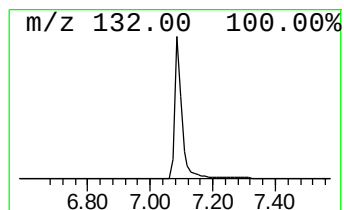
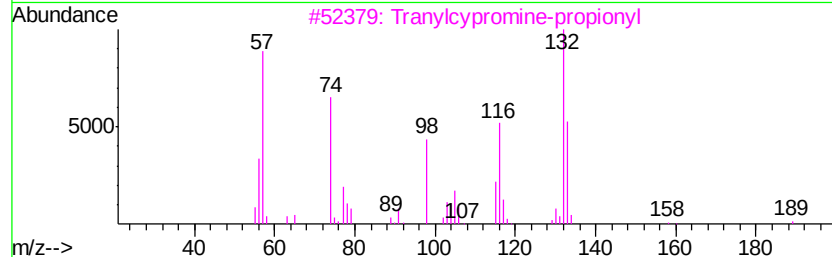
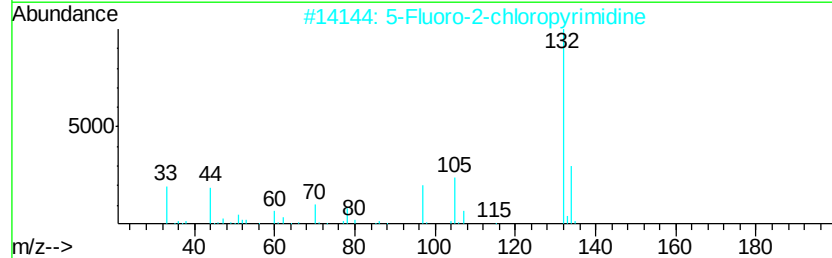
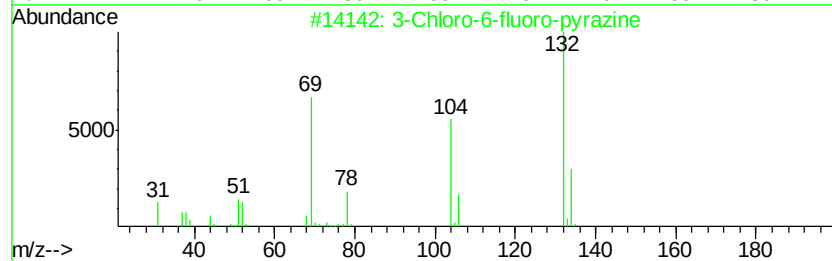
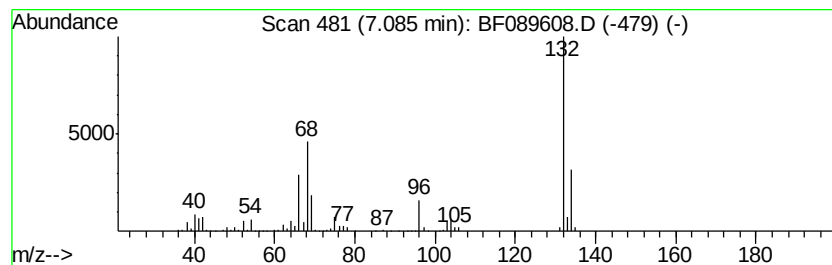
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Peak Number 2 unknown7.08 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	85.40 ng	1020110	1,4-Dichlorobenzene-d4	7.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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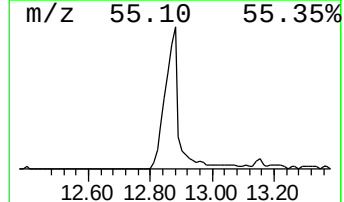
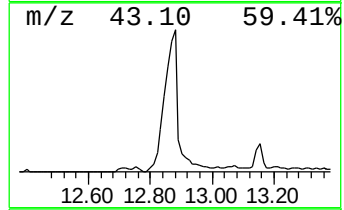
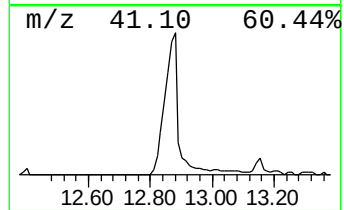
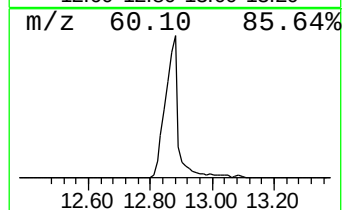
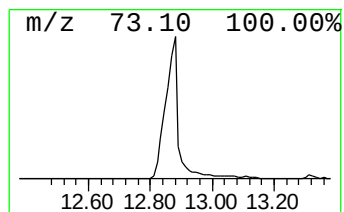
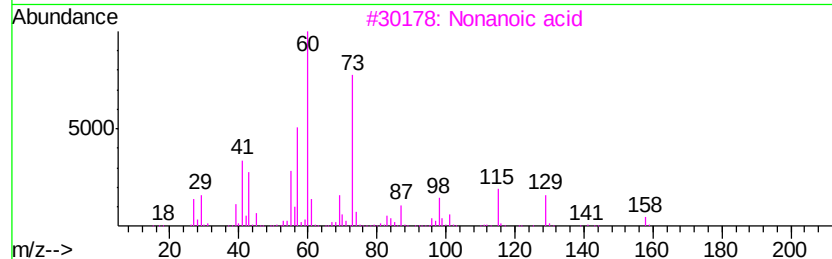
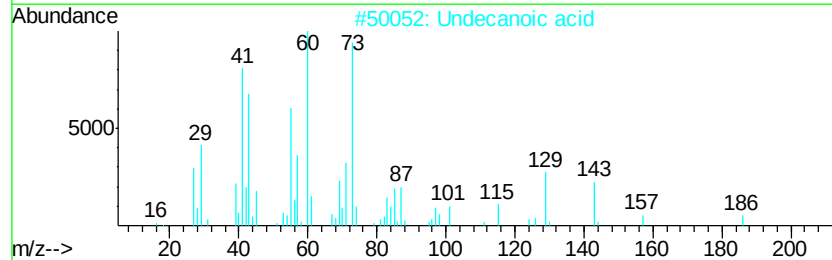
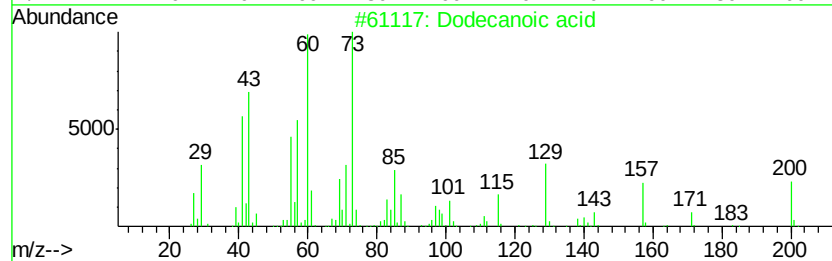
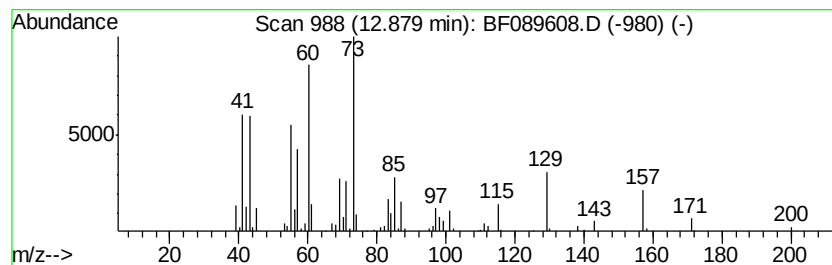
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Peak Number 4 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.88	33.49 ng	687095	Acenaphthene-d10	12.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecanoic acid	200 C12H24O2	000143-07-7	93
2	Undecanoic acid	186 C11H22O2	000112-37-8	64
3	Nonanoic acid	158 C9H18O2	000112-05-0	53
4	Maltose	342 C12H22O11	000069-79-4	50
5	.alpha.-D-Glucopyranose, 4-O-.be...	342 C12H22O11	014641-93-1	43



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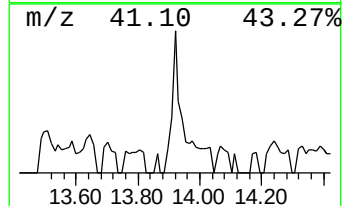
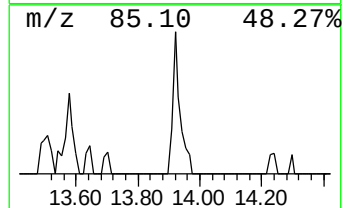
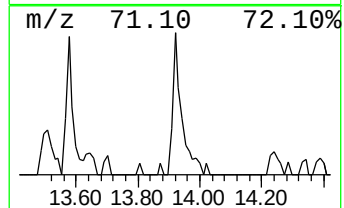
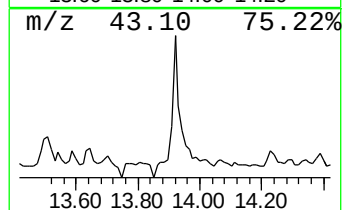
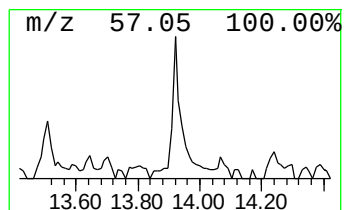
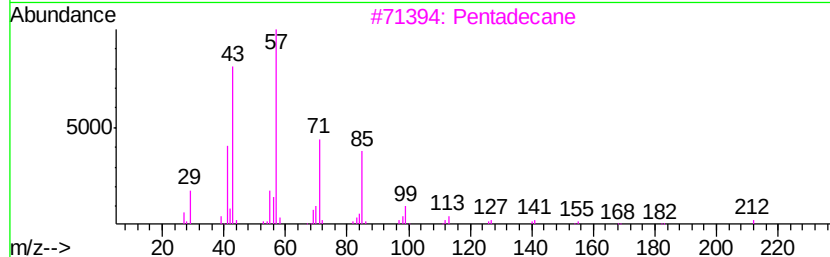
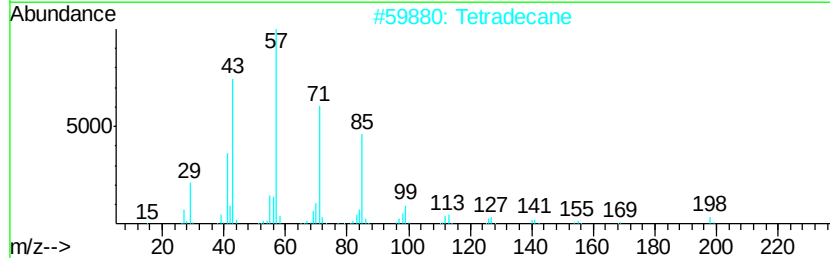
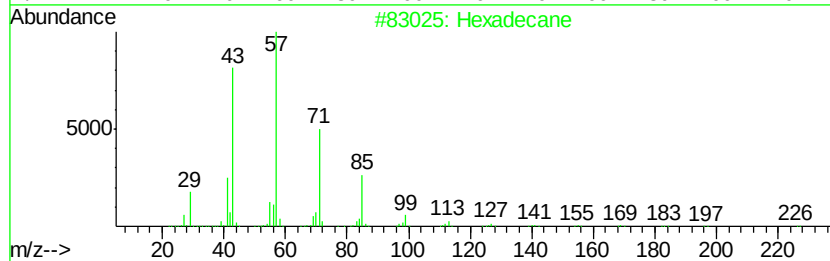
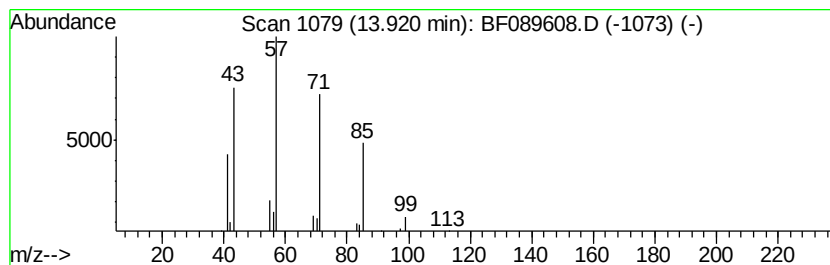
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Peak Number 5 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.92	2.51 ng	51248	Phenanthrene-d10	14.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	78
2	Tetradecane	198	C14H30	000629-59-4	64
3	Pentadecane	212	C15H32	000629-62-9	64
4	Tridecane	184	C13H28	000629-50-5	64
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	59



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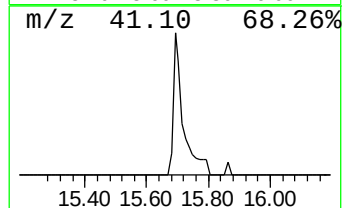
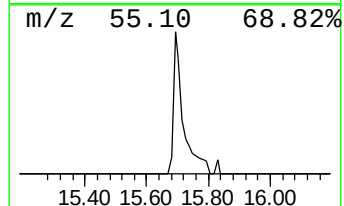
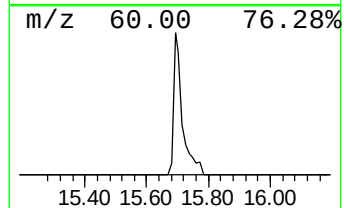
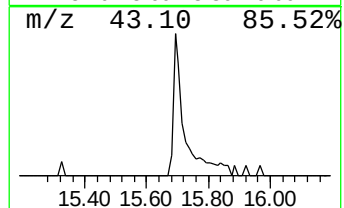
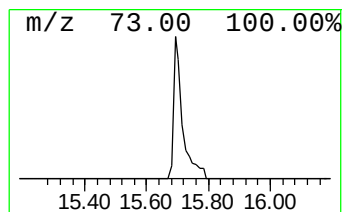
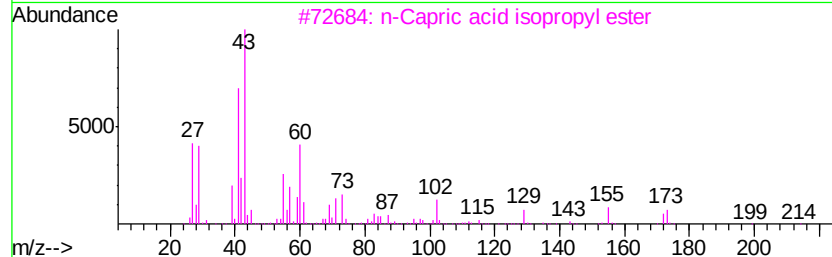
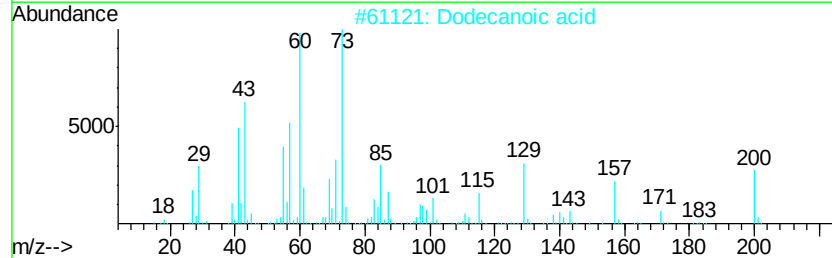
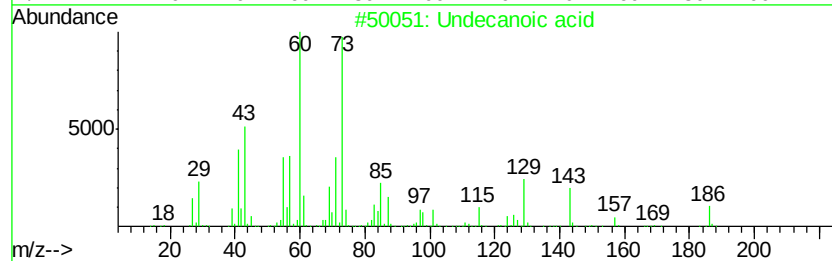
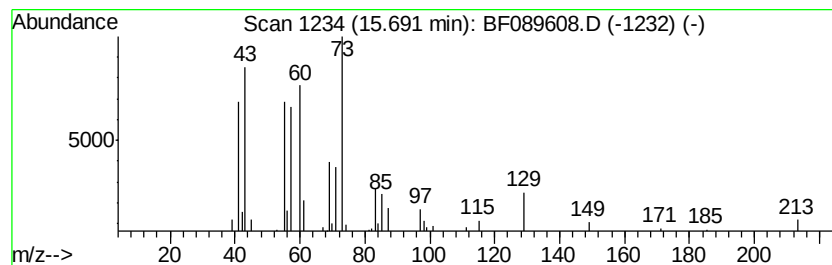
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Peak Number 6 Undecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	3.97 ng	81097	Phenanthrene-d10	14.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	Dodecanoic acid	200	C12H24O2	000143-07-7	59
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	53
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	.beta.-D-Glucopyranoside, methyl...	292	C14H28O6	1000157-04-9	50



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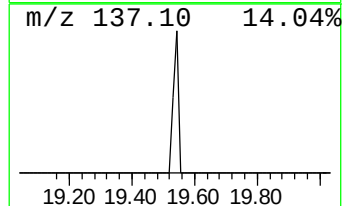
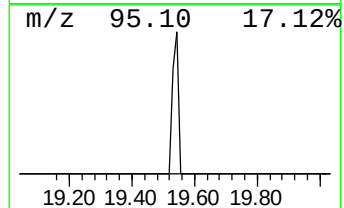
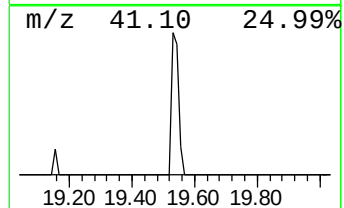
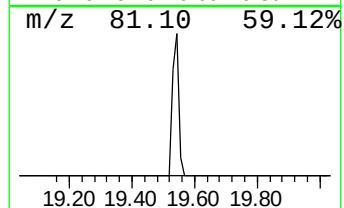
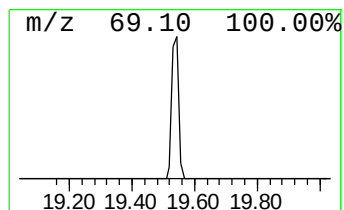
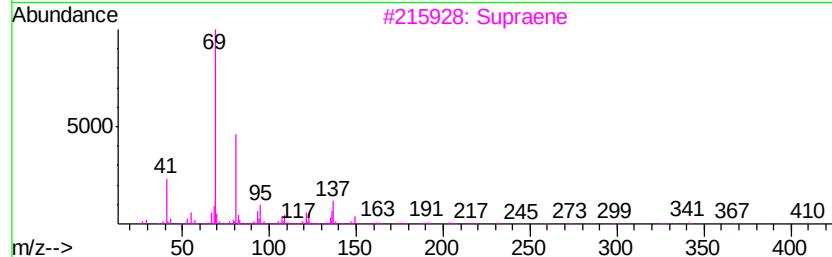
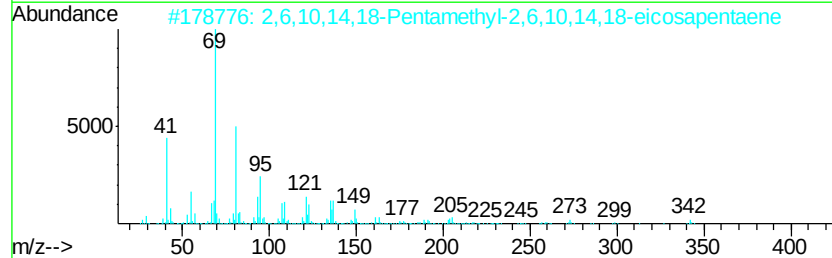
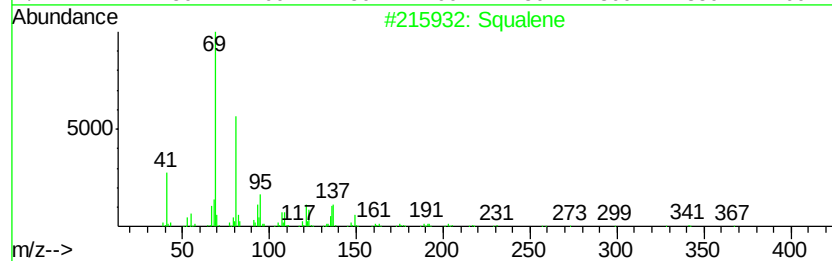
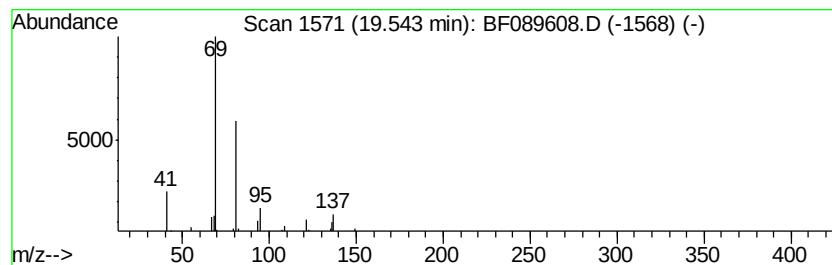
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.54	2.37 ng	29014	Perylene-d12	20.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	90
2		2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	90
3		Supraene	410	C30H50	007683-64-9	90
4		trans-Farnesol	222	C15H26O	000106-28-5	72
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	56



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080416\
Data File : BF089608.D
Acq On : 5 Aug 2016 2:26
Operator : UM/SJ
Sample : H4348-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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
2-Pentanone, 4-hy...	4.64	13.9	ng	165404	1	7.44	238890	20.0
unknown7.08	7.08	85.4	ng	1020110	1	7.44	238890	20.0
Dodecanoic acid	12.88	33.5	ng	687095	3	12.29	410305	20.0
Hexadecane	13.92	2.5	ng	51248	4	14.69	408972	20.0
Undecanoic acid	15.69	4.0	ng	81097	4	14.69	408972	20.0
Squalene	19.54	2.4	ng	29014	6	20.05	244927	20.0