

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090116\
 Data File : BF089967.D
 Acq On : 1 Sep 2016 13:07
 Operator : UM/SJ
 Sample : H4635-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GW-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-BF083116.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	1.633	3	4	13	rVV	405624	805568	12.98%	1.674%
2	1.747	13	14	50	rVB	2266555	6204503	100.00%	12.889%
3	4.764	275	278	284	rBV	566313	778777	12.55%	1.618%
4	5.210	314	317	320	rBV	2691591	3285455	52.95%	6.825%
5	6.273	407	410	412	rBV	2567403	2310637	37.24%	4.800%
6	6.399	418	421	424	rBV	3906447	4092532	65.96%	8.502%
7	6.639	439	442	444	rBV	1029787	1124217	18.12%	2.335%
8	6.787	453	455	458	rVB	2855842	3836442	61.83%	7.970%
9	6.925	463	467	471	rVB2	37693	62263	1.00%	0.129%
10	7.199	488	491	493	rBV	2385623	3095949	49.90%	6.432%
11	7.668	526	532	537	rBV2	39102	90728	1.46%	0.188%
12	7.919	552	554	556	rBV	1692391	1448314	23.34%	3.009%
13	7.999	560	561	563	rVV	61041	84902	1.37%	0.176%
14	8.045	563	565	567	rVB3	50702	63671	1.03%	0.132%
15	8.296	582	587	591	rBV7	18330	66975	1.08%	0.139%
16	8.365	591	593	595	rBV	193554	190222	3.07%	0.395%
17	8.959	642	645	646	rBV	183088	172203	2.78%	0.358%
18	9.005	646	649	651	rVB	4636044	5792195	93.35%	12.033%
19	9.073	653	655	657	rBV3	32164	66958	1.08%	0.139%
20	9.393	681	683	686	rVB2	491547	582326	9.39%	1.210%
21	9.519	691	694	697	rBV2	47538	76540	1.23%	0.159%
22	9.668	704	707	709	rBV	1593616	1645366	26.52%	3.418%
23	10.342	763	766	767	rBV	114657	150157	2.42%	0.312%
24	10.445	772	775	778	rBV	2574495	2813816	45.35%	5.845%
25	10.571	784	786	787	rBV	211829	219895	3.54%	0.457%
26	10.605	787	789	791	rVB	352047	364544	5.88%	0.757%
27	10.891	812	814	816	rVB	113921	98880	1.59%	0.205%
28	11.062	828	829	832	rVB	117724	103007	1.66%	0.214%
29	11.131	833	835	838	rVV	1312432	1400647	22.57%	2.910%
30	11.691	881	884	887	rBV2	53694	106979	1.72%	0.222%
31	11.988	908	910	915	rVB	52889	67142	1.08%	0.139%
32	12.342	938	941	943	rBV	604194	671352	10.82%	1.395%
33	12.388	943	945	947	rVB2	48151	62359	1.01%	0.130%
34	12.559	958	960	962	rBV	73859	63670	1.03%	0.132%

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Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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35	12.719	971	974	976	rBV	3878685	3591250	57.88%	7.461%
36	13.634	1052	1054	1061	rVB	63215	91488	1.47%	0.190%
37	13.748	1061	1064	1072	rBV	1418128	1290592	20.80%	2.681%
38	15.097	1179	1182	1185	rBV	1068423	1164092	18.76%	2.418%

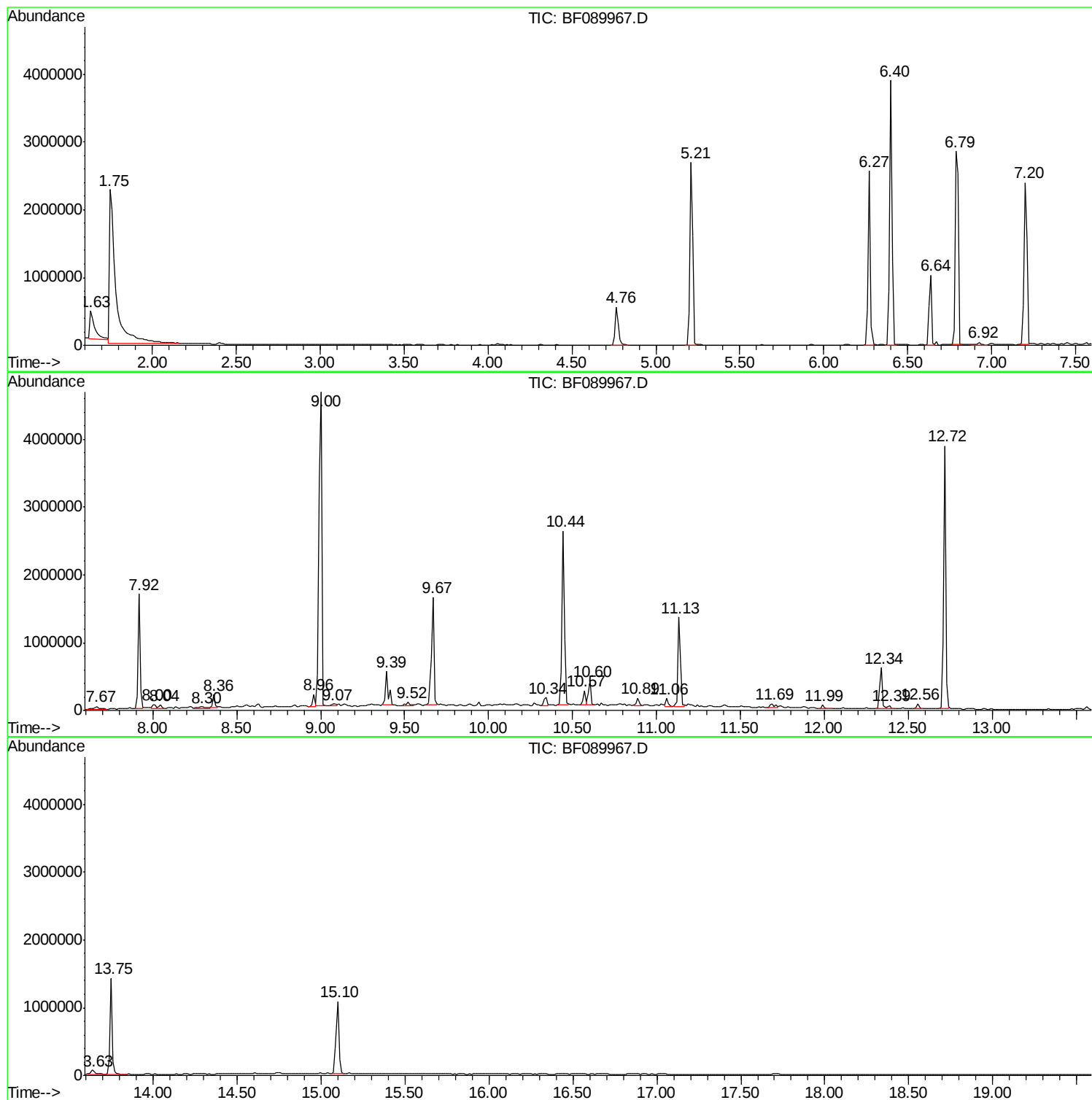
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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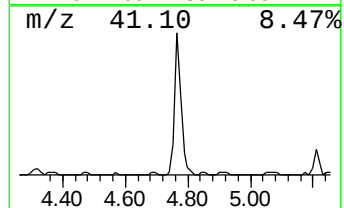
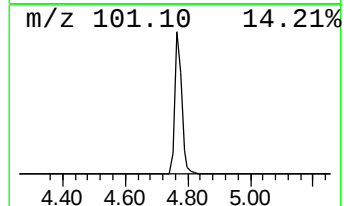
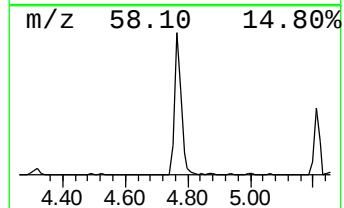
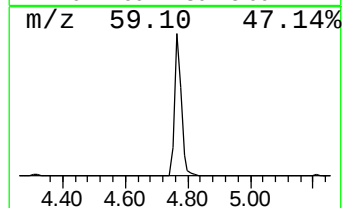
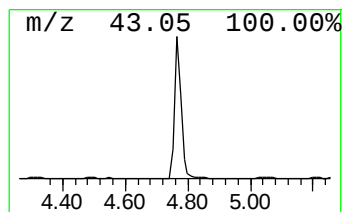
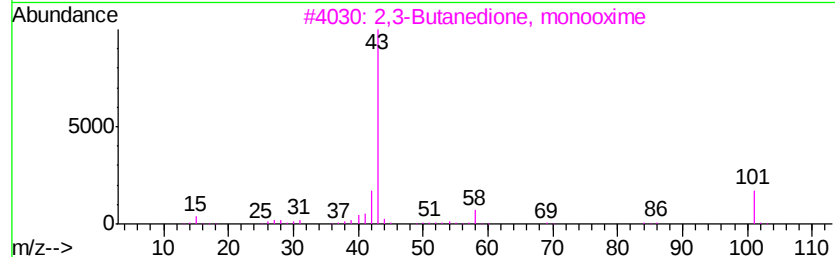
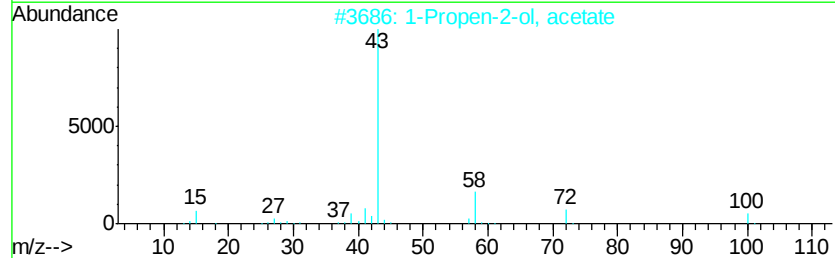
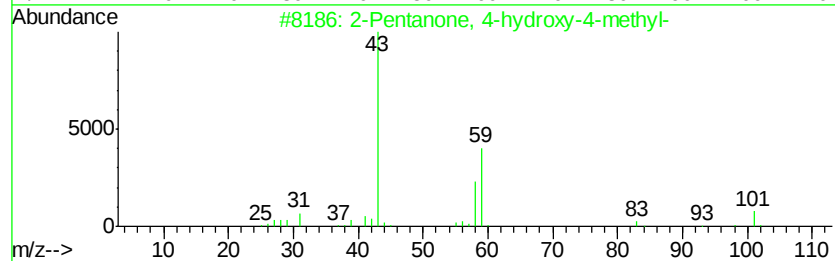
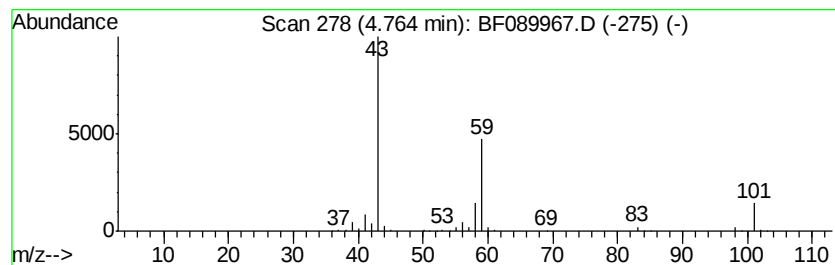
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	13.85 ng	778777	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	7



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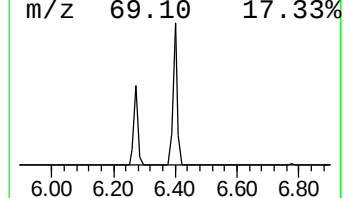
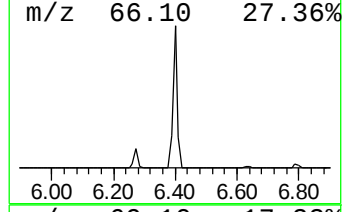
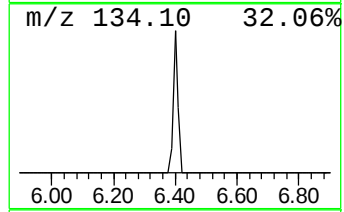
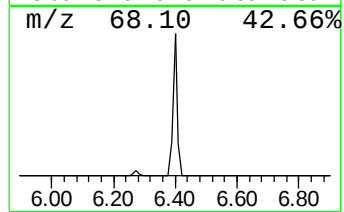
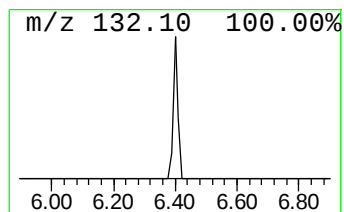
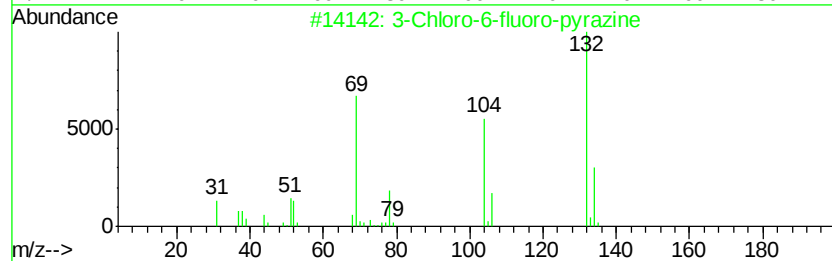
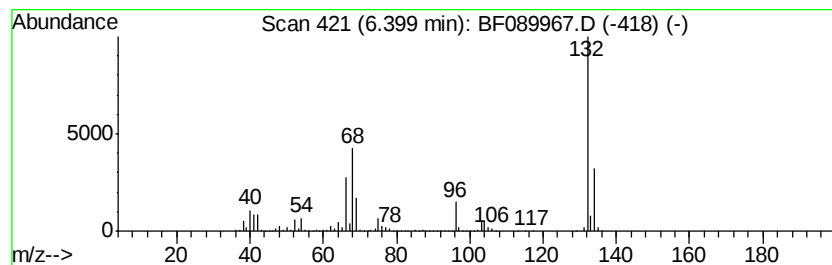
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	72.81 ng	4092530	1,4-Dichlorobenzene-d4	6.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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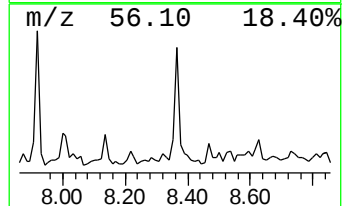
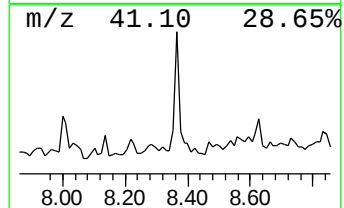
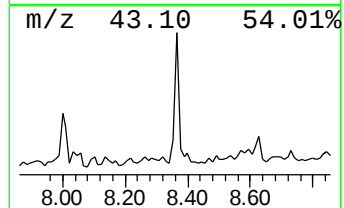
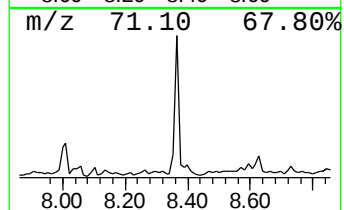
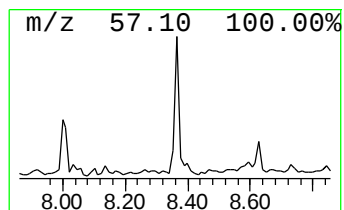
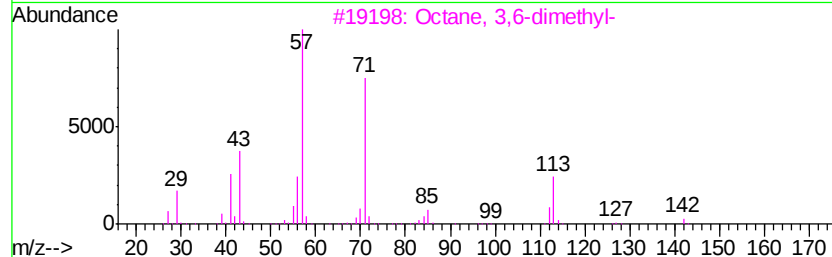
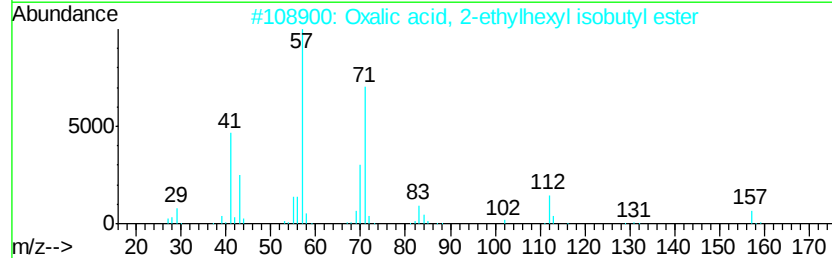
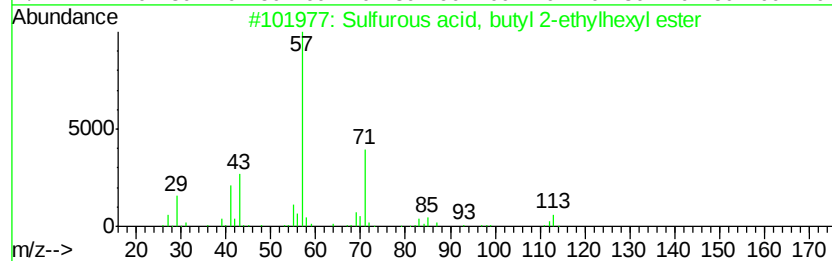
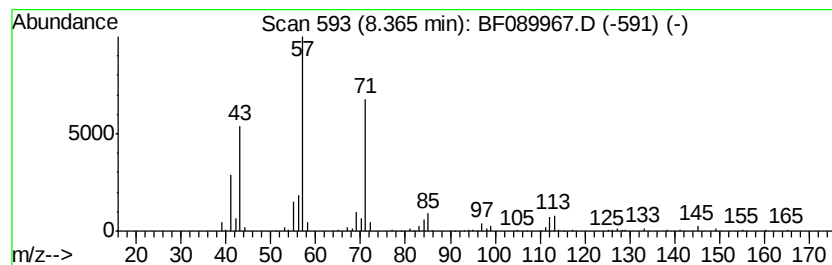
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Peak Number 6 Sulfurous acid, butyl 2-eth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.36	2.63 ng	190222	Napthalene-d8	7.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	78
2			Oxalic acid, 2-ethylhexyl isobut...	258	C14H26O4	1000309-38-5	72
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	72
4			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	64
5			Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	64



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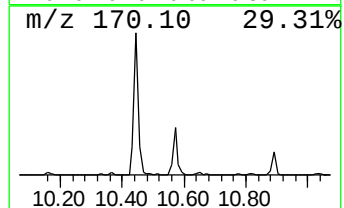
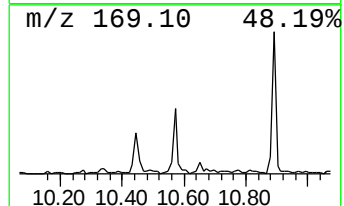
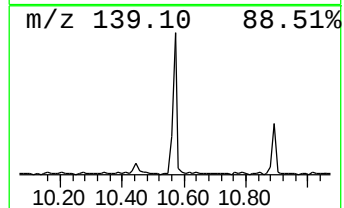
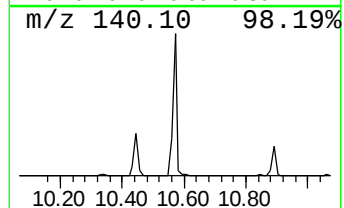
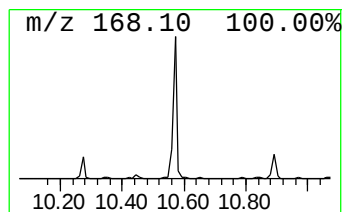
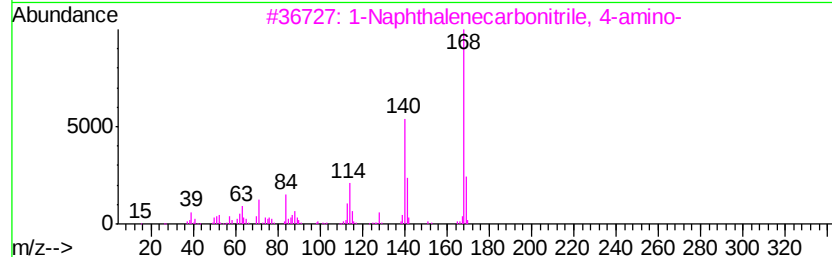
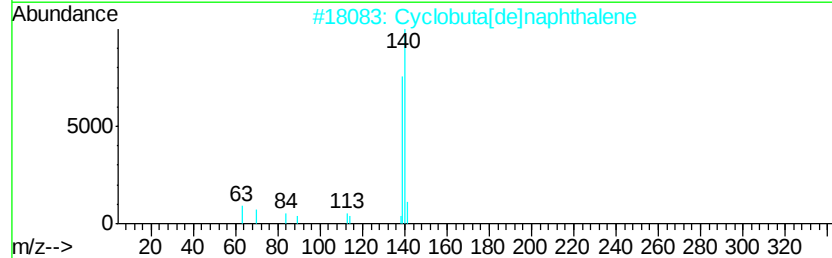
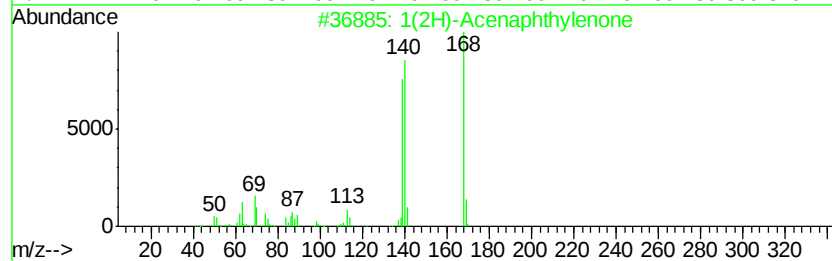
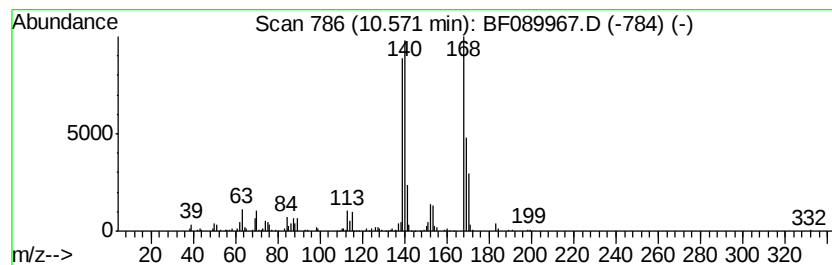
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Peak Number 7 1(2H)-Acenaphthylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	3.14 ng	219895	Phenanthrene-d10	11.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1(2H)-Acenaphthylene	168	C12H8O	002235-15-6	76
2		Cyclobuta[de]naphthalene	140	C11H8	024973-91-9	45
3		1-Naphthalenecarbonitrile, 4-amino-	168	C11H8N2	058728-64-6	38
4		Benzoic acid, 2-chloro-, methyl ...	170	C8H7ClO2	000610-96-8	25
5		3-Chlorobenzoic acid, 2-biphenyl...	308	C19H13ClO2	1000357-40-2	22



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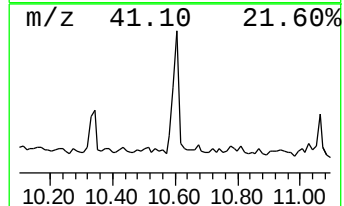
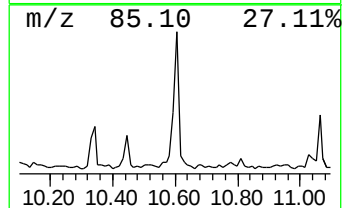
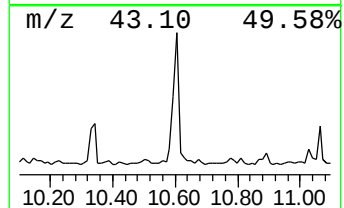
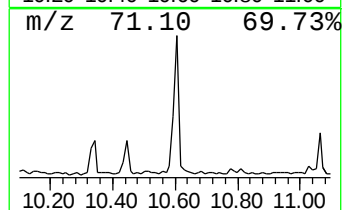
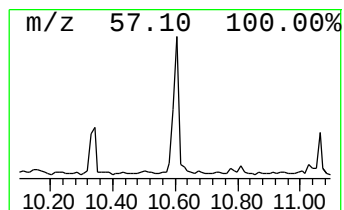
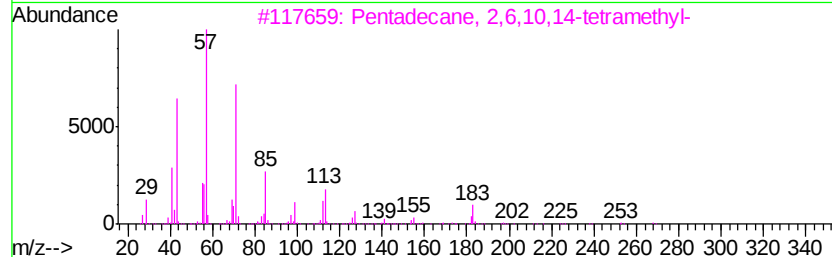
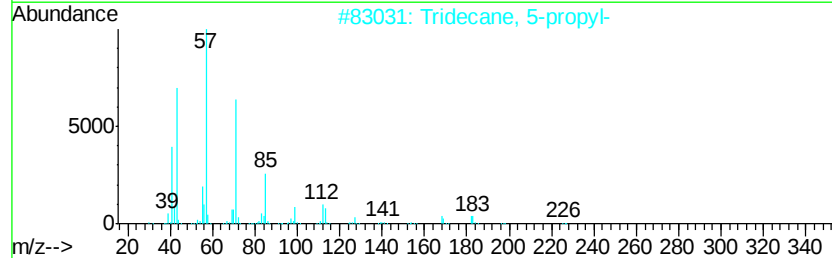
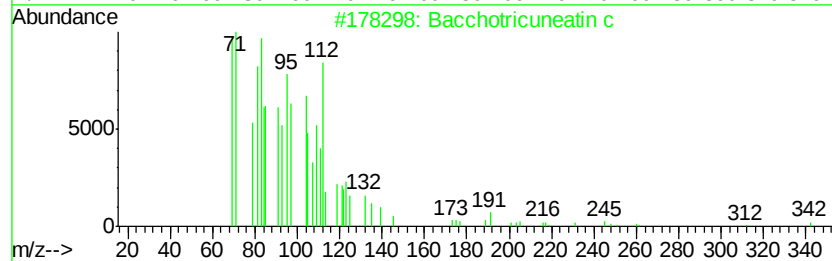
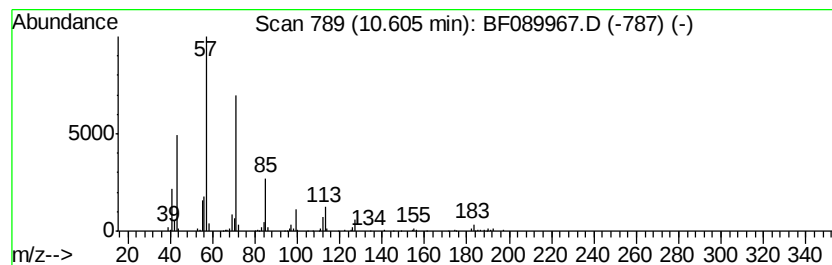
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Peak Number 8 Bacchotricuneatin c Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	5.21 ng	364544	Phenanthrene-d10	11.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bacchotricuneatin c	342	C20H22O5	066563-30-2	97
2		Tridecane, 5-propyl-	226	C16H34	055045-11-9	86
3		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	86
4		Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	72
5		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64



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ClientSampleId :
GW-1

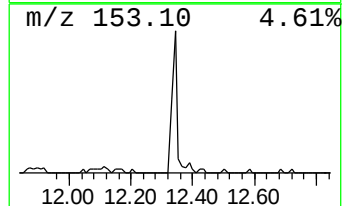
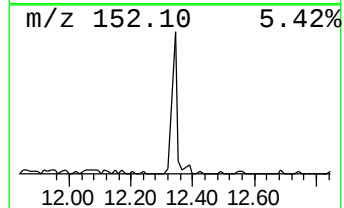
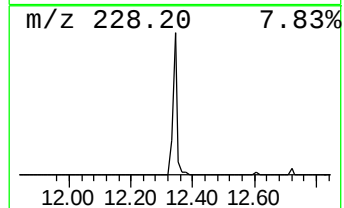
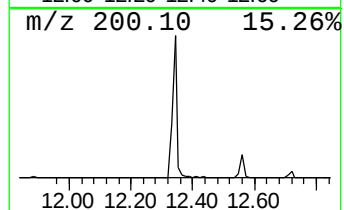
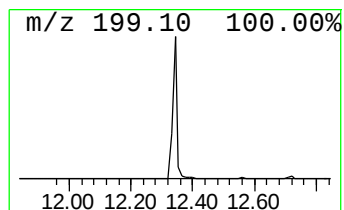
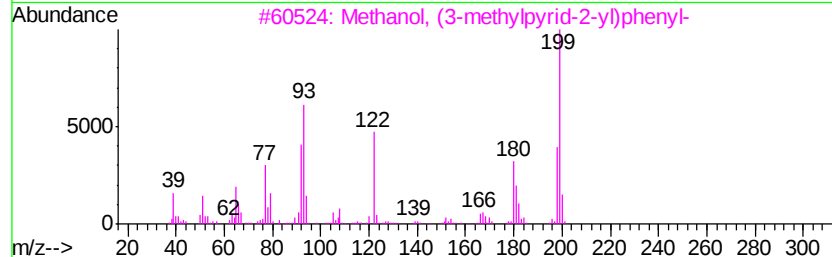
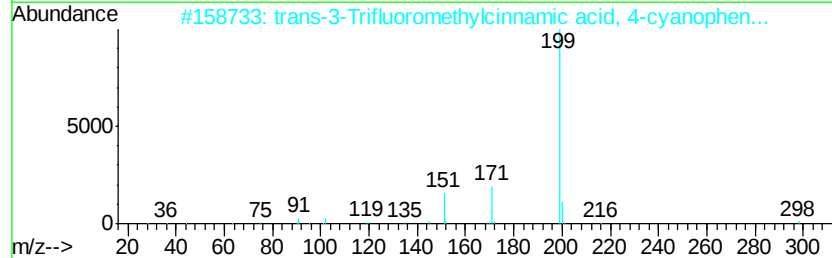
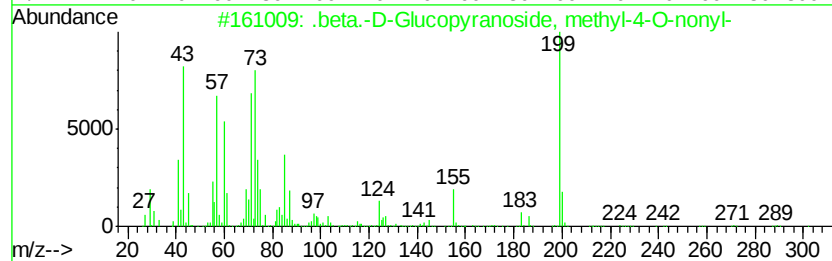
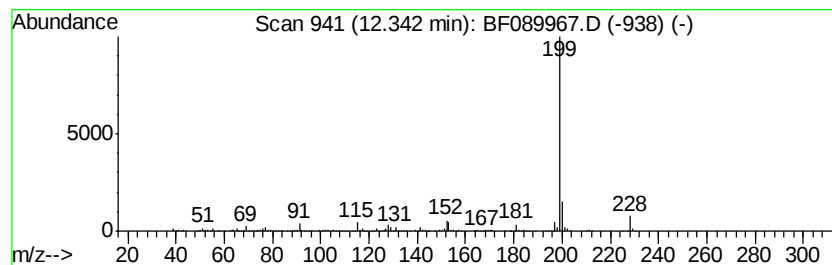
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 .beta.-D-Glucopyranoside, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	9.59 ng	671352	Phenanthrene-d10	11.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-D-Glucopyranoside, methyl...	320	C16H32O6	1000157-04-8	50
2		trans-3-Trifluoromethylcinnamic ...	317	C17H10F3NO2	1000307-81-1	45
3		Methanol, (3-methylpyrid-2-yl)ph...	199	C13H13NO	1000262-43-8	42
4		1,3-Benzenediol, 2-(phenylmethyl)-	200	C13H12O2	003769-40-2	42
5		s-Indacene, 1,2,3,5,6,7-hexahydr...	214	C16H22	006047-64-9	39



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090116\
Data File : BF089967.D
Acq On : 1 Sep 2016 13:07
Operator : UM/SJ
Sample : H4635-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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...	4.76	13.9	ng	778777	1	6.64	1124220	20.0
unknown6.40	6.40	72.8	ng	4092530	1	6.64	1124220	20.0
Sulfurous acid, b...	8.36	2.6	ng	190222	2	7.92	1448310	20.0
1(2H)-Acenaphthyl...	10.57	3.1	ng	219895	4	11.13	1400650	20.0
Bacchotricuneatin c	10.60	5.2	ng	364544	4	11.13	1400650	20.0
.beta.-D-Glucopyr...	12.34	9.6	ng	671352	4	11.13	1400650	20.0