

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032717\
 Data File : BF093972.D
 Acq On : 28 Mar 2017 5:12
 Operator : SJ/MA
 Sample : I2422-01
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HHD-S1

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-BF032217.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	4.069	368	371	379	rVB	196245	239602	7.39%	0.774%
2	4.463	433	438	441	rBV	2637855	2545340	78.55%	8.220%
3	5.534	614	620	625	rBV2	2464368	3240450	100.00%	10.465%
4	5.681	639	645	648	rBV	2832196	2864845	88.41%	9.252%
5	5.939	684	689	692	rBV	1047422	1013368	31.27%	3.273%
6	6.116	714	719	723	rBV	2172543	2085486	64.36%	6.735%
7	6.410	765	769	777	rVB	281154	255891	7.90%	0.826%
8	6.586	792	799	802	rBV	1760073	1814444	55.99%	5.860%
9	7.439	939	944	948	rBV	1358907	1384554	42.73%	4.472%
10	8.422	1104	1111	1118	rBV2	55918	73418	2.27%	0.237%
11	8.769	1161	1170	1173	rBV	3074216	3136747	96.80%	10.130%
12	9.257	1249	1253	1257	rBV	168507	169824	5.24%	0.548%
13	9.557	1300	1304	1305	rBV2	59715	55880	1.72%	0.180%
14	9.586	1305	1309	1313	rVB2	1413355	1422601	43.90%	4.594%
15	10.174	1404	1409	1413	rVB	99769	94602	2.92%	0.306%
16	10.451	1448	1456	1458	rBV	34257	59838	1.85%	0.193%
17	10.557	1468	1474	1478	rBV	1768046	1796689	55.45%	5.803%
18	10.757	1505	1508	1511	rBV	97184	106624	3.29%	0.344%
19	11.316	1599	1603	1606	rBV	50316	46938	1.45%	0.152%
20	11.410	1613	1619	1622	rBV	1297487	1277208	39.41%	4.125%
21	11.433	1622	1623	1627	rVB	93340	74026	2.28%	0.239%
22	12.163	1744	1747	1750	rBV2	30882	34427	1.06%	0.111%
23	12.898	1868	1872	1876	rBV	198948	187587	5.79%	0.606%
24	13.174	1914	1919	1923	rBV2	164988	186294	5.75%	0.602%
25	13.251	1929	1932	1938	rVB2	69488	69152	2.13%	0.223%
26	13.386	1950	1955	1959	rBV	2020358	2068181	63.82%	6.679%
27	14.292	2105	2109	2113	rBV	174912	176109	5.43%	0.569%
28	14.545	2148	2152	2161	rBV2	240237	346862	10.70%	1.120%
29	14.657	2166	2171	2175	rVV	848483	1033364	31.89%	3.337%
30	14.686	2175	2176	2179	rVB	69587	57510	1.77%	0.186%
31	15.098	2242	2246	2250	rBV	130064	140322	4.33%	0.453%
32	15.333	2283	2286	2294	rBV3	58057	91664	2.83%	0.296%
33	15.768	2357	2360	2363	rBV	75192	76313	2.36%	0.246%
34	15.845	2370	2373	2376	rBV2	64350	67567	2.09%	0.218%

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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-BF032217.M
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35	15.880	2376	2379	2382	rBV	57243	73245	2.26%	0.237%
36	16.227	2436	2438	2443	rVB	66619	73240	2.26%	0.237%
37	16.292	2445	2449	2457	rVV	687017	866303	26.73%	2.798%
38	18.309	2786	2792	2804	rVB2	354303	766731	23.66%	2.476%
39	18.545	2825	2832	2844	rVB3	369908	890516	27.48%	2.876%

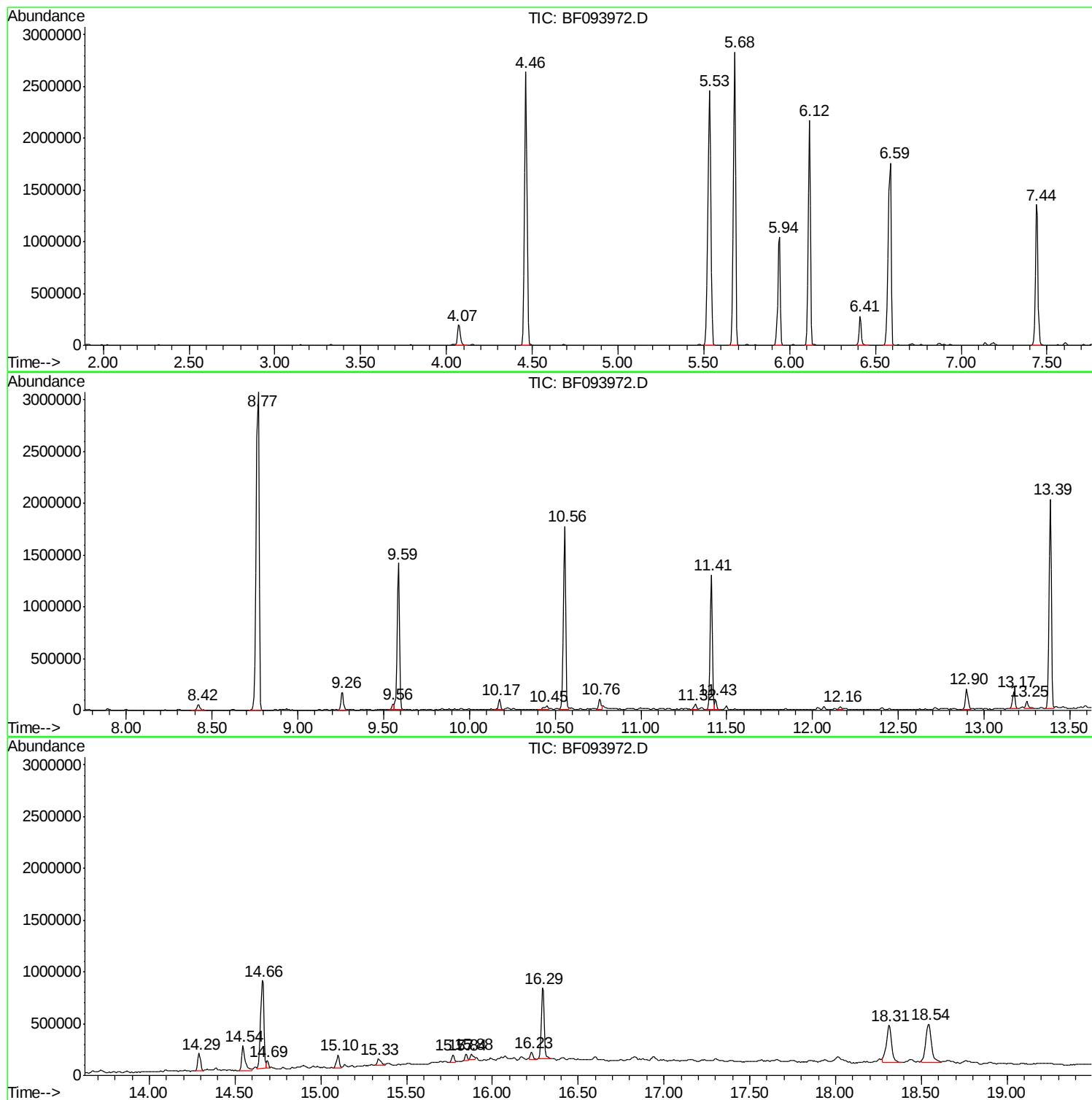
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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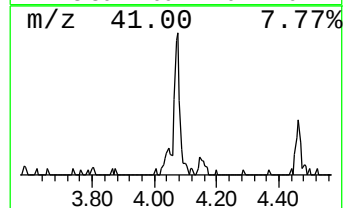
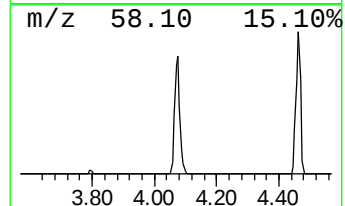
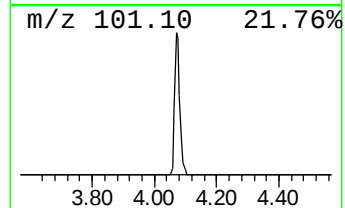
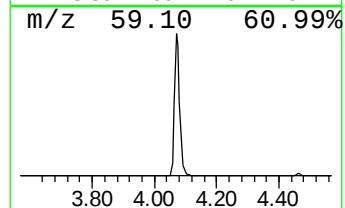
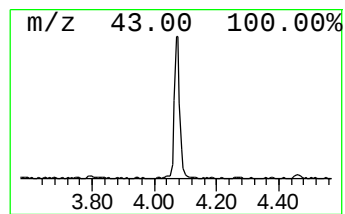
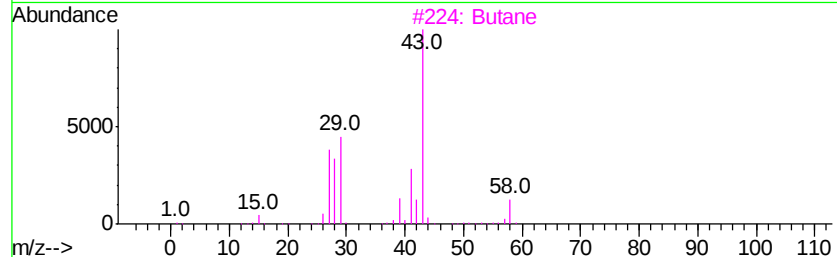
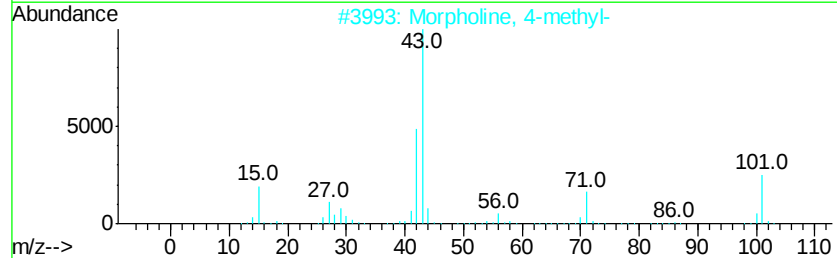
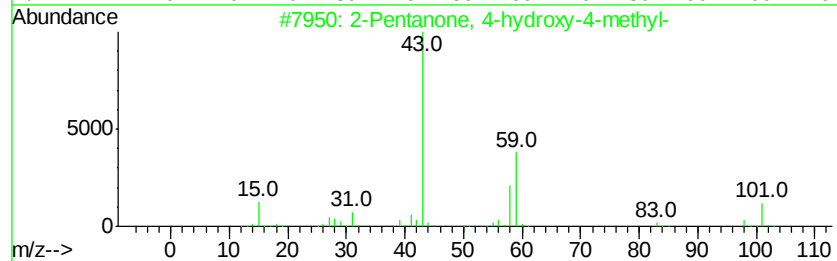
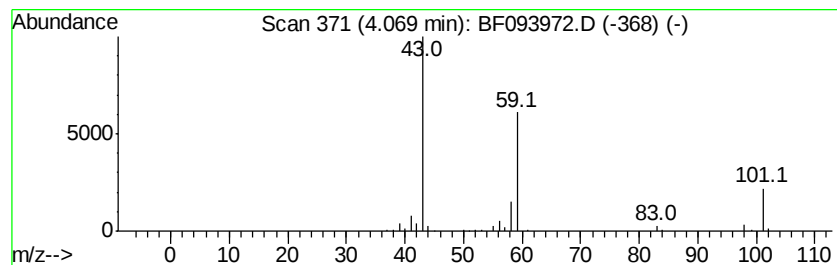
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.07	4.73 ng	239602	1,4-Dichlorobenzene-d4	5.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	64
2	Morpholine, 4-methyl-	101	C5H11NO		000109-02-4	9
3	Butane	58	C4H10		000106-97-8	9
4	Guanidine	59	CH5N3		000113-00-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2		000057-71-6	9



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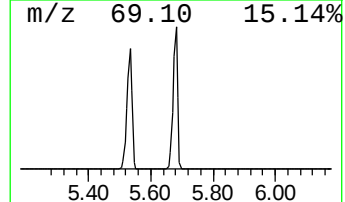
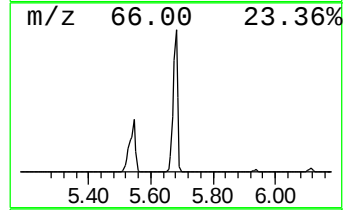
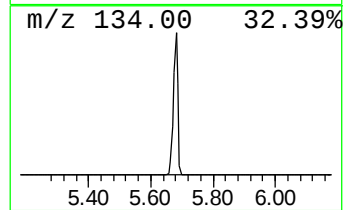
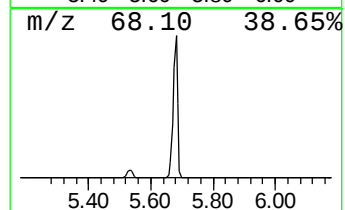
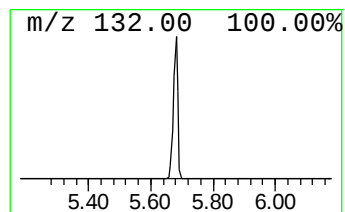
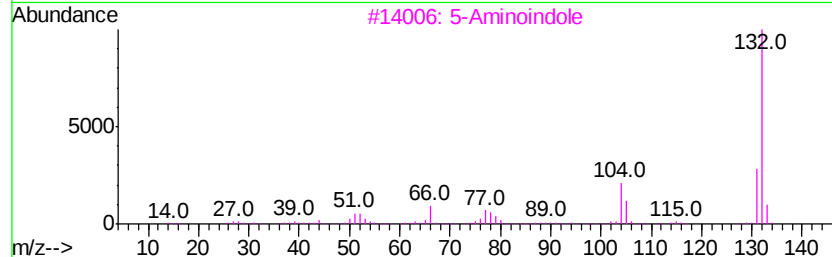
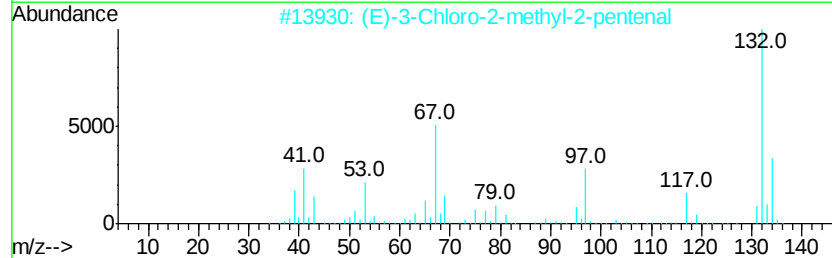
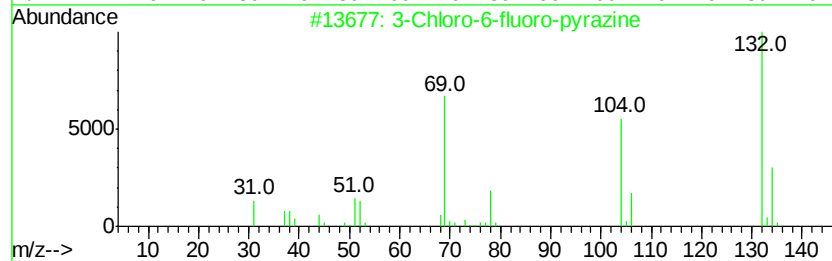
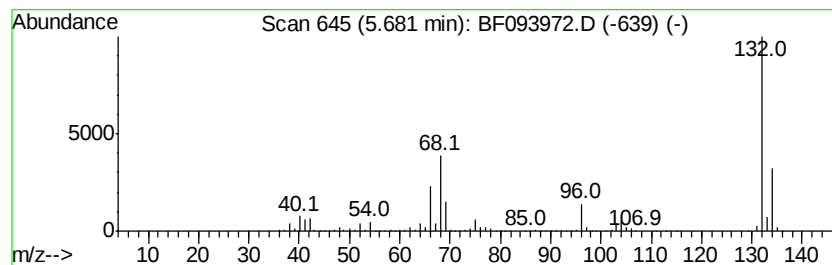
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown5.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.68	56.54 ng	2864850	1,4-Dichlorobenzene-d4	5.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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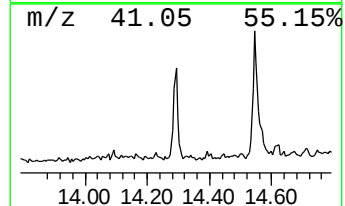
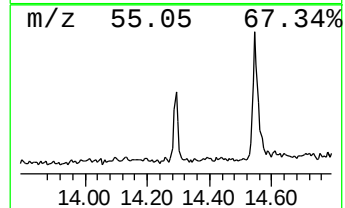
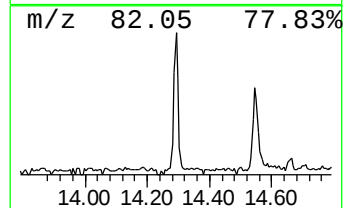
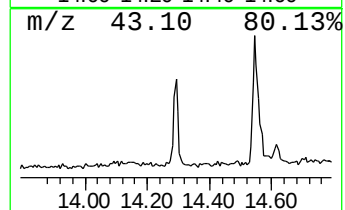
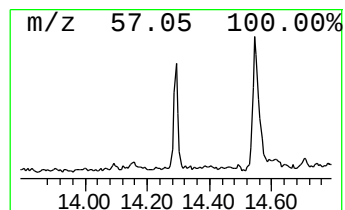
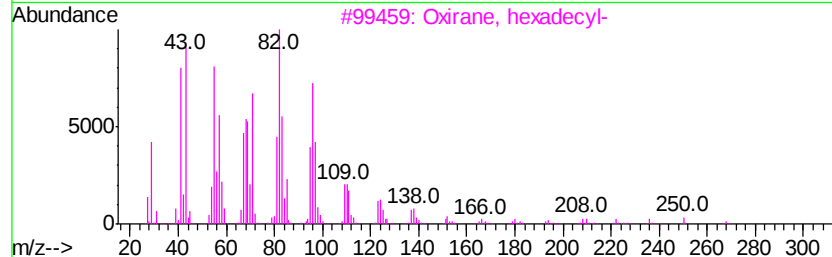
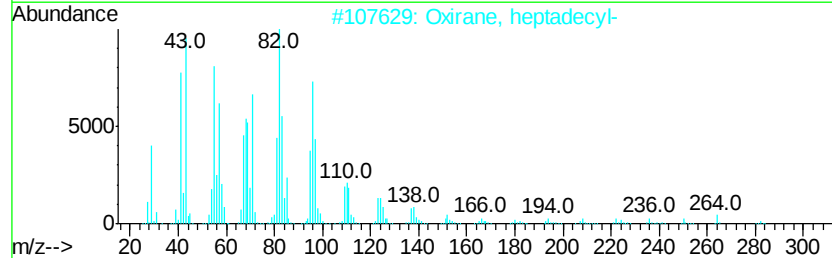
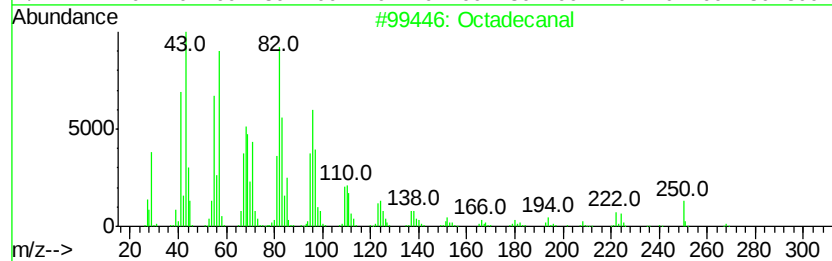
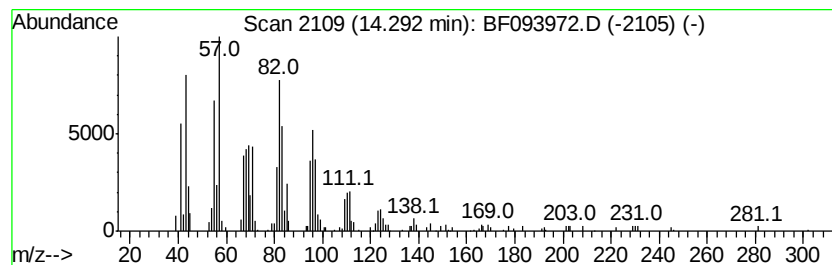
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	3.41 ng	176109	Chrysene-d12	14.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4	Tetradecanal	212	C14H28O	000124-25-4	91
5	Hexadecanal	240	C16H32O	000629-80-1	91



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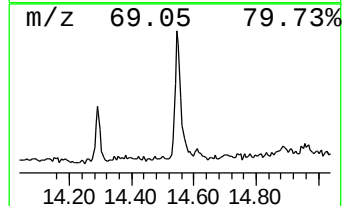
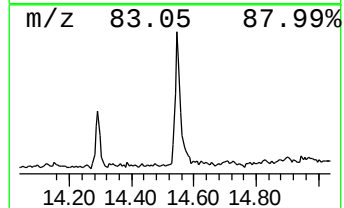
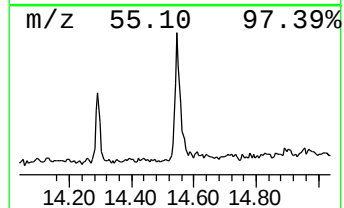
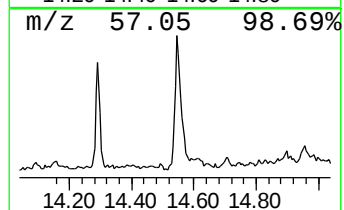
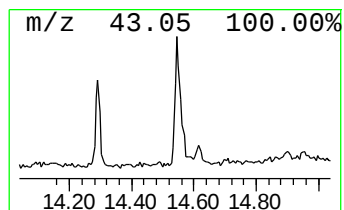
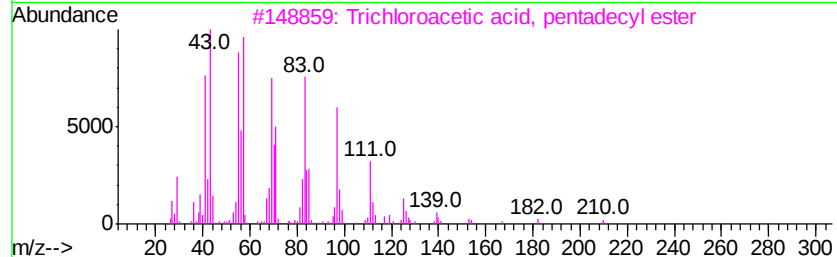
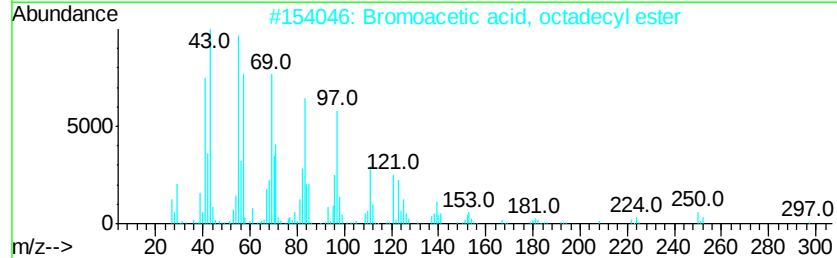
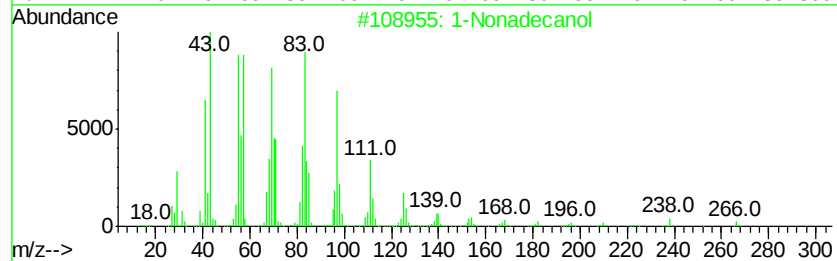
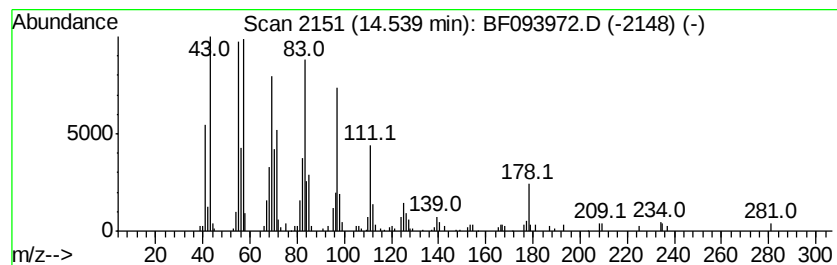
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Nonadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	6.71 ng	346862	Chrysene-d12	14.66
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonadecanol	284 C19H40O	001454-84-8	93
2	Bromoacetic acid, octadecyl ester	390 C20H39BrO2	018992-03-5	91
3	Trichloroacetic acid, pentadecyl...	372 C17H31Cl3O2	074339-53-0	90
4	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	90
5	Trifluoroacetic acid, n-octadecy...	366 C20H37F3O2	079392-43-1	87



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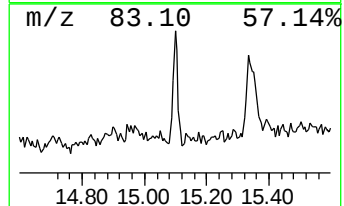
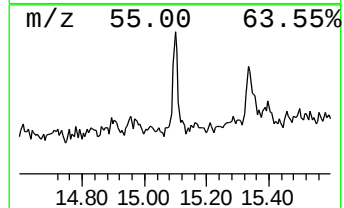
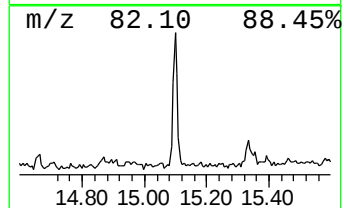
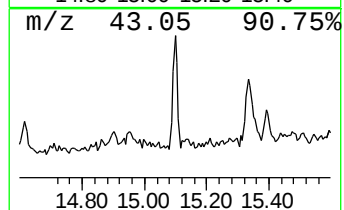
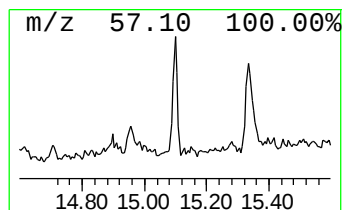
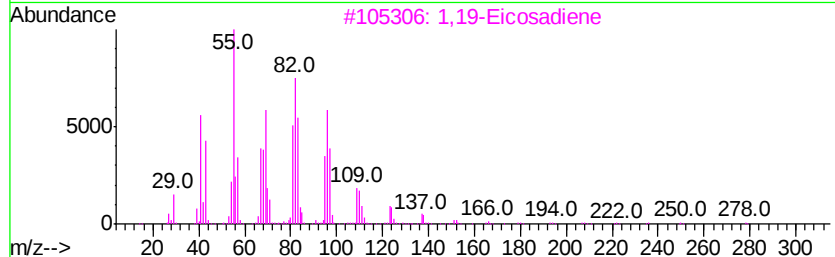
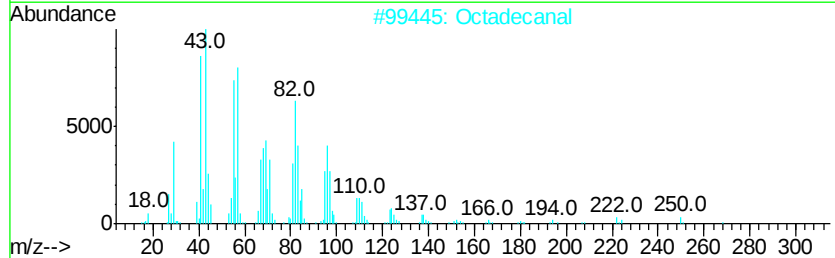
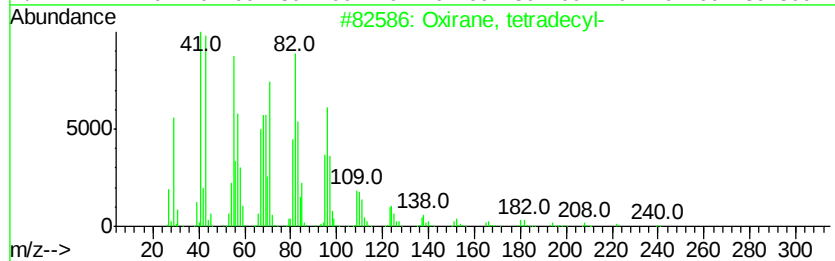
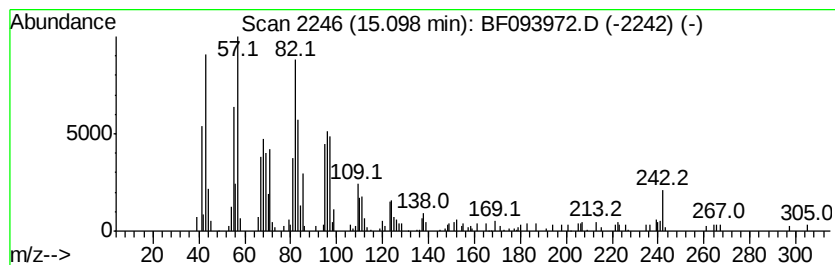
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Peak Number 6 Oxirane, tetradecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.10	2.72 ng	140322	Chrysene-d12		14.66
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	92
2	Octadecanal	268	C18H36O	000638-66-4	90
3	1,19-Eicosadiene	278	C20H38	014811-95-1	81
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	80
5	16-Heptadecenal	252	C17H32O	1000144-57-9	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032717\
Data File : BF093972.D
Acq On : 28 Mar 2017 5:12
Operator : SJ/MA
Sample : I2422-01
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
HHD-S1

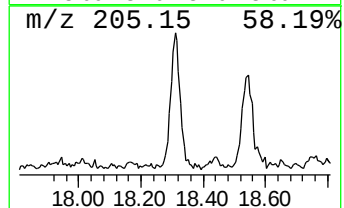
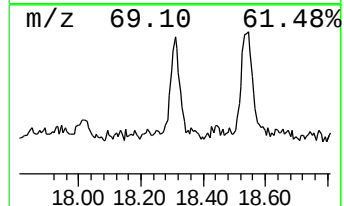
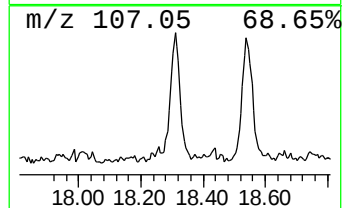
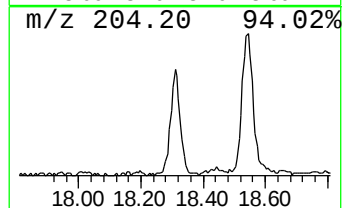
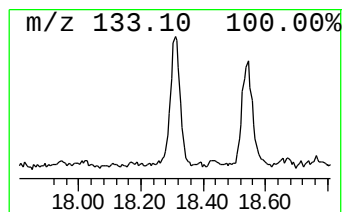
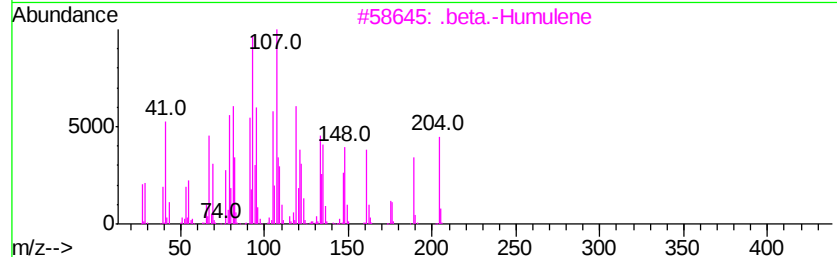
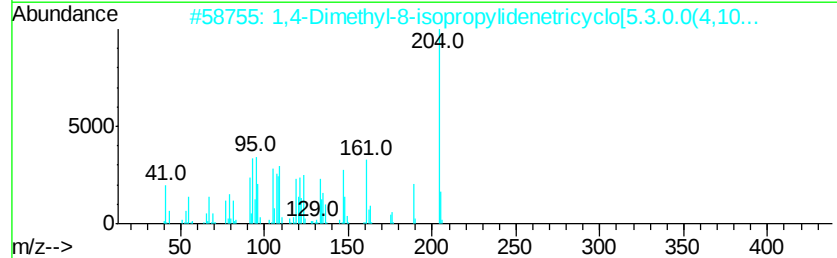
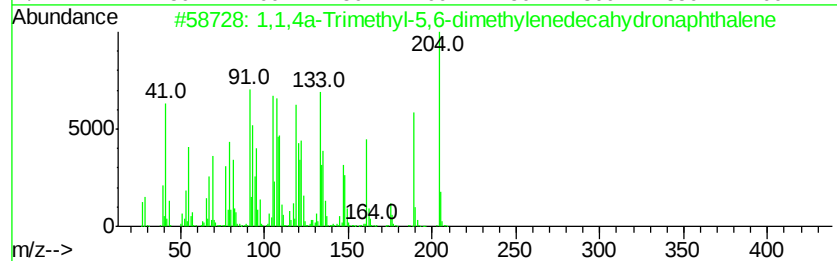
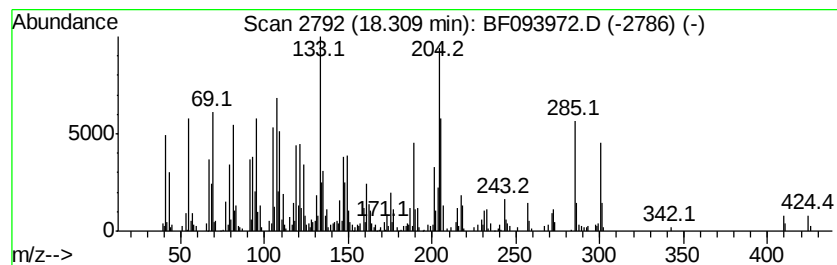
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown18.31 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	17.70 ng	766731	Perylene-d12	16.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	49
2		1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	38
3		.beta.-Humulene	204	C15H24	000116-04-1	35
4		1H-Cycloprop[elazulene, 1a,2,3,4...	204	C15H24	000489-40-7	30
5		1,3-Dimethyl-5-(propen-1-yl)adam...	204	C15H24	057040-48-9	30



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Sample : I2422-01
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HHD-S1

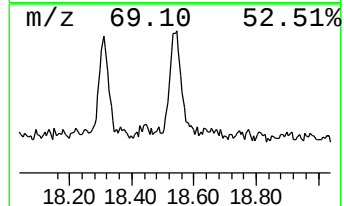
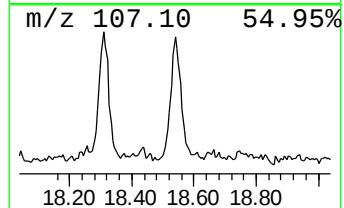
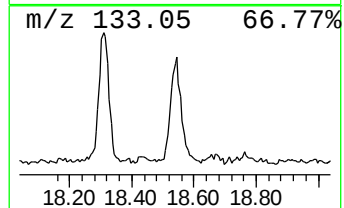
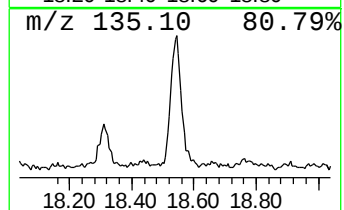
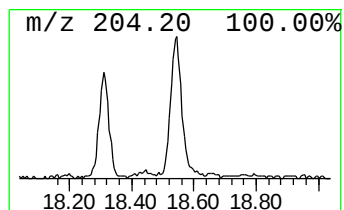
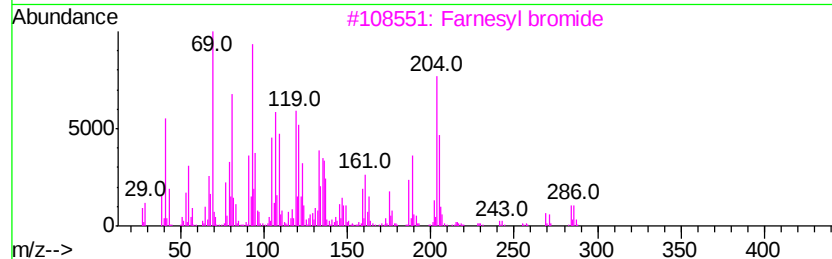
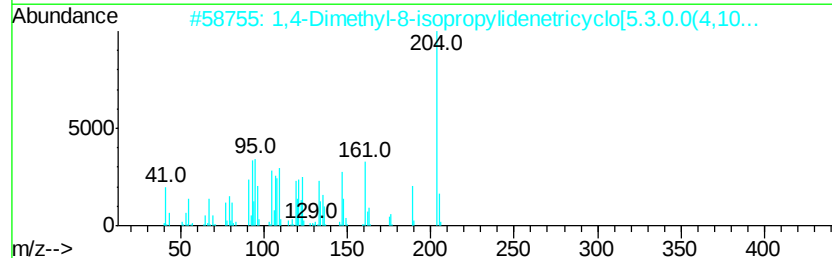
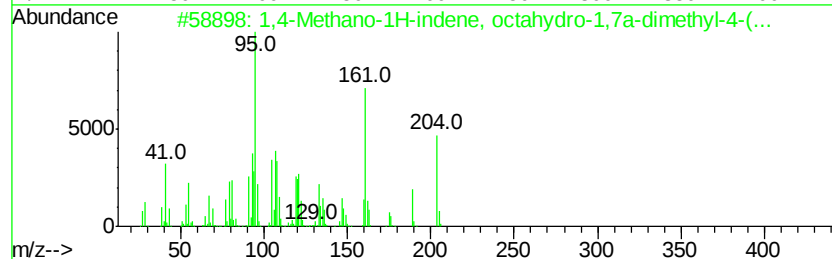
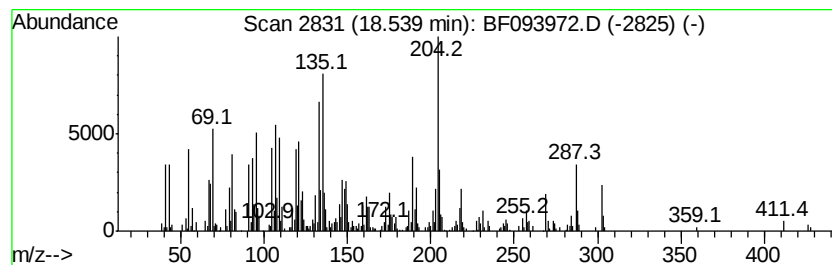
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,4-Methano-1H-indene, octa... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.54	20.56 ng	890516	Perylene-d12	16.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Methano-1H-indene, octahydro...	204	C15H24	087064-18-4	53
2		1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	52
3		Farnesyl bromide	284	C15H25Br	006874-67-5	45
4		Aciphyllene	204	C15H24	087745-31-1	43
5		3-Cyclohexene-1-methanol, .alpha...	222	C15H26O	023178-88-3	30



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Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HHD-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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
2-Pentanone, 4-hy...	4.07	4.7	ng	239602	1	5.94	1013370	20.0
unknown5.68	5.68	56.5	ng	2864850	1	5.94	1013370	20.0
Octadecanal	14.29	3.4	ng	176109	5	14.66	1033360	20.0
1-Nonadecanol	14.54	6.7	ng	346862	5	14.66	1033360	20.0
Oxirane, tetradecyl-	15.10	2.7	ng	140322	5	14.66	1033360	20.0
unknown18.31	18.31	17.7	ng	766731	6	16.29	866303	20.0
1,4-Methano-1H-in...	18.54	20.6	ng	890516	6	16.29	866303	20.0