

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
 Data File : BM010031.D
 Acq On : 12 May 2017 19:40
 Operator : SJ/MA
 Sample : I3100-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PMW-2-051017

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_M\METHODS\8270-BM051117.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	3.516	68	73	80	rVB5	10401	18518	1.15%	0.134%
2	4.904	303	309	318	rBV2	35632	63479	3.96%	0.458%
3	5.351	379	385	399	rVB2	203316	351966	21.95%	2.538%
4	6.945	650	656	666	rBV3	153379	357284	22.28%	2.576%
5	7.293	710	715	729	rVB	378953	635151	39.60%	4.579%
6	7.622	766	771	775	rVB4	22545	36146	2.25%	0.261%
7	7.757	788	794	801	rBV	257603	425683	26.54%	3.069%
8	7.892	813	817	824	rVB3	16416	25920	1.62%	0.187%
9	8.075	840	848	858	rVB	326642	555352	34.63%	4.004%
10	8.510	916	922	928	rBV4	20705	39946	2.49%	0.288%
11	8.798	965	971	976	rBV6	24598	51565	3.22%	0.372%
12	8.934	988	994	1004	rBV	293562	545031	33.99%	3.930%
13	9.069	1011	1017	1022	rBV6	13704	23223	1.45%	0.167%
14	9.163	1029	1033	1042	rVB7	15303	35124	2.19%	0.253%
15	9.304	1053	1057	1063	rVB5	10882	17074	1.06%	0.123%
16	10.551	1262	1269	1281	rBV	337036	595823	37.15%	4.296%
17	11.216	1375	1382	1385	rBV5	19447	33842	2.11%	0.244%
18	12.227	1548	1554	1566	rBV2	121469	349068	21.77%	2.517%
19	13.022	1682	1689	1696	rBV	718524	1054868	65.78%	7.606%
20	13.869	1828	1833	1845	rVB	344771	515176	32.12%	3.714%
21	14.280	1898	1903	1909	rBV2	33364	49312	3.07%	0.356%
22	14.410	1918	1925	1936	rVB2	493895	781421	48.73%	5.634%
23	14.833	1993	1997	2001	rVV6	13448	23000	1.43%	0.166%
24	14.898	2005	2008	2014	rVB6	13799	19752	1.23%	0.142%
25	15.233	2061	2065	2071	rBV	100855	134882	8.41%	0.972%
26	15.639	2125	2134	2138	rBV4	30298	74321	4.63%	0.536%
27	15.733	2146	2150	2156	rVB6	11981	18830	1.17%	0.136%
28	15.792	2156	2160	2168	rBV3	17411	30718	1.92%	0.221%
29	15.857	2168	2171	2175	rBV4	15384	20516	1.28%	0.148%
30	15.916	2175	2181	2190	rBV	595412	925135	57.69%	6.670%
31	16.098	2207	2212	2220	rBV2	139594	244555	15.25%	1.763%
32	16.439	2263	2270	2274	rBV6	22033	47503	2.96%	0.342%
33	16.557	2287	2290	2295	rBV4	21823	34097	2.13%	0.246%
34	16.668	2305	2309	2313	rBV2	57509	82550	5.15%	0.595%

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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

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35	16.892	2342	2347	2350	rBV	86525	104211	6.50%	0.751%
36	16.933	2352	2354	2359	rVB4	17104	27433	1.71%	0.198%
37	17.168	2385	2394	2402	rBV	680923	998432	62.26%	7.199%
38	17.633	2469	2473	2478	rVB	25080	33934	2.12%	0.245%
39	17.933	2517	2524	2528	rBV7	12656	28065	1.75%	0.202%
40	17.980	2528	2532	2536	rBV7	10561	16050	1.00%	0.116%
41	18.045	2538	2543	2548	rBV	258384	327070	20.39%	2.358%
42	18.086	2548	2550	2554	rVB4	14110	16236	1.01%	0.117%
43	19.180	2731	2736	2738	rBV4	19798	22472	1.40%	0.162%
44	19.321	2755	2760	2767	rBV2	116024	176035	10.98%	1.269%
45	19.492	2787	2789	2793	rVB5	16023	19660	1.23%	0.142%
46	19.580	2801	2804	2808	rVB5	14764	21364	1.33%	0.154%
47	19.792	2834	2840	2845	rBV	1302942	1603717	100.00%	11.563%
48	20.056	2882	2885	2889	rBV6	18186	26859	1.67%	0.194%
49	20.362	2935	2937	2941	rBV5	16011	18903	1.18%	0.136%
50	20.580	2971	2974	2977	rVB3	30179	35290	2.20%	0.254%
51	21.045	3049	3053	3059	rBV3	189753	248914	15.52%	1.795%
52	21.356	3101	3106	3112	rBV	854105	1097169	68.41%	7.910%
53	23.650	3490	3496	3504	rVB2	415995	831146	51.83%	5.992%

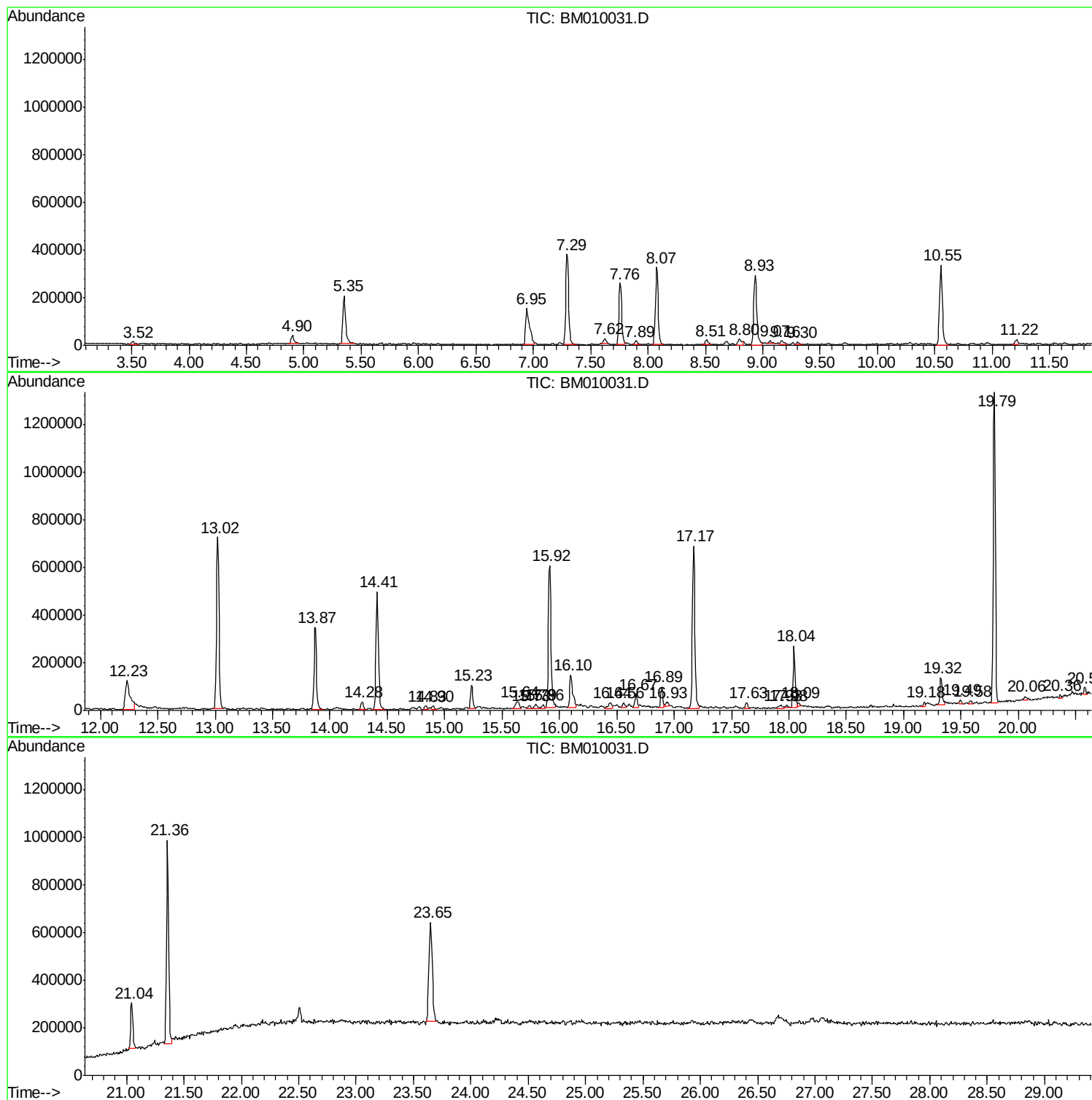
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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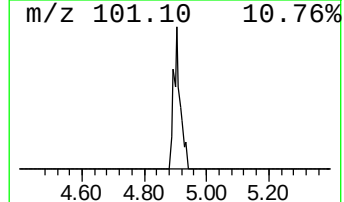
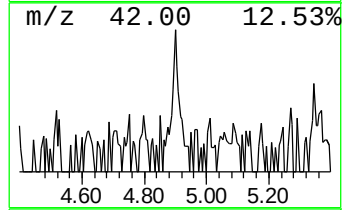
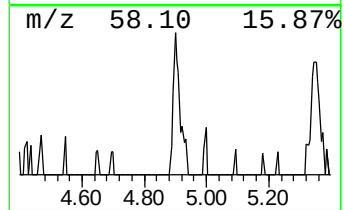
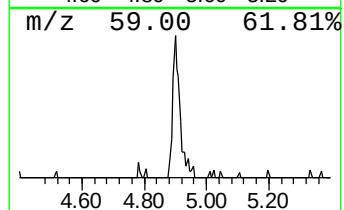
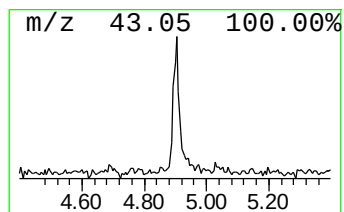
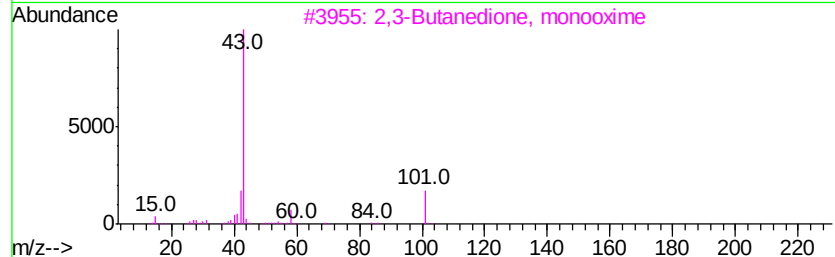
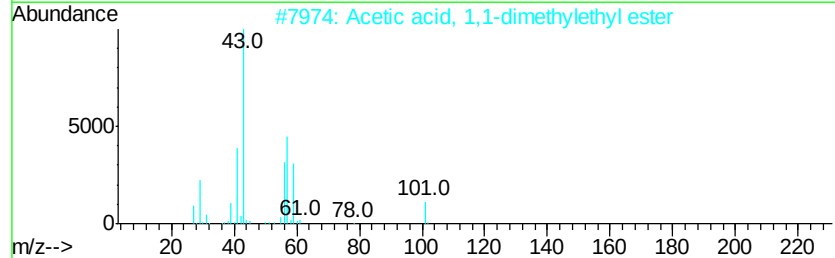
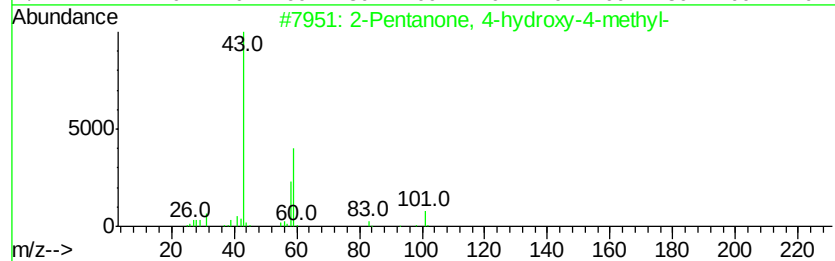
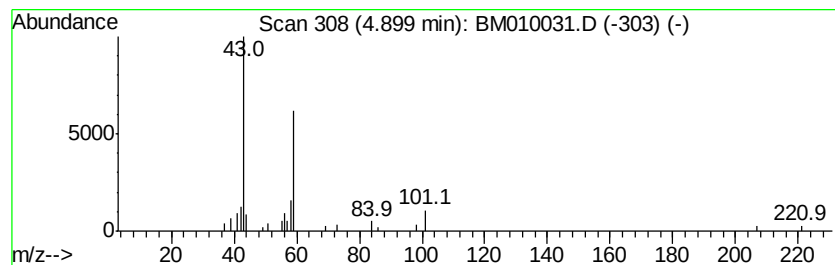
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.98 ng	63479	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5		2-Pentanone	86	C5H10O	000107-87-9	9



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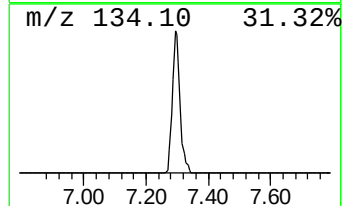
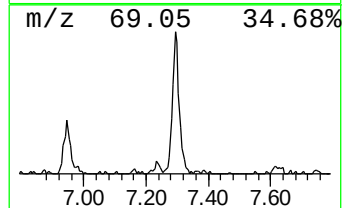
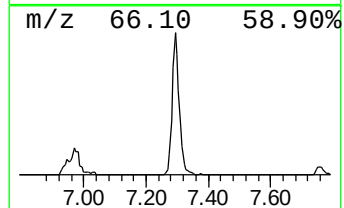
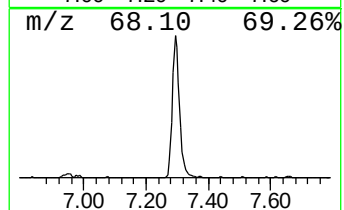
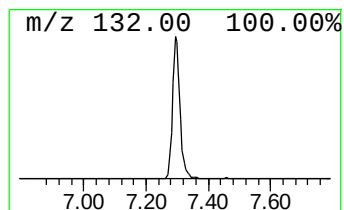
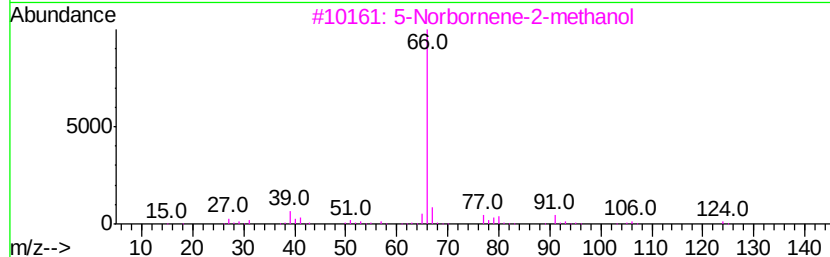
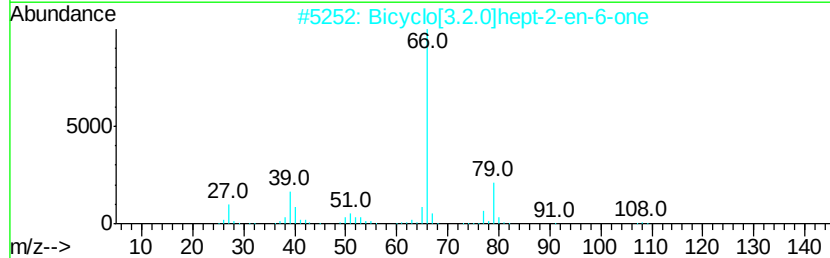
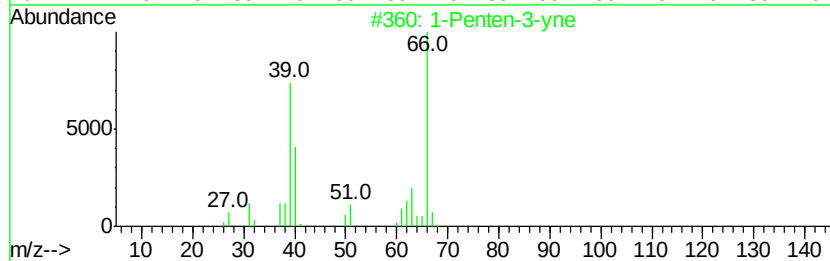
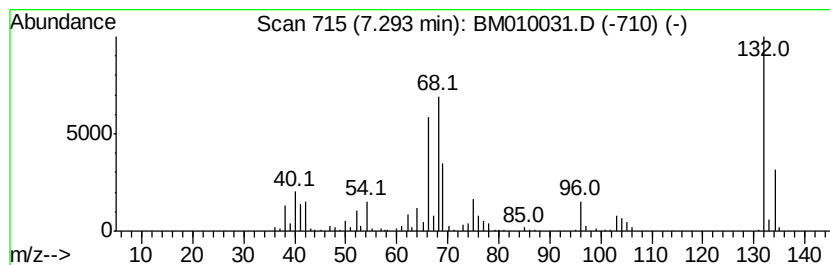
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	29.84 ng	635151	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Penten-3-yne	66	C5H6	000646-05-9	35
2		Bicyclo[3.2.0]hept-2-en-6-one	108	C7H8O	013173-09-6	25
3		5-Norbornene-2-methanol	124	C8H12O	000095-12-5	25
4		Silane, bicyclo[2.2.1]hept-5-en-...	226	C7H9Cl3Si	014319-64-3	25
5		3-Butenenitrile, 3-chloro-	101	C4H4ClN	021031-46-9	23



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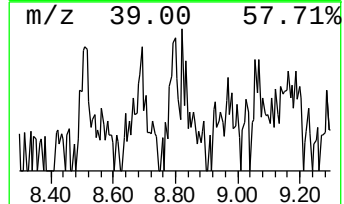
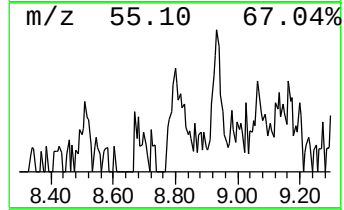
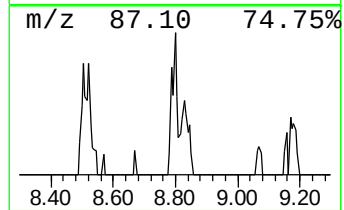
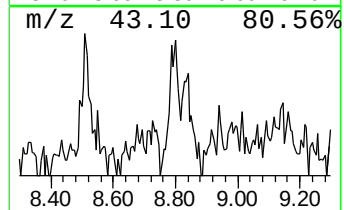
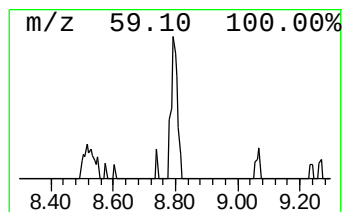
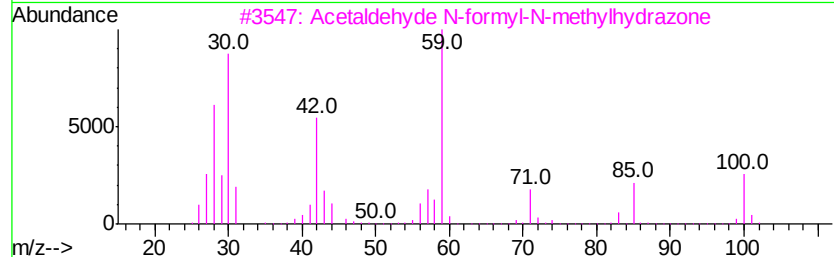
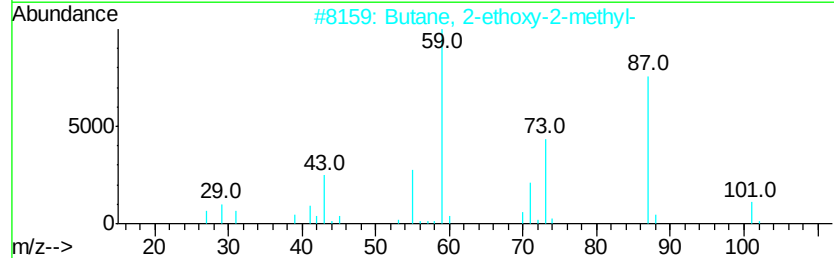
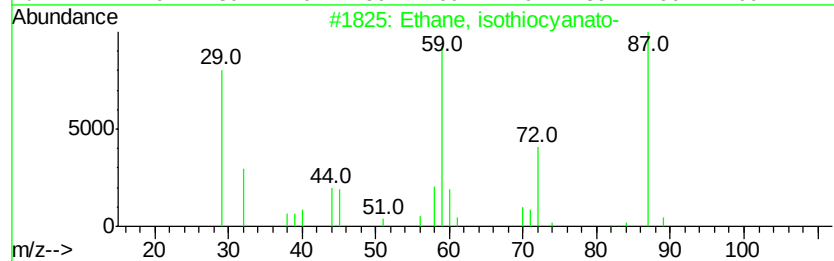
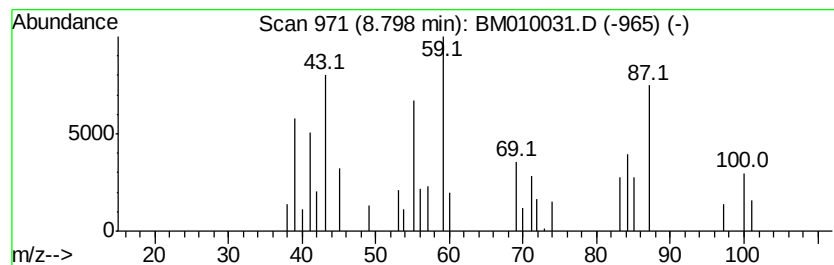
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown8.80 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.80	2.42 ng	51565	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	37
2		Butane, 2-ethoxy-2-methyl-	116	C7H16O	000919-94-8	37
3		Acetaldehyde N-formyl-N-methylhyv...	100	C4H8N2O	016568-02-8	30
4		1,3-Propanediol, 2,2-diethyl-	132	C7H16O2	000115-76-4	12
5		Ethanol, 2-(2-butoxyethoxy)-, ac...	204	C10H20O4	000124-17-4	12



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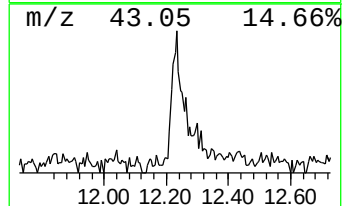
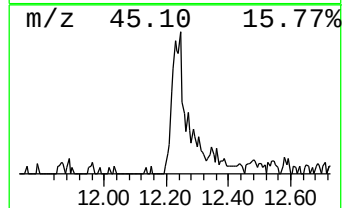
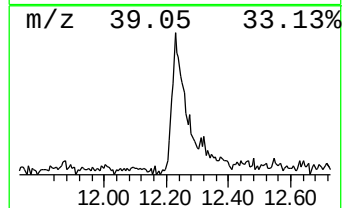
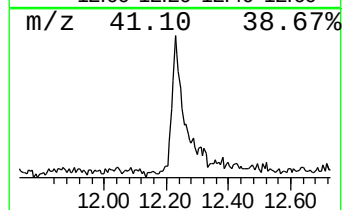
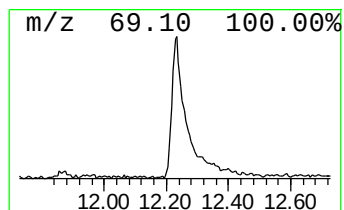
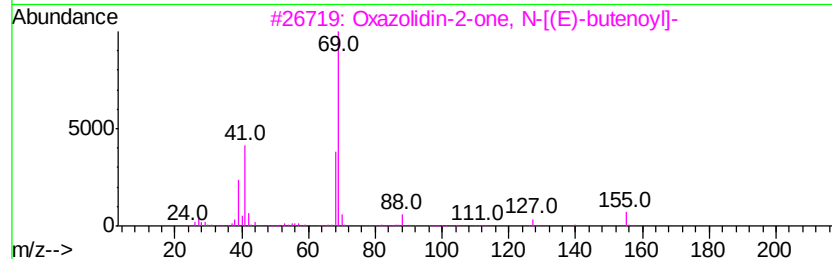
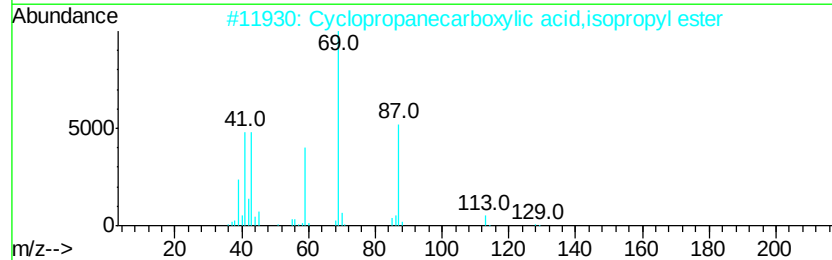
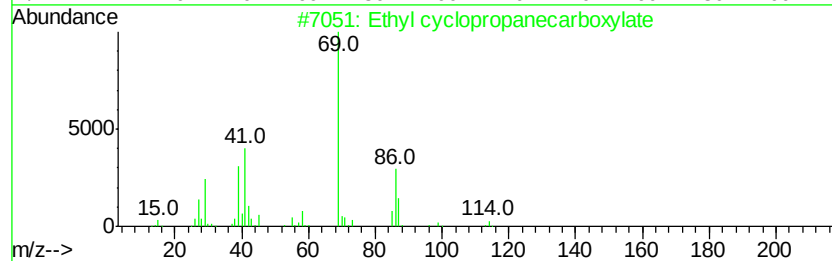
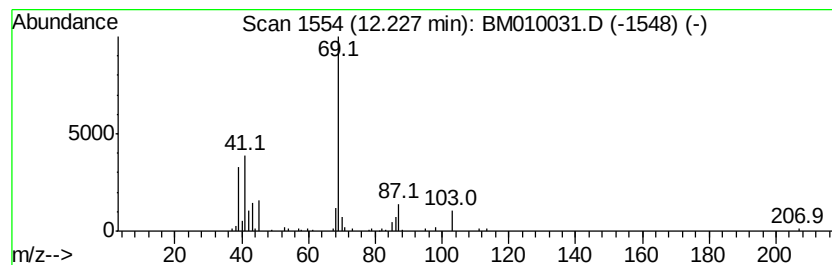
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown12.23 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.23	11.72 ng	349068	Naphthalene-d8	10.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	36
2		Cyclopropanecarboxylic acid,isop...	128	C7H12O2	006887-83-8	36
3		Oxazolidin-2-one, N-[(E)-butenoyl]-	155	C7H9NO3	1000156-45-5	28
4		Oxazole	69	C3H3NO	000288-42-6	9
5		Cyclopentane, ethyl-	98	C7H14	001640-89-7	9



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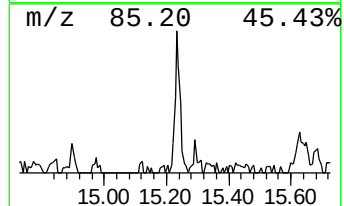
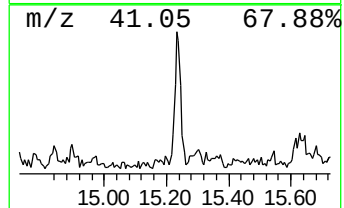
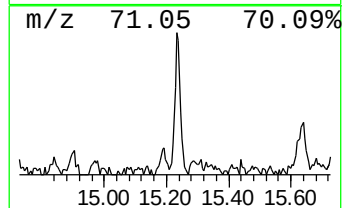
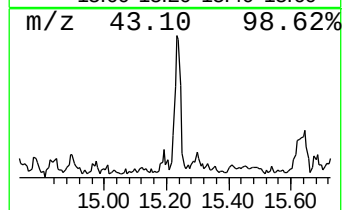
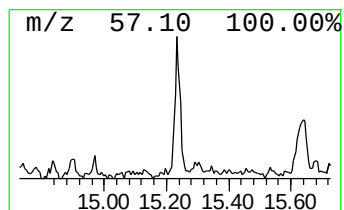
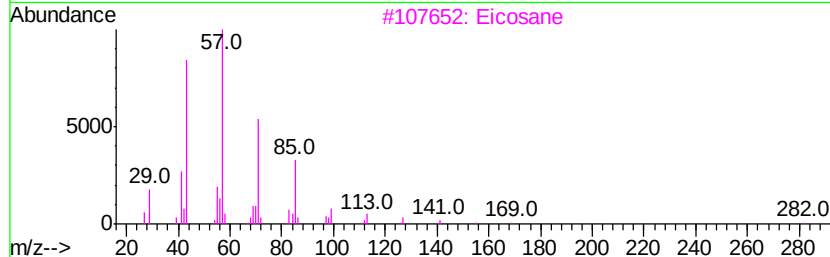
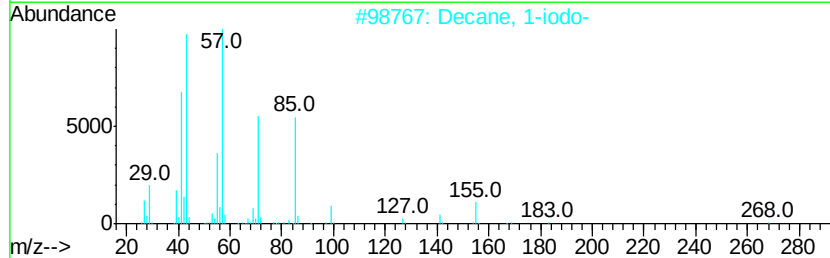
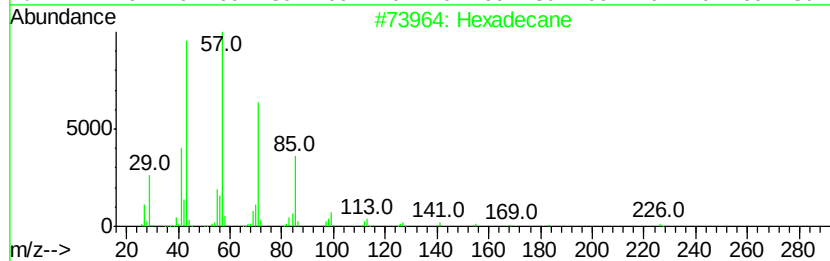
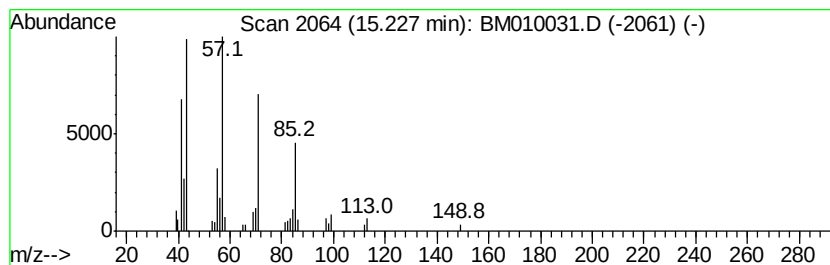
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	3.45 ng	134882	Acenaphthene-d10	14.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	72
2		Decane, 1-iodo-	268	C10H21I	002050-77-3	64
3		Eicosane	282	C20H42	000112-95-8	64
4		Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	64
5		Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	64



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010031.D
Acq On : 12 May 2017 19:40
Operator : SJ/MA
Sample : I3100-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

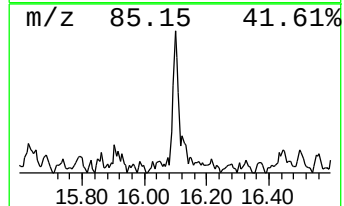
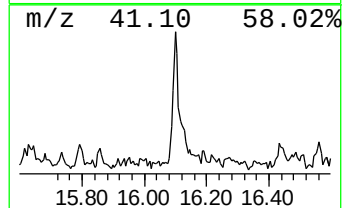
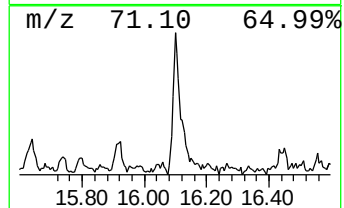
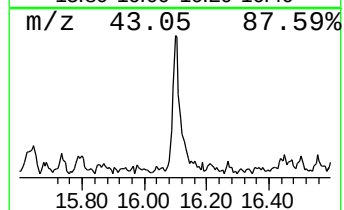
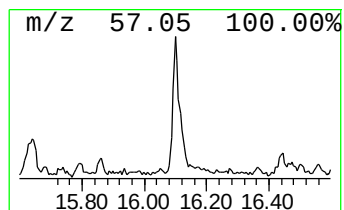
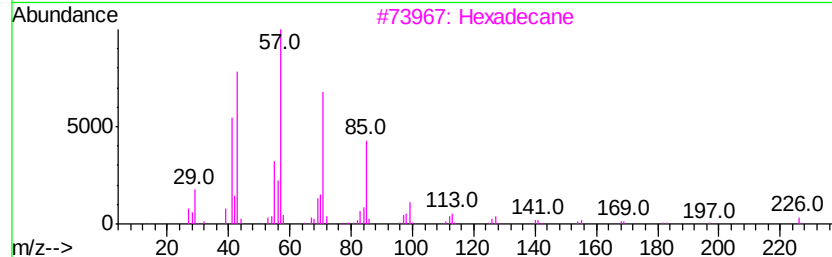
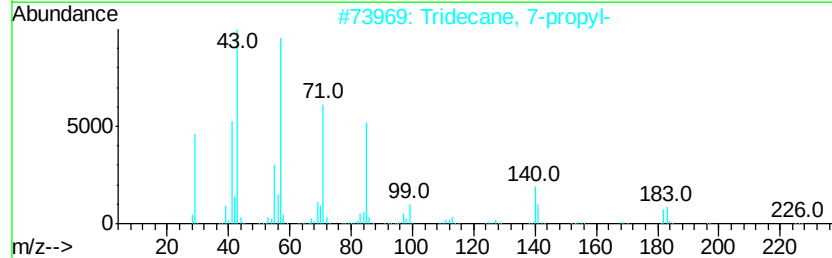
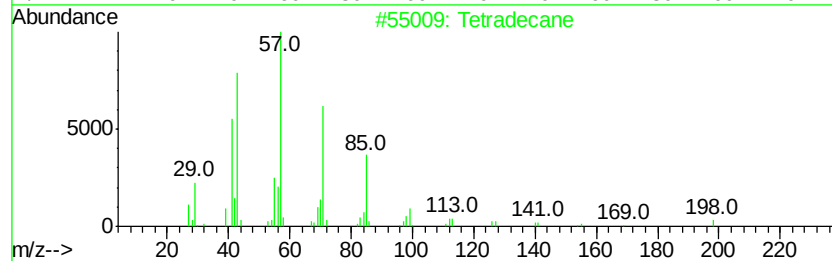
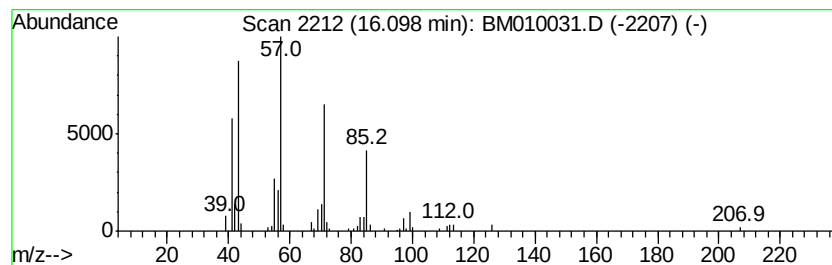
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.10	4.90 ng	244555	Phenanthrene-d10		17.17
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Tridecane, 7-propyl-	226	C16H34	055045-09-5	86
3	Hexadecane	226	C16H34	000544-76-3	83
4	Eicosane	282	C20H42	000112-95-8	78
5	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	72



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
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Sample : I3100-01
Misc :
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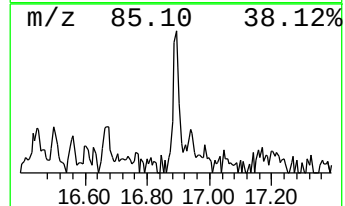
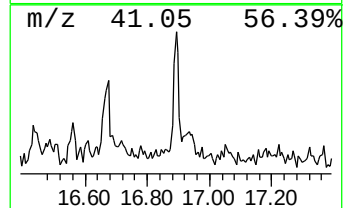
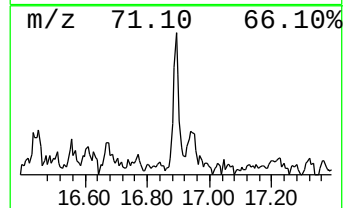
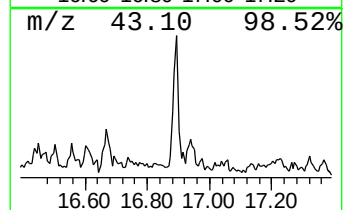
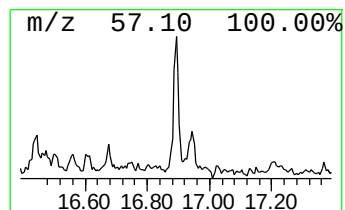
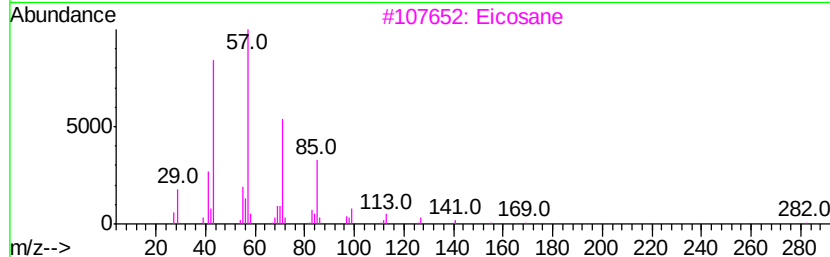
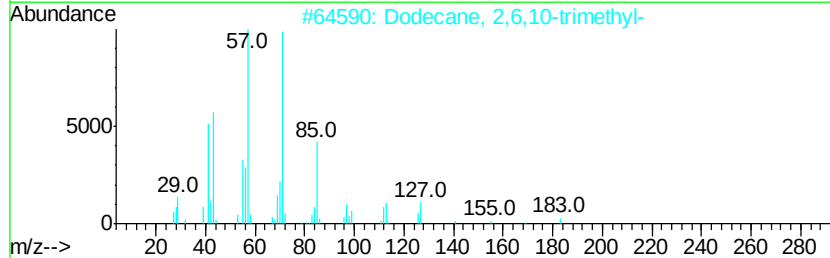
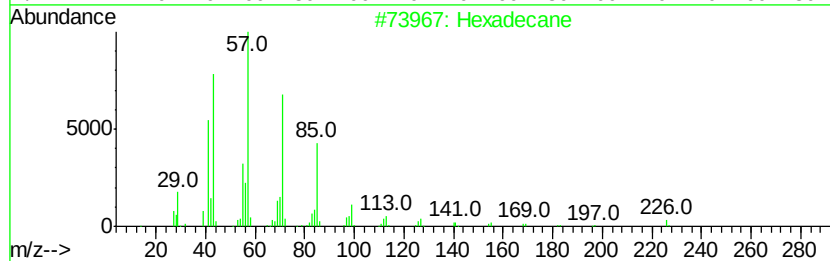
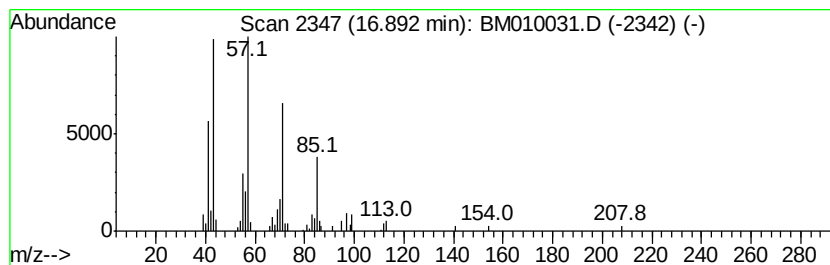
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.89	2.09 ng	104211	Phenanthrene-d10	17.17	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	86
3	Eicosane	282	C20H42	000112-95-8	83
4	Nonadecane	268	C19H40	000629-92-5	80
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	78



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010031.D
Acq On : 12 May 2017 19:40
Operator : SJ/MA
Sample : I3100-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PMW-2-051017

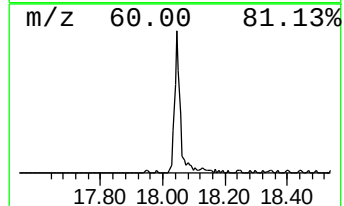
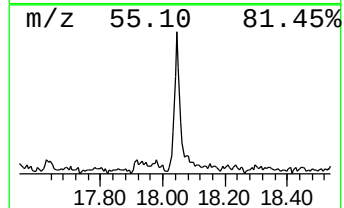
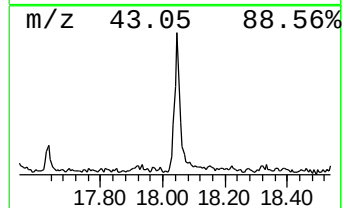
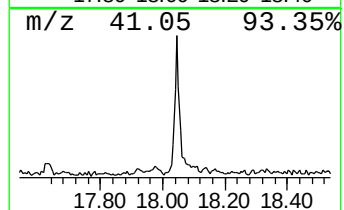
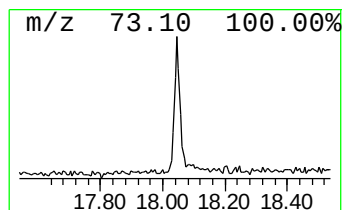
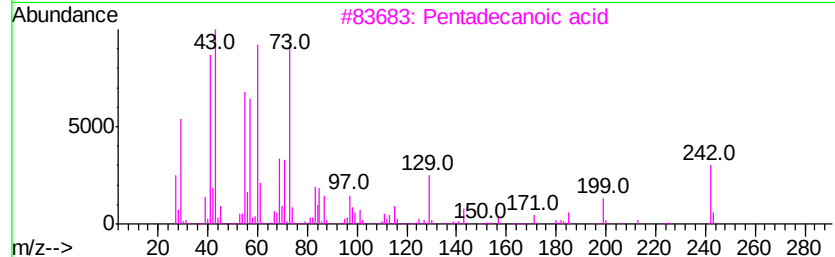
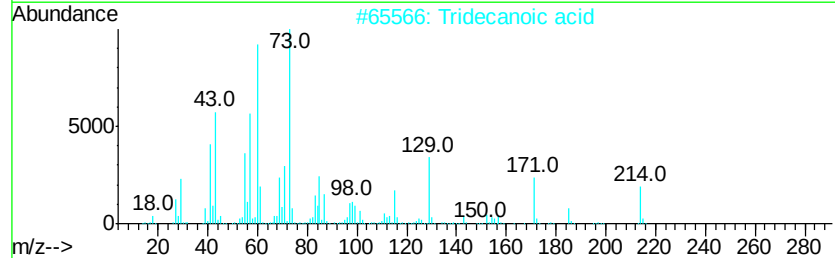
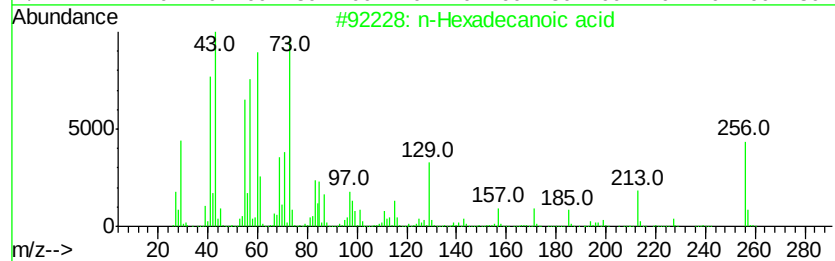
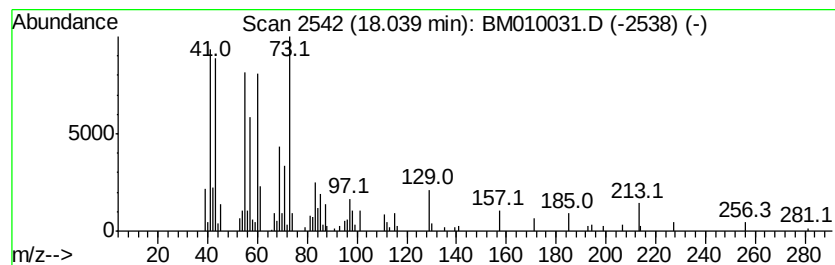
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	6.55 ng	327070	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Undecanoic acid	186	C11H22O2	000112-37-8	86



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010031.D
Acq On : 12 May 2017 19:40
Operator : SJ/MA
Sample : I3100-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PMW-2-051017

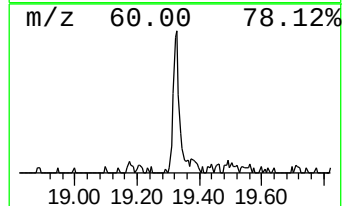
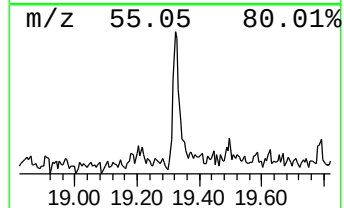
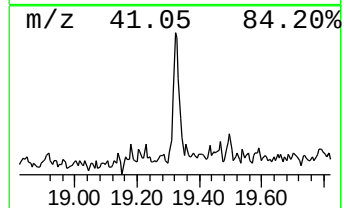
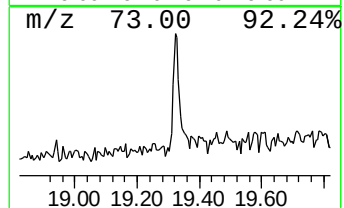
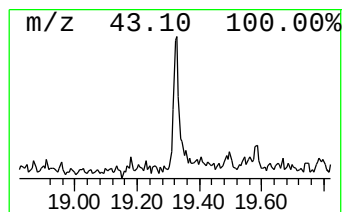
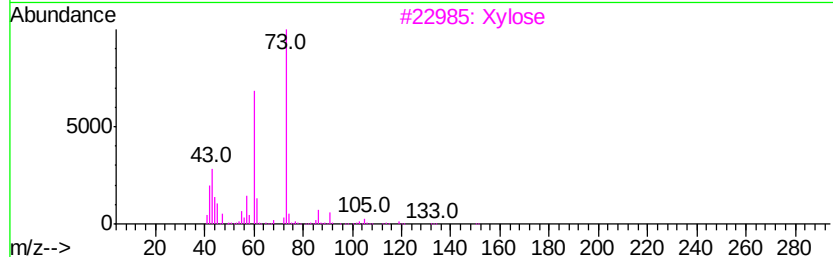
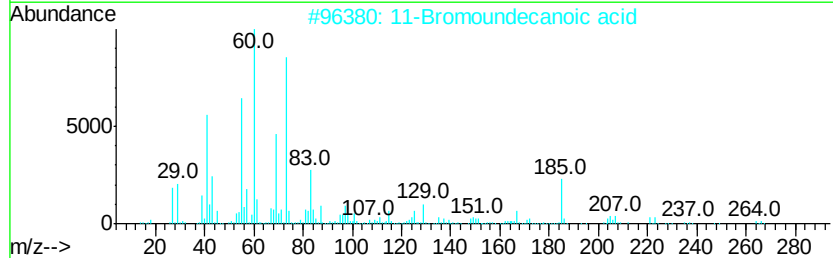
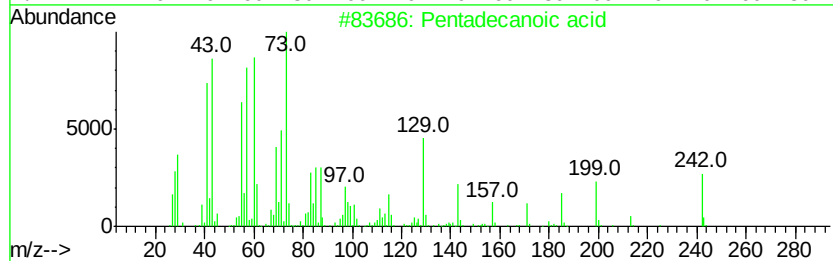
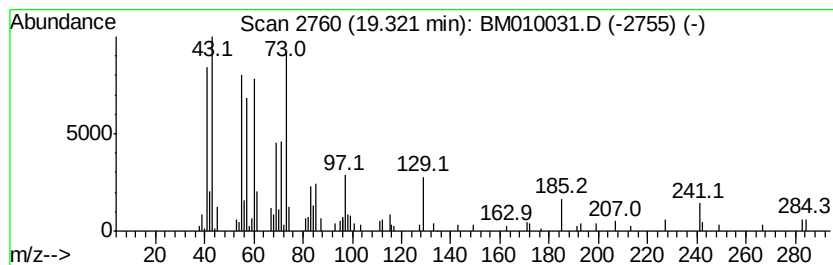
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.32	3.21 ng	176035	Chrysene-d12	21.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	38
3		Xylose	150	C5H10O5	000058-86-6	35
4		N-Acetylisoaxazolidine	115	C5H9NO2	115615-36-6	27
5		n-Decanoic acid	172	C10H20O2	000334-48-5	14



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010031.D
Acq On : 12 May 2017 19:40
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Sample : I3100-01
Misc :
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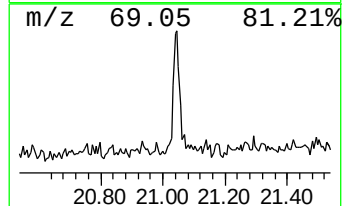
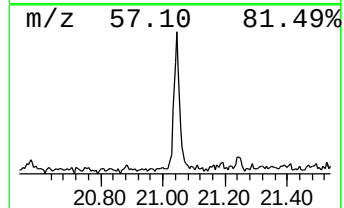
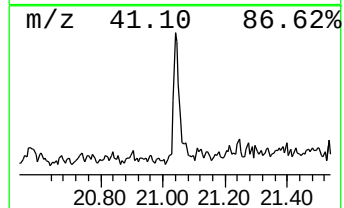
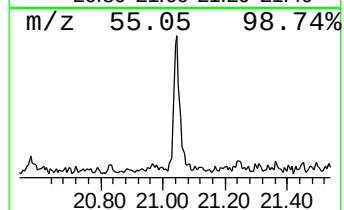
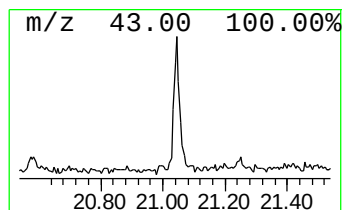
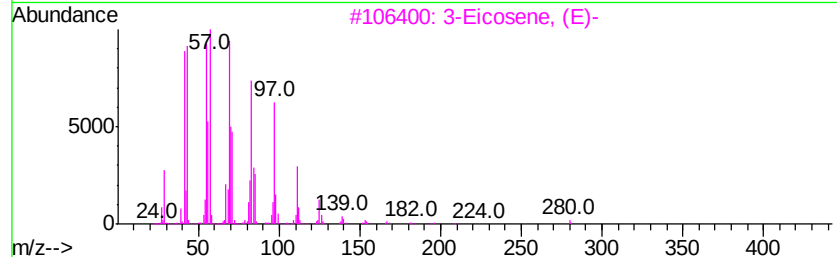
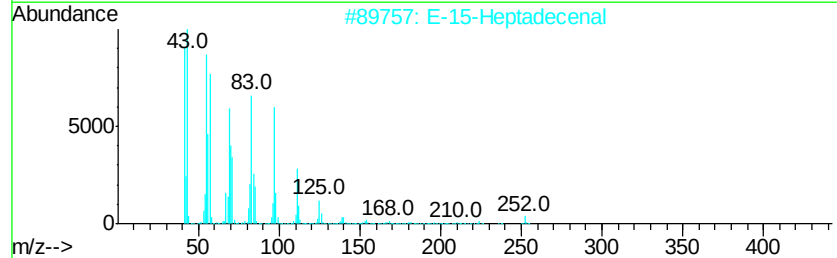
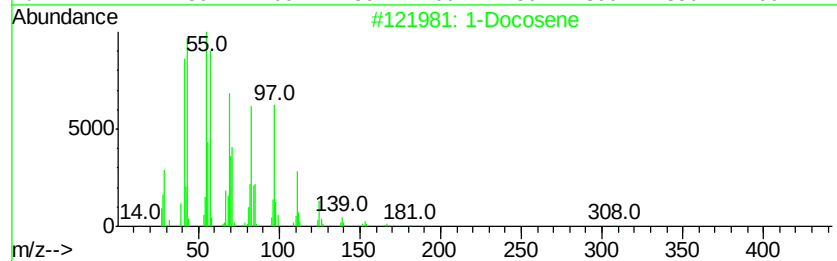
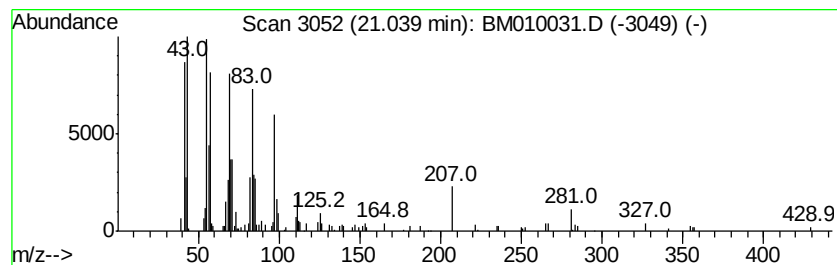
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.04	4.54 ng	248914	Chrysene-d12	21.36	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	74
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	72
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	68
4	Heptafluorobutyric acid, n-octadecyl-	466	C22H37F7O2	000400-57-7	68
5	Trichloroacetic acid, tetradecyl-	358	C16H29Cl3O2	074339-52-9	64



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM051217\
Data File : BM010031.D
Acq On : 12 May 2017 19:40
Operator : SJ/MA
Sample : I3100-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PMW-2-051017

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.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
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unknown8.80	8.80	2.4	ng	51565	1	7.76	425683	20.0
unknown12.23	12.23	11.7	ng	349068	2	10.55	595823	20.0
Hexadecane	15.23	3.5	ng	134882	3	14.41	781421	20.0
Tetradecane	16.10	4.9	ng	244555	4	17.17	998432	20.0
Eicosane	16.89	2.1	ng	104211	4	17.17	998432	20.0
n-Hexadecanoic acid	18.04	6.5	ng	327070	4	17.17	998432	20.0
Pentadecanoic acid	19.32	3.2	ng	176035	5	21.36	1097170	20.0
1-Docosene	21.04	4.5	ng	248914	5	21.36	1097170	20.0