

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032916\
 Data File : BF085864.D
 Acq On : 29 Mar 2016 22:25
 Operator : UM/SJ
 Sample : H1970-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-6

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-BF032416.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	4.996	235	237	243	rBV	39449	65829	2.18%	0.227%
2	5.407	270	273	275	rBV	2614569	3020774	100.00%	10.439%
3	6.447	361	364	367	rBV	2349582	2698516	89.33%	9.325%
4	6.573	373	375	378	rBV	2644342	2724429	90.19%	9.415%
5	6.802	393	395	398	rBV	771548	692256	22.92%	2.392%
6	6.962	407	409	411	rBV	2515014	2247430	74.40%	7.767%
7	7.373	442	445	447	rBV	1873442	1857394	61.49%	6.419%
8	7.407	447	448	450	rVV	144149	116783	3.87%	0.404%
9	7.476	450	454	459	rVB	45356	65608	2.17%	0.227%
10	7.842	484	486	491	rBV	18277	30819	1.02%	0.107%
11	8.093	505	508	510	rBV	940498	900026	29.79%	3.110%
12	9.168	599	602	605	rBV	2836312	2466355	81.65%	8.523%
13	9.568	635	637	639	rBV	485594	462179	15.30%	1.597%
14	9.762	652	654	658	rBV2	64477	114706	3.80%	0.396%
15	9.842	659	661	663	rVV	970013	873130	28.90%	3.017%
16	10.048	677	679	682	rBV4	23744	39494	1.31%	0.136%
17	10.276	698	699	701	rVB	115032	84968	2.81%	0.294%
18	10.493	715	718	721	rBV	29257	52123	1.73%	0.180%
19	10.631	728	730	733	rBV	1399479	1517236	50.23%	5.243%
20	10.745	739	740	745	rBV	96920	149273	4.94%	0.516%
21	10.962	755	759	761	rBV2	32681	57202	1.89%	0.198%
22	11.202	776	780	781	rBV2	38098	64644	2.14%	0.223%
23	11.225	781	782	786	rVB	44120	37006	1.23%	0.128%
24	11.328	789	791	792	rBV	888447	783402	25.93%	2.707%
25	11.408	795	798	799	rVB	47487	76365	2.53%	0.264%
26	11.568	808	812	815	rBV2	26274	47166	1.56%	0.163%
27	11.625	815	817	822	rVB4	37109	59181	1.96%	0.205%
28	11.831	833	835	836	rBV	45907	43951	1.45%	0.152%
29	11.865	836	838	840	rVV2	298419	390912	12.94%	1.351%
30	11.934	843	844	848	rVB3	49483	95996	3.18%	0.332%
31	12.128	858	861	862	rBV	27952	39702	1.31%	0.137%
32	12.151	862	863	865	rBV2	29877	32077	1.06%	0.111%
33	12.368	880	882	884	rBV2	47114	69984	2.32%	0.242%
34	12.414	884	886	889	rVB2	71978	94744	3.14%	0.327%

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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

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35	12.459	889	890	894	rVB2	31346	46778	1.55%	0.162%
36	12.539	894	897	898	rBV	395422	353896	11.72%	1.223%
37	12.642	904	906	909	rBV	151815	178881	5.92%	0.618%
38	12.768	913	917	919	rBV	325738	347466	11.50%	1.201%
39	12.916	927	930	932	rBV	1176786	1602409	53.05%	5.538%
40	12.996	933	937	940	rBV4	33927	76837	2.54%	0.266%
41	13.088	942	945	947	rVB	26581	59434	1.97%	0.205%
42	13.191	951	954	958	rVB2	61087	109744	3.63%	0.379%
43	13.294	961	963	964	rBV	27637	32697	1.08%	0.113%
44	13.328	964	966	968	rBV	66899	101547	3.36%	0.351%
45	13.477	977	979	982	rBV2	48245	85813	2.84%	0.297%
46	13.625	989	992	994	rVB3	98558	168502	5.58%	0.582%
47	13.717	997	1000	1001	rBV	41662	66161	2.19%	0.229%
48	13.762	1003	1004	1007	rVV	155492	196944	6.52%	0.681%
49	13.808	1007	1008	1013	rVB2	159107	209533	6.94%	0.724%
50	13.957	1018	1021	1026	rBV3	551141	1183087	39.17%	4.088%
51	14.128	1034	1036	1038	rBV2	44851	61190	2.03%	0.211%
52	14.437	1061	1063	1065	rBV3	48051	70981	2.35%	0.245%
53	14.985	1108	1111	1114	rBV	183857	391520	12.96%	1.353%
54	15.042	1114	1116	1118	rVB3	61097	77159	2.55%	0.267%
55	15.260	1134	1135	1138	rVB	104234	138607	4.59%	0.479%
56	15.328	1138	1141	1143	rVV	129980	192104	6.36%	0.664%
57	15.385	1143	1146	1152	rVB	506733	755661	25.02%	2.611%
58	16.425	1235	1237	1245	rVB3	58826	139352	4.61%	0.482%
59	16.757	1264	1266	1270	rBV2	58581	102918	3.41%	0.356%
60	17.180	1300	1303	1309	rVB	51141	116215	3.85%	0.402%

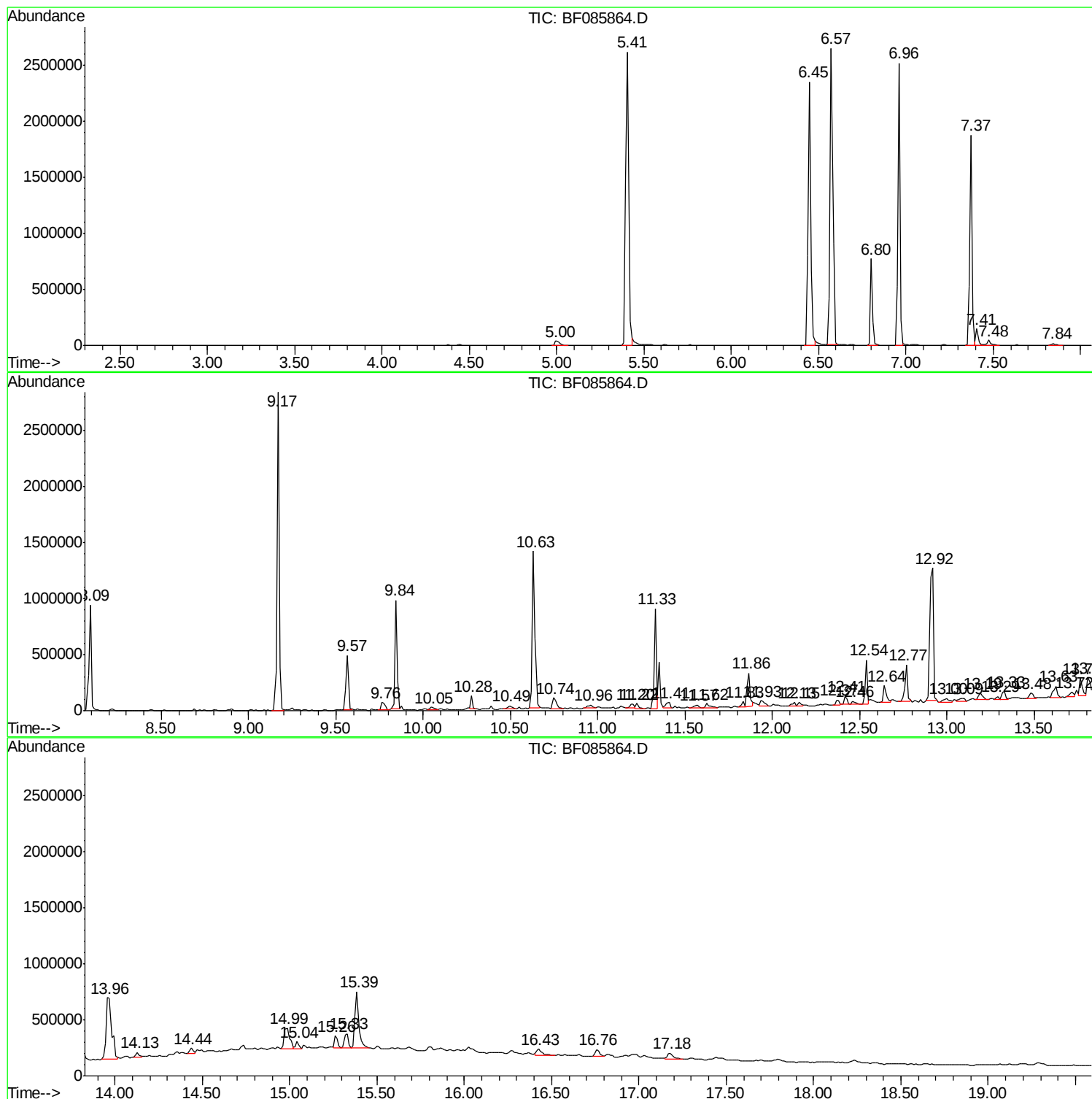
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampleId :
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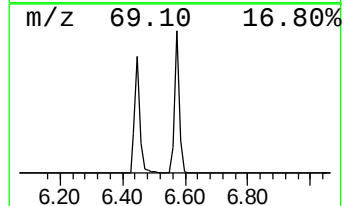
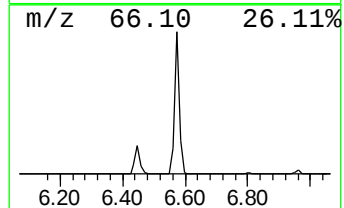
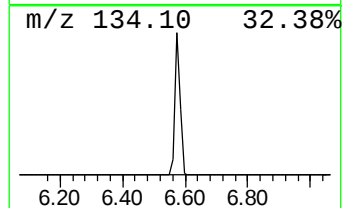
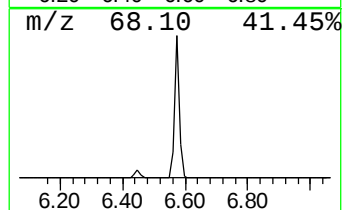
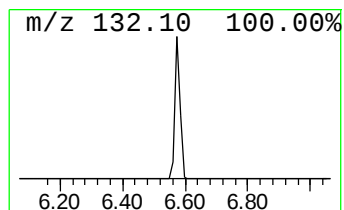
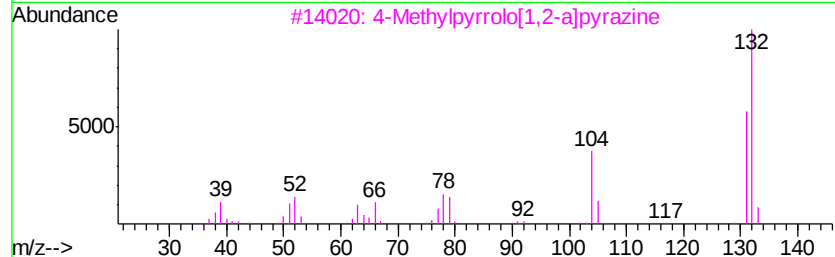
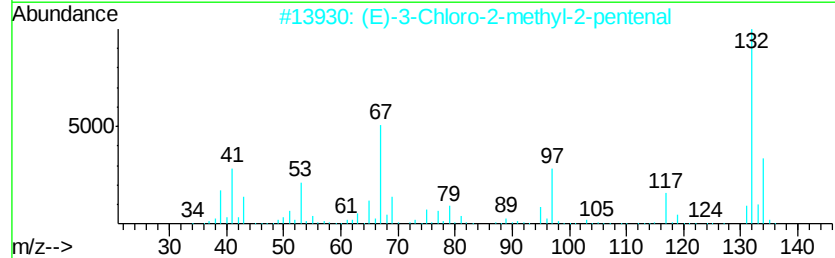
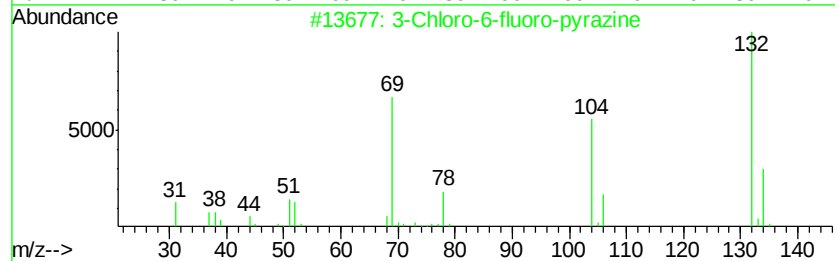
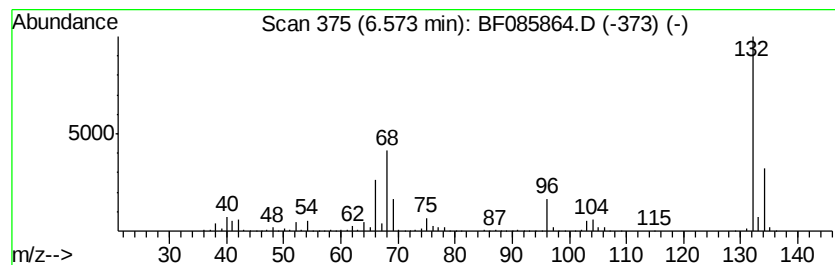
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	78.71 ng	2724430	1,4-Dichlorobenzene-d4	6.80

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	9
3		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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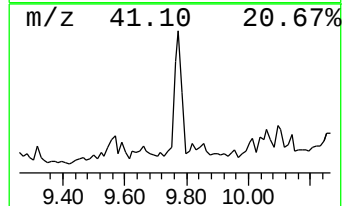
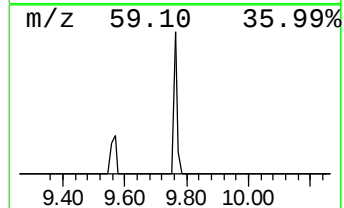
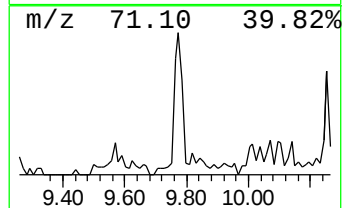
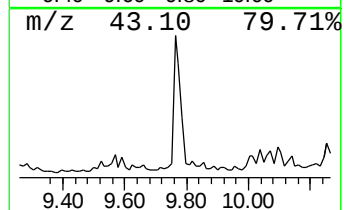
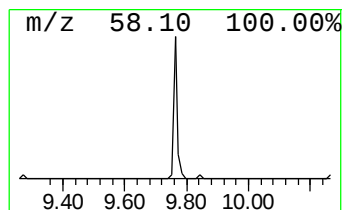
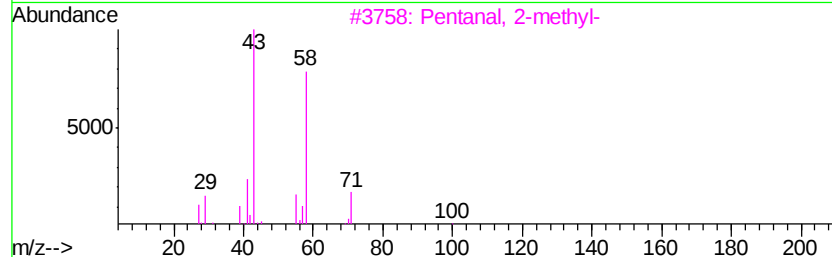
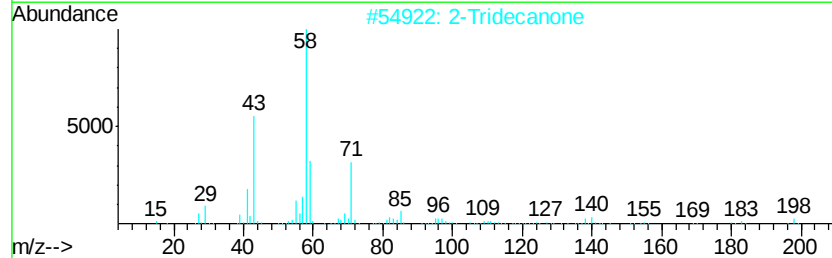
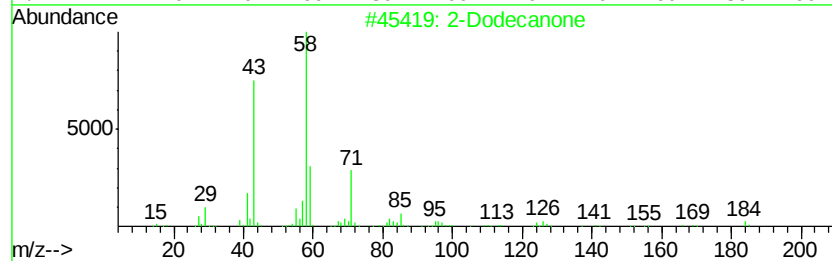
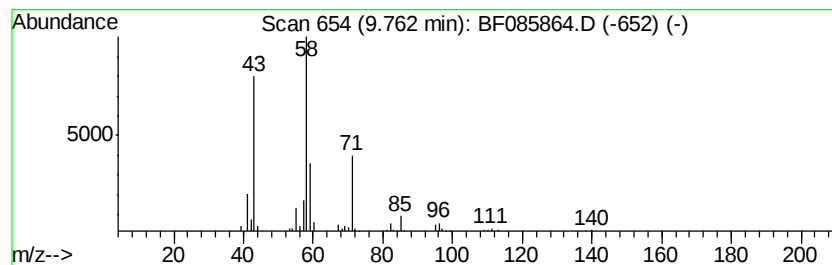
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Dodecanone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	2.63 ng	114706	Acenaphthene-d10	9.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Dodecanone	184	C12H24O	006175-49-1	90
2			2-Tridecanone	198	C13H26O	000593-08-8	72
3			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	59
4			Pentanal, 2,4-dimethyl-	114	C7H14O	027944-79-2	47
5			2-Octanone	128	C8H16O	000111-13-7	42



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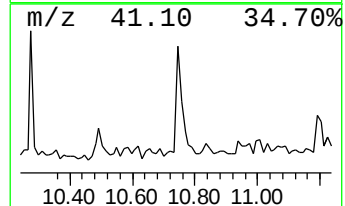
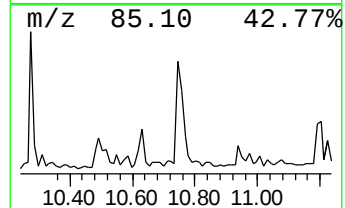
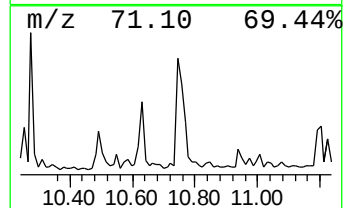
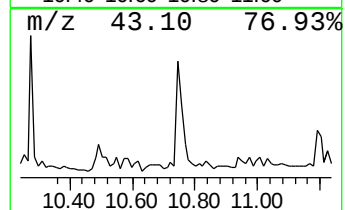
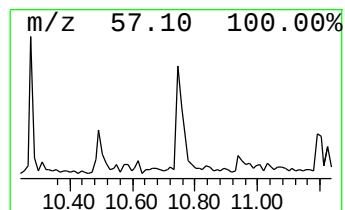
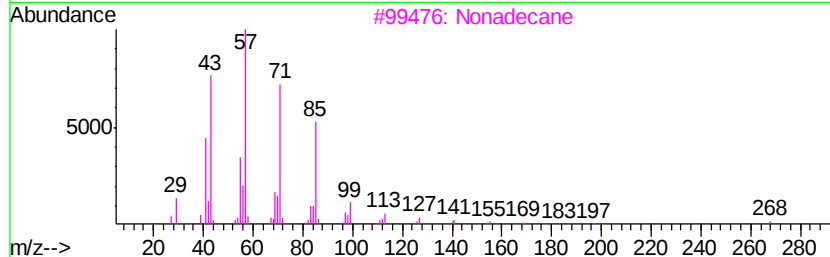
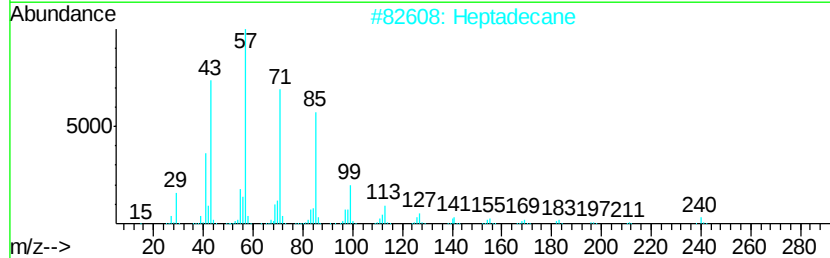
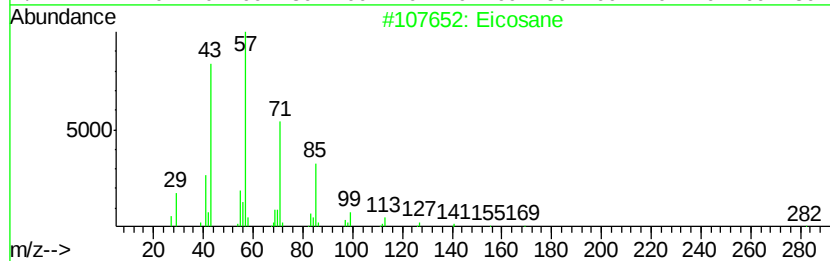
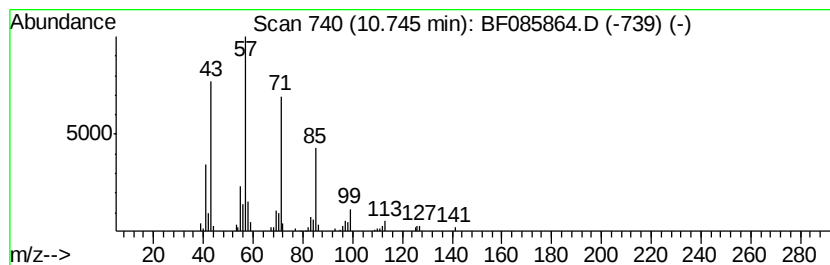
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	3.81 ng	149273	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Heptadecane		240	C17H36	000629-78-7	87
3	Nonadecane		268	C19H40	000629-92-5	86
4	Pentadecane		212	C15H32	000629-62-9	86
5	Tetradecane		198	C14H30	000629-59-4	86



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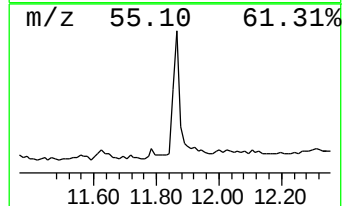
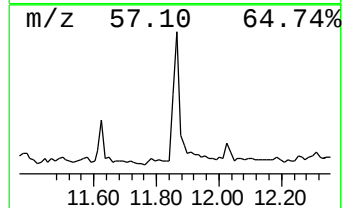
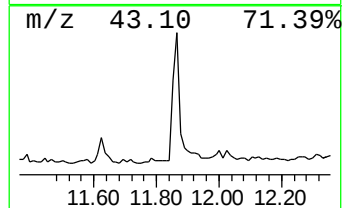
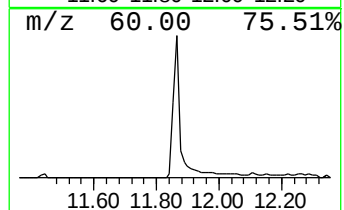
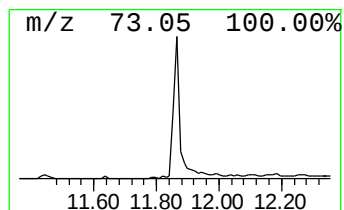
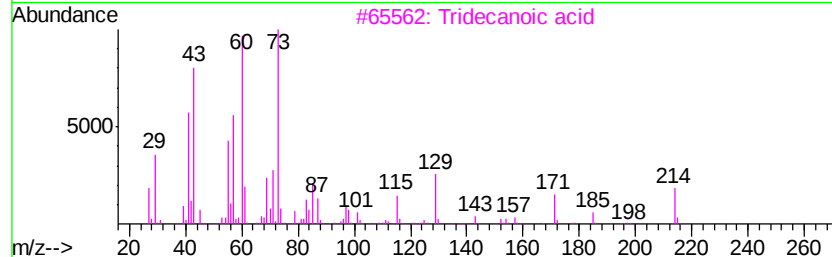
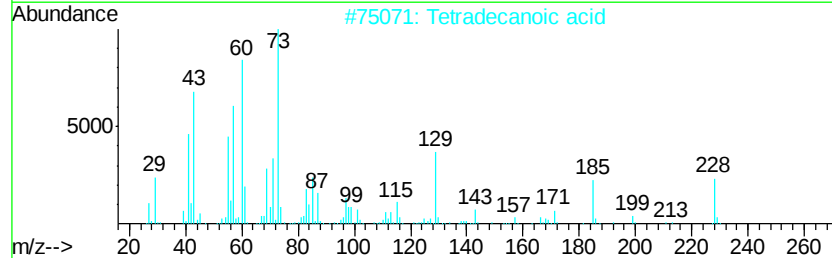
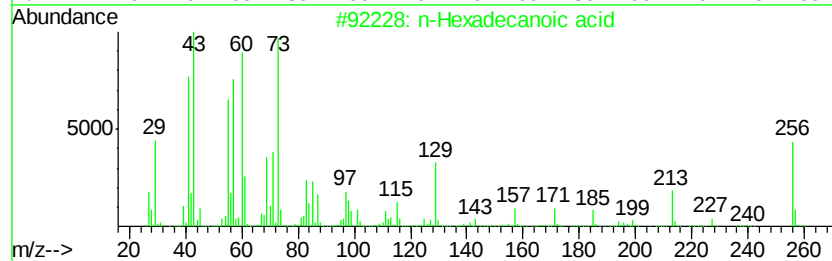
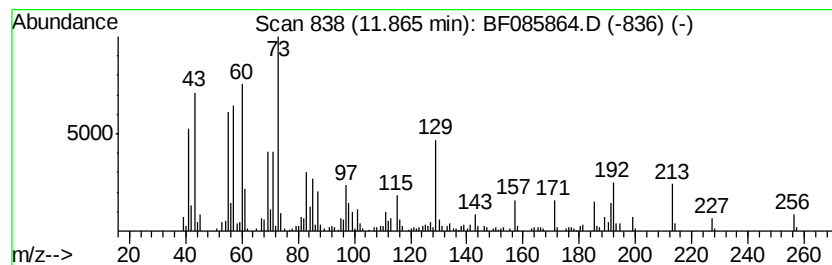
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.86	9.98 ng	390912	Phenanthrene-d10		11.33	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	86
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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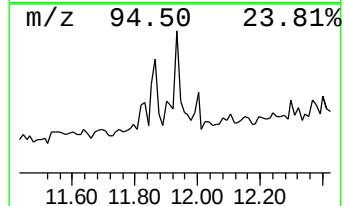
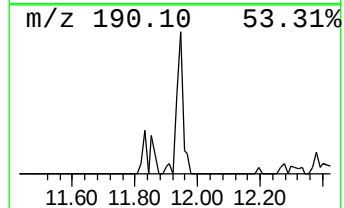
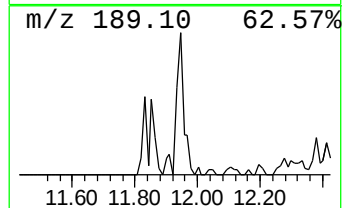
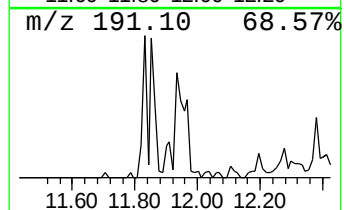
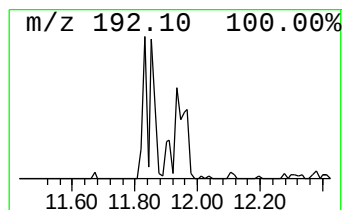
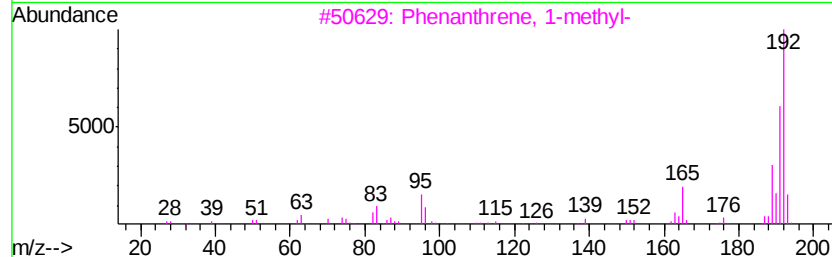
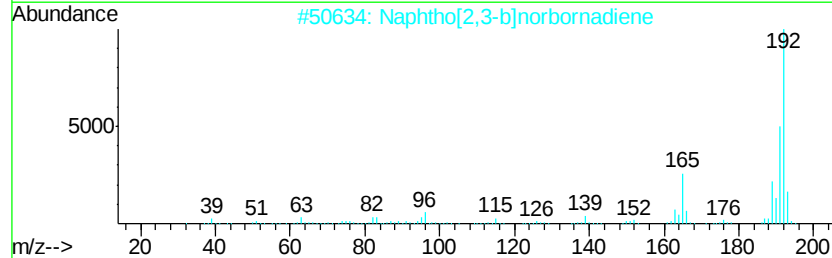
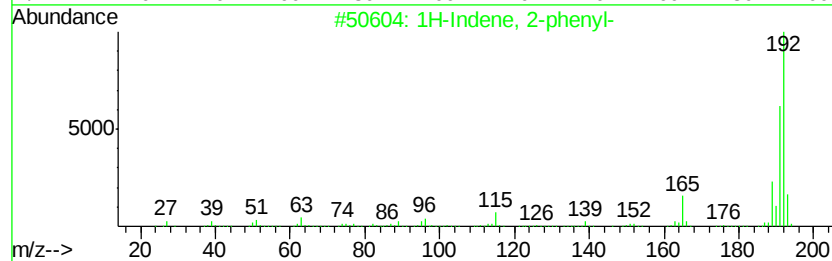
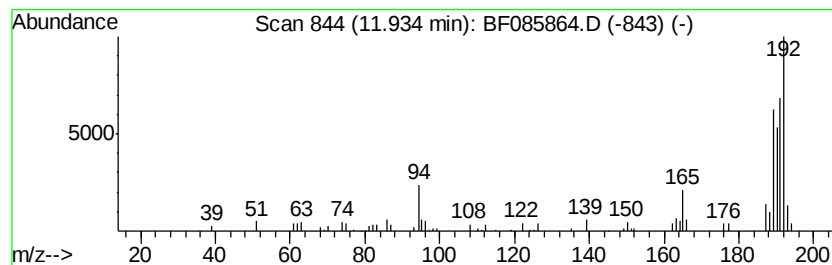
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1H-Indene, 2-phenyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.		
11.93	2.45 ng	95996	Phenanthrene-d10		11.33		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	53
2			Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	50
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	49
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	49
5			Anthracene, 2-methyl-	192	C15H12	000613-12-7	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032916\
Data File : BF085864.D
Acq On : 29 Mar 2016 22:25
Operator : UM/SJ
Sample : H1970-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

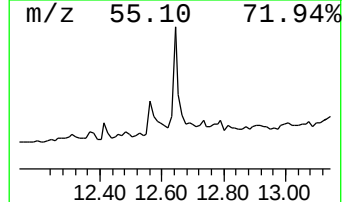
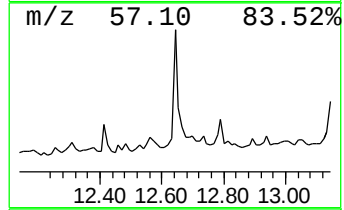
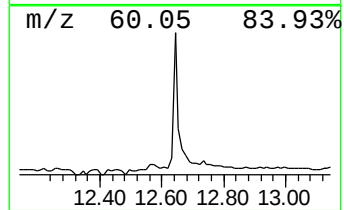
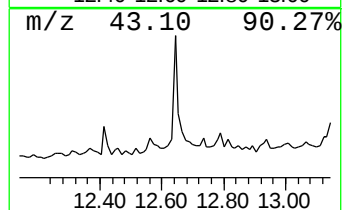
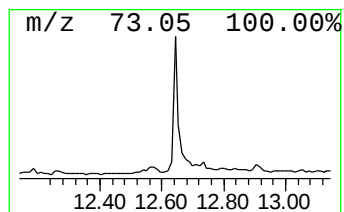
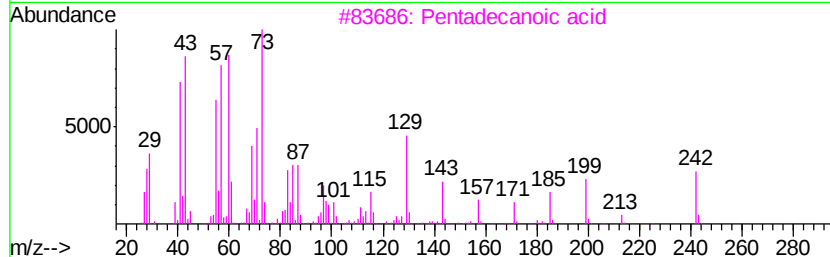
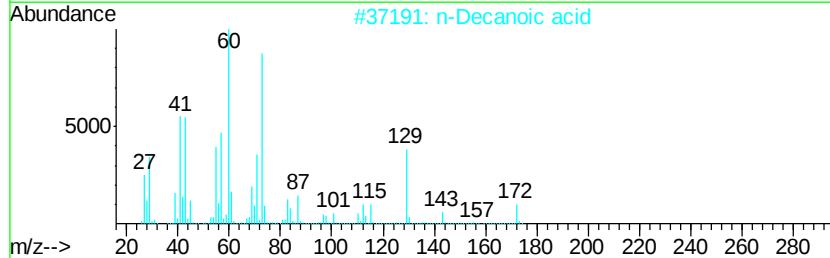
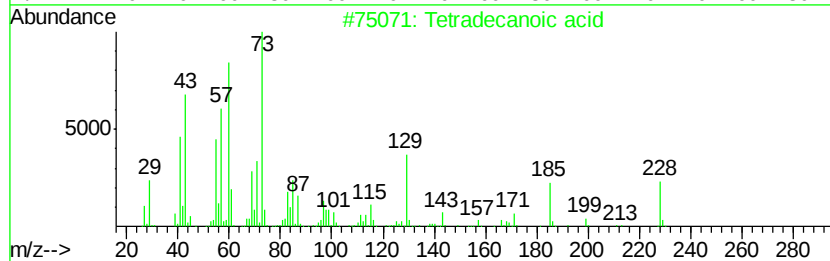
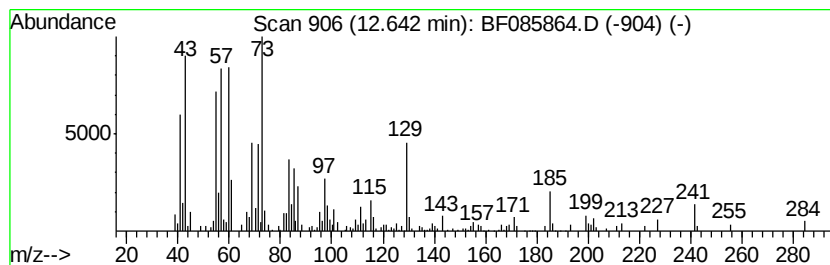
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	4.57 ng	178881	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
2	n-Decanoic acid	172	C10H20O2	000334-48-5	76
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4	Dodecane	170	C12H26	000112-40-3	11
5	Undecane	156	C11H24	001120-21-4	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032916\
Data File : BF085864.D
Acq On : 29 Mar 2016 22:25
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Sample : H1970-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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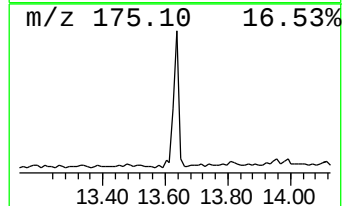
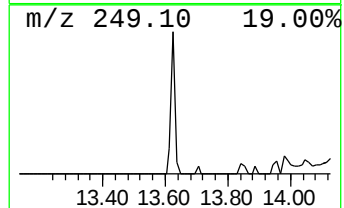
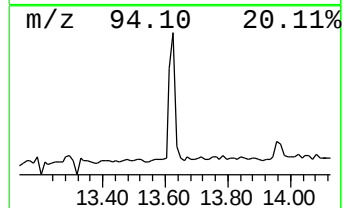
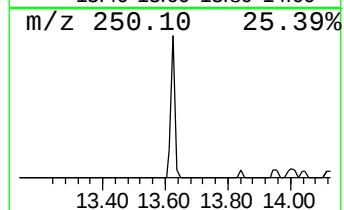
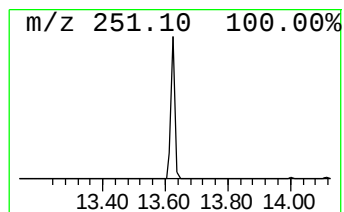
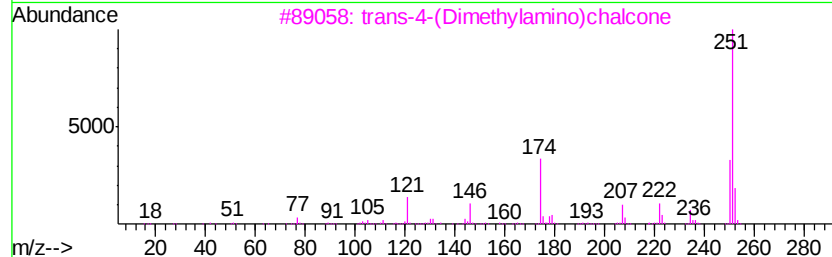
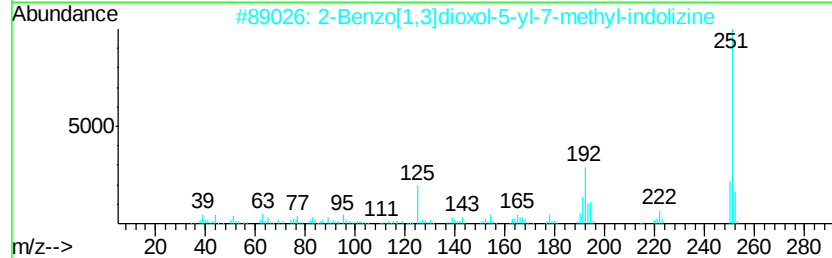
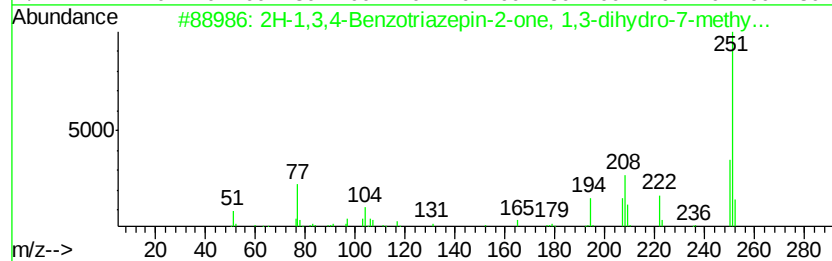
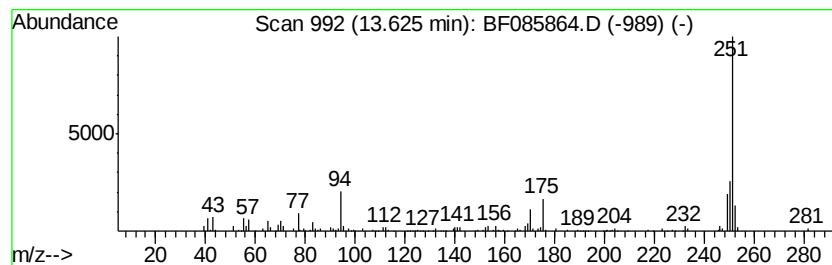
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2H-1,3,4-Benzotriazepin-2-o... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	2.85 ng	168502	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-1,3,4-Benzotriazepin-2-one, 1...	251	C15H13N3O	002855-57-4	50
2		2-Benzo[1,3]dioxol-5-yl-7-methyl...	251	C16H13N02	1000274-75-9	50
3		trans-4-(Dimethylamino)chalcone	251	C17H17NO	022965-98-6	50
4		Phosphoric acid, isodecyl diphen...	390	C22H31O4P	029761-21-5	43
5		2-(4-Cyanophenyl)-5-dimethylamin...	251	C14H13N5	150405-58-6	40



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Acq On : 29 Mar 2016 22:25
Operator : UM/SJ
Sample : H1970-06
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ClientSampleId :
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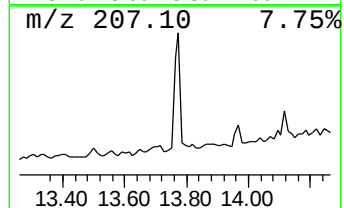
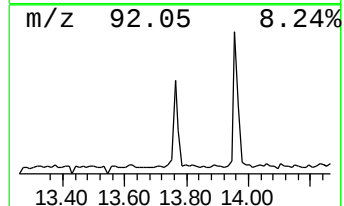
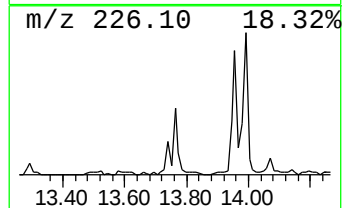
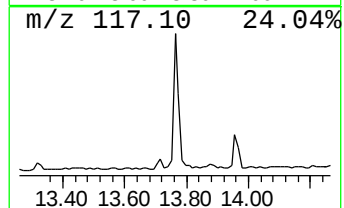
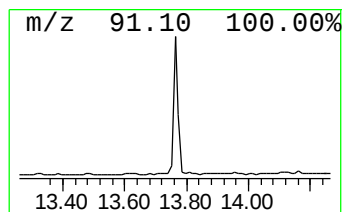
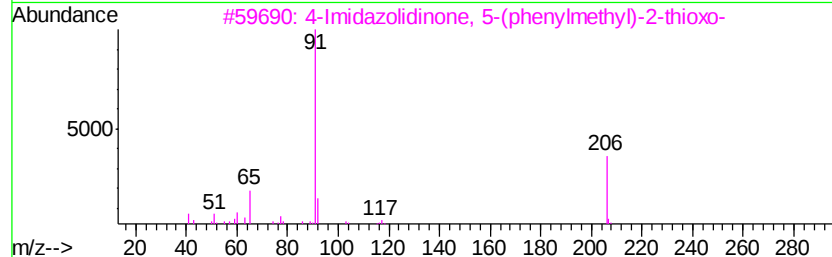
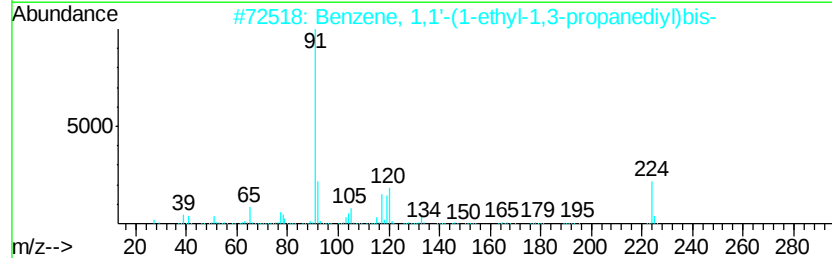
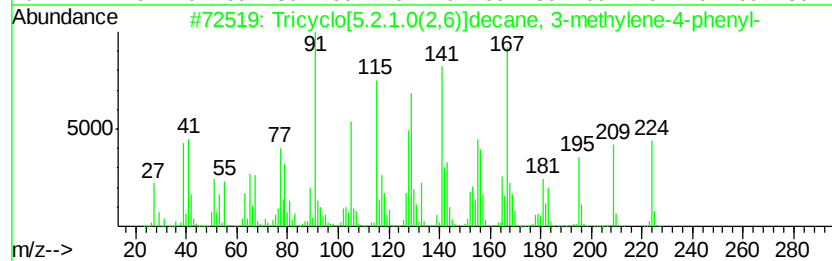
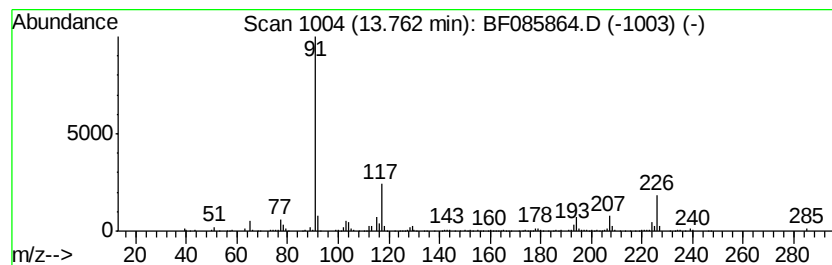
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tricyclo[5.2.1.0(2,6)]decan... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	3.33 ng	196944	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricyclo[5.2.1.0(2,6)]decane, 3-...	224	C17H20	1000150-37-1	64
2		Benzene, 1,1'-(1-ethyl-1,3-propa...	224	C17H20	000838-45-9	27
3		4-Imidazolidinone, 5-(phenylmeth...	206	C10H10N2OS	006330-09-2	16
4		Bicyclo[2.2.1]heptane, 3-methyle...	224	C17H20	1000150-36-8	14
5		3-Phenylthiane, S-oxide	194	C11H14OS	058121-26-9	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032916\
Data File : BF085864.D
Acq On : 29 Mar 2016 22:25
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Misc :
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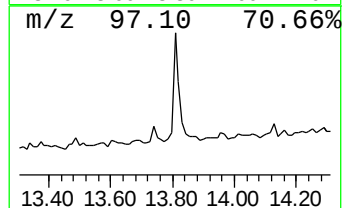
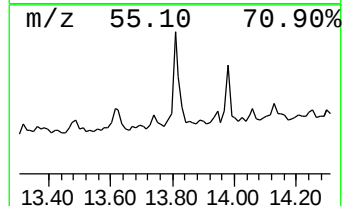
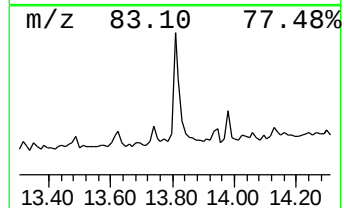
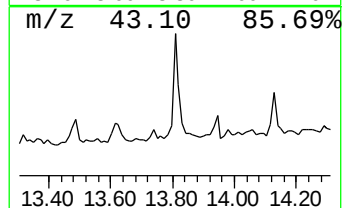
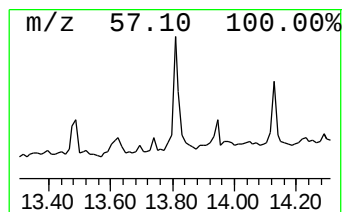
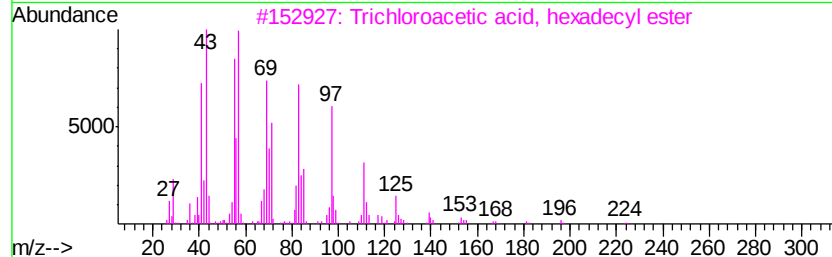
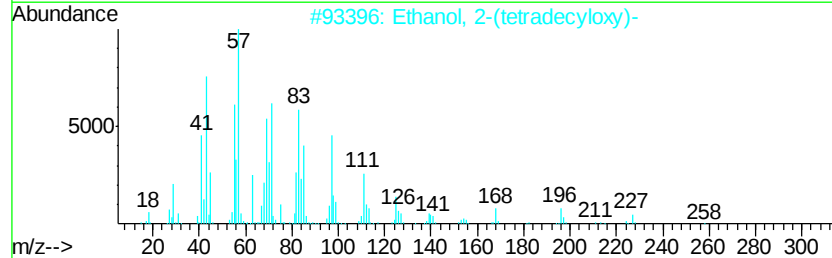
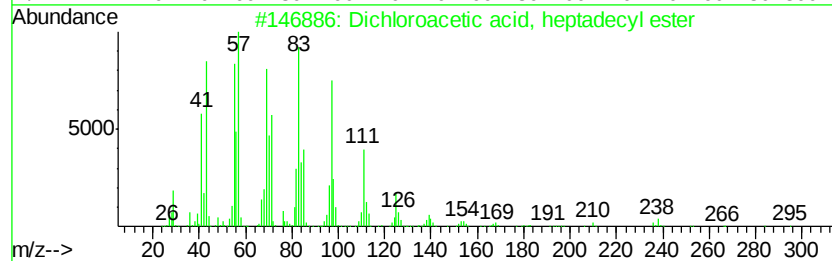
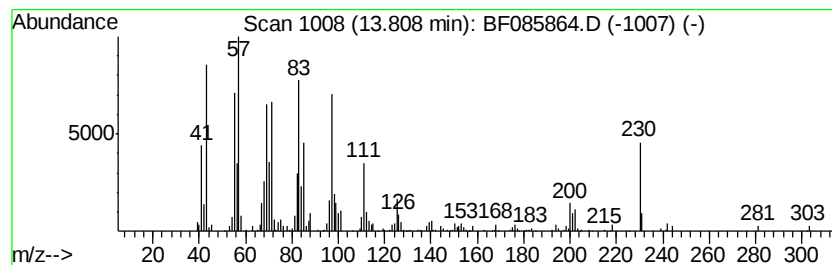
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Dichloroacetic acid, heptad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.54 ng	209533	Chrysene-d12	13.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	92
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	76
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	70
4			2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	70
5			Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	70



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032916\
Data File : BF085864.D
Acq On : 29 Mar 2016 22:25
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Sample : H1970-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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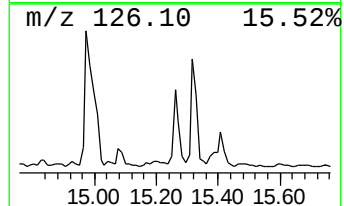
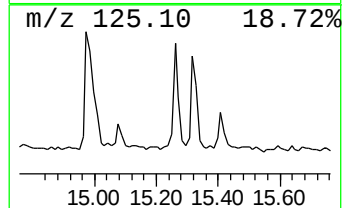
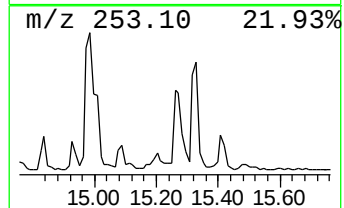
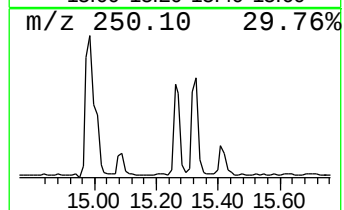
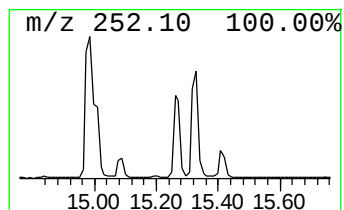
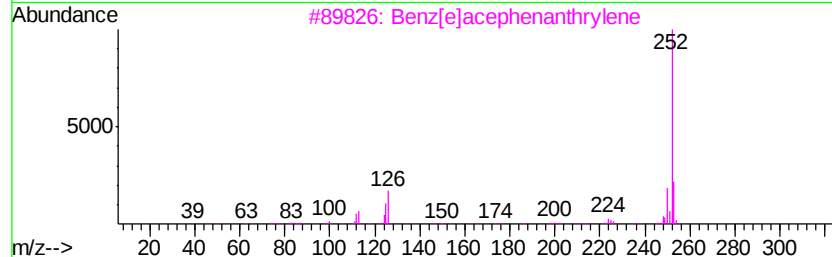
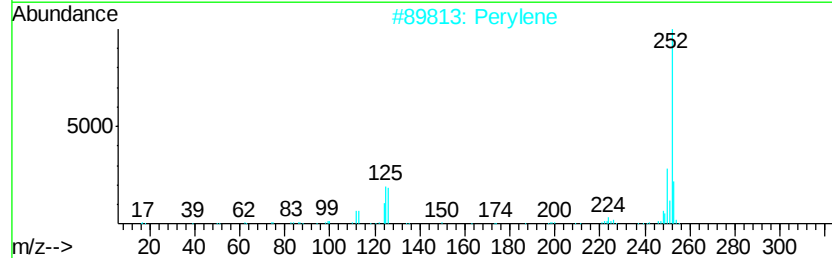
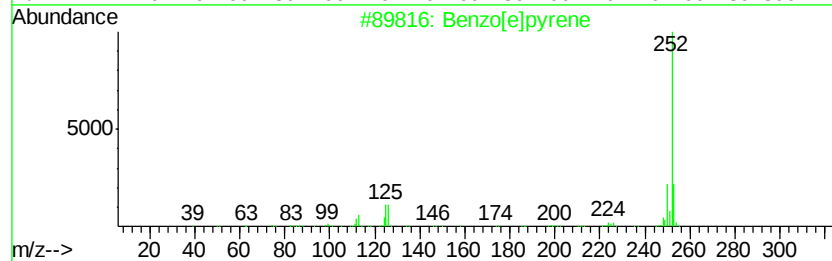
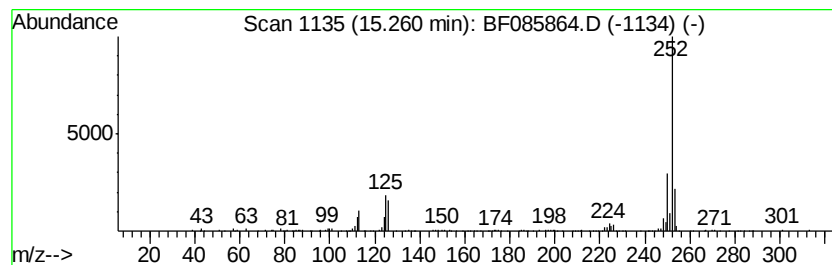
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.26	3.67 ng	138607	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Perylene	252	C20H12	000198-55-0	97
3		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	95



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032916\
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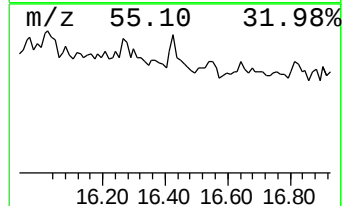
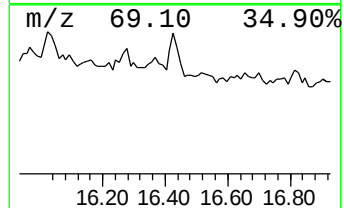
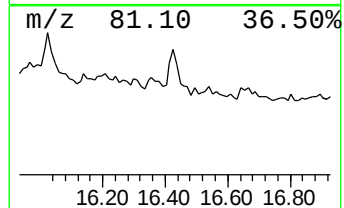
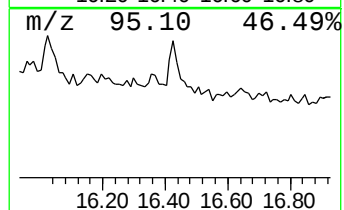
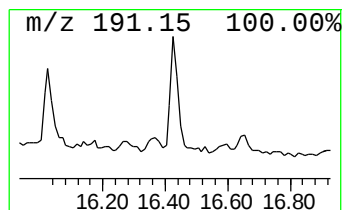
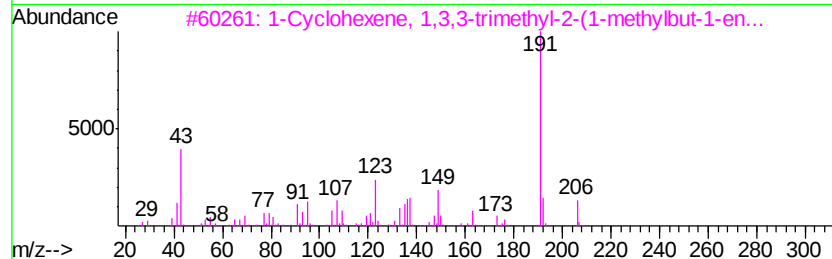
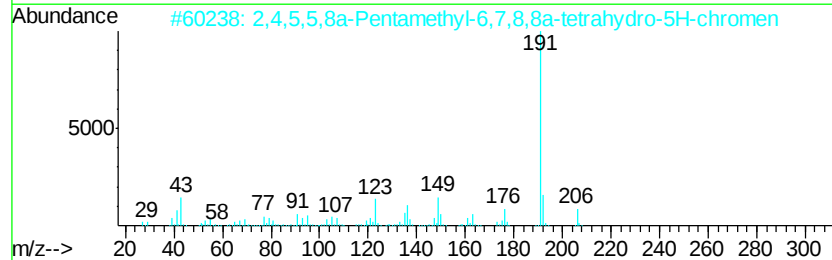
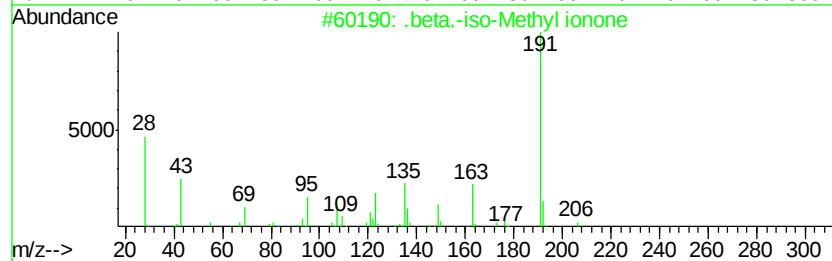
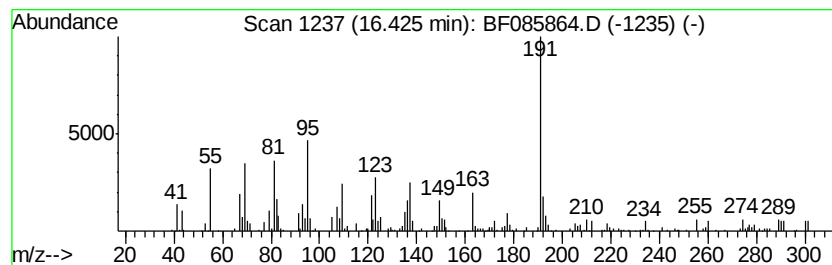
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 .beta.-iso-Methyl ionone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.43	3.69 ng	139352	Perylene-d12	15.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	60
2	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	47
3	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	38
4	Amiphenazole	191	C9H9N3S	000490-55-1	35
5	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032916\
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Operator : UM/SJ
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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
unknown6.57	6.57	78.7	ng	2724430	1	6.80	692256	20.0
2-Dodecanone	9.76	2.6	ng	114706	3	9.84	873130	20.0
Eicosane	10.74	3.8	ng	149273	4	11.33	783402	20.0
n-Hexadecanoic acid	11.86	10.0	ng	390912	4	11.33	783402	20.0
1H-Indene, 2-phenyl-	11.93	2.5	ng	95996	4	11.33	783402	20.0
Tetradecanoic acid	12.64	4.6	ng	178881	4	11.33	783402	20.0
2H-1,3,4-Benzotri...	13.63	2.9	ng	168502	5	13.97	1183090	20.0
Tricyclo[5.2.1.0(...	13.76	3.3	ng	196944	5	13.97	1183090	20.0
Dichloroacetic ac...	13.81	3.5	ng	209533	5	13.97	1183090	20.0
Benzo[e]pyrene	15.26	3.7	ng	138607	6	15.39	755661	20.0
.beta.-iso-Methyl...	16.43	3.7	ng	139352	6	15.39	755661	20.0