

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
 Data File : BF093026.D
 Acq On : 17 Feb 2017 22:26
 Operator : SJ/MA
 Sample : I1884-01 2X
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PIT-A-COMP

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-BF013017.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	3.756	144	146	149	rVB	29648	48651	1.91%	0.166%
2	4.487	208	210	214	rVB	46970	58729	2.31%	0.201%
3	5.013	254	256	266	rVB	712765	863525	33.90%	2.948%
4	5.402	288	290	292	rBV	27392	45442	1.78%	0.155%
5	5.447	292	294	297	rVB	2227745	2091929	82.12%	7.142%
6	6.499	383	386	395	rVB	2287711	2547491	100.00%	8.698%
7	6.625	395	397	399	rVV	2622327	2232587	87.64%	7.623%
8	6.682	399	402	405	rVB2	22115	37246	1.46%	0.127%
9	6.853	415	417	420	rVB	1115368	948694	37.24%	3.239%
10	7.013	429	431	433	rBV	1875135	1735490	68.13%	5.925%
11	7.425	464	467	469	rBV	1458527	1441332	56.58%	4.921%
12	7.459	469	470	472	rVB	33360	25784	1.01%	0.088%
13	8.145	527	530	532	rBV	1255864	1282644	50.35%	4.379%
14	8.568	565	567	569	rBV	30781	41338	1.62%	0.141%
15	8.728	579	581	584	rBV	41044	54345	2.13%	0.186%
16	9.219	621	624	626	rBV	2415155	2278573	89.44%	7.780%
17	9.299	629	631	633	rVV	94100	103512	4.06%	0.353%
18	9.368	634	637	640	rVB3	20648	30745	1.21%	0.105%
19	9.550	652	653	654	rBV	34766	28771	1.13%	0.098%
20	9.608	656	658	660	rVV	247912	264801	10.39%	0.904%
21	9.756	669	671	673	rBV	57997	53848	2.11%	0.184%
22	9.825	673	677	679	rBV	141129	137748	5.41%	0.470%
23	9.893	681	683	685	rVB	1404157	1200507	47.13%	4.099%
24	10.053	694	697	698	rBV2	19416	28112	1.10%	0.096%
25	10.099	698	701	703	rVB2	36446	50087	1.97%	0.171%
26	10.145	703	705	707	rBV3	25892	35212	1.38%	0.120%
27	10.213	707	711	712	rBV3	22683	54695	2.15%	0.187%
28	10.328	717	721	722	rBV	105796	157884	6.20%	0.539%
29	10.431	729	730	734	rVB3	18786	37041	1.45%	0.126%
30	10.545	737	740	743	rBV	49945	75990	2.98%	0.259%
31	10.591	743	744	746	rBV2	22902	29211	1.15%	0.100%
32	10.682	749	752	754	rBV	1154672	1112134	43.66%	3.797%
33	10.796	760	762	766	rBV	210273	265251	10.41%	0.906%
34	10.991	776	779	780	rBV2	31226	52699	2.07%	0.180%

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35	11.139	788	792	794	rBV4	28802	68377	2.68%	0.233%
36	11.242	798	801	803	rBV	181825	191860	7.53%	0.655%
37	11.276	803	804	807	rVB	60320	50145	1.97%	0.171%
38	11.379	811	813	814	rBV	1121081	1096419	43.04%	3.743%
39	11.448	818	819	821	rVB	66418	62021	2.43%	0.212%
40	11.608	830	833	836	rBV5	30955	95124	3.73%	0.325%
41	11.665	836	838	840	rVV	112906	123515	4.85%	0.422%
42	11.711	840	842	845	rVB2	24376	33161	1.30%	0.113%
43	11.768	845	847	848	rBV	31676	46309	1.82%	0.158%
44	11.836	851	853	855	rBV3	28060	40723	1.60%	0.139%
45	11.882	855	857	858	rBV	56432	85126	3.34%	0.291%
46	11.905	858	859	861	rVV	116596	93496	3.67%	0.319%
47	11.951	862	863	865	rVV2	31648	44318	1.74%	0.151%
48	11.985	865	866	870	rVB2	115010	179390	7.04%	0.612%
49	12.076	872	874	876	rVV	89460	81316	3.19%	0.278%
50	12.179	880	883	886	rVV3	63874	131733	5.17%	0.450%
51	12.316	893	895	897	rBV3	41725	65885	2.59%	0.225%
52	12.431	903	905	906	rBV	84407	92476	3.63%	0.316%
53	12.465	906	908	911	rVB	105058	128734	5.05%	0.440%
54	12.591	916	919	921	rBV	625005	583365	22.90%	1.992%
55	12.625	921	922	926	rBV4	46911	80825	3.17%	0.276%
56	12.819	936	939	942	rBV	536237	674773	26.49%	2.304%
57	12.957	949	951	954	rVB	1323687	1360804	53.42%	4.646%
58	13.037	956	958	962	rBV4	47283	93135	3.66%	0.318%
59	13.242	975	976	980	rBV3	54179	72175	2.83%	0.246%
60	13.528	999	1001	1003	rBV	61444	100028	3.93%	0.342%
61	13.654	1009	1012	1014	rBV	496104	561414	22.04%	1.917%
62	13.860	1027	1030	1033	rVB2	191905	242651	9.53%	0.828%
63	13.905	1033	1034	1036	rBV	70130	83407	3.27%	0.285%
64	14.008	1040	1043	1050	rVV2	843822	1530168	60.07%	5.224%
65	14.294	1067	1068	1070	rVB	151233	176207	6.92%	0.602%
66	15.037	1131	1133	1137	rBV	269507	441072	17.31%	1.506%
67	15.391	1161	1164	1167	rBV	225983	295343	11.59%	1.008%
68	15.448	1167	1169	1176	rVB	585879	831569	32.64%	2.839%

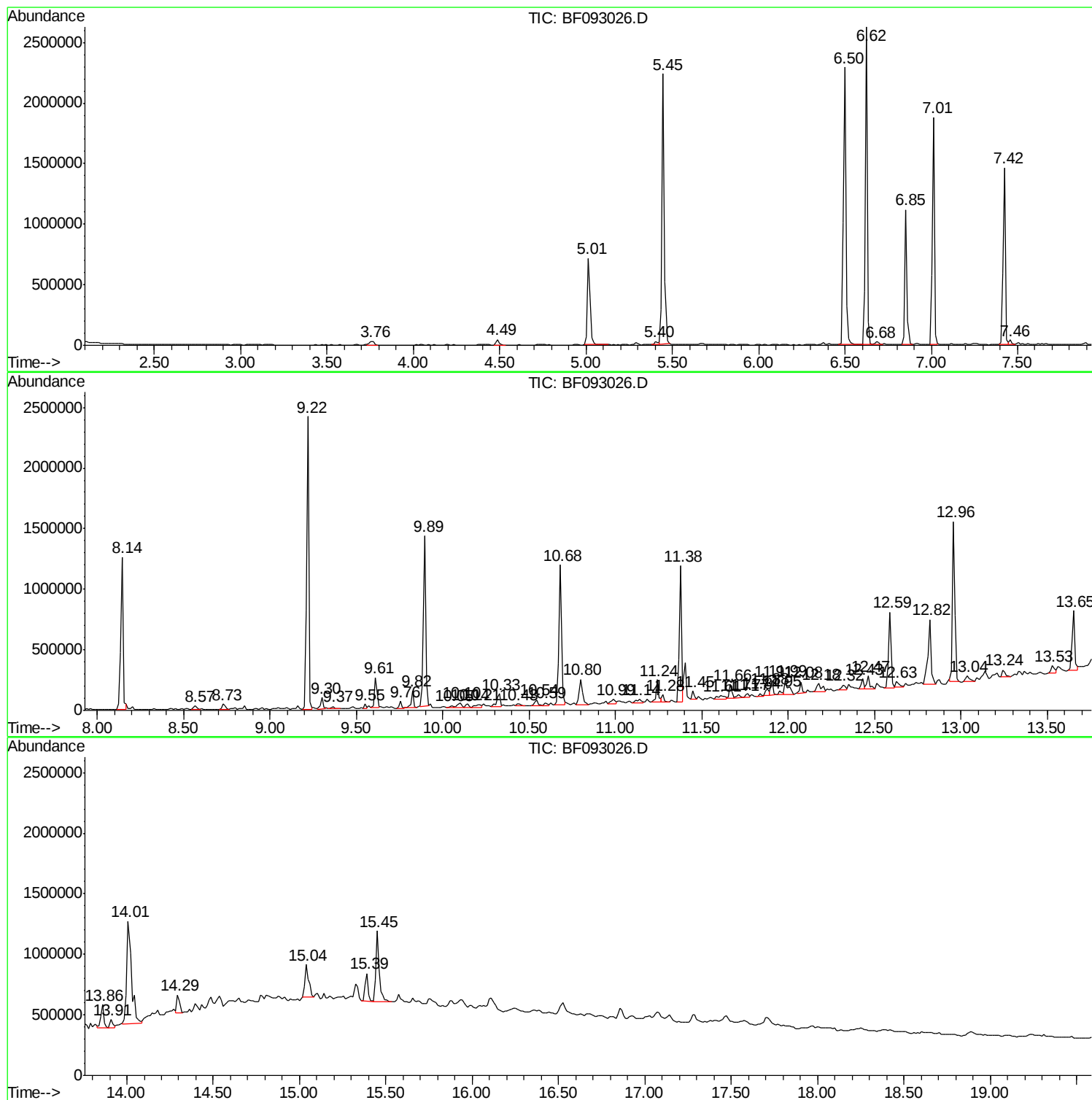
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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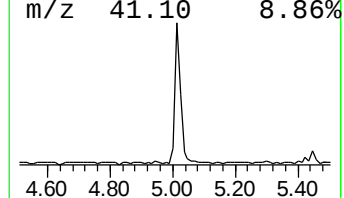
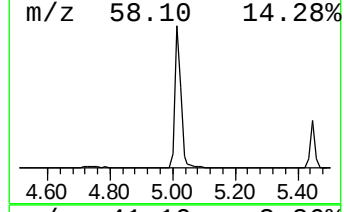
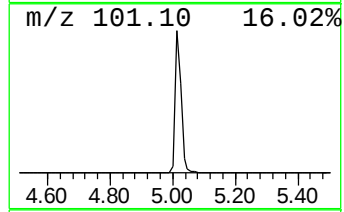
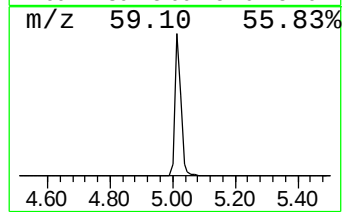
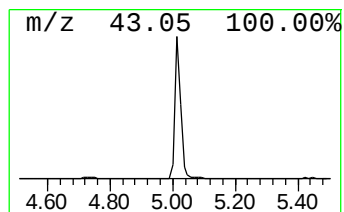
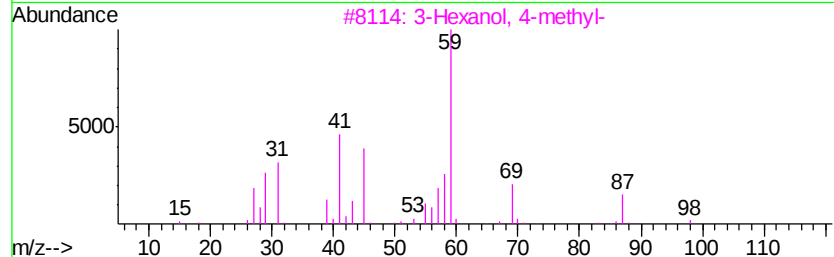
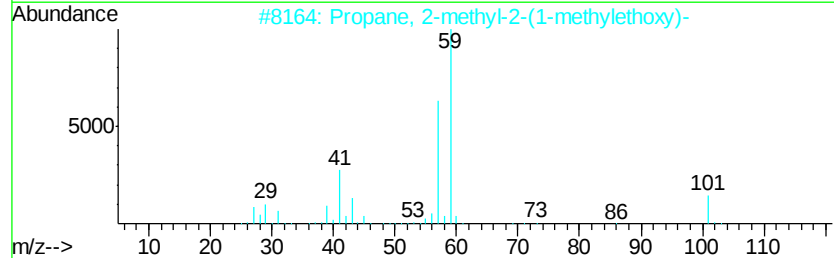
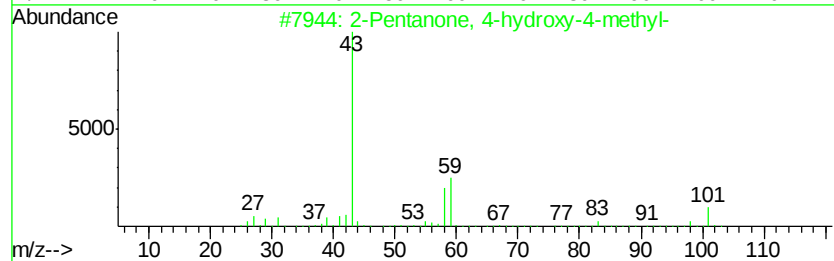
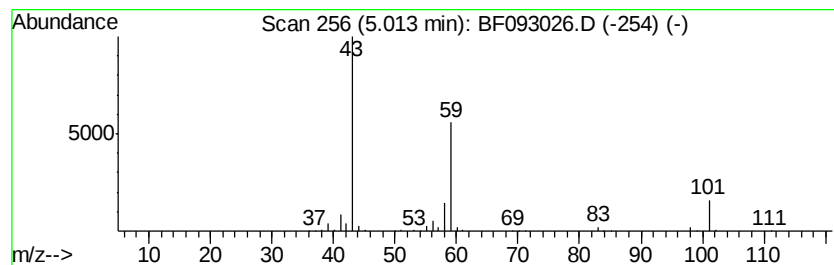
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	18.20 ng	863525	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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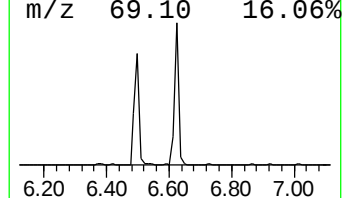
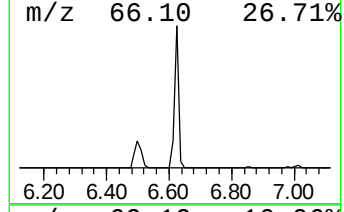
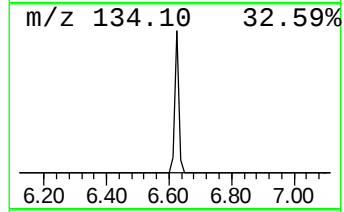
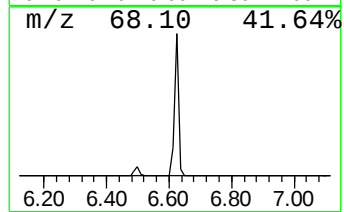
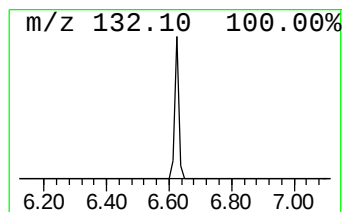
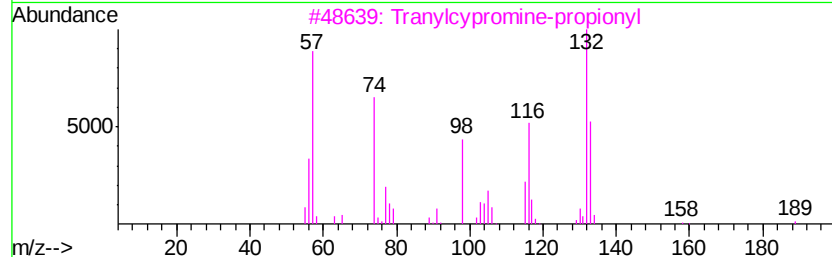
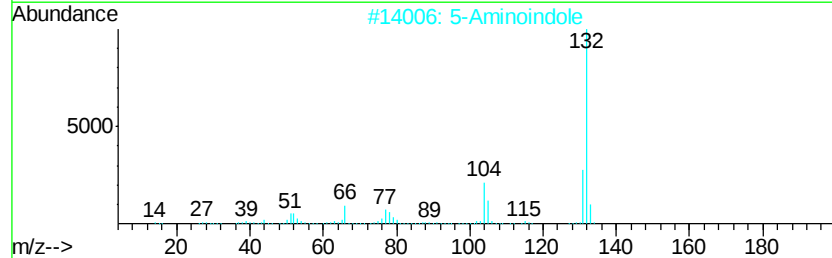
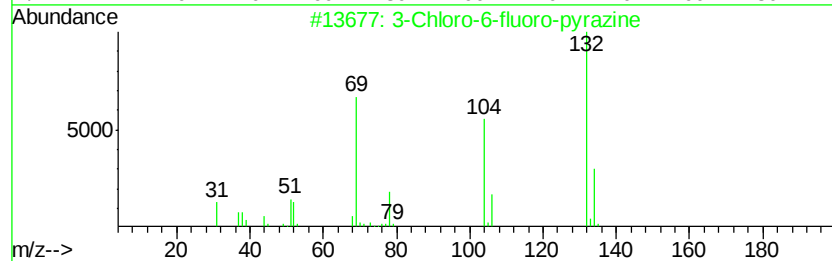
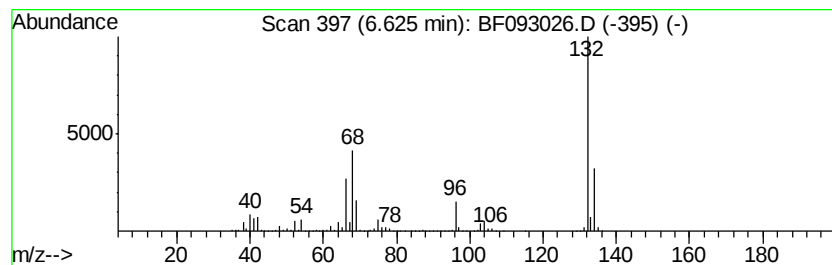
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	47.07 ng	2232590	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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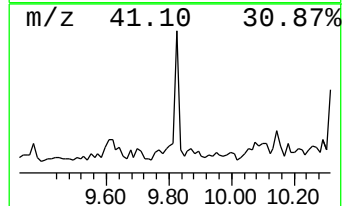
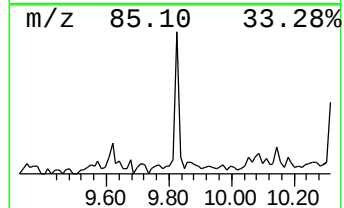
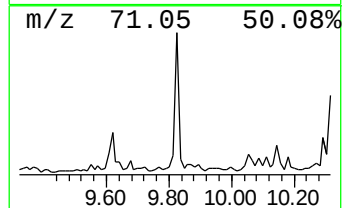
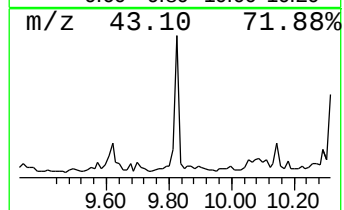
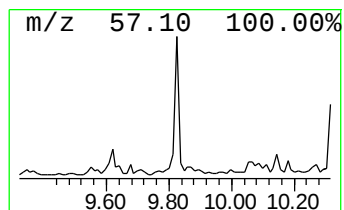
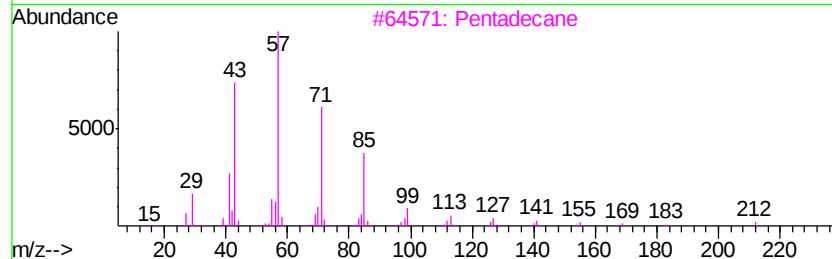
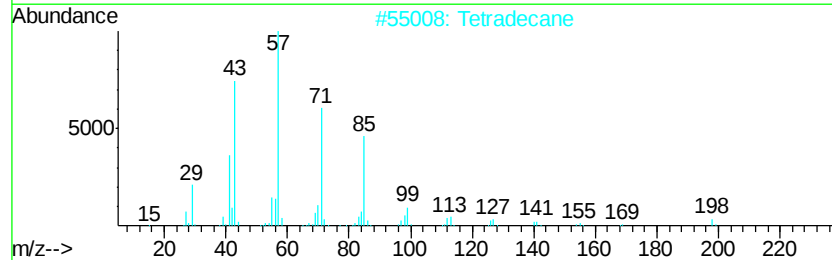
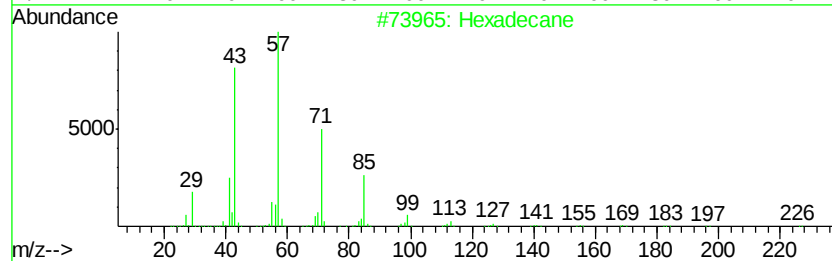
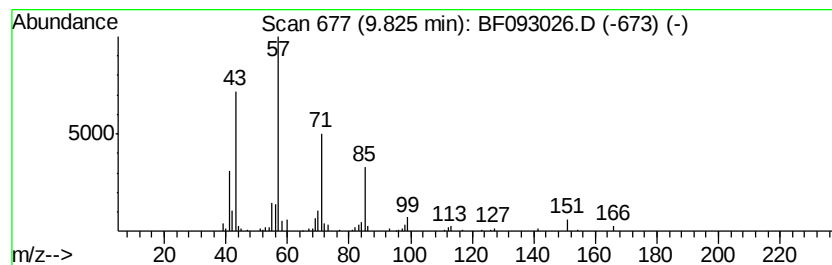
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	2.29 ng	137748	Acenaphthene-d10	9.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	87
2		Tetradecane	198	C14H30	000629-59-4	80
3		Pentadecane	212	C15H32	000629-62-9	78
4		Undecane	156	C11H24	001120-21-4	72
5		Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	64



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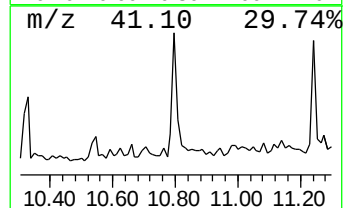
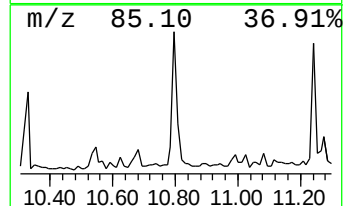
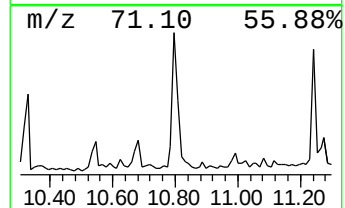
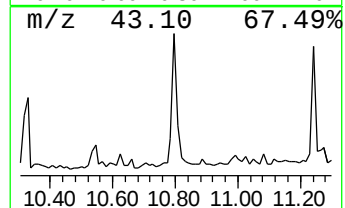
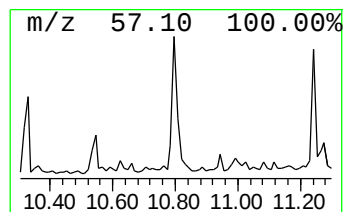
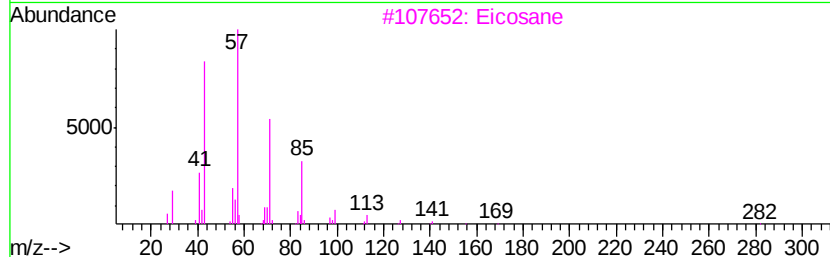
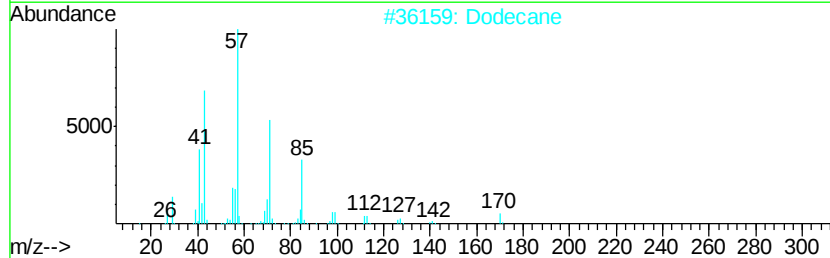
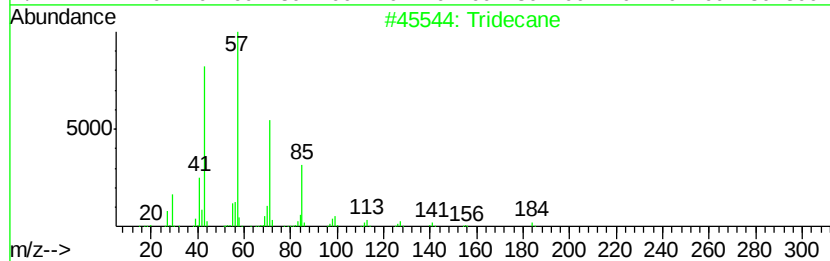
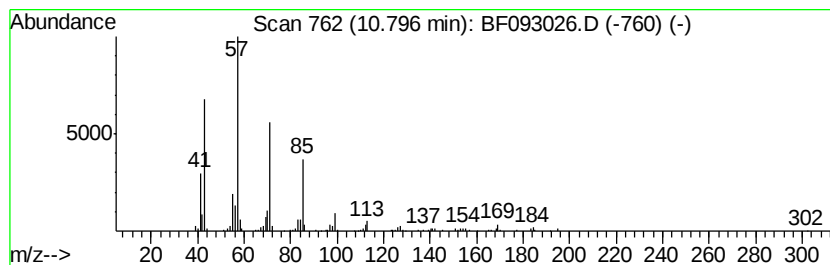
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.80	4.84 ng	265251	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Dodecane	170	C12H26	000112-40-3	91
3	Eicosane	282	C20H42	000112-95-8	91
4	Hexadecane	226	C16H34	000544-76-3	90
5	Heptadecane	240	C17H36	000629-78-7	90



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PIT-A-COMP

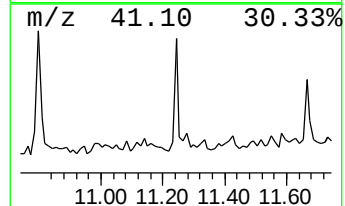
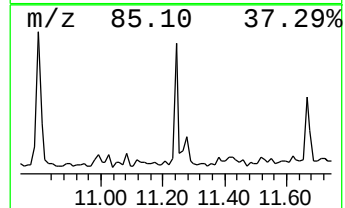
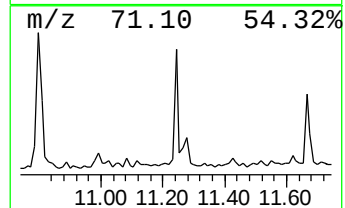
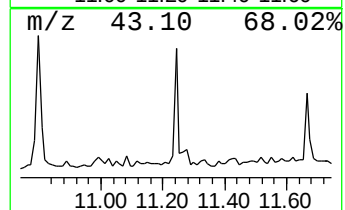
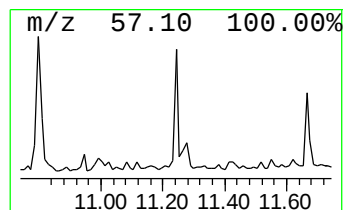
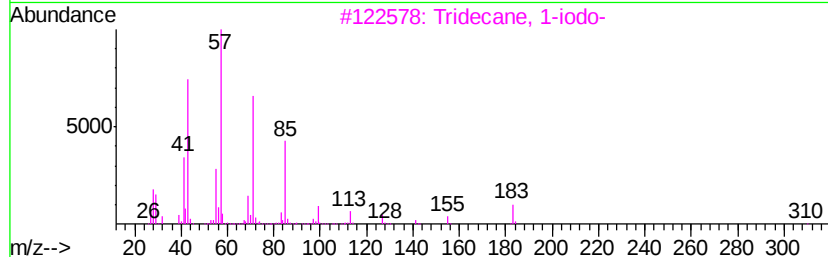
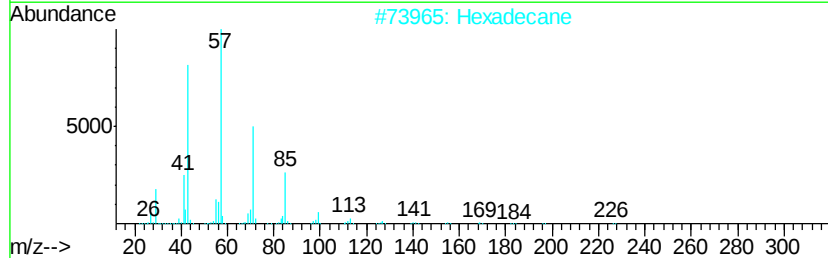
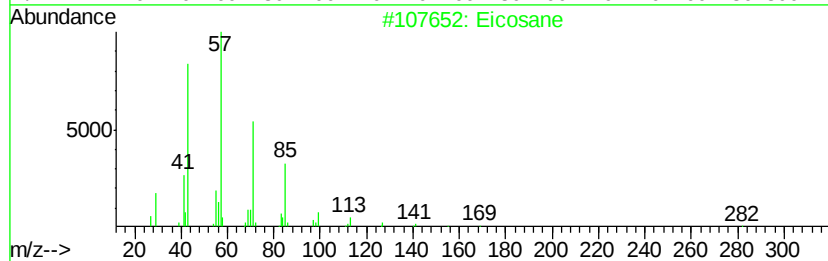
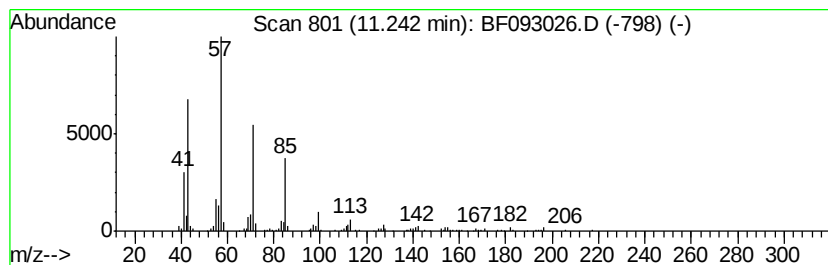
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	3.50 ng	191860	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Hexadecane		226	C16H34	000544-76-3	90
3	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	90
4	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	86
5	2-Bromo dodecane		248	C12H25Br	013187-99-0	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093026.D
Acq On : 17 Feb 2017 22:26
Operator : SJ/MA
Sample : I1884-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIT-A-COMP

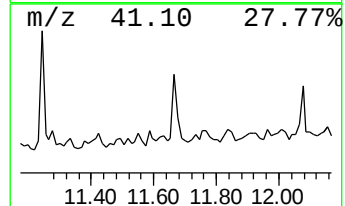
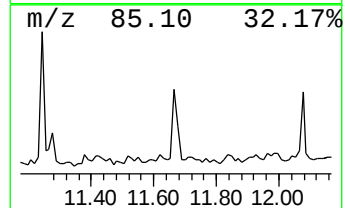
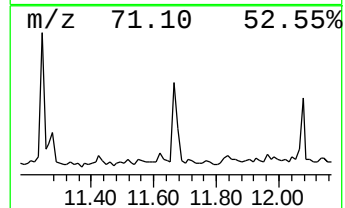
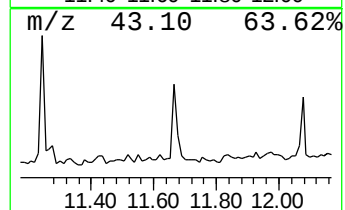
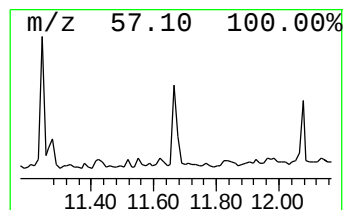
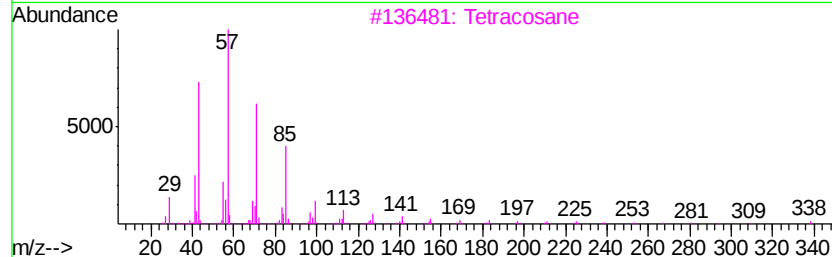
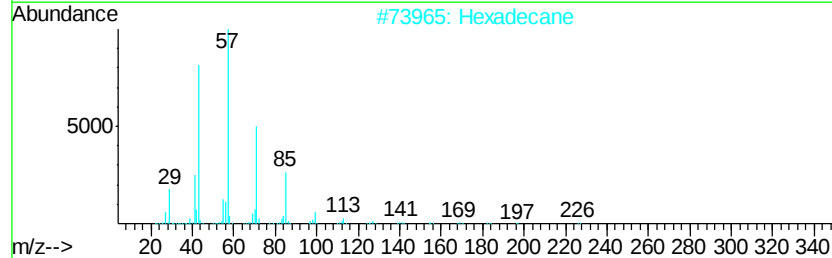
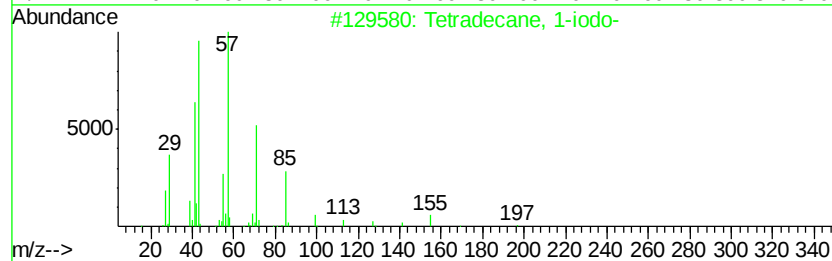
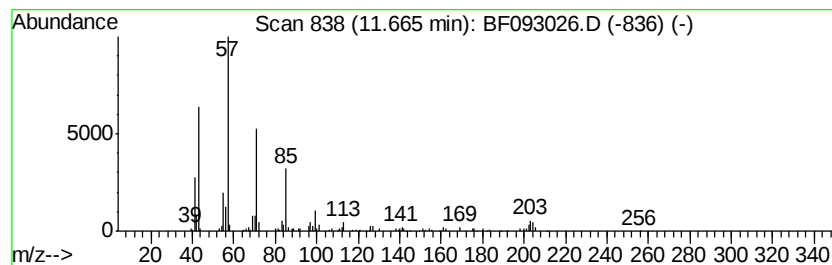
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecane, 1-iodo- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	2.25 ng	123515	Phenanthrene-d10	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
2		Hexadecane	226	C16H34	000544-76-3	72
3		Tetracosane	338	C24H50	000646-31-1	64
4		Nonadecane	268	C19H40	000629-92-5	64
5		Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
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Sample : I1884-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

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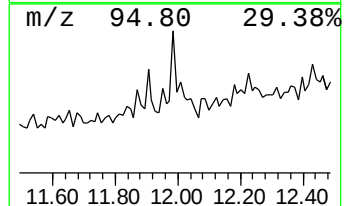
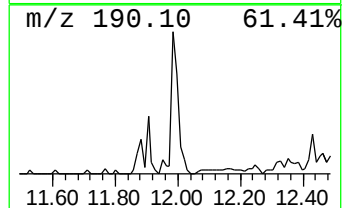
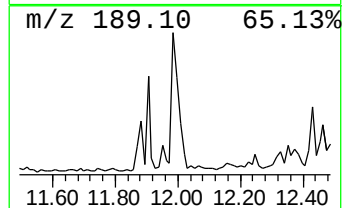
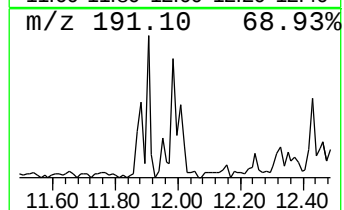
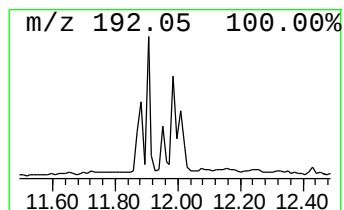
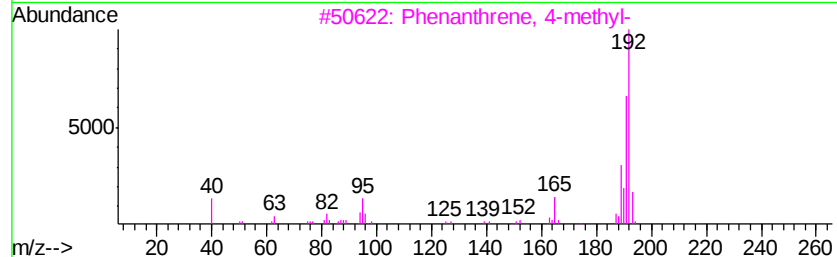
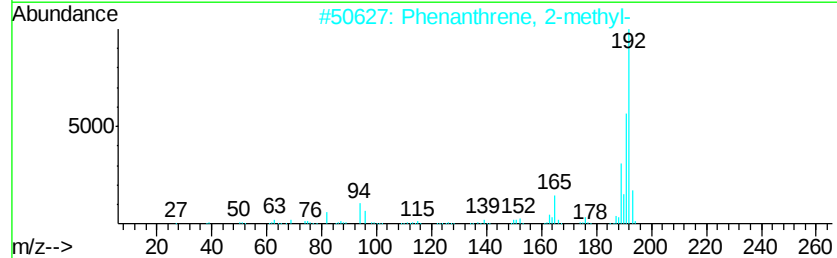
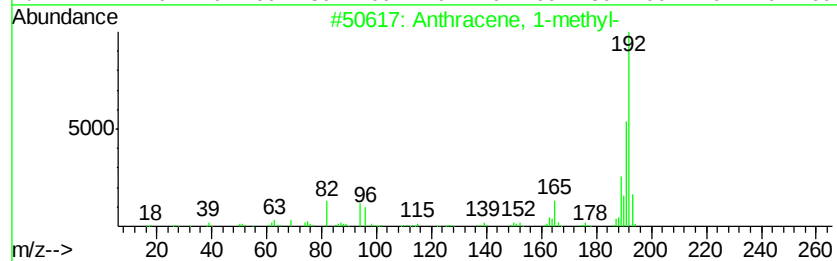
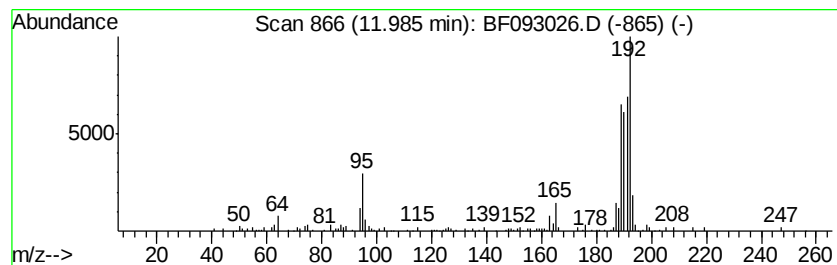
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Anthracene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	3.27 ng	179390	Phenanthrene-d10	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	60
2		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	60
3		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	60
4		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	55
5		Anthracene, 2-methyl-	192	C15H12	000613-12-7	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093026.D
Acq On : 17 Feb 2017 22:26
Operator : SJ/MA
Sample : I1884-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIT-A-COMP

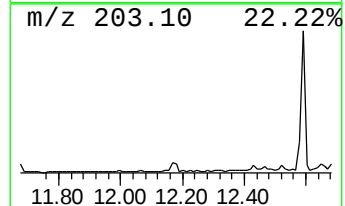
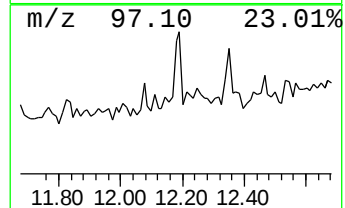
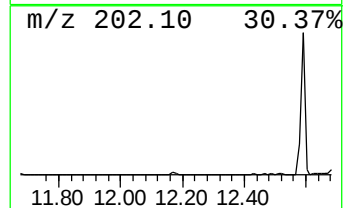
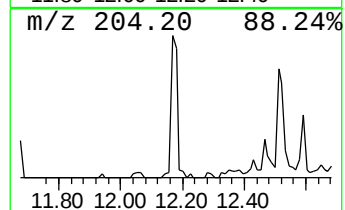
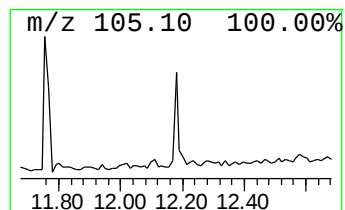
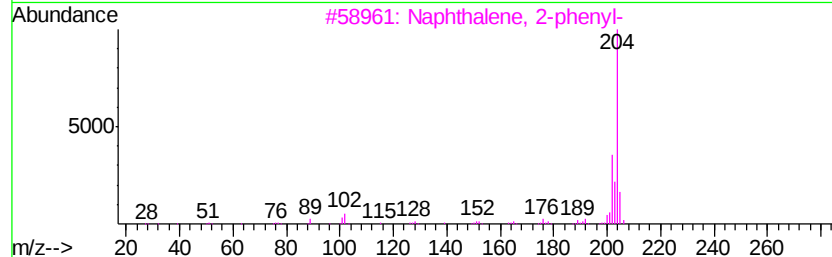
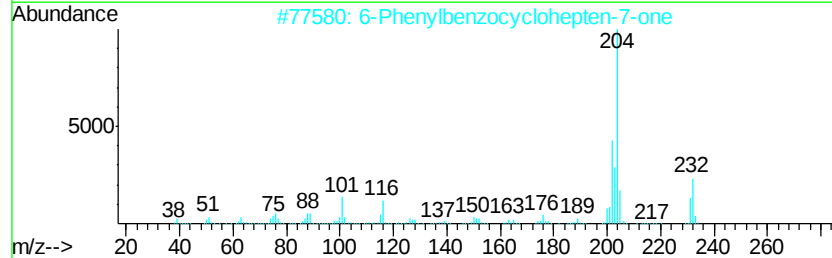
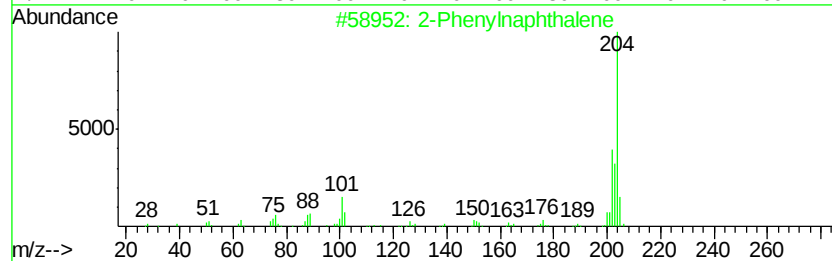
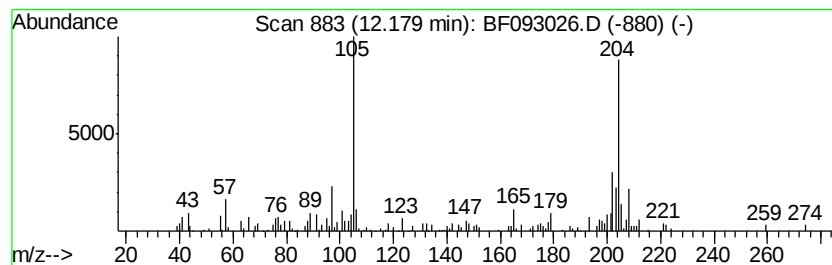
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Phenylnaphthalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.18	2.40 ng	131733	Phenanthrene-d10	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Phenylnaphthalene	204	C16H12	035465-71-5	90
2		6-Phenylbenzocyclohepten-7-one	232	C17H12O	093327-56-1	58
3		Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	53
4		Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	53
5		9,10-di(Chloromethyl)anthracene	274	C16H12Cl2	010387-13-0	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
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ALS Vial : 23 Sample Multiplier: 1

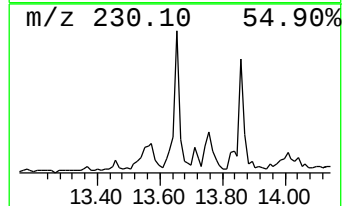
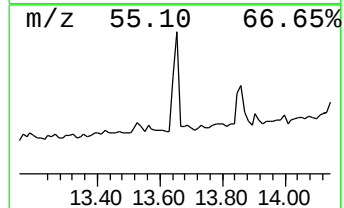
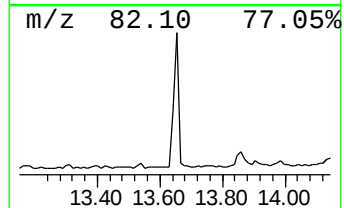
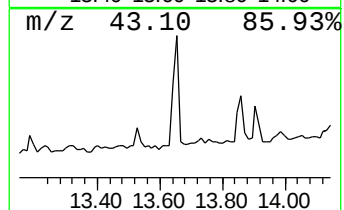
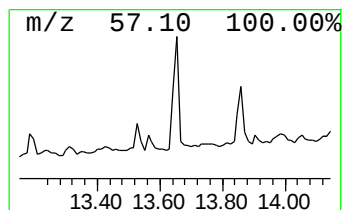
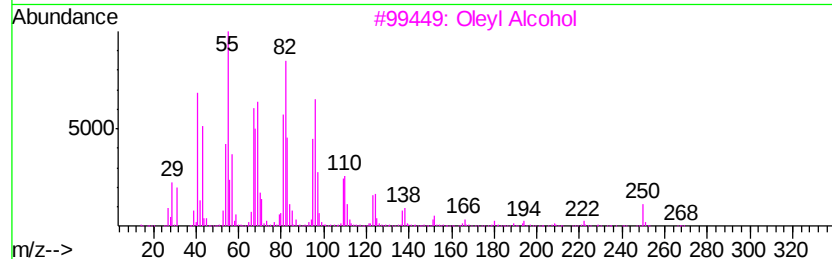
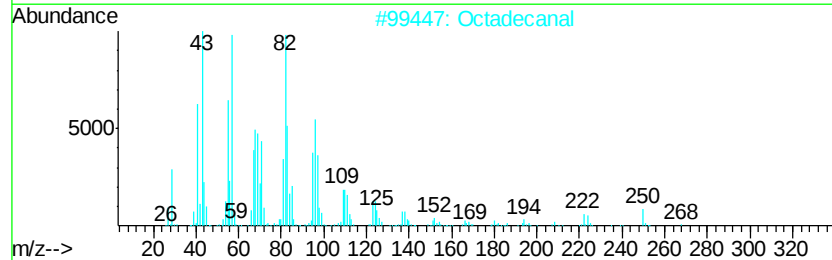
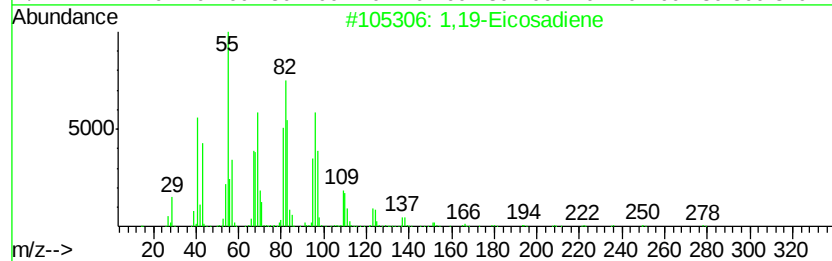
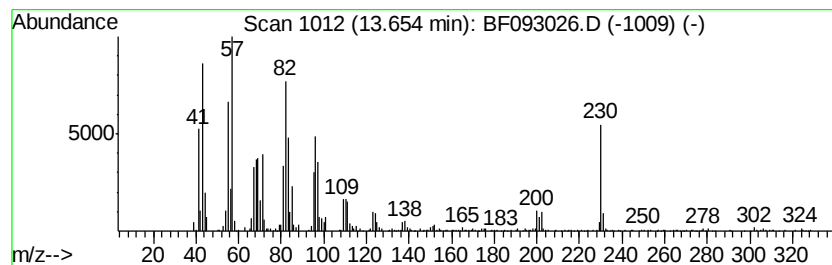
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1,19-Eicosadiene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.65	7.34 ng	561414	Chrysene-d12	14.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	93
2	Octadecanal	268	C18H36O	000638-66-4	81
3	Oleyl Alcohol	268	C18H36O	000143-28-2	80
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	76
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093026.D
Acq On : 17 Feb 2017 22:26
Operator : SJ/MA
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PIT-A-COMP

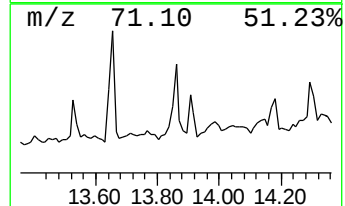
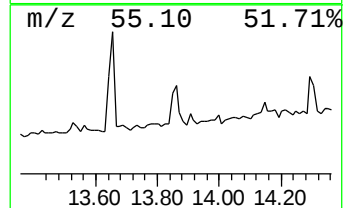
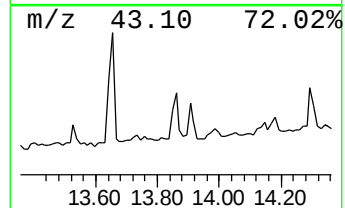
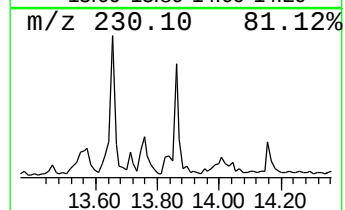
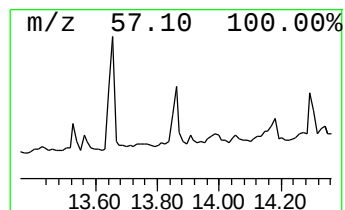
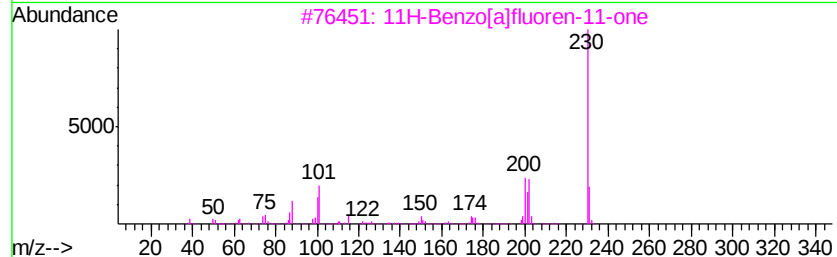
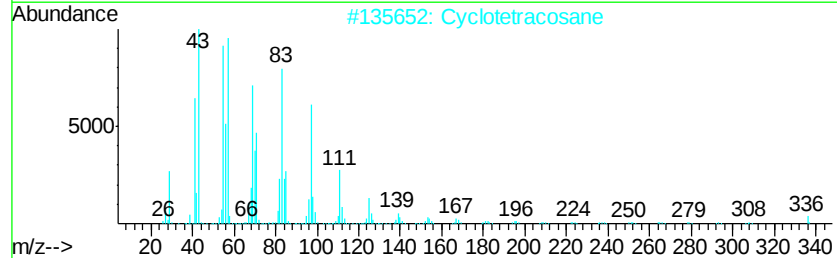
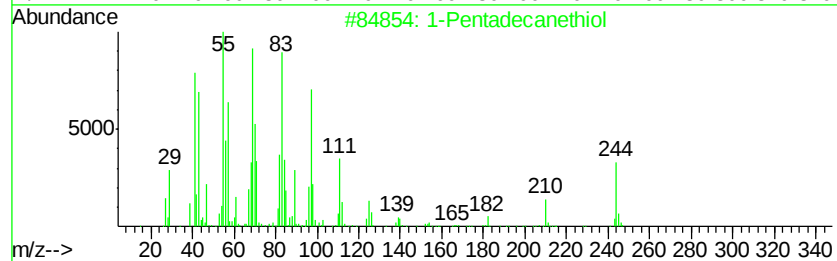
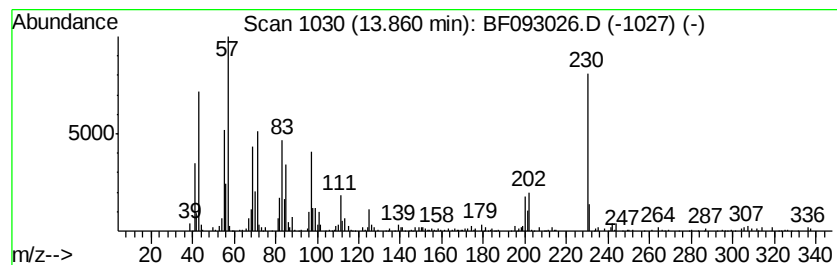
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Pentadecanethiol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.17 ng	242651	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Pentadecanethiol	244	C15H32S	025276-70-4	74
2		Cyclotetracosane	336	C24H48	000297-03-0	59
3		11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	46
4		7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	46
5		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
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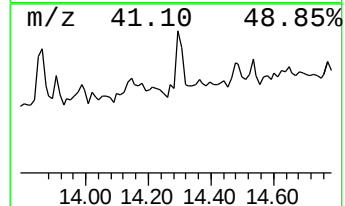
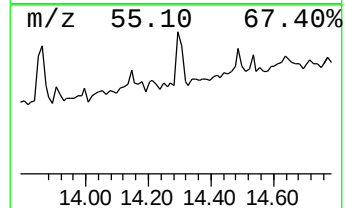
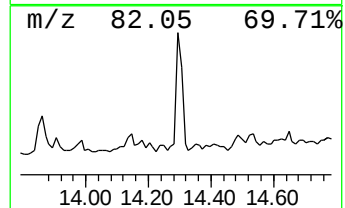
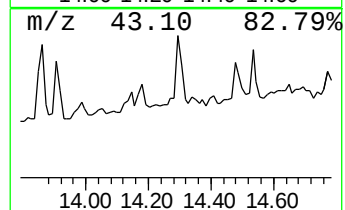
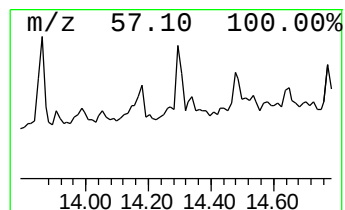
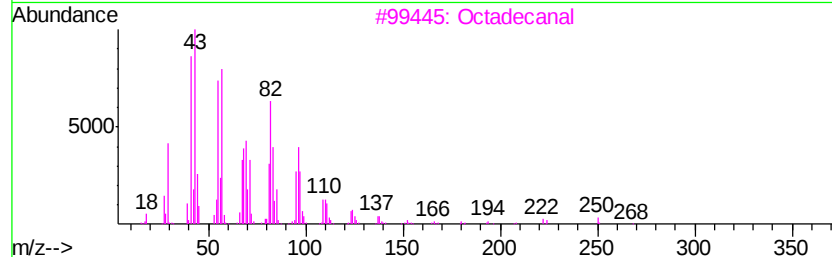
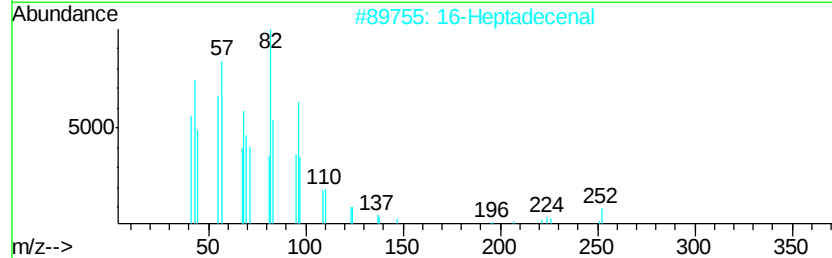
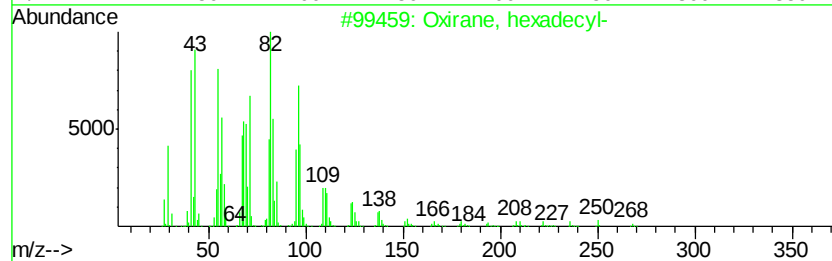
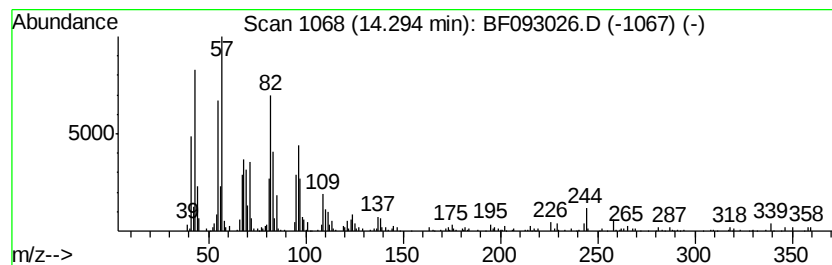
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Oxirane, hexadecyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.29	2.30 ng	176207	Chrysene-d12	14.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	95
2	16-Heptadecenal	252	C17H32O	1000144-57-9	93
3	Octadecanal	268	C18H36O	000638-66-4	90
4	1,19-Eicosadiene	278	C20H38	014811-95-1	87
5	Tetradecanal	212	C14H28O	000124-25-4	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
 Data File : BF093026.D
 Acq On : 17 Feb 2017 22:26
 Operator : SJ/MA
 Sample : I1884-01 2X
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PIT-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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...	5.01	18.2	ng	863525	1	6.85	948694	20.0
unknown6.62	6.62	47.1	ng	2232590	1	6.85	948694	20.0
Hexadecane	9.82	2.3	ng	137748	3	9.89	1200510	20.0
Tridecane	10.80	4.8	ng	265251	4	11.38	1096420	20.0
Eicosane	11.24	3.5	ng	191860	4	11.38	1096420	20.0
Tetradecane, 1-iodo-	11.67	2.3	ng	123515	4	11.38	1096420	20.0
Anthracene, 1-met...	11.99	3.3	ng	179390	4	11.38	1096420	20.0
2-Phenylnaphthalene	12.18	2.4	ng	131733	4	11.38	1096420	20.0
1,19-Eicosadiene	13.65	7.3	ng	561414	5	14.01	1530170	20.0
1-Pentadecanethiol	13.86	3.2	ng	242651	5	14.01	1530170	20.0
Oxirane, hexadecyl-	14.29	2.3	ng	176207	5	14.01	1530170	20.0