

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
 Data File : BF097154.D
 Acq On : 28 Jul 2017 15:06
 Operator : SJ/JU
 Sample : I4420-13
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 2A-6-7-8-9-10-COMP-(0-10)

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-BF072517.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	4.634	464	467	480	rBV	178666	273000	10.79%	1.174%
2	5.092	540	545	561	rBV	2278056	2529807	100.00%	10.881%
3	5.734	650	654	660	rBV	55297	61234	2.42%	0.263%
4	5.792	660	664	671	rBV	60249	69154	2.73%	0.297%
5	5.934	680	688	693	rBV	29163	43629	1.72%	0.188%
6	5.998	697	699	702	rVV2	48750	48625	1.92%	0.209%
7	6.028	702	704	711	rVB	60884	65040	2.57%	0.280%
8	6.086	711	714	717	rBV	46607	45120	1.78%	0.194%
9	6.151	720	725	735	rBV	2226173	2461193	97.29%	10.586%
10	6.263	740	744	747	rVV	2469094	2332433	92.20%	10.033%
11	6.339	754	757	762	rVB	303169	277830	10.98%	1.195%
12	6.445	768	775	778	rBV5	25200	52005	2.06%	0.224%
13	6.486	778	782	786	rVV	786640	699043	27.63%	3.007%
14	6.522	786	788	791	rVB	265937	194374	7.68%	0.836%
15	6.563	791	795	799	rBV3	33042	47421	1.87%	0.204%
16	6.645	803	809	814	rBV	1860204	1774096	70.13%	7.631%
17	6.786	830	833	836	rVB	85114	81702	3.23%	0.351%
18	6.816	836	838	841	rVB	76276	57052	2.26%	0.245%
19	6.851	841	844	847	rBV	132741	120795	4.77%	0.520%
20	6.898	847	852	857	rVB	88464	115292	4.56%	0.496%
21	7.022	868	873	874	rBV4	30879	38483	1.52%	0.166%
22	7.057	874	879	882	rVV	1636197	1566294	61.91%	6.737%
23	7.110	885	888	891	rVV	634867	530483	20.97%	2.282%
24	7.145	892	894	899	rVB3	40061	51476	2.03%	0.221%
25	7.192	899	902	904	rBV2	33357	40942	1.62%	0.176%
26	7.222	904	907	911	rVB2	63783	73767	2.92%	0.317%
27	7.292	917	919	925	rVB	99409	98884	3.91%	0.425%
28	7.345	925	928	934	rVB4	20214	31673	1.25%	0.136%
29	7.410	934	939	943	rBV4	41495	65502	2.59%	0.282%
30	7.481	946	951	954	rBV2	58473	75390	2.98%	0.324%
31	7.510	954	956	959	rVB	42129	32909	1.30%	0.142%
32	7.545	959	962	966	rVB	84958	76778	3.03%	0.330%
33	7.592	966	970	972	rBV	43740	40292	1.59%	0.173%
34	7.769	996	1000	1004	rBV	1098051	1051726	41.57%	4.524%

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35	7.857	1012	1015	1018	rVB	71065	54413	2.15%	0.234%
36	8.216	1072	1076	1085	rVB	23606	26939	1.06%	0.116%
37	8.851	1179	1184	1187	rBV	2540189	2370251	93.69%	10.195%
38	9.245	1248	1251	1256	rBV	216569	172377	6.81%	0.741%
39	9.516	1292	1297	1304	rVB	864424	765374	30.25%	3.292%
40	9.969	1371	1374	1377	rVB	43448	34368	1.36%	0.148%
41	10.186	1405	1411	1414	rBV2	19179	28027	1.11%	0.121%
42	10.298	1427	1430	1439	rBV	1032848	1018225	40.25%	4.380%
43	10.439	1450	1454	1460	rBV	62082	66379	2.62%	0.286%
44	10.886	1521	1530	1533	rBV2	26529	28523	1.13%	0.123%
45	10.986	1544	1547	1551	rBV	659416	583705	23.07%	2.511%
46	11.545	1639	1642	1645	rBV	57413	53543	2.12%	0.230%
47	12.327	1772	1775	1780	rBV2	40767	42545	1.68%	0.183%
48	12.574	1812	1817	1820	rBV	1560616	1460566	57.73%	6.282%
49	13.486	1968	1972	1977	rBV	91122	119298	4.72%	0.513%
50	13.610	1989	1993	1997	rBV	621448	585630	23.15%	2.519%
51	14.115	2076	2079	2083	rBV5	20050	27844	1.10%	0.120%
52	14.962	2218	2223	2227	rBV	438273	492933	19.49%	2.120%
53	15.809	2364	2367	2373	rBV7	27417	75094	2.97%	0.323%
54	17.433	2642	2643	2646	rBV3	24706	32890	1.30%	0.141%
55	17.956	2729	2732	2733	rBV3	25061	26161	1.03%	0.113%
56	18.339	2795	2797	2800	rBV3	26717	28926	1.14%	0.124%
57	18.721	2858	2862	2863	rBV4	24621	31283	1.24%	0.135%

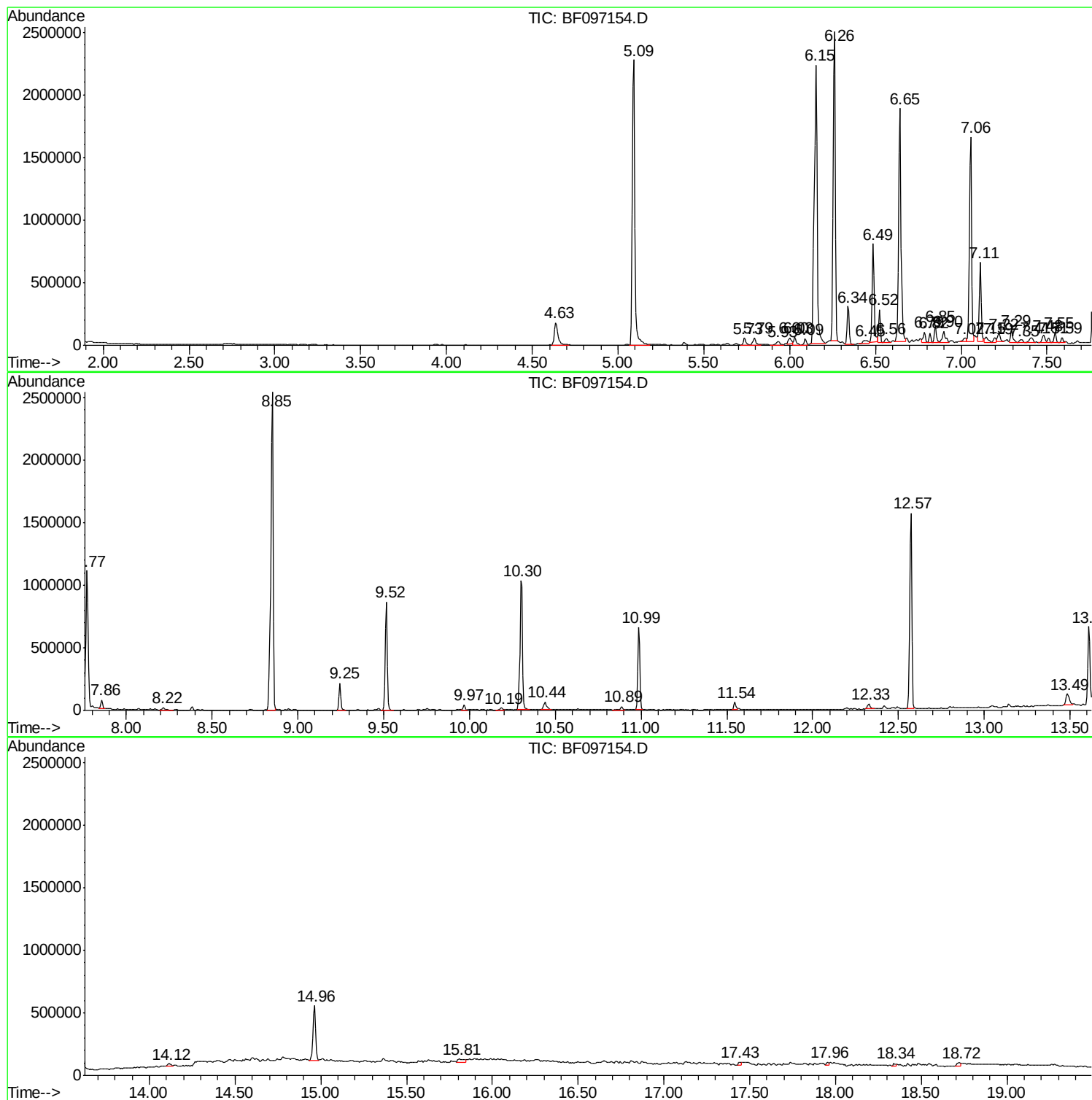
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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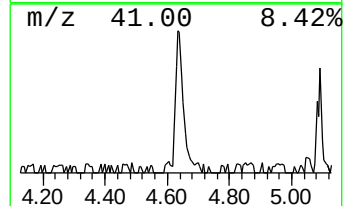
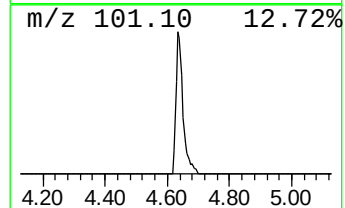
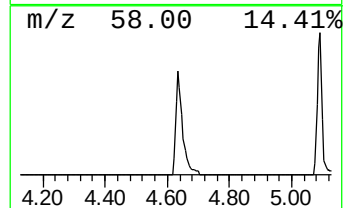
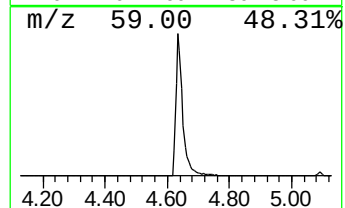
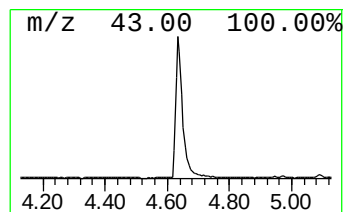
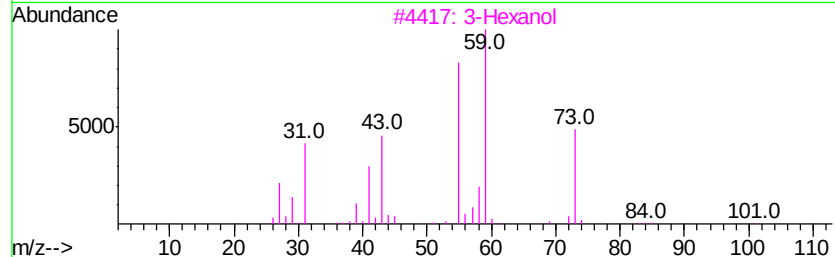
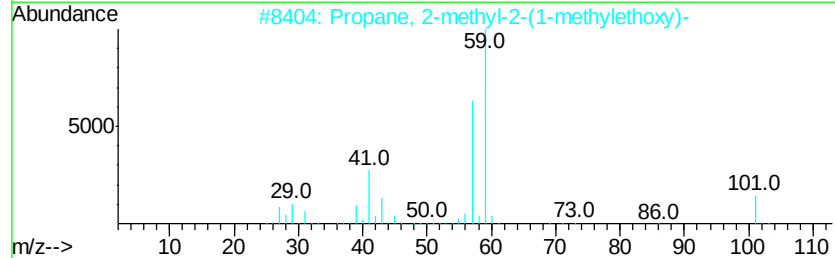
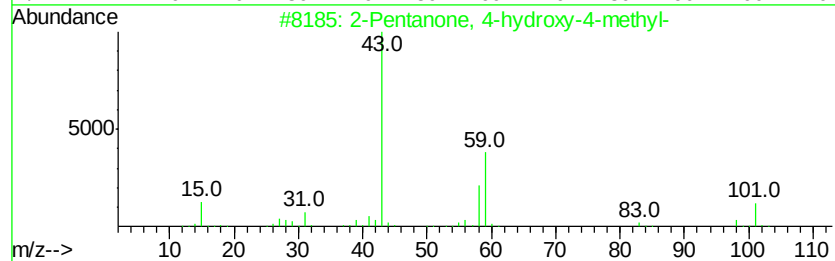
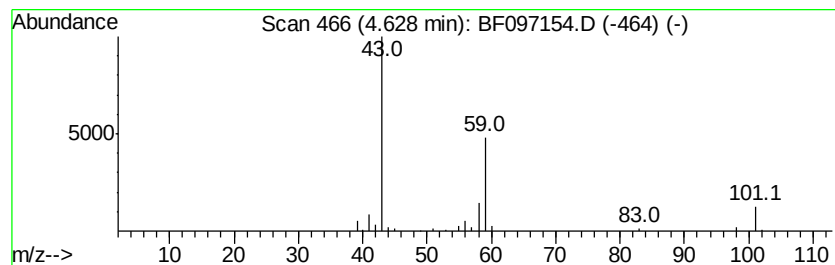
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.63	7.81 ng	273000	1,4-Dichlorobenzene-d4	6.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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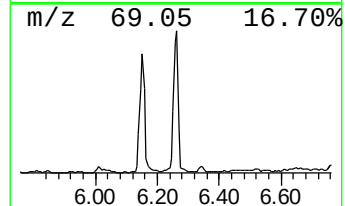
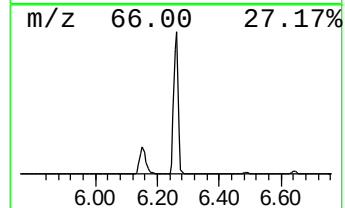
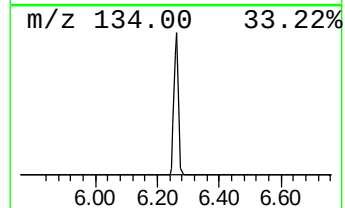
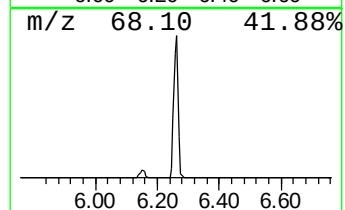
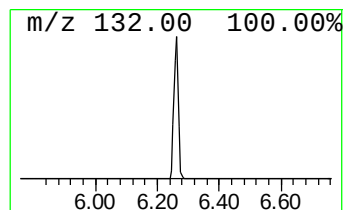
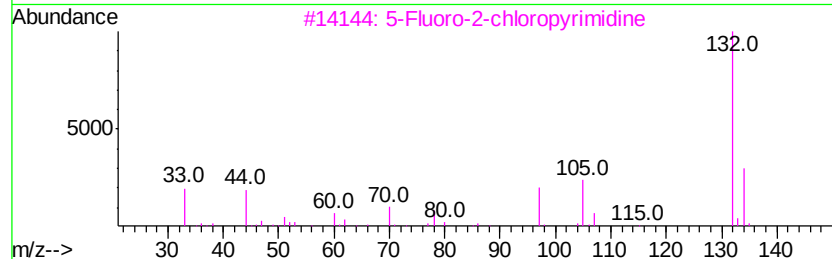
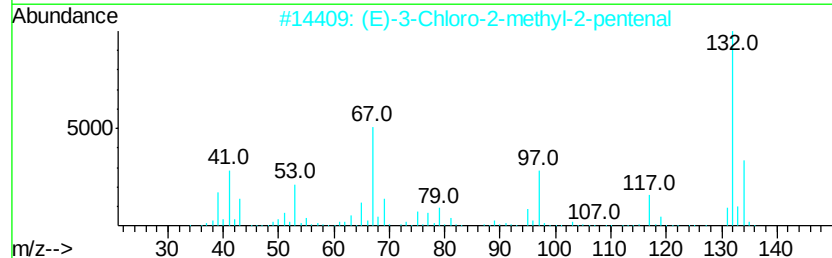
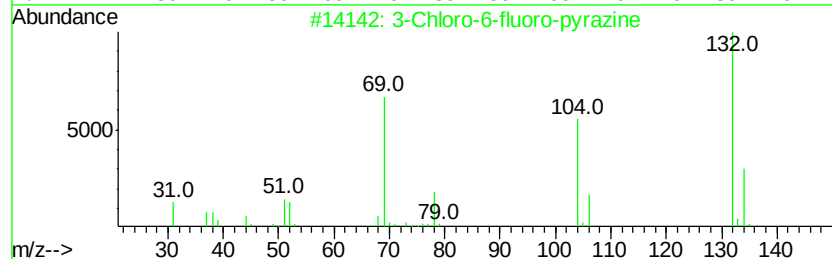
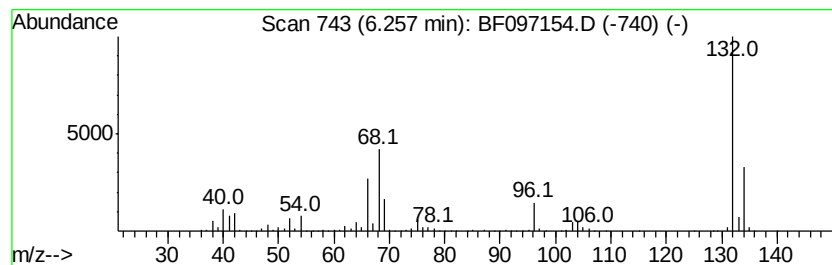
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	66.73 ng	2332430	1,4-Dichlorobenzene-d4	6.49

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	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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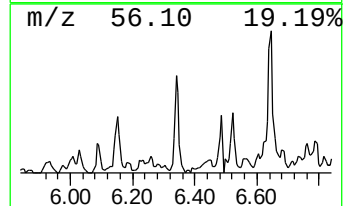
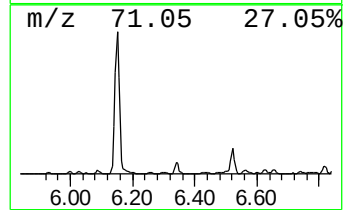
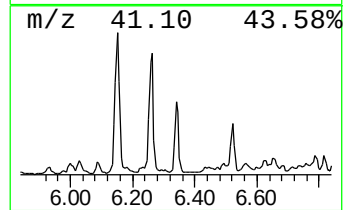
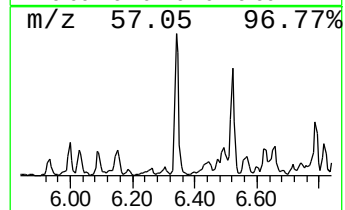
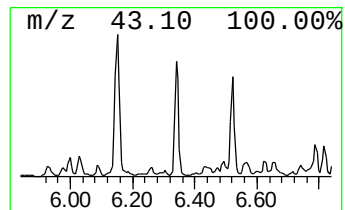
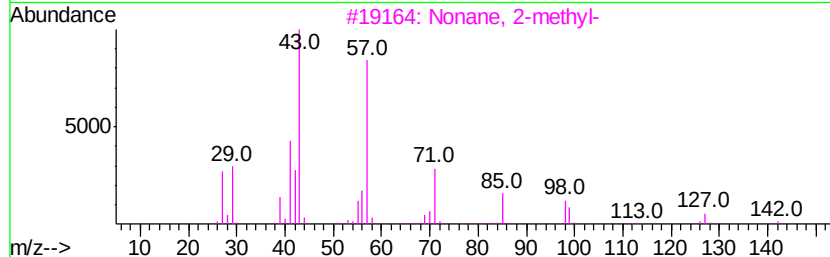
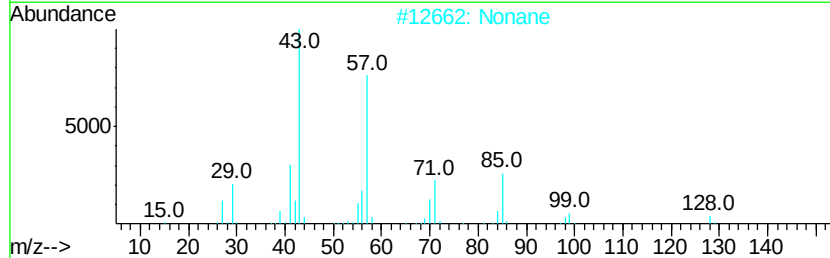
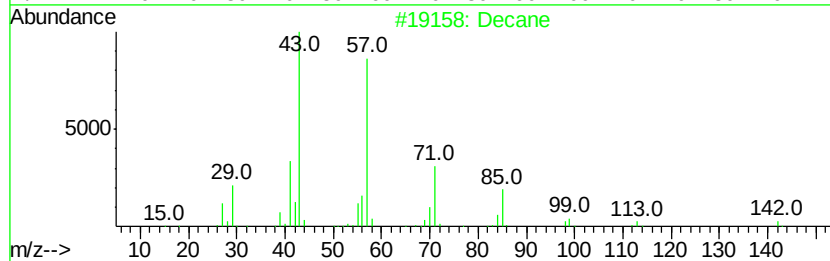
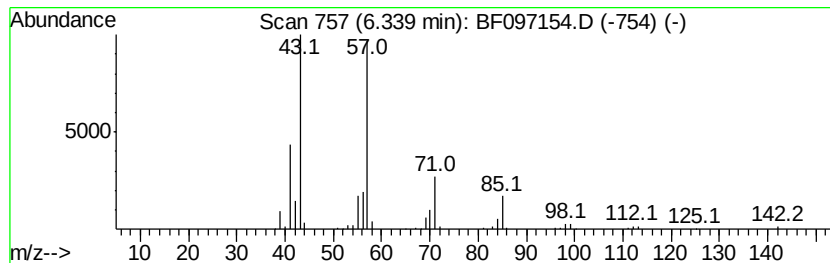
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Decane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	7.95 ng	277830	1,4-Dichlorobenzene-d4	6.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane			142	C10H22	000124-18-5	83
2	Nonane			128	C9H20	000111-84-2	83
3	Nonane, 2-methyl-			142	C10H22	000871-83-0	80
4	Oxalic acid, isobutyl pentyl ester			216	C11H20O4	1000309-37-0	72
5	Oxalic acid, isobutyl nonyl ester			272	C15H28O4	1000309-37-4	64



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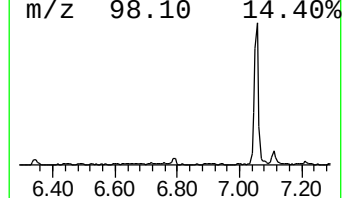
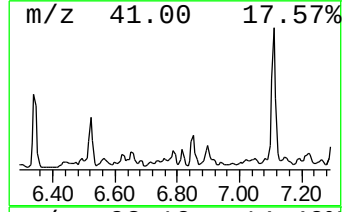
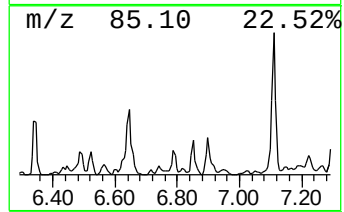
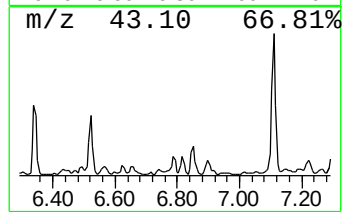
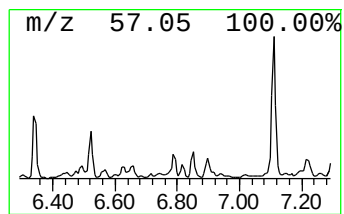
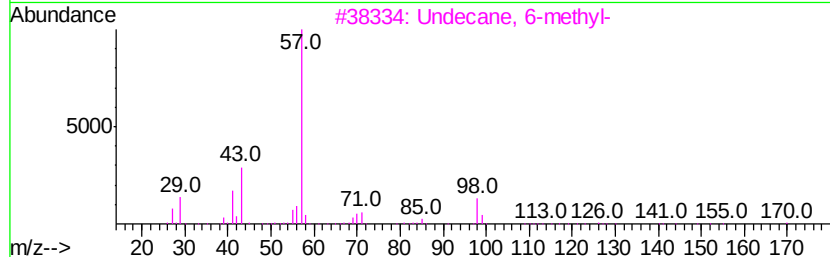
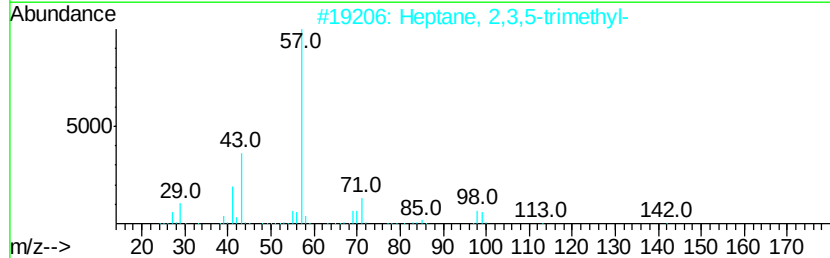
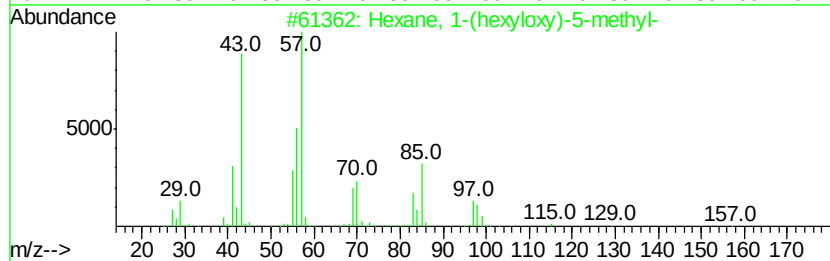
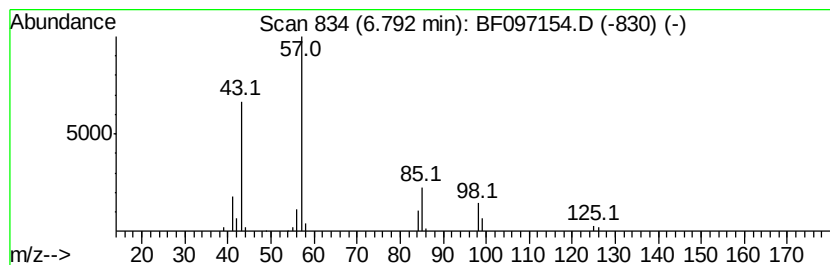
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexane, 1-(hexyloxy)-5-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.79	2.34 ng	81702	1,4-Dichlorobenzene-d4	6.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 1-(hexyloxy)-5-methyl-	200	C13H28O	074421-19-5	56
2	Heptane, 2,3,5-trimethyl-	142	C10H22	020278-85-7	53
3	Undecane, 6-methyl-	170	C12H26	017302-33-9	50
4	Hexadecane	226	C16H34	000544-76-3	50
5	Heptane, 4-ethyl-	128	C9H20	002216-32-2	42



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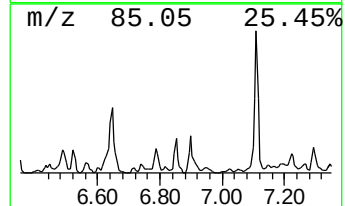
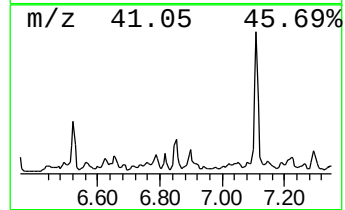
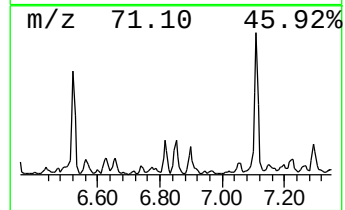
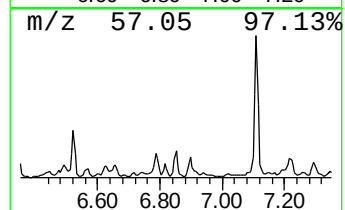
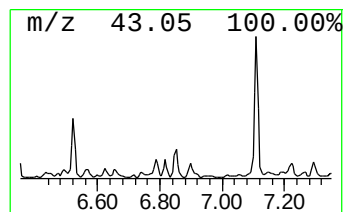
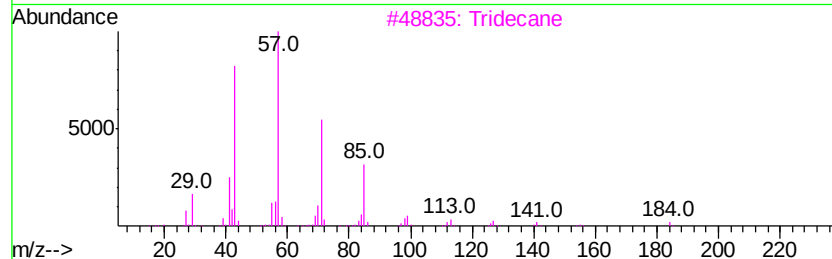
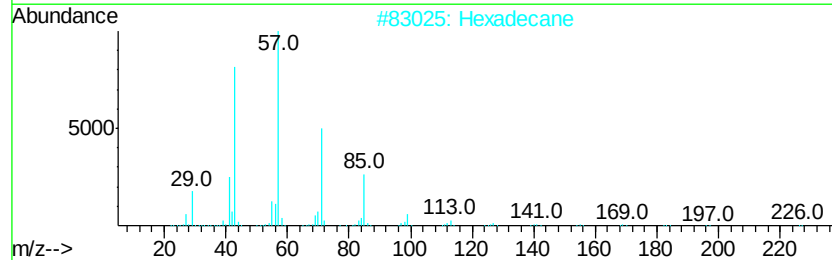
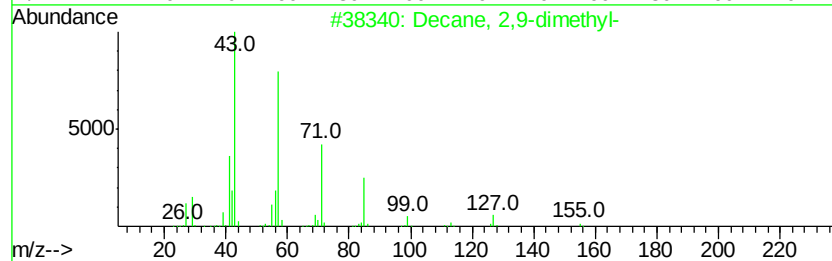
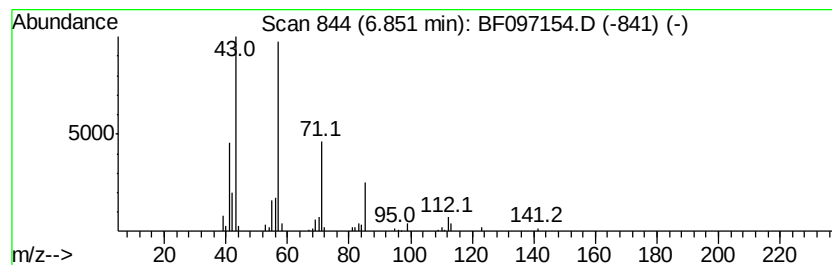
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2A-6-7-8-9-10-COMP-(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Decane, 2,9-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.85	3.46 ng	120795	1,4-Dichlorobenzene-d4	6.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	78
2	Hexadecane	226	C16H34	000544-76-3	72
3	Tridecane	184	C13H28	000629-50-5	72
4	Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	64
5	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097154.D
Acq On : 28 Jul 2017 15:06
Operator : SJ/JU
Sample : I4420-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

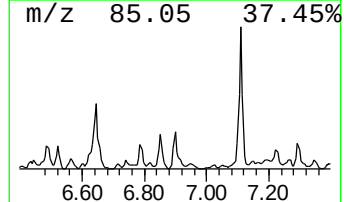
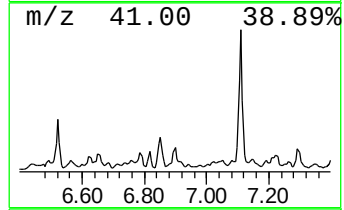
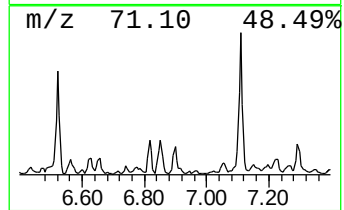
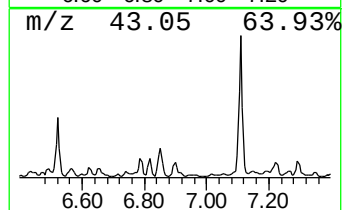
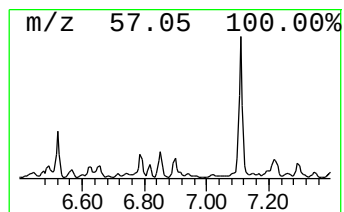
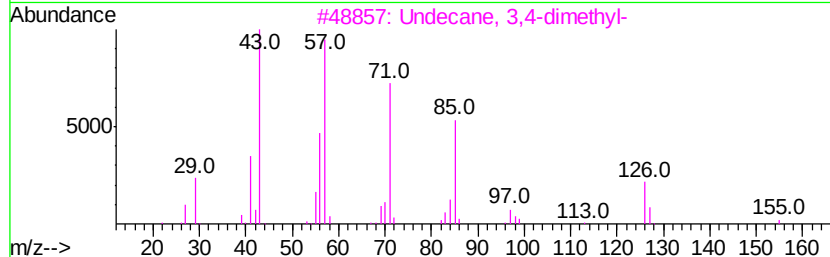
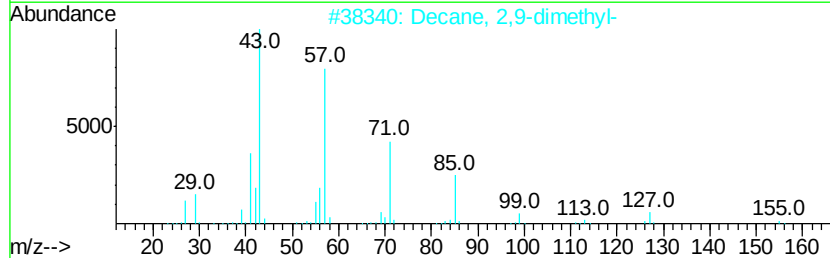
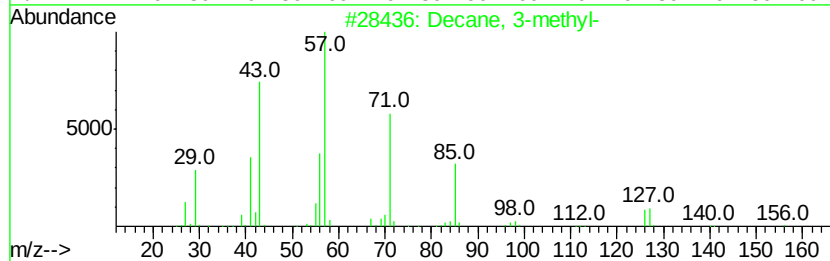
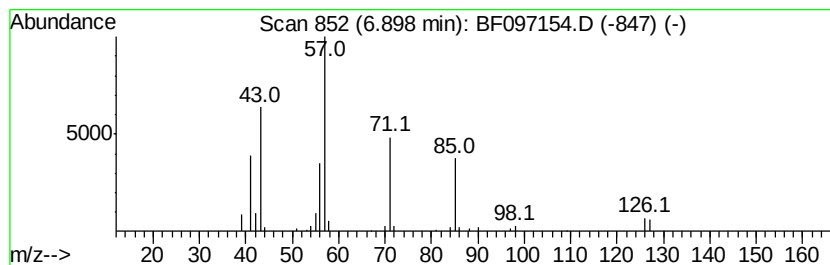
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Decane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.90	3.30 ng	115292	1,4-Dichlorobenzene-d4	6.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3-methyl-	156	C11H24	013151-34-3	78
2	Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	64
3	Undecane, 3,4-dimethyl-	184	C13H28	017312-78-6	59
4	Dodecane, 2,5-dimethyl-	198	C14H30	056292-65-0	59
5	Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
Data File : BF097154.D
Acq On : 28 Jul 2017 15:06
Operator : SJ/JU
Sample : I4420-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

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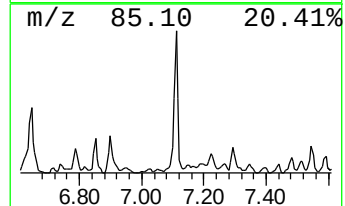
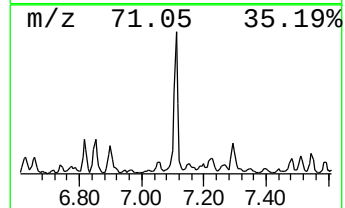
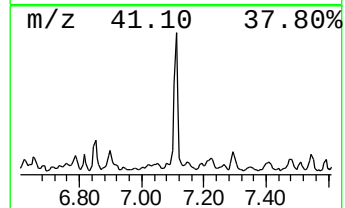
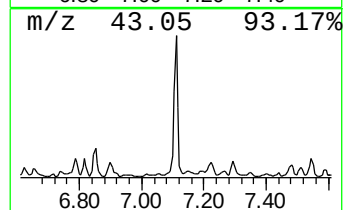
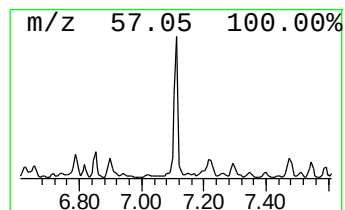
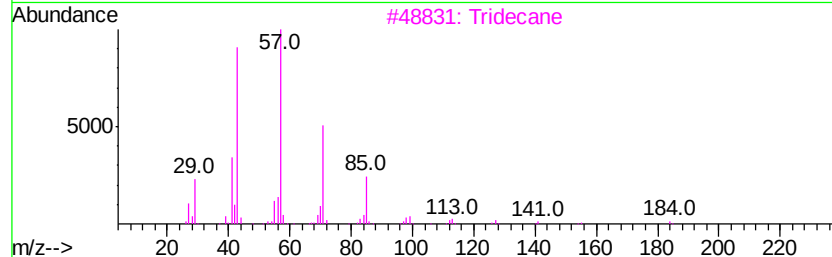
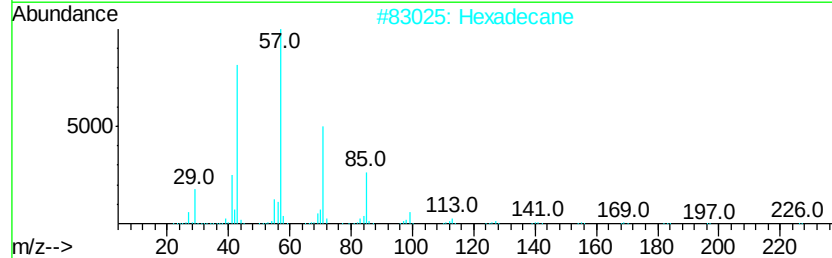
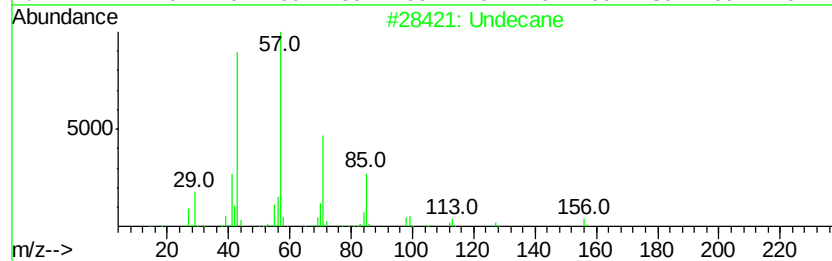
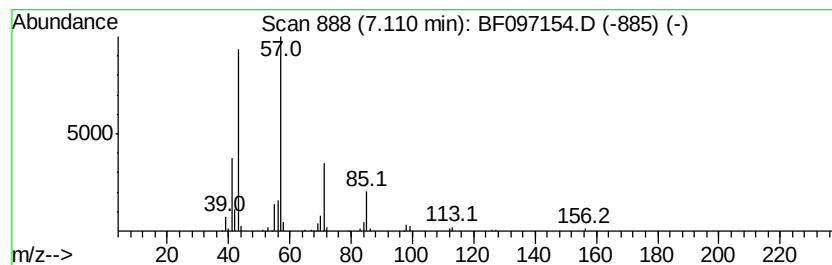
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.11	15.18 ng	530483	1,4-Dichlorobenzene-d4	6.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane		156	C11H24	001120-21-4	83
2	Hexadecane		226	C16H34	000544-76-3	83
3	Tridecane		184	C13H28	000629-50-5	78
4	Tetradecane		198	C14H30	000629-59-4	78
5	Octane, 2,7-dimethyl-		142	C10H22	001072-16-8	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
Data File : BF097154.D
Acq On : 28 Jul 2017 15:06
Operator : SJ/JU
Sample : I4420-13
Misc :
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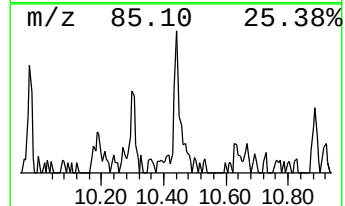
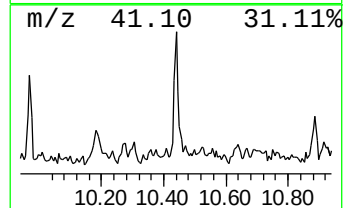
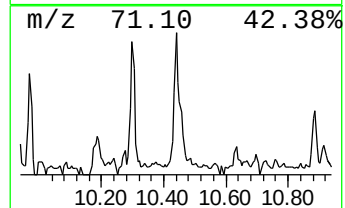
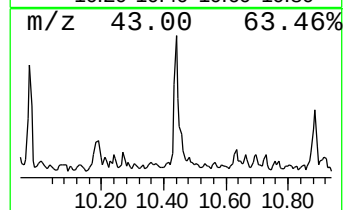
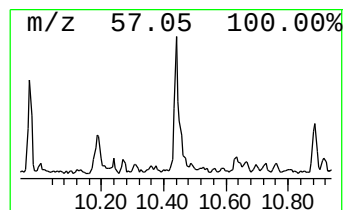
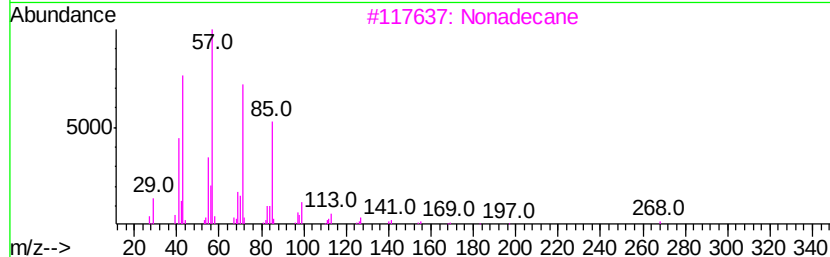
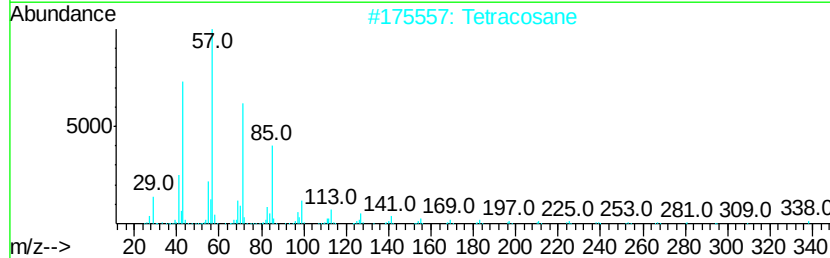
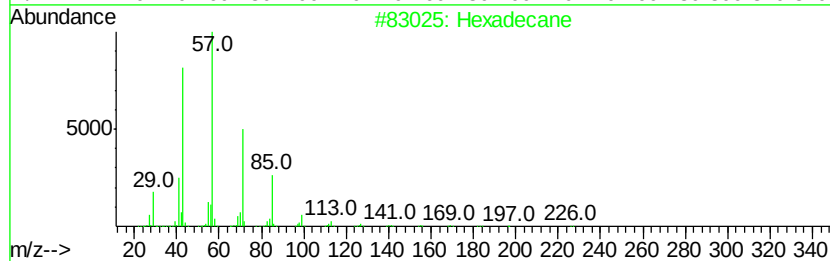
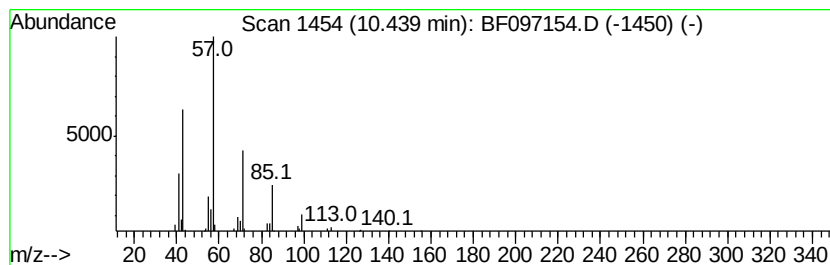
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.44	2.27 ng	66379	Phenanthrene-d10		10.99
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Nonadecane	268	C19H40	000629-92-5	86
4	Octacosane	394	C28H58	000630-02-4	86
5	Heptacosane	380	C27H56	000593-49-7	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
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Sample : I4420-13
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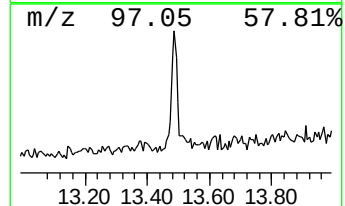
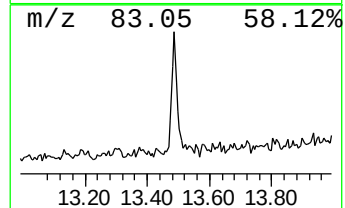
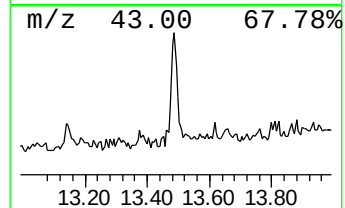
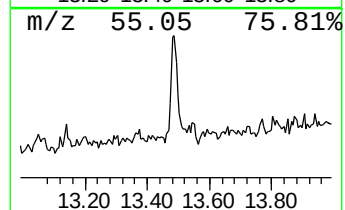
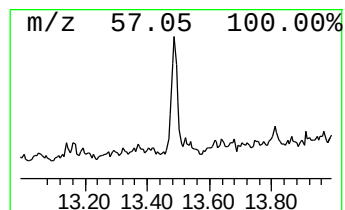
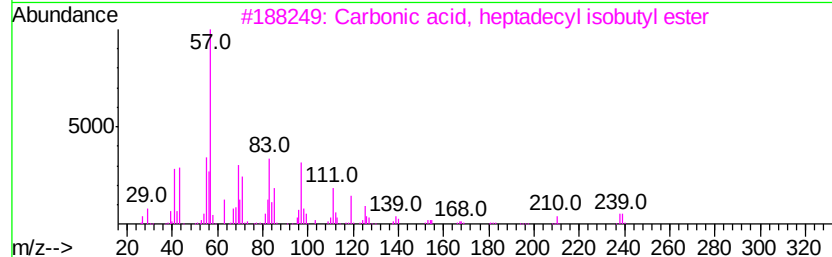
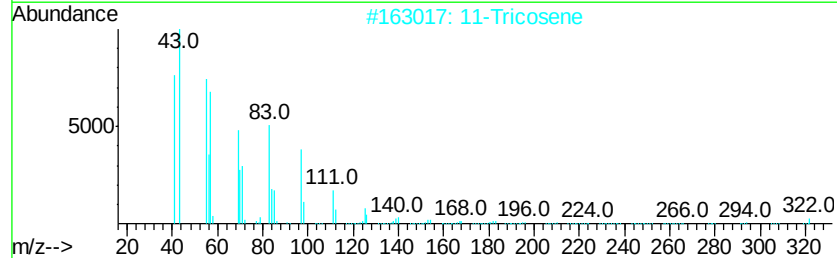
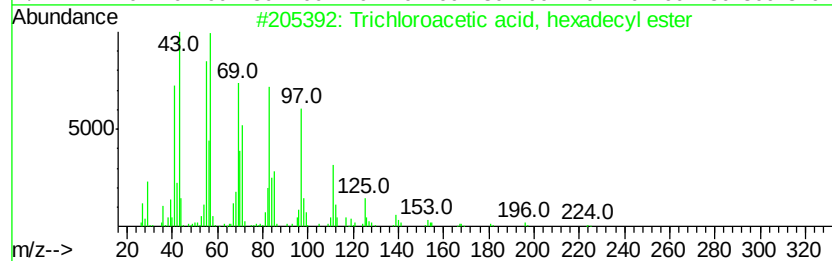
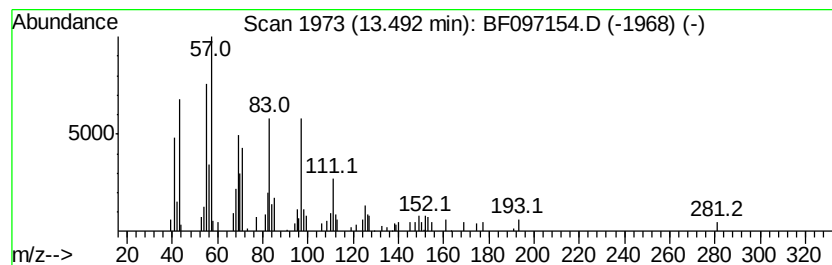
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.49	4.07 ng	119298	Chrysene-d12	13.61		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2		11-Tricosene	322	C23H46	052078-56-5	83
3		Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	72
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	64
5		1,2-Octadecanediol	286	C18H38O2	020294-76-2	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
Data File : BF097154.D
Acq On : 28 Jul 2017 15:06
Operator : SJ/JU
Sample : I4420-13
Misc :
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Instrument :
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ClientSampleId :
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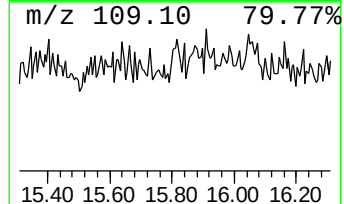
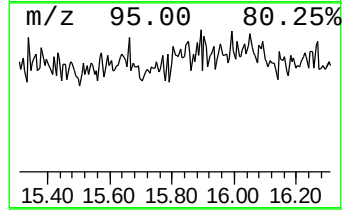
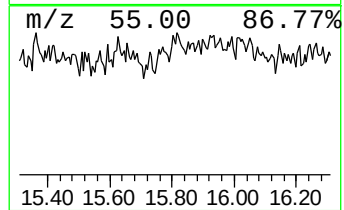
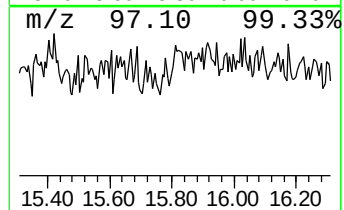
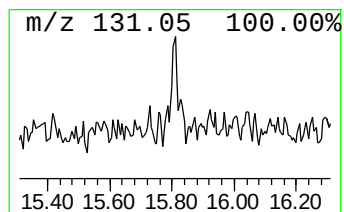
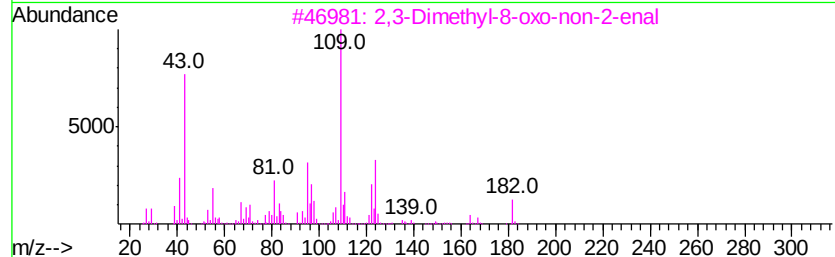
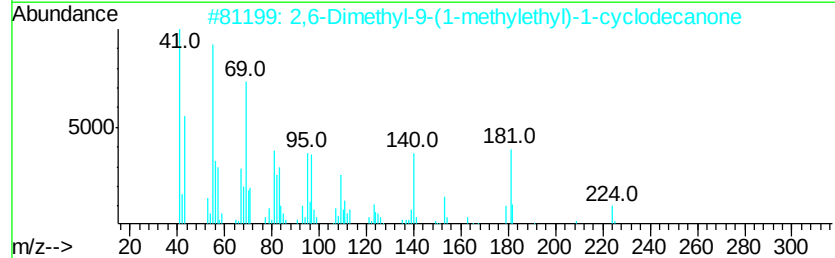
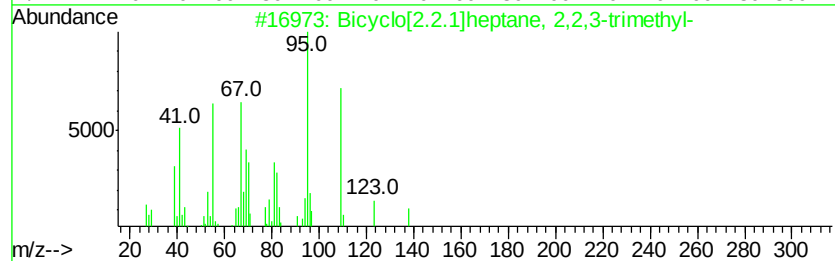
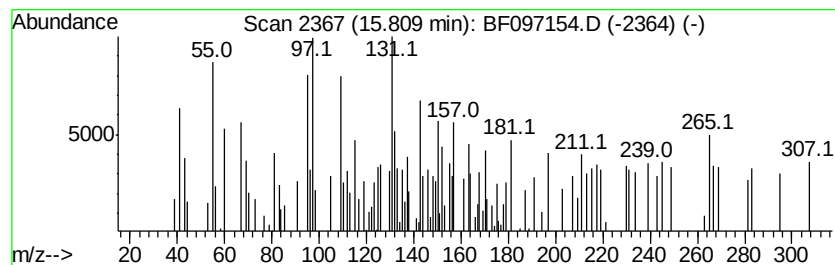
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.81 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	3.05 ng	75094	Perylene-d12	14.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	22
2			2,6-Dimethyl-9-(1-methylethyl)-1...	224	C15H28O	038601-98-8	16
3			2,3-Dimethyl-8-oxo-non-2-enal	182	C11H18O2	1000186-82-6	16
4			4-Isobenzofuranol, octahydro-3a,...	170	C10H18O2	054382-58-0	14
5			Cyclohexaneacetic acid, 3-oxo-, ...	170	C9H14O3	002808-12-0	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
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Acq On : 28 Jul 2017 15:06
Operator : SJ/JU
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.26	6.26	66.7	ng	2332430	1	6.49	699043	20.0
Decane	6.34	8.0	ng	277830	1	6.49	699043	20.0
Hexane, 1-(hexylo...	6.79	2.3	ng	81702	1	6.49	699043	20.0
Decane, 2,9-dimet...	6.85	3.5	ng	120795	1	6.49	699043	20.0
Decane, 3-methyl-	6.90	3.3	ng	115292	1	6.49	699043	20.0
Undecane	7.11	15.2	ng	530483	1	6.49	699043	20.0
Hexadecane	10.44	2.3	ng	66379	4	10.99	583705	20.0
Trichloroacetic a...	13.49	4.1	ng	119298	5	13.61	585630	20.0
unknown15.81	15.81	3.0	ng	75094	6	14.96	492933	20.0