

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121516\
 Data File : BF091634.D
 Acq On : 15 Dec 2016 17:56
 Operator : UM/SJ
 Sample : H6012-04
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-5-8-9

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-BF120916.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	4.956	248	251	263	rVB	1960070	2857844	34.80%	3.799%
2	5.390	286	289	291	rBV	6817721	7087216	86.29%	9.421%
3	6.430	377	380	382	rBV	6718130	8213257	100.00%	10.918%
4	6.556	388	391	393	rBV	7325420	7633092	92.94%	10.146%
5	6.784	409	411	413	rBV	2138214	1870588	22.78%	2.487%
6	6.944	422	425	427	rBV	5023691	5700123	69.40%	7.577%
7	7.344	457	460	463	rBV	3604271	4811495	58.58%	6.396%
8	8.065	521	523	526	rBV	2261135	2448841	29.82%	3.255%
9	9.150	615	618	620	rBV	7559244	7154304	87.11%	9.510%
10	9.539	650	652	655	rBV	949318	935551	11.39%	1.244%
11	9.825	674	677	679	rBV	2922664	2780148	33.85%	3.696%
12	10.236	711	713	714	rBV	109063	95345	1.16%	0.127%
13	10.259	714	715	717	rVB	162596	163775	1.99%	0.218%
14	10.488	732	735	737	rBV	64171	106634	1.30%	0.142%
15	10.613	743	746	748	rBV	4234770	4729954	57.59%	6.287%
16	10.739	755	757	760	rBV	189435	277422	3.38%	0.369%
17	11.185	794	796	797	rBV	223829	202033	2.46%	0.269%
18	11.299	804	806	810	rVB	2518835	2511850	30.58%	3.339%
19	11.608	831	833	835	rBV	227812	212632	2.59%	0.283%
20	11.836	851	853	855	rBV2	159149	217438	2.65%	0.289%
21	11.916	858	860	865	rVB2	95062	185669	2.26%	0.247%
22	12.019	865	869	870	rBV	66595	104504	1.27%	0.139%
23	12.511	910	912	914	rBV	914920	791809	9.64%	1.053%
24	12.739	929	932	934	rBV	781288	882865	10.75%	1.174%
25	12.888	943	945	948	rVV	5145029	5172596	62.98%	6.876%
26	12.956	948	951	955	rVV2	62224	111686	1.36%	0.148%
27	13.071	957	961	962	rVB	86844	185708	2.26%	0.247%
28	13.174	968	970	973	rBV2	83377	138333	1.68%	0.184%
29	13.471	991	996	999	rBV6	42821	128548	1.57%	0.171%
30	13.574	1002	1005	1007	rVB2	58560	90781	1.11%	0.121%
31	13.677	1012	1014	1016	rBV2	68369	111447	1.36%	0.148%
32	13.791	1021	1024	1028	rVB3	223532	296764	3.61%	0.394%
33	13.928	1033	1036	1042	rBV2	1593605	2692800	32.79%	3.579%
34	14.042	1043	1046	1047	rVB2	63714	91864	1.12%	0.122%

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ClientSampleId :
SB-5-8-9

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.317	1068	1070	1072	rBV	83146	88984	1.08%	0.118%
36	14.785	1108	1111	1115	rBV	283183	335296	4.08%	0.446%
37	14.945	1122	1125	1130	rVB	367988	751687	9.15%	0.999%
38	15.037	1131	1133	1136	rVB2	72301	99161	1.21%	0.132%
39	15.220	1147	1149	1152	rVB	191350	255283	3.11%	0.339%
40	15.277	1152	1154	1157	rBV	318295	387044	4.71%	0.514%
41	15.345	1157	1160	1162	rBV	1221568	1713847	20.87%	2.278%
42	16.683	1274	1277	1282	rVB2	146718	312493	3.80%	0.415%
43	17.094	1309	1313	1320	rVB	120739	290969	3.54%	0.387%

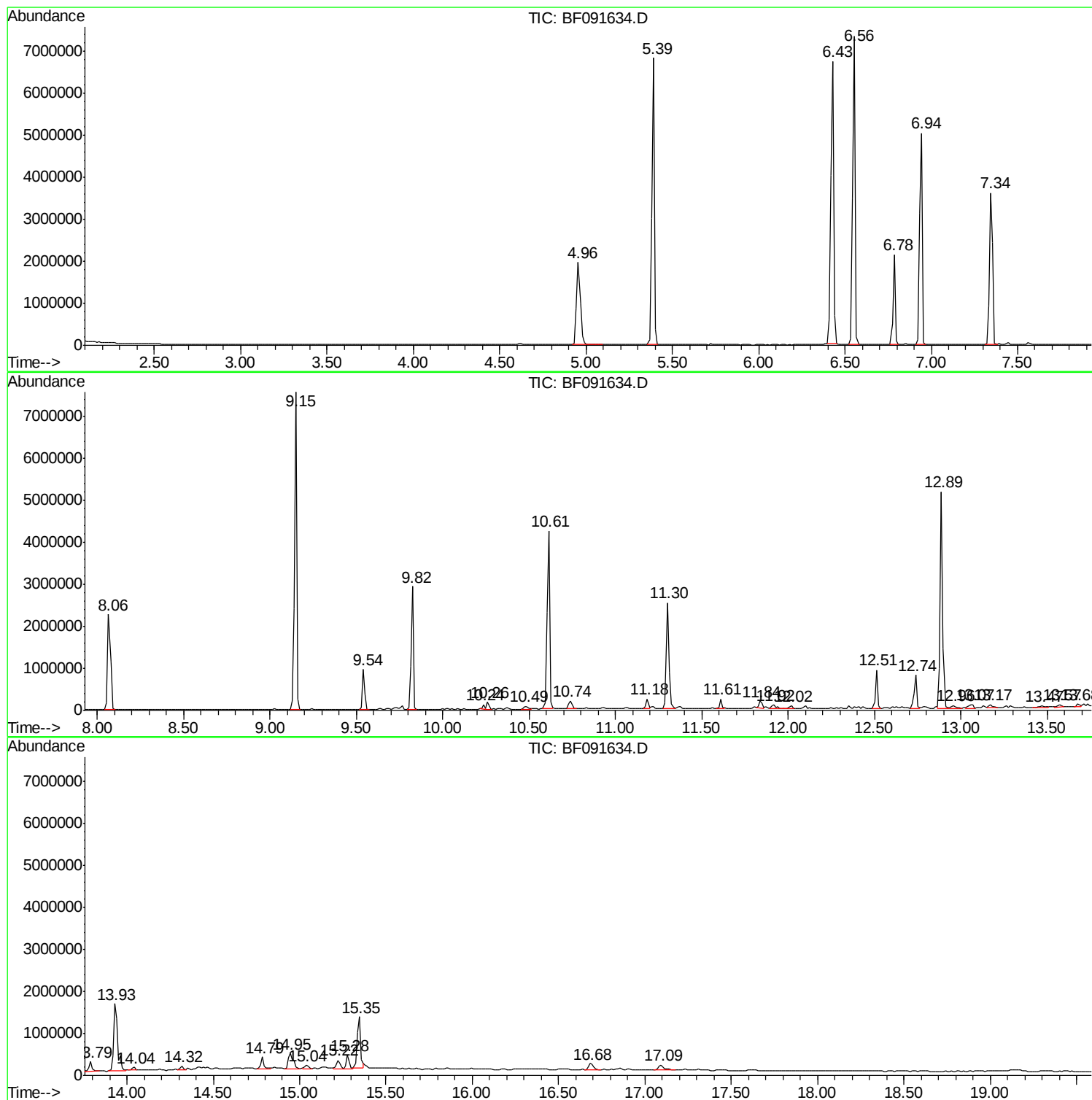
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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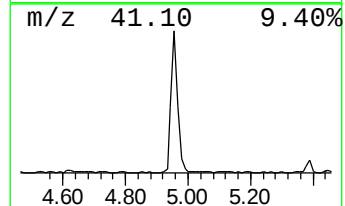
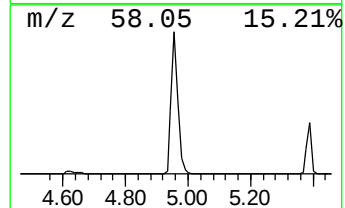
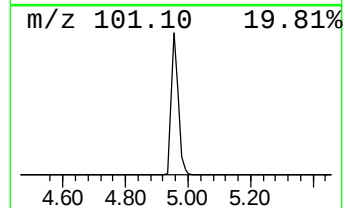
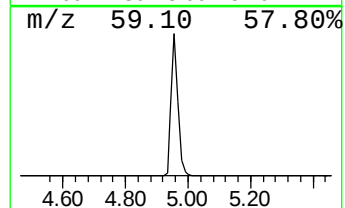
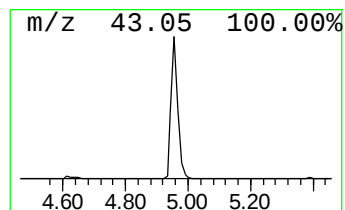
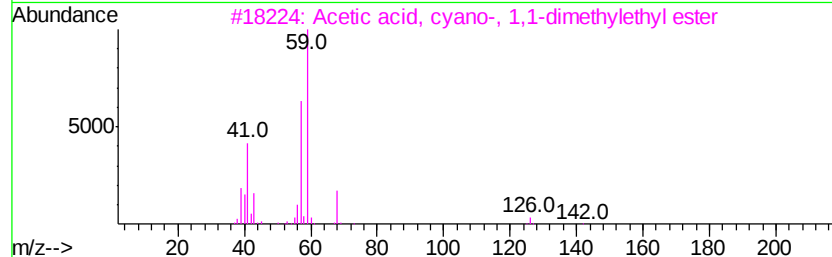
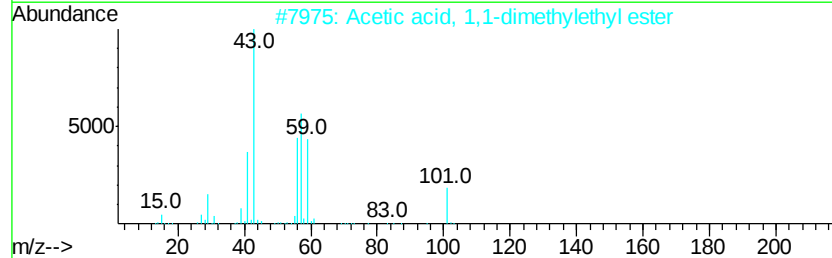
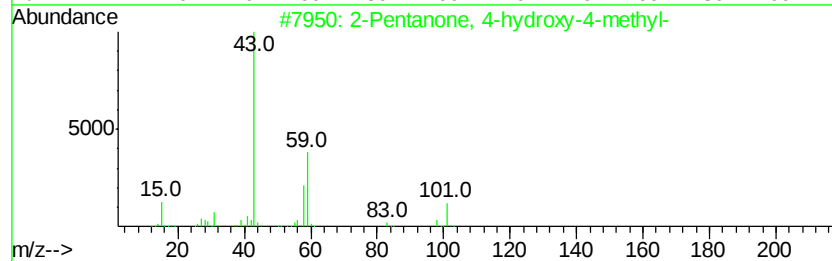
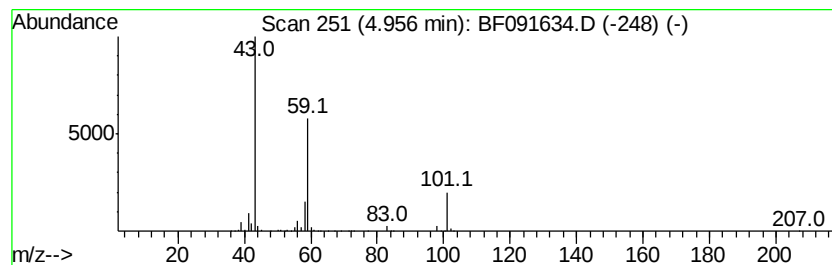
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	30.56 ng	2857840	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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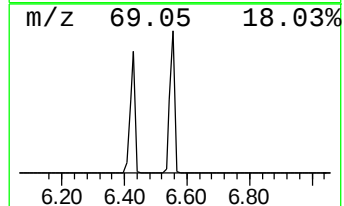
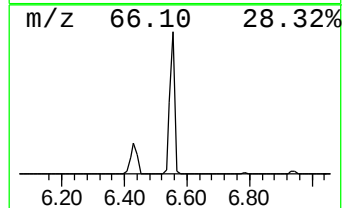
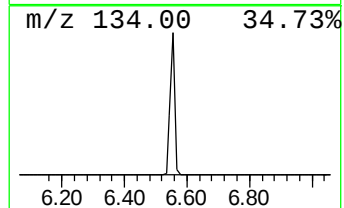
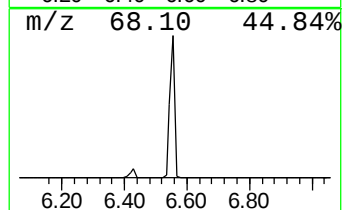
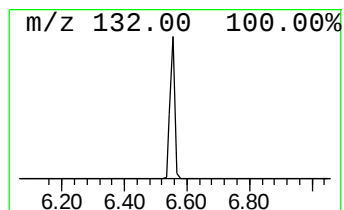
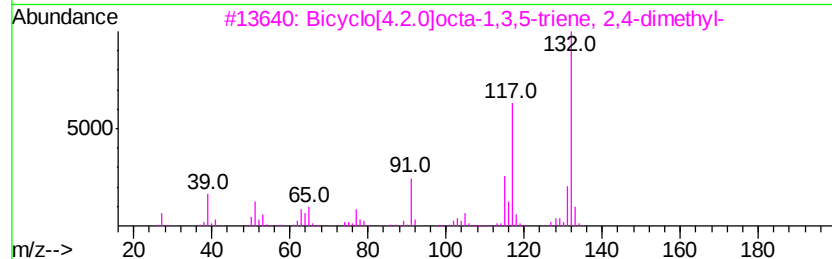
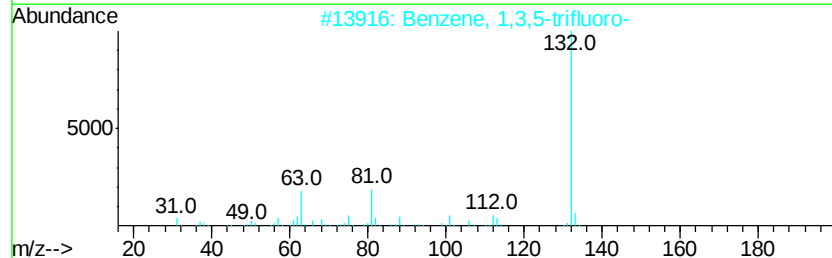
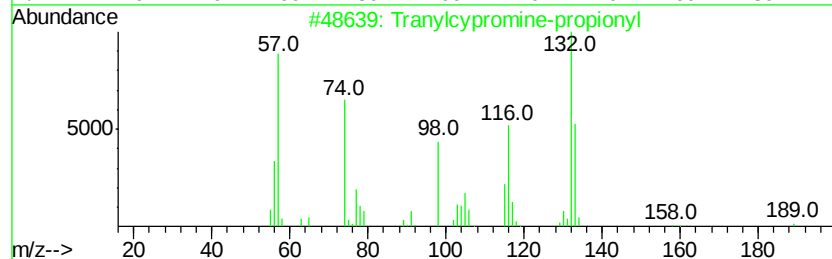
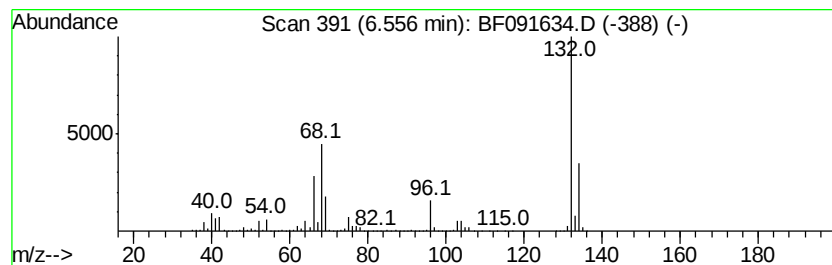
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	81.61 ng	7633090	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
2		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
3		Bicvclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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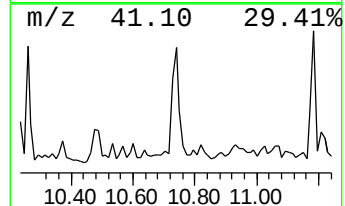
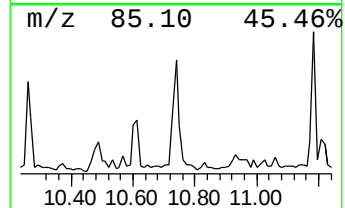
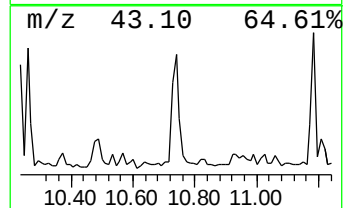
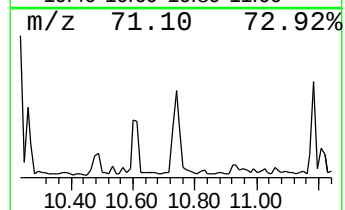
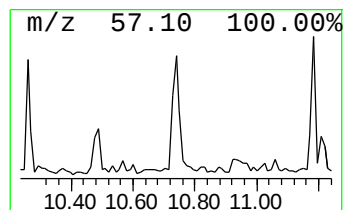
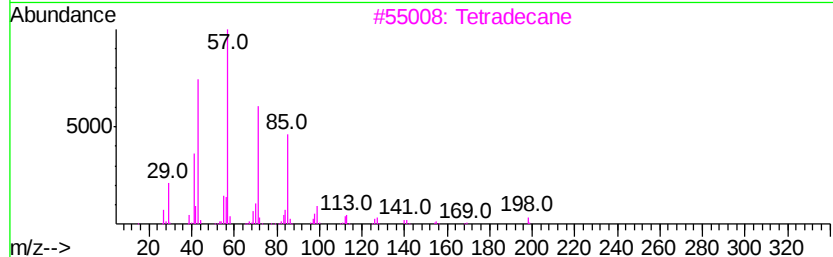
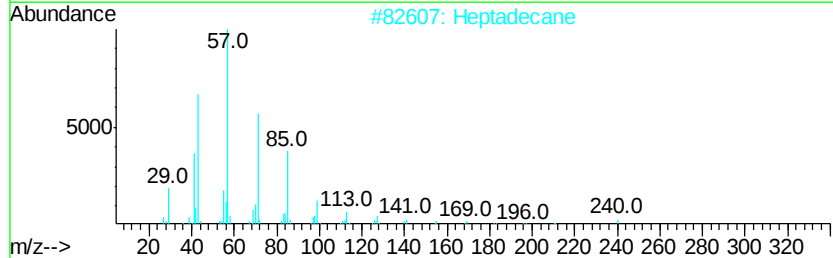
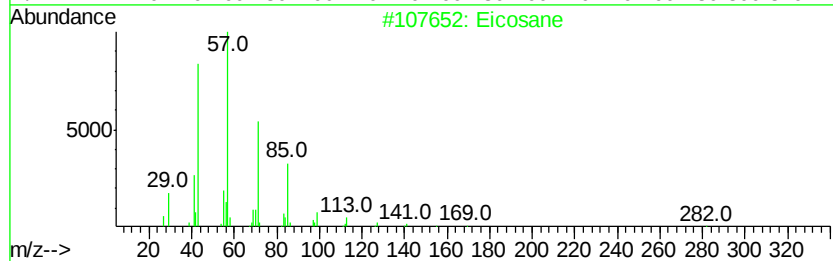
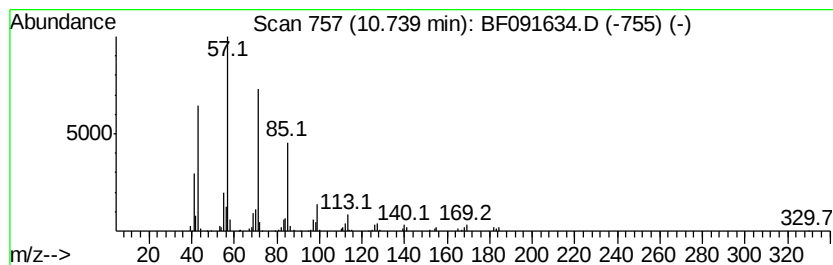
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.21 ng	277422	Phenanthrene-d10	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Heptadecane		240	C17H36	000629-78-7	91
3	Tetradecane		198	C14H30	000629-59-4	91
4	Hexadecane		226	C16H34	000544-76-3	91
5	Heneicosane		296	C21H44	000629-94-7	90



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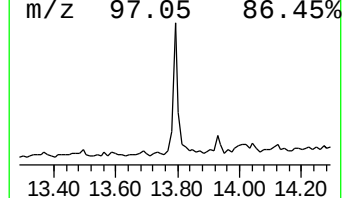
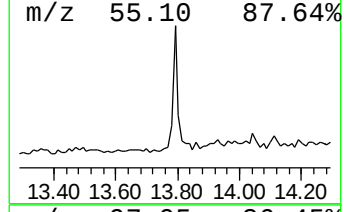
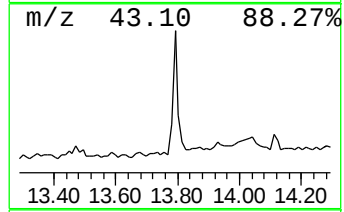
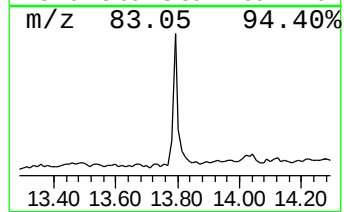
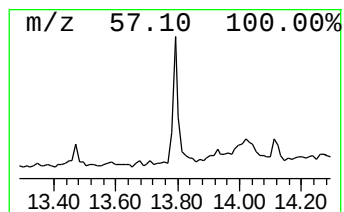
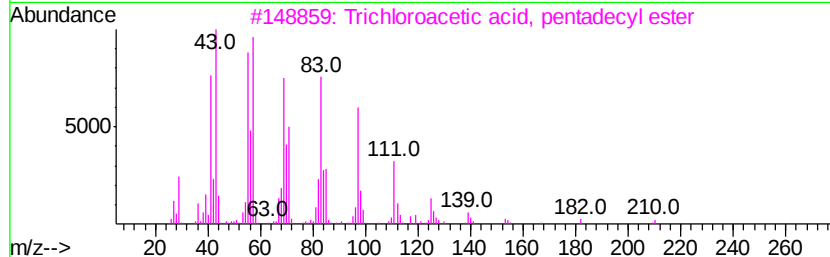
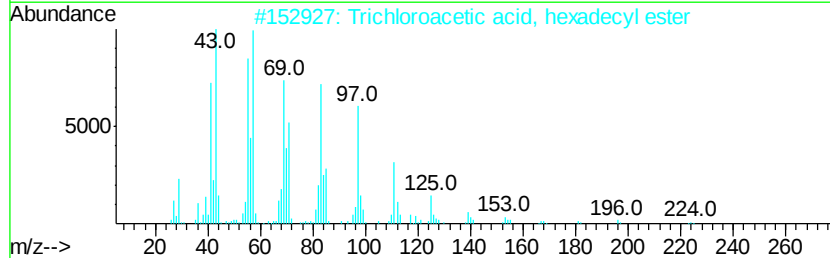
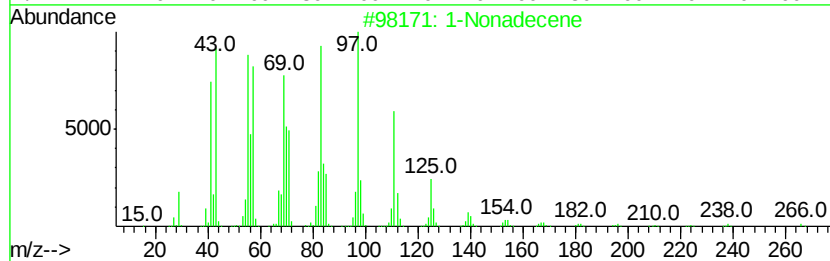
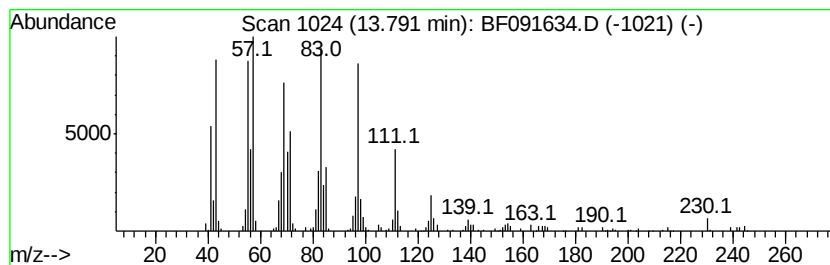
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	2.20 ng	296764	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Nonadecene	266	C19H38	018435-45-5	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
4		1-Docosene	308	C22H44	001599-67-3	81
5		1-Nonadecanol	284	C19H40O	001454-84-8	81



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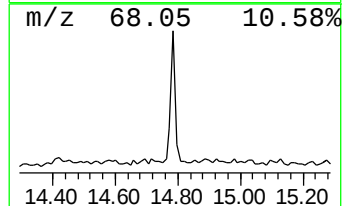
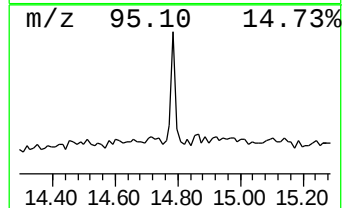
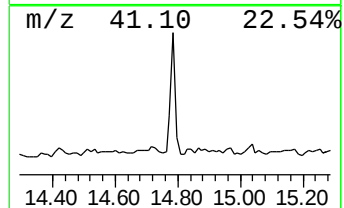
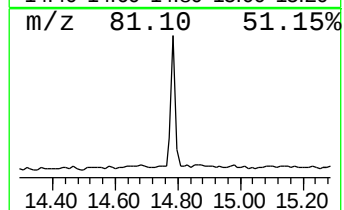
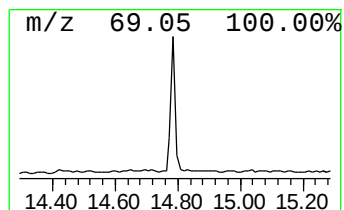
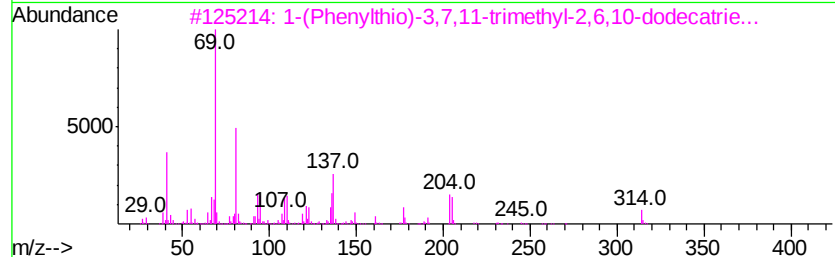
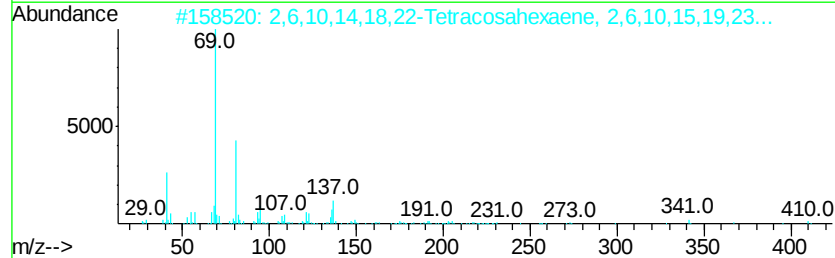
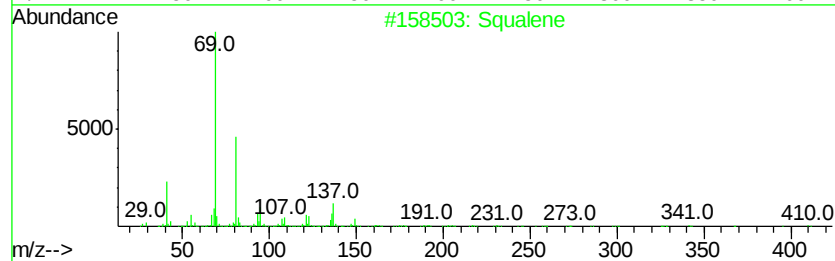
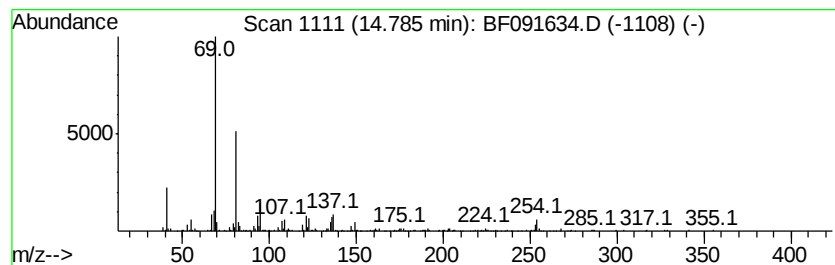
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	3.91 ng	335296	Perylene-d12	15.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	007683-64-9	80
2			2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	80
3			1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	72
4			Farnesol isomer a	222	C15H26O	1000108-92-4	64
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121516\
Data File : BF091634.D
Acq On : 15 Dec 2016 17:56
Operator : UM/SJ
Sample : H6012-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5-8-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.96	30.6	ng	2857840	1	6.78	1870590	20.0
unknown6.56	6.56	81.6	ng	7633090	1	6.78	1870590	20.0
Eicosane	10.74	2.2	ng	277422	4	11.30	2511850	20.0
1-Nonadecene	13.79	2.2	ng	296764	5	13.94	2692800	20.0
Squalene	14.79	3.9	ng	335296	6	15.35	1713850	20.0