

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092916\
 Data File : BF090291.D
 Acq On : 29 Sep 2016 14:20
 Operator : UM/SJ
 Sample : H4982-06
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-17

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-BF092016.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	1.644	3	5	30	rVB	722685	1875486	51.37%	5.243%
2	4.547	256	259	273	rVB	391964	793399	21.73%	2.218%
3	5.027	298	301	303	rBV	2952144	3650963	100.00%	10.206%
4	6.125	394	397	400	rBV	2668084	3409628	93.39%	9.531%
5	6.227	403	406	409	rVB	3013569	3399384	93.11%	9.503%
6	6.456	424	426	429	rBV	727757	757395	20.75%	2.117%
7	6.616	437	440	443	rBV	2810042	2768502	75.83%	7.739%
8	7.039	473	477	479	rBV	2235109	2542021	69.63%	7.106%
9	7.748	537	539	542	rBV	1133116	1022125	28.00%	2.857%
10	8.833	631	634	637	rBV	3373181	3601475	98.64%	10.068%
11	9.233	667	669	672	rVB	857951	762562	20.89%	2.132%
12	9.462	687	689	690	rBV	48035	46033	1.26%	0.129%
13	9.496	690	692	694	rVV	1298343	1128248	30.90%	3.154%
14	9.919	726	729	731	rBV3	13434	38283	1.05%	0.107%
15	9.953	731	732	734	rVB	63905	84849	2.32%	0.237%
16	10.182	748	752	755	rBV	40765	92421	2.53%	0.258%
17	10.285	758	761	763	rBV	2027521	2199452	60.24%	6.148%
18	10.434	771	774	777	rBV	101357	162835	4.46%	0.455%
19	10.479	777	778	780	rVV	48731	43577	1.19%	0.122%
20	10.514	780	781	783	rVV2	58303	59610	1.63%	0.167%
21	10.548	783	784	788	rVV3	37624	59168	1.62%	0.165%
22	10.616	788	790	792	rVV2	30469	56770	1.55%	0.159%
23	10.651	792	793	795	rVV2	46960	55435	1.52%	0.155%
24	10.696	795	797	799	rVV	41529	67659	1.85%	0.189%
25	10.731	799	800	803	rVB2	30541	38748	1.06%	0.108%
26	10.879	810	813	814	rBV2	42060	58116	1.59%	0.162%
27	10.959	818	820	824	rBV	671233	1039066	28.46%	2.905%
28	11.039	824	827	830	rVB2	40291	52254	1.43%	0.146%
29	11.531	868	870	872	rVV2	110619	136917	3.75%	0.383%
30	11.565	872	873	878	rVB2	40875	91944	2.52%	0.257%
31	12.159	923	925	928	rBV	176982	232984	6.38%	0.651%
32	12.308	936	938	942	rBV4	45106	98781	2.71%	0.276%
33	12.388	942	945	947	rBV	258633	262864	7.20%	0.735%
34	12.559	957	960	962	rBV	1979986	2724567	74.63%	7.616%

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35	12.617	962	965	966	rVB2	21215	49405	1.35%	0.138%
36	12.822	981	983	984	rBV2	36124	49094	1.34%	0.137%
37	13.474	1037	1040	1044	rBV2	186121	276635	7.58%	0.773%
38	13.577	1047	1049	1055	rBV	665763	976272	26.74%	2.729%
39	14.102	1093	1095	1098	rBV3	68123	94149	2.58%	0.263%
40	14.571	1134	1136	1140	rBV	106126	238328	6.53%	0.666%
41	14.857	1159	1161	1163	rBV	88035	126472	3.46%	0.354%
42	14.903	1163	1165	1168	rVV	417873	548591	15.03%	1.534%

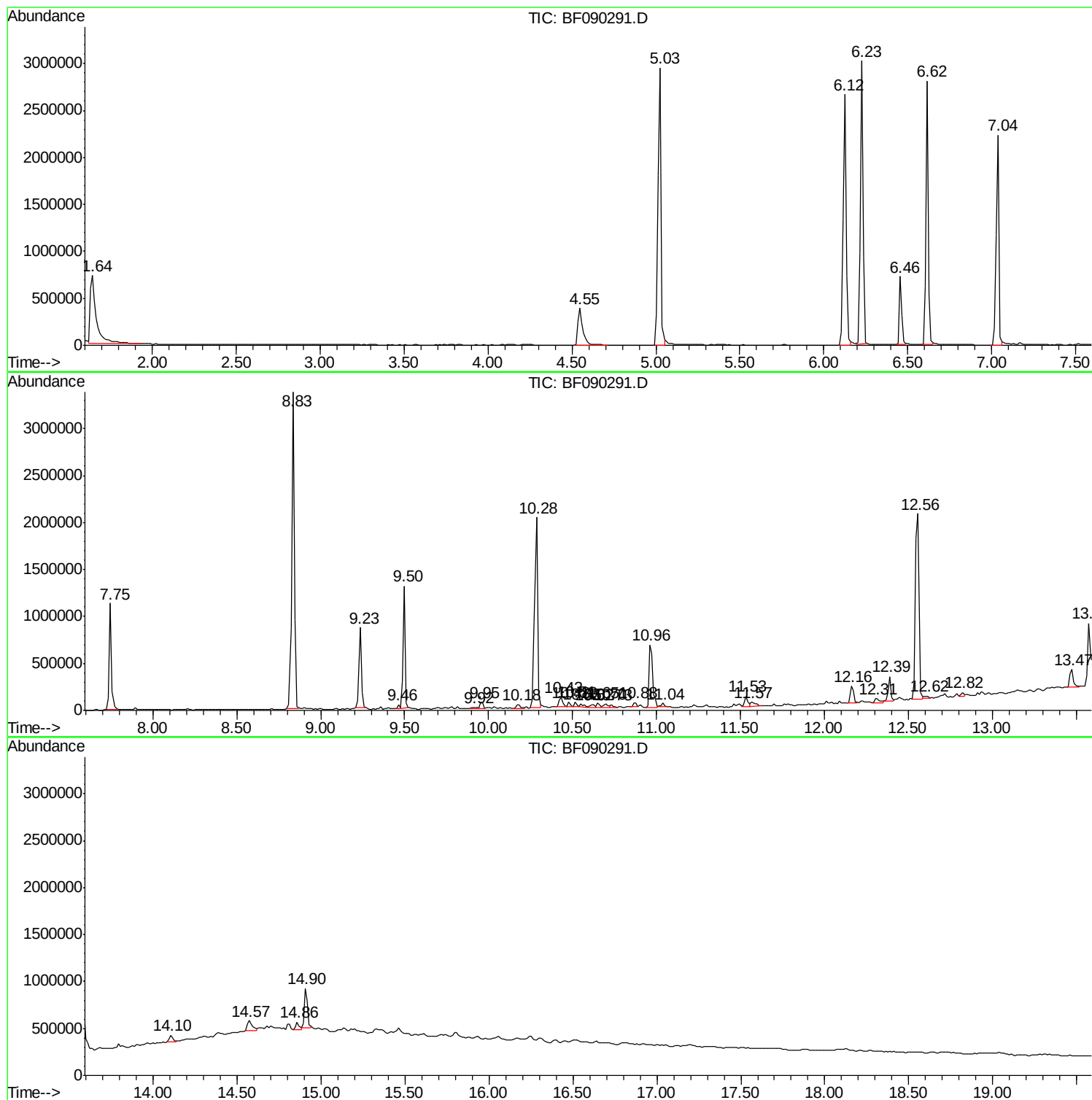
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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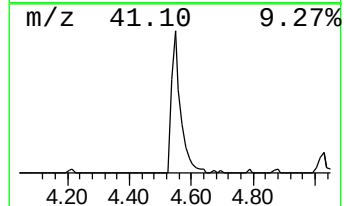
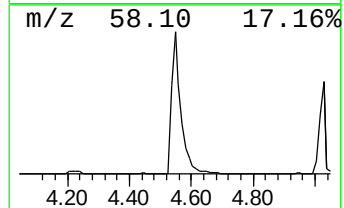
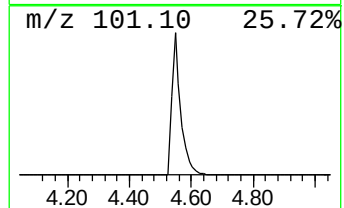
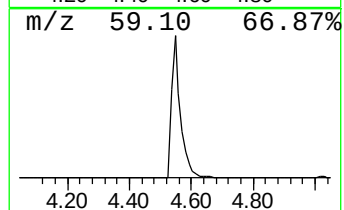
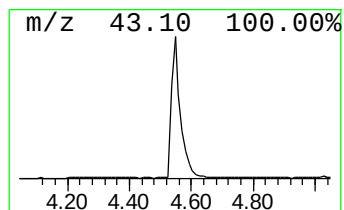
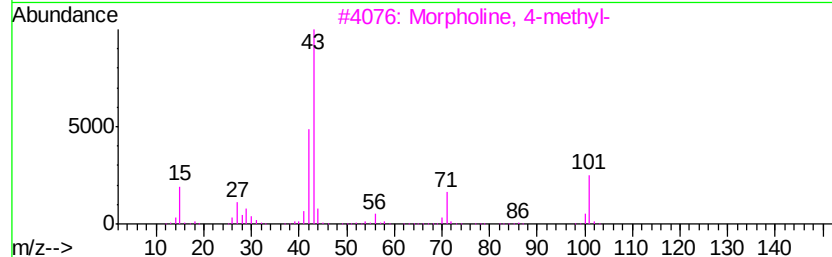
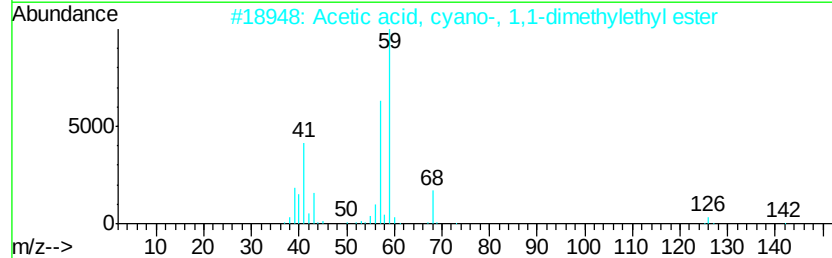
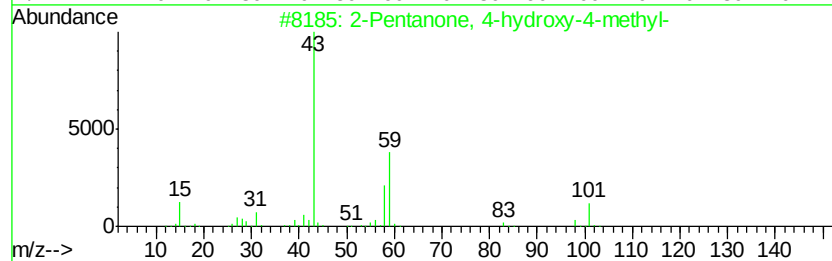
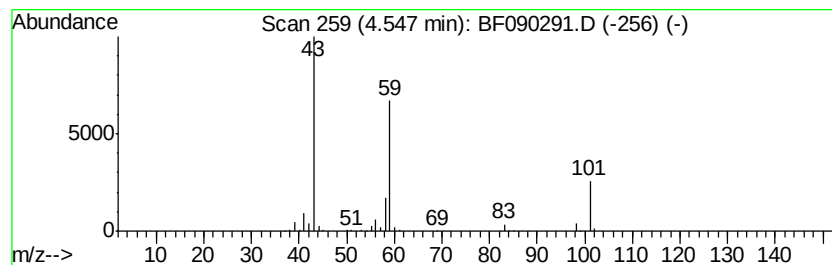
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	20.95 ng	793399	1,4-Dichlorobenzene-d4	6.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Acetone	58	C3H6O	000067-64-1	9



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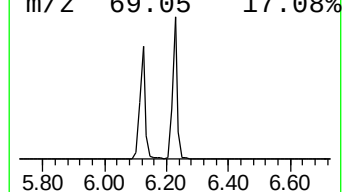
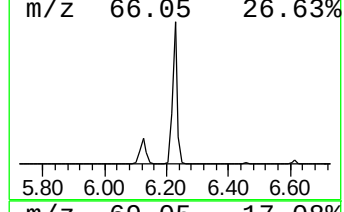
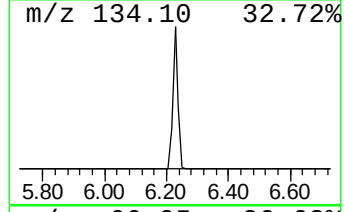
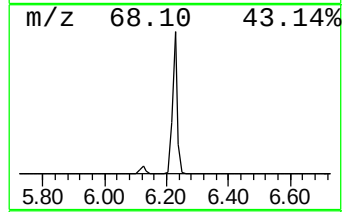
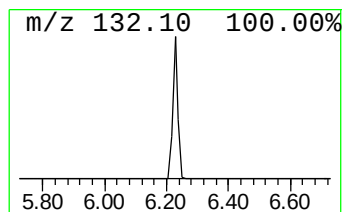
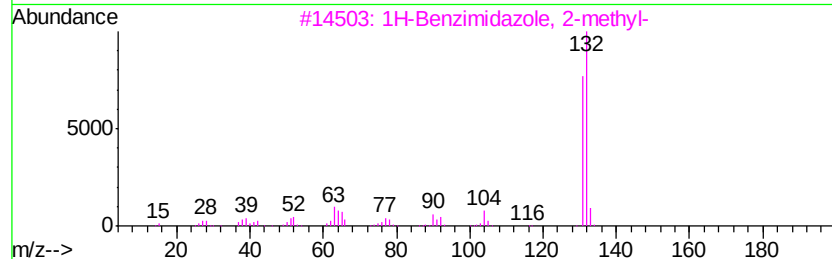
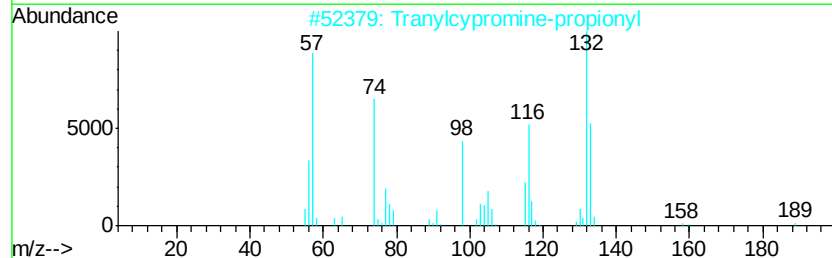
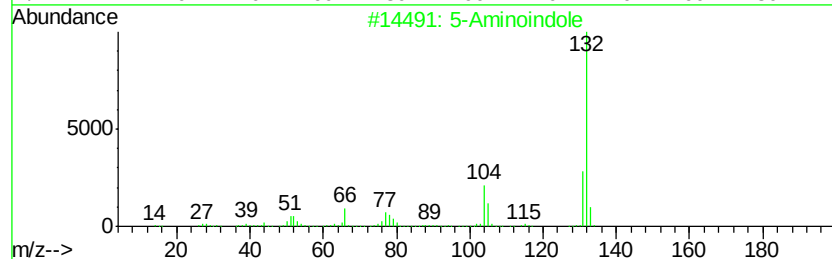
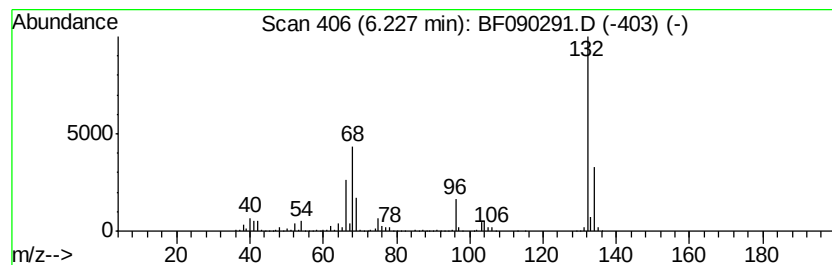
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Peak Number 3 unknown6.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.23	89.77 ng	3399380	1,4-Dichlorobenzene-d4	6.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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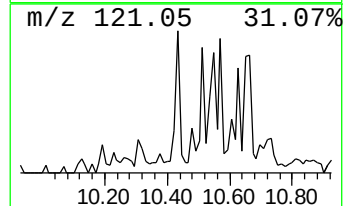
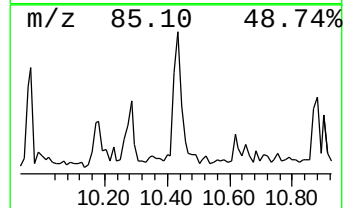
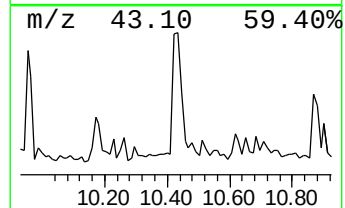
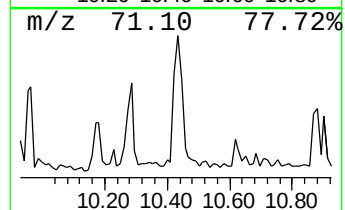
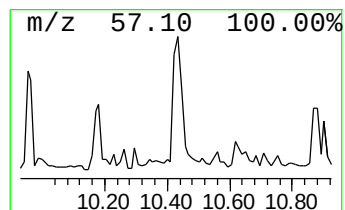
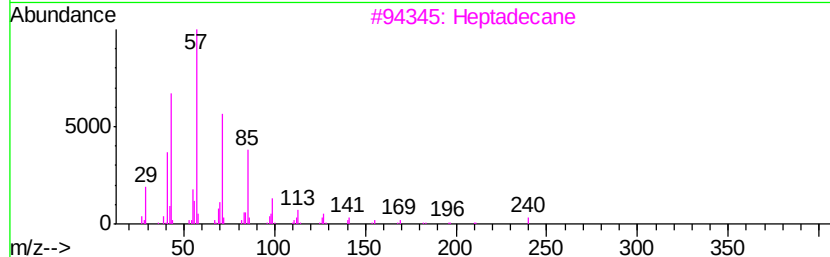
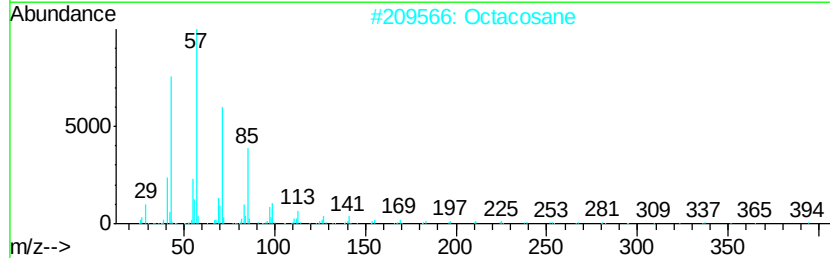
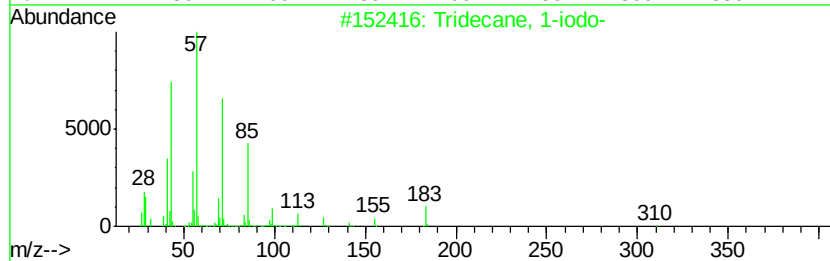
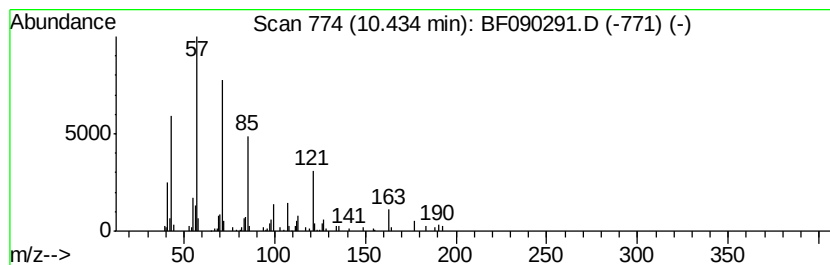
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.43	3.13 ng	162835	Phenanthrene-d10	10.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
2	Octacosane	394	C28H58	000630-02-4	72
3	Heptadecane	240	C17H36	000629-78-7	72
4	Hexadecane	226	C16H34	000544-76-3	72
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72



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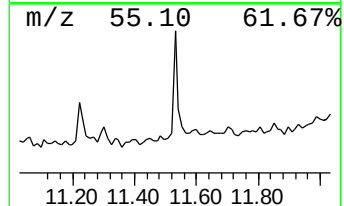
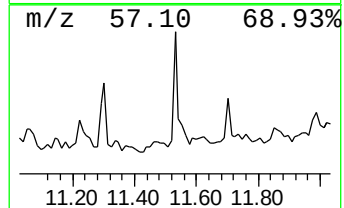
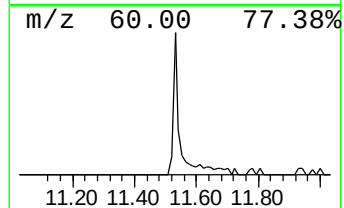
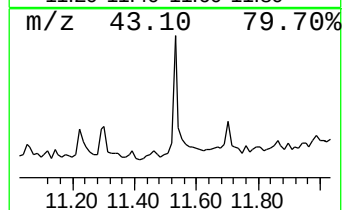
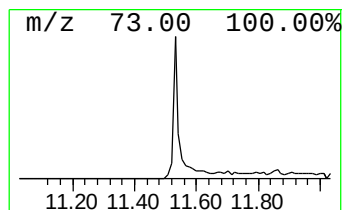
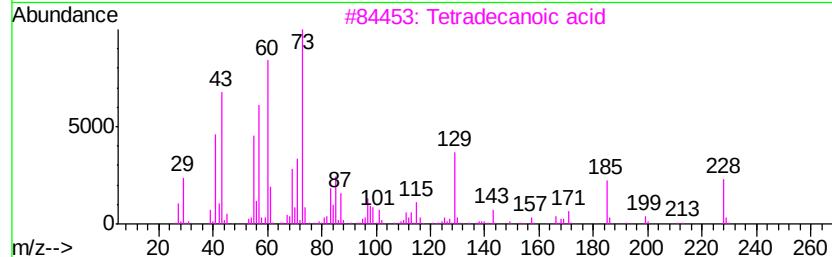
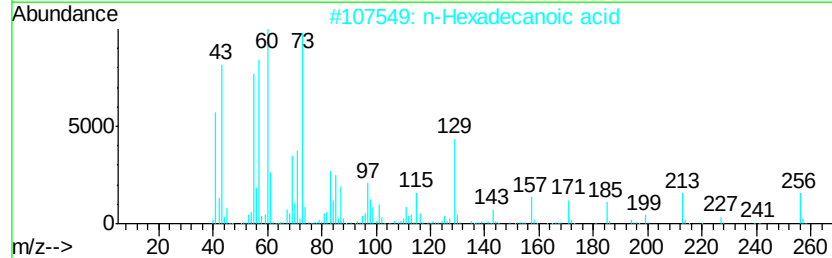
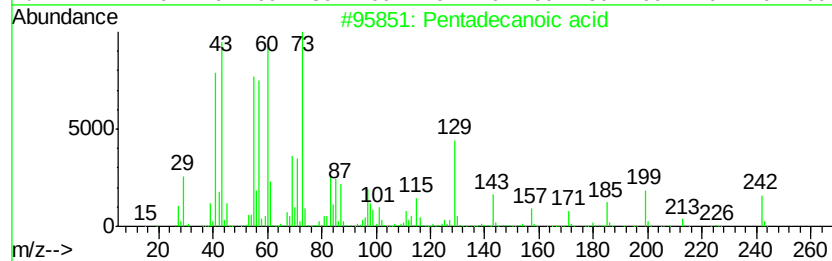
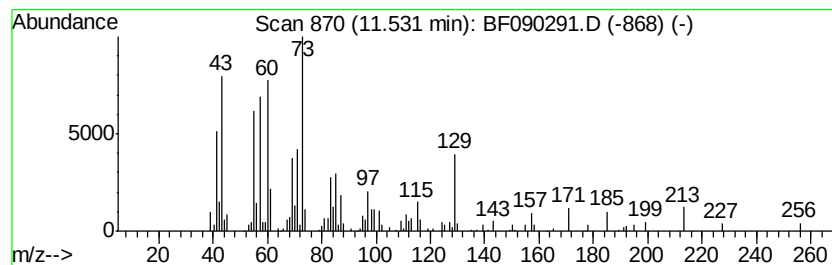
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.53	2.64 ng	136917	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



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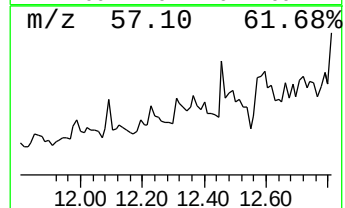
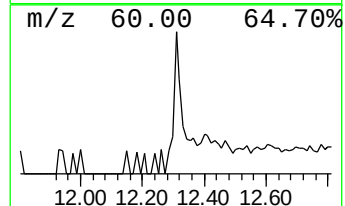
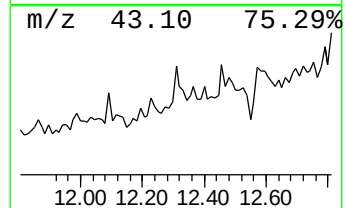
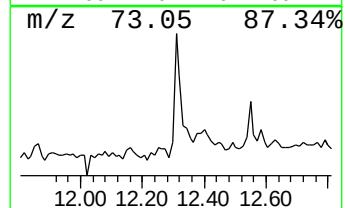
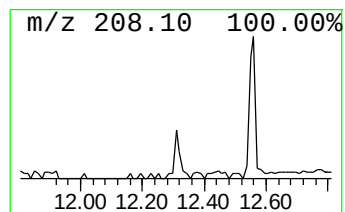
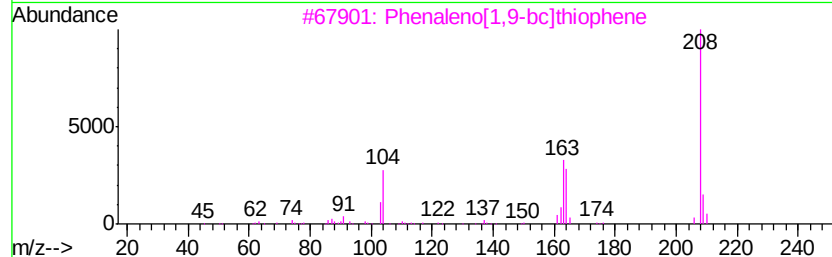
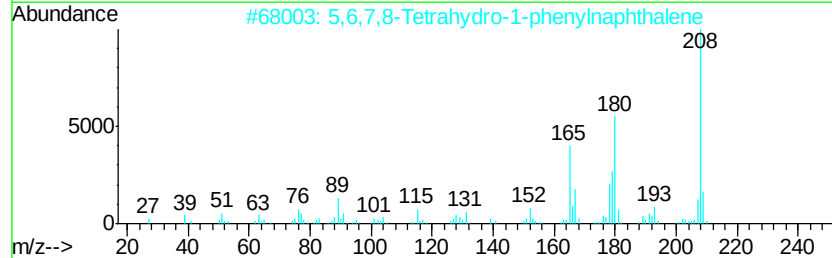
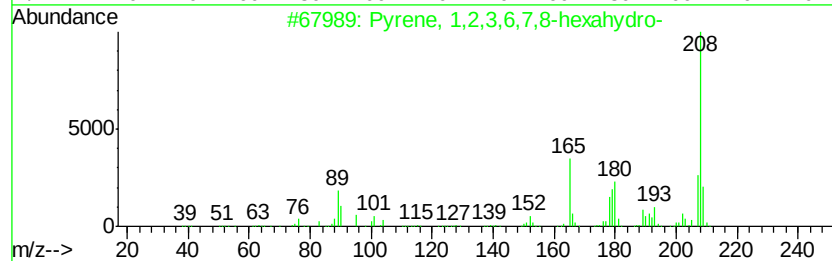
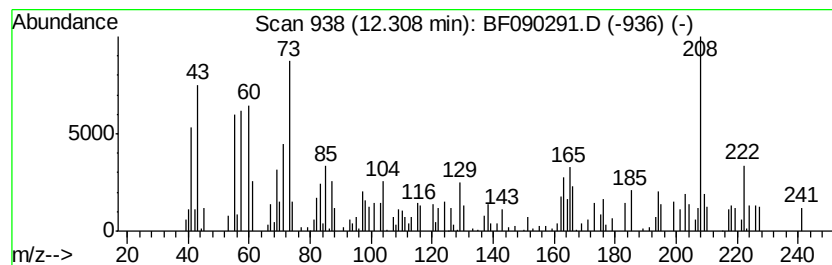
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 unknown12.31 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.31	2.02 ng	98781	Chrysene-d12	13.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1,2,3,6,7,8-hexahydro-	208	C16H16	001732-13-4	47
2		5,6,7,8-Tetrahydro-1-phenylnapht...	208	C16H16	067064-63-5	38
3		Phenalenof[1,9-bcl]thiophene	208	C14H8S	079965-99-4	38
4		2-Adamantylamine, N-trimethylsilyl-	223	C13H25NSi	1000333-95-7	38
5		.beta.-Asarone	208	C12H16O3	005273-86-9	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
Data File : BF090291.D
Acq On : 29 Sep 2016 14:20
Operator : UM/SJ
Sample : H4982-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

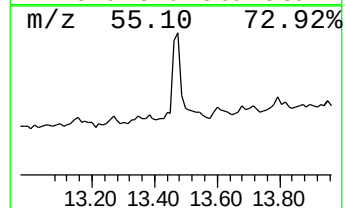
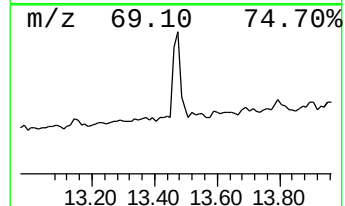
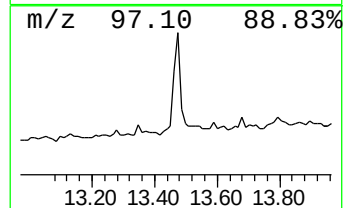
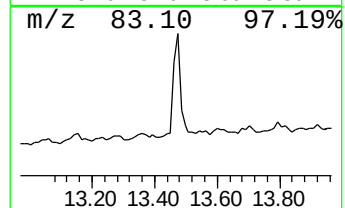
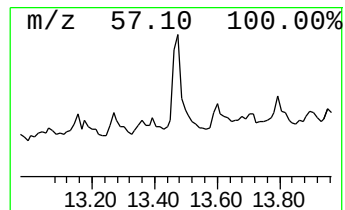
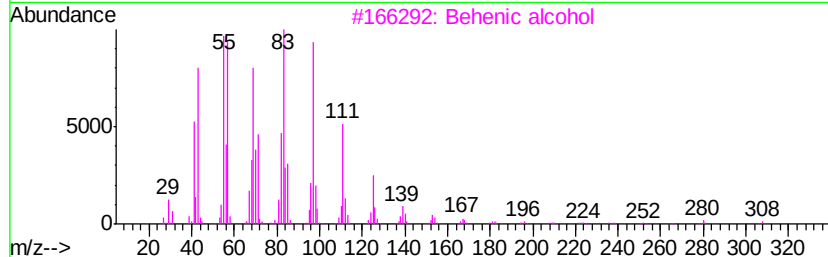
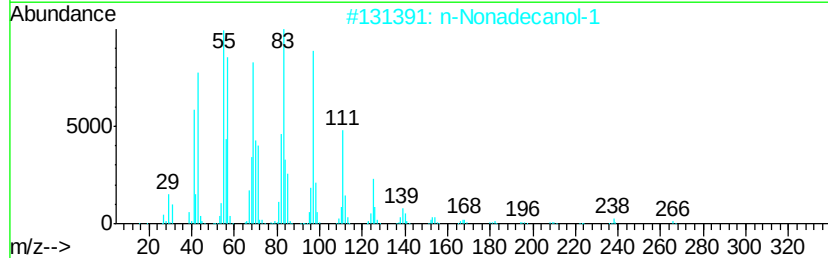
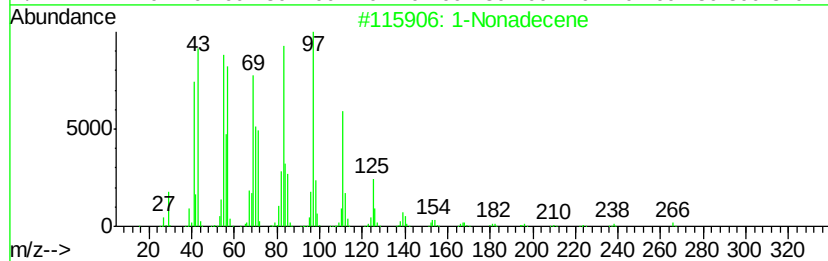
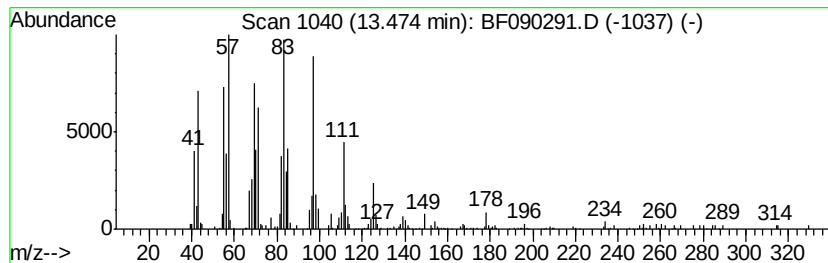
Instrument :
BNA_F
ClientSampleId :
S-17

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	5.67 ng	276635	Chrysene-d12	13.58
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonadecene	266 C19H38	018435-45-5	99
2	n-Nonadecanol-1	284 C19H40O	001454-84-8	93
3	Behenic alcohol	326 C22H46O	000661-19-8	93
4	5-Octadecene, (E)-	252 C18H36	007206-21-5	93
5	3-Eicosene, (E)-	280 C20H40	074685-33-9	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092916\
Data File : BF090291.D
Acq On : 29 Sep 2016 14:20
Operator : UM/SJ
Sample : H4982-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.55	20.9	ng	793399	1	6.46	757395	20.0
unknown6.23	6.23	89.8	ng	3399380	1	6.46	757395	20.0
Tridecane, 1-iodo-	10.43	3.1	ng	162835	4	10.97	1039070	20.0
Pentadecanoic acid	11.53	2.6	ng	136917	4	10.97	1039070	20.0
unknown12.31	12.31	2.0	ng	98781	5	13.58	976272	20.0
1-Nonadecene	13.47	5.7	ng	276635	5	13.58	976272	20.0