

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112215\
 Data File : BF083191.D
 Acq On : 23 Nov 2015 6:58
 Operator : UM/IZ
 Sample : G4437-04
 Misc :
 ALS Vial : 77 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-37

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-BF112115.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	4.787	243	245	256	rVB	960857	1373884	18.60%	2.561%
2	5.256	283	286	293	rBV	2571928	3480949	47.14%	6.488%
3	6.307	376	378	386	rBV	1957665	2313052	31.32%	4.311%
4	6.422	386	388	391	rBV	5255845	5616448	76.06%	10.468%
5	6.650	406	408	410	rBV	1438847	1414553	19.16%	2.637%
6	6.810	419	422	424	rBV	5253417	5647364	76.47%	10.526%
7	7.004	436	439	441	rVB	82086	94869	1.28%	0.177%
8	7.096	445	447	450	rVV	89278	95297	1.29%	0.178%
9	7.176	451	454	455	rVV	176824	194469	2.63%	0.362%
10	7.222	455	458	461	rVV	4202480	4788563	64.84%	8.925%
11	7.267	461	462	464	rVV	170953	157145	2.13%	0.293%
12	7.359	467	470	474	rVV2	88752	133495	1.81%	0.249%
13	7.484	474	481	482	rVV4	46364	116811	1.58%	0.218%
14	7.519	482	484	486	rVB2	129426	146036	1.98%	0.272%
15	7.667	495	497	500	rBV2	44578	119112	1.61%	0.222%
16	7.850	511	513	514	rBV2	75427	86257	1.17%	0.161%
17	7.885	514	516	518	rVB	58935	76458	1.04%	0.143%
18	7.942	518	521	523	rBV	1438032	1747338	23.66%	3.257%
19	8.090	532	534	536	rBV	60921	84825	1.15%	0.158%
20	8.422	561	563	565	rVV	73090	96395	1.31%	0.180%
21	8.467	565	567	570	rVB	288942	311761	4.22%	0.581%
22	8.776	591	594	597	rBV3	62663	81941	1.11%	0.153%
23	9.016	612	615	618	rBV	5818272	7384647	100.00%	13.764%
24	9.188	626	630	632	rVB4	47348	92683	1.26%	0.173%
25	9.359	643	645	647	rBV2	46220	78763	1.07%	0.147%
26	9.416	647	650	654	rVV2	102277	147093	1.99%	0.274%
27	9.485	654	656	660	rVB	85926	94863	1.28%	0.177%
28	9.633	667	669	671	rBV	86879	81163	1.10%	0.151%
29	9.679	671	673	676	rBV	1292231	1825366	24.72%	3.402%
30	10.033	702	704	706	rBV	90191	121396	1.64%	0.226%
31	10.136	709	713	715	rBV2	113596	134026	1.81%	0.250%
32	10.479	740	743	745	rBV	2809509	4068504	55.09%	7.583%
33	10.605	752	754	758	rVB	110872	144986	1.96%	0.270%
34	11.051	789	793	794	rBV3	63537	93336	1.26%	0.174%

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35	11.165	800	803	805	rBV	1239991	1582983	21.44%	2.951%
36	11.713	848	851	853	rBV	401995	413042	5.59%	0.770%
37	12.411	908	912	917	rBV5	43325	115971	1.57%	0.216%
38	12.491	917	919	922	rBV	475324	561148	7.60%	1.046%
39	12.754	939	942	944	rBV	4251637	5956957	80.67%	11.103%
40	13.668	1019	1022	1025	rBV	91974	152418	2.06%	0.284%
41	13.782	1030	1032	1035	rBV	1447947	1405441	19.03%	2.620%
42	15.154	1149	1152	1154	rBV	706781	1019137	13.80%	1.900%

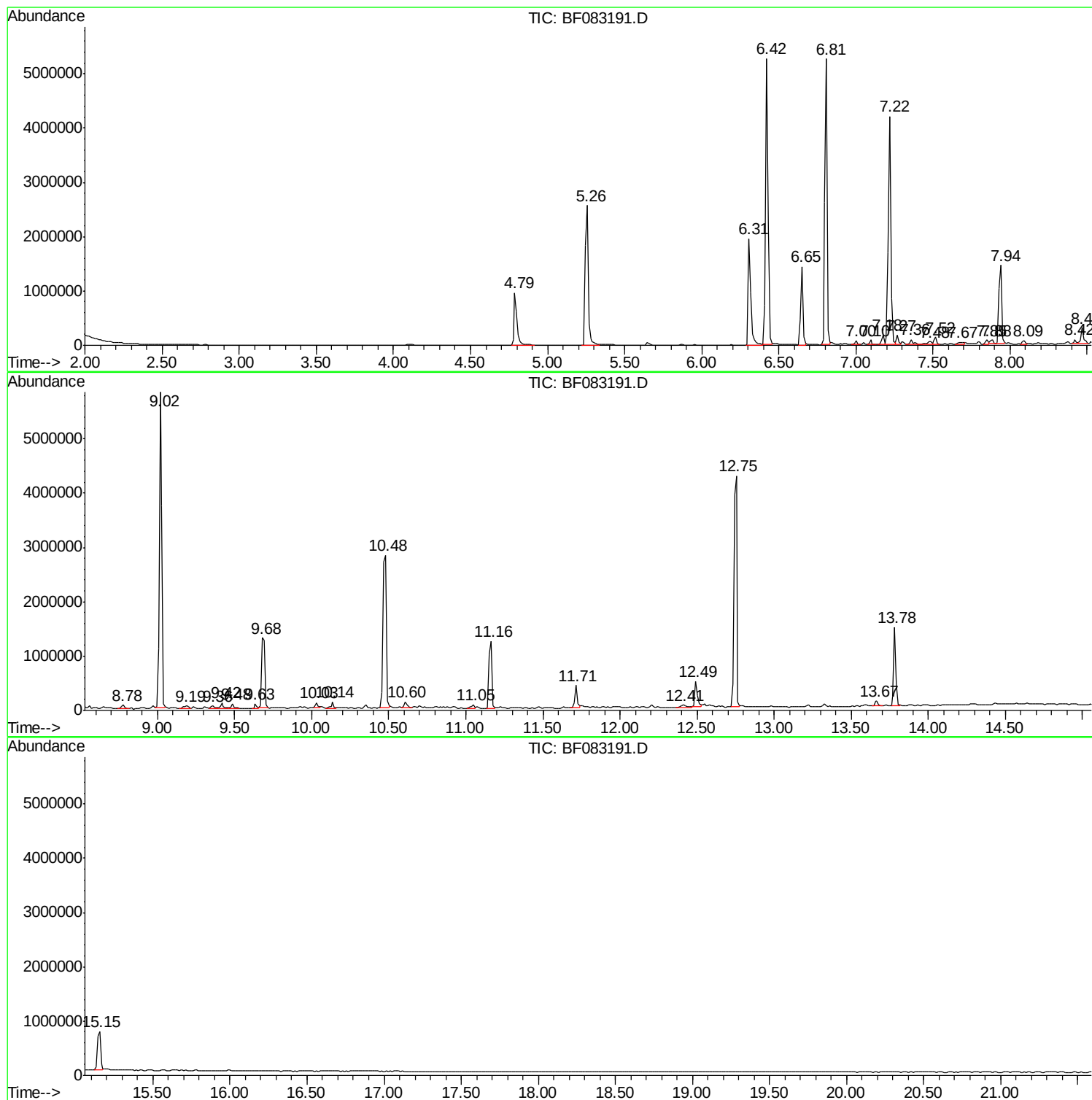
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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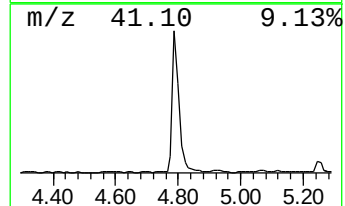
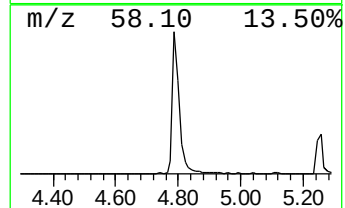
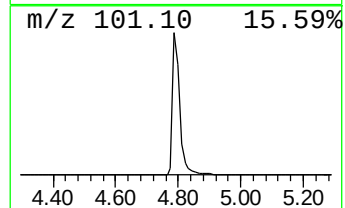
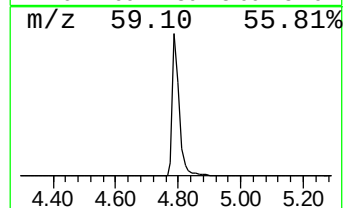
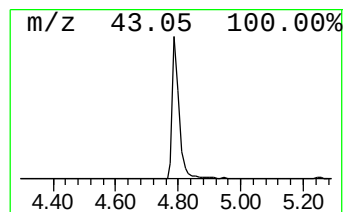
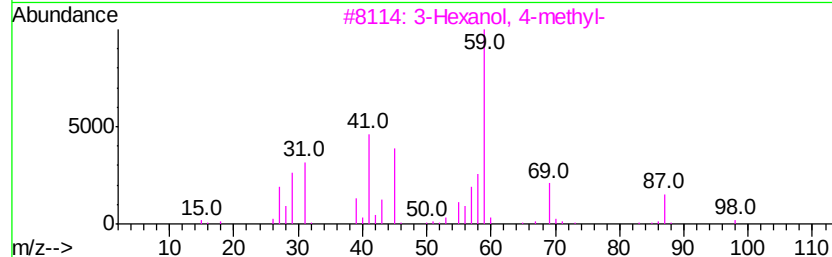
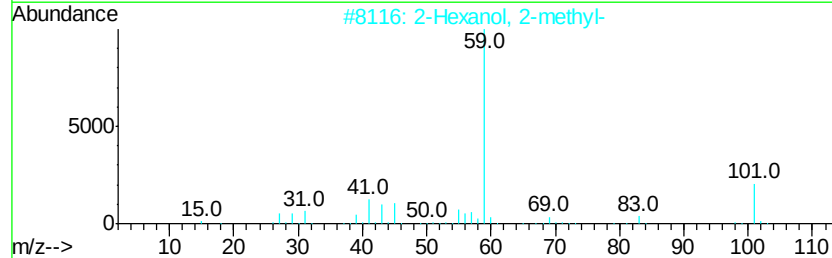
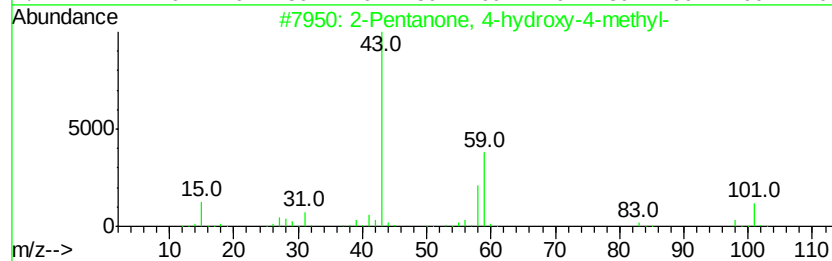
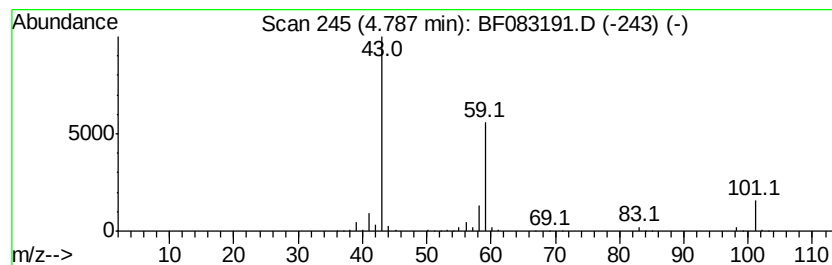
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	19.43 ng	1373880	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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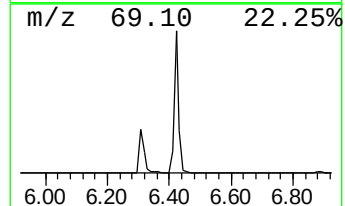
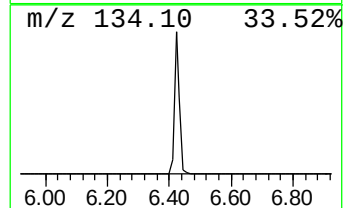
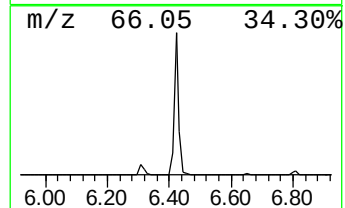
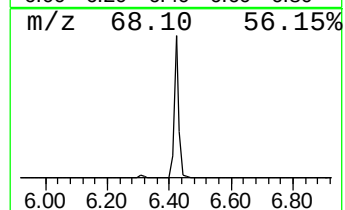
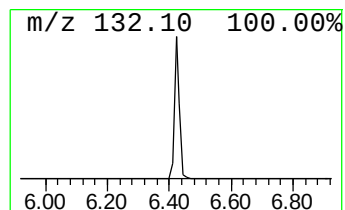
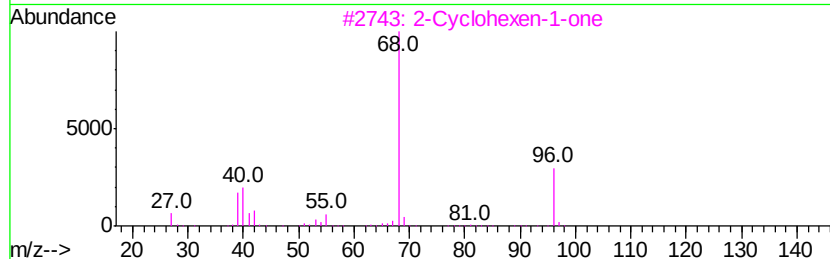
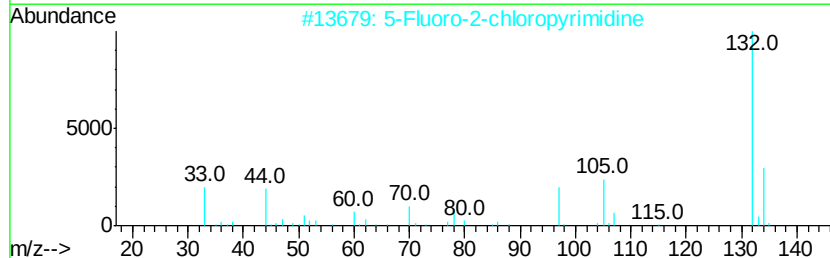
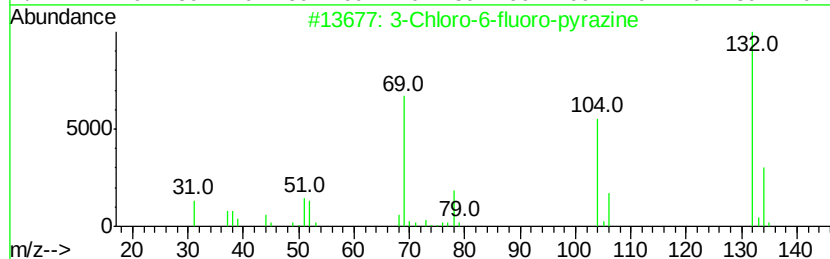
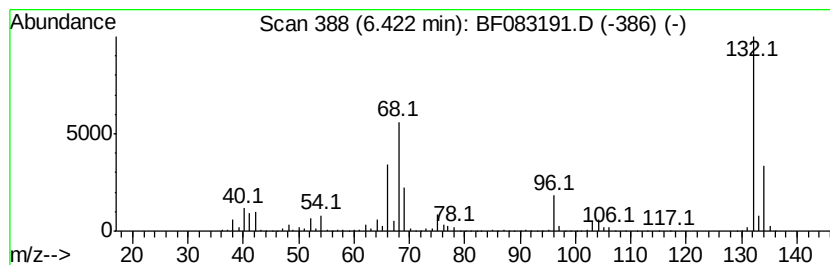
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.42 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	79.41 ng	5616450	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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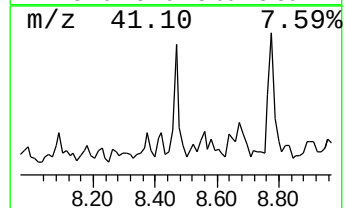
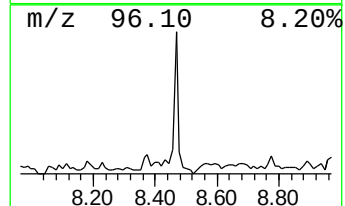
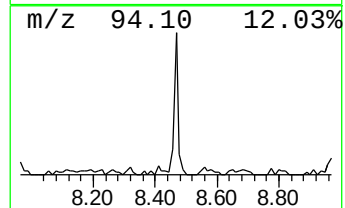
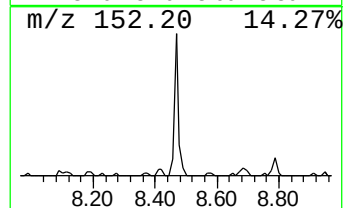
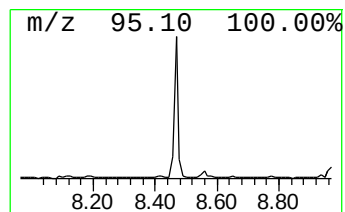
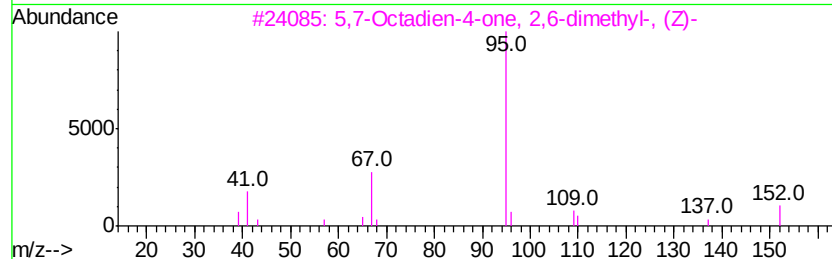
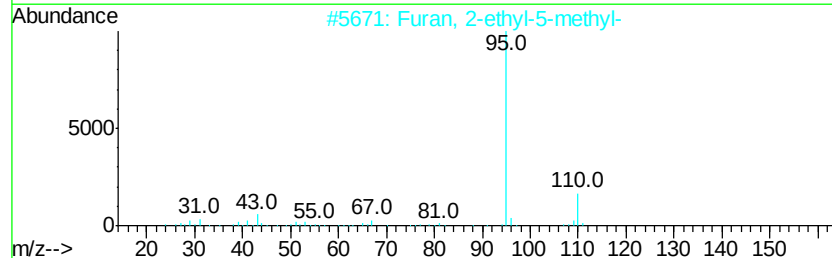
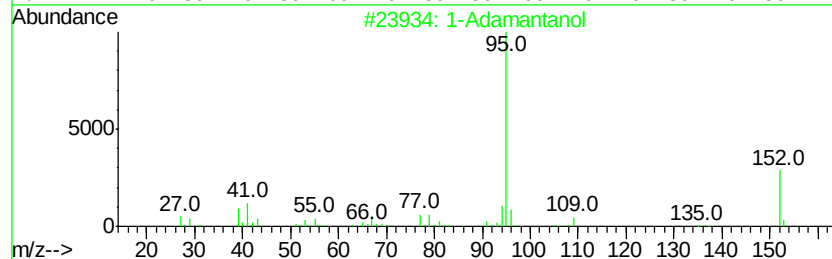
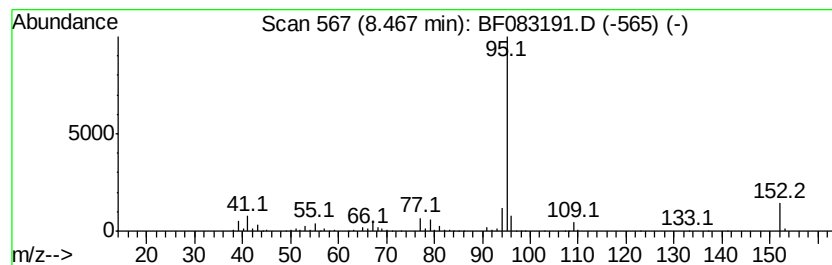
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 1-Adamantanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	3.57 ng	311761	Napthalene-d8	7.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Adamantanol	152	C10H16O	000768-95-6	91
2		Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	45
3		5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	003588-18-9	42
4		Cyclohexene, 1-methyl-3-(1-methyl...	138	C10H18	013828-31-4	39
5		3-Hydroxypyridine monoacetate	137	C7H7NO2	017747-43-2	25



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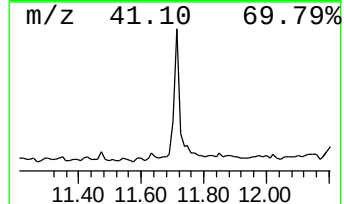
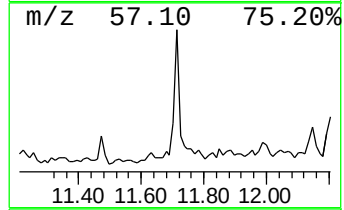
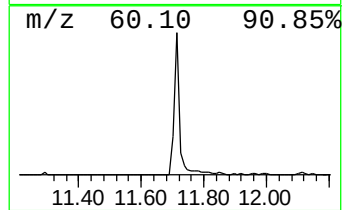
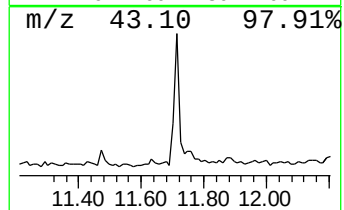
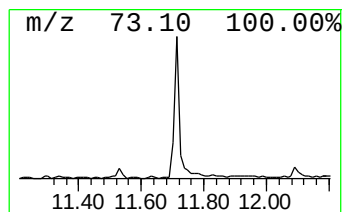
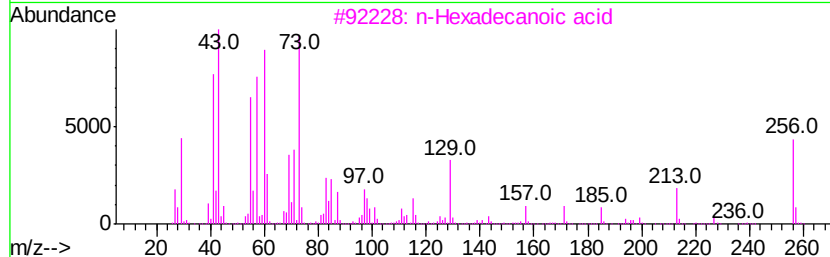
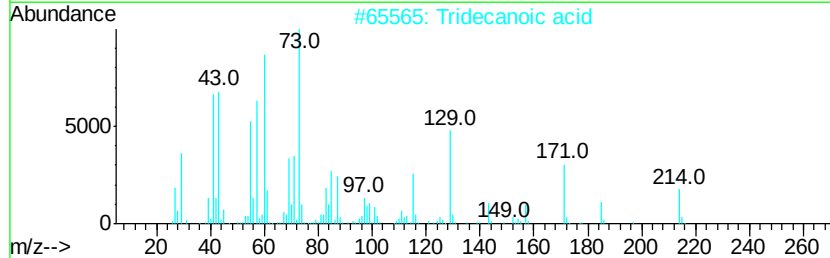
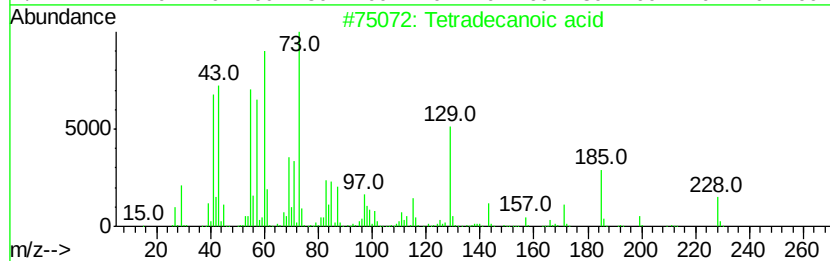
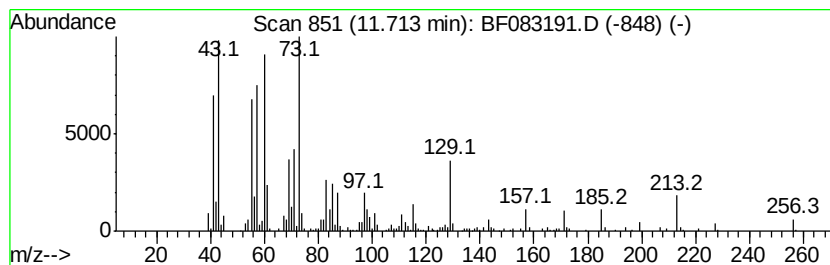
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.71	5.22 ng	413042	Phenanthrene-d10		11.16
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Nonanoic acid	158	C9H18O2	000112-05-0	43



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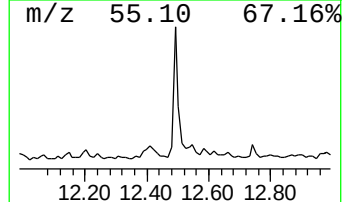
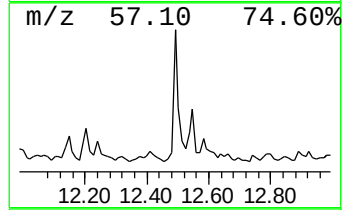
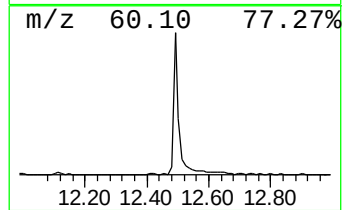
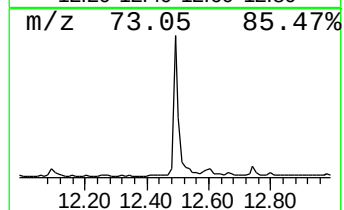
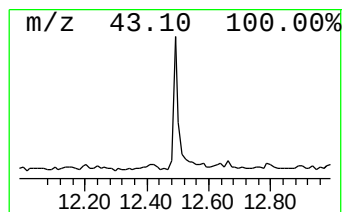
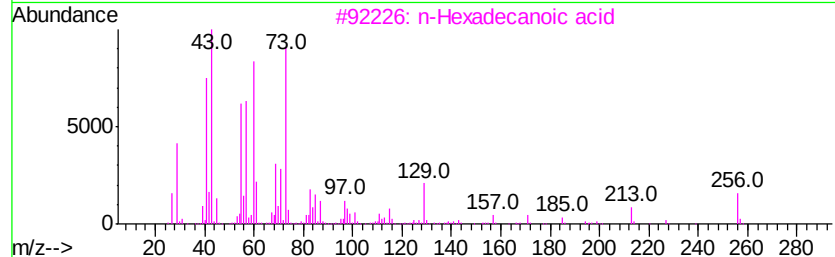
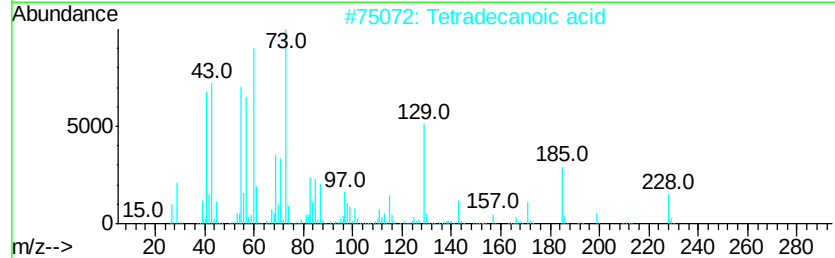
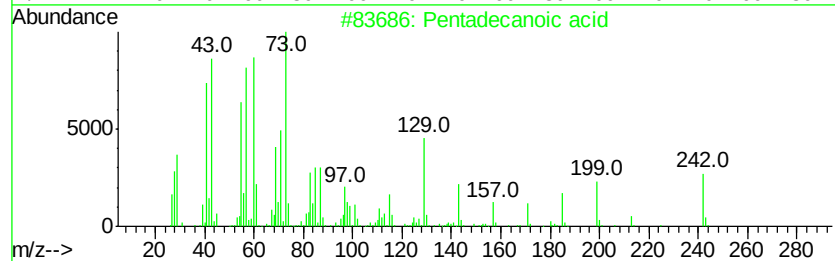
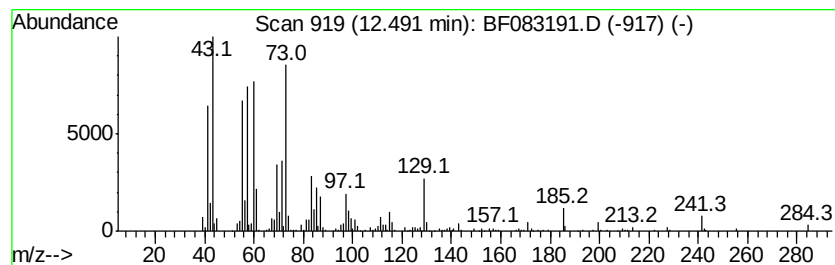
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	7.99 ng	561148	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	50
5	Octanoic Acid	144	C8H16O2	000124-07-2	50



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Sample : G4437-04
Misc :
ALS Vial : 77 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-37

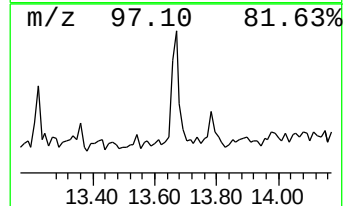
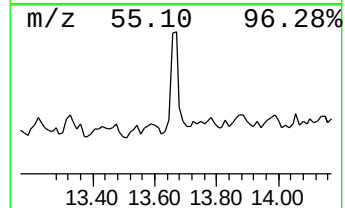
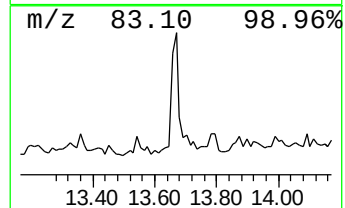
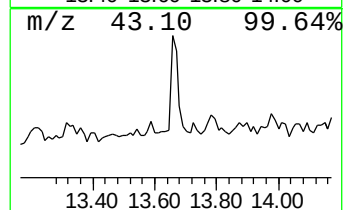
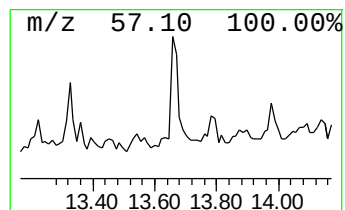
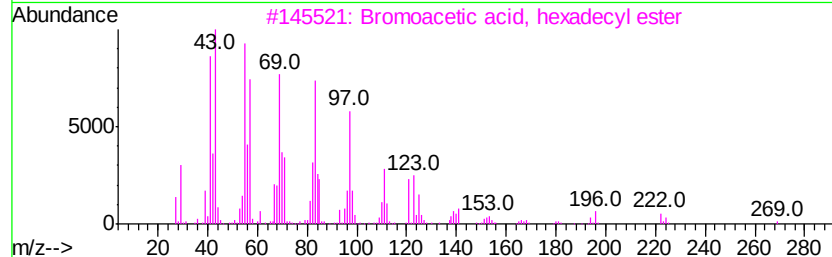
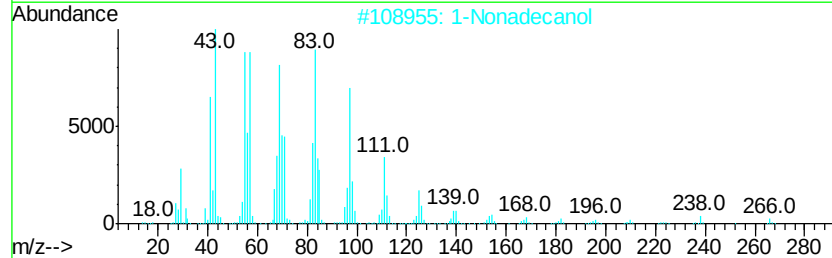
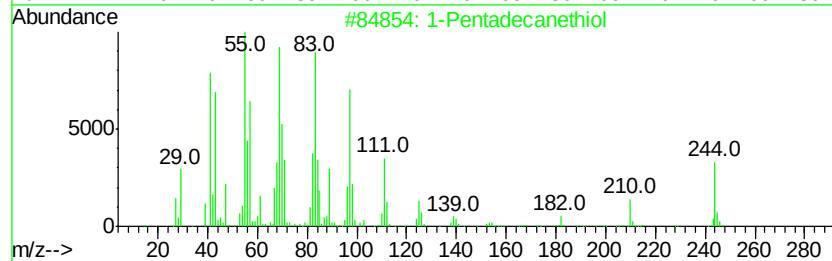
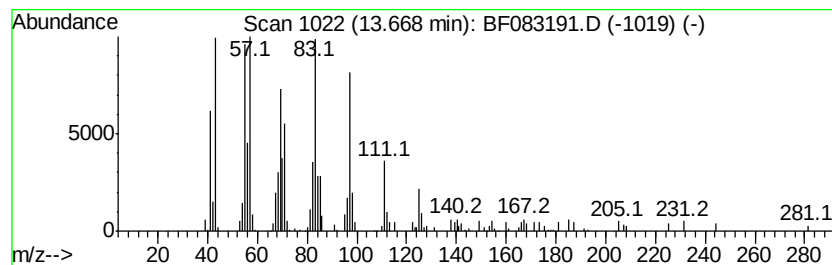
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Pentadecanethiol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	2.17 ng	152418	Chrysene-d12	13.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Pentadecanethiol	244	C15H32S	025276-70-4	94
2		1-Nonadecanol	284	C19H40O	001454-84-8	94
3		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112215\
Data File : BF083191.D
Acq On : 23 Nov 2015 6:58
Operator : UM/IZ
Sample : G4437-04
Misc :
ALS Vial : 77 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-37

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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...	4.79	19.4	ng	1373880	1	6.65	1414550	20.0
unknown6.42	6.42	79.4	ng	5616450	1	6.65	1414550	20.0
1-Adamantanol	8.47	3.6	ng	311761	2	7.94	1747340	20.0
Tetradecanoic acid	11.71	5.2	ng	413042	4	11.16	1582980	20.0
Pentadecanoic acid	12.49	8.0	ng	561148	5	13.78	1405440	20.0
1-Pentadecanethiol	13.67	2.2	ng	152418	5	13.78	1405440	20.0