

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
 Data File : BF092558.D
 Acq On : 27 Jan 2017 6:32
 Operator : SJ/MA
 Sample : I1364-02
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-26

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-BF012417.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	5.150	266	268	271	rBV	668232	738547	14.67%	1.673%
2	5.561	302	304	307	rBV	1791783	2544556	50.55%	5.765%
3	6.590	392	394	397	rBV	1750368	1620338	32.19%	3.671%
4	6.739	404	407	409	rBV	3974349	4287217	85.17%	9.714%
5	6.967	425	427	429	rBV	1361907	1158777	23.02%	2.625%
6	7.127	438	441	443	rBV	3722639	3531186	70.15%	8.001%
7	7.539	474	477	479	rBV	3091204	3348033	66.51%	7.586%
8	8.259	537	540	543	rBV	1518824	1479155	29.38%	3.351%
9	9.345	632	635	638	rBV	4380706	5008338	99.49%	11.348%
10	9.745	666	670	673	rVB	38747	74709	1.48%	0.169%
11	10.030	692	695	696	rBV	1698372	1732700	34.42%	3.926%
12	10.053	696	697	699	rVB	148571	193163	3.84%	0.438%
13	10.236	710	713	715	rBV	95310	128319	2.55%	0.291%
14	10.328	718	721	724	rBV	48222	121445	2.41%	0.275%
15	10.453	730	732	736	rVB2	78946	117845	2.34%	0.267%
16	10.682	749	752	755	rVB	1146676	1730097	34.37%	3.920%
17	10.819	761	764	766	rBV	2503328	3007425	59.74%	6.814%
18	10.888	766	770	772	rVV	1401507	1595775	31.70%	3.616%
19	10.933	772	774	779	rVB2	92548	158048	3.14%	0.358%
20	11.116	787	790	792	rVB3	30897	57148	1.14%	0.129%
21	11.379	811	813	815	rBV2	59203	69614	1.38%	0.158%
22	11.516	822	825	827	rBV	1880480	1665536	33.09%	3.774%
23	11.722	841	843	848	rVB2	115451	144363	2.87%	0.327%
24	12.133	877	879	881	rBV2	41603	58494	1.16%	0.133%
25	12.236	886	888	891	rVB2	35050	54858	1.09%	0.124%
26	12.739	930	932	934	rBV	59164	64764	1.29%	0.147%
27	12.876	942	944	946	rBV	85343	111352	2.21%	0.252%
28	12.922	946	948	950	rVV	546625	487637	9.69%	1.105%
29	13.002	952	955	957	rVV2	111128	175072	3.48%	0.397%
30	13.105	961	964	967	rBV	3543995	5033886	100.00%	11.405%
31	13.631	1007	1010	1012	rVB	336511	320088	6.36%	0.725%
32	13.676	1012	1014	1015	rBV	39674	61194	1.22%	0.139%
33	13.882	1030	1032	1040	rVB3	59512	122964	2.44%	0.279%
34	13.996	1040	1042	1050	rVB	126321	196694	3.91%	0.446%

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35	14.156	1053	1056	1058	rBV	1448724	1363620	27.09%	3.090%
36	14.317	1068	1070	1075	rVB	82120	87756	1.74%	0.199%
37	14.625	1094	1097	1099	rBV2	54658	70919	1.41%	0.161%
38	14.934	1122	1124	1126	rBV	64196	68310	1.36%	0.155%
39	15.277	1152	1154	1156	rVB	63946	72901	1.45%	0.165%
40	15.631	1182	1185	1188	rBV	637293	1075915	21.37%	2.438%
41	16.111	1224	1227	1235	rVB	52999	101750	2.02%	0.231%
42	16.625	1269	1272	1278	rBV	39881	95268	1.89%	0.216%

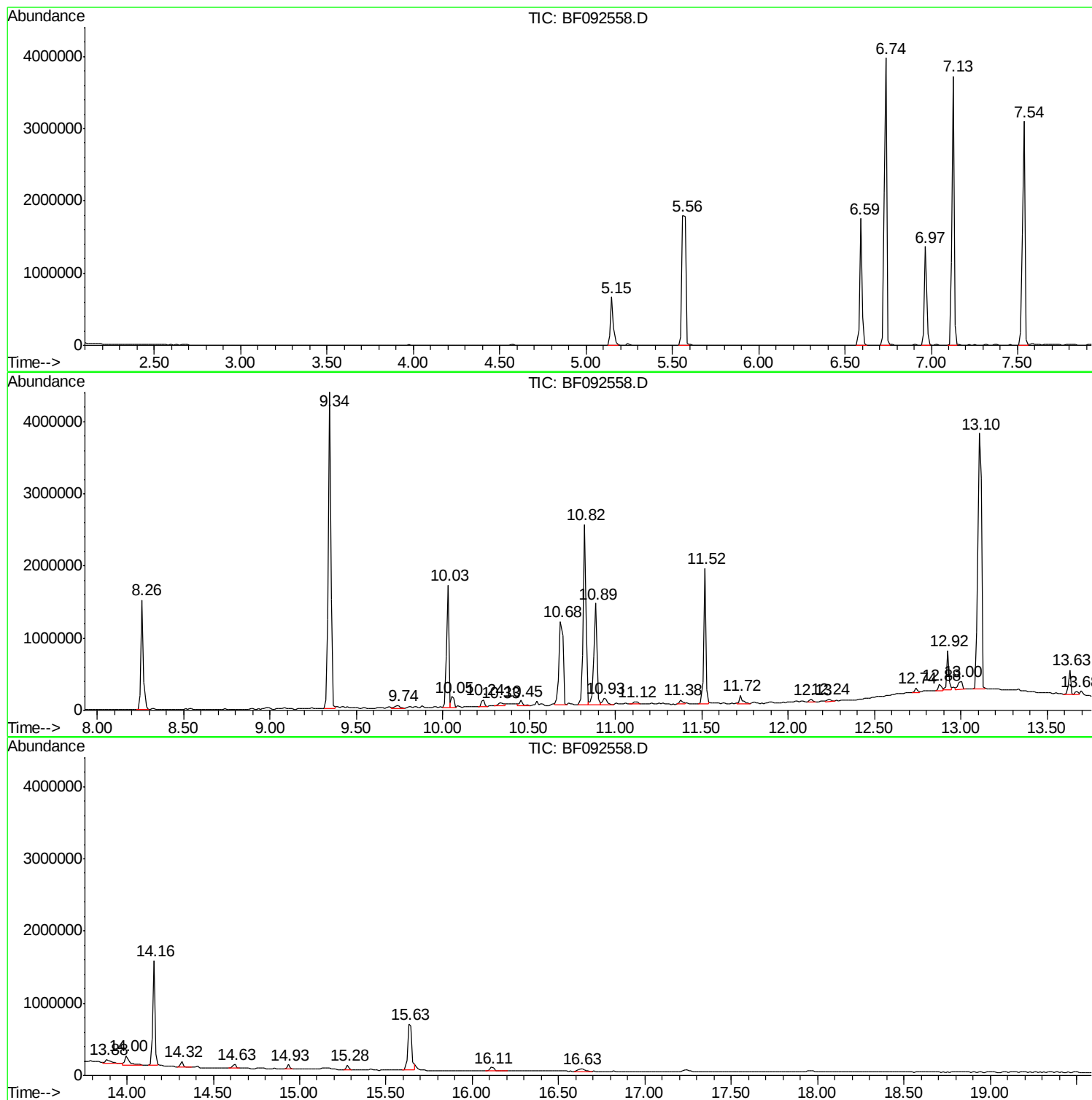
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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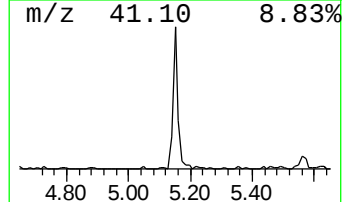
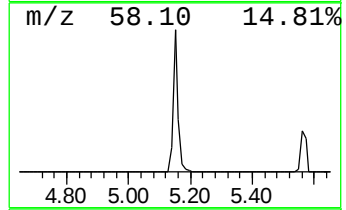
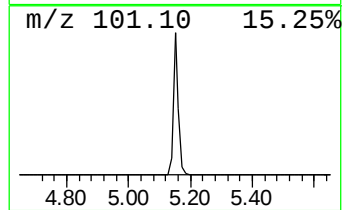
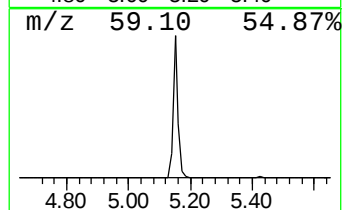
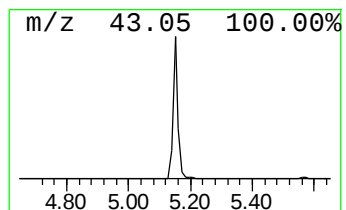
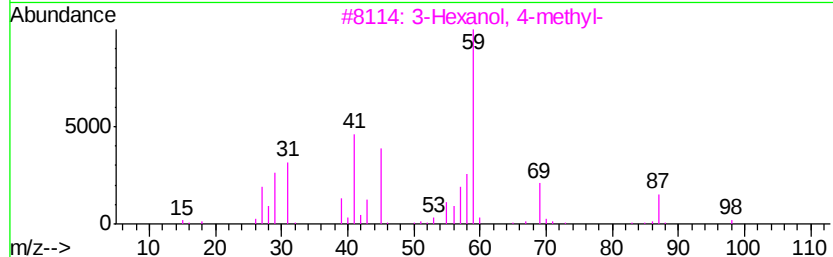
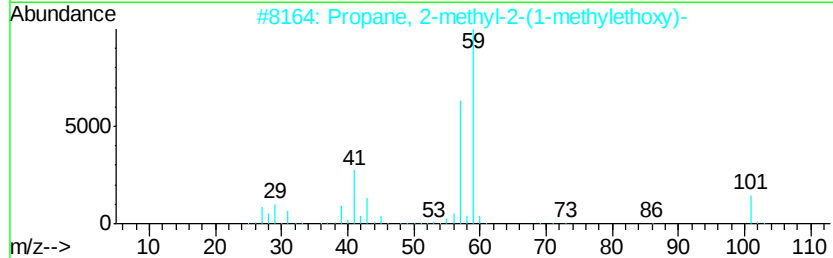
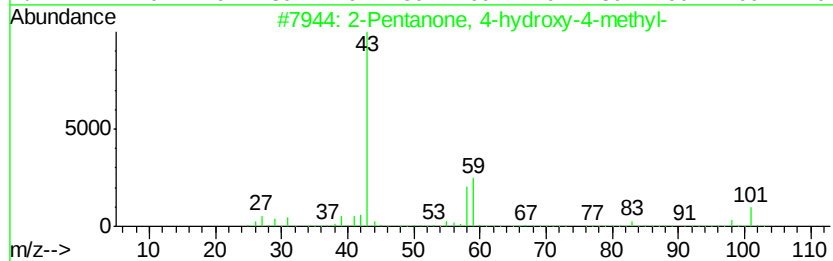
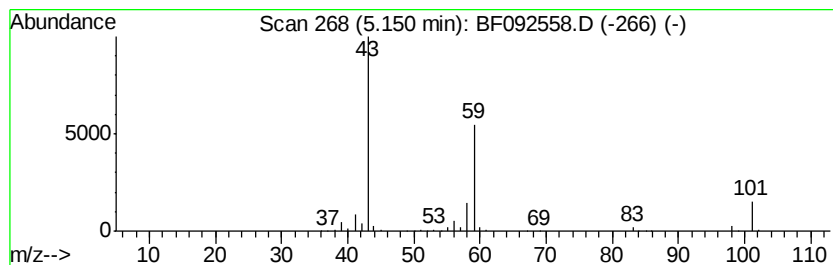
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	12.75 ng	738547	1,4-Dichlorobenzene-d4	6.97

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	42
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-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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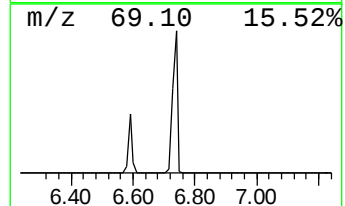
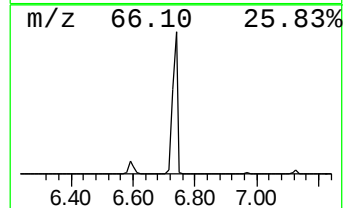
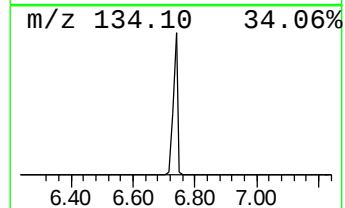
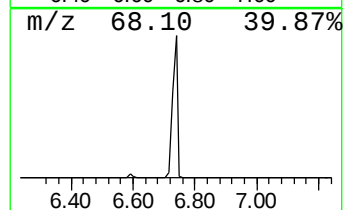
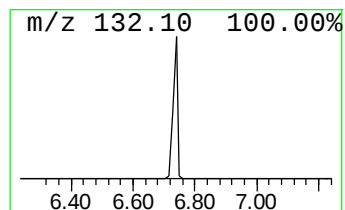
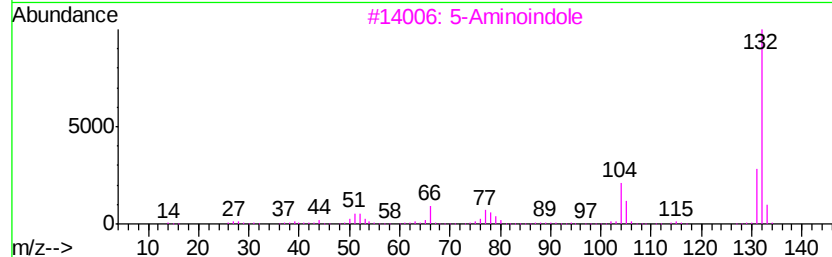
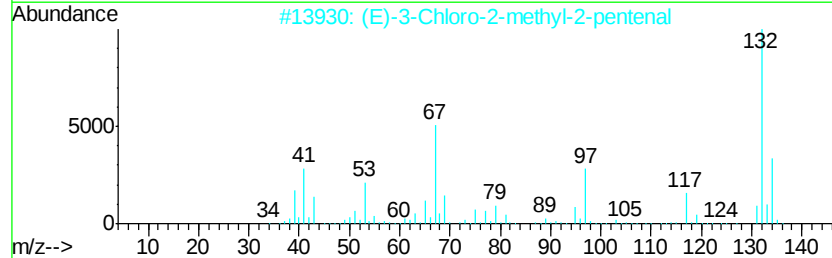
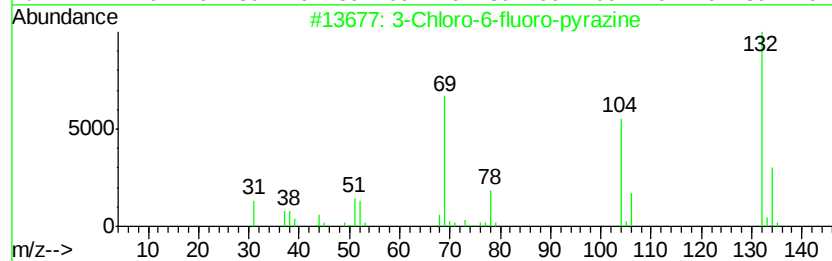
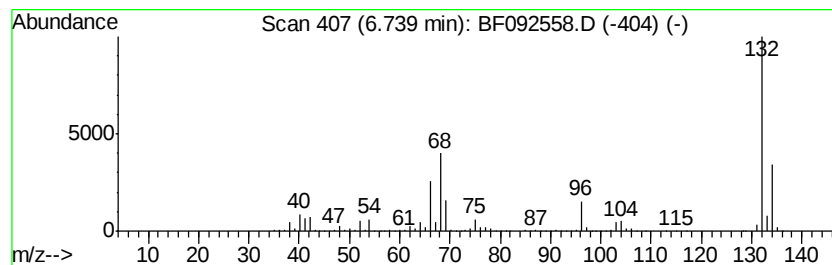
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	74.00 ng	4287220	1,4-Dichlorobenzene-d4	6.97

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-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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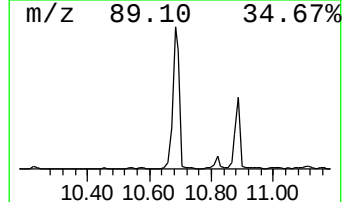
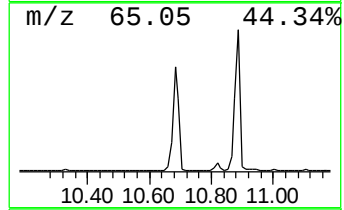
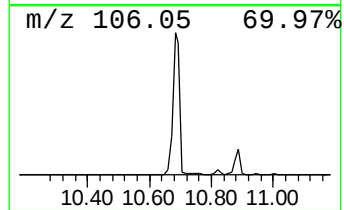
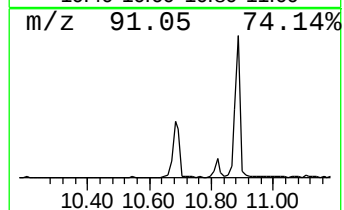
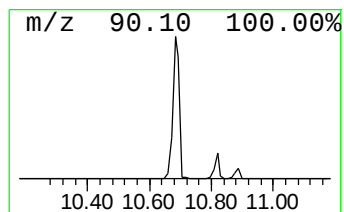
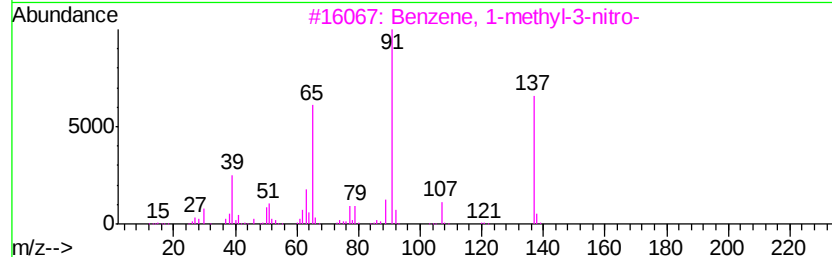
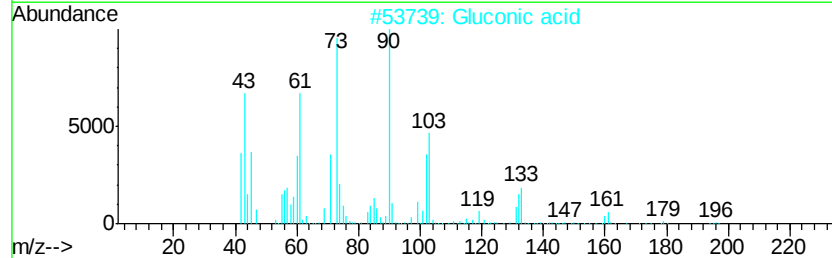
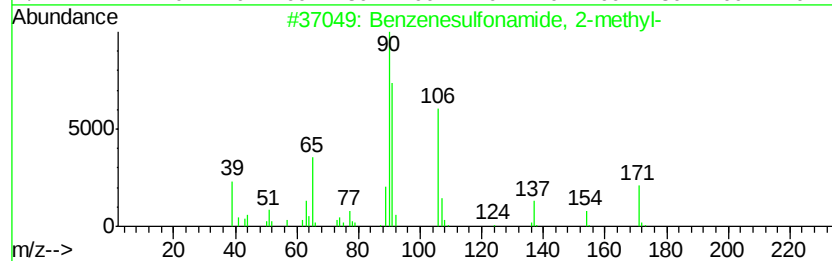
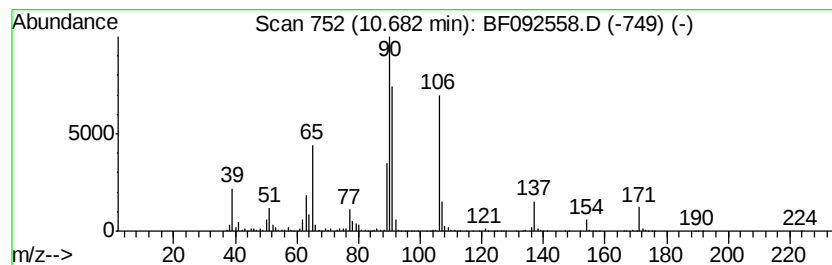
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzenesulfonamide, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	19.97 ng	1730100	Acenaphthene-d10	10.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzenesulfonamide, 2-methyl-	171 C7H9NO2S	000088-19-7 97
2		Gluconic acid	196 C6H12O7	000526-95-4 38
3		Benzene, 1-methyl-3-nitro-	137 C7H7NO2	000099-08-1 38
4		Benzenemethanesulfonamide	171 C7H9NO2S	004563-33-1 38
5		1,3,5-Norcaratriene	90 C7H6	004646-69-9 37



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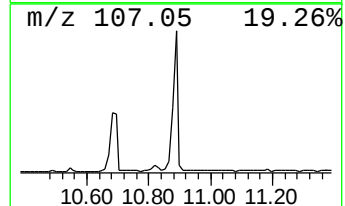
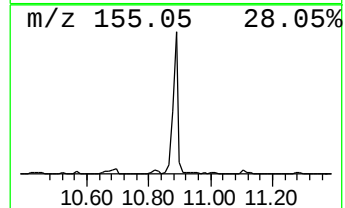
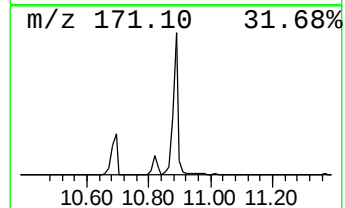
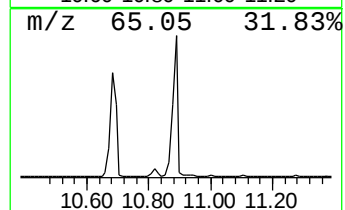
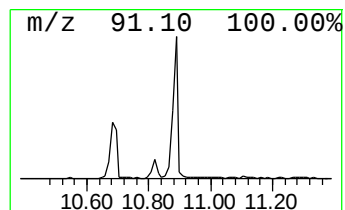
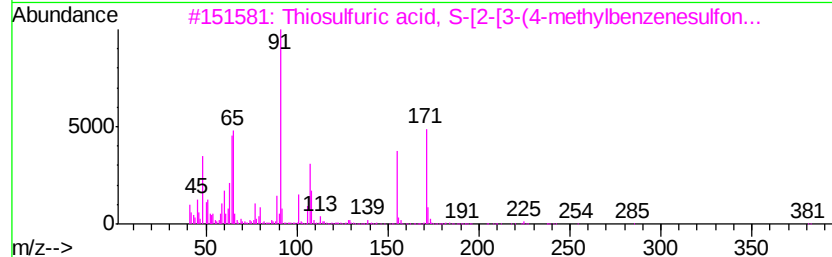
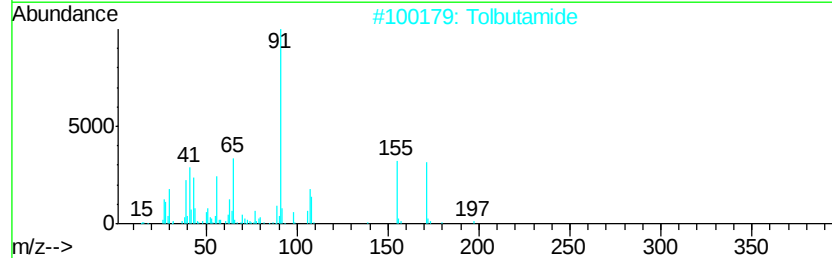
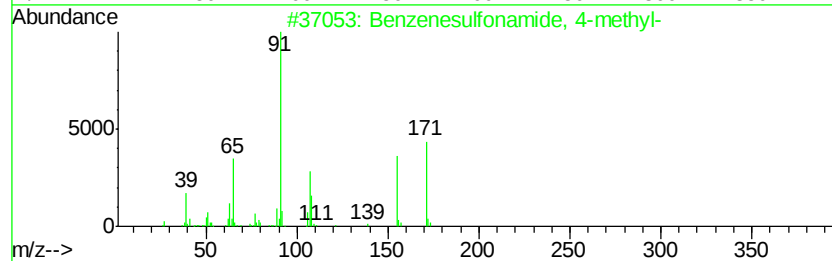
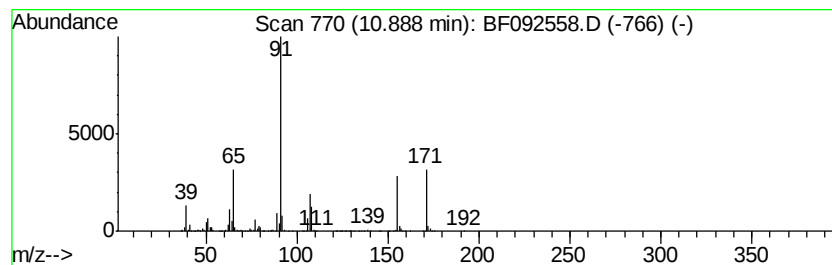
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Peak Number 5 Benzenesulfonamide, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.89	19.16 ng	1595780	Phenanthrene-d10	11.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	98
2		Tolbutamide	270	C12H18N2O3S	000064-77-7	91
3		Thiosulfuric acid, S-[2-[3-(4-methyl-...]	381	C12H19N3O5S3	1000255-60-3	80
4		O-p-toluenesulfonyl-N-acetylserine	315	C13H17NO6S	1000126-44-8	72
5		N-p-toluenesulfonyl-L-threonine,...	363	C18H21NO5S	1000130-34-4	58



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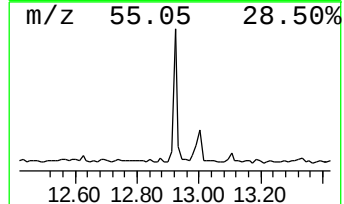
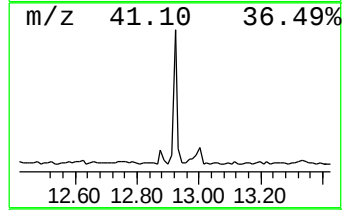
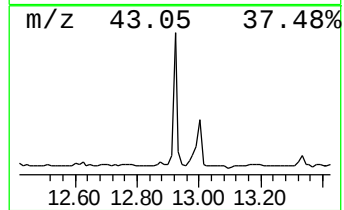
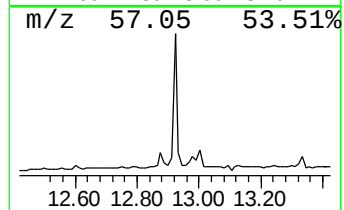
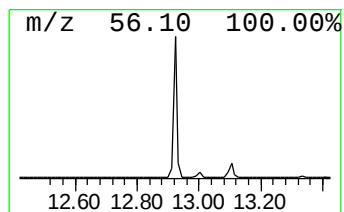
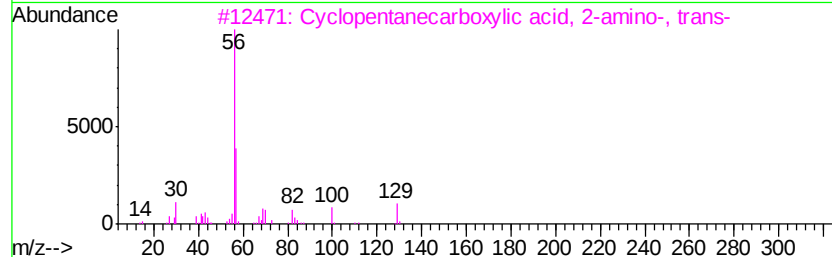
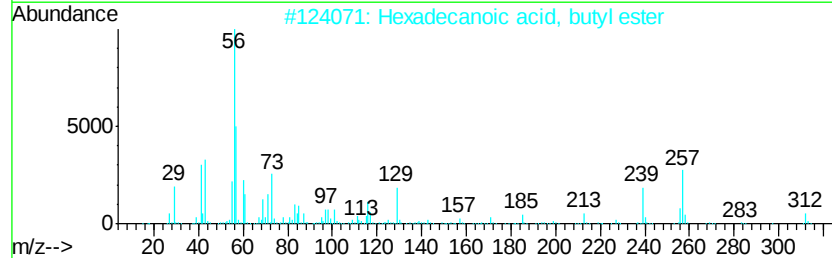
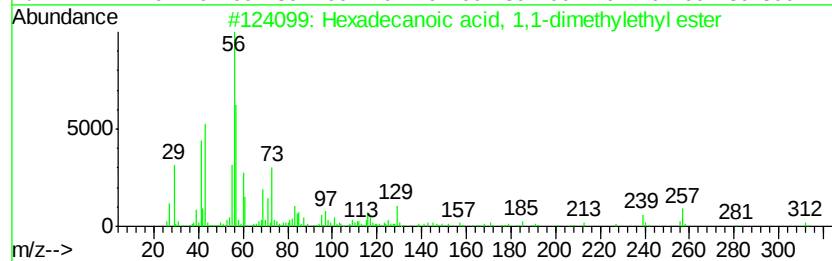
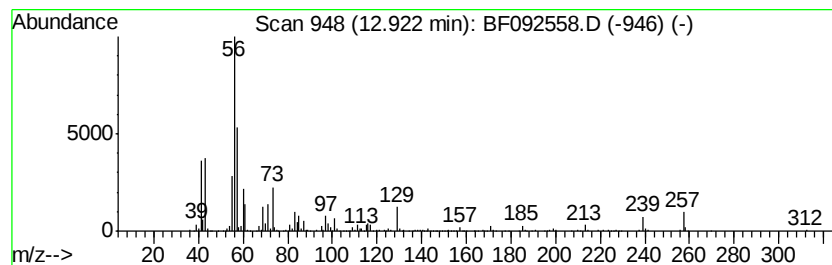
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.92	7.15 ng	487637	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	46
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5		Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092558.D
Acq On : 27 Jan 2017 6:32
Operator : SJ/MA
Sample : I1364-02
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-26

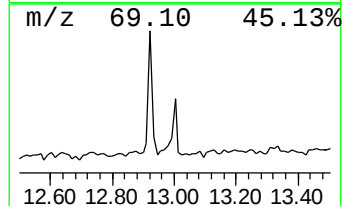
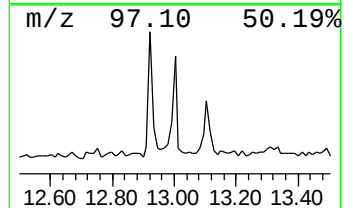
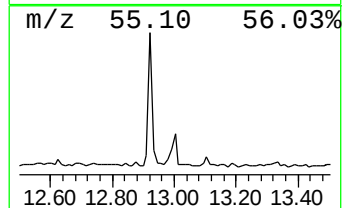
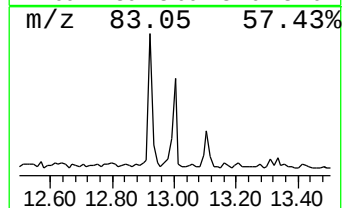
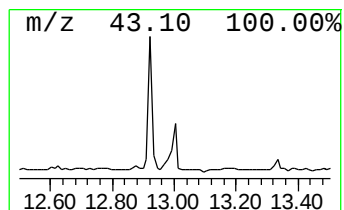
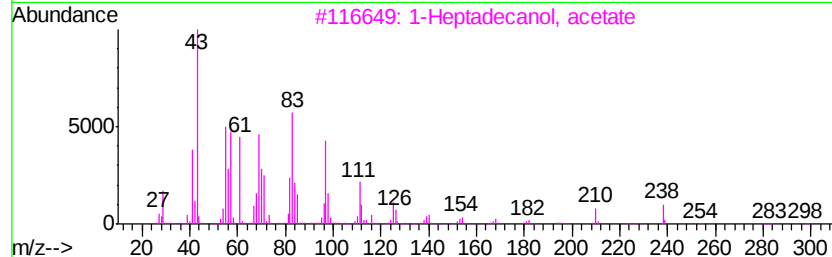
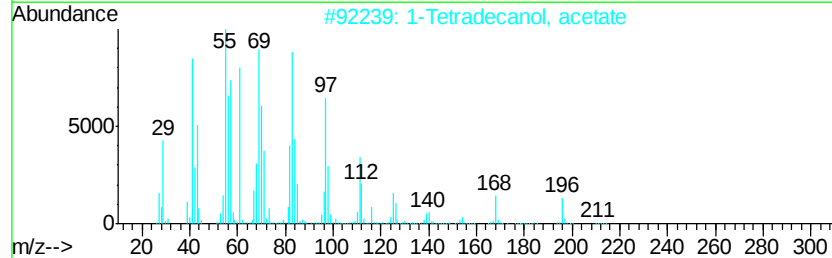
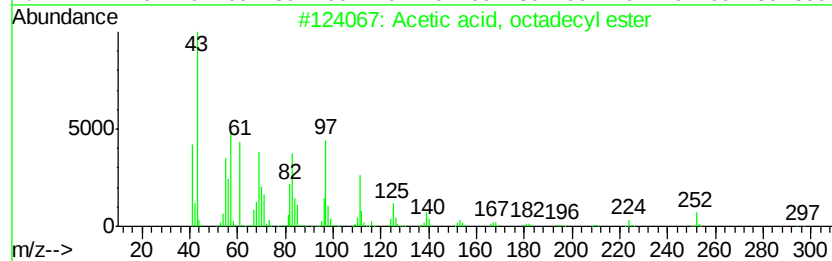
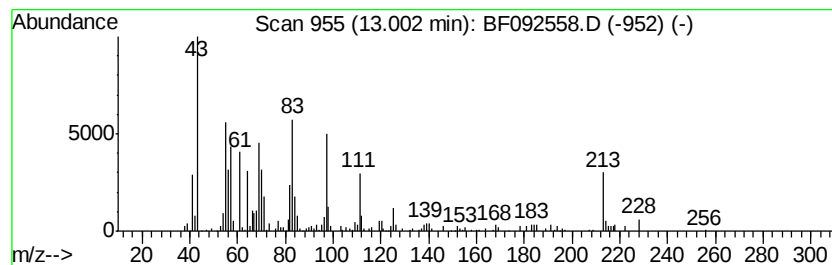
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Acetic acid, octadecyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.00	2.57 ng	175072	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	58
2		1-Tetradecanol, acetate	256	C16H32O2	000638-59-5	46
3		1-Heptadecanol, acetate	298	C19H38O2	000822-20-8	35
4		9-Octadecene, (E)-	252	C18H36	007206-25-9	25
5		Cyclotetradecane	196	C14H28	000295-17-0	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
Data File : BF092558.D
Acq On : 27 Jan 2017 6:32
Operator : SJ/MA
Sample : I1364-02
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-26

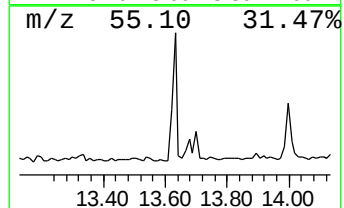
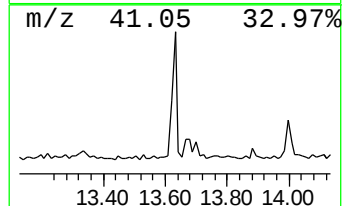
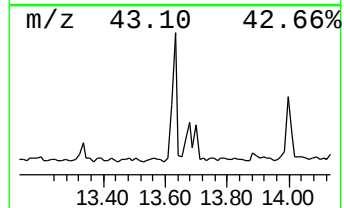
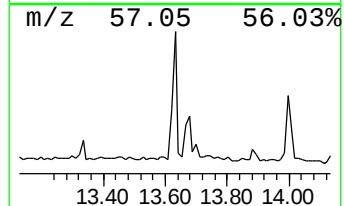
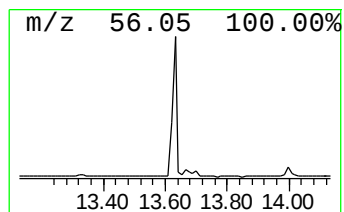
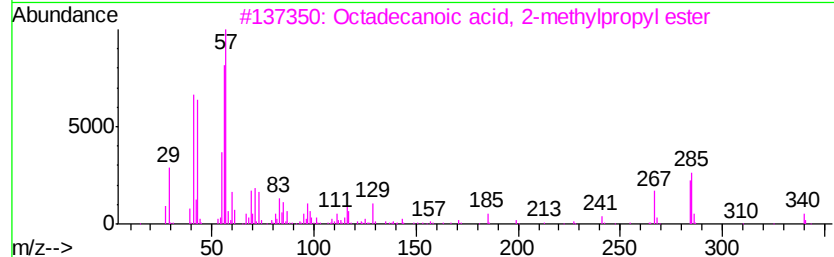
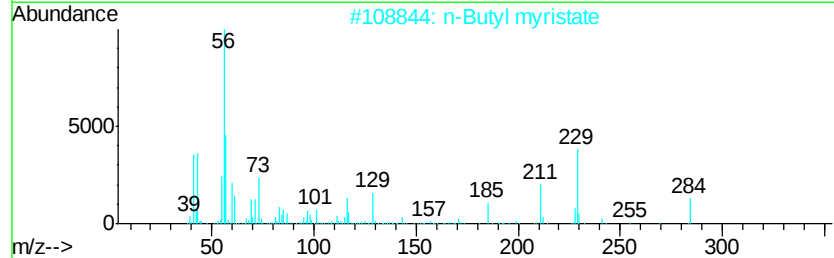
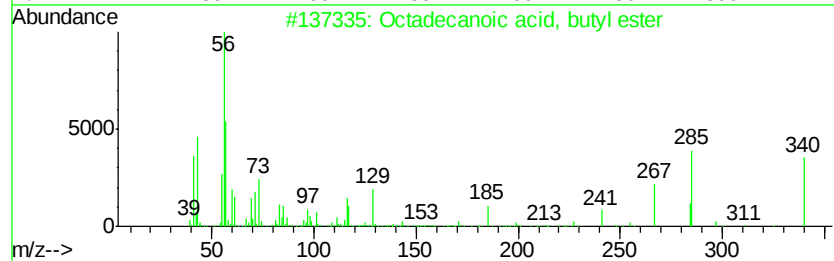
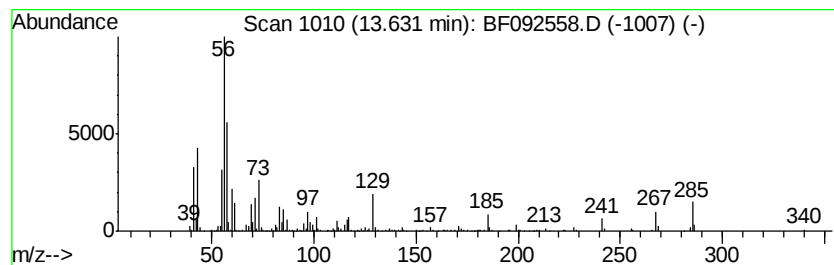
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	4.69 ng	320088	Chrysene-d12	14.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		n-Butyl myristate	284	C18H36O2	000110-36-1	83
3		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	46
4		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37
5		Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
Data File : BF092558.D
Acq On : 27 Jan 2017 6:32
Operator : SJ/MA
Sample : I1364-02
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-26

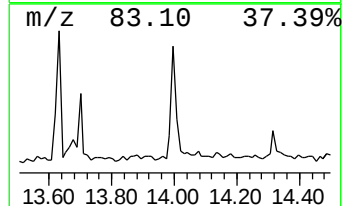
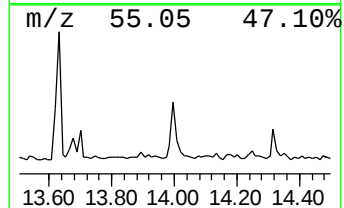
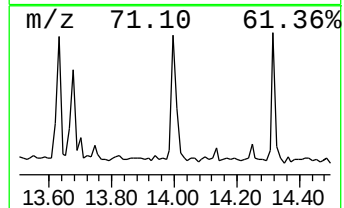
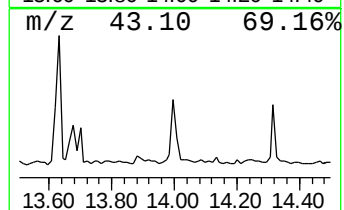
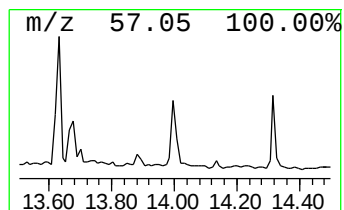
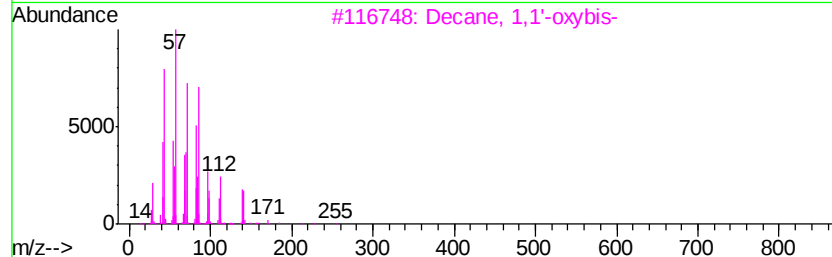
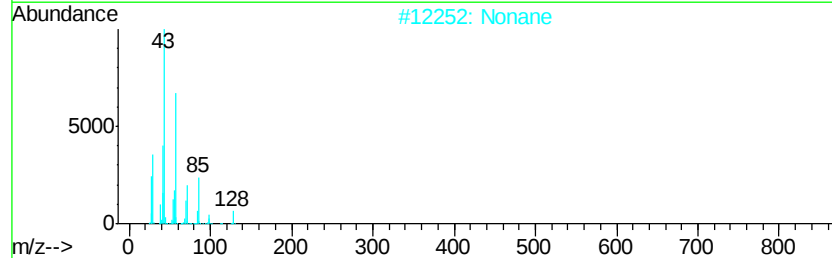
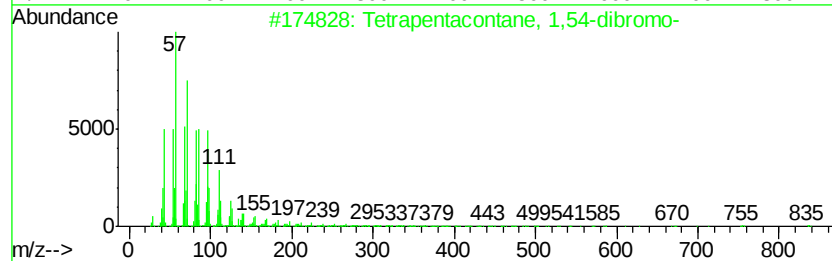
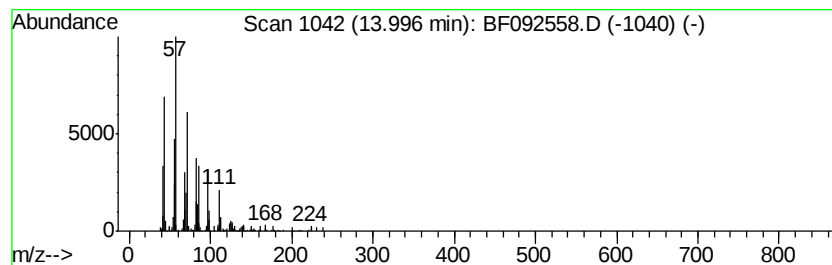
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetrapentacontane, 1,54-dib... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	2.88 ng	196694	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	80
2		Nonane	128	C9H20	000111-84-2	60
3		Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	58
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	49
5		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
Data File : BF092558.D
Acq On : 27 Jan 2017 6:32
Operator : SJ/MA
Sample : I1364-02
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-26

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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...	5.15	12.8	ng	738547	1	6.97	1158780	20.0
unknown6.74	6.74	74.0	ng	4287220	1	6.97	1158780	20.0
Benzenesulfonamid...	10.68	20.0	ng	1730100	3	10.03	1732700	20.0
Benzenesulfonamid...	10.89	19.2	ng	1595780	4	11.52	1665540	20.0
Hexadecanoic acid...	12.92	7.2	ng	487637	5	14.16	1363620	20.0
Acetic acid, octa...	13.00	2.6	ng	175072	5	14.16	1363620	20.0
Octadecanoic acid...	13.63	4.7	ng	320088	5	14.16	1363620	20.0
Tetrapentacontane...	14.00	2.9	ng	196694	5	14.16	1363620	20.0