

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
 Data File : BF082902.D
 Acq On : 13 Nov 2015 17:32
 Operator : UM/IZ
 Sample : G4362-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-14

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-BF110715.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	3.595	128	132	137	rBV	98264	189321	2.70%	0.385%
2	4.967	249	252	254	rVB	646051	851227	12.14%	1.731%
3	5.401	287	290	292	rBV	2976856	2696978	38.45%	5.486%
4	6.430	378	380	383	rBV	1527893	1986676	28.33%	4.041%
5	6.567	389	392	394	rBV	4074139	3563036	50.80%	7.247%
6	6.727	404	406	410	rBV	69444	78518	1.12%	0.160%
7	6.796	410	412	414	rBV	1520225	1254613	17.89%	2.552%
8	6.956	423	426	428	rBV	4866437	4294054	61.22%	8.734%
9	7.367	458	462	464	rBV	3398042	4257459	60.70%	8.659%
10	7.607	477	483	486	rVB3	39520	79517	1.13%	0.162%
11	7.824	501	502	504	rVB2	98082	97764	1.39%	0.199%
12	8.087	522	525	526	rVV	1756756	1653215	23.57%	3.363%
13	8.110	526	527	531	rVB2	73528	76677	1.09%	0.156%
14	8.396	550	552	554	rBV	168606	219718	3.13%	0.447%
15	8.636	572	573	578	rVB2	33062	79197	1.13%	0.161%
16	9.173	616	620	622	rVV	5620011	7013766	100.00%	14.266%
17	9.299	629	631	634	rVB2	49493	71606	1.02%	0.146%
18	9.562	649	654	656	rBV2	117236	143065	2.04%	0.291%
19	9.756	669	671	673	rBV	134255	150463	2.15%	0.306%
20	9.790	673	674	676	rVB	118003	83289	1.19%	0.169%
21	9.836	676	678	681	rBV	1717044	1832944	26.13%	3.728%
22	10.053	693	697	700	rVV4	75175	161578	2.30%	0.329%
23	10.282	716	717	719	rVB	112581	125047	1.78%	0.254%
24	10.476	733	734	736	rBV2	62018	84996	1.21%	0.173%
25	10.625	745	747	749	rVB	2827076	2686712	38.31%	5.465%
26	10.670	749	751	753	rVB	100154	89239	1.27%	0.182%
27	10.762	757	759	762	rVB	125969	157569	2.25%	0.320%
28	10.922	770	773	775	rVB4	36178	70489	1.01%	0.143%
29	11.196	795	797	799	rBV2	133932	167588	2.39%	0.341%
30	11.322	805	808	810	rBV	2062808	1837369	26.20%	3.737%
31	11.516	824	825	832	rVB2	54929	85588	1.22%	0.174%
32	11.699	839	841	846	rVB4	80478	110860	1.58%	0.225%
33	11.859	853	855	859	rBV2	282610	484291	6.90%	0.985%
34	12.373	898	900	902	rBV	70115	94391	1.35%	0.192%

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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-BF110715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.419	902	904	909	rVV3	67923	179063	2.55%	0.364%
36	12.556	914	916	918	rVV3	64309	106351	1.52%	0.216%
37	12.602	918	920	922	rVV	51101	82222	1.17%	0.167%
38	12.648	922	924	928	rVV	291889	324514	4.63%	0.660%
39	12.796	935	937	939	rVB	103233	126925	1.81%	0.258%
40	12.910	944	947	950	rVV	5474226	6413014	91.43%	13.044%
41	13.825	1024	1027	1033	rVB2	212247	371962	5.30%	0.757%
42	13.951	1036	1038	1041	rBV	1360049	1585616	22.61%	3.225%
43	15.368	1159	1162	1165	rBV	1041688	1220679	17.40%	2.483%
44	16.522	1254	1263	1280	rVB	314501	1788212	25.50%	3.637%
45	16.922	1295	1298	1305	rVB7	43560	137947	1.97%	0.281%

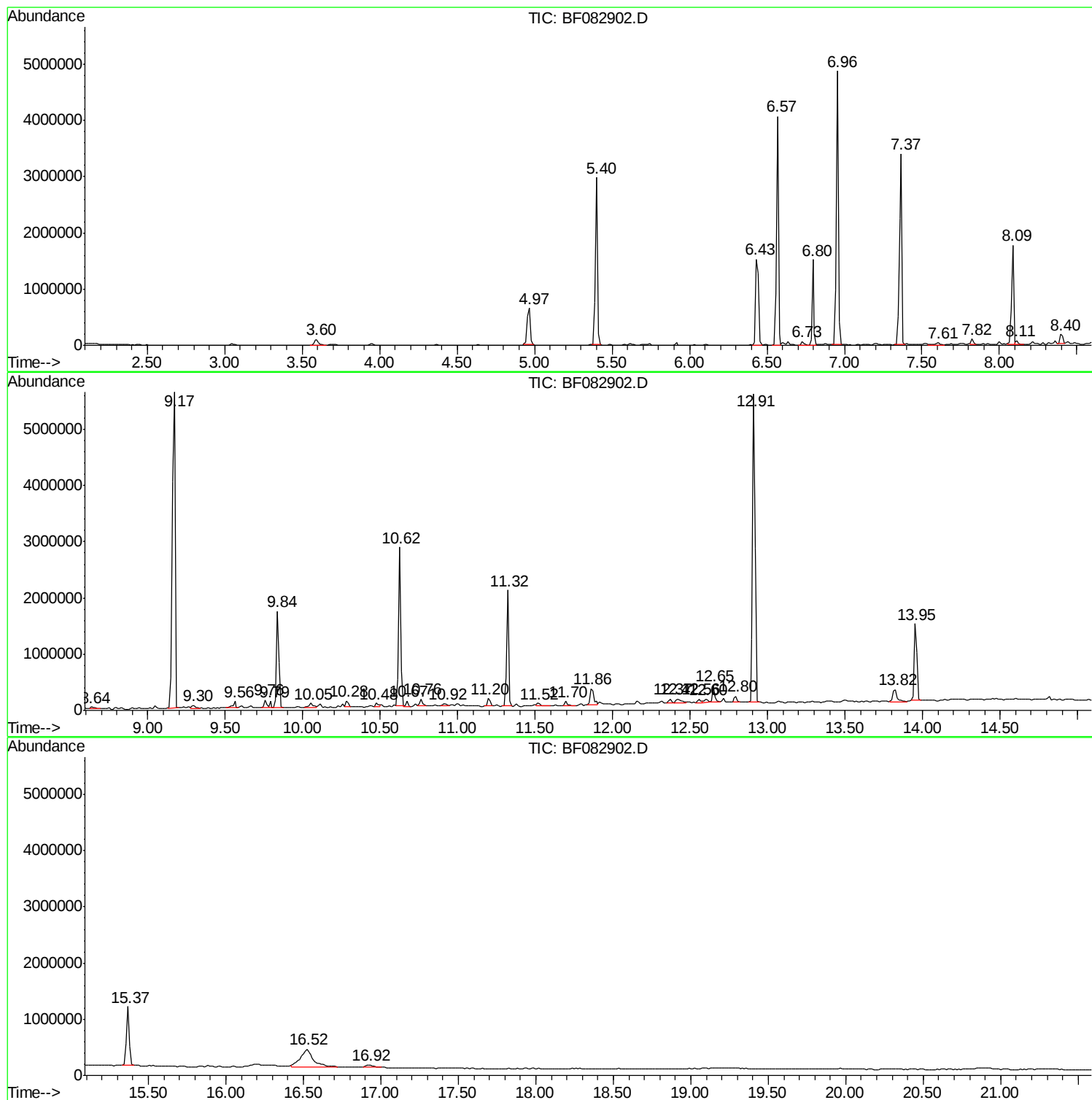
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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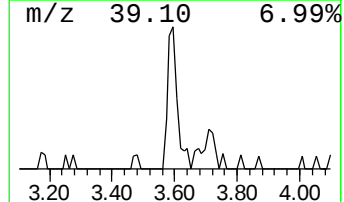
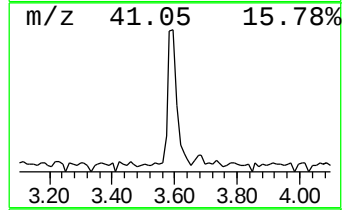
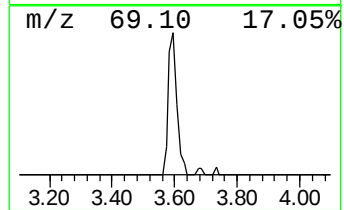
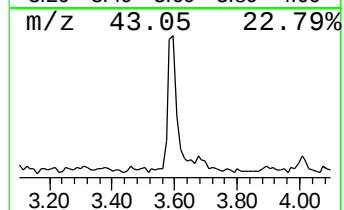
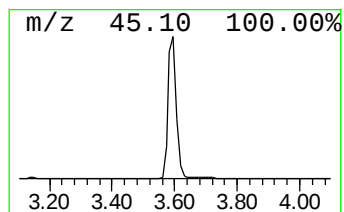
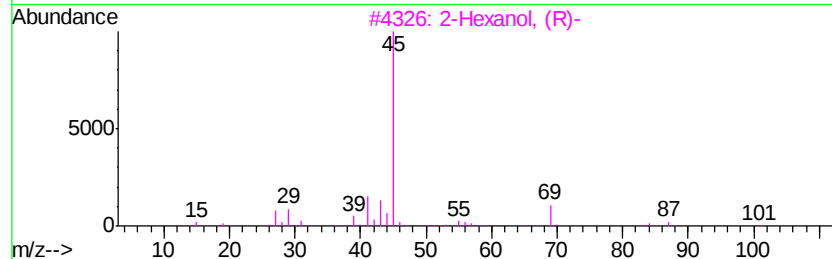
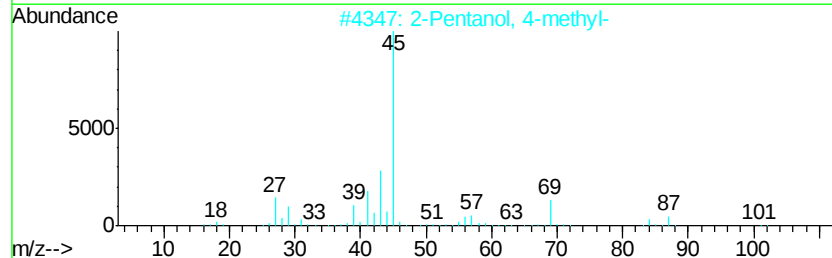
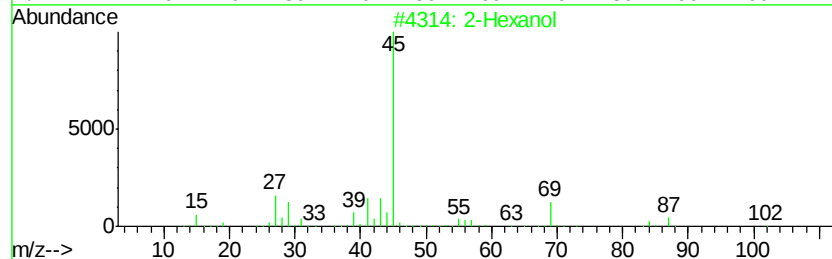
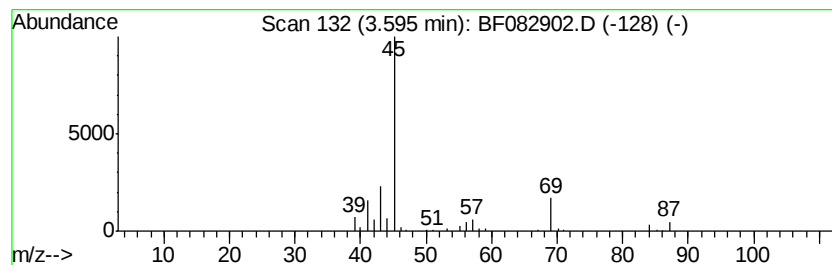
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Hexanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	3.02 ng	189321	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol	102	C6H14O	000626-93-7	83
2			2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	83
3			2-Hexanol, (R)-	102	C6H14O	026549-24-6	78
4			2-Hexanol, (S)-	102	C6H14O	052019-78-0	64
5			2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	50



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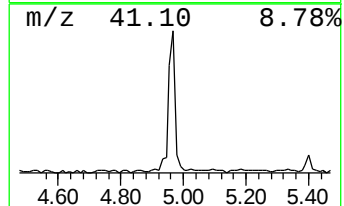
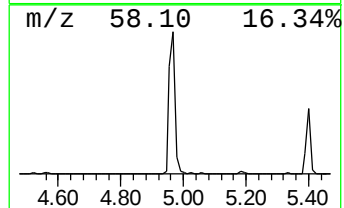
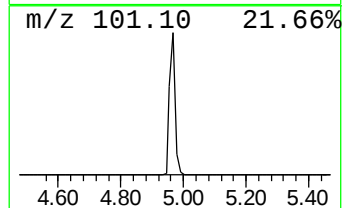
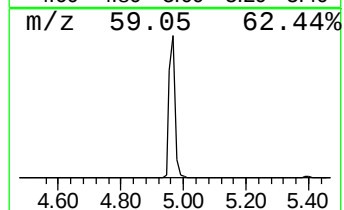
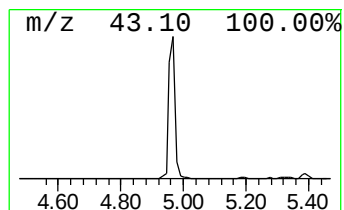
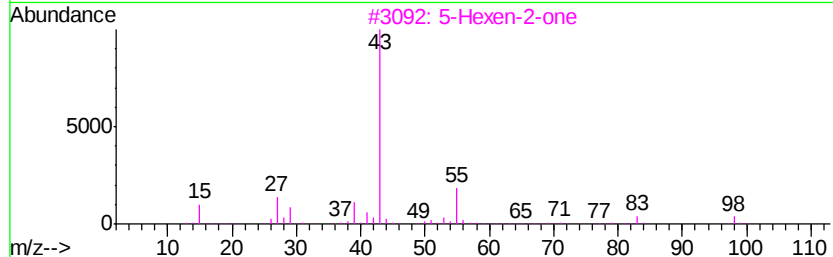
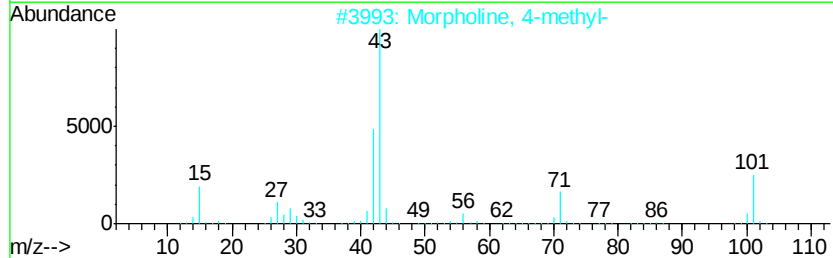
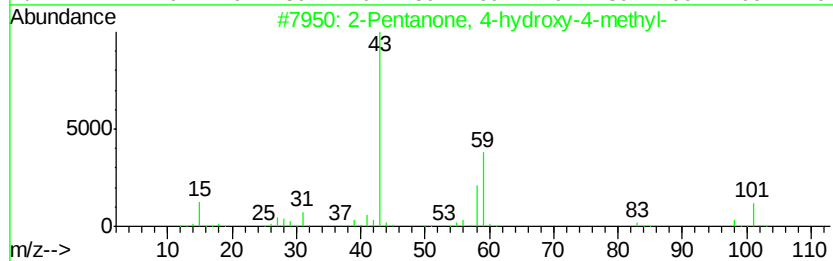
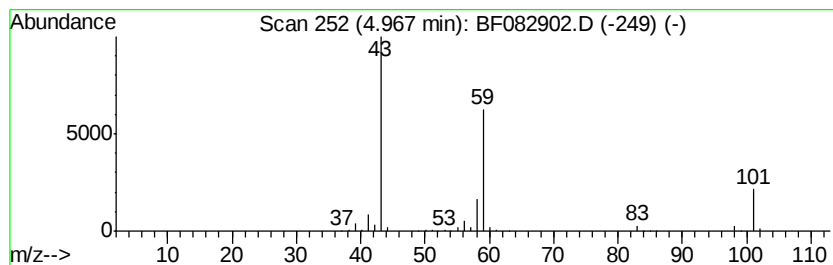
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	13.57 ng	851227	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Acetone	58	C3H6O	000067-64-1	9
5		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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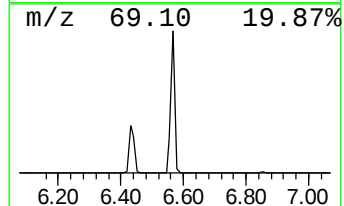
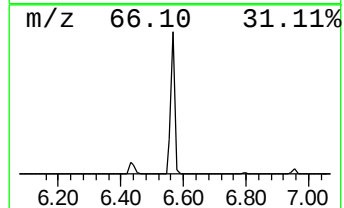
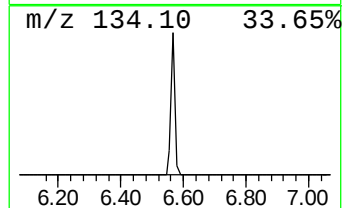
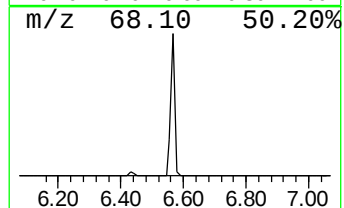
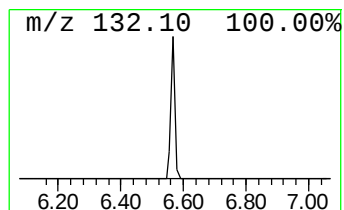
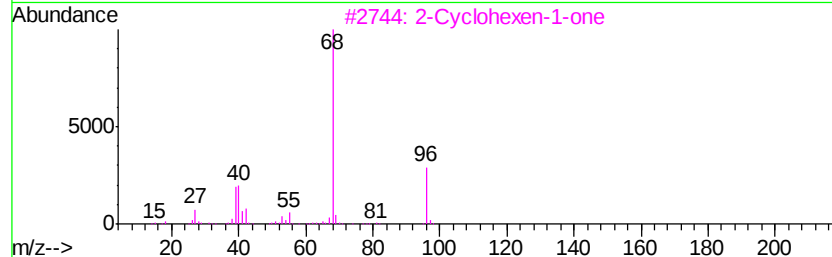
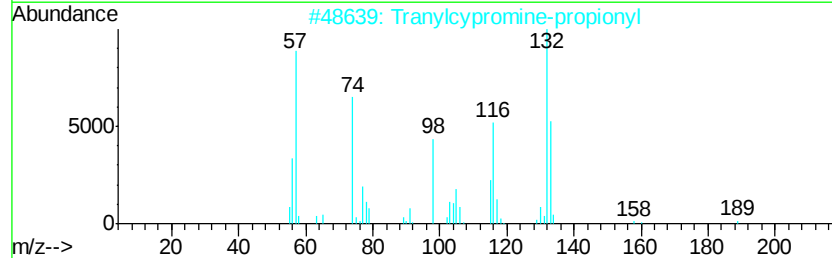
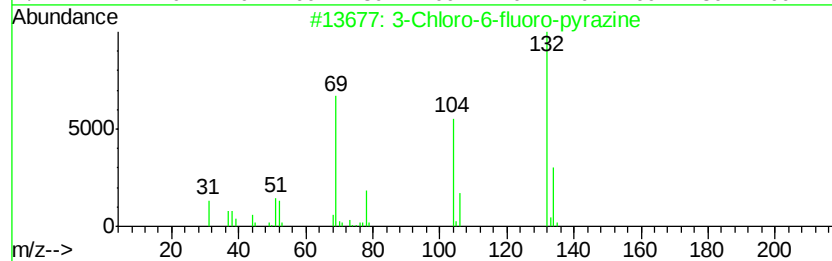
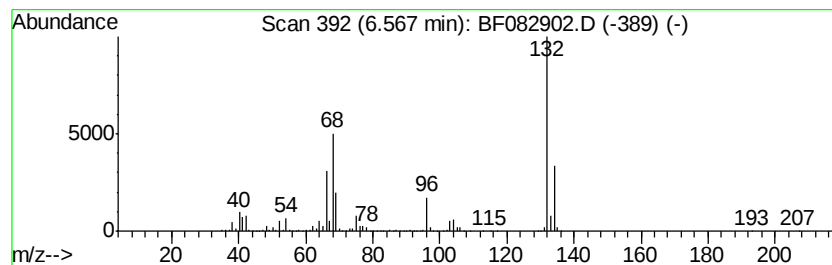
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	56.80 ng	3563040	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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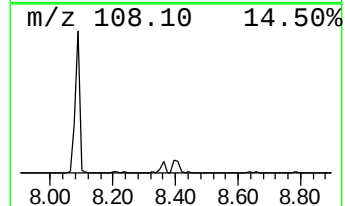
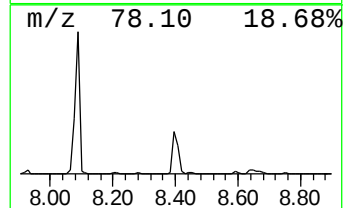
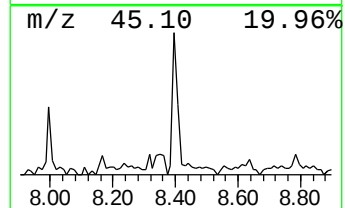
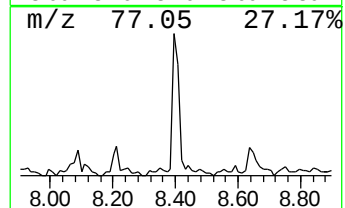
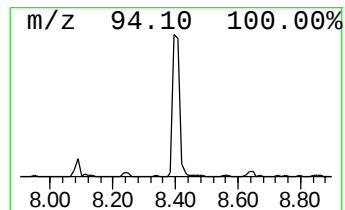
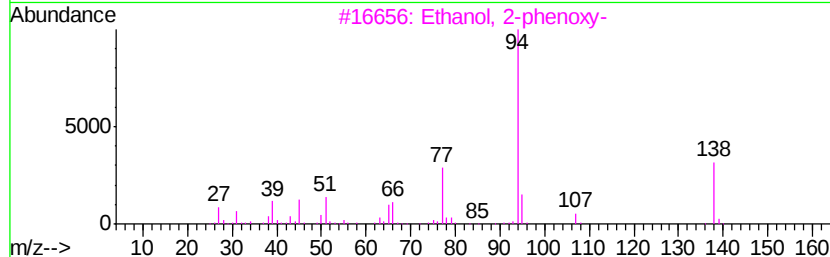
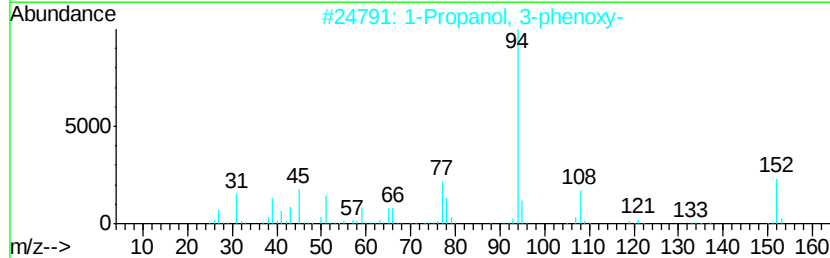
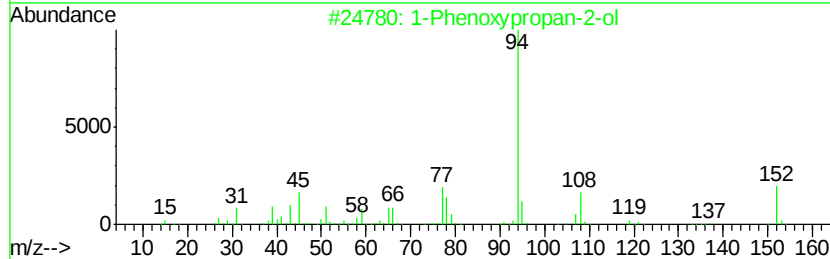
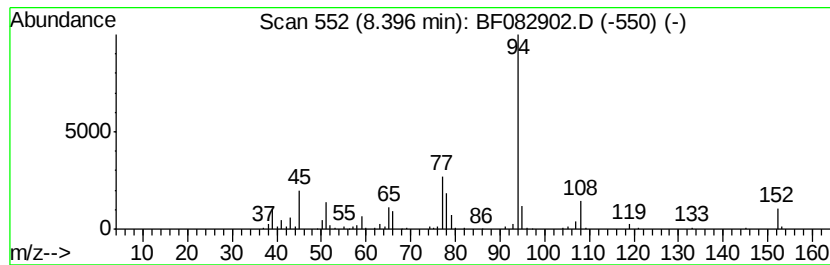
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	2.66 ng	219718	Napthalene-d8	8.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	90
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	86
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Benzene, (1-methylpropoxy)-	150	C10H14O	010574-17-1	50
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	50



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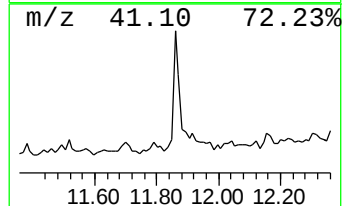
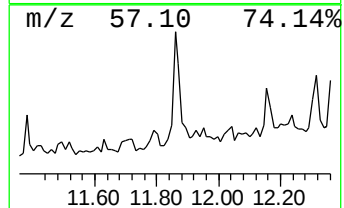
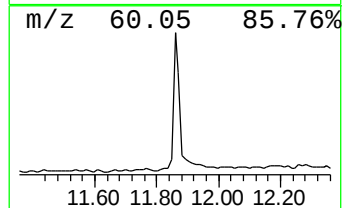
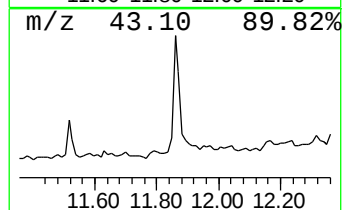
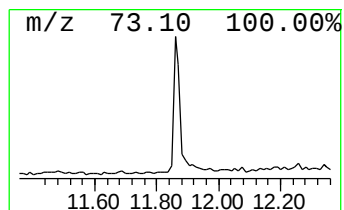
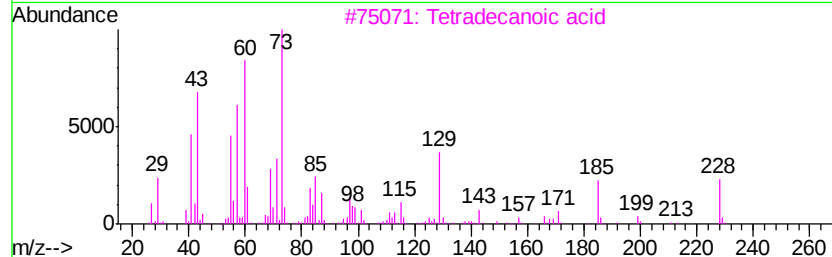
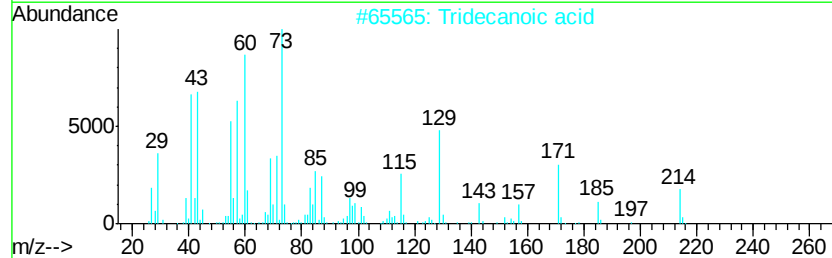
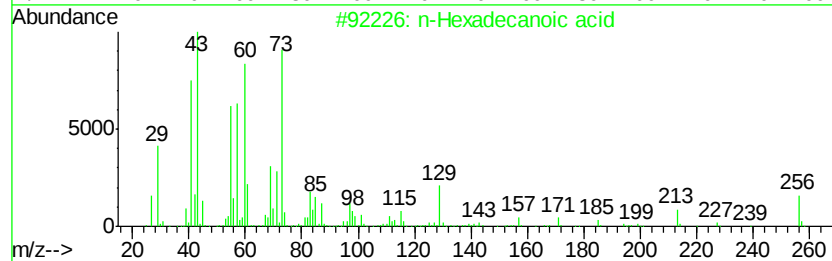
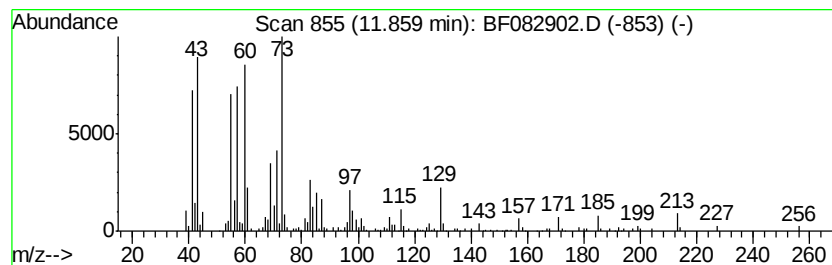
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.86	5.27 ng	484291	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5	Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111315\
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Acq On : 13 Nov 2015 17:32
Operator : UM/IZ
Sample : G4362-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

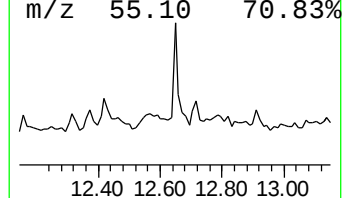
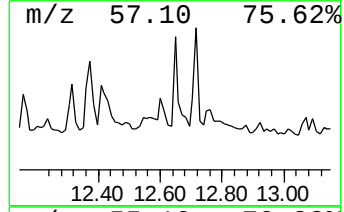
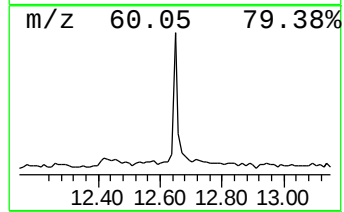
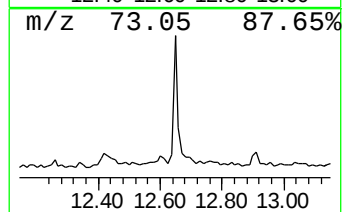
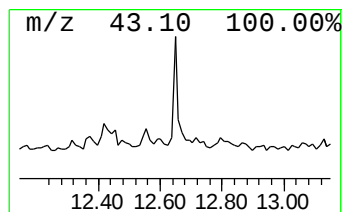
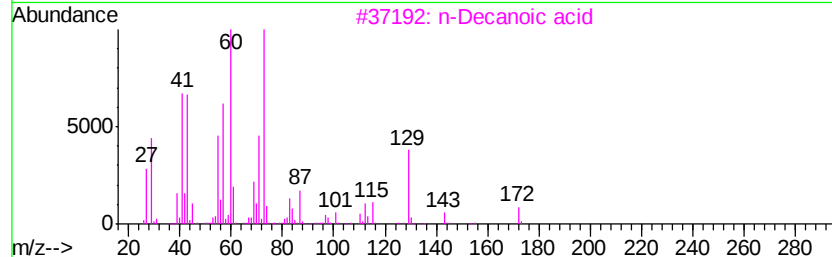
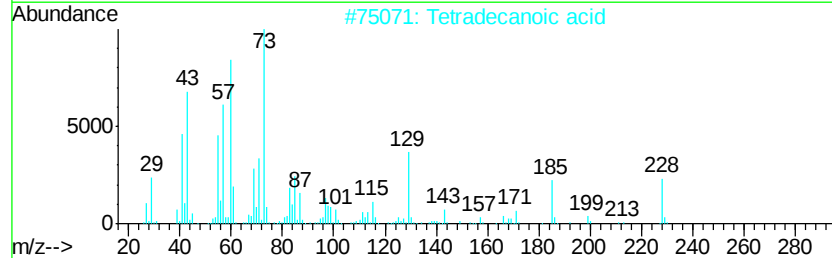
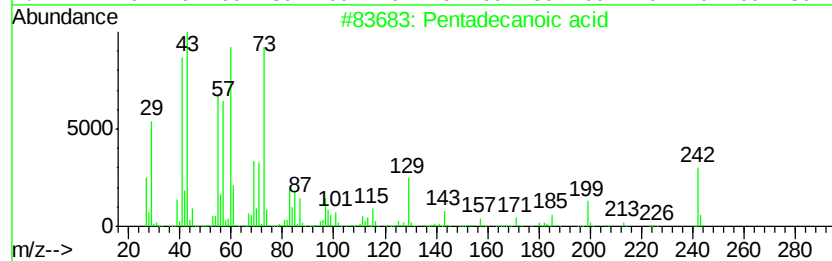
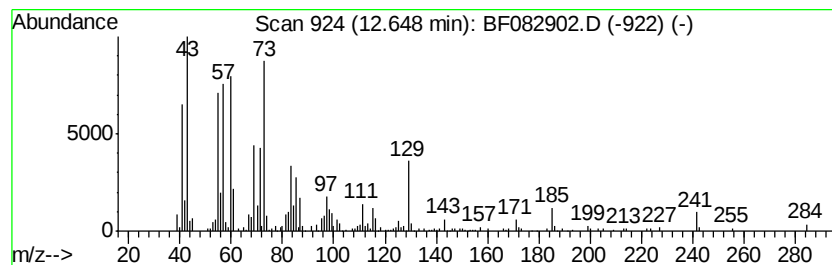
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	4.09 ng	324514	Chrysene-d12	13.95
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pentadecanoic acid	242 C15H30O2	001002-84-2 81
2		Tetradecanoic acid	228 C14H28O2	000544-63-8 80
3		n-Decanoic acid	172 C10H20O2	000334-48-5 70
4		Tridecanoic acid	214 C13H26O2	000638-53-9 64
5		Amyl Nitrite	117 C5H11NO2	000110-46-3 27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111315\
Data File : BF082902.D
Acq On : 13 Nov 2015 17:32
Operator : UM/IZ
Sample : G4362-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-14

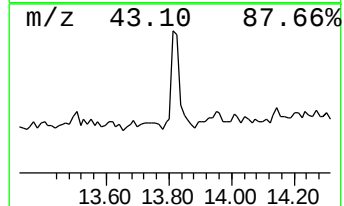
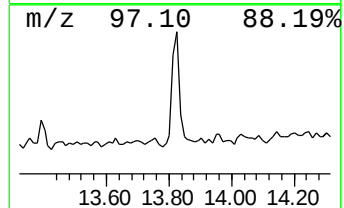
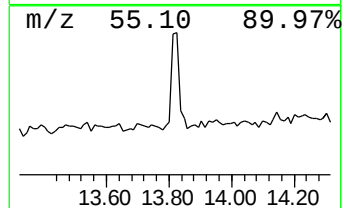
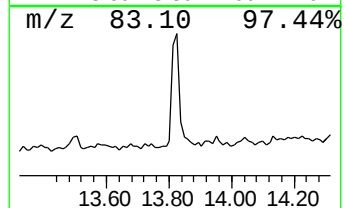
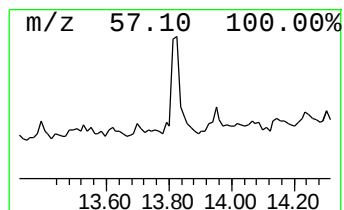
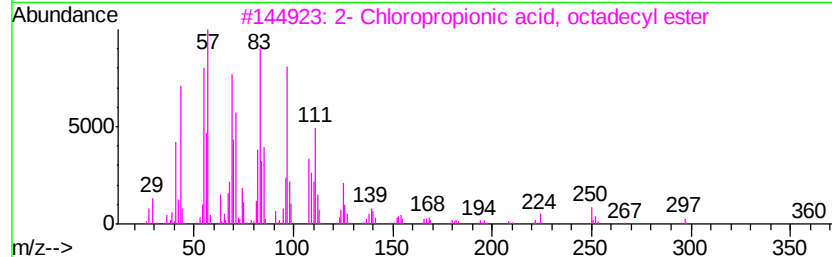
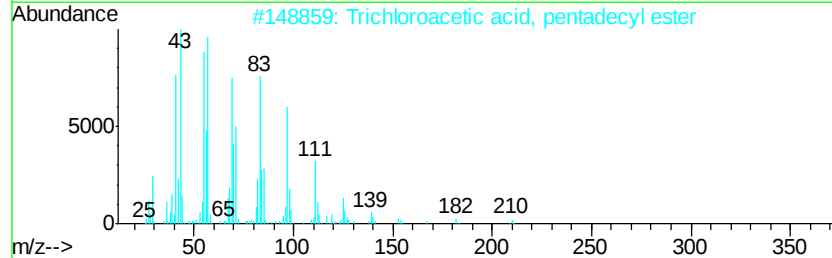
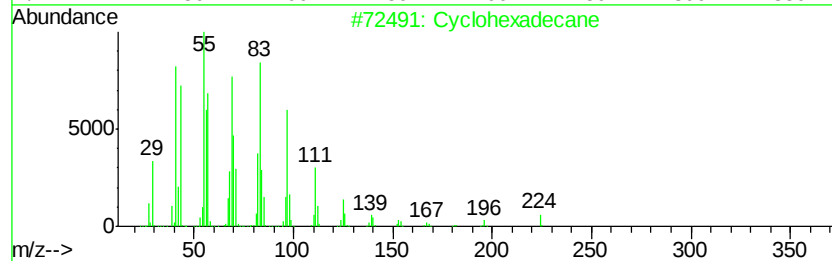
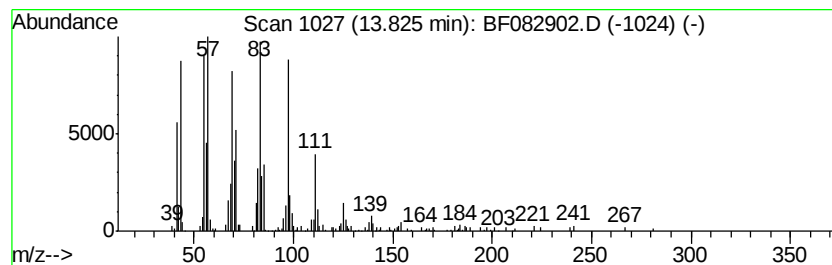
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	4.69 ng	371962	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexadecane	224	C16H32	000295-65-8	93
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
3		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	87
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81



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Operator : UM/IZ
Sample : G4362-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-14

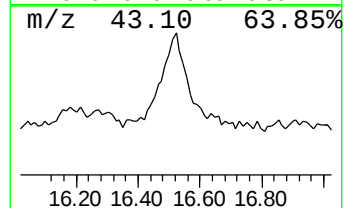
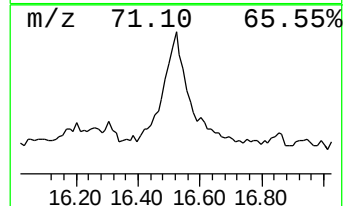
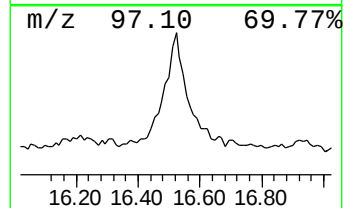
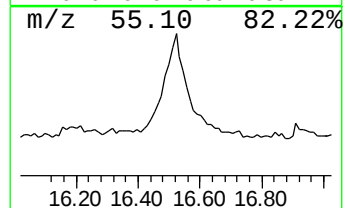
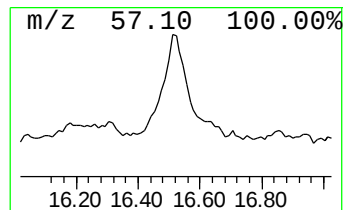
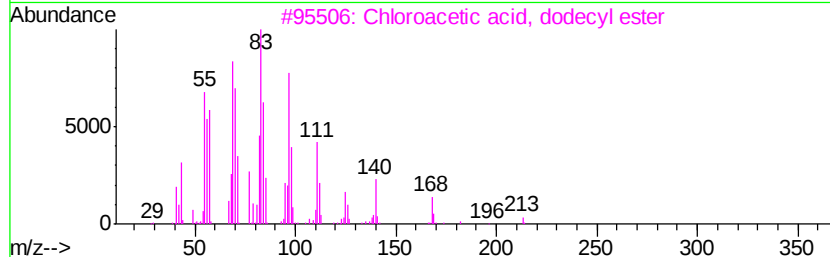
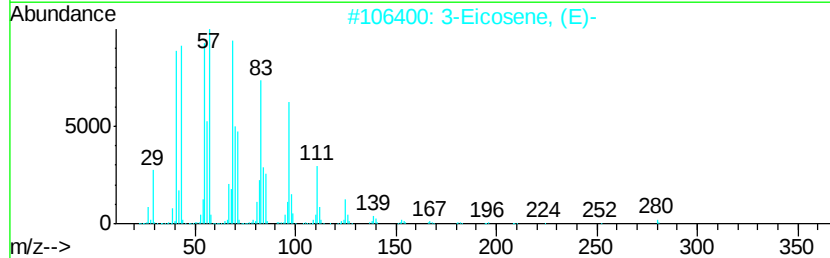
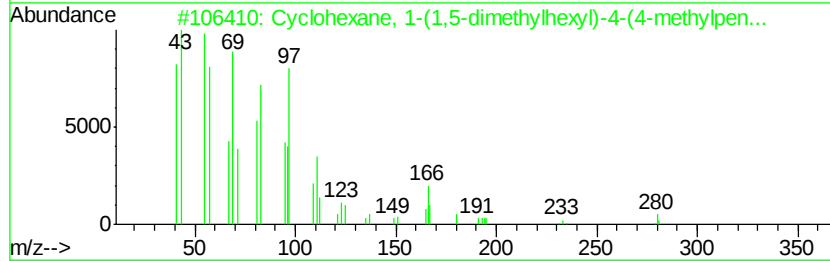
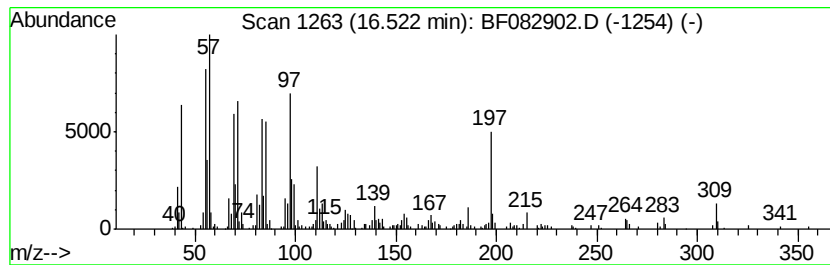
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclohexane, 1-(1,5-dimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.52	29.30 ng	1788210	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-(1,5-dimethylhexyl)-4-(4-methylphenyl)-	280	C20H40	056009-20-2	50
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	45
3		Chloroacetic acid, dodecyl ester	262	C14H27ClO2	006316-04-7	43
4		5-Eicosene, (E)-	280	C20H40	074685-30-6	38
5		Docosane	310	C22H46	000629-97-0	38



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Acq On : 13 Nov 2015 17:32
Operator : UM/IZ
Sample : G4362-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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-Hexanol	3.60	3.0	ng	189321	1	6.80	1254610	20.0
2-Pentanone, 4-hy...	4.97	13.6	ng	851227	1	6.80	1254610	20.0
unknown6.57	6.57	56.8	ng	3563040	1	6.80	1254610	20.0
1-Phenoxypropan-2-ol	8.40	2.7	ng	219718	2	8.09	1653220	20.0
n-Hexadecanoic acid	11.86	5.3	ng	484291	4	11.32	1837370	20.0
Pentadecanoic acid	12.65	4.1	ng	324514	5	13.95	1585620	20.0
Cyclohexadecane	13.82	4.7	ng	371962	5	13.95	1585620	20.0
Cyclohexane, 1-(1...	16.52	29.3	ng	1788210	6	15.37	1220680	20.0