

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100217\
 Data File : BF099006.D
 Acq On : 2 Oct 2017 18:15
 Operator : SJ/JU
 Sample : I5534-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-ENV-114-1(5-10)

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-BF092317.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	2.210	16	21	28	rVB	124829	158970	6.12%	0.662%
2	5.128	514	517	528	rVB	363254	449665	17.32%	1.874%
3	5.522	579	584	587	rBV	2567994	2452345	94.47%	10.220%
4	6.528	750	755	758	rBV	2463993	2384976	91.88%	9.939%
5	6.669	775	779	783	rBV	2575575	2528395	97.40%	10.537%
6	6.904	815	819	822	rBV	890771	792626	30.53%	3.303%
7	7.057	841	845	848	rBV	2241903	1917766	73.88%	7.992%
8	7.463	909	914	917	rBV	1665179	1528639	58.89%	6.370%
9	7.540	923	927	933	rBV	52677	62926	2.42%	0.262%
10	8.181	1032	1036	1040	rBV	1069995	993734	38.28%	4.141%
11	9.257	1214	1219	1222	rBV	2955299	2595877	100.00%	10.818%
12	9.651	1282	1286	1289	rBV	421313	370566	14.28%	1.544%
13	9.939	1331	1335	1339	rBV2	1185582	985732	37.97%	4.108%
14	10.363	1404	1407	1409	rVB	42435	34831	1.34%	0.145%
15	10.728	1465	1469	1479	rVB	1331717	1162781	44.79%	4.846%
16	10.833	1484	1487	1491	rBV	62593	68740	2.65%	0.286%
17	11.280	1560	1563	1565	rBV	40059	29297	1.13%	0.122%
18	11.310	1565	1568	1575	rVB4	33098	33963	1.31%	0.142%
19	11.427	1584	1588	1591	rBV	996197	837844	32.28%	3.492%
20	11.939	1671	1675	1680	rBV4	25451	39582	1.52%	0.165%
21	12.639	1791	1794	1797	rBV	78411	60036	2.31%	0.250%
22	12.686	1799	1802	1806	rVB	93969	78144	3.01%	0.326%
23	12.869	1828	1833	1836	rBV	74573	72115	2.78%	0.301%
24	13.010	1853	1857	1865	rVB	2037350	1788037	68.88%	7.451%
25	13.480	1933	1937	1941	rVB	37539	38985	1.50%	0.162%
26	13.898	2004	2008	2018	rVB	129212	164633	6.34%	0.686%
27	14.033	2028	2031	2033	rBV	231492	194573	7.50%	0.811%
28	14.069	2033	2037	2040	rVB	700180	670026	25.81%	2.792%
29	14.216	2059	2062	2066	rBV2	31396	37114	1.43%	0.155%
30	14.521	2111	2114	2118	rBV	118421	118526	4.57%	0.494%
31	14.680	2139	2141	2145	rBV	80808	75927	2.92%	0.316%
32	14.916	2177	2181	2186	rBV2	65100	87785	3.38%	0.366%
33	15.027	2197	2200	2204	rVB	48479	53748	2.07%	0.224%
34	15.115	2212	2215	2218	rBV	34700	47845	1.84%	0.199%

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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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.174	2223	2225	2229	rVB	38400	33303	1.28%	0.139%
36	15.321	2247	2250	2257	rVB	85757	117314	4.52%	0.489%
37	15.486	2276	2278	2283	rVB	24426	29444	1.13%	0.123%
38	15.557	2285	2290	2298	rVB	609192	785642	30.26%	3.274%
39	16.010	2363	2367	2372	rVB2	35966	55306	2.13%	0.230%
40	16.515	2449	2453	2460	rBV5	27583	58638	2.26%	0.244%

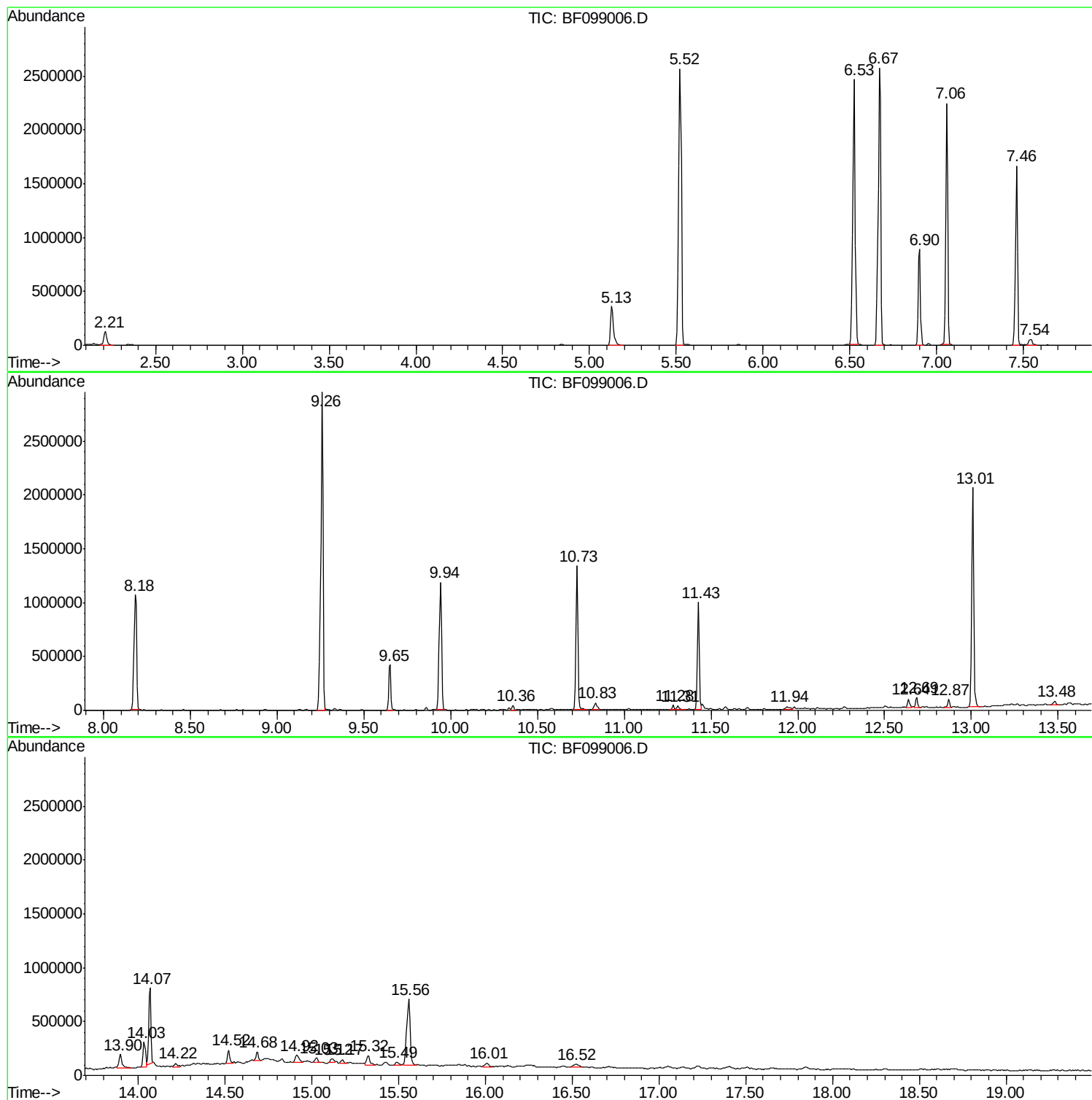
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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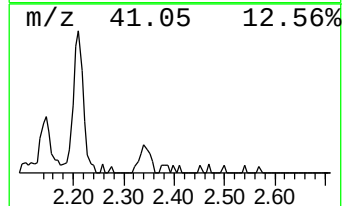
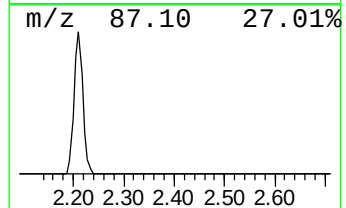
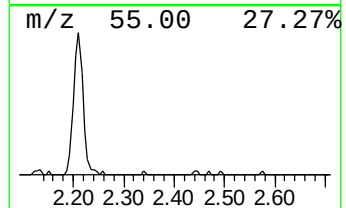
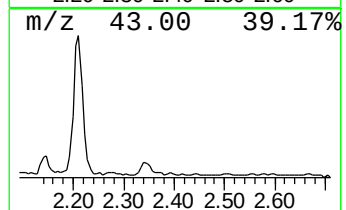
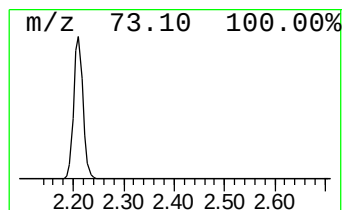
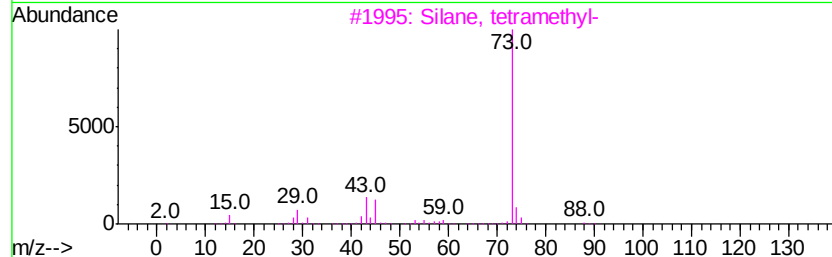
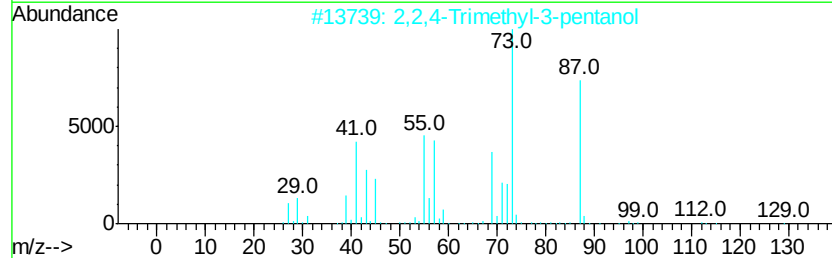
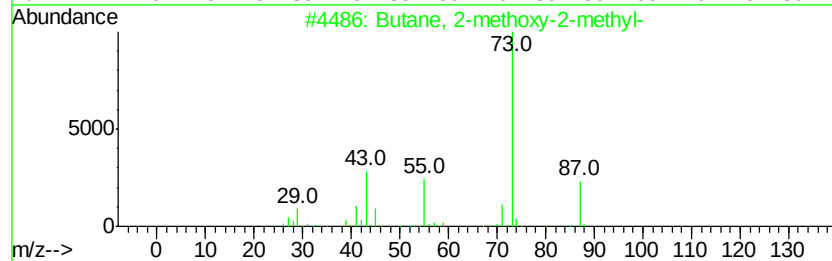
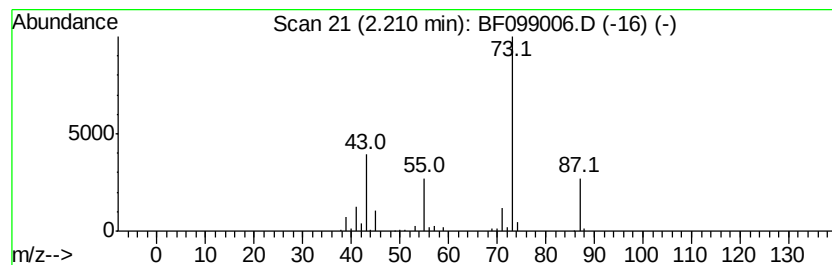
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	4.01 ng	158970	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25



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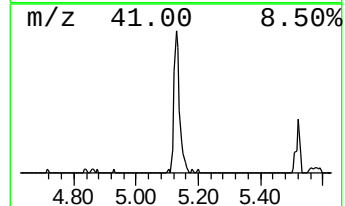
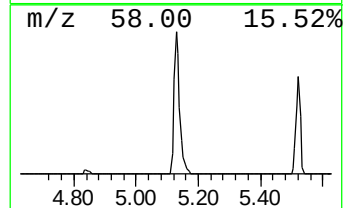
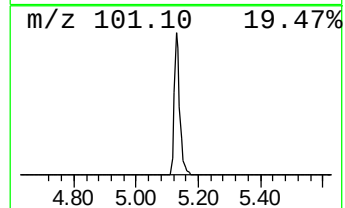
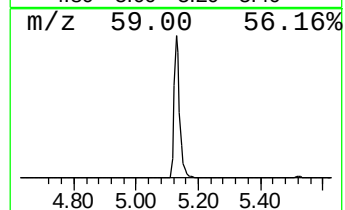
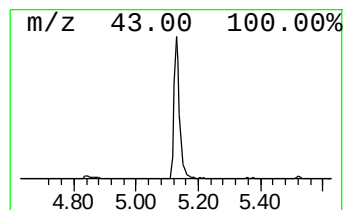
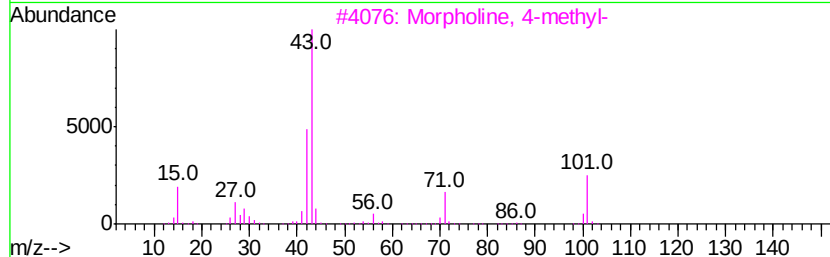
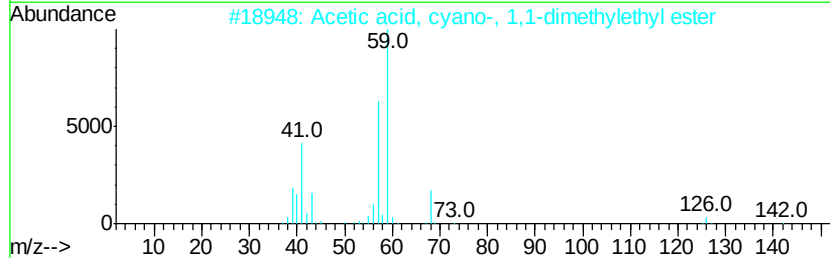
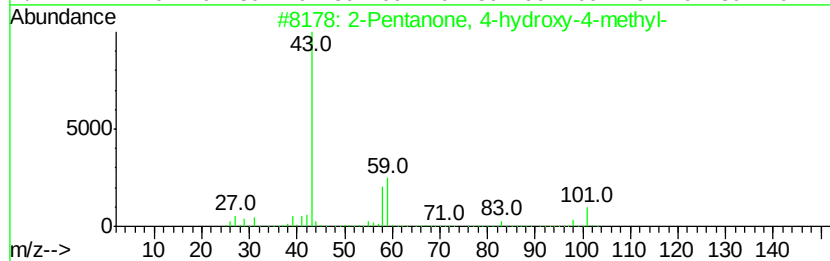
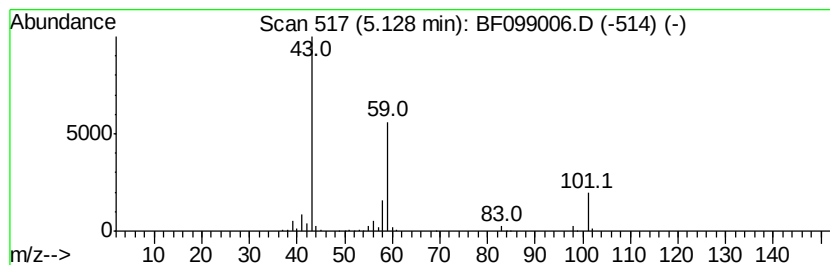
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	11.35 ng	449665	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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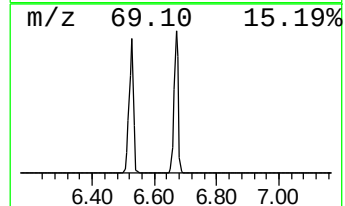
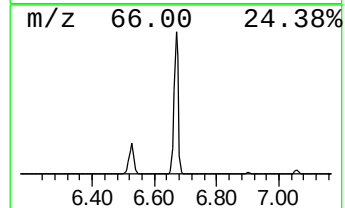
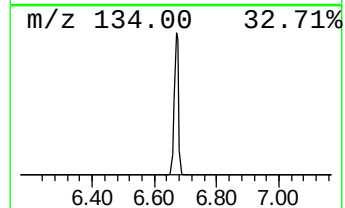
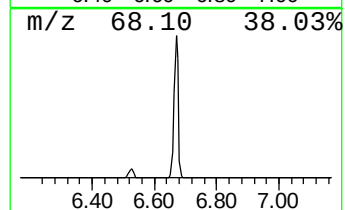
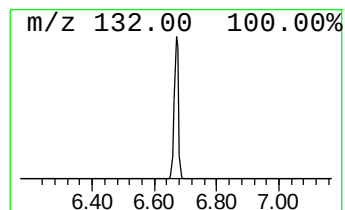
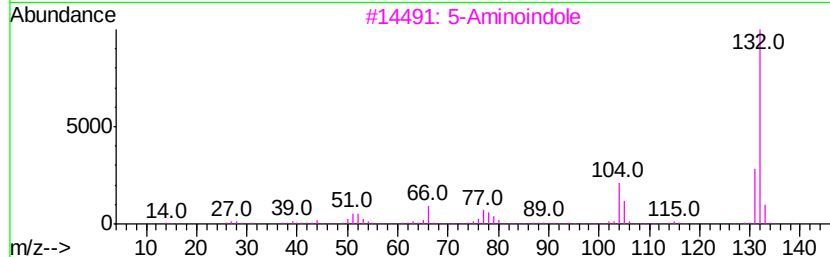
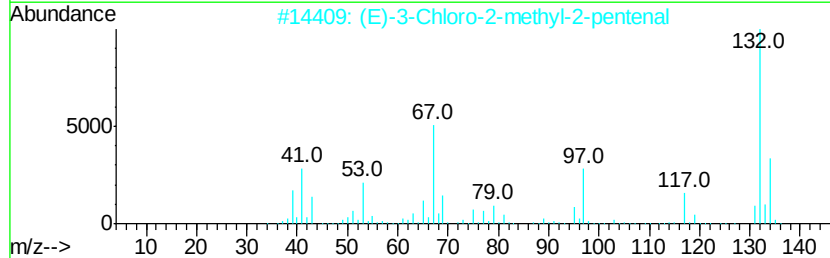
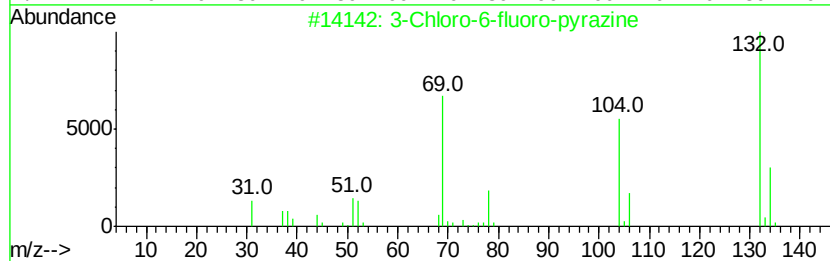
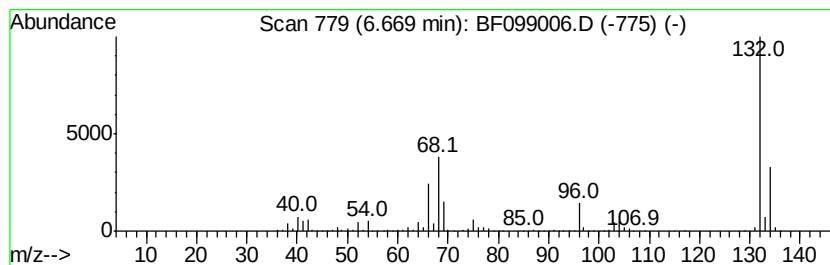
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	63.80 ng	2528400	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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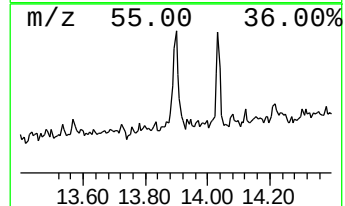
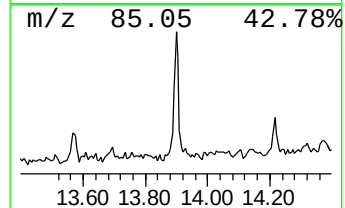
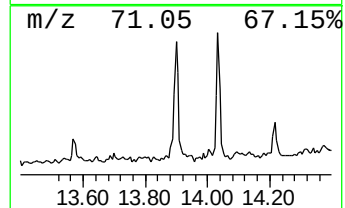
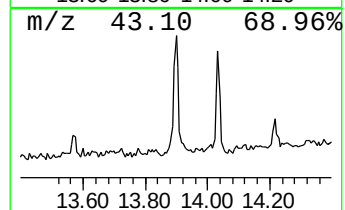
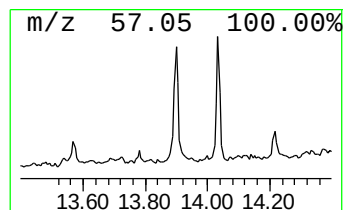
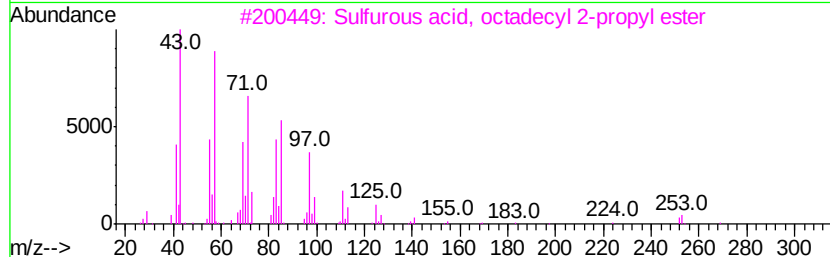
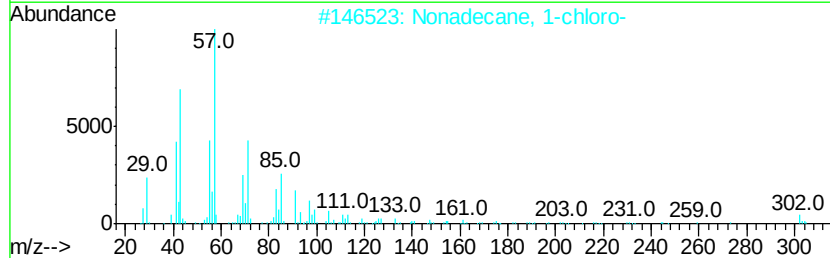
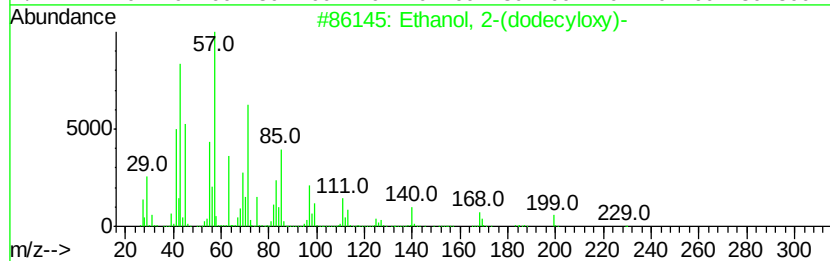
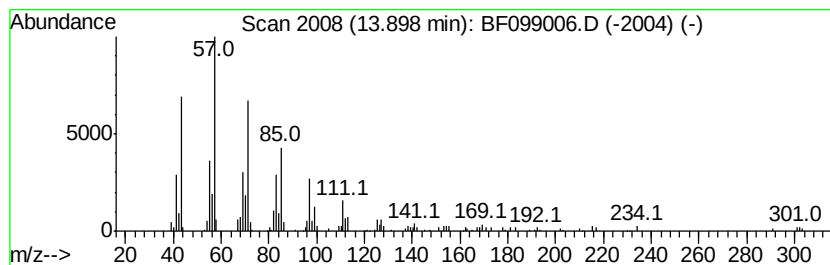
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Ethanol, 2-(dodecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	4.91 ng	164633	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	93
2	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	90
3	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
4	Tritetracontane	605	C43H88	007098-21-7	87
5	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	87



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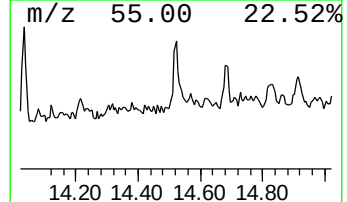
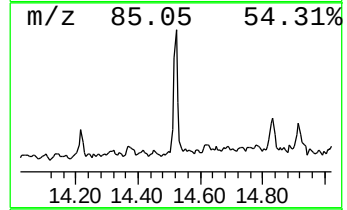
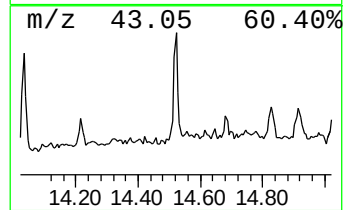
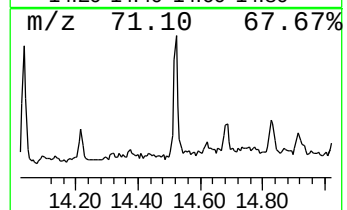
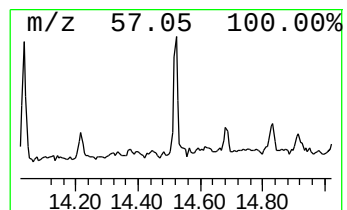
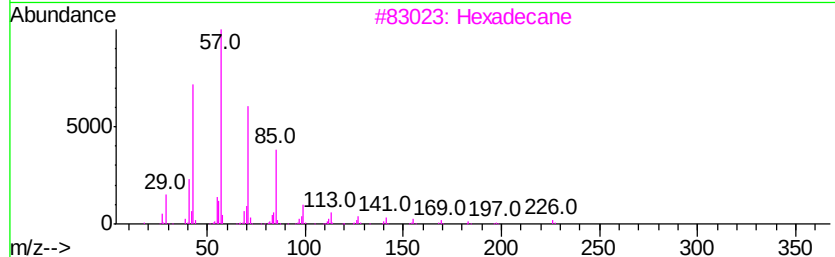
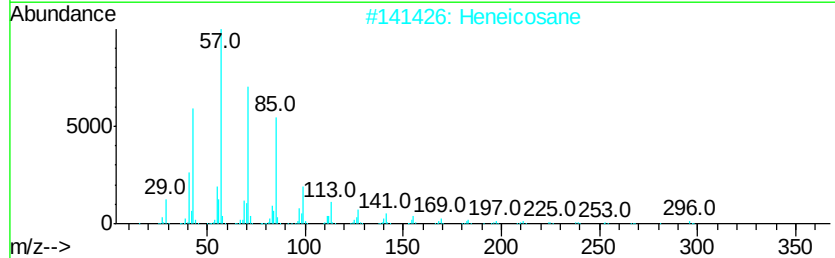
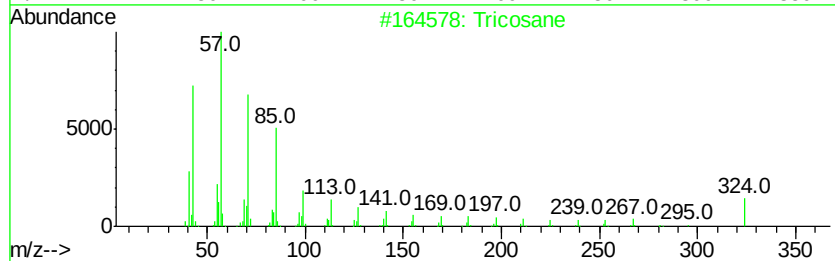
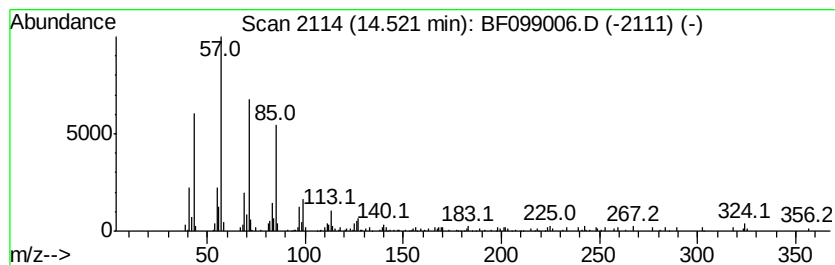
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tricosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	3.54 ng	118526	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Hexadecane	226	C16H34	000544-76-3	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
Data File : BF099006.D
Acq On : 2 Oct 2017 18:15
Operator : SJ/JU
Sample : I5534-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-114-1(5-10)

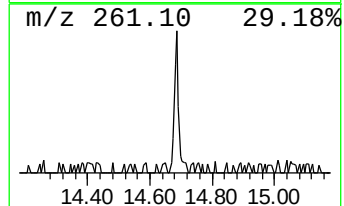
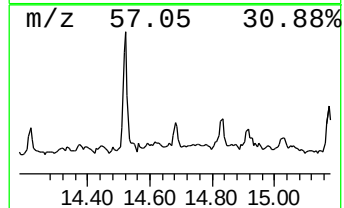
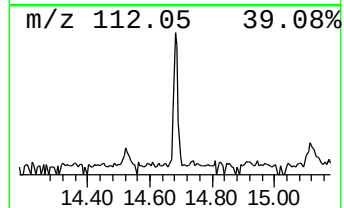
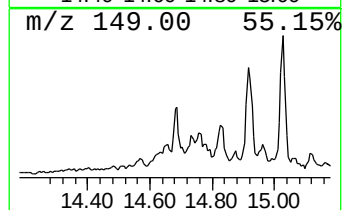
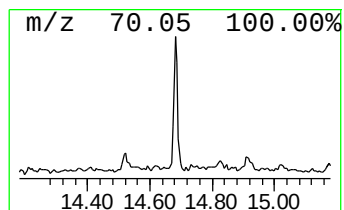
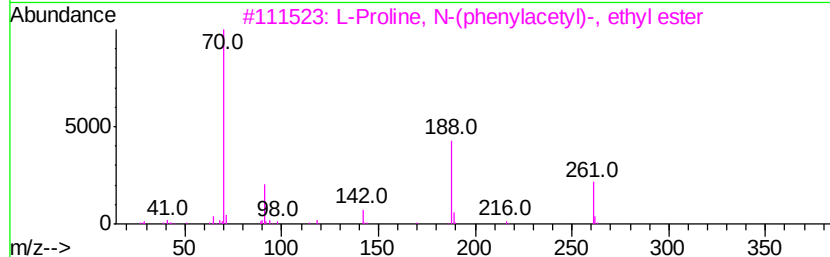
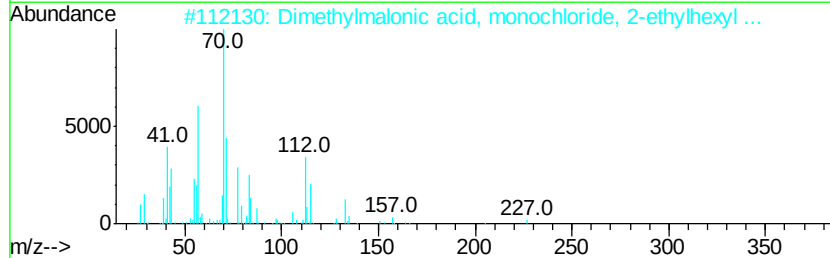
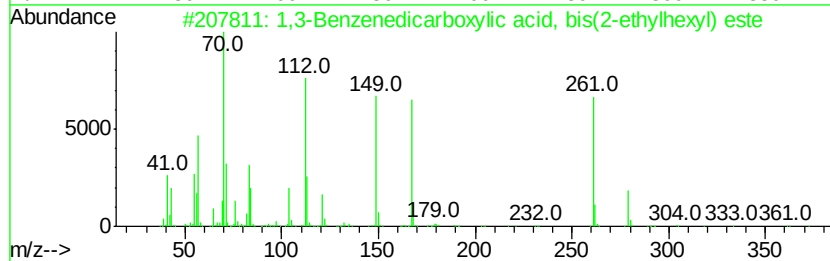
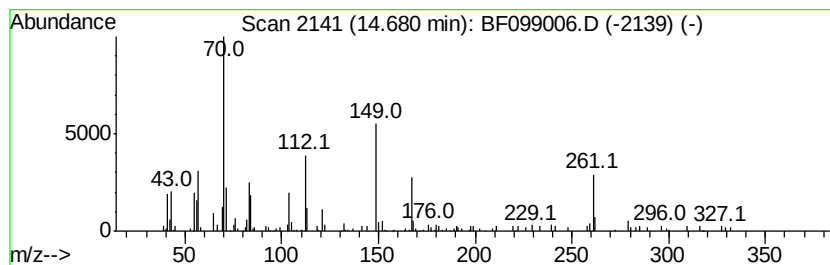
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.68 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.68	2.27 ng	75927	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	38
2		Dimethylmalonic acid, monochlori...	262	C13H23ClO3	1000361-64-8	32
3		L-Proline, N-(phenylacetyl)-, et...	261	C15H19NO3	1000346-18-9	27
4		Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	16
5		2-Undecene, 3-methyl-, (Z)-	168	C12H24	057024-90-5	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
Data File : BF099006.D
Acq On : 2 Oct 2017 18:15
Operator : SJ/JU
Sample : I5534-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-114-1(5-10)

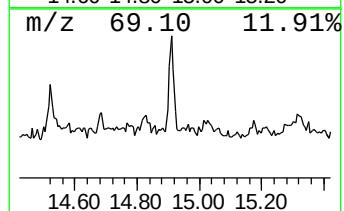
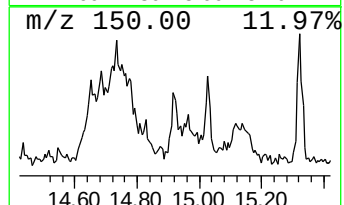
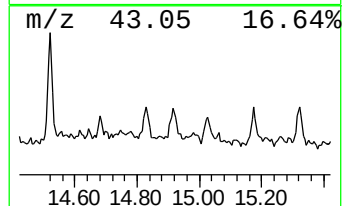
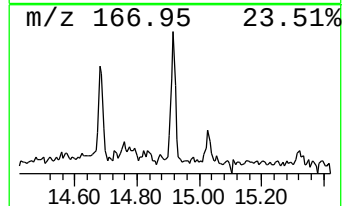
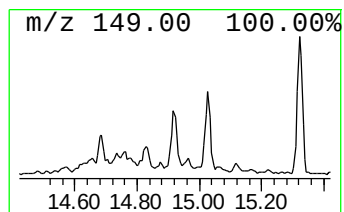
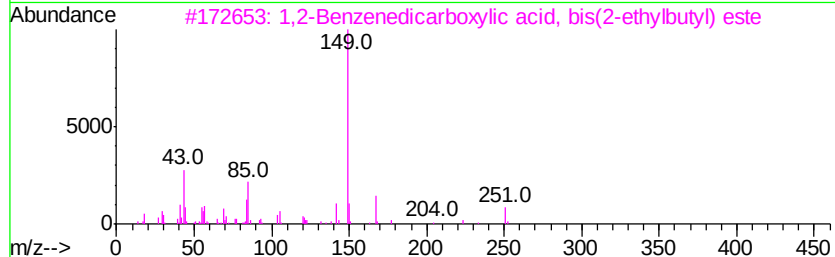
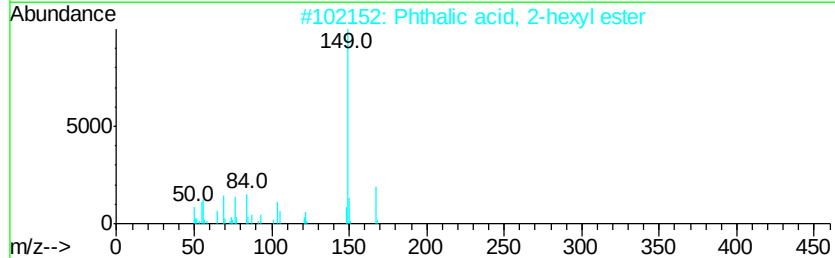
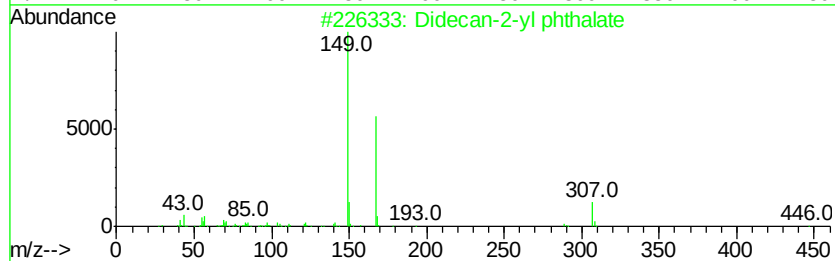
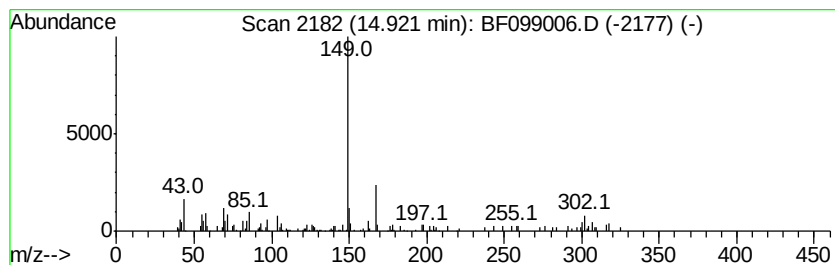
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Didecan-2-yl phthalate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.23 ng	87785	Perylene-d12	15.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Didecan-2-yl phthalate	446	C28H46O4	028029-89-2	72
2			Phthalic acid, 2-hexyl ester	250	C14H18O4	079107-80-5	64
3			1,2-Benzenedicarboxylic acid, bi...	334	C20H30O4	007299-89-0	59
4			Phthalic acid, monocyclohexyl ester	248	C14H16O4	007517-36-4	59
5			4-Methoxyanthranilic acid	167	C8H9NO3	004294-95-5	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
Data File : BF099006.D
Acq On : 2 Oct 2017 18:15
Operator : SJ/JU
Sample : I5534-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

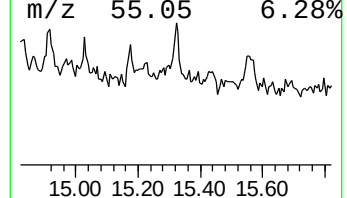
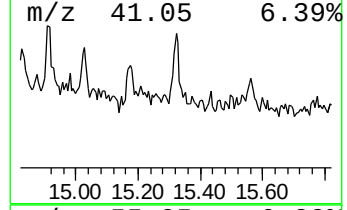
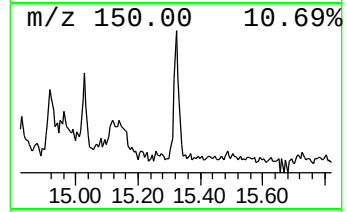
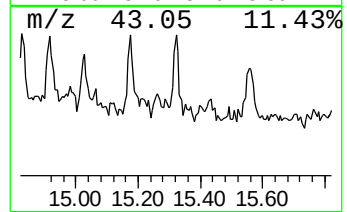
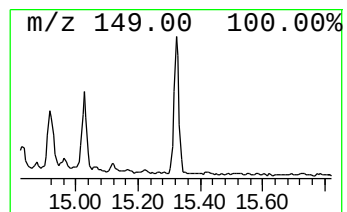
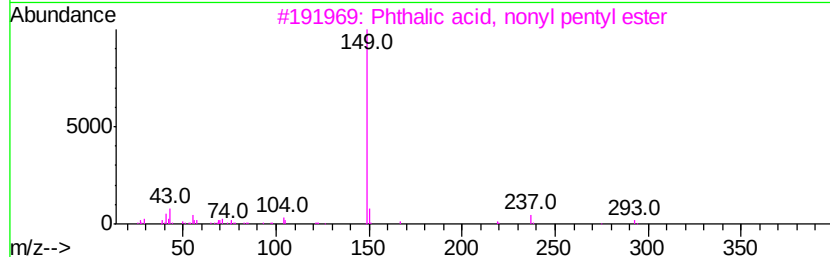
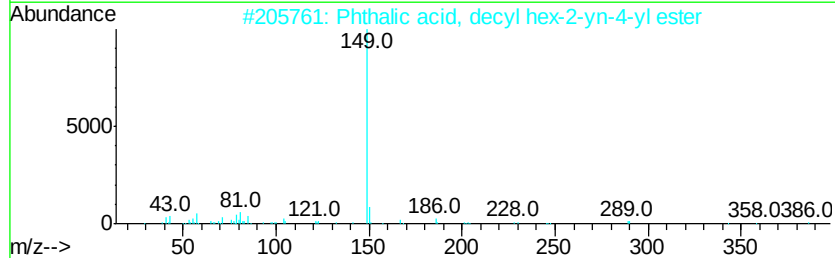
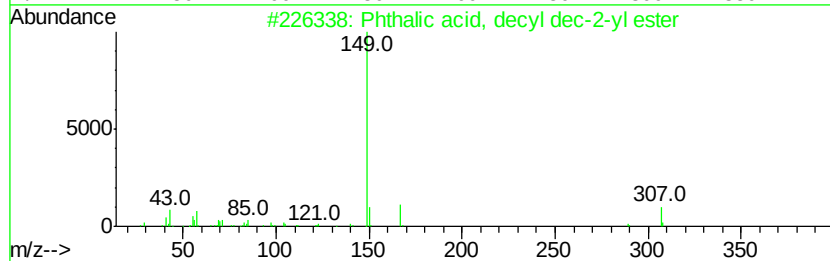
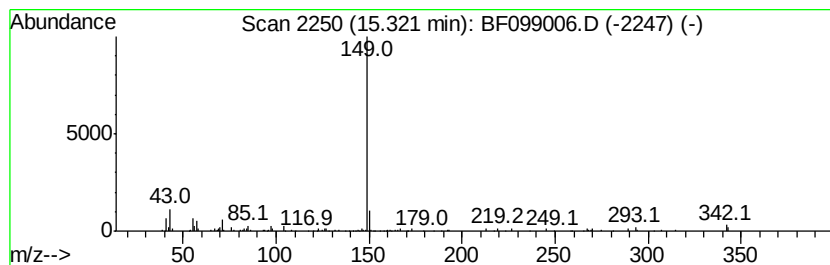
Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-114-1(5-10)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Phthalic acid, decyl dec-2-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.32	2.99 ng	117314	Perylene-d12	15.56		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, decyl dec-2-yl ester	446	C28H46O4	1000356-94-5	72	
2	Phthalic acid, decyl hex-2-yn-4-...	386	C24H34O4	1000315-19-6	72	
3	Phthalic acid, nonyl pentyl ester	362	C22H34O4	1000308-93-1	72	
4	1,2-Benzenedicarboxylic acid, di...	418	C26H42O4	000084-76-4	72	
5	Phthalic acid, 2-methylbutyl pro...	278	C16H22O4	1000322-81-1	64	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100217\
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Operator : SJ/JU
Sample : I5534-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-114-1(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.21	4.0	ng	158970	1	6.90	792626	20.0
2-Pentanone, 4-hy...	5.13	11.4	ng	449665	1	6.90	792626	20.0
unknown6.67	6.67	63.8	ng	2528400	1	6.90	792626	20.0
Ethanol, 2-(dodec...	13.90	4.9	ng	164633	5	14.07	670026	20.0
Tricosane	14.52	3.5	ng	118526	5	14.07	670026	20.0
unknown14.68	14.68	2.3	ng	75927	5	14.07	670026	20.0
Didecan-2-yl phth...	14.92	2.2	ng	87785	6	15.56	785642	20.0
Phthalic acid, de...	15.32	3.0	ng	117314	6	15.56	785642	20.0