

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
 Data File : BF097689.D
 Acq On : 15 Aug 2017 14:21
 Operator : SJ/JU
 Sample : I4705-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-B-COMP

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-BF081517.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	4.981	487	492	500	rVB	208260	262056	8.06%	0.816%
2	5.387	555	561	564	rBV	2921605	3007936	92.55%	9.368%
3	6.363	721	727	729	rBV2	33456	47473	1.46%	0.148%
4	6.410	729	735	739	rVB	3059520	3249929	100.00%	10.122%
5	6.551	754	759	762	rBV	2938663	3012257	92.69%	9.382%
6	6.781	794	798	801	rBV	1107718	870585	26.79%	2.711%
7	6.940	821	825	828	rVB	2293074	2035951	62.65%	6.341%
8	7.345	888	894	897	rBV	2039587	1919796	59.07%	5.979%
9	7.422	903	907	911	rBV	45948	49051	1.51%	0.153%
10	8.063	1012	1016	1019	rBV	1402448	1129099	34.74%	3.517%
11	9.145	1195	1200	1203	rBV	3027679	3026797	93.13%	9.427%
12	9.534	1262	1266	1269	rBV	751456	614293	18.90%	1.913%
13	9.816	1310	1314	1318	rBV2	1330639	1180858	36.33%	3.678%
14	10.257	1387	1389	1392	rVB	76645	58717	1.81%	0.183%
15	10.480	1420	1427	1429	rBV2	24172	34213	1.05%	0.107%
16	10.604	1443	1448	1451	rBV	2061107	1925504	59.25%	5.997%
17	10.728	1466	1469	1478	rVB2	94059	117120	3.60%	0.365%
18	11.180	1542	1546	1549	rBV2	65365	62027	1.91%	0.193%
19	11.298	1562	1566	1569	rBV	1469649	1239074	38.13%	3.859%
20	11.322	1569	1570	1573	rVV	87609	42141	1.30%	0.131%
21	11.369	1575	1578	1581	rVB	60067	53949	1.66%	0.168%
22	11.527	1600	1605	1609	rBV4	31501	41654	1.28%	0.130%
23	11.704	1632	1635	1639	rVB	56462	47731	1.47%	0.149%
24	11.839	1653	1658	1662	rBV	376409	380553	11.71%	1.185%
25	11.910	1666	1670	1679	rVB3	37123	65244	2.01%	0.203%
26	12.392	1748	1752	1753	rBV2	36108	38909	1.20%	0.121%
27	12.410	1753	1755	1763	rVB3	84774	108269	3.33%	0.337%
28	12.504	1768	1771	1776	rBV	184252	178404	5.49%	0.556%
29	12.563	1779	1781	1786	rVV	35666	34803	1.07%	0.108%
30	12.622	1788	1791	1804	rVV2	270823	341750	10.52%	1.064%
31	12.733	1804	1810	1815	rVV	121373	136935	4.21%	0.426%
32	12.892	1832	1837	1840	rBV	2809176	2948608	90.73%	9.183%
33	13.045	1860	1863	1865	rBV2	31879	41781	1.29%	0.130%
34	13.069	1865	1867	1870	rVB2	56640	49241	1.52%	0.153%

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35	13.451	1928	1932	1934	rBV5	19463	33516	1.03%	0.104%
36	13.727	1977	1979	1985	rVB2	59154	69155	2.13%	0.215%
37	13.786	1986	1989	1994	rVV	255724	256132	7.88%	0.798%
38	13.827	1994	1996	1998	rVB	57941	43394	1.34%	0.135%
39	13.933	2005	2014	2017	rBV	1038384	1211764	37.29%	3.774%
40	14.033	2028	2031	2038	rVB	85680	92608	2.85%	0.288%
41	14.192	2055	2058	2061	rBV3	32694	33607	1.03%	0.105%
42	14.427	2095	2098	2102	rBV2	74863	81041	2.49%	0.252%
43	14.616	2127	2130	2133	rBV4	25940	35236	1.08%	0.110%
44	14.692	2140	2143	2146	rBV3	27655	38094	1.17%	0.119%
45	14.945	2182	2186	2190	rBV	252296	386010	11.88%	1.202%
46	15.051	2201	2204	2207	rBV2	65442	68758	2.12%	0.214%
47	15.239	2232	2236	2242	rVB	143438	177096	5.45%	0.552%
48	15.298	2242	2246	2250	rBV	143279	170484	5.25%	0.531%
49	15.363	2252	2257	2260	rBV	622514	732146	22.53%	2.280%
50	15.886	2343	2346	2356	rVB8	45359	81100	2.50%	0.253%
51	16.745	2487	2492	2499	rBV2	49473	99364	3.06%	0.309%
52	16.821	2501	2505	2514	rVB4	36973	64859	2.00%	0.202%
53	17.162	2559	2563	2572	rVB2	40031	80907	2.49%	0.252%

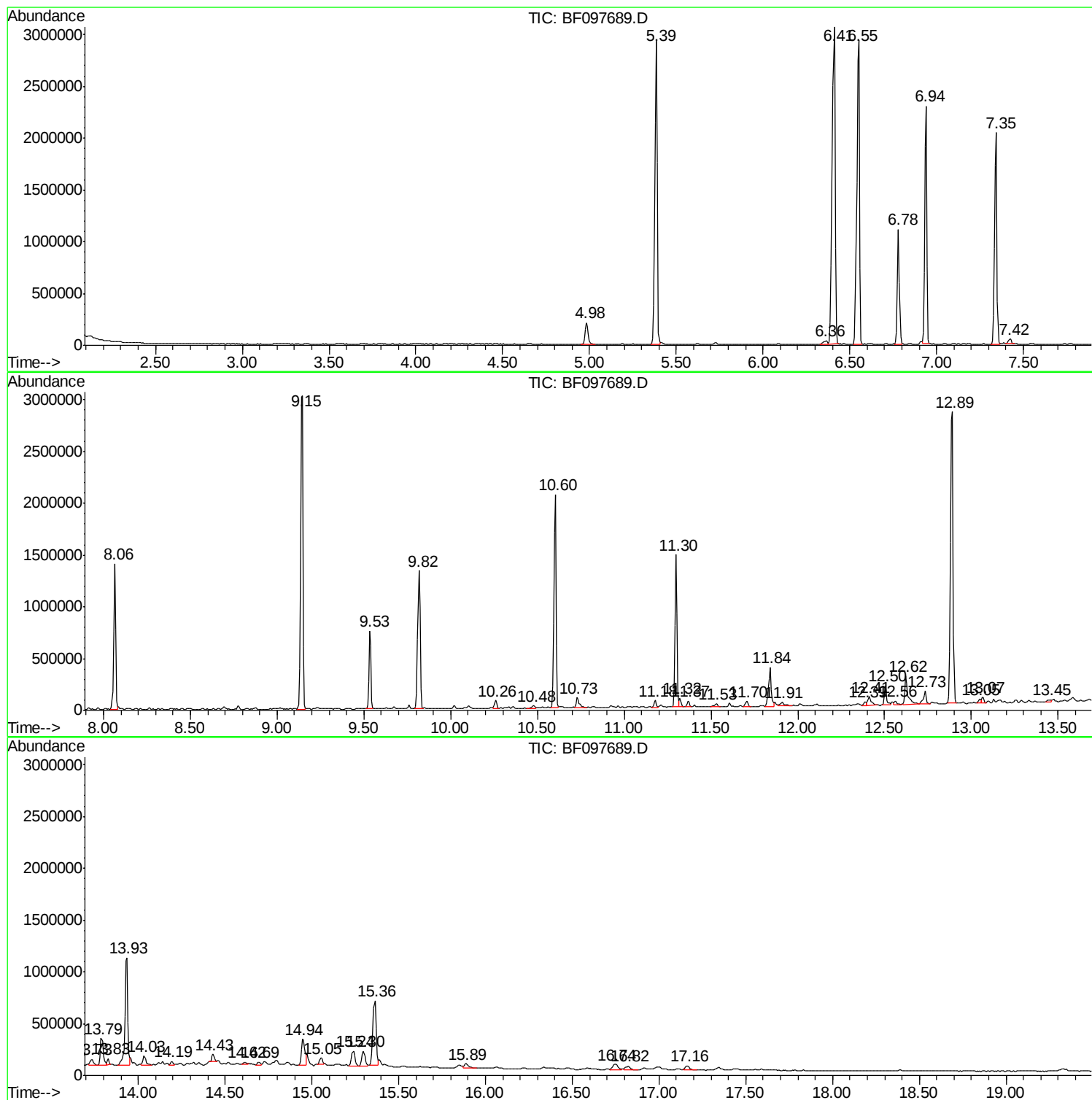
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ClientSampled :
SP-B-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.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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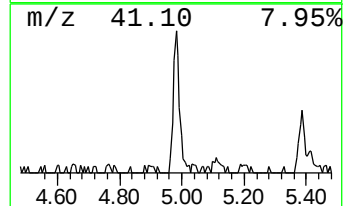
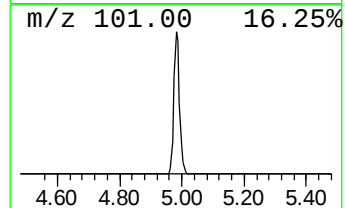
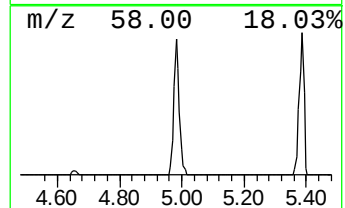
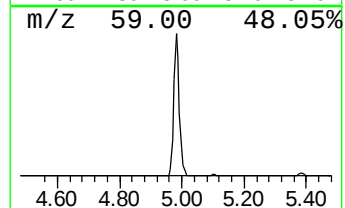
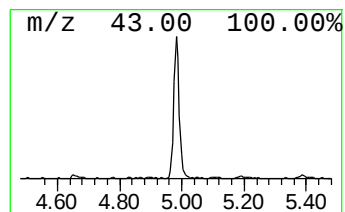
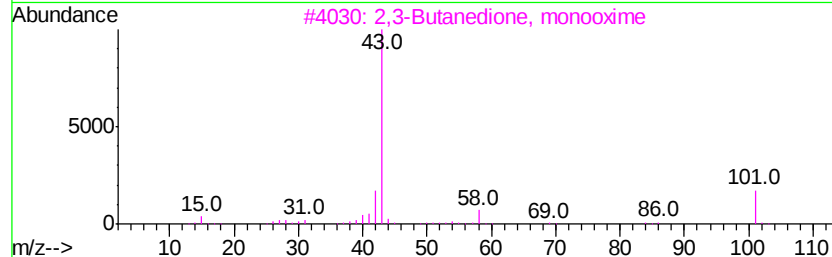
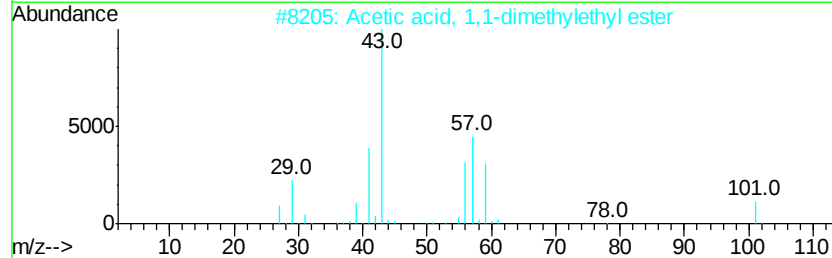
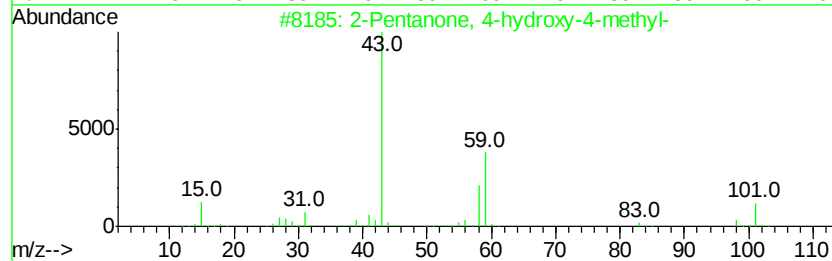
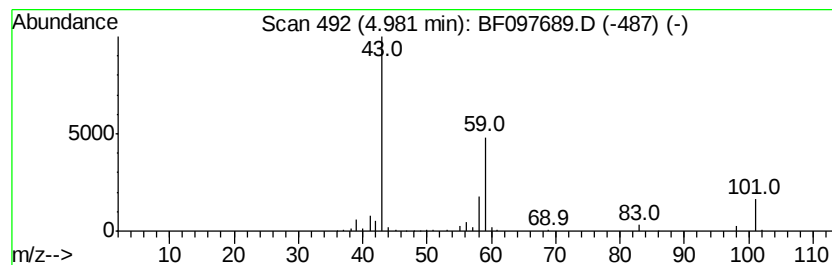
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	6.02 ng	262056	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		Acetone	58	C3H6O	000067-64-1	12
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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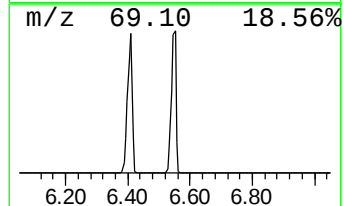
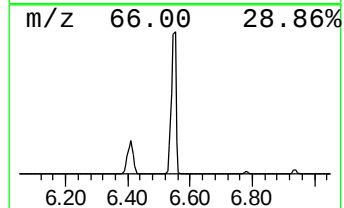
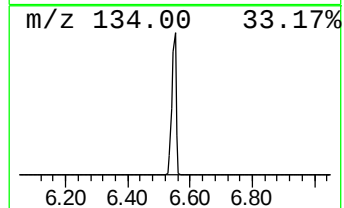
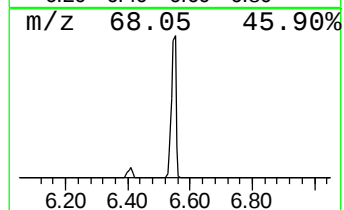
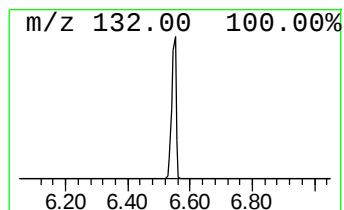
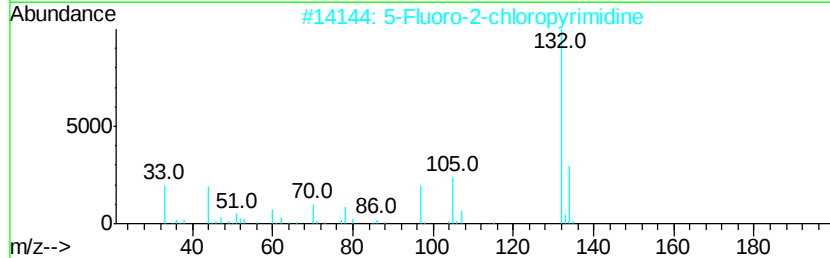
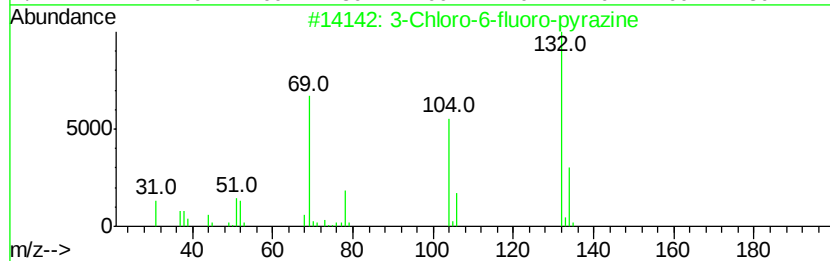
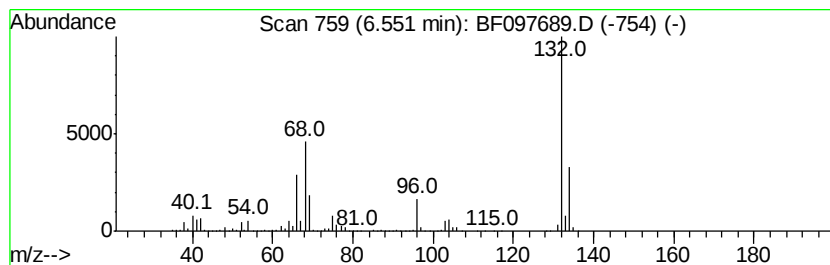
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	69.20 ng	3012260	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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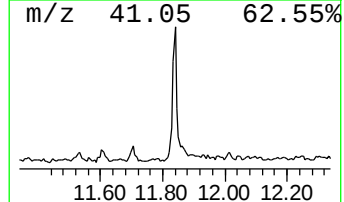
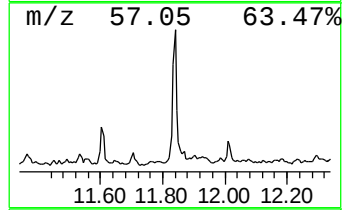
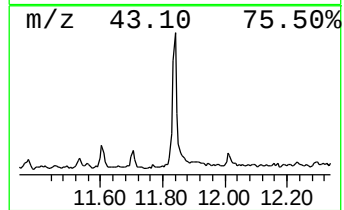
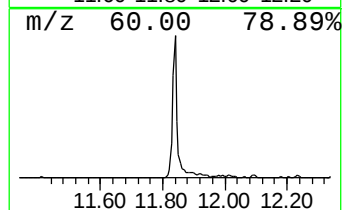
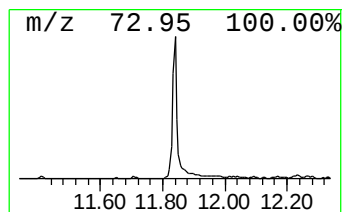
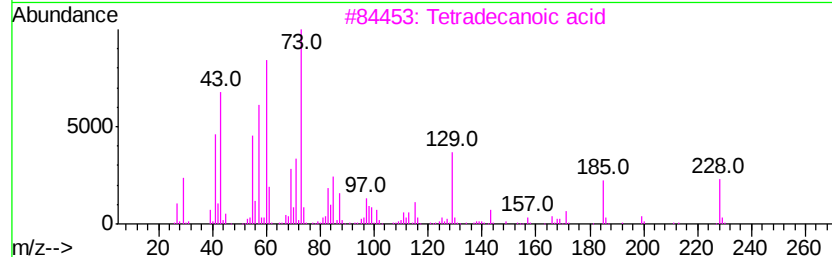
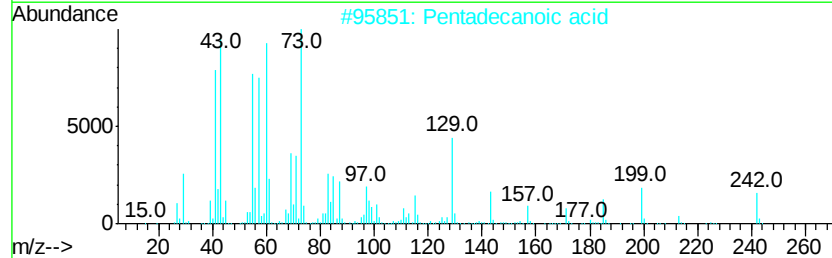
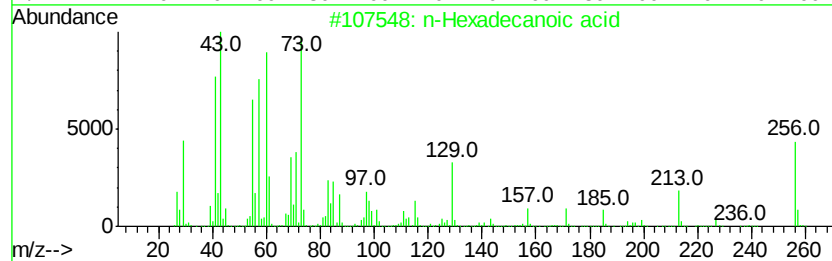
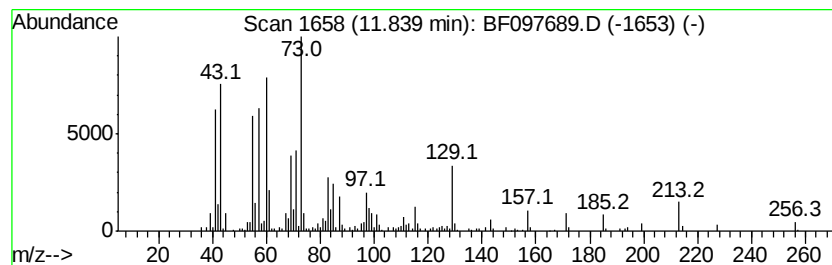
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	6.14 ng	380553	Phenanthrene-d10	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	25



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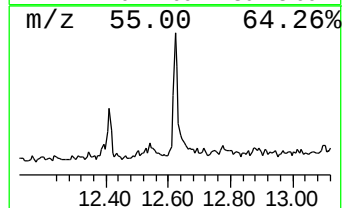
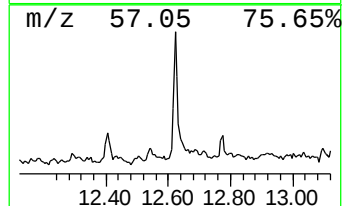
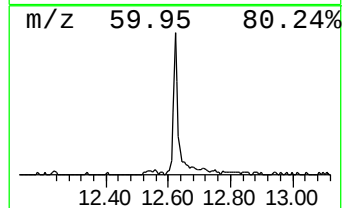
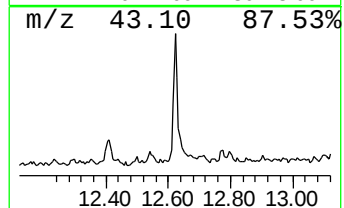
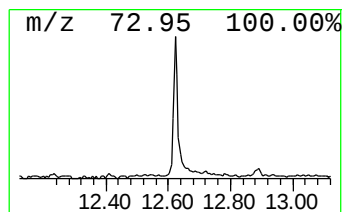
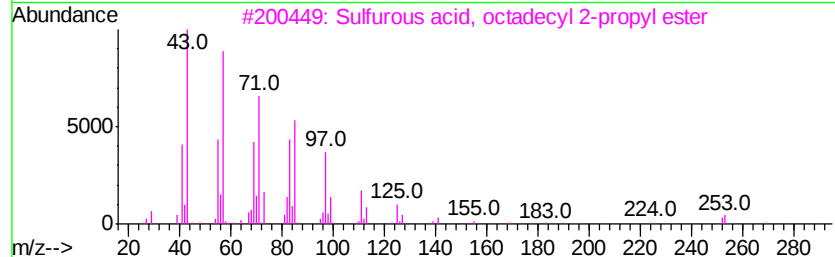
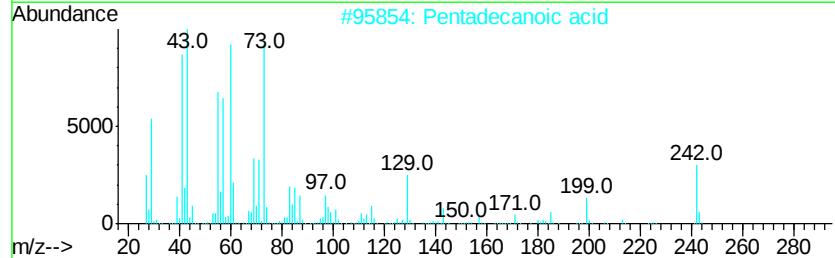
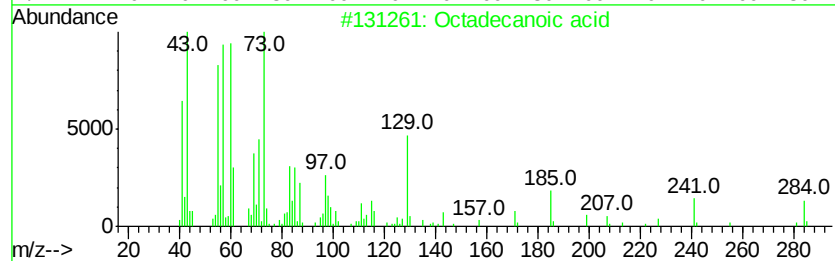
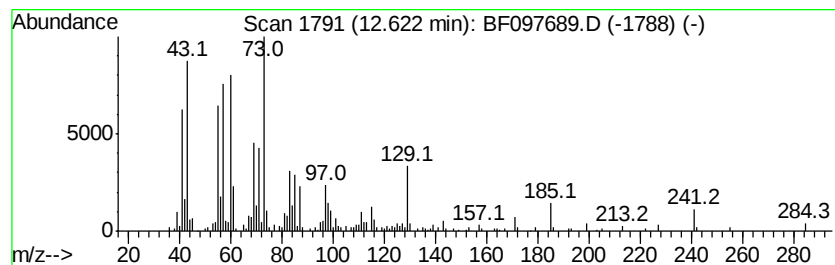
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.62	5.64 ng	341750	Chrysene-d12	13.93	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25
4	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	25
5	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	20



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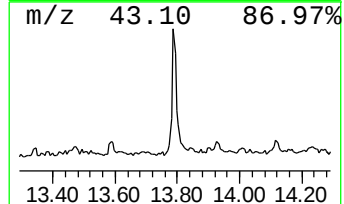
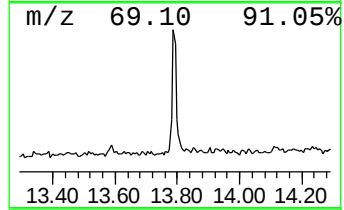
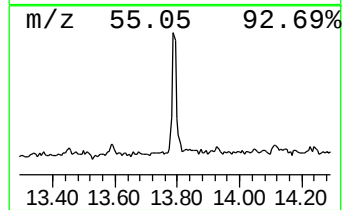
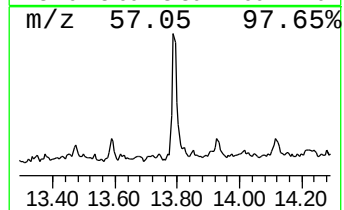
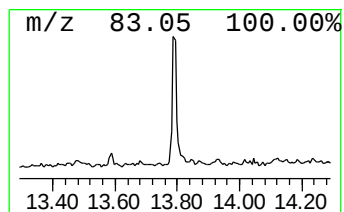
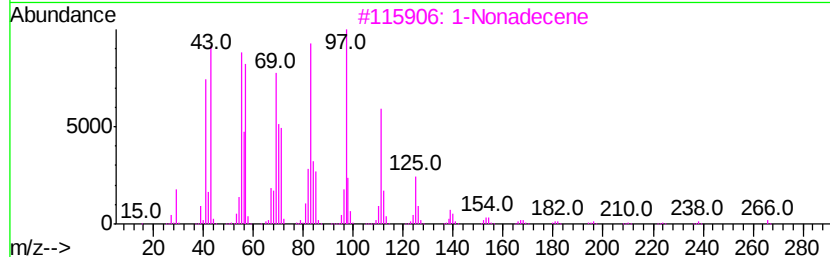
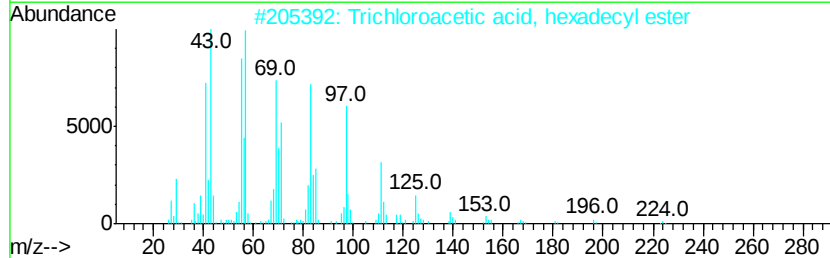
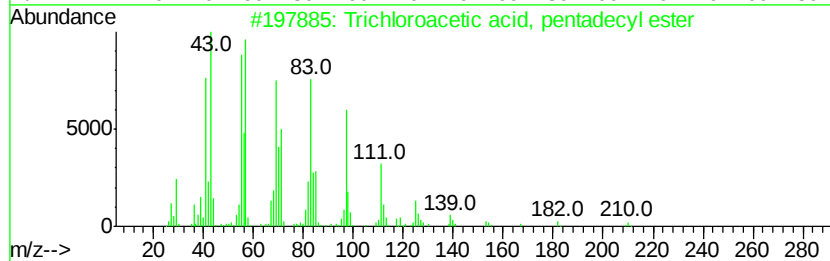
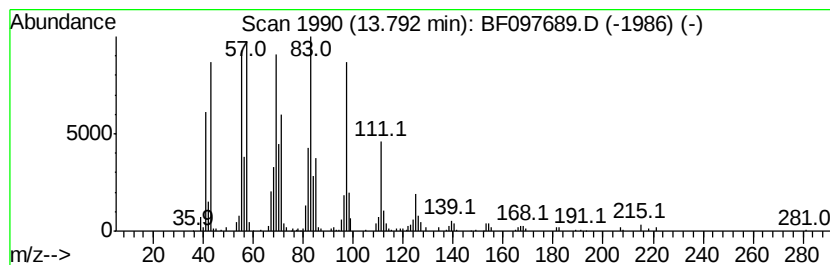
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trichloroacetic acid, penta... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	4.23 ng	256132	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		1-Heneicosanol	312	C21H44O	015594-90-8	91
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
Data File : BF097689.D
Acq On : 15 Aug 2017 14:21
Operator : SJ/JU
Sample : I4705-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-B-COMP

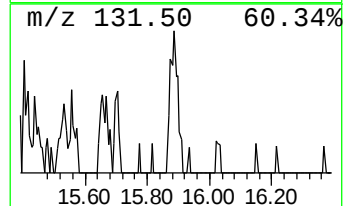
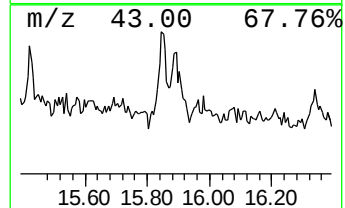
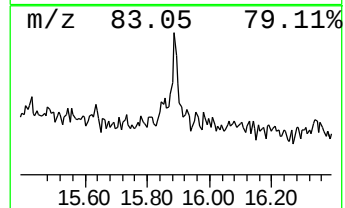
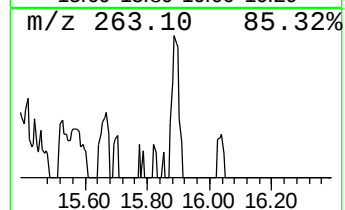
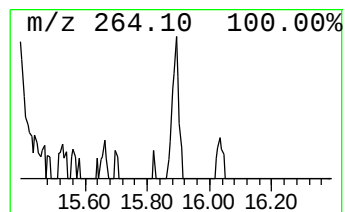
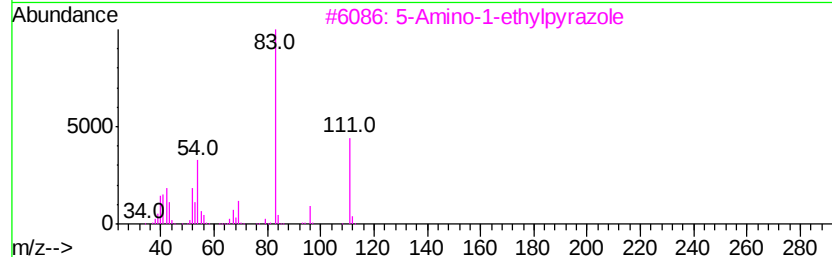
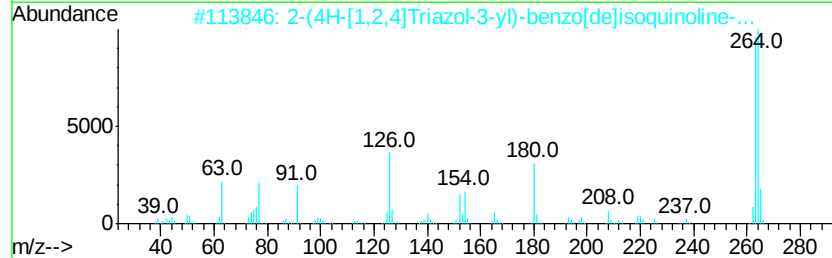
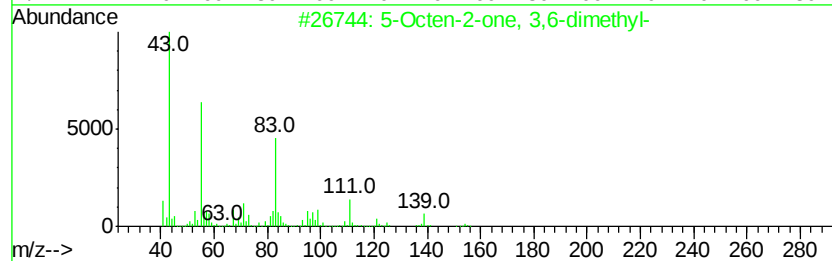
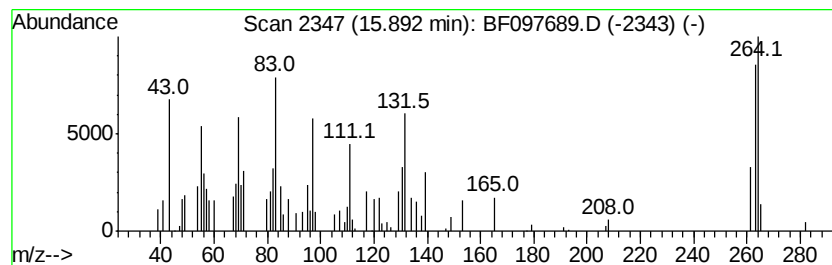
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.89 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	2.22 ng	81100	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octen-2-one, 3,6-dimethyl-	154	C10H18O	064165-21-5	27
2		2-(4H-[1,2,4]Triazol-3-yl)-benzo...	264	C14H8N4O2	1000318-09-6	25
3		5-Amino-1-ethylpyrazole	111	C5H9N3	003528-58-3	25
4		2-Methyl-6-phenylimidazo[2,1-b]-...	263	C11H9N3Se	034602-63-6	25
5		7,12a-Dimethyl-1,2,3,4,4a,11,12,...	264	C20H24	075758-27-9	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081517\
Data File : BF097689.D
Acq On : 15 Aug 2017 14:21
Operator : SJ/JU
Sample : I4705-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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...	4.98	6.0	ng	262056	1	6.78	870585	20.0
unknown6.55	6.55	69.2	ng	3012260	1	6.78	870585	20.0
n-Hexadecanoic acid	11.84	6.1	ng	380553	4	11.30	1239070	20.0
Octadecanoic acid	12.62	5.6	ng	341750	5	13.93	1211760	20.0
Trichloroacetic a...	13.79	4.2	ng	256132	5	13.93	1211760	20.0
unknown15.89	15.89	2.2	ng	81100	6	15.36	732146	20.0