

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
 Data File : BF097216.D
 Acq On : 31 Jul 2017 19:05
 Operator : SJ/JU
 Sample : I4488-13
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CL-02-072717-E

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-BF072517.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	4.622	461	465	479	rBV	190666	304293	10.67%	1.179%
2	5.092	541	545	561	rBV	2544416	2748637	96.40%	10.650%
3	6.157	722	726	739	rBV	2367080	2851202	100.00%	11.047%
4	6.257	739	743	754	rVB	2916845	2828677	99.21%	10.960%
5	6.481	777	781	790	rBV	863998	771732	27.07%	2.990%
6	6.633	803	807	811	rBV	2070601	1877670	65.86%	7.275%
7	7.051	873	878	881	rBV	1950830	1852178	64.96%	7.176%
8	7.763	995	999	1002	rBV	1226520	1068566	37.48%	4.140%
9	8.839	1177	1182	1186	rBV	2310170	2374606	83.28%	9.201%
10	9.239	1246	1250	1254	rBV	547299	458940	16.10%	1.778%
11	9.369	1266	1272	1279	rVB	36773	36630	1.28%	0.142%
12	9.510	1291	1296	1300	rBV	1294249	1151640	40.39%	4.462%
13	9.963	1370	1373	1376	rVB	58303	47210	1.66%	0.183%
14	10.180	1404	1410	1417	rBV2	20756	41266	1.45%	0.160%
15	10.298	1426	1430	1438	rVB	1477614	1383402	48.52%	5.360%
16	10.433	1450	1453	1462	rVB	84599	98456	3.45%	0.381%
17	10.880	1524	1529	1531	rBV2	52246	46182	1.62%	0.179%
18	10.986	1543	1547	1550	rBV	960334	854348	29.96%	3.310%
19	11.063	1555	1560	1564	rVB	38029	41699	1.46%	0.162%
20	11.545	1639	1642	1648	rBV2	134727	147544	5.17%	0.572%
21	12.033	1722	1725	1728	rBV	27840	30601	1.07%	0.119%
22	12.192	1748	1752	1757	rBV	154958	144458	5.07%	0.560%
23	12.327	1772	1775	1778	rBV3	27920	32281	1.13%	0.125%
24	12.415	1785	1790	1793	rBV	185596	173624	6.09%	0.673%
25	12.574	1812	1817	1820	rBV	1676267	1780977	62.46%	6.901%
26	12.645	1824	1829	1832	rBV4	30644	51010	1.79%	0.198%
27	12.733	1840	1844	1845	rBV3	22296	32314	1.13%	0.125%
28	12.745	1845	1846	1850	rVB	44621	37320	1.31%	0.145%
29	12.810	1855	1857	1861	rBV2	28358	29459	1.03%	0.114%
30	12.851	1861	1864	1867	rVV	32706	29705	1.04%	0.115%
31	12.939	1876	1879	1882	rVB	30955	33084	1.16%	0.128%
32	12.968	1882	1884	1888	rBV2	29528	29207	1.02%	0.113%
33	13.115	1905	1909	1910	rBV4	28560	30716	1.08%	0.119%
34	13.492	1970	1973	1979	rVB2	146813	185808	6.52%	0.720%

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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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.610	1988	1993	1996	rBV	801750	897370	31.47%	3.477%
36	13.633	1996	1997	2001	rVB	104316	93142	3.27%	0.361%
37	14.604	2159	2162	2165	rBV	114910	145408	5.10%	0.563%
38	14.857	2202	2205	2211	rVB	86793	125111	4.39%	0.485%
39	14.909	2211	2214	2219	rBV2	140893	207483	7.28%	0.804%
40	14.962	2219	2223	2226	rBV	521933	594727	20.86%	2.304%
41	16.086	2412	2414	2417	rBV4	27295	37087	1.30%	0.144%
42	16.545	2490	2492	2498	rBV3	44031	60837	2.13%	0.236%
43	17.009	2569	2571	2573	rBV3	35027	42331	1.48%	0.164%

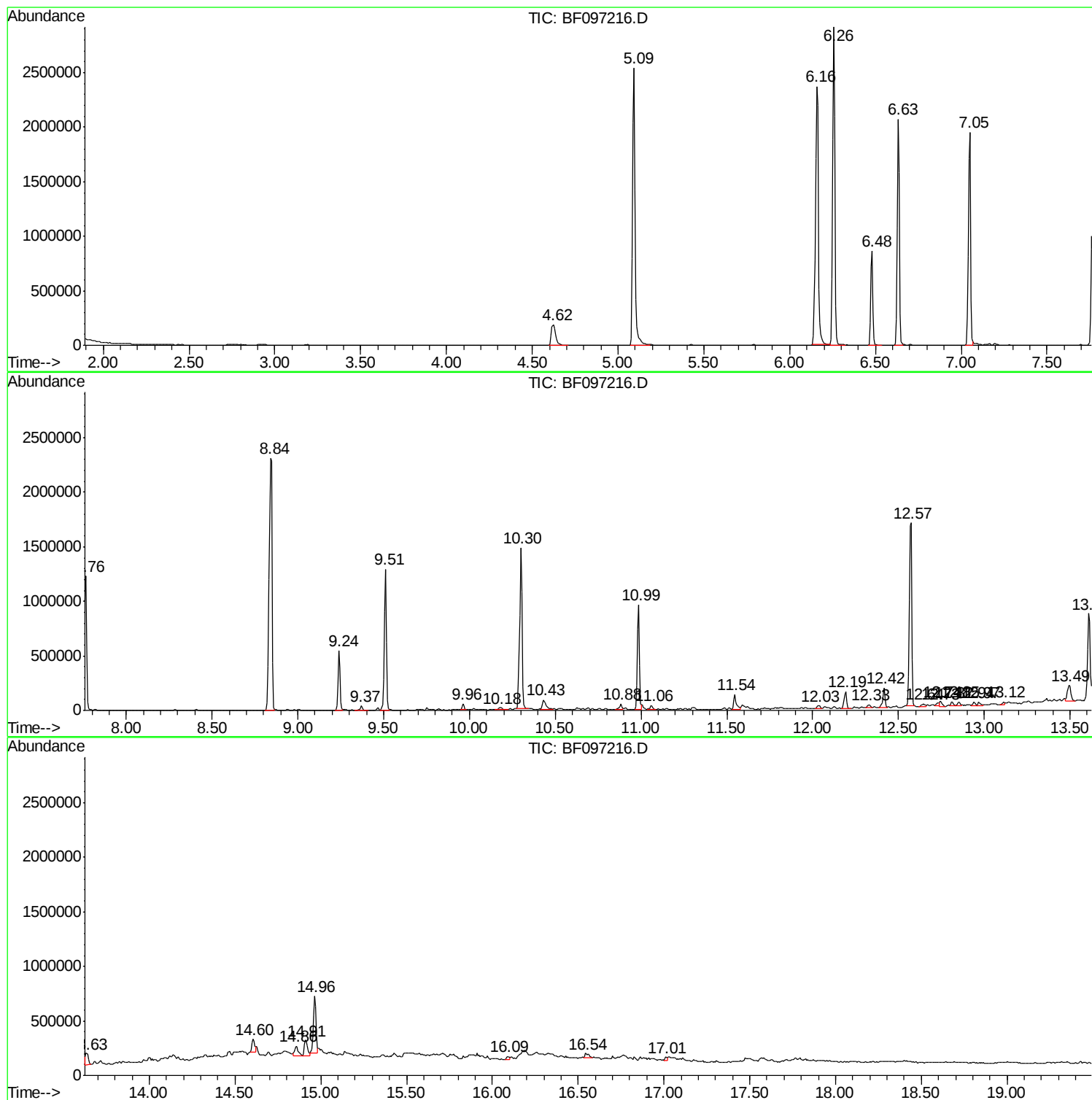
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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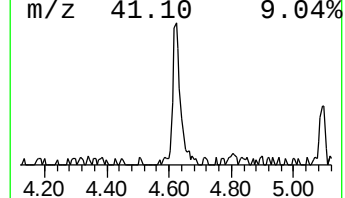
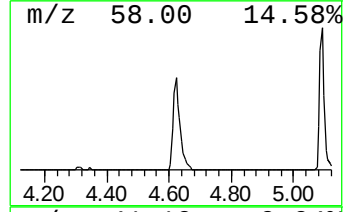
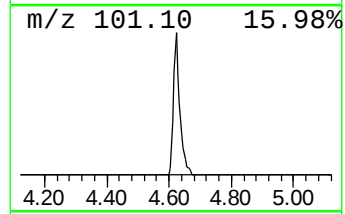
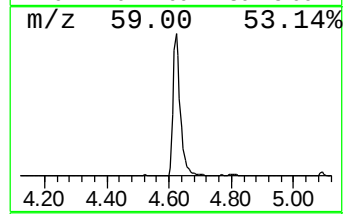
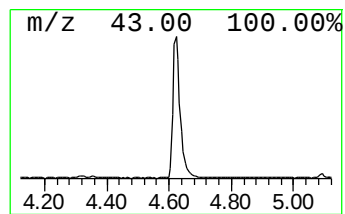
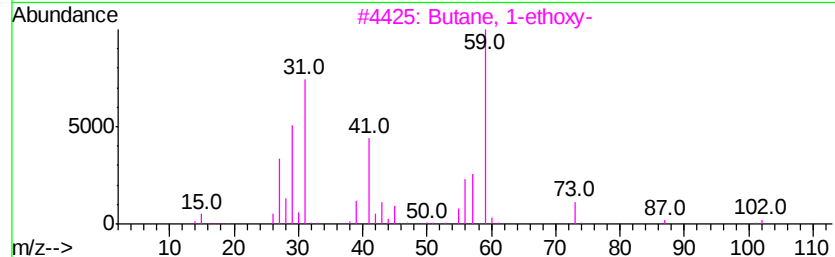
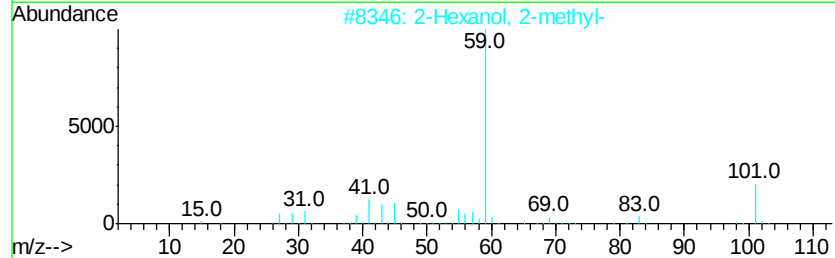
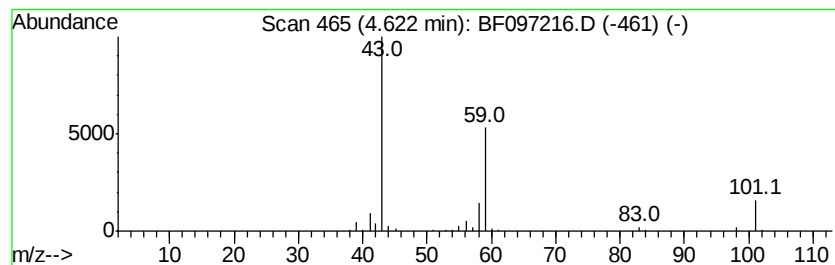
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	7.89 ng	304293	1,4-Dichlorobenzene-d4	6.48

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9



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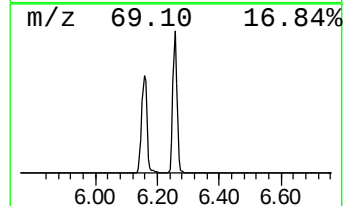
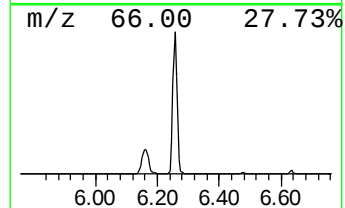
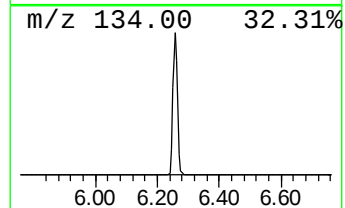
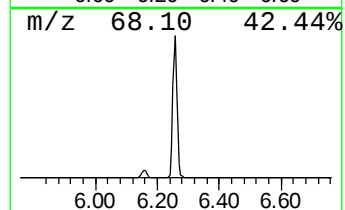
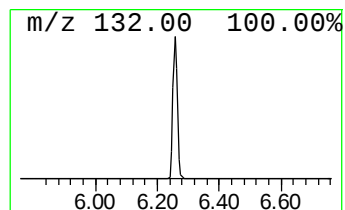
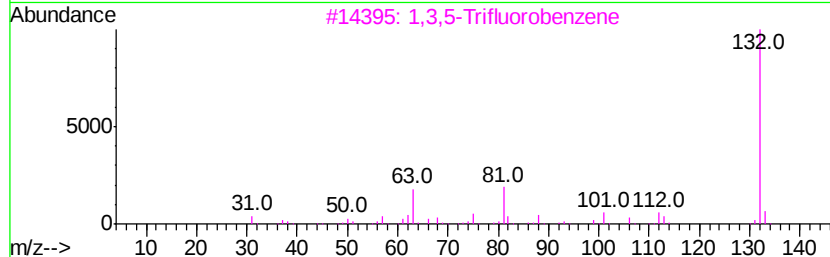
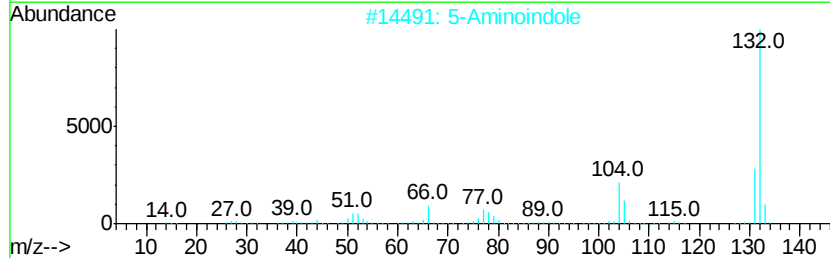
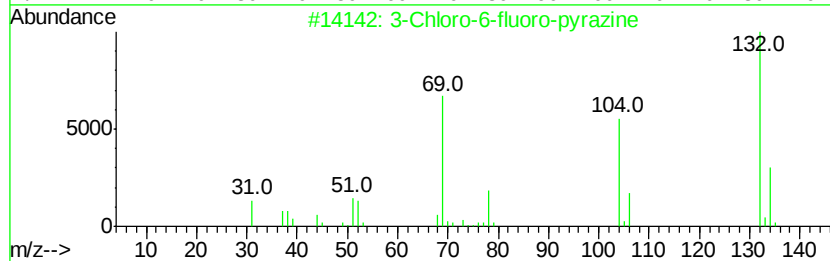
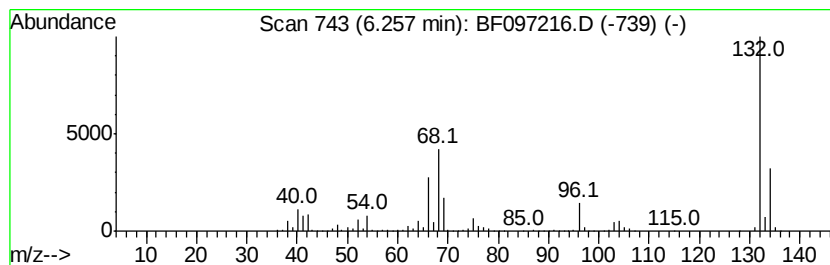
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Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	73.31 ng	2828680	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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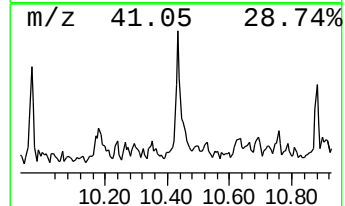
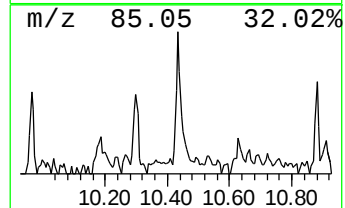
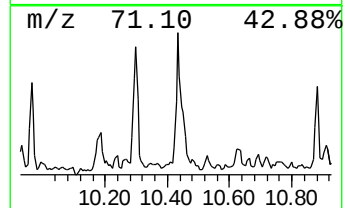
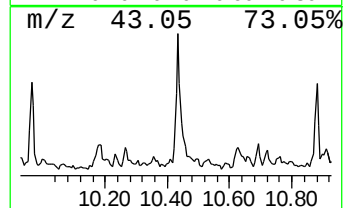
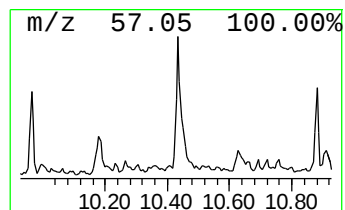
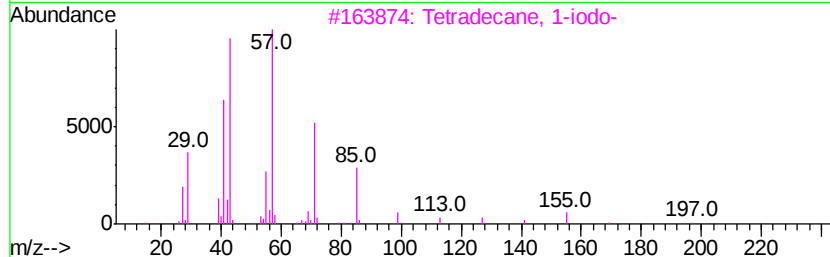
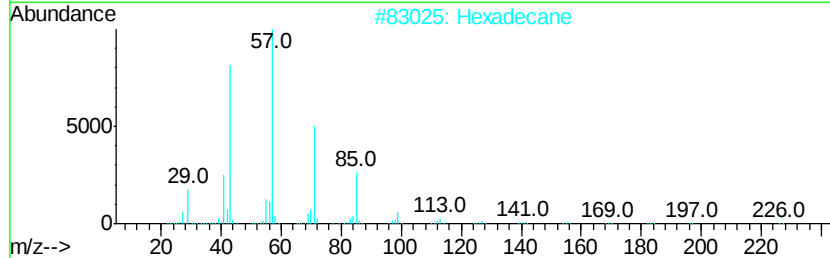
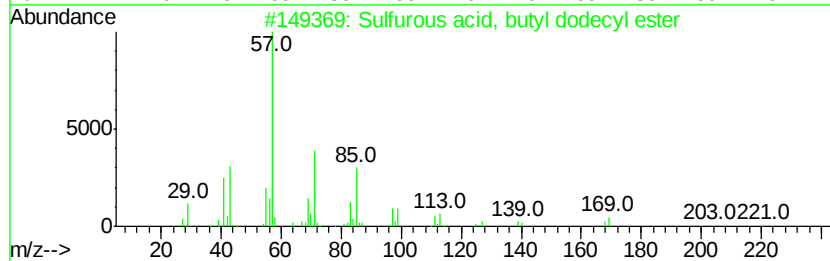
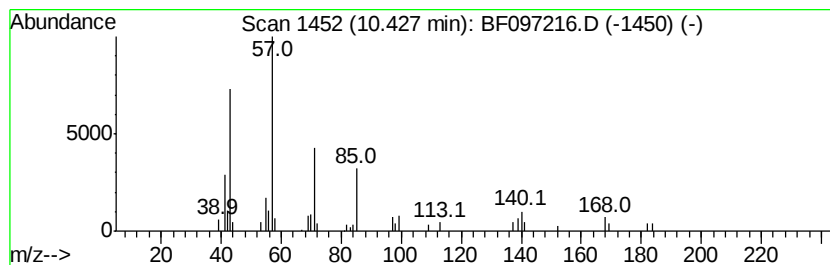
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Sulfurous acid, butyl dodec... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.43	2.30 ng	98456	Phenanthrene-d10	10.99		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	78
2		Hexadecane	226	C16H34	000544-76-3	78
3		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72
4		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	59
5		Octacosane	394	C28H58	000630-02-4	59



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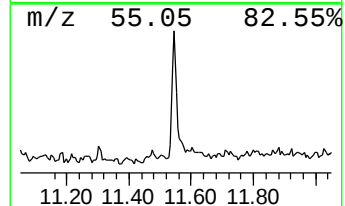
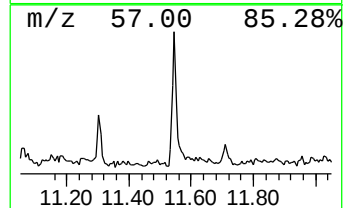
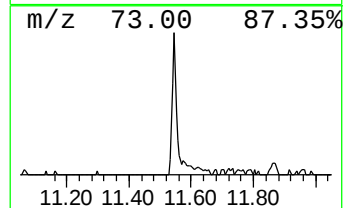
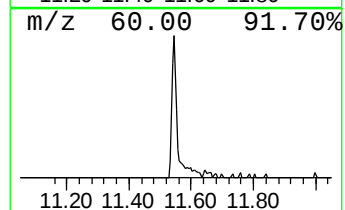
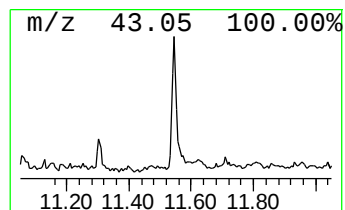
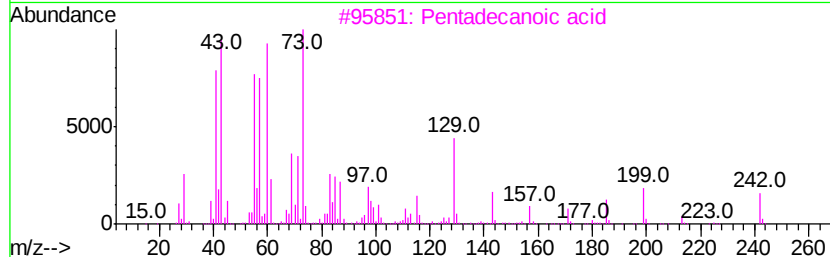
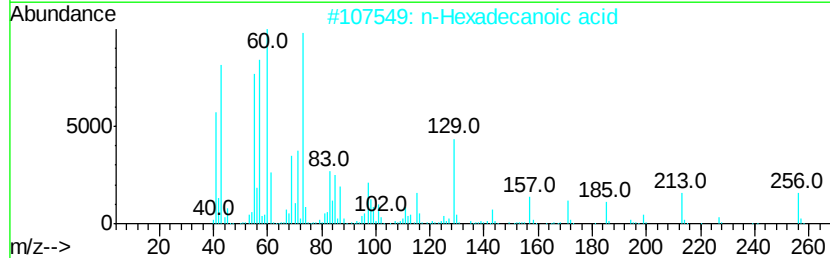
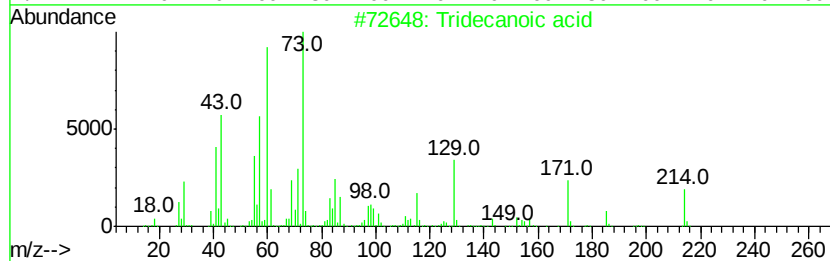
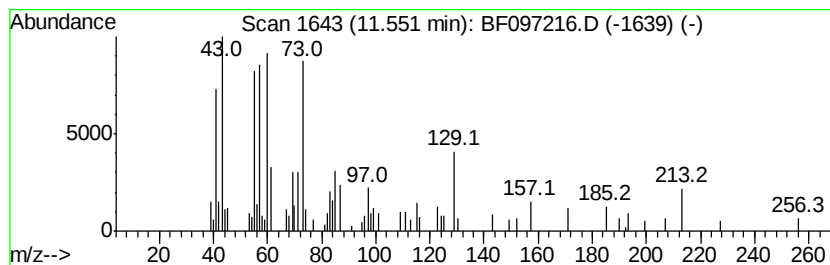
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	3.45 ng	147544	Phenanthrene-d10	10.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	93
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5		Undecanoic acid	186	C11H22O2	000112-37-8	58



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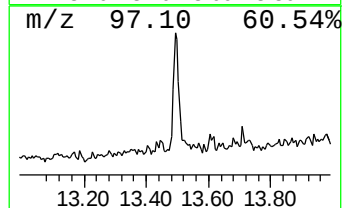
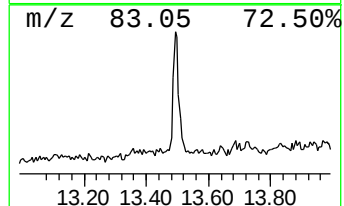
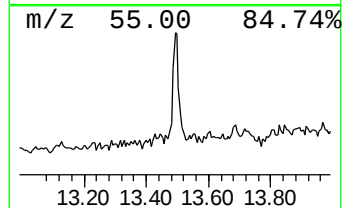
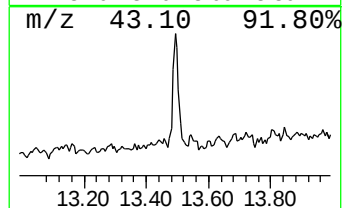
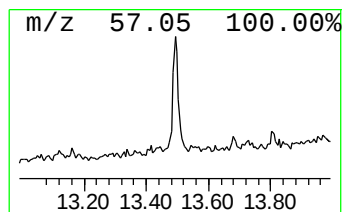
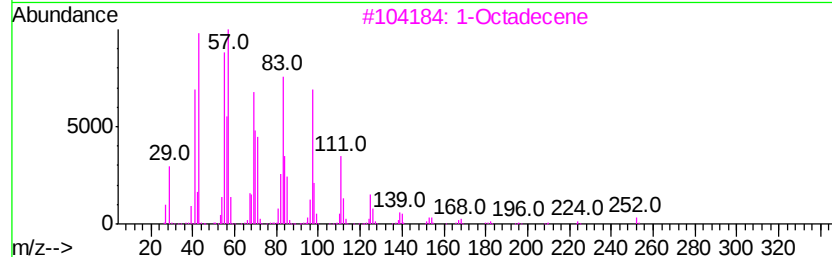
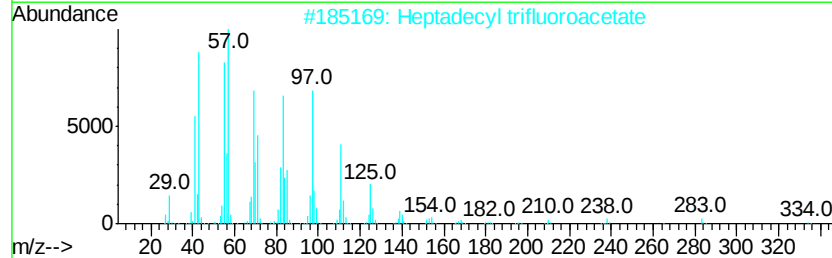
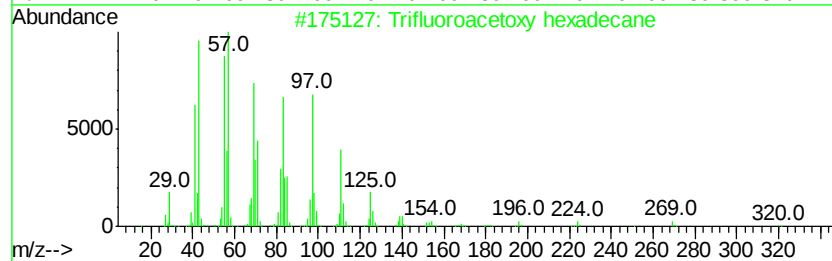
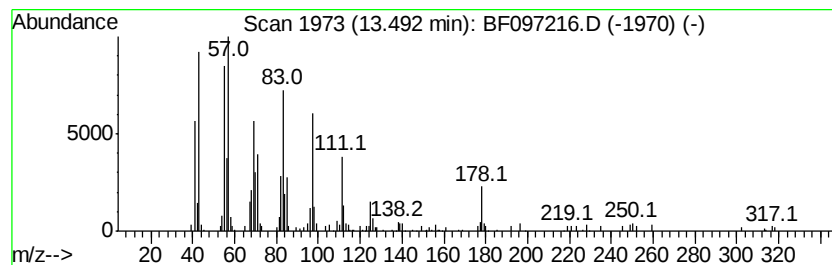
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	4.14 ng	185808	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3	1-Octadecene	252	C18H36	000112-88-9	90
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073117\
Data File : BF097216.D
Acq On : 31 Jul 2017 19:05
Operator : SJ/JU
Sample : I4488-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-072717-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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...	4.62	7.9	ng	304293	1	6.48	771732	20.0
unknown6.26	6.26	73.3	ng	2828680	1	6.48	771732	20.0
Sulfurous acid, b...	10.43	2.3	ng	98456	4	10.99	854348	20.0
Tridecanoic acid	11.55	3.5	ng	147544	4	10.99	854348	20.0
Trifluoroacetoxy ...	13.49	4.1	ng	185808	5	13.61	897370	20.0