

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032217\
 Data File : BF093870.D
 Acq On : 23 Mar 2017 9:03
 Operator : SJ/MA
 Sample : I2350-11
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11937-VNJ-205-COMP

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-BF032217.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	2.116	35	39	45	rVB	146821	170954	2.91%	0.338%
2	4.145	379	384	396	rVB	694355	1066283	18.15%	2.107%
3	4.522	441	448	451	rBV	4702984	5447410	92.71%	10.762%
4	4.910	511	514	522	rVB	64885	65902	1.12%	0.130%
5	5.575	619	627	631	rBV	3927672	5875617	100.00%	11.608%
6	5.734	647	654	657	rBV	4557198	5664974	96.41%	11.192%
7	5.987	693	697	701	rBV	1289402	1150682	19.58%	2.273%
8	6.169	722	728	731	rVB	4129531	4330358	73.70%	8.555%
9	6.634	800	807	811	rBV	2794475	3744101	63.72%	7.397%
10	7.486	947	952	956	rBV	1519661	1548165	26.35%	3.059%
11	8.816	1171	1178	1182	rBV	4811496	5819839	99.05%	11.498%
12	9.304	1256	1261	1265	rBV	573309	516049	8.78%	1.020%
13	9.633	1308	1317	1321	rBV2	1589003	1662144	28.29%	3.284%
14	10.222	1413	1417	1421	rVB	109769	101778	1.73%	0.201%
15	10.498	1457	1464	1467	rBV	45598	62328	1.06%	0.123%
16	10.604	1476	1482	1486	rBV	2624052	3205413	54.55%	6.333%
17	10.810	1513	1517	1519	rBV	139412	152171	2.59%	0.301%
18	11.363	1607	1611	1614	rBV	126001	112854	1.92%	0.223%
19	11.457	1622	1627	1630	rBV	1488703	1476328	25.13%	2.917%
20	11.480	1630	1631	1636	rVB	156397	132355	2.25%	0.261%
21	11.545	1639	1642	1645	rVB	80943	72886	1.24%	0.144%
22	11.892	1694	1701	1705	rVB2	95418	134500	2.29%	0.266%
23	12.174	1744	1749	1752	rBV2	132508	141424	2.41%	0.279%
24	12.945	1875	1880	1884	rBV	259233	247885	4.22%	0.490%
25	13.221	1922	1927	1930	rBV	223598	227015	3.86%	0.449%
26	13.439	1957	1964	1967	rBV	3648435	4169059	70.96%	8.237%
27	14.592	2156	2160	2170	rBV	199482	282304	4.80%	0.558%
28	14.704	2174	2179	2183	rBV	1009868	1148596	19.55%	2.269%
29	15.380	2291	2294	2302	rVB	58247	78979	1.34%	0.156%
30	15.927	2384	2387	2390	rBV	58778	76609	1.30%	0.151%
31	16.098	2412	2416	2426	rBV	121443	200514	3.41%	0.396%
32	16.280	2443	2447	2451	rVB	52491	67368	1.15%	0.133%
33	16.345	2453	2458	2466	rVB	748282	925774	15.76%	1.829%
34	16.656	2507	2511	2517	rBV3	46373	62666	1.07%	0.124%

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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

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35	16.892	2547	2551	2555	rBV	57892	91546	1.56%	0.181%
36	17.645	2673	2679	2688	rBV4	48517	93816	1.60%	0.185%
37	17.939	2724	2729	2735	rBV7	31203	68822	1.17%	0.136%
38	18.239	2771	2780	2781	rBV7	30787	62553	1.06%	0.124%
39	18.339	2793	2797	2805	rVB5	72477	157489	2.68%	0.311%

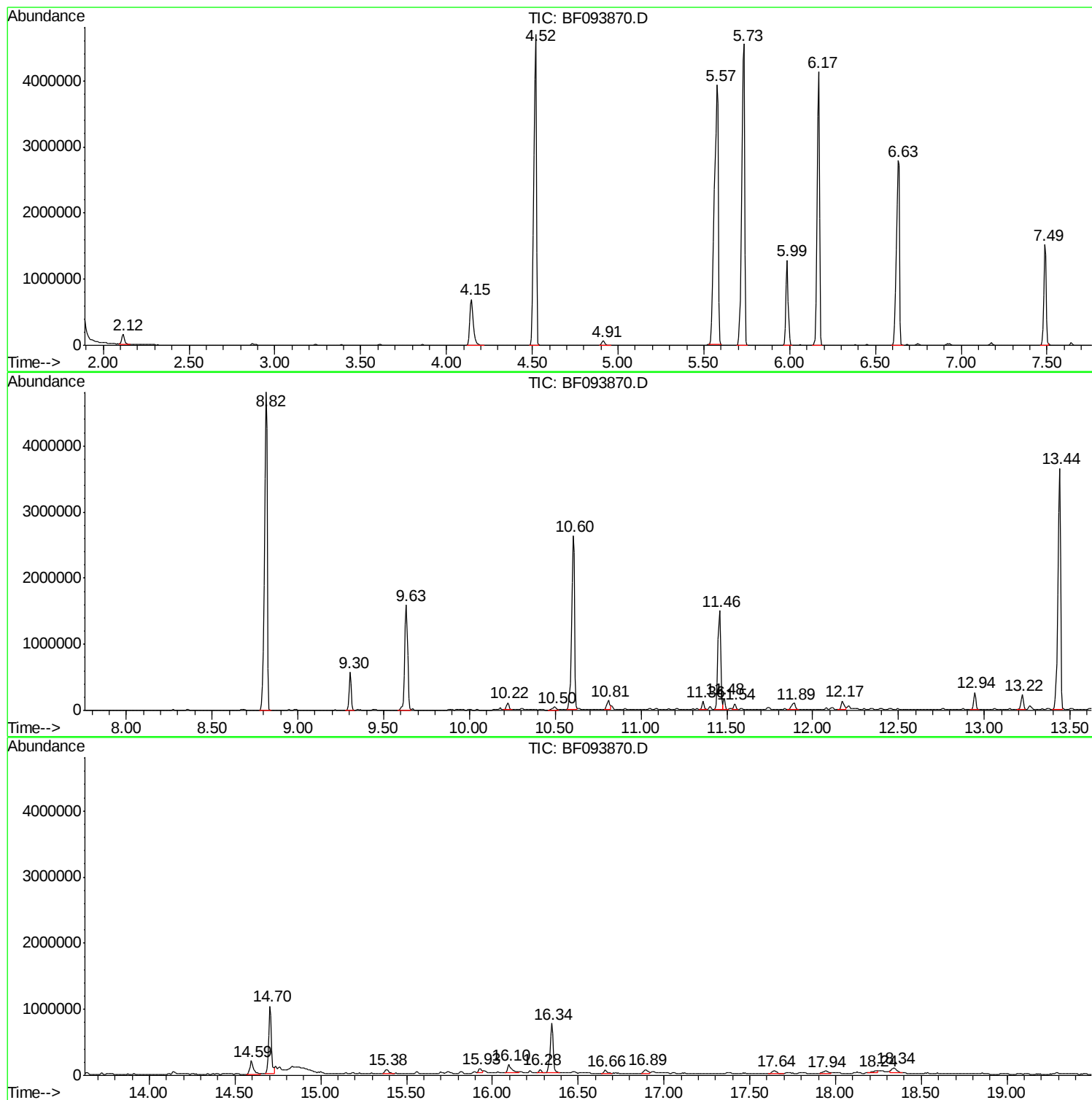
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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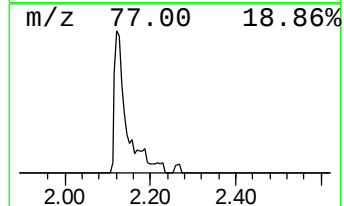
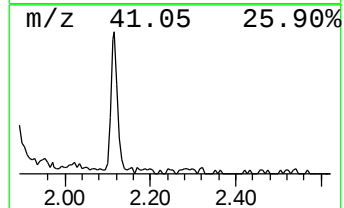
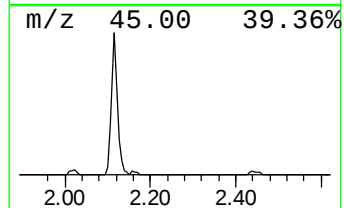
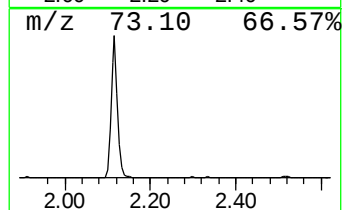
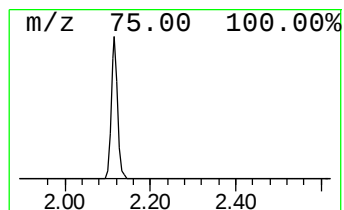
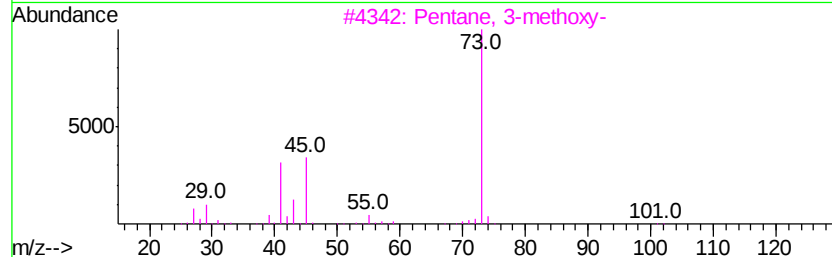
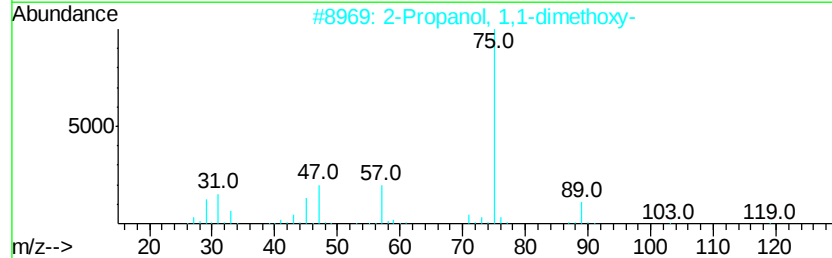
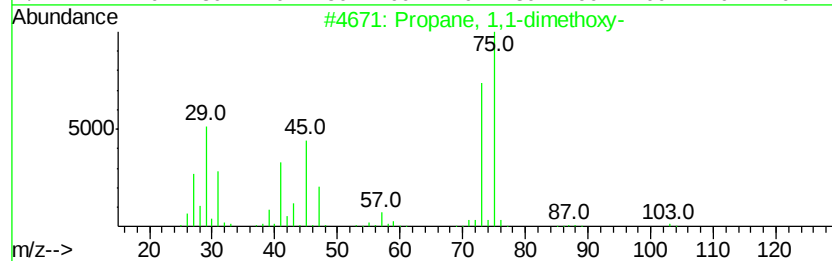
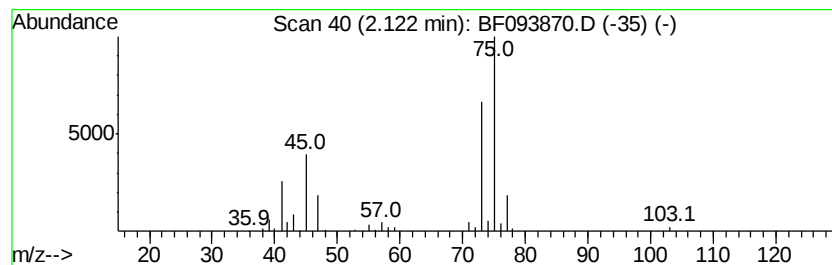
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	2.97 ng	170954	1,4-Dichlorobenzene-d4	5.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	28
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
5		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9



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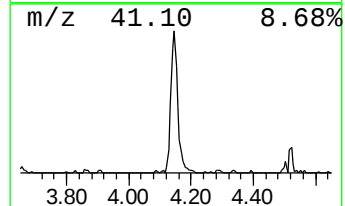
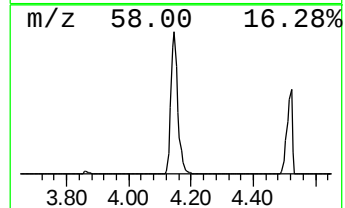
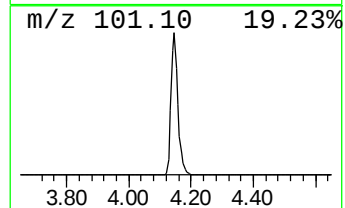
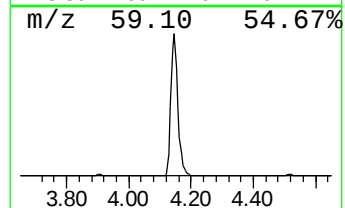
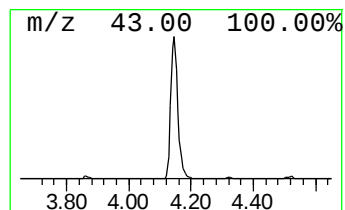
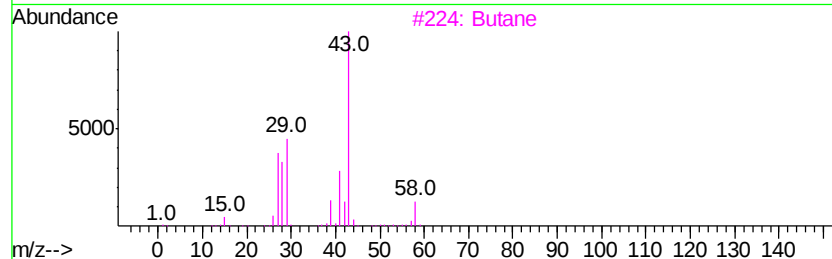
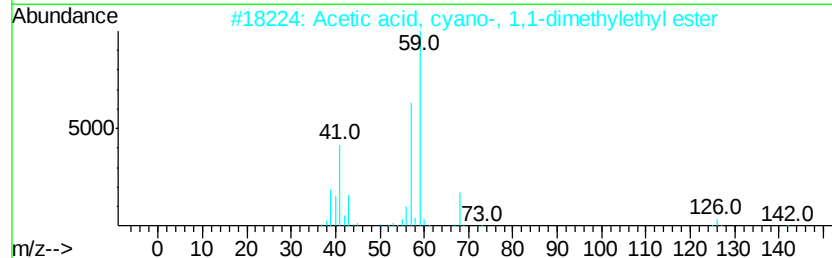
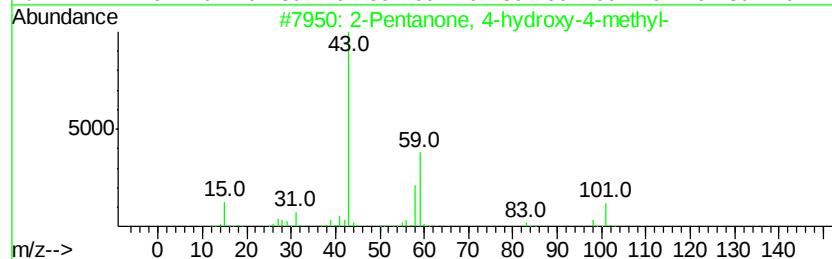
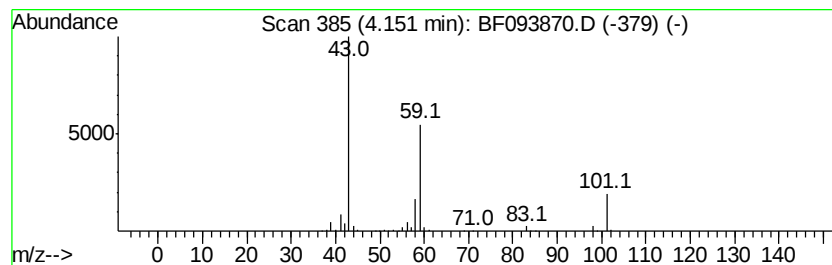
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.15	18.53 ng	1066280	1,4-Dichlorobenzene-d4	5.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Butane	58	C4H10	000106-97-8	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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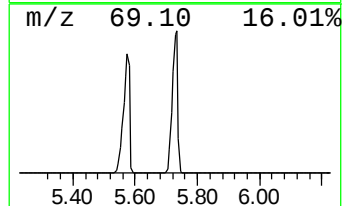
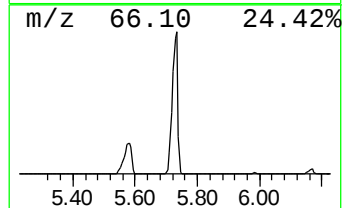
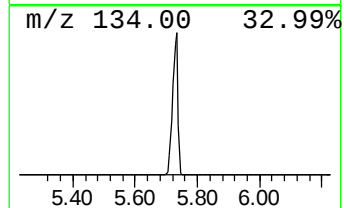
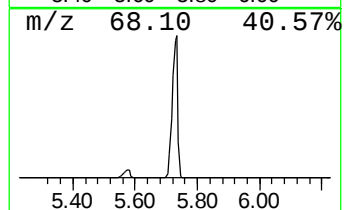
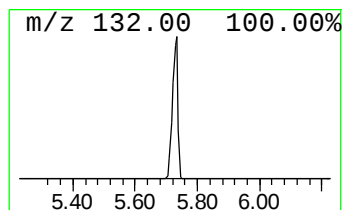
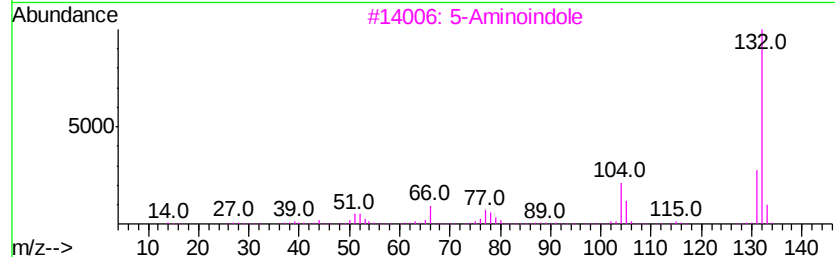
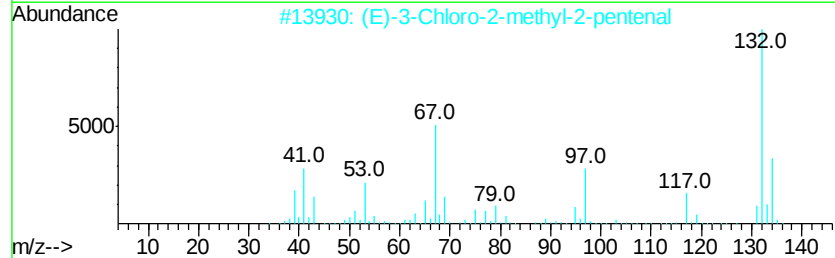
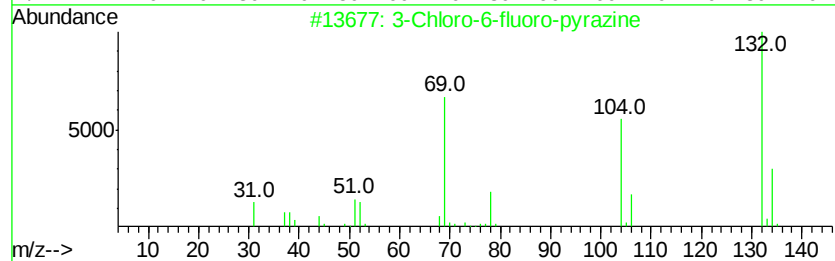
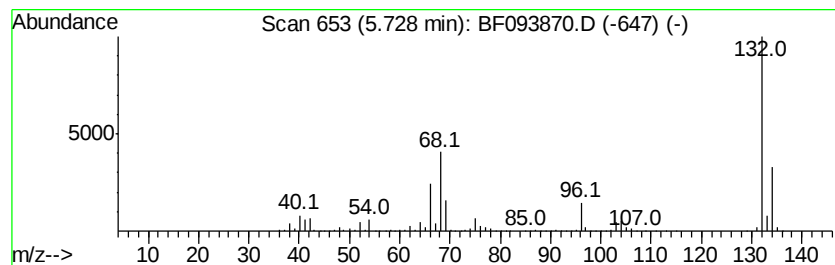
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	98.46 ng	5664970	1,4-Dichlorobenzene-d4	5.99

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		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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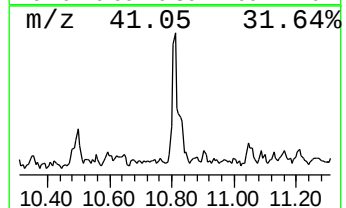
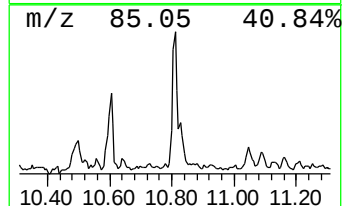
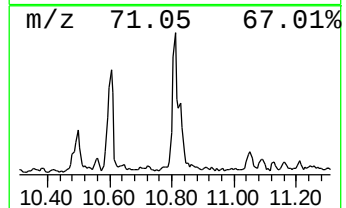
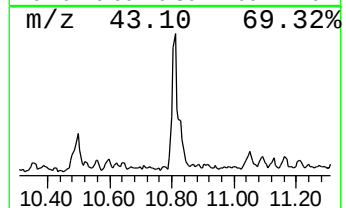
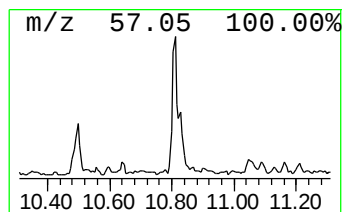
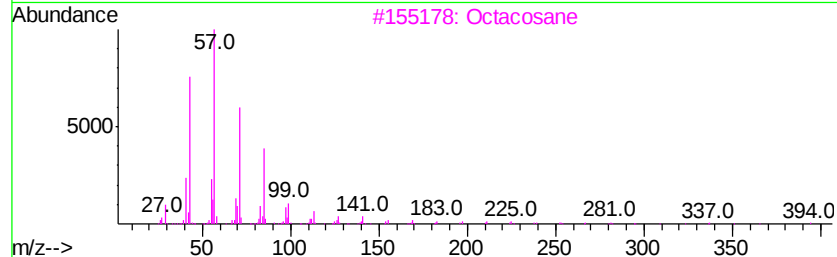
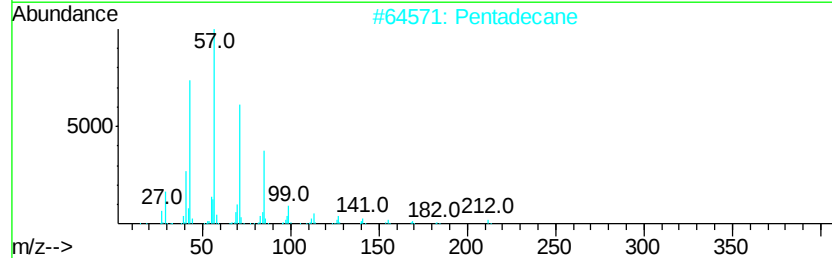
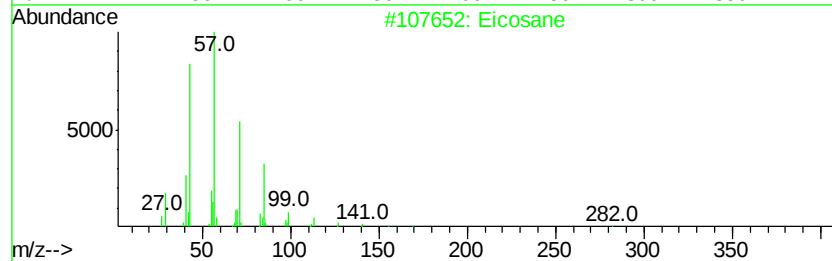
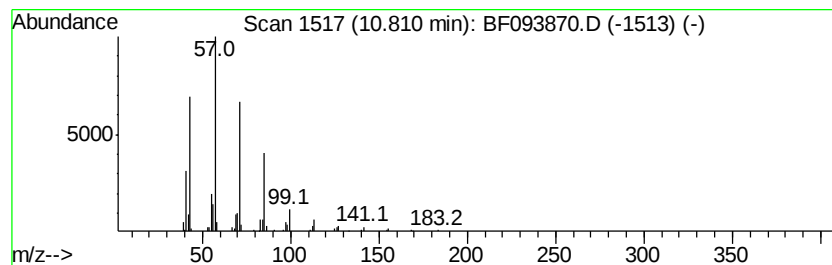
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Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	2.06 ng	152171	Phenanthrene-d10	11.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Pentadecane		212	C15H32	000629-62-9	91
3	Octacosane		394	C28H58	000630-02-4	90
4	Hexadecane		226	C16H34	000544-76-3	90
5	Heptacosane		380	C27H56	000593-49-7	90



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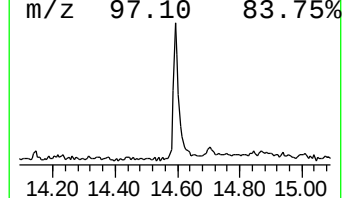
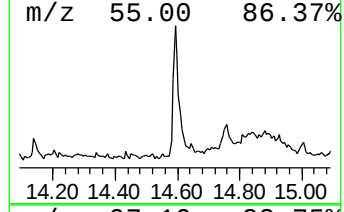
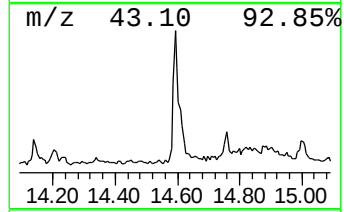
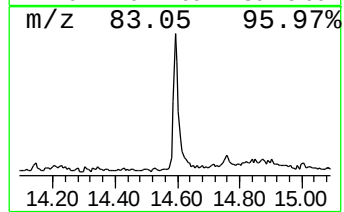
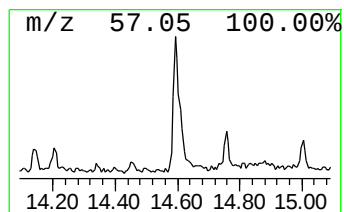
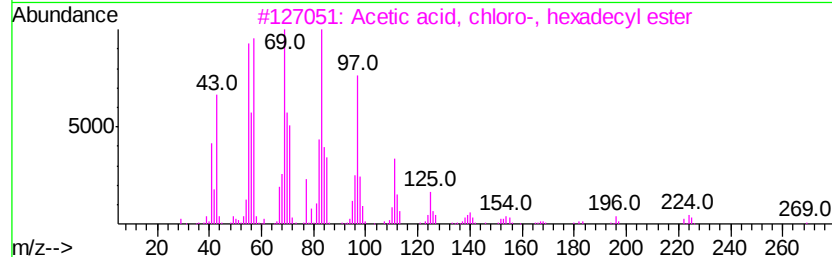
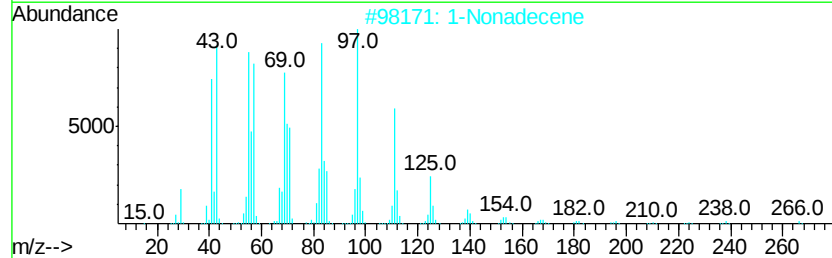
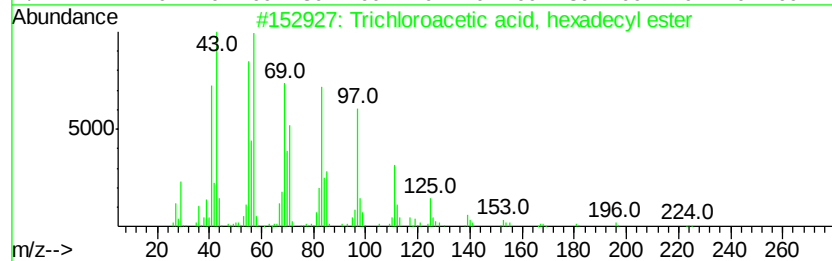
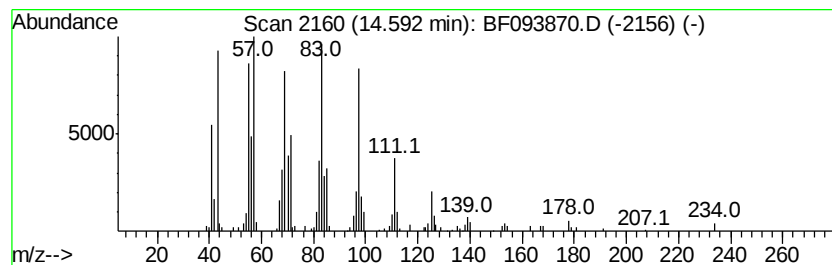
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.59	4.92 ng	282304	Chrysene-d12	14.70	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2	1-Nonadecene	266	C19H38	018435-45-5	87
3	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	87
4	Cyclopentadecane	210	C15H30	000295-48-7	86
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032217\
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Operator : SJ/MA
Sample : I2350-11
Misc :
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Instrument :
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ClientSampleId :
72-11937-VNJ-205-COMP

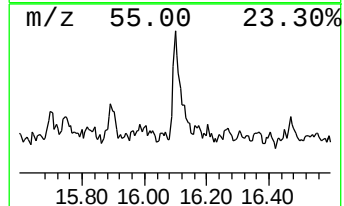
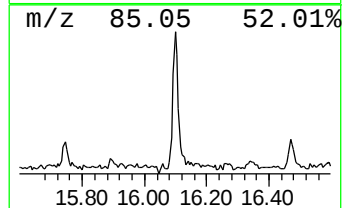
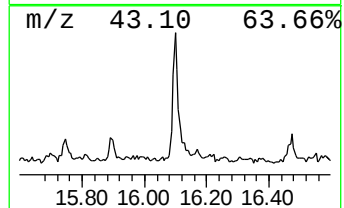
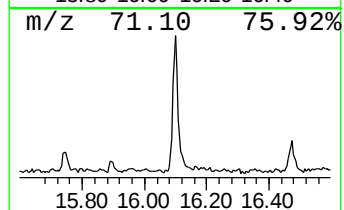
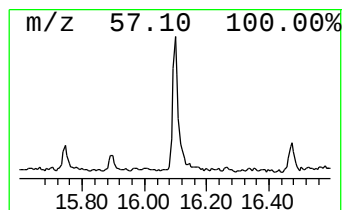
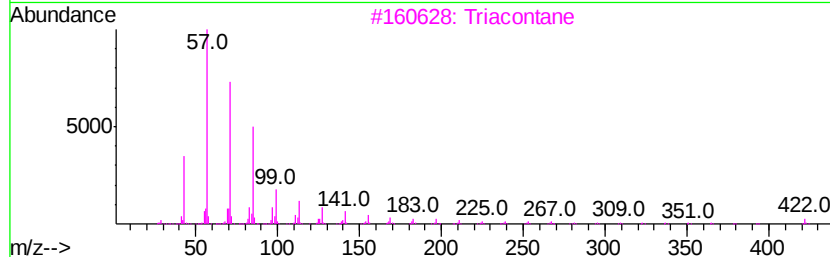
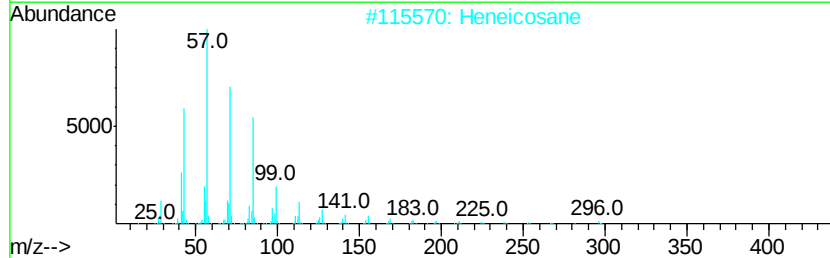
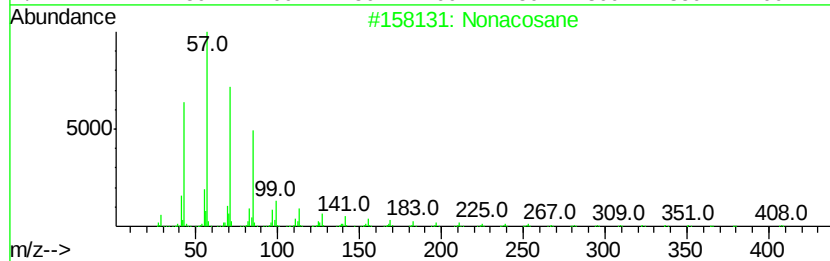
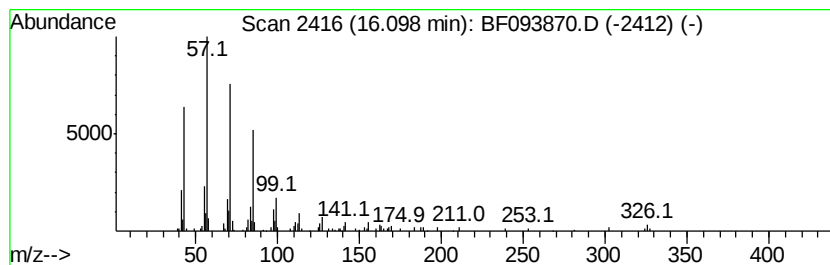
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	4.33 ng	200514	Perylene-d12	16.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacosane		408	C29H60	000630-03-5	90
2	Heneicosane		296	C21H44	000629-94-7	90
3	Triacontane		422	C30H62	000638-68-6	90
4	Nonadecane, 2-methyl-		282	C20H42	001560-86-7	87
5	Docosane		310	C22H46	000629-97-0	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032217\
Data File : BF093870.D
Acq On : 23 Mar 2017 9:03
Operator : SJ/MA
Sample : I2350-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11937-VNJ-205-COMP

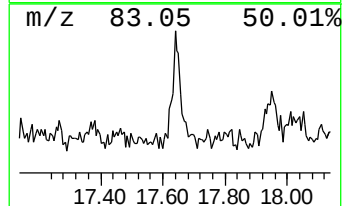
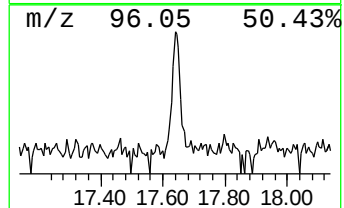
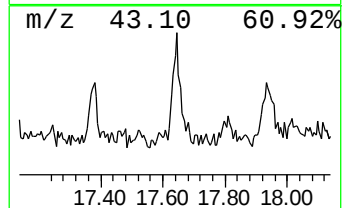
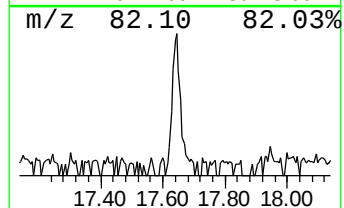
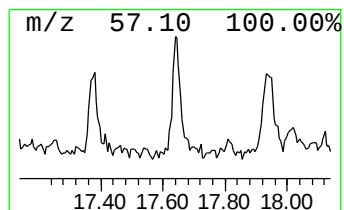
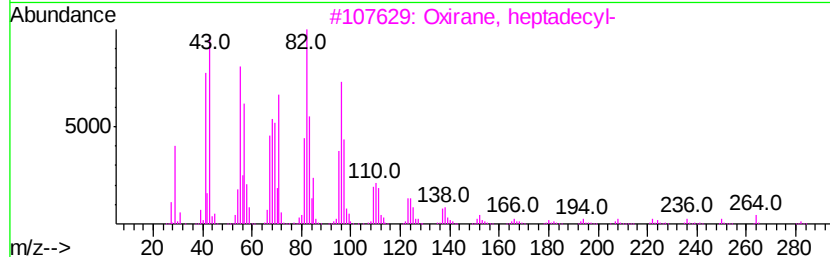
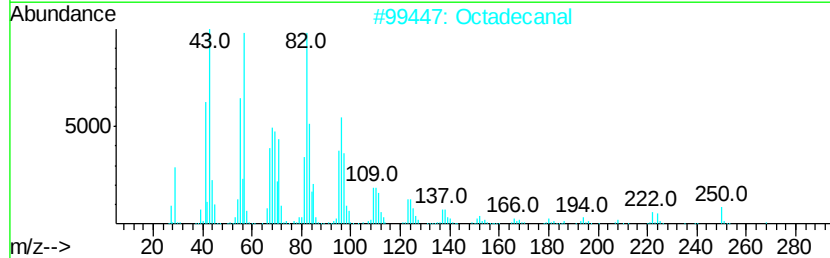
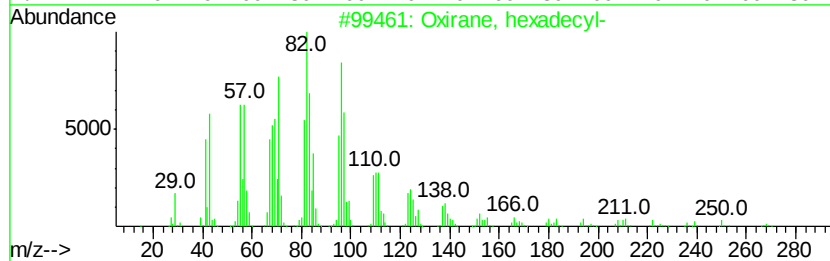
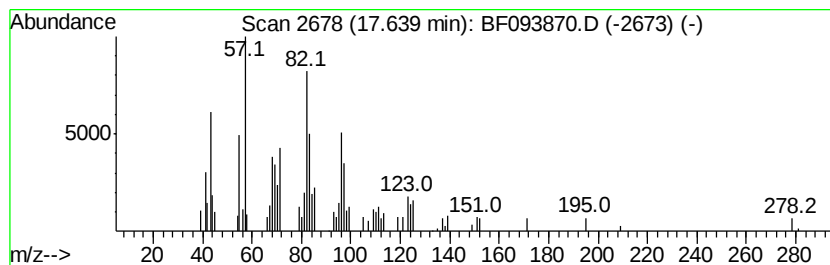
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, hexadecyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.64	2.03 ng	93816	Perylene-d12	16.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	62
2		Octadecanal	268	C18H36O	000638-66-4	58
3		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	49
4		Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	46
5		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032217\
Data File : BF093870.D
Acq On : 23 Mar 2017 9:03
Operator : SJ/MA
Sample : I2350-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11937-VNJ-205-COMP

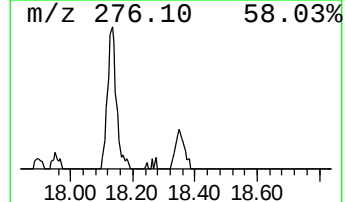
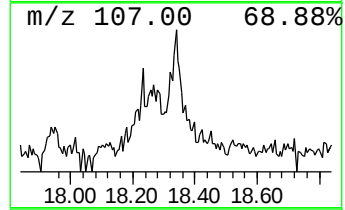
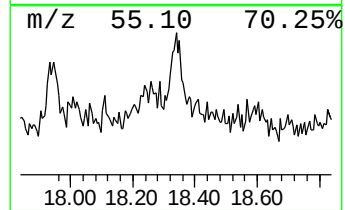
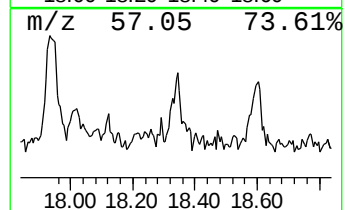
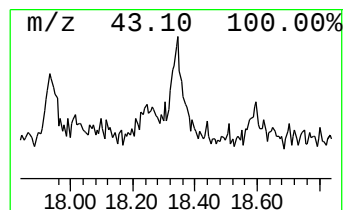
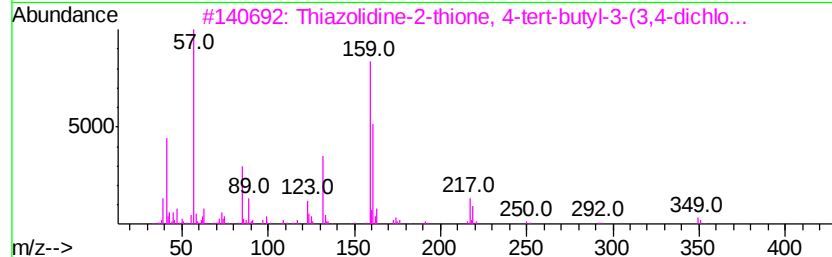
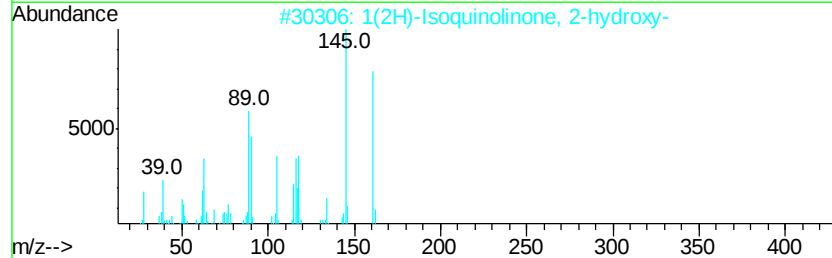
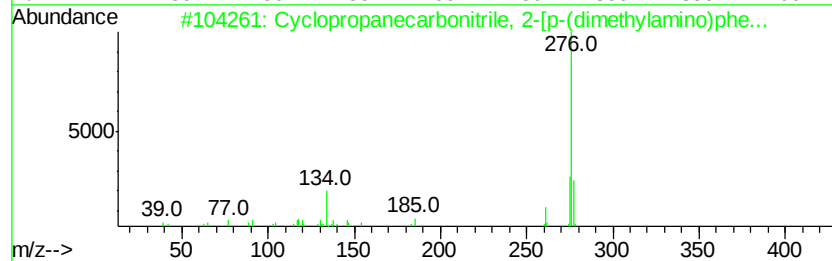
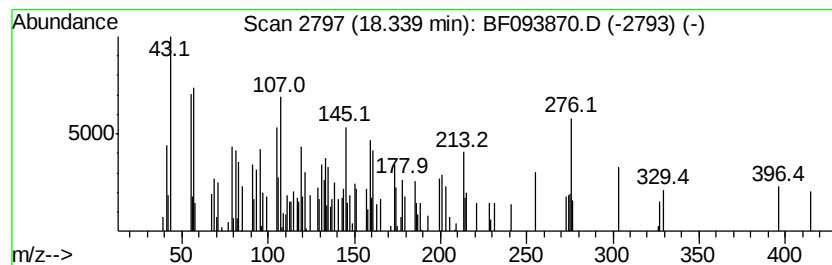
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown18.34 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	3.40 ng	157489	Perylene-d12	16.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropanecarbonitrile, 2-[p-(...	276	C19H20N2	032589-51-8	10
2		1(2H)-Isoquinolinone, 2-hydroxy-	161	C9H7NO2	021201-50-3	10
3		Thiazolidine-2-thione, 4-tert-bu...	349	C14H17Cl2NOS2	1000264-76-3	10
4		Pyrrol-5-amine, 4-(2-benzoxazolyl...	276	C16H12N4O	039116-39-7	9
5		2,3,5a,6,9,10-Hexahydro-1H-cyclo...	276	C14H16N2S2	1000148-50-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032217\
Data File : BF093870.D
Acq On : 23 Mar 2017 9:03
Operator : SJ/MA
Sample : I2350-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11937-VNJ-205-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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
Propane, 1,1-dime...	2.12	3.0	ng	170954	1	5.99	1150680	20.0
2-Pentanone, 4-hy...	4.15	18.5	ng	1066280	1	5.99	1150680	20.0
unknown5.73	5.73	98.5	ng	5664970	1	5.99	1150680	20.0
Eicosane	10.81	2.1	ng	152171	4	11.46	1476330	20.0
Trichloroacetic a...	14.59	4.9	ng	282304	5	14.70	1148600	20.0
Nonacosane	16.10	4.3	ng	200514	6	16.34	925774	20.0
Oxirane, hexadecyl-	17.64	2.0	ng	93816	6	16.34	925774	20.0
unknown18.34	18.34	3.4	ng	157489	6	16.34	925774	20.0