

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042517\  
 Data File : BF094615.D  
 Acq On : 25 Apr 2017 19:47  
 Operator : SJ/MA  
 Sample : I2832-01  
 Misc :  
 ALS Vial : 20 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TEST-PIT-RD-(0-3)

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-BF041717.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	3.907	331	335	345	rBV	281972	341805	10.51%	1.184%
2	4.301	398	402	421	rBV	2814076	2952824	90.77%	10.226%
3	5.378	580	585	602	rBV	2513411	3016605	92.73%	10.447%
4	5.507	602	607	610	rBV	3047307	3062415	94.14%	10.605%
5	5.754	645	649	652	rBV	806380	771564	23.72%	2.672%
6	5.931	674	679	682	rBV	2626801	2381653	73.21%	8.248%
7	6.401	754	759	762	rBV	1902420	1897790	58.34%	6.572%
8	7.007	860	862	873	rVB2	19730	34037	1.05%	0.118%
9	7.242	898	902	906	rBV	1105578	1027292	31.58%	3.558%
10	8.431	1101	1104	1116	rBV2	26812	38038	1.17%	0.132%
11	8.572	1123	1128	1131	rBV	3064535	3253164	100.00%	11.266%
12	9.066	1209	1212	1217	rBV	200477	185842	5.71%	0.644%
13	9.377	1258	1265	1274	rBV2	1056175	1079899	33.20%	3.740%
14	9.977	1364	1367	1371	rVB	86315	73364	2.26%	0.254%
15	10.248	1406	1413	1416	rBV	27669	47210	1.45%	0.163%
16	10.301	1419	1422	1427	rVB	69384	68676	2.11%	0.238%
17	10.354	1427	1431	1437	rBV	1432822	1479970	45.49%	5.125%
18	10.560	1463	1466	1469	rBV	92092	102994	3.17%	0.357%
19	11.119	1557	1561	1563	rBV	44239	41986	1.29%	0.145%
20	11.201	1571	1575	1578	rBV	893709	886359	27.25%	3.069%
21	11.224	1578	1579	1585	rVB	84422	72954	2.24%	0.253%
22	11.448	1614	1617	1621	rBV	40221	41551	1.28%	0.144%
23	11.554	1631	1635	1643	rBV	348634	435389	13.38%	1.508%
24	11.936	1697	1700	1707	rBV4	38548	56047	1.72%	0.194%
25	12.248	1747	1753	1756	rBV	46913	48068	1.48%	0.166%
26	12.689	1824	1828	1833	rVB	83493	97260	2.99%	0.337%
27	12.813	1845	1849	1854	rBV	30447	33677	1.04%	0.117%
28	12.966	1872	1875	1880	rVB	95284	99176	3.05%	0.343%
29	13.148	1902	1906	1908	rBV	356497	363227	11.17%	1.258%
30	13.177	1908	1911	1915	rVB	2000118	2187550	67.24%	7.576%
31	13.283	1926	1929	1933	rVB2	45345	42298	1.30%	0.146%
32	13.383	1935	1946	1949	rBV3	17706	32875	1.01%	0.114%
33	13.607	1980	1984	1989	rBV	392672	391884	12.05%	1.357%
34	14.048	2055	2059	2064	rVB	82072	85076	2.62%	0.295%

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Integration Parameters: rteint.p  
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 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 >  
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35	14.348	2105	2110	2118	rBV3	63643	114648	3.52%	0.397%
36	14.448	2122	2127	2135	rBV	707130	883032	27.14%	3.058%
37	14.654	2160	2162	2169	rVB	48279	50679	1.56%	0.176%
38	15.389	2285	2287	2292	rVB5	25396	35230	1.08%	0.122%
39	15.677	2333	2336	2339	rBV	38604	59547	1.83%	0.206%
40	15.959	2381	2384	2390	rVB2	39556	54264	1.67%	0.188%
41	16.024	2391	2395	2399	rBV	33480	48623	1.49%	0.168%
42	16.077	2399	2404	2411	rBV	632784	733710	22.55%	2.541%
43	16.201	2421	2425	2429	rBV6	21922	33847	1.04%	0.117%
44	16.659	2500	2503	2506	rBV3	36258	51651	1.59%	0.179%
45	16.695	2507	2509	2517	rVB4	52276	80806	2.48%	0.280%

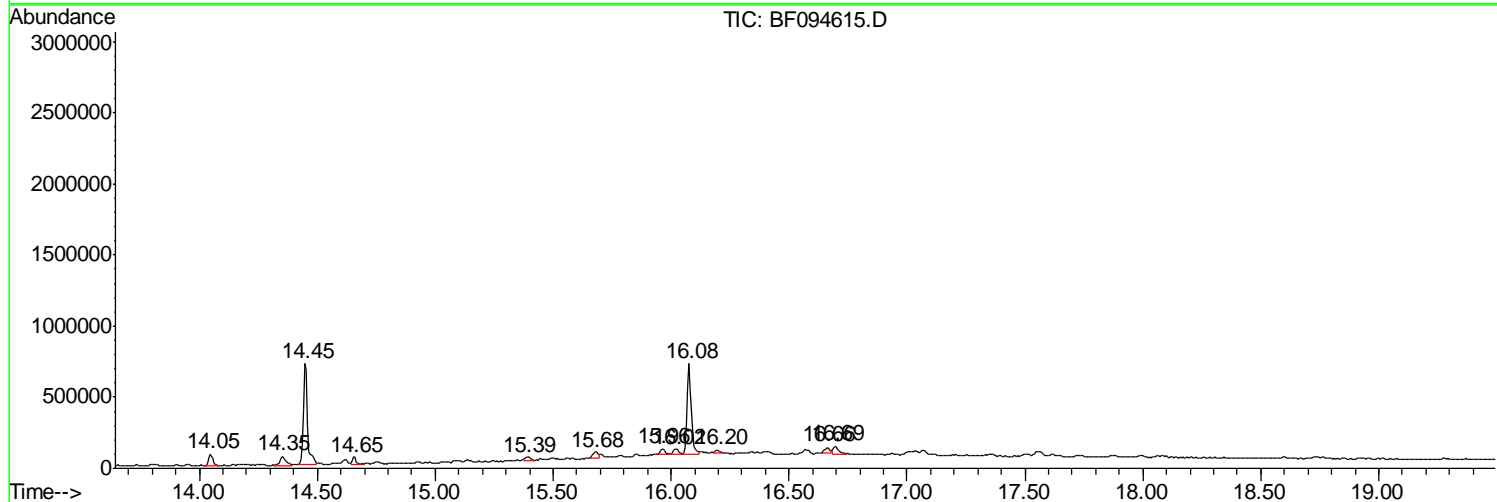
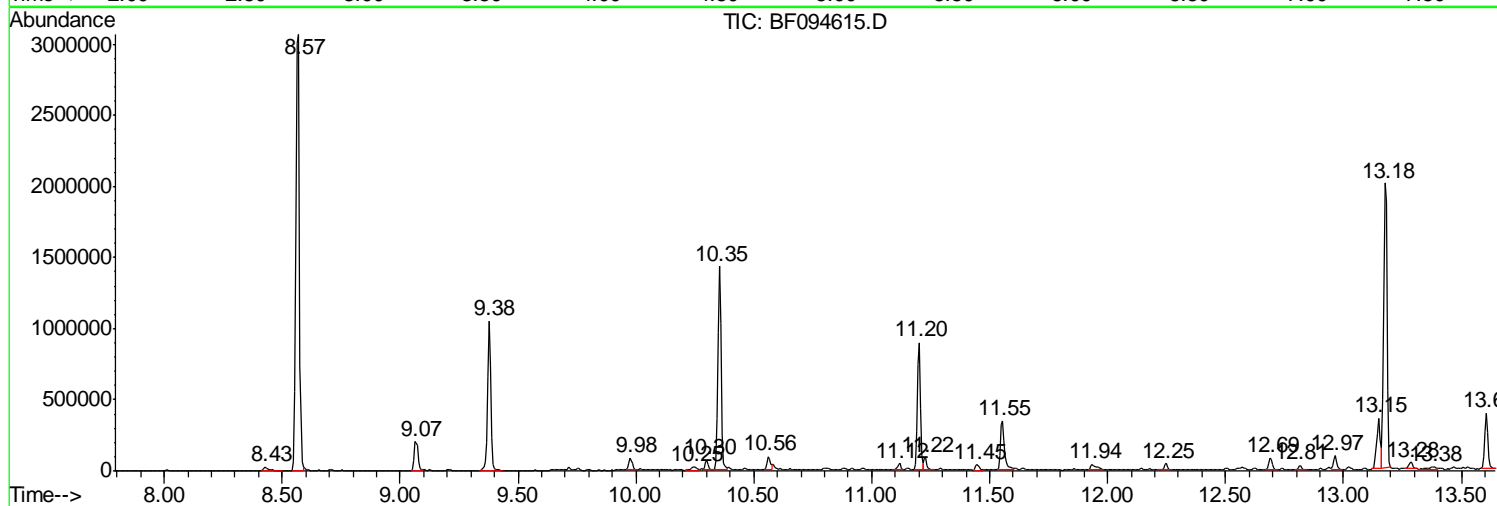
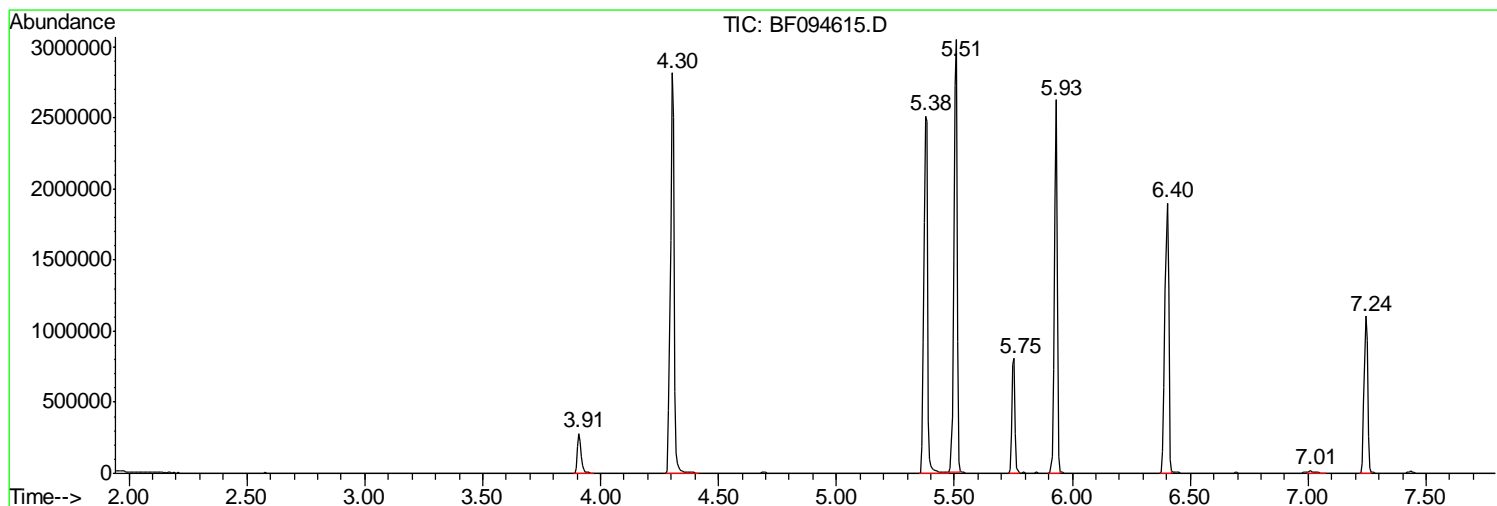
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**Instrument :**  
 BNA\_F  
**ClientSampled :**  
 TEST-PIT-RD-(0-3)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.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-BF041717.M  
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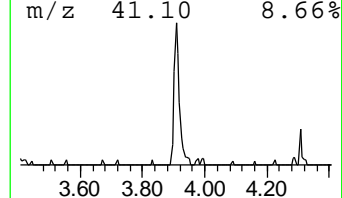
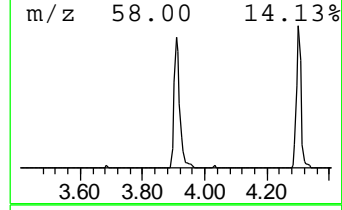
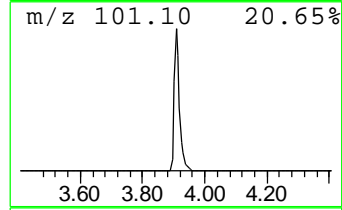
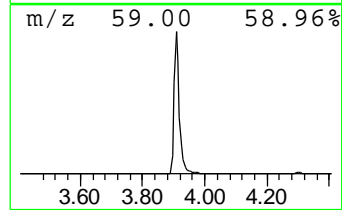
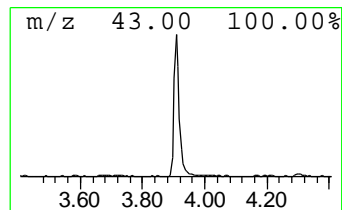
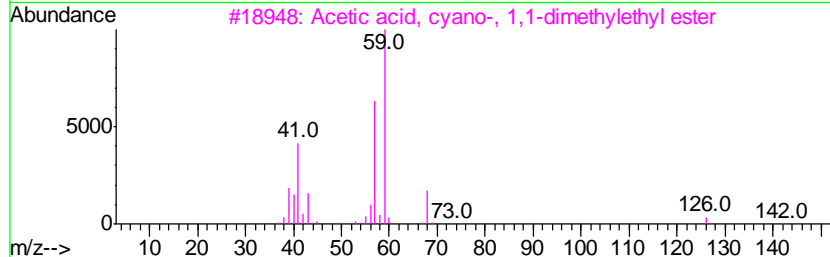
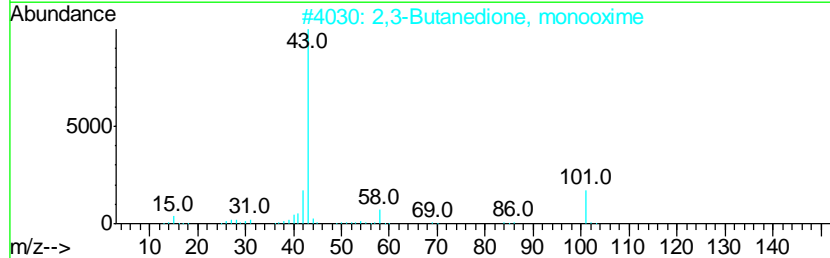
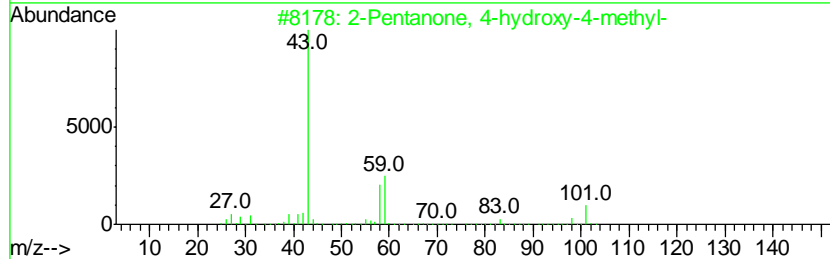
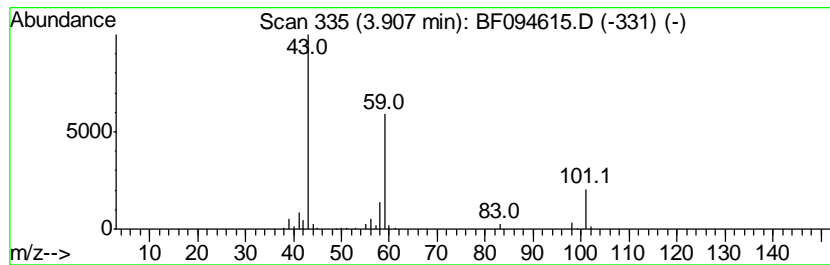
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.91	8.86 ng	341805	1,4-Dichlorobenzene-d4	5.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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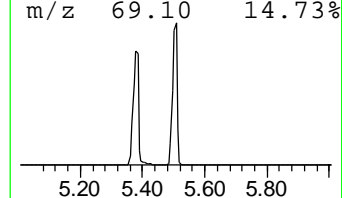
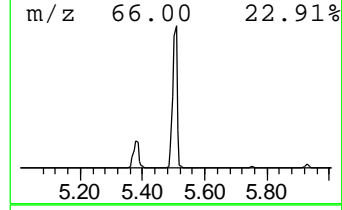
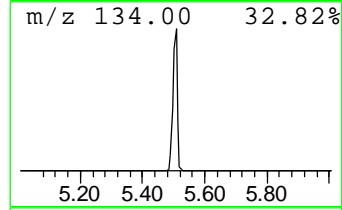
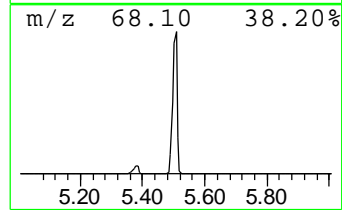
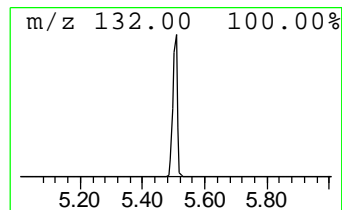
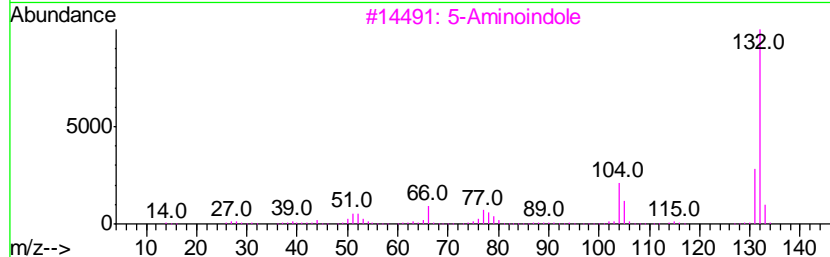
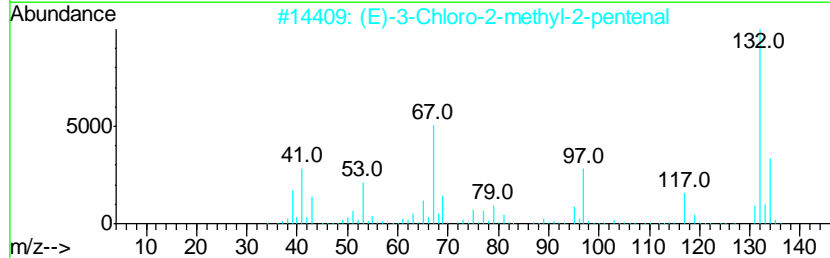
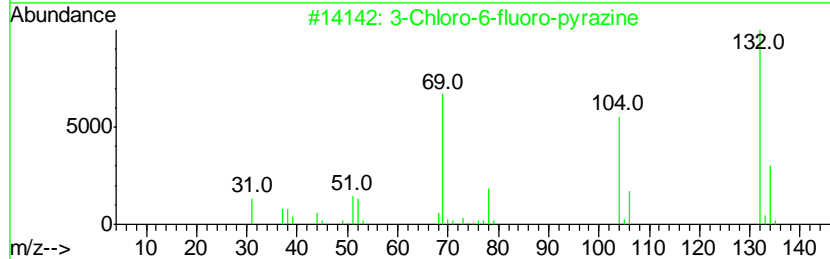
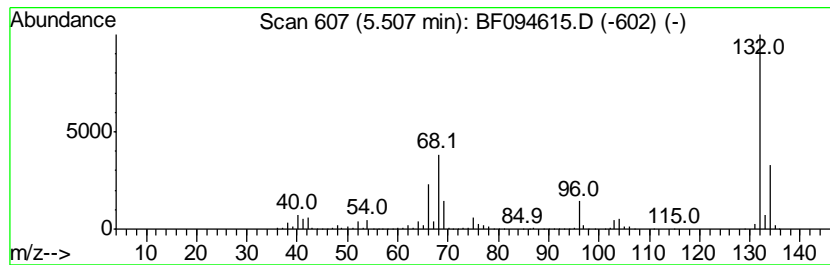
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
 Peak Number 2 unknown5.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	79.38 ng	3062420	1,4-Dichlorobenzene-d4	5.75

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

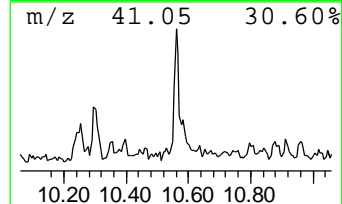
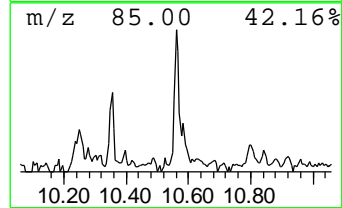
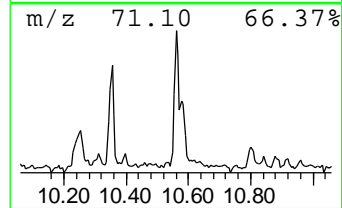
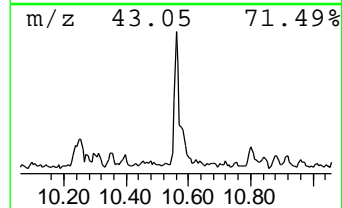
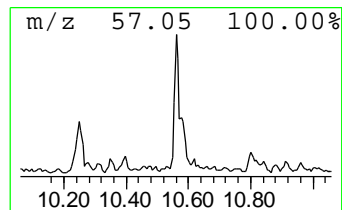
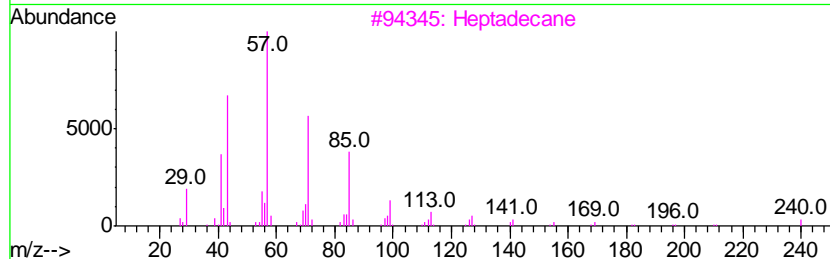
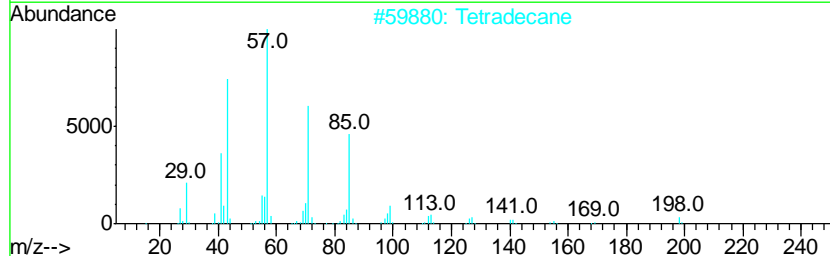
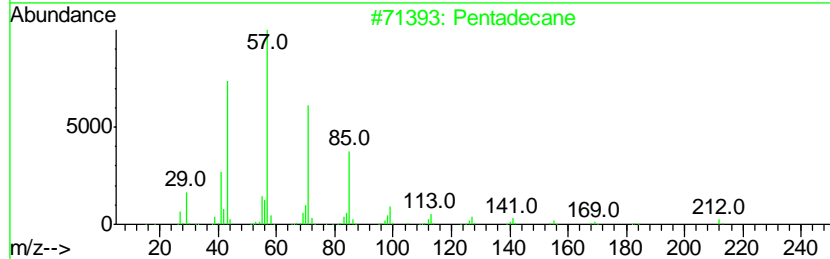
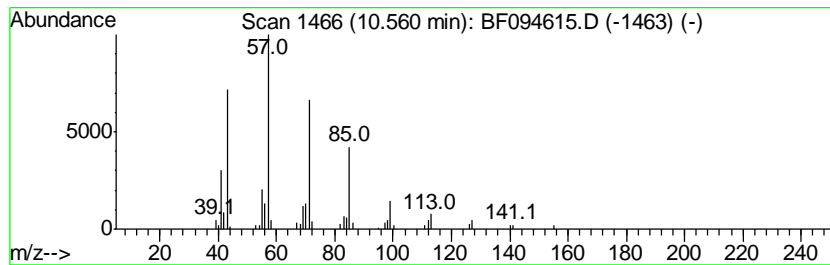
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 4 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	2.32 ng	102994	Phenanthrene-d10	11.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	91
2		Tetradecane	198	C14H30	000629-59-4	91
3		Heptadecane	240	C17H36	000629-78-7	90
4		Hexadecane	226	C16H34	000544-76-3	90
5		Tetracosane	338	C24H50	000646-31-1	90



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

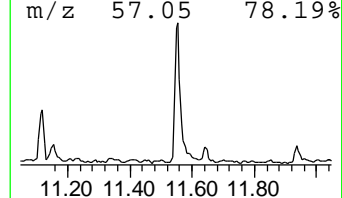
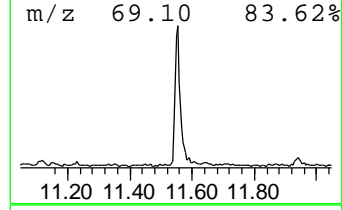
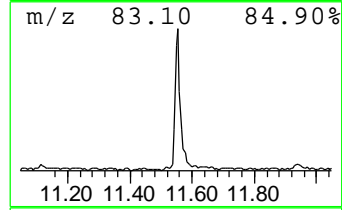
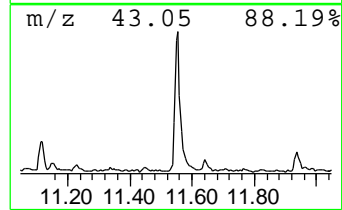
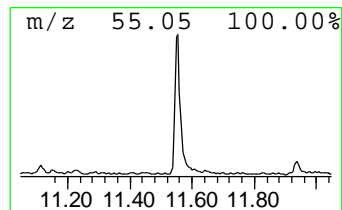
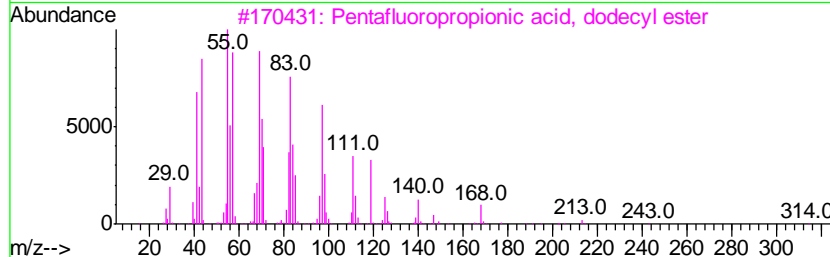
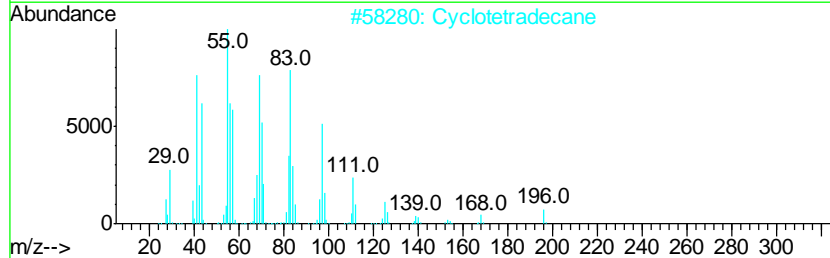
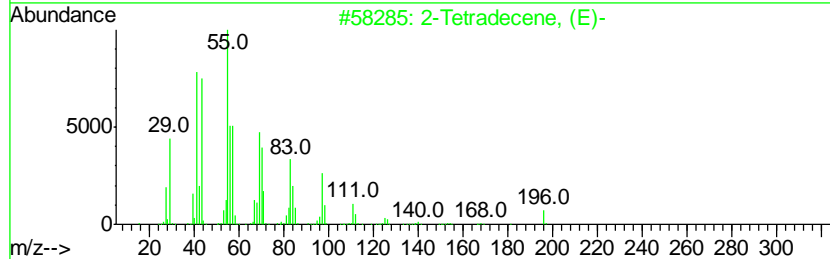
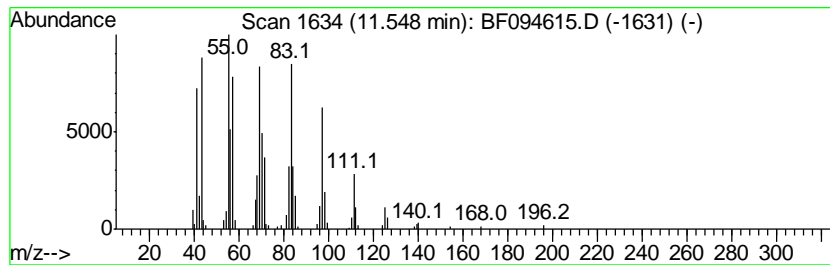
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 5 2-Tetradecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	9.82 ng	435389	Phenanthrene-d10	11.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Tetradecene, (E)-	196	C14H28	035953-54-9	96
2		Cyclotetradecane	196	C14H28	000295-17-0	96
3		Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	94
4		1-Hexadecanol	242	C16H34O	036653-82-4	94
5		1-Tetradecene	196	C14H28	001120-36-1	93



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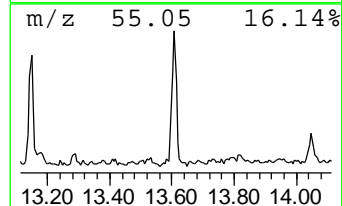
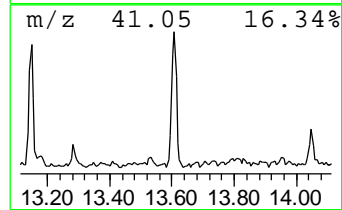
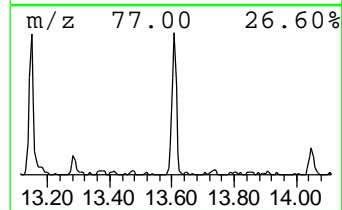
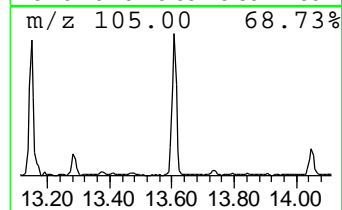
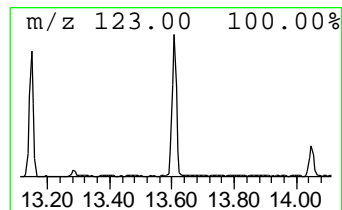
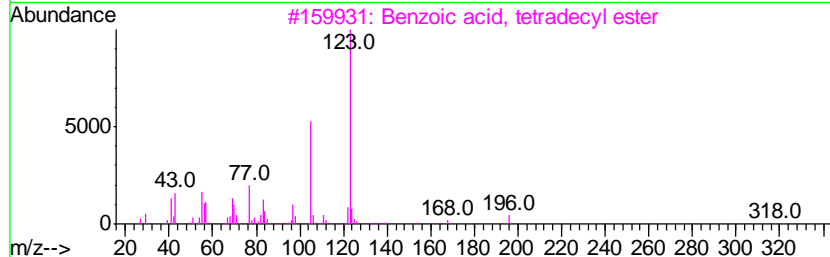
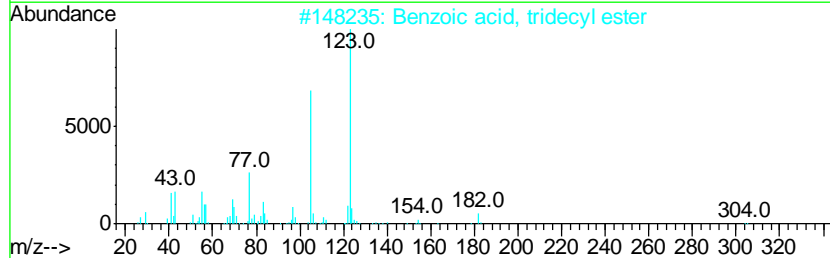
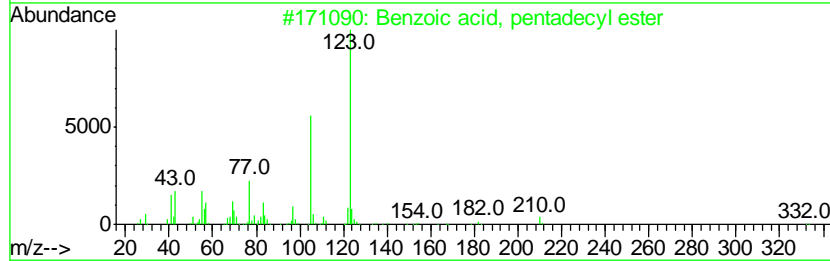
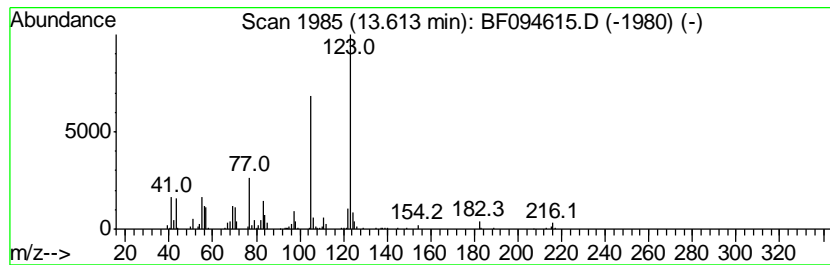
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 8 Benzoic acid, pentadecyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	8.88 ng	391884	Chrysene-d12	14.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, pentadecyl ester	332	C22H36O2	1000340-22-8	91
2		Benzoic acid, tridecyl ester	304	C20H32O2	1000340-22-6	91
3		Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	91
4		Benzoic acid, octadecyl ester	374	C25H42O2	1000340-23-1	91
5		Benzoic acid, heptadecyl ester	360	C24H40O2	1000340-23-0	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042517\  
 Data File : BF094615.D  
 Acq On : 25 Apr 2017 19:47  
 Operator : SJ/MA  
 Sample : I2832-01  
 Misc :  
 ALS Vial : 20 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TEST-PIT-RD-(0-3)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

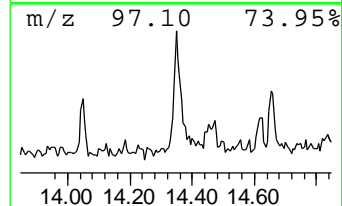
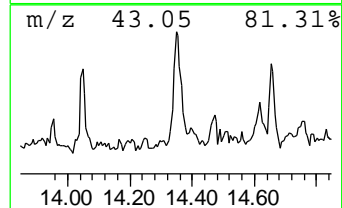
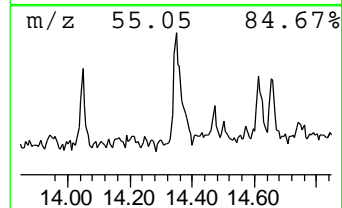
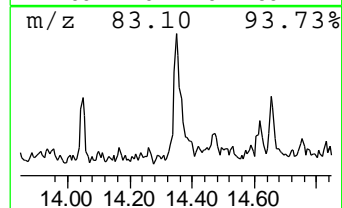
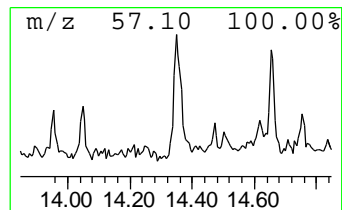
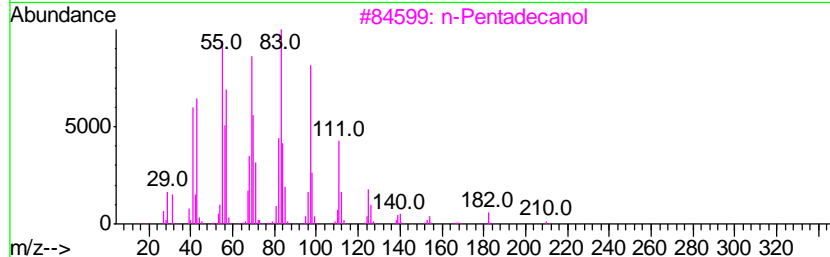
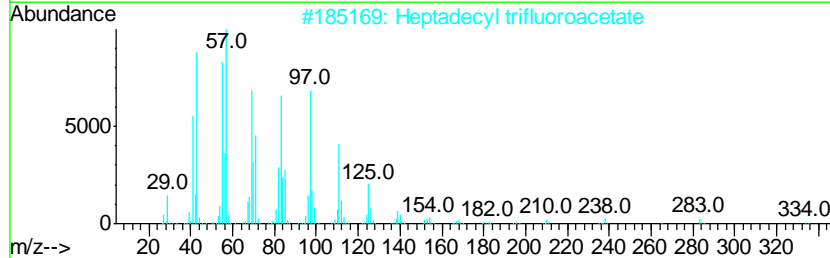
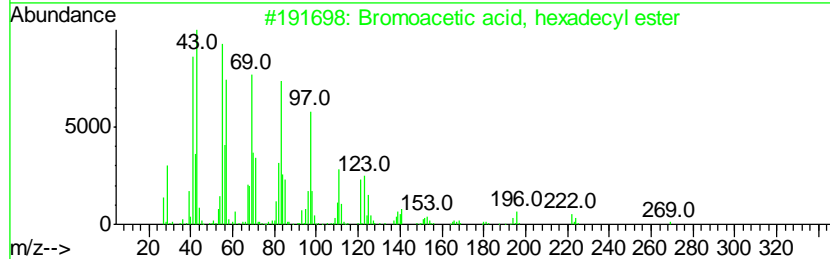
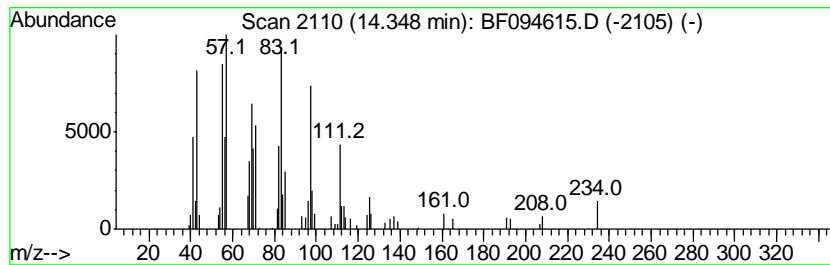
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 9 Bromoacetic acid, hexadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.60 ng	114648	Chrysene-d12	14.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3		n-Pentadecanol	228	C15H32O	000629-76-5	90
4		1-Nonadecene	266	C19H38	018435-45-5	90
5		1-Eicosanol	298	C20H42O	000629-96-9	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042517\  
 Data File : BF094615.D  
 Acq On : 25 Apr 2017 19:47  
 Operator : SJ/MA  
 Sample : I2832-01  
 Misc :  
 ALS Vial : 20 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TEST-PIT-RD-(0-3)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

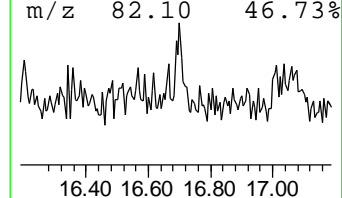
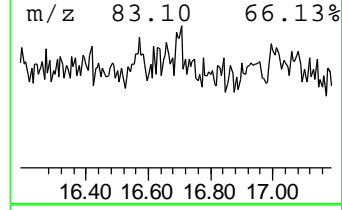
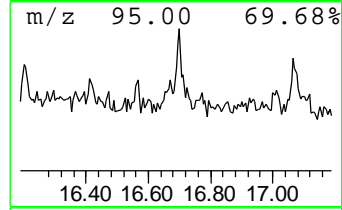
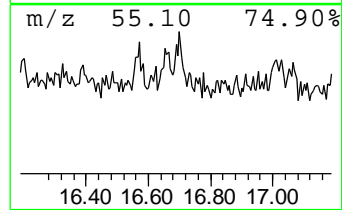
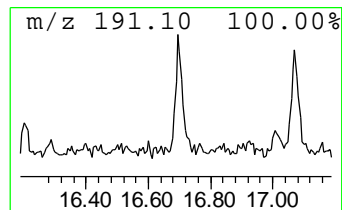
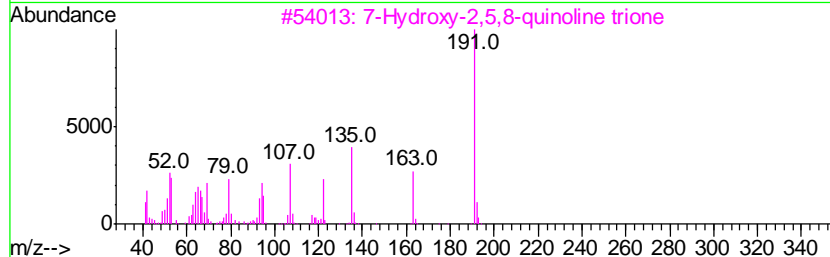
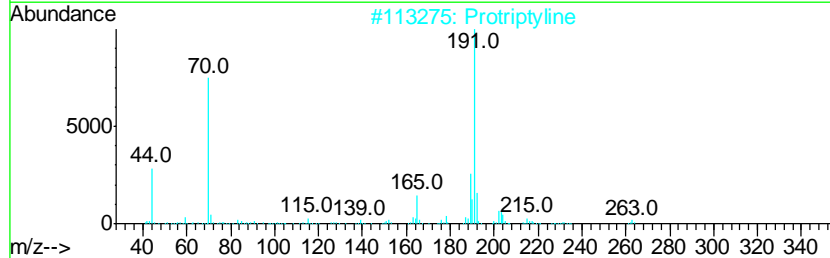
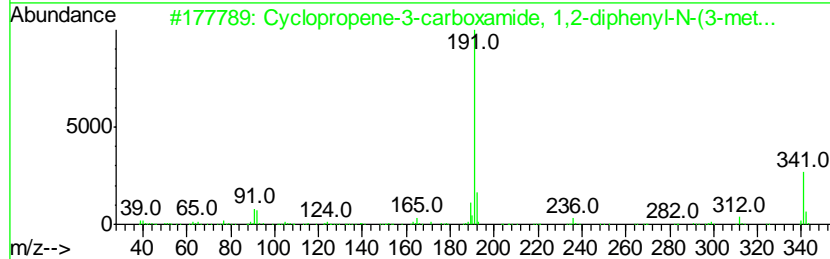
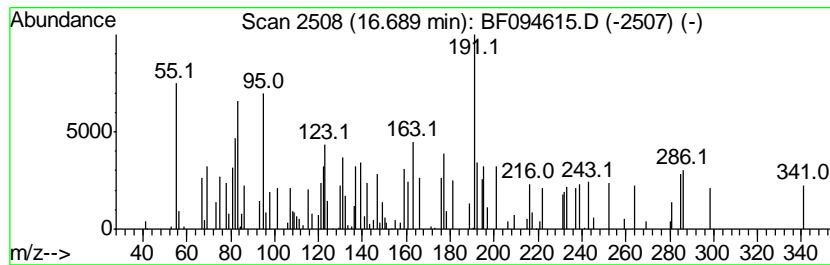
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 10 unknown16.69 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	2.20 ng	80806	Perylene-d12	16.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropene-3-carboxamide, 1,2-...	341	C23H19NO2	1000264-18-3	38
2		Protriptyline	263	C19H21N	000438-60-8	35
3		7-Hydroxy-2,5,8-quinoline trione	191	C9H5NO4	015544-54-4	35
4		Silane, 1,3-decadiynyltrimethyl-	206	C13H22Si	084751-17-7	32
5		(3-Cyano-6-ethyl-5-methyl-pyridi...	264	C13H16N2O2S	1000300-45-4	32



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF042517\  
Data File : BF094615.D  
Acq On : 25 Apr 2017 19:47  
Operator : SJ/MA  
Sample : I2832-01  
Misc :  
ALS Vial : 20 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TEST-PIT-RD-(0-3)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF041717.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...	3.91	8.9	ng	341805	1	5.75	771564	20.0
unknown5.51	5.51	79.4	ng	3062420	1	5.75	771564	20.0
Pentadecane	10.56	2.3	ng	102994	4	11.20	886359	20.0
2-Tetradecene, (E)-	11.55	9.8	ng	435389	4	11.20	886359	20.0
Benzoic acid, pen...	13.61	8.9	ng	391884	5	14.45	883032	20.0
Bromoacetic acid,...	14.35	2.6	ng	114648	5	14.45	883032	20.0
unknown16.69	16.69	2.2	ng	80806	6	16.08	733710	20.0