

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
 Data File : BF097650.D
 Acq On : 12 Aug 2017 23:40
 Operator : SJ/JU
 Sample : I4649-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-13(0-10)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-BF081117.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	4.769	520	524	542	rBV	91070	251192	9.09%	1.096%
2	5.451	636	640	675	rBV	1403667	2763888	100.00%	12.060%
3	7.098	915	920	929	rBV	1525214	2415953	87.41%	10.541%
4	7.175	929	933	954	rVB	1625800	2730970	98.81%	11.916%
5	7.398	968	971	978	rVB3	19337	32469	1.17%	0.142%
6	7.504	985	989	1003	rBV	580318	764666	27.67%	3.336%
7	7.739	1024	1029	1048	rVB	1205604	1660093	60.06%	7.243%
8	8.416	1140	1144	1163	rBV	992873	1503355	54.39%	6.560%
9	9.533	1329	1334	1346	rBV	727704	1045635	37.83%	4.562%
10	9.639	1349	1352	1364	rVB5	16328	33402	1.21%	0.146%
11	11.310	1630	1636	1647	rBV	1466511	1925841	69.68%	8.403%
12	12.004	1749	1754	1764	rBV	292716	382751	13.85%	1.670%
13	12.357	1809	1814	1831	rVB2	744691	1000860	36.21%	4.367%
14	13.204	1952	1958	1964	rBV2	33327	45642	1.65%	0.199%
15	13.562	2010	2019	2022	rBV4	16515	36557	1.32%	0.160%
16	13.657	2030	2035	2047	rBV	722790	1061978	38.42%	4.634%
17	13.974	2085	2089	2092	rBV	52903	70705	2.56%	0.309%
18	14.704	2209	2213	2217	rBV	34216	47771	1.73%	0.208%
19	14.756	2217	2222	2226	rVV	622477	824614	29.84%	3.598%
20	14.792	2226	2228	2236	rVB	75323	111546	4.04%	0.487%
21	14.892	2241	2245	2248	rVV	23333	29247	1.06%	0.128%
22	15.598	2362	2365	2369	rBV3	23628	31363	1.13%	0.137%
23	15.703	2380	2383	2387	rBV3	36935	50438	1.82%	0.220%
24	16.533	2521	2524	2525	rBV	41670	42855	1.55%	0.187%
25	16.562	2525	2529	2533	rVB	205420	248667	9.00%	1.085%
26	16.862	2576	2580	2586	rBV	257111	307025	11.11%	1.340%
27	17.033	2606	2609	2612	rBV2	41314	46882	1.70%	0.205%
28	17.109	2617	2622	2629	rVV	941478	1091569	39.49%	4.763%
29	17.503	2687	2689	2694	rVB	50028	52536	1.90%	0.229%
30	18.362	2832	2835	2838	rVB2	50600	68933	2.49%	0.301%
31	18.456	2846	2851	2854	rBV2	484898	662100	23.96%	2.889%
32	18.486	2854	2856	2865	rVB2	105989	180580	6.53%	0.788%
33	18.727	2895	2897	2899	rBV3	45701	35872	1.30%	0.157%
34	18.750	2899	2901	2902	rBV	57282	39204	1.42%	0.171%

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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	19.721	3063	3066	3075	rBV	146759	352376	12.75%	1.538%
36	20.015	3113	3116	3120	rBV	72696	92502	3.35%	0.404%
37	20.074	3124	3126	3130	rVV	79939	94363	3.41%	0.412%
38	20.127	3131	3135	3143	rVB	411899	535019	19.36%	2.334%
39	20.950	3273	3275	3276	rBV2	50676	40044	1.45%	0.175%
40	22.591	3553	3554	3556	rBV2	35912	32630	1.18%	0.142%
41	22.691	3567	3571	3572	rBV4	43272	60262	2.18%	0.263%
42	22.844	3595	3597	3598	rBV2	42895	43250	1.56%	0.189%
43	23.644	3732	3733	3735	rBV2	40620	40173	1.45%	0.175%
44	23.821	3761	3763	3764	rBV2	30628	30908	1.12%	0.135%

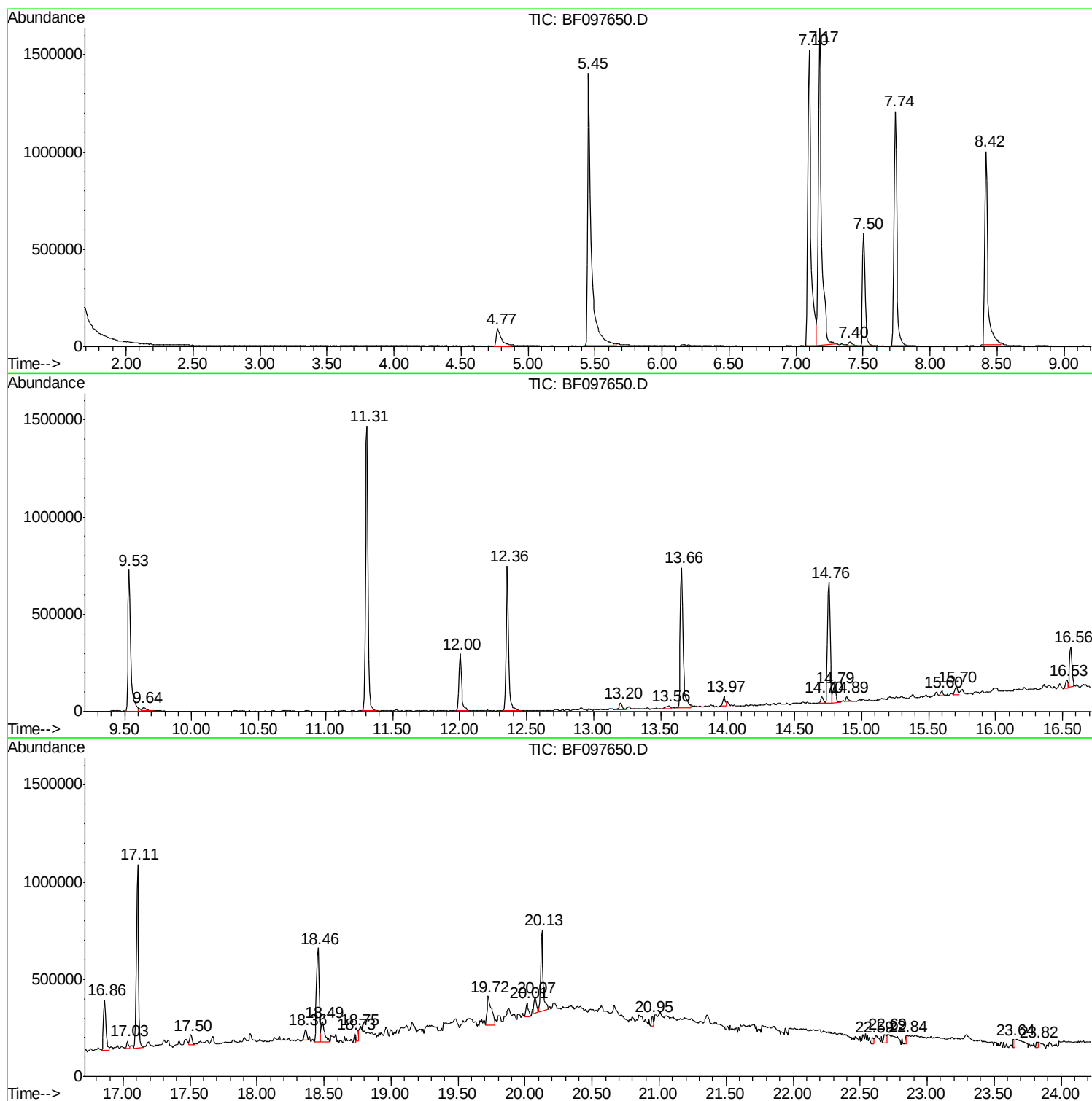
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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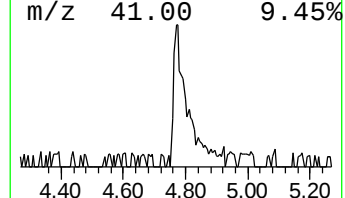
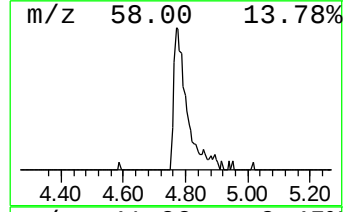
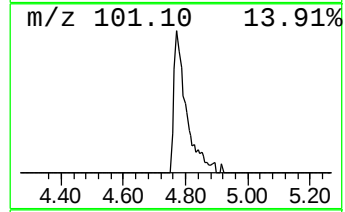
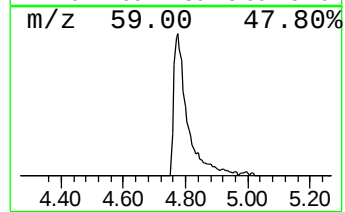
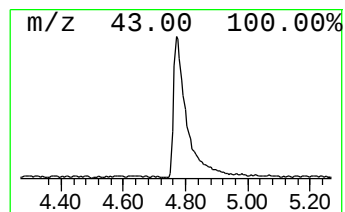
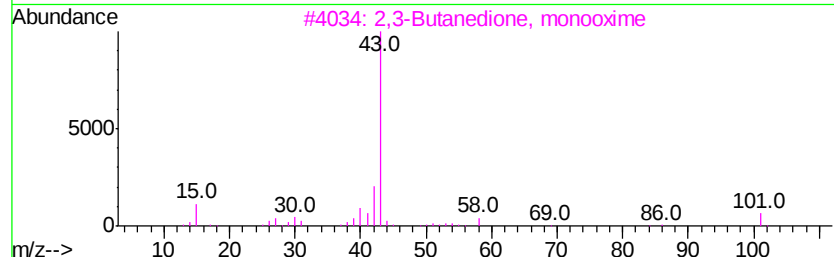
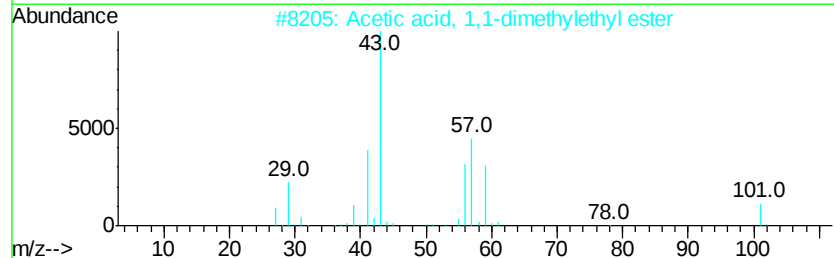
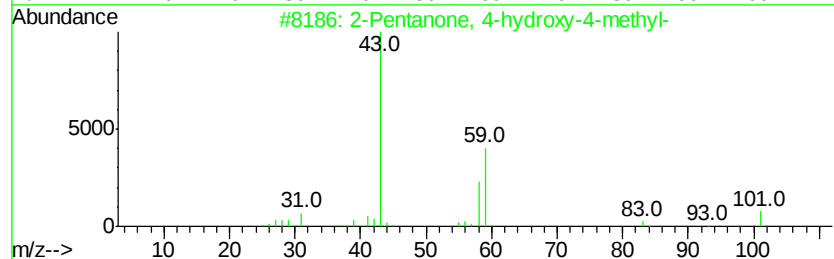
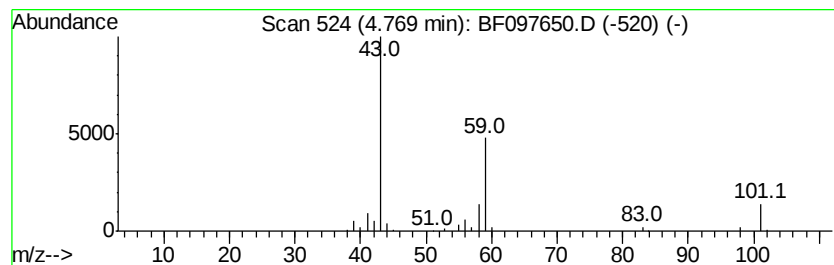
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	6.57 ng	251192	1,4-Dichlorobenzene-d4	7.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



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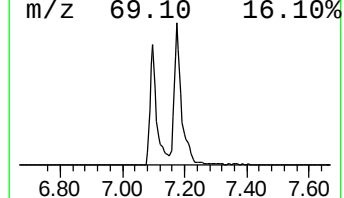
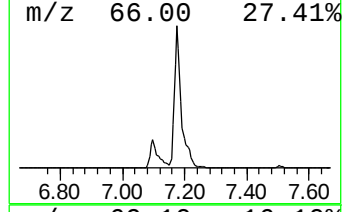
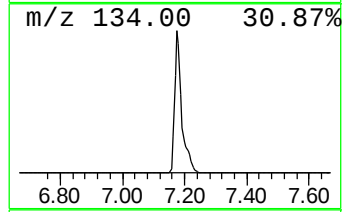
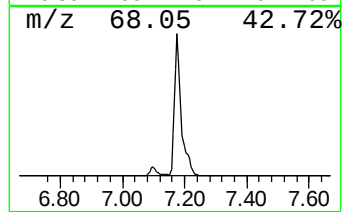
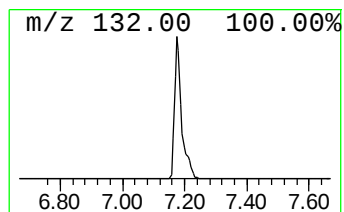
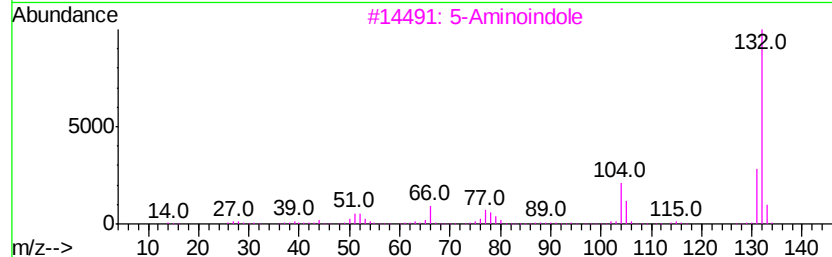
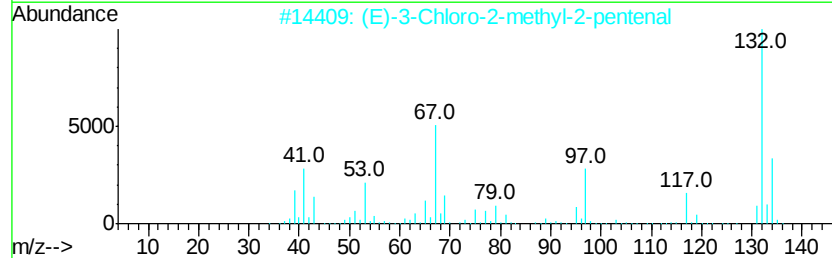
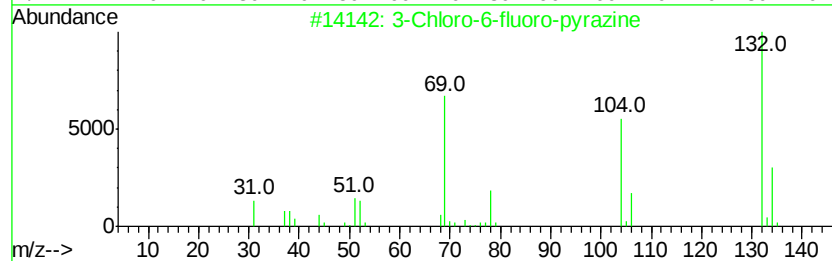
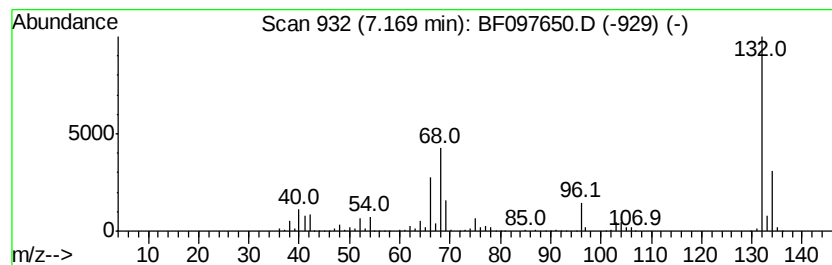
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Peak Number 2 unknown7.17 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.17	71.43 ng	2730970	1,4-Dichlorobenzene-d4	7.50

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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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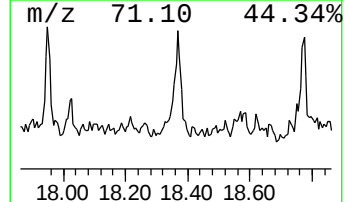
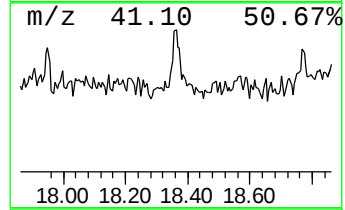
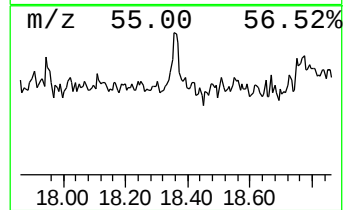
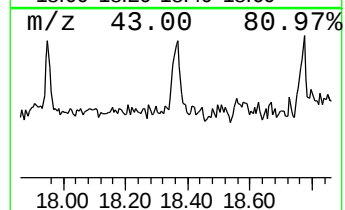
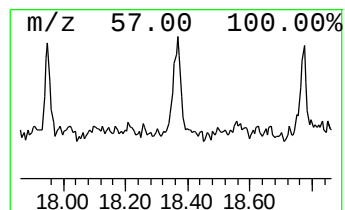
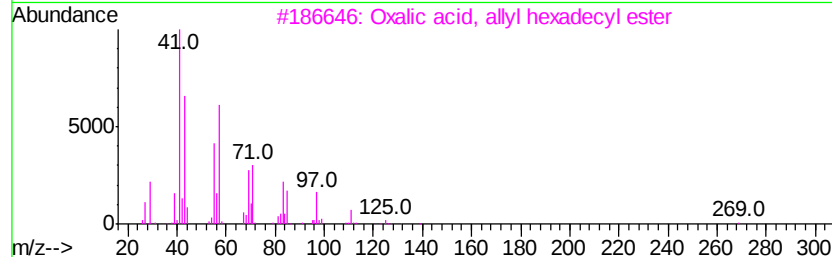
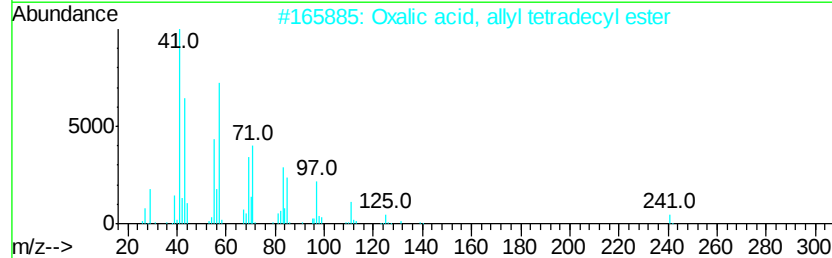
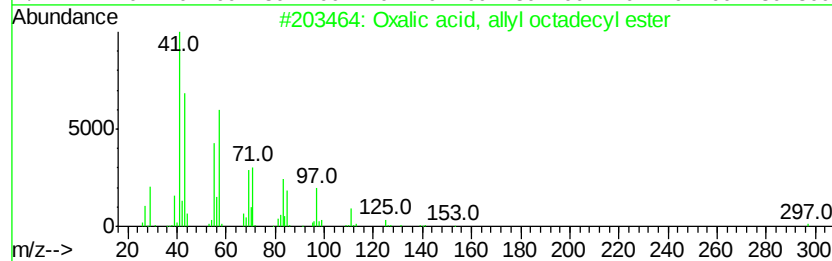
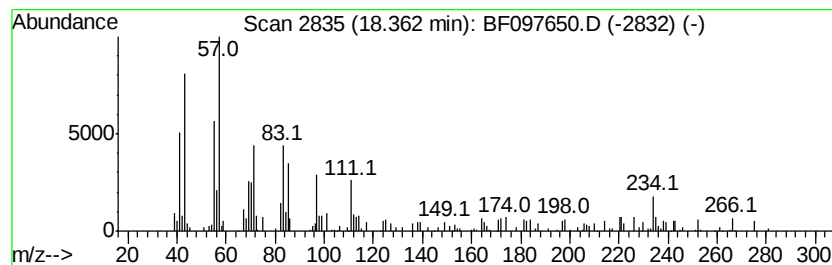
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Oxalic acid, allyl octadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	2.08 ng	68933	Chrysene-d12	18.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	64
2		Oxalic acid, allyl tetradecyl ester	326	C19H34O4	1000309-24-2	64
3		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	64
4		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	52
5		Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	50



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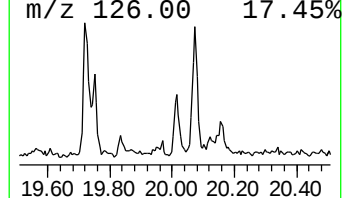
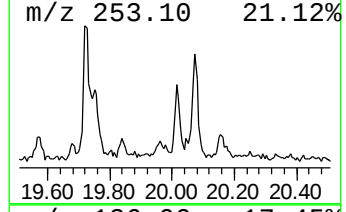
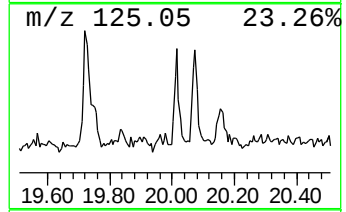
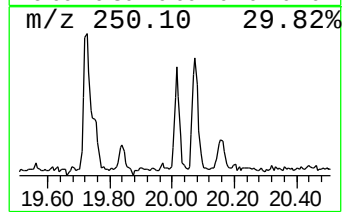
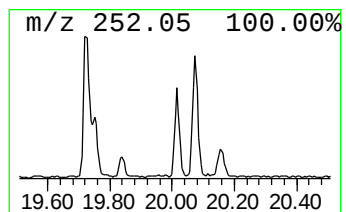
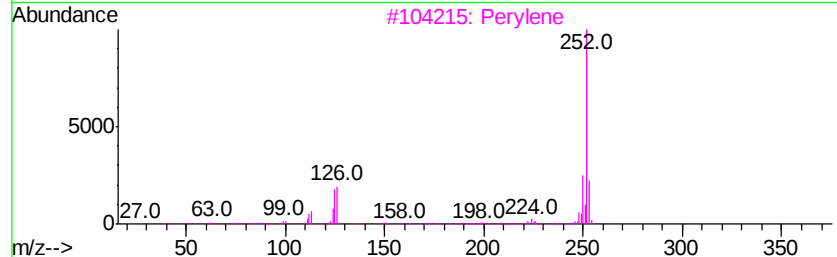
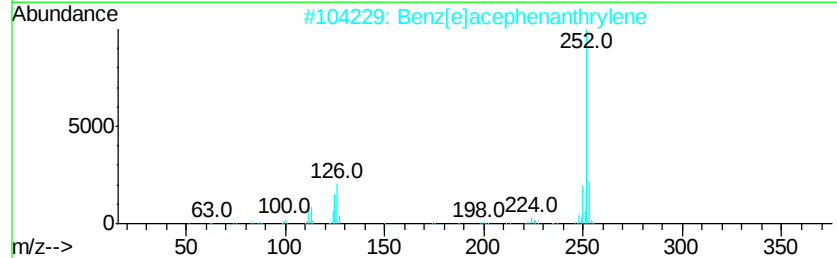
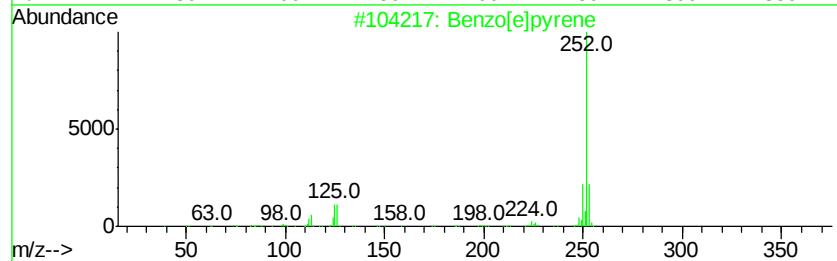
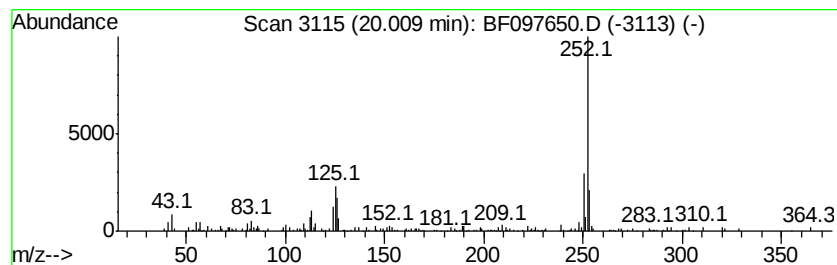
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.01	3.46 ng	92502	Perylene-d12	20.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
3		Perylene	252	C20H12	000198-55-0	89
4		Benzo[a]pyrene	252	C20H12	000050-32-8	83
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	81



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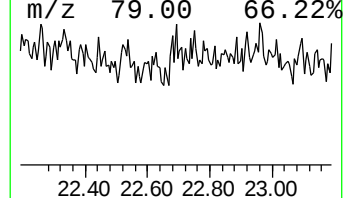
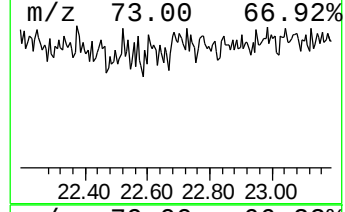
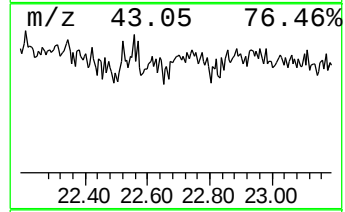
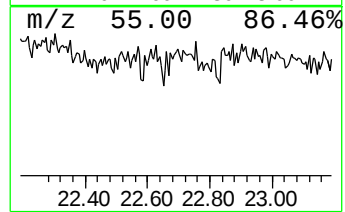
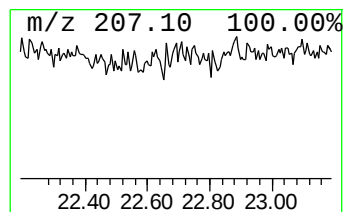
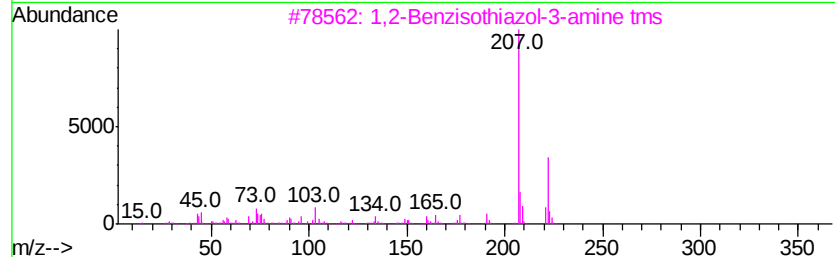
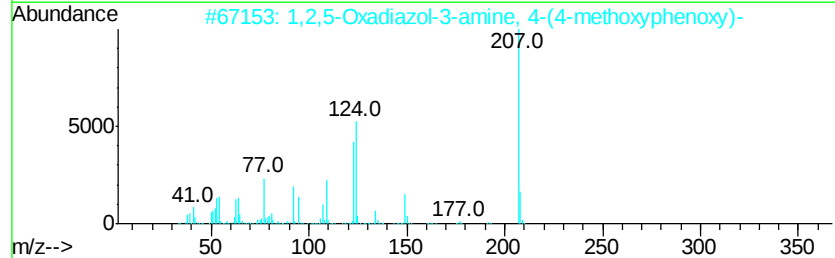
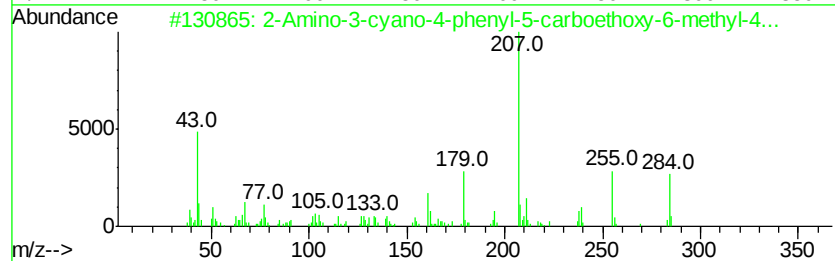
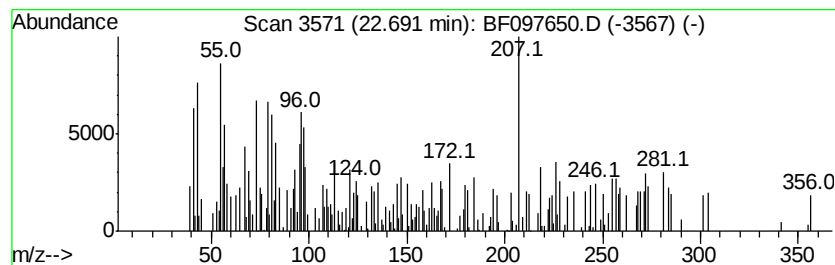
Instrument :
BNA_F
ClientSampleId :
B-13(0-10)COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown22.69 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
22.69	2.25 ng	60262	Perylene-d12	20.13		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-3-cvano-4-phenyl-5-carbo...	284	C16H16N2O3	1000301-54-4	22	
2	1,2,5-Oxadiazol-3-amine, 4-(4-me...	207	C9H9N3O3	1000351-72-7	14	
3	1,2-Benzisothiazol-3-amine tms	222	C10H14N2SSi	1000332-66-2	14	
4	1H-Indole, 3-ethyl-2-(2-pyridyl)-	222	C15H14N2	093732-43-5	14	
5	Pyrido[2,3-d]pyrimidine, 4-phenyl-	207	C13H9N3	028732-75-4	14	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081217\
Data File : BF097650.D
Acq On : 12 Aug 2017 23:40
Operator : SJ/JU
Sample : I4649-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-13(0-10)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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...	4.77	6.6	ng	251192	1	7.50	764666	20.0
unknown7.17	7.17	71.4	ng	2730970	1	7.50	764666	20.0
Oxalic acid, ally...	18.36	2.1	ng	68933	5	18.46	662100	20.0
Benzo[e]pyrene	20.01	3.5	ng	92502	6	20.13	535019	20.0
unknown22.69	22.69	2.3	ng	60262	6	20.13	535019	20.0