

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050817\
 Data File : BF094988.D
 Acq On : 8 May 2017 19:32
 Operator : SJ/MA
 Sample : I2947-14
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-05-0-2.0

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-BF050217.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	5.019	521	524	541	rBV	112262	226912	9.91%	1.022%
2	5.654	628	632	656	rBV	1252927	2100880	91.73%	9.461%
3	7.248	898	903	919	rBV	1293488	1908251	83.32%	8.593%
4	7.372	919	924	937	rVB	1603662	2114375	92.32%	9.521%
5	7.713	978	982	992	rBV	452893	516804	22.56%	2.327%
6	7.948	1017	1022	1037	rBV	1288110	1529530	66.78%	6.888%
7	8.613	1130	1135	1156	rBV	869413	1227634	53.60%	5.528%
8	9.736	1321	1326	1342	rBV	511403	739826	32.30%	3.332%
9	11.507	1622	1627	1646	rBV	1888672	2290296	100.00%	10.314%
10	12.201	1740	1745	1752	rBV	238947	321879	14.05%	1.449%
11	12.342	1764	1769	1775	rBV	30317	41292	1.80%	0.186%
12	12.560	1802	1806	1817	rBV2	637808	911557	39.80%	4.105%
13	13.407	1945	1950	1955	rBV	42976	49504	2.16%	0.223%
14	13.854	2021	2026	2042	rBV	913491	1363421	59.53%	6.140%
15	14.177	2077	2081	2084	rBV	34828	41235	1.80%	0.186%
16	14.965	2210	2215	2227	rVB	558398	769589	33.60%	3.466%
17	15.930	2376	2379	2389	rVB3	71703	105790	4.62%	0.476%
18	16.548	2480	2484	2488	rBV	23417	27699	1.21%	0.125%
19	16.706	2508	2511	2514	rBV	32464	31271	1.37%	0.141%
20	16.748	2514	2518	2523	rBV	159391	184524	8.06%	0.831%
21	16.883	2538	2541	2547	rBV	17813	23009	1.00%	0.104%
22	17.047	2565	2569	2579	rVB	203292	237811	10.38%	1.071%
23	17.136	2579	2584	2588	rBV	146800	148071	6.47%	0.667%
24	17.242	2599	2602	2605	rVV	33405	33480	1.46%	0.151%
25	17.289	2605	2610	2617	rVB	1589765	1726709	75.39%	7.776%
26	17.365	2619	2623	2627	rVV3	17076	24585	1.07%	0.111%
27	17.477	2638	2642	2645	rBV3	21030	34844	1.52%	0.157%
28	17.512	2645	2648	2652	rVB	33225	40884	1.79%	0.184%
29	17.600	2660	2663	2667	rVB	21788	23798	1.04%	0.107%
30	17.647	2667	2671	2673	rBV2	29013	37208	1.62%	0.168%
31	17.677	2673	2676	2681	rVB	59030	60753	2.65%	0.274%
32	18.059	2737	2741	2747	rBV	103762	114872	5.02%	0.517%
33	18.124	2747	2752	2755	rBV2	28777	32203	1.41%	0.145%
34	18.342	2786	2789	2792	rVB2	22127	24078	1.05%	0.108%

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35	18.542	2818	2823	2826	rBV2	36146	45667	1.99%	0.206%
36	18.577	2826	2829	2832	rVV4	17570	33288	1.45%	0.150%
37	18.630	2832	2838	2842	rVV2	611818	867957	37.90%	3.909%
38	18.665	2842	2844	2855	rVB2	133840	204392	8.92%	0.920%
39	18.853	2871	2876	2884	rBV7	11236	29132	1.27%	0.131%
40	19.141	2919	2925	2929	rBV	32597	48559	2.12%	0.219%
41	19.183	2929	2932	2936	rVB	25800	30567	1.33%	0.138%
42	19.324	2953	2956	2960	rVB2	31689	35750	1.56%	0.161%
43	19.694	3016	3019	3023	rBV2	23813	26496	1.16%	0.119%
44	19.765	3028	3031	3035	rVB	26817	30680	1.34%	0.138%
45	19.894	3049	3053	3056	rBV	165758	220623	9.63%	0.994%
46	19.924	3056	3058	3063	rVB	74507	90697	3.96%	0.408%
47	20.012	3069	3073	3076	rBV	31477	34418	1.50%	0.155%
48	20.053	3076	3080	3084	rVB2	31997	37174	1.62%	0.167%
49	20.188	3099	3103	3107	rBV	106309	120758	5.27%	0.544%
50	20.241	3109	3112	3117	rVV	137127	156416	6.83%	0.704%
51	20.300	3117	3122	3131	rVV	490218	674301	29.44%	3.037%
52	20.394	3135	3138	3146	rVB5	36476	55400	2.42%	0.249%
53	20.765	3198	3201	3205	rVB2	20694	29345	1.28%	0.132%
54	21.600	3338	3343	3351	rBV2	62863	120945	5.28%	0.545%
55	21.683	3353	3357	3364	rVB7	13568	26358	1.15%	0.119%
56	21.747	3364	3368	3373	rBV5	12434	26464	1.16%	0.119%
57	21.977	3402	3407	3416	rBV	45375	94695	4.13%	0.426%
58	23.724	3697	3704	3712	rVB6	37201	101822	4.45%	0.459%

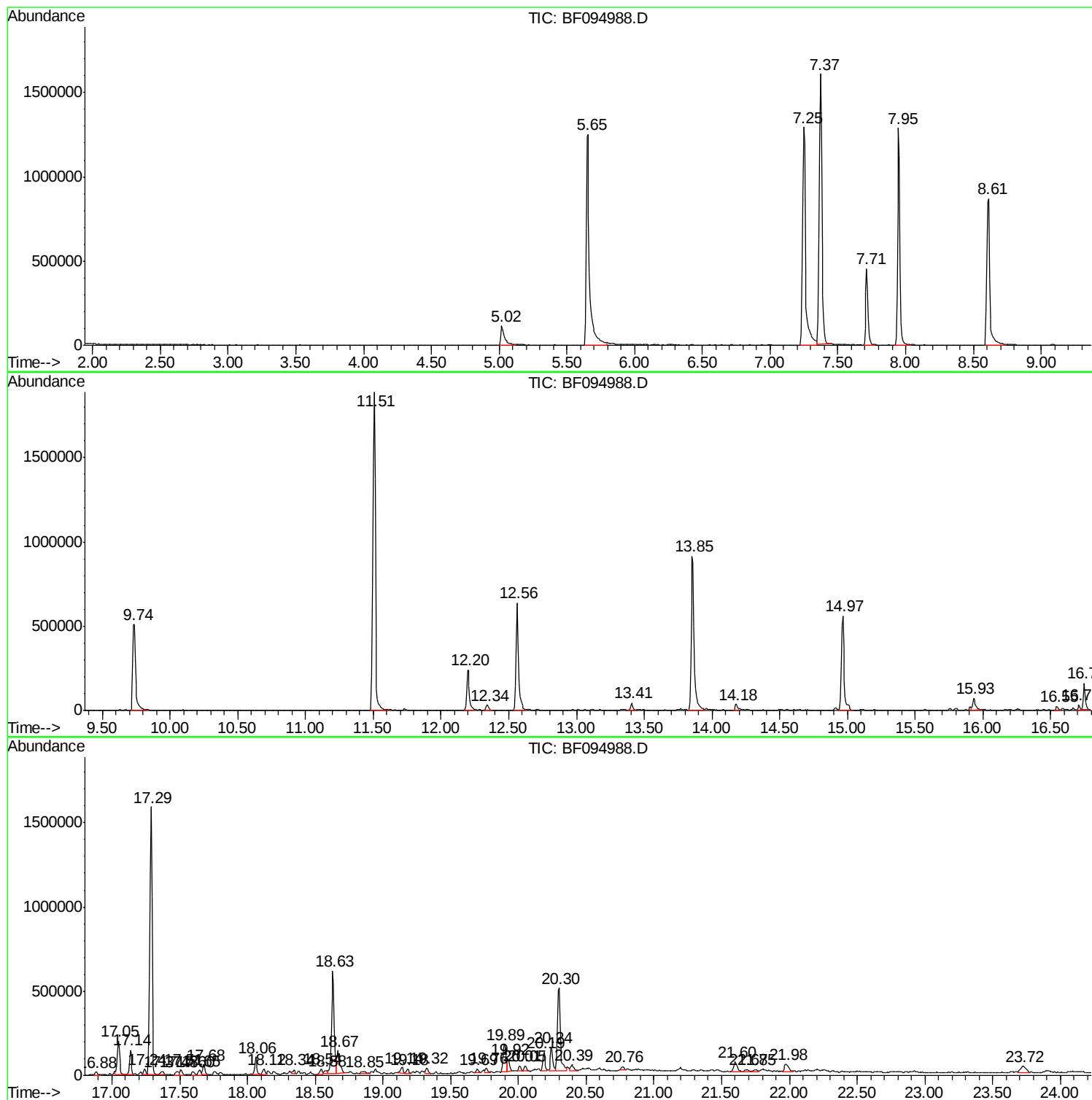
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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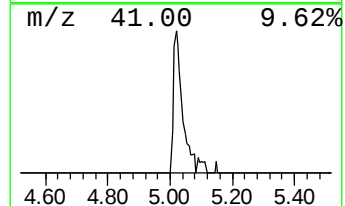
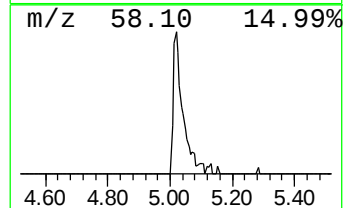
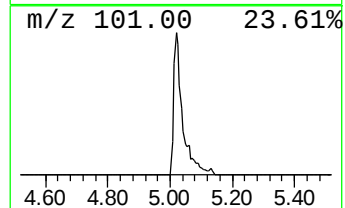
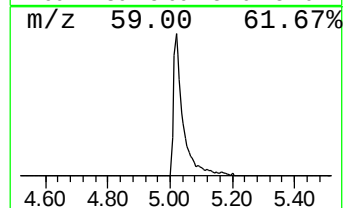
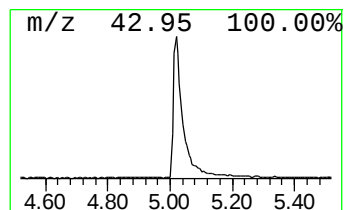
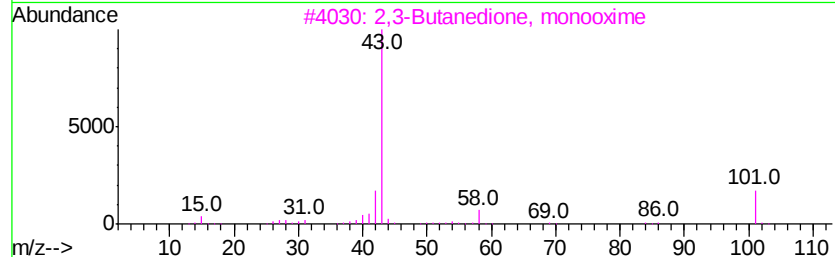
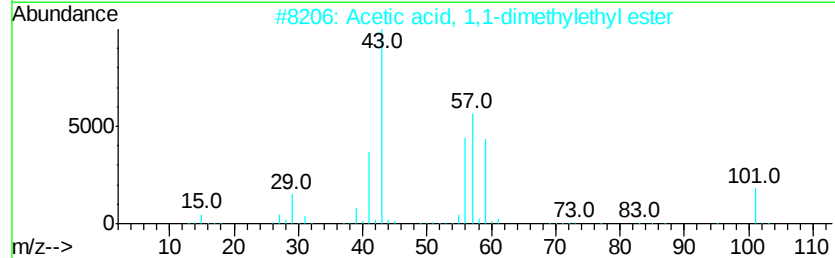
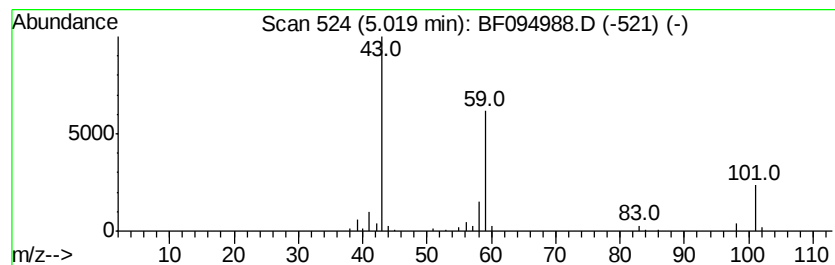
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	8.78 ng	226912	1,4-Dichlorobenzene-d4	7.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			3-Hexanol	102	C6H14O	000623-37-0	28



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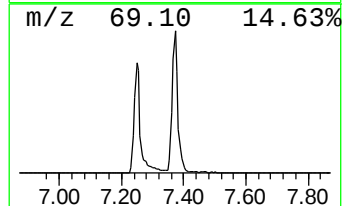
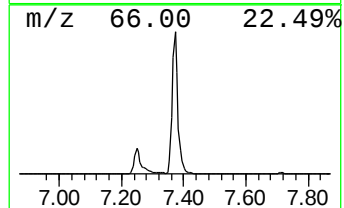
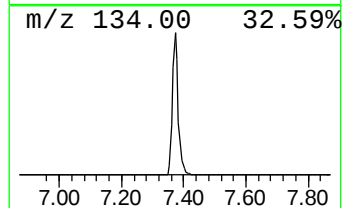
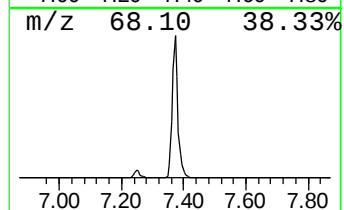
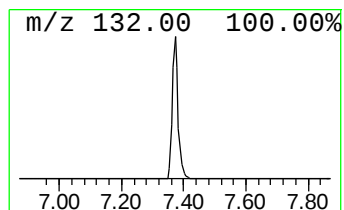
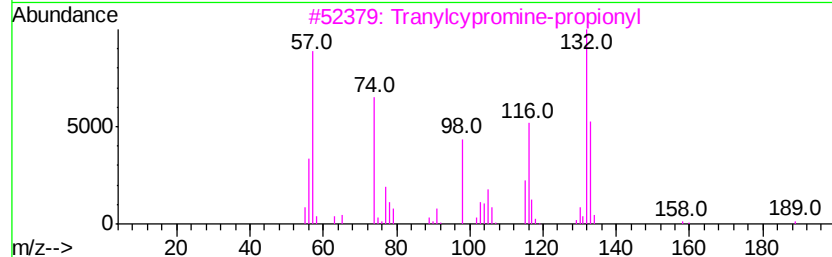
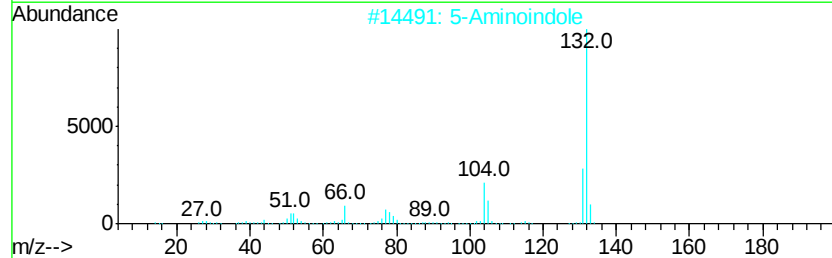
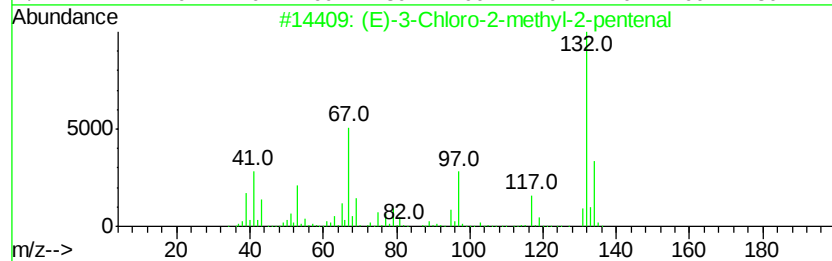
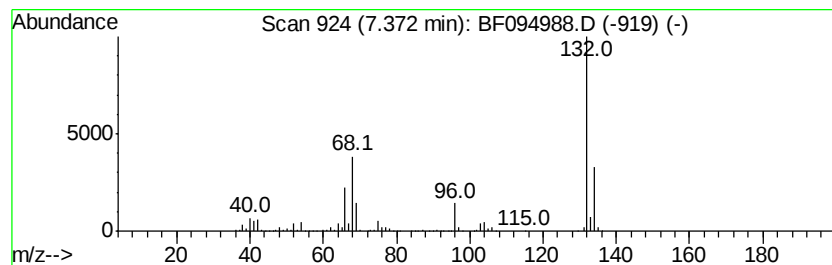
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	81.83 ng	2114380	1,4-Dichlorobenzene-d4	7.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10	
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9	
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9	



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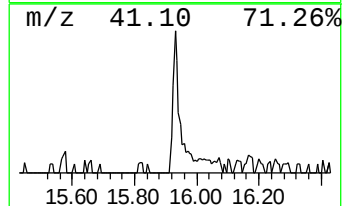
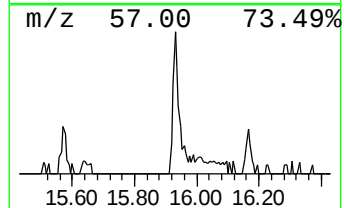
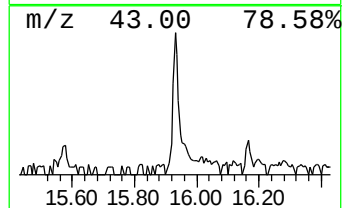
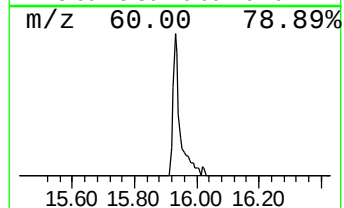
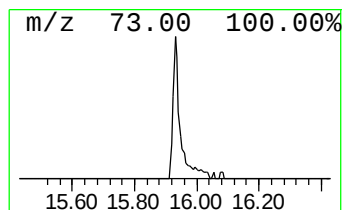
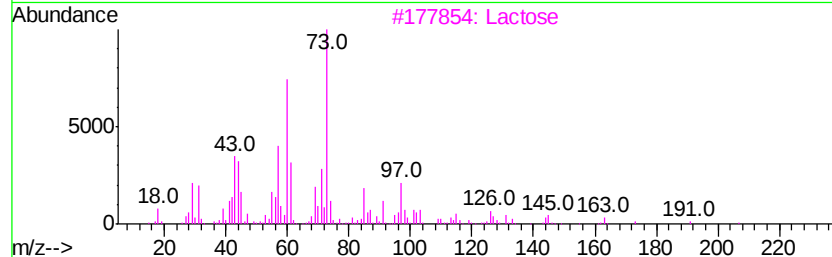
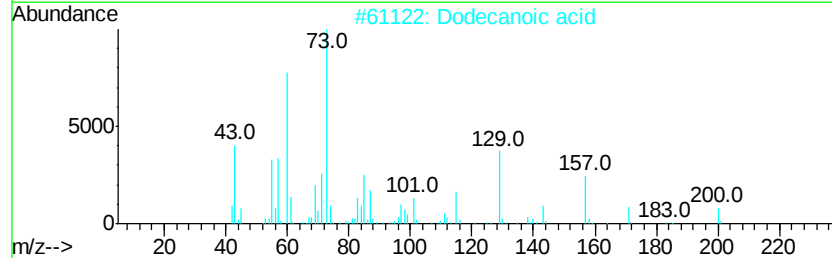
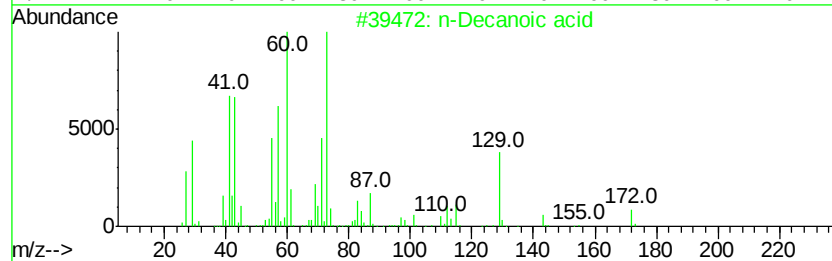
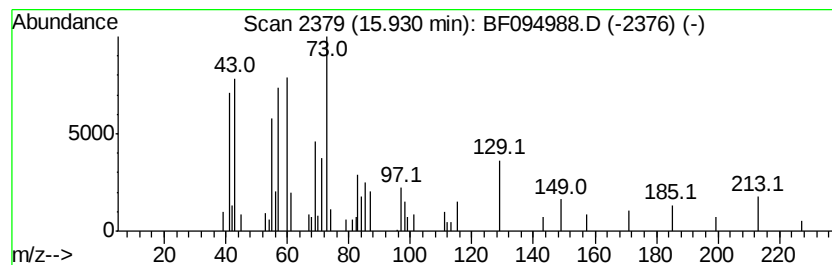
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Decanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	2.75 ng	105790	Phenanthrene-d10	14.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Decanoic acid	172	C10H20O2	000334-48-5	53
2		Dodecanoic acid	200	C12H24O2	000143-07-7	50
3		Lactose	342	C12H22O11	000063-42-3	47
4		Tridecanoic acid	214	C13H26O2	000638-53-9	45
5		d-Glucohexodialdose	178	C6H10O6	1000149-19-1	43



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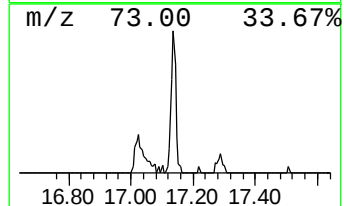
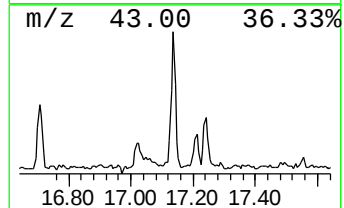
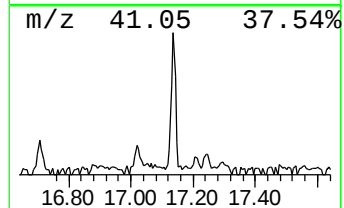
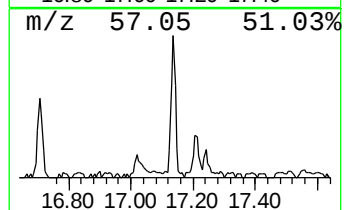
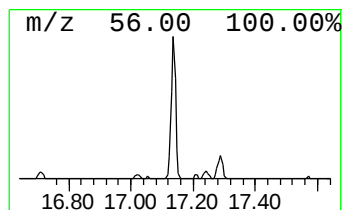
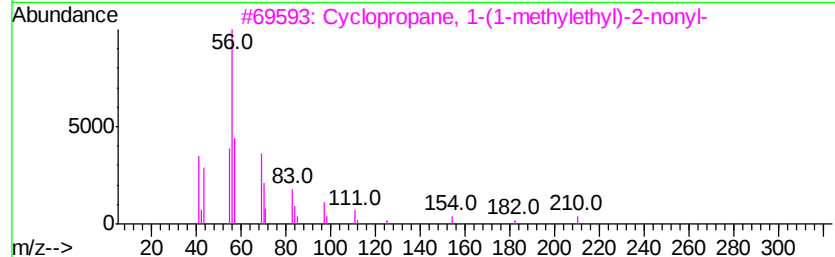
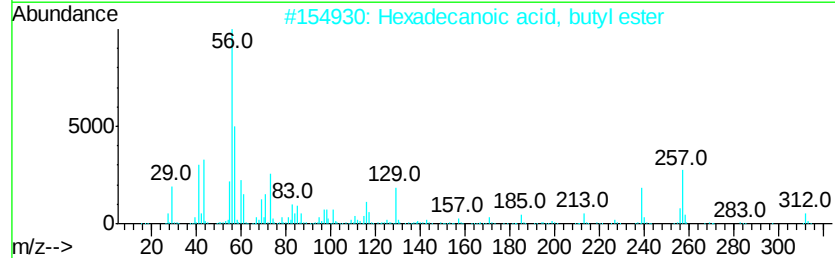
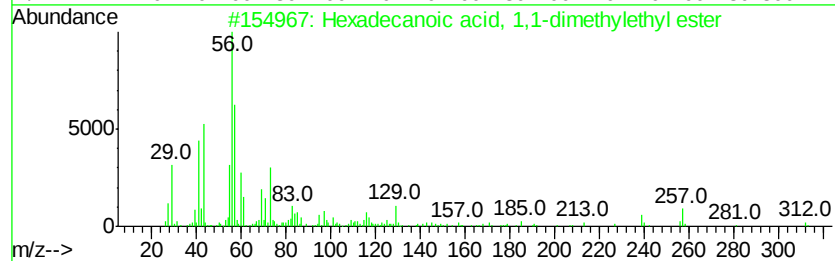
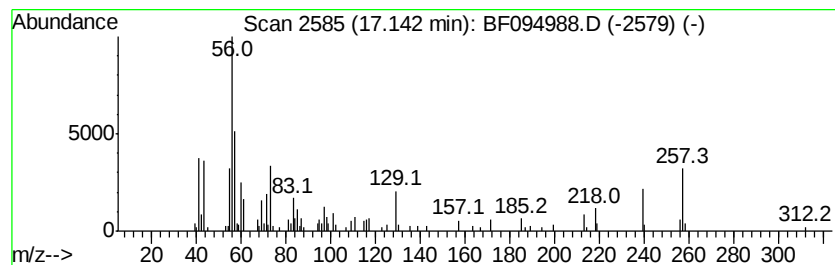
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.14	3.41 ng	148071	Chrysene-d12	18.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	97
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	96
3		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
4		Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	32
5		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27



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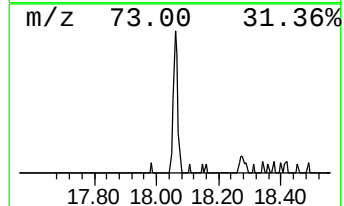
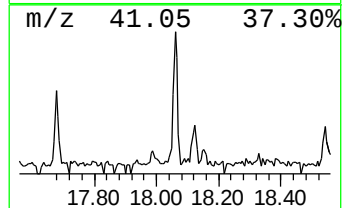
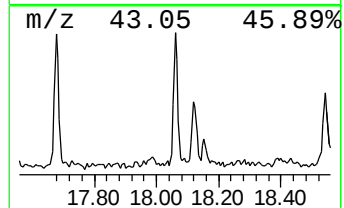
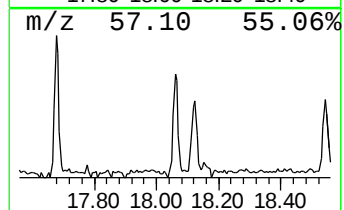
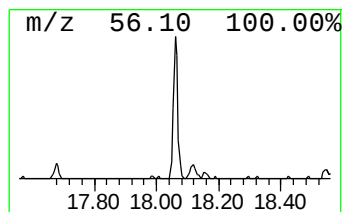
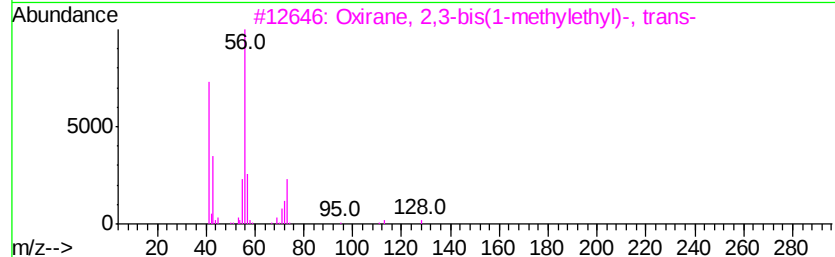
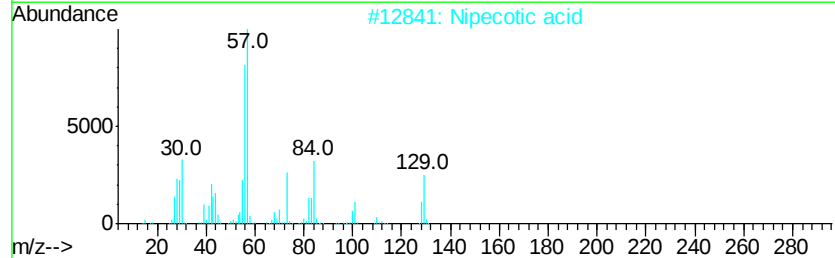
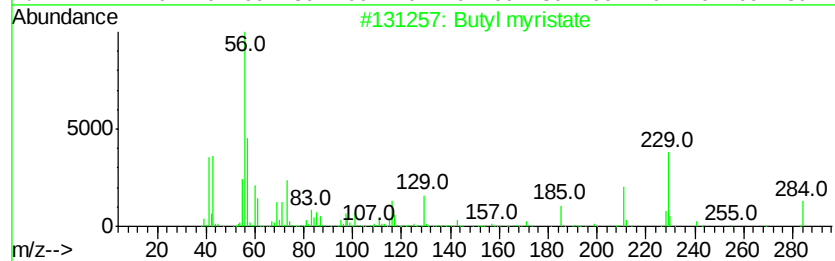
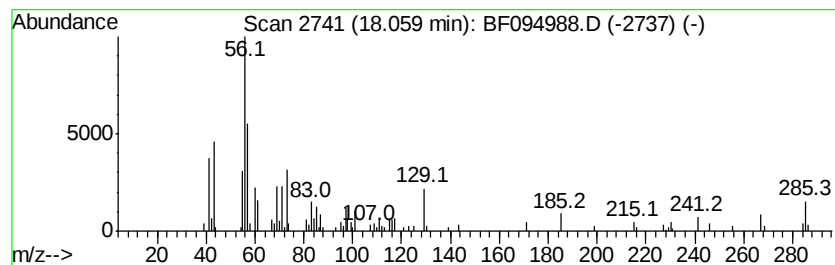
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BNA_F
ClientSampleId :
SB-05-0-2.0

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Butyl myristate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.06	2.65 ng	114872	Chrysene-d12	18.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	64
2	Nipecotic acid	129	C6H11NO2	000498-95-3	53
3	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37
4	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050817\
Data File : BF094988.D
Acq On : 8 May 2017 19:32
Operator : SJ/MA
Sample : I2947-14
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-0-2.0

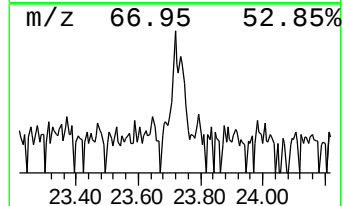
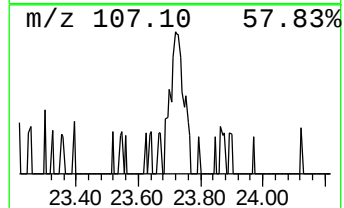
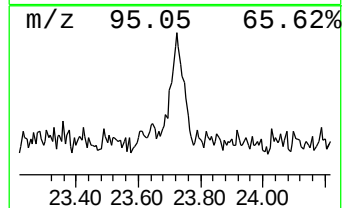
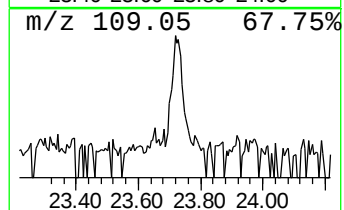
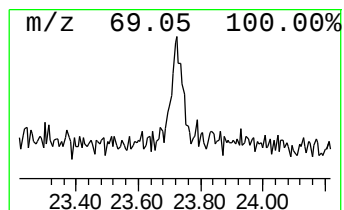
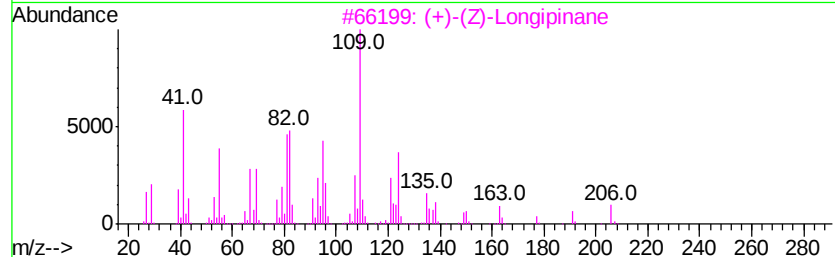
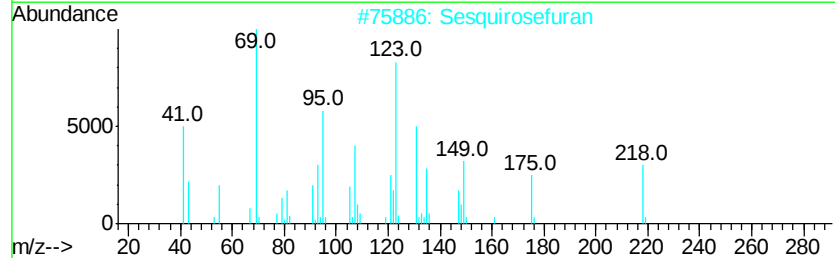
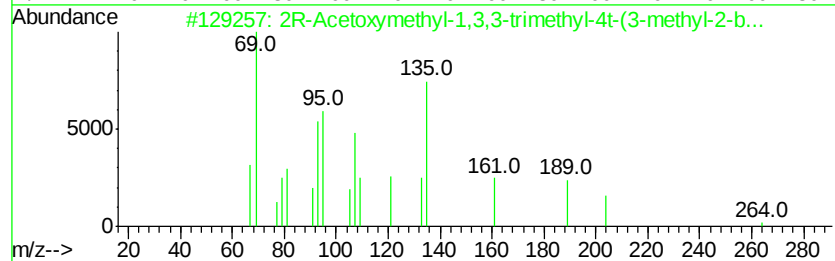
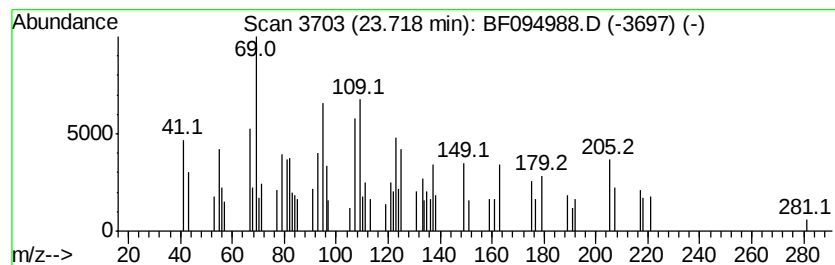
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown23.72 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.72	3.02 ng	101822	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2R-Acetoxyethyl-1,3,3-trimethyl...	282	C17H30O3	1000144-12-4	43
2		Sesquirosefuran	218	C15H22O	039007-93-7	38
3		(+)-(Z)-Longipinane	206	C15H26	1000156-12-3	27
4		(4R*,5R*,9S*)-5,9-Dimethylspiro[...	166	C11H18O	063088-19-7	22
5		3-Fluorobenzoic acid, 3,5-dimeth...	250	C15H19FO2	1000279-01-8	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050817\
Data File : BF094988.D
Acq On : 8 May 2017 19:32
Operator : SJ/MA
Sample : I2947-14
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	5.02	8.8	ng	226912	1	7.71	516804	20.0
unknown7.37	7.37	81.8	ng	2114380	1	7.71	516804	20.0
n-Decanoic acid	15.93	2.8	ng	105790	4	14.97	769589	20.0
Hexadecanoic acid...	17.14	3.4	ng	148071	5	18.63	867957	20.0
Butyl myristate	18.06	2.6	ng	114872	5	18.63	867957	20.0
unknown23.72	23.72	3.0	ng	101822	6	20.30	674301	20.0