

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
 Data File : BF095276.D
 Acq On : 19 May 2017 22:11
 Operator : SJ/MA
 Sample : I3202-09
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-9COMP

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	5.113	536	540	564	rBV	184920	538604	24.10%	2.633%
2	5.731	641	645	679	rBV	738621	1850350	82.79%	9.046%
3	6.319	741	745	752	rBV	13864	25816	1.16%	0.126%
4	7.301	909	912	929	rBV	957145	1795247	80.33%	8.776%
5	7.431	929	934	954	rVB	1304544	2232398	99.89%	10.914%
6	7.766	987	991	1003	rBV	380075	488279	21.85%	2.387%
7	8.001	1026	1031	1052	rBV	1178986	1538194	68.83%	7.520%
8	8.666	1140	1144	1177	rBV	587351	1187919	53.15%	5.807%
9	9.783	1330	1334	1360	rBV	372575	683359	30.58%	3.341%
10	11.548	1630	1634	1652	rBV	1456165	2234907	100.00%	10.926%
11	12.254	1750	1754	1774	rBV	228620	402146	17.99%	1.966%
12	12.613	1811	1815	1828	rBV2	524730	836606	37.43%	4.090%
13	13.448	1953	1957	1962	rVB	21970	24981	1.12%	0.122%
14	13.907	2031	2035	2057	rBV	812957	1442197	64.53%	7.050%
15	14.218	2084	2088	2092	rBV2	21653	31749	1.42%	0.155%
16	14.954	2207	2213	2217	rBV	20669	27302	1.22%	0.133%
17	15.018	2217	2224	2247	rVV2	493595	865811	38.74%	4.233%
18	15.977	2380	2387	2402	rBV3	124140	242805	10.86%	1.187%
19	16.748	2515	2518	2521	rVB2	47599	45647	2.04%	0.223%
20	16.824	2527	2531	2537	rBV	26492	38258	1.71%	0.187%
21	16.954	2544	2553	2559	rBV6	9856	25474	1.14%	0.125%
22	17.059	2568	2571	2578	rBV2	29867	53172	2.38%	0.260%
23	17.118	2578	2581	2588	rVB	31149	48840	2.19%	0.239%
24	17.336	2613	2618	2627	rBV	1749563	2057143	92.05%	10.057%
25	18.042	2735	2738	2744	rBV	112156	124749	5.58%	0.610%
26	18.112	2746	2750	2755	rVV	42488	44508	1.99%	0.218%
27	18.577	2825	2829	2842	rBV3	46528	109653	4.91%	0.536%
28	18.689	2844	2848	2863	rVV	457856	733120	32.80%	3.584%
29	18.983	2894	2898	2904	rVB	24591	28451	1.27%	0.139%
30	19.365	2959	2963	2967	rBV	29921	30505	1.36%	0.149%
31	19.730	3022	3025	3030	rBV	23173	27223	1.22%	0.133%
32	19.806	3034	3038	3042	rVV	34584	37434	1.67%	0.183%
33	20.089	3083	3086	3090	rVB3	34801	37212	1.67%	0.182%
34	20.371	3130	3134	3143	rBV	251136	442183	19.79%	2.162%

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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-9COMP

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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	20.436	3143	3145	3152	rVB4	30671	41515	1.86%	0.203%
36	20.818	3206	3210	3217	rVB2	27104	33245	1.49%	0.163%
37	21.253	3280	3284	3289	rVB4	16556	24113	1.08%	0.118%
38	22.330	3464	3467	3479	rVB10	10518	24164	1.08%	0.118%

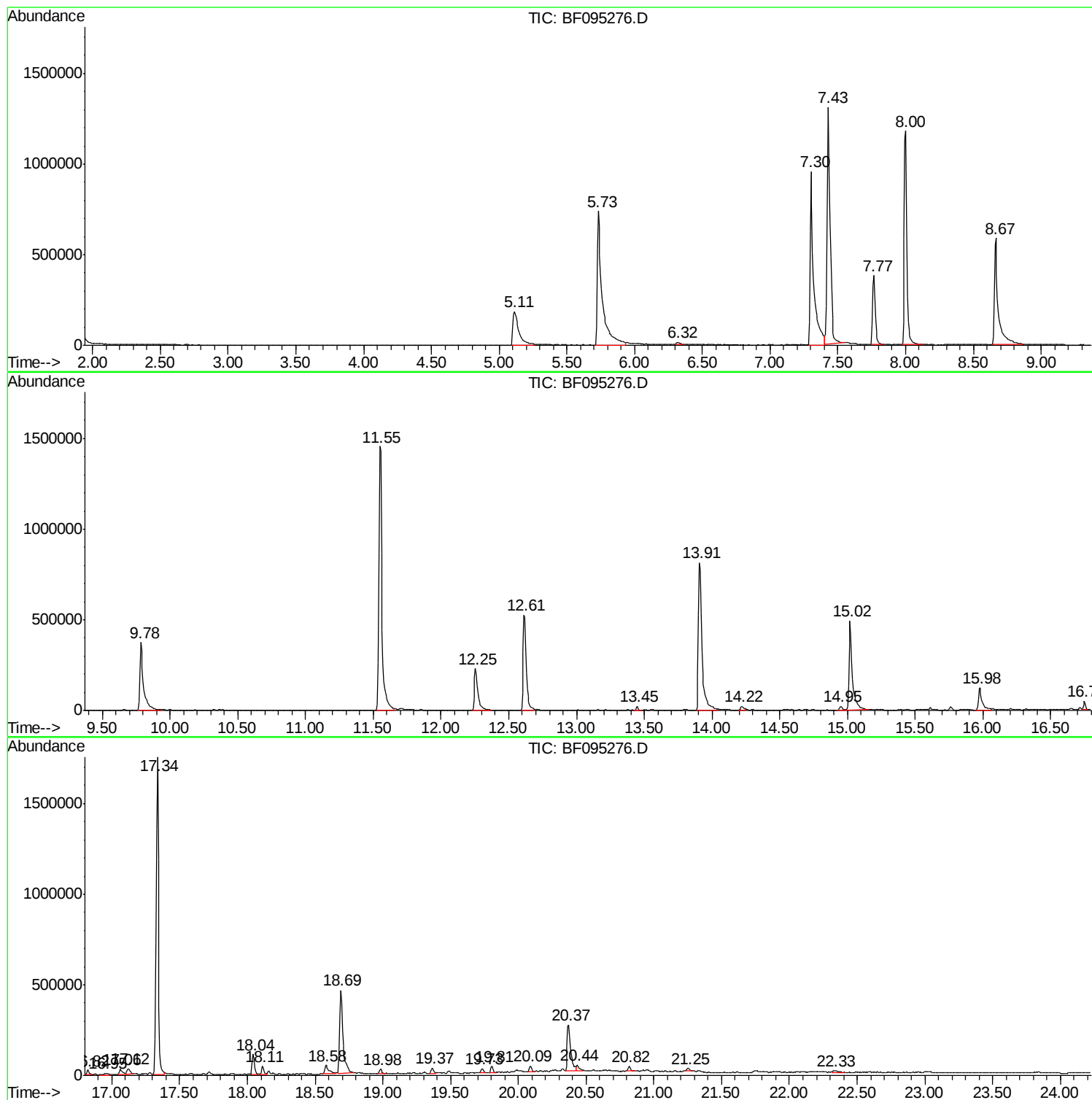
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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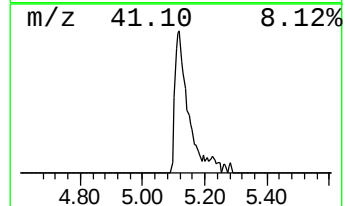
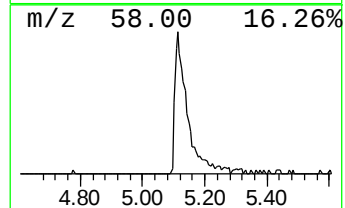
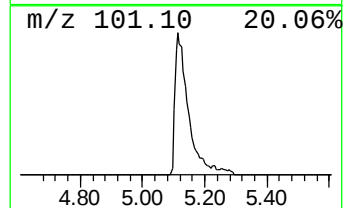
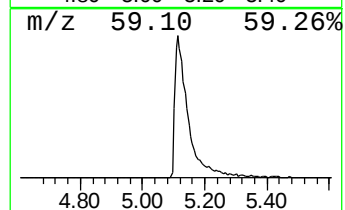
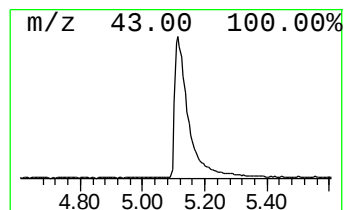
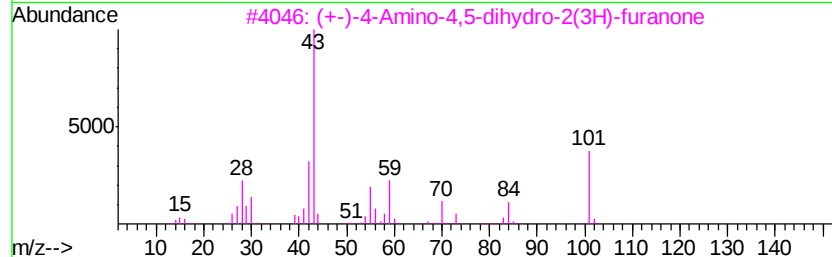
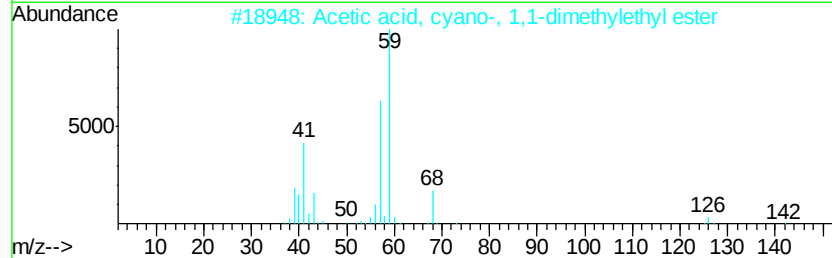
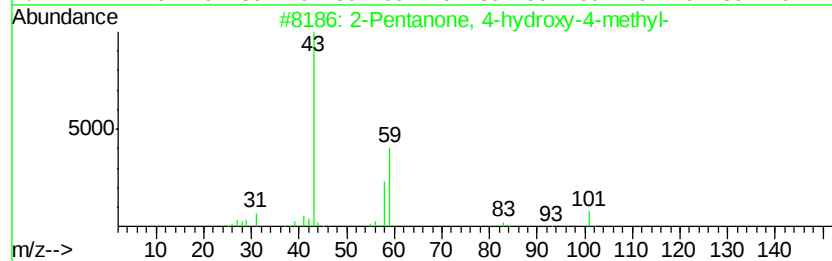
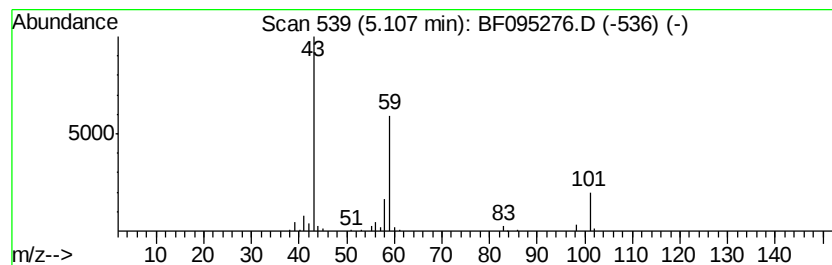
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.11	22.06 ng	538604	1,4-Dichlorobenzene-d4	7.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Acetone	58	C3H6O	000067-64-1	9



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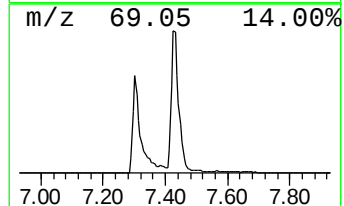
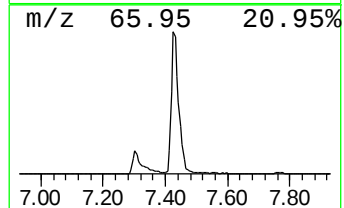
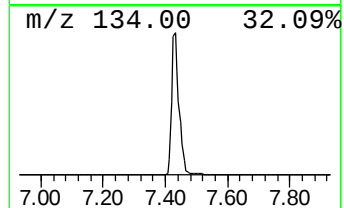
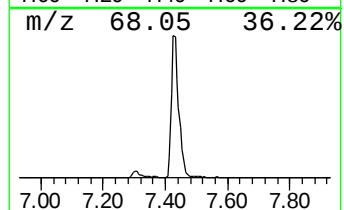
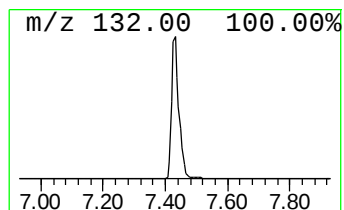
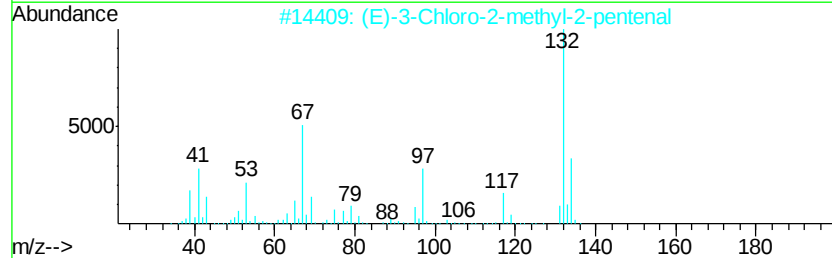
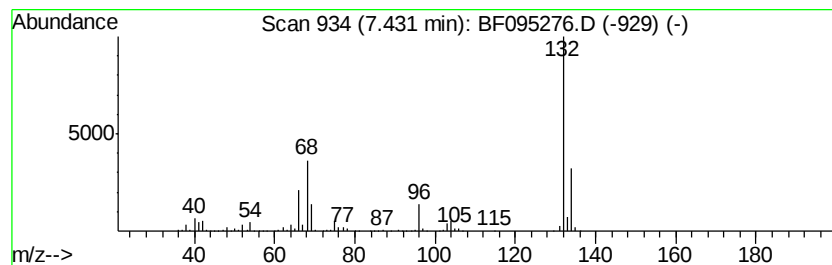
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.43	91.44 ng	2232400	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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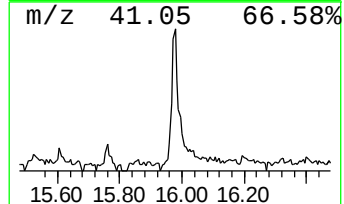
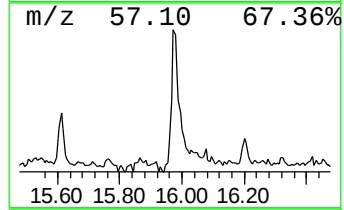
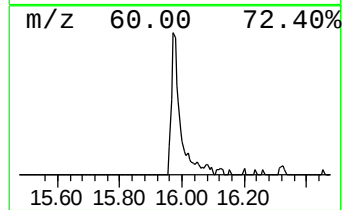
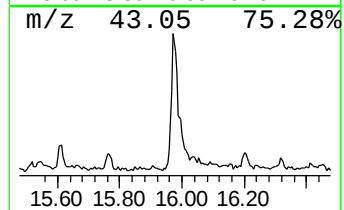
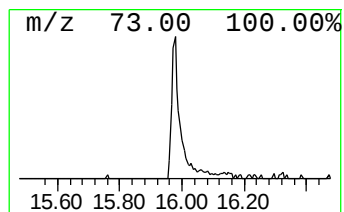
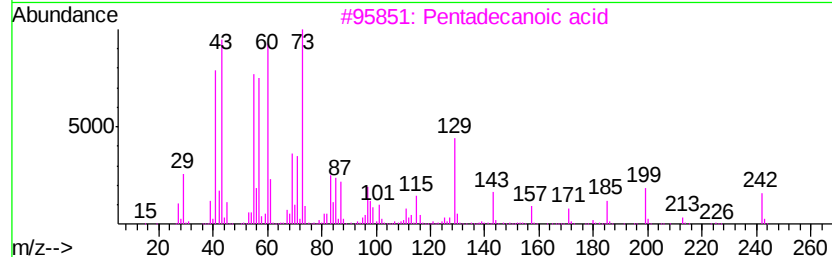
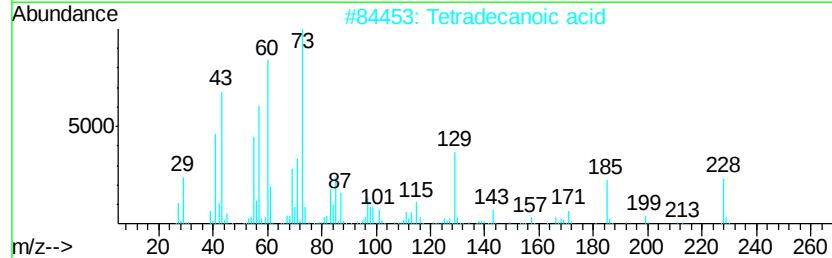
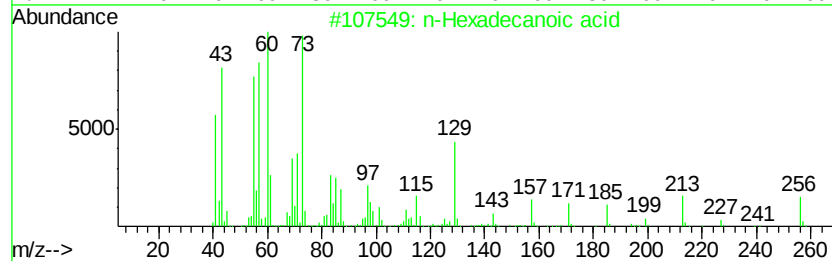
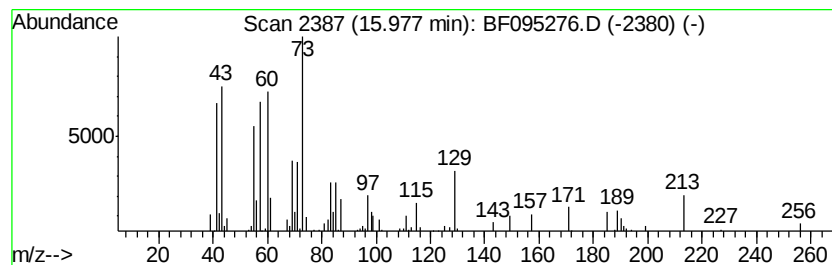
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.98	5.61 ng	242805	Phenanthrene-d10		15.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95	
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58	
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58	
4	Tridecanoic acid	214	C13H26O2	000638-53-9	45	
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43	



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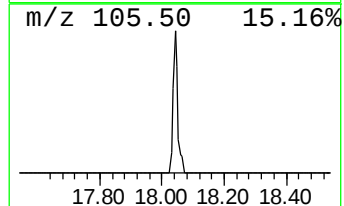
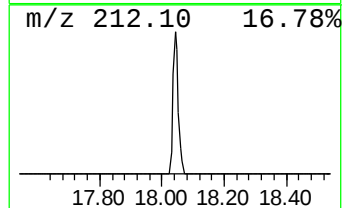
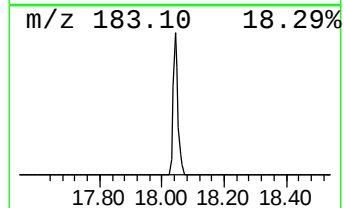
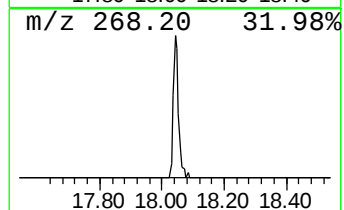
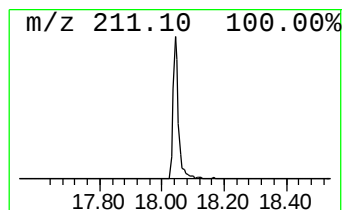
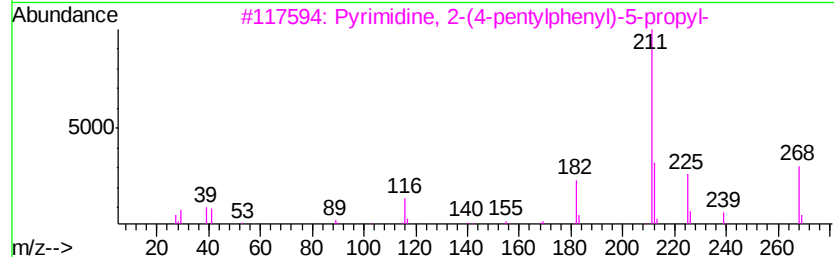
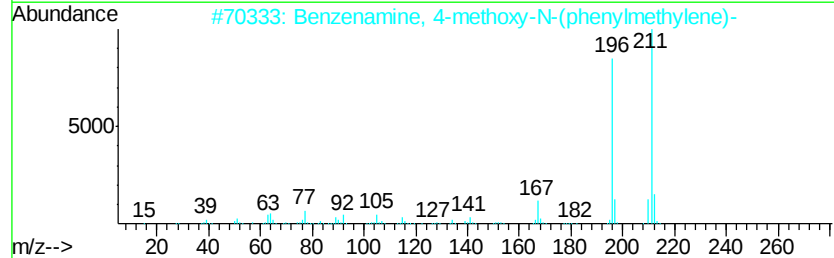
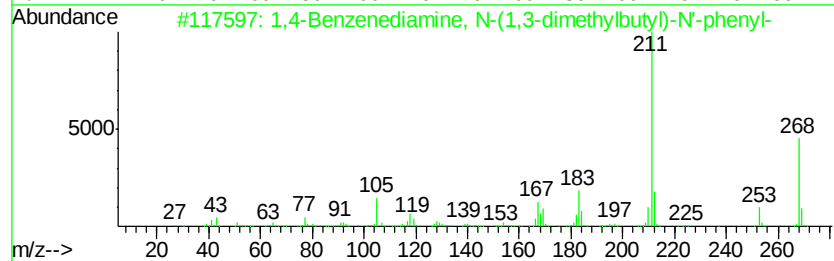
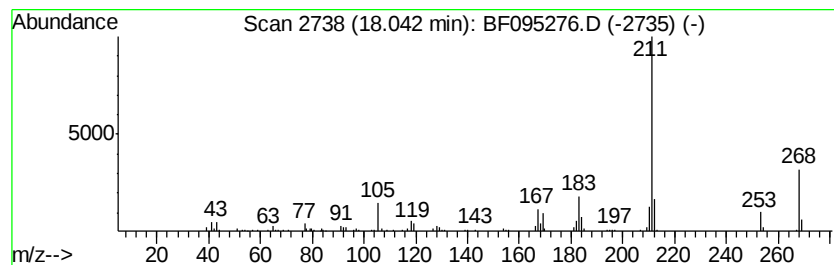
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,4-Benzenediamine, N-(1,3-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	3.40 ng	124749	Chrysene-d12	18.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenediamine, N-(1,3-dimet...	268	C18H24N2	000793-24-8	98
2		Benzenamine, 4-methoxy-N-(phenyl...	211	C14H13NO	000783-08-4	58
3		Pyrimidine, 2-(4-pentylphenyl)-5...	268	C18H24N2	094320-32-8	50
4		Milrinone	211	C12H9N3O	078415-72-2	50
5		4-Amino-1-phenylpyrazolo(3,4-e)p...	211	C11H9N5	005334-30-5	50



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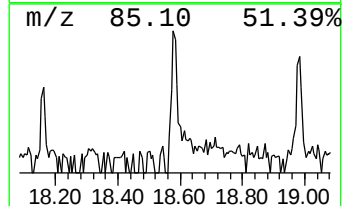
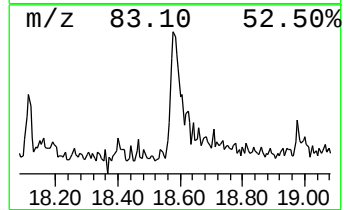
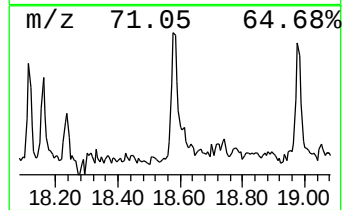
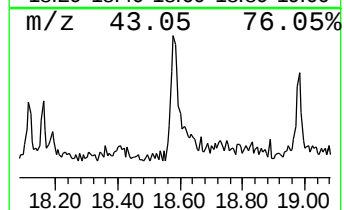
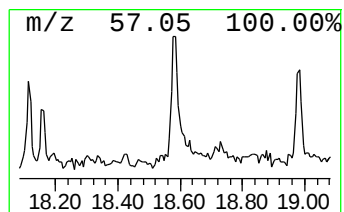
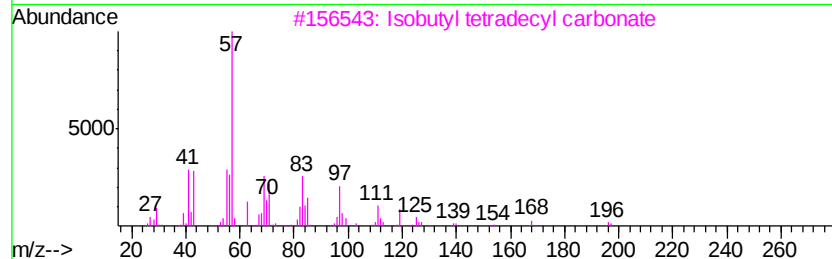
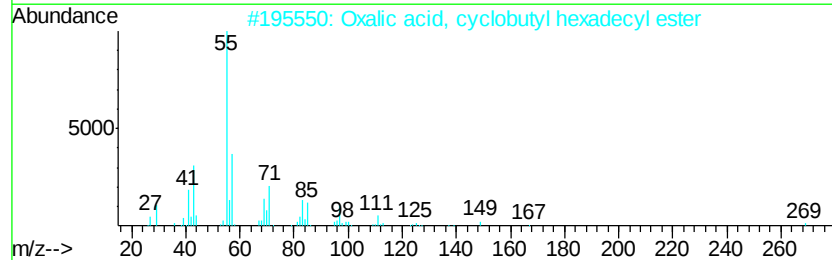
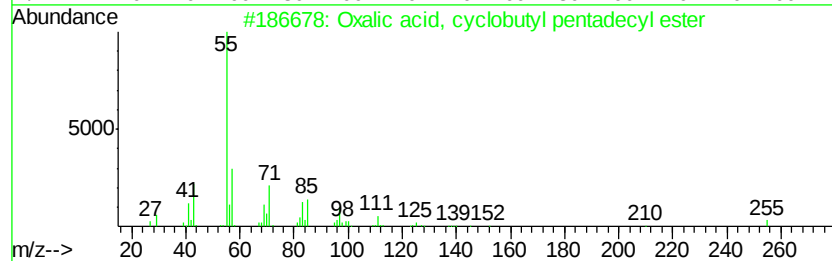
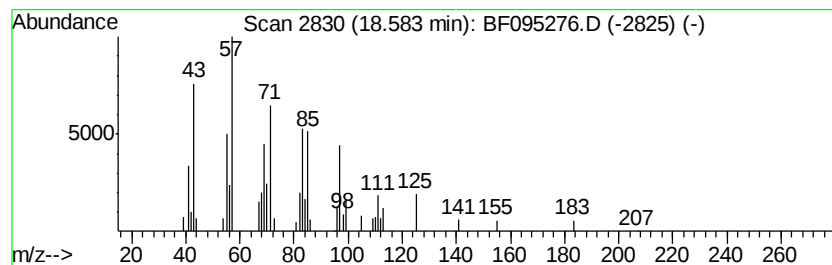
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Oxalic acid, cyclobutyl pen... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.58	2.99 ng	109653	Chrysene-d12	18.69		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	78	
2	Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	78	
3	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	53	
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	52	
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	43	



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BNA_F
ClientSampleId :
SB-9COMP

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...	5.11	22.1	ng	538604	1	7.77	488279	20.0
unknown7.43	7.43	91.4	ng	2232400	1	7.77	488279	20.0
n-Hexadecanoic acid	15.98	5.6	ng	242805	4	15.02	865811	20.0
1,4-Benzenediamin...	18.04	3.4	ng	124749	5	18.69	733120	20.0
Oxalic acid, cycl...	18.58	3.0	ng	109653	5	18.69	733120	20.0