

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051717\
 Data File : BF095207.D
 Acq On : 18 May 2017 3:06
 Operator : SJ/MA
 Sample : I3184-06 5X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE2

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	537	540	548	rBV3	11441	27145	4.44%	0.518%
2	5.784	651	654	655	rBV	38471	34588	5.66%	0.660%
3	7.360	918	922	935	rBV	45844	158741	25.98%	3.027%
4	7.454	935	938	952	rVB	114805	272673	44.63%	5.200%
5	7.772	987	992	1002	rBV	352708	465352	76.17%	8.874%
6	8.007	1028	1032	1043	rBV	163294	226807	37.13%	4.325%
7	8.689	1144	1148	1160	rBV2	38779	103814	16.99%	1.980%
8	9.784	1330	1334	1347	rBV	385902	610904	100.00%	11.650%
9	10.848	1512	1515	1522	rBV3	4486	8586	1.41%	0.164%
10	11.560	1632	1636	1658	rBV	140734	243163	39.80%	4.637%
11	11.778	1670	1673	1683	rVB4	5805	11321	1.85%	0.216%
12	12.266	1751	1756	1760	rBV3	12804	21109	3.46%	0.403%
13	12.477	1786	1792	1796	rBV3	5331	7095	1.16%	0.135%
14	12.619	1812	1816	1831	rBV2	351198	553527	90.61%	10.556%
15	13.172	1906	1910	1913	rBV3	5439	6492	1.06%	0.124%
16	13.454	1953	1958	1964	rBV2	10878	15701	2.57%	0.299%
17	13.813	2012	2019	2023	rBV3	6858	12155	1.99%	0.232%
18	13.936	2036	2040	2051	rBV3	32076	61025	9.99%	1.164%
19	14.230	2083	2090	2092	rBV2	11776	16883	2.76%	0.322%
20	14.254	2092	2094	2101	rVB3	11627	14017	2.29%	0.267%
21	14.960	2209	2214	2217	rBV	11441	14487	2.37%	0.276%
22	15.024	2217	2225	2244	rVV2	318363	520138	85.14%	9.919%
23	15.618	2323	2326	2332	rBV4	10524	13031	2.13%	0.248%
24	15.765	2348	2351	2356	rVB	28403	31592	5.17%	0.602%
25	15.818	2356	2360	2362	rBV2	5115	6202	1.02%	0.118%
26	15.854	2364	2366	2369	rVB4	5275	6334	1.04%	0.121%
27	15.965	2382	2385	2388	rBV3	6776	12055	1.97%	0.230%
28	16.001	2388	2391	2397	rVB7	7359	12347	2.02%	0.235%
29	16.095	2403	2407	2412	rBV5	3888	7682	1.26%	0.146%
30	16.207	2423	2426	2430	rBV4	8917	9599	1.57%	0.183%
31	16.418	2460	2462	2466	rVB4	6374	7555	1.24%	0.144%
32	16.607	2490	2494	2497	rBV3	14664	19056	3.12%	0.363%
33	16.724	2510	2514	2517	rBV	93415	104465	17.10%	1.992%
34	16.760	2517	2520	2523	rVV	158152	165828	27.14%	3.162%

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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	16.812	2527	2529	2534	rVV	24113	27152	4.44%	0.518%
36	16.883	2538	2541	2548	rVB	35819	40379	6.61%	0.770%
37	16.948	2550	2552	2554	rBV3	7600	6612	1.08%	0.126%
38	17.112	2576	2580	2584	rBV2	30227	42788	7.00%	0.816%
39	17.224	2596	2599	2602	rBV4	6707	10073	1.65%	0.192%
40	17.259	2602	2605	2609	rVV5	11775	12914	2.11%	0.246%
41	17.342	2615	2619	2625	rBV	180107	225787	36.96%	4.306%
42	17.783	2690	2694	2697	rBV4	16241	27925	4.57%	0.533%
43	18.289	2776	2780	2781	rBV4	17640	22366	3.66%	0.427%
44	18.695	2844	2849	2855	rBV	425655	574988	94.12%	10.965%
45	20.371	3130	3134	3142	rVB	298811	381266	62.41%	7.271%
46	22.283	3455	3459	3464	rBV7	33887	70191	11.49%	1.339%

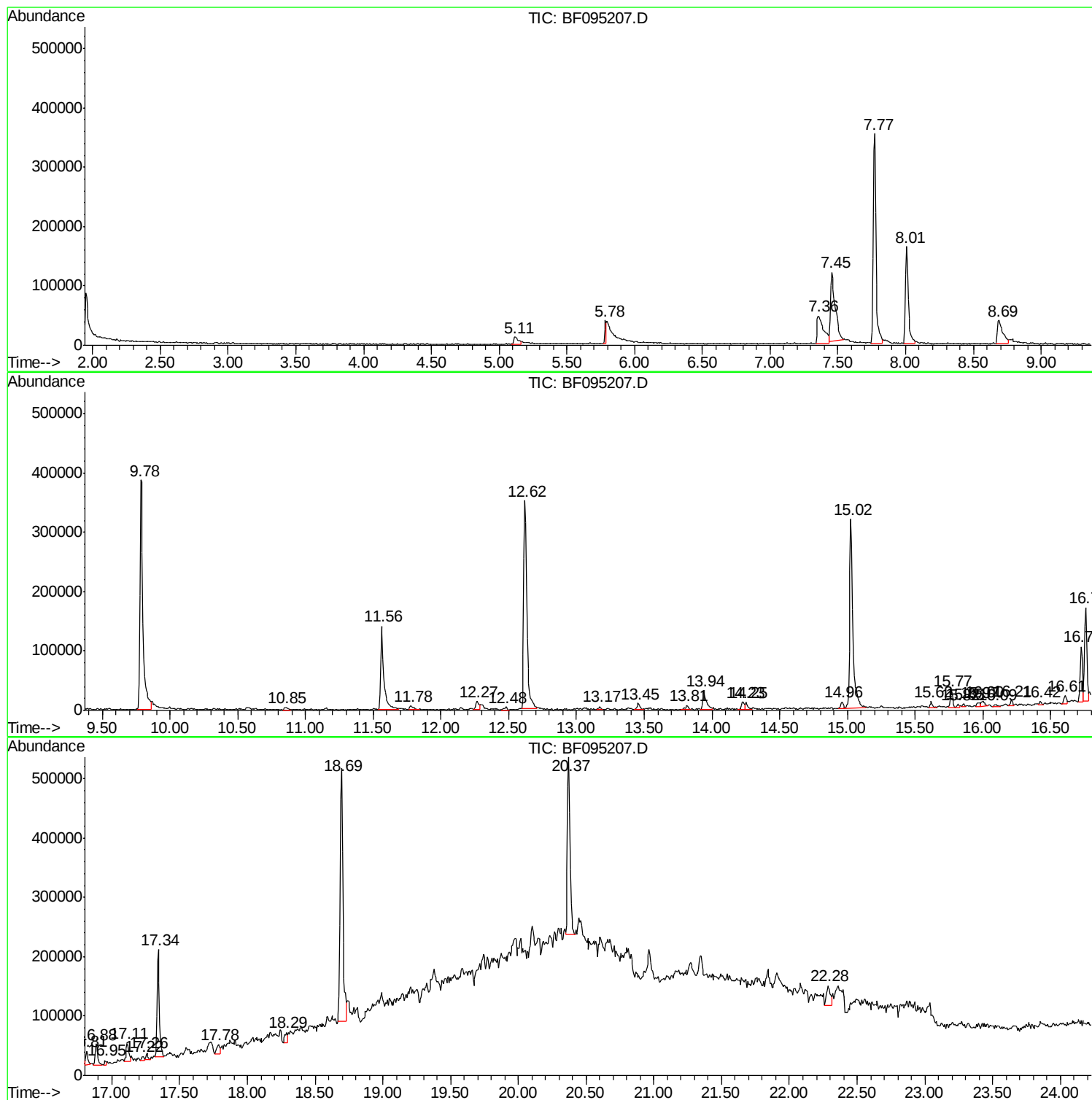
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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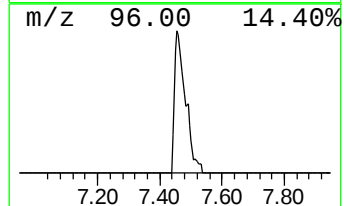
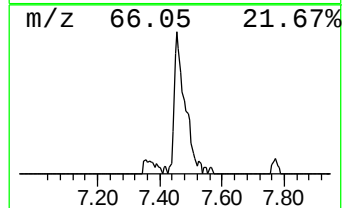
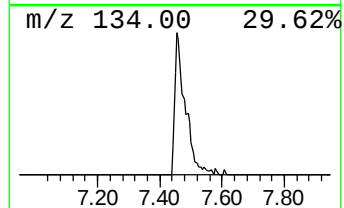
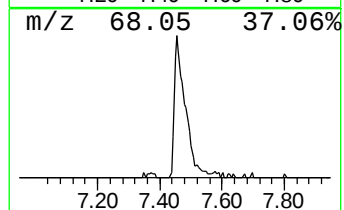
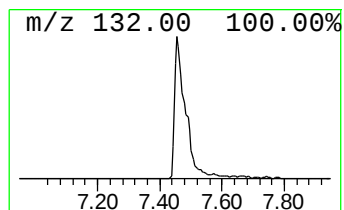
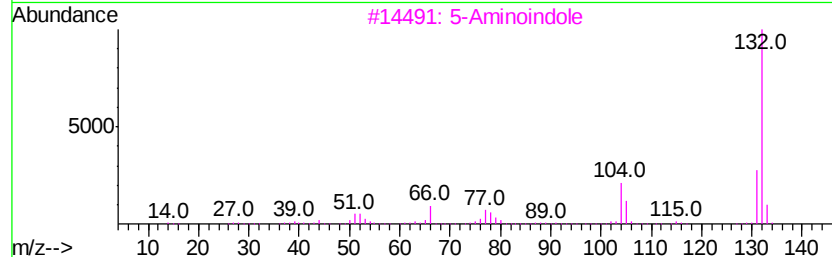
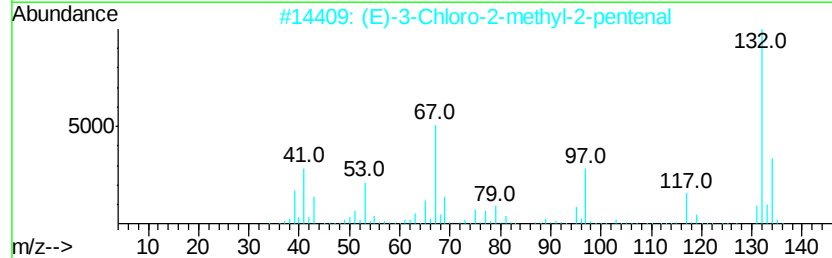
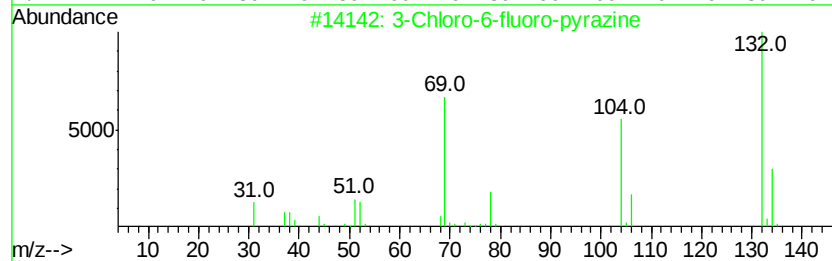
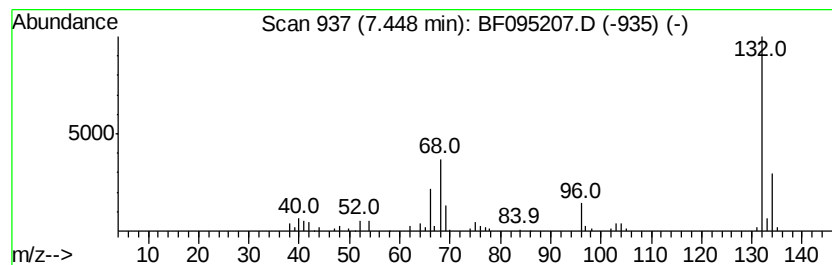
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.45	11.72 ng	272673	1,4-Dichlorobenzene-d4	7.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	23
3			5-Aminoindole	132	C8H8N2	005192-03-0	16
4			1H-Indol-4-amine	132	C8H8N2	005192-23-4	12
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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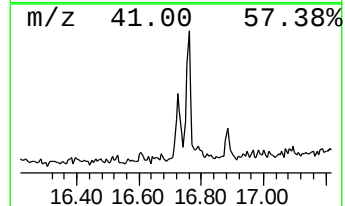
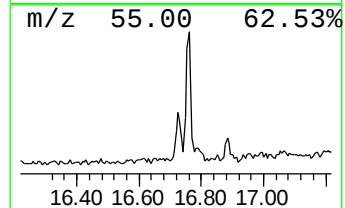
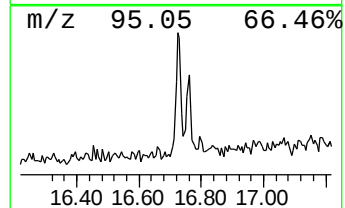
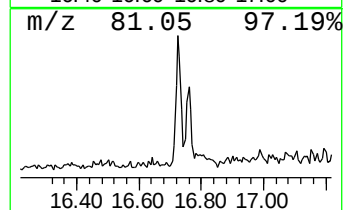
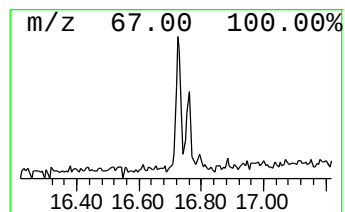
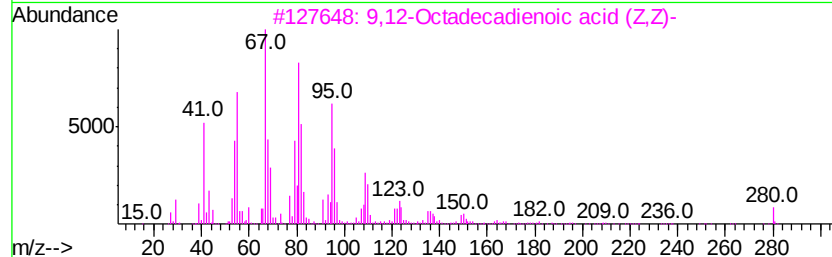
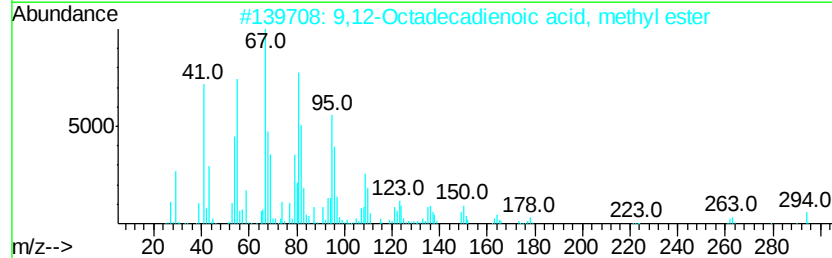
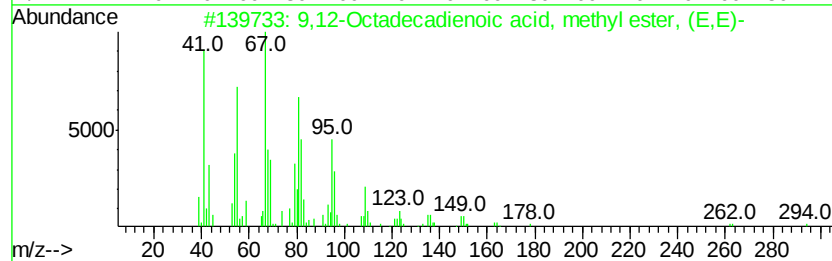
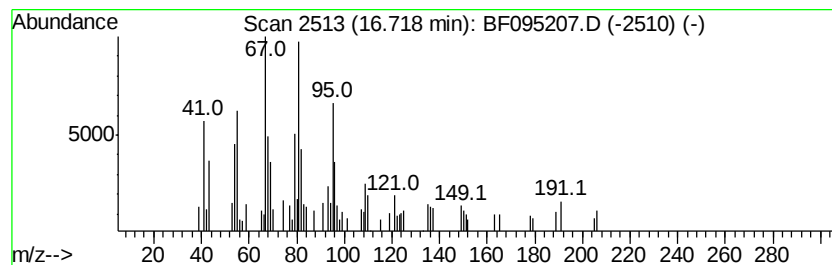
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	4.02 ng	104465	Phenanthrene-d10	15.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
2		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	98
3		9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
4		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	93
5		2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	91



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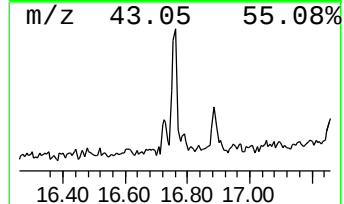
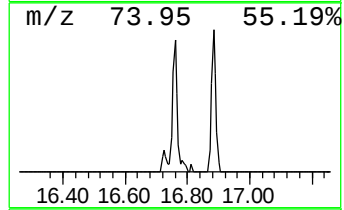
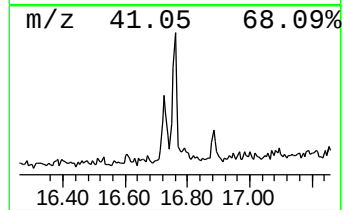
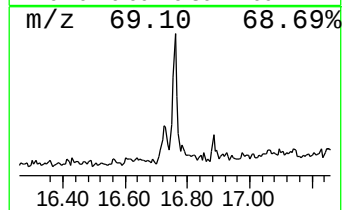
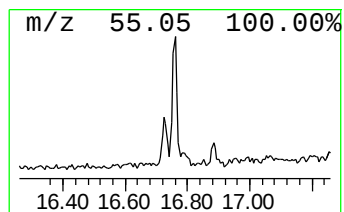
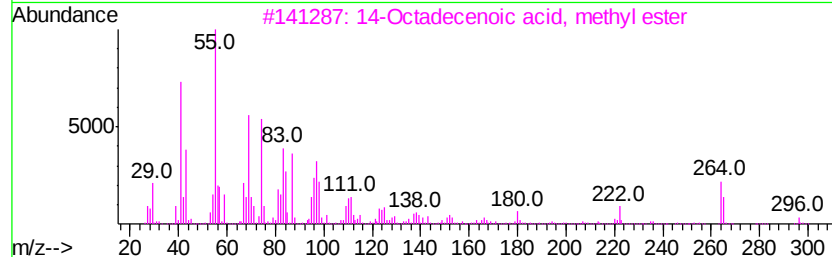
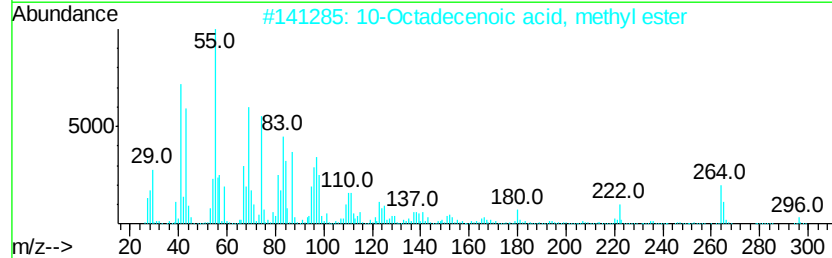
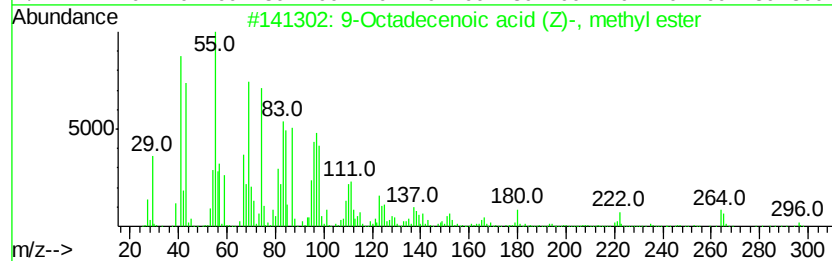
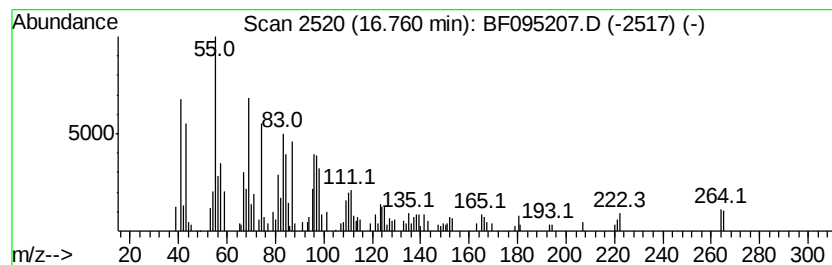
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.76	6.38 ng	165828	Phenanthrene-d10	15.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	87
5	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	87



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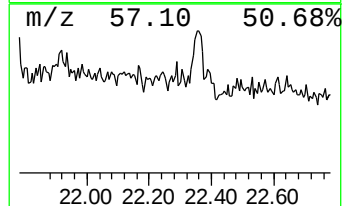
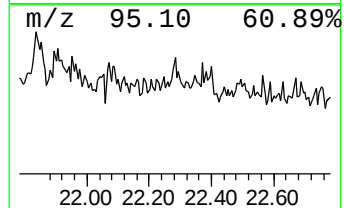
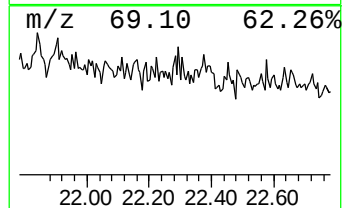
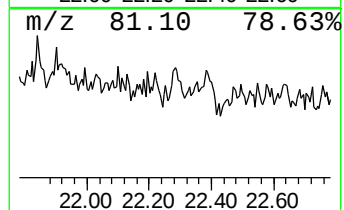
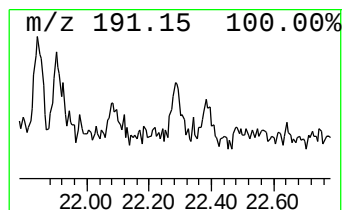
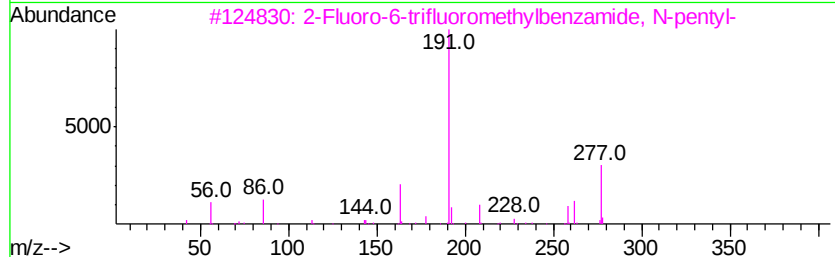
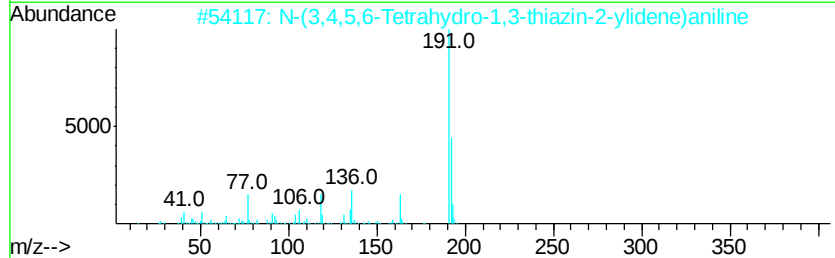
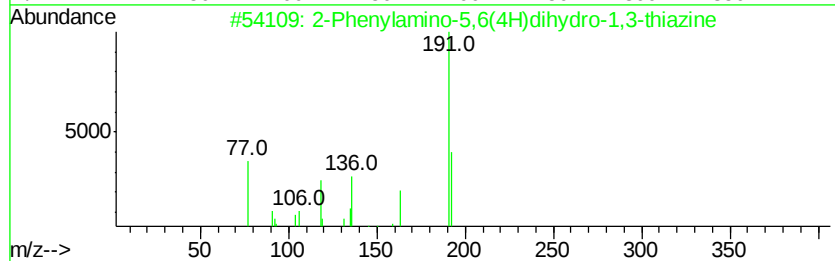
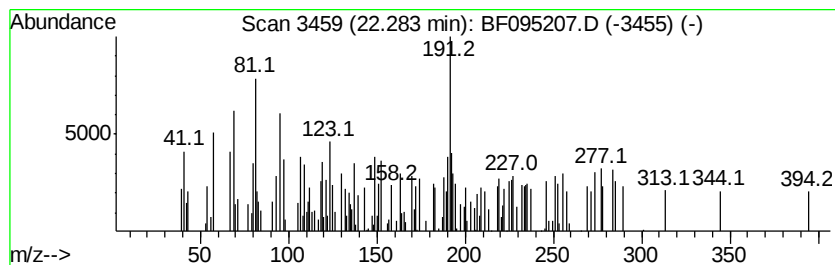
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Peak Number 5 unknown22.28 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	3.68 ng	70191	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	30	
2	N-(3,4,5,6-Tetrahydro-1,3-thiazi...	192	C10H12N2S	003420-40-4	27	
3	2-Fluoro-6-trifluoromethylbenzam...	277	C13H15F4NO	1000358-11-1	25	
4	9-(Chloromethyl)anthracene	226	C15H11Cl	024463-19-2	22	
5	Benzoic acid, 4-nitro-2-[(triflu...	278	C9H5F3N2O5	091533-09-4	22	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.45	7.45	11.7	ng	272673	1	7.77	465352	20.0
9,12-Octadecadien...	16.72	4.0	ng	104465	4	15.02	520138	20.0
9-Octadecenoic ac...	16.76	6.4	ng	165828	4	15.02	520138	20.0
unknown22.28	22.28	3.7	ng	70191	6	20.37	381266	20.0