

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082919\
 Data File : BM022427.D
 Acq On : 30 Aug 2019 02:51
 Operator : HP/JU
 Sample : K4514-14
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 S301A-J-2.0-2.5-082319

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.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	5.140	361	366	381	rBV	410973	612115	43.42%	7.315%
2	6.722	629	635	653	rBV	413630	683117	48.46%	8.163%
3	7.057	686	692	705	rBB	460162	710010	50.37%	8.485%
4	7.522	765	771	778	rBB	76651	117152	8.31%	1.400%
5	7.834	817	824	832	rVB	296797	475008	33.70%	5.676%
6	8.692	964	970	987	rBV	209625	379088	26.89%	4.530%
7	10.292	1236	1242	1255	rBB	75915	136834	9.71%	1.635%
8	12.786	1660	1666	1683	rBV	470410	694347	49.26%	8.297%
9	13.663	1810	1815	1822	rBV	53248	76117	5.40%	0.910%
10	14.186	1898	1904	1912	rBB	123501	181794	12.90%	2.172%
11	15.698	2155	2161	2173	rBV	608370	839759	59.57%	10.035%
12	16.951	2369	2374	2379	rBV	164242	234556	16.64%	2.803%
13	16.998	2379	2382	2387	rVB	23803	28803	2.04%	0.344%
14	17.845	2519	2526	2530	rBV2	42238	55994	3.97%	0.669%
15	19.027	2722	2727	2732	rBV	69088	90258	6.40%	1.079%
16	19.139	2742	2746	2750	rBV3	14575	20322	1.44%	0.243%
17	19.368	2780	2785	2786	rBV3	8998	14543	1.03%	0.174%
18	19.392	2786	2789	2795	rVB	63426	81522	5.78%	0.974%
19	19.598	2819	2824	2830	rBV	1281180	1409629	100.00%	16.845%
20	19.898	2864	2875	2880	rBV2	15087	39073	2.77%	0.467%
21	20.056	2897	2902	2906	rBV3	9101	17190	1.22%	0.205%
22	20.445	2965	2968	2973	rVB5	27214	32457	2.30%	0.388%
23	20.621	2994	2998	3001	rBV6	14077	22086	1.57%	0.264%
24	20.733	3014	3017	3021	rBV5	23022	29544	2.10%	0.353%
25	20.792	3023	3027	3034	rVV6	19678	46218	3.28%	0.552%
26	20.862	3035	3039	3051	rVB4	82545	139087	9.87%	1.662%
27	20.992	3058	3061	3066	rVB3	39002	47507	3.37%	0.568%
28	21.068	3069	3074	3077	rBV2	36715	57108	4.05%	0.682%
29	21.168	3085	3091	3095	rBV2	334995	470224	33.36%	5.619%
30	21.203	3095	3097	3102	rVB	50288	58962	4.18%	0.705%
31	21.903	3213	3216	3222	rBV2	37985	59582	4.23%	0.712%
32	22.709	3349	3353	3357	rBV	51856	88524	6.28%	1.058%
33	23.356	3457	3463	3469	rBV	234634	419749	29.78%	5.016%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

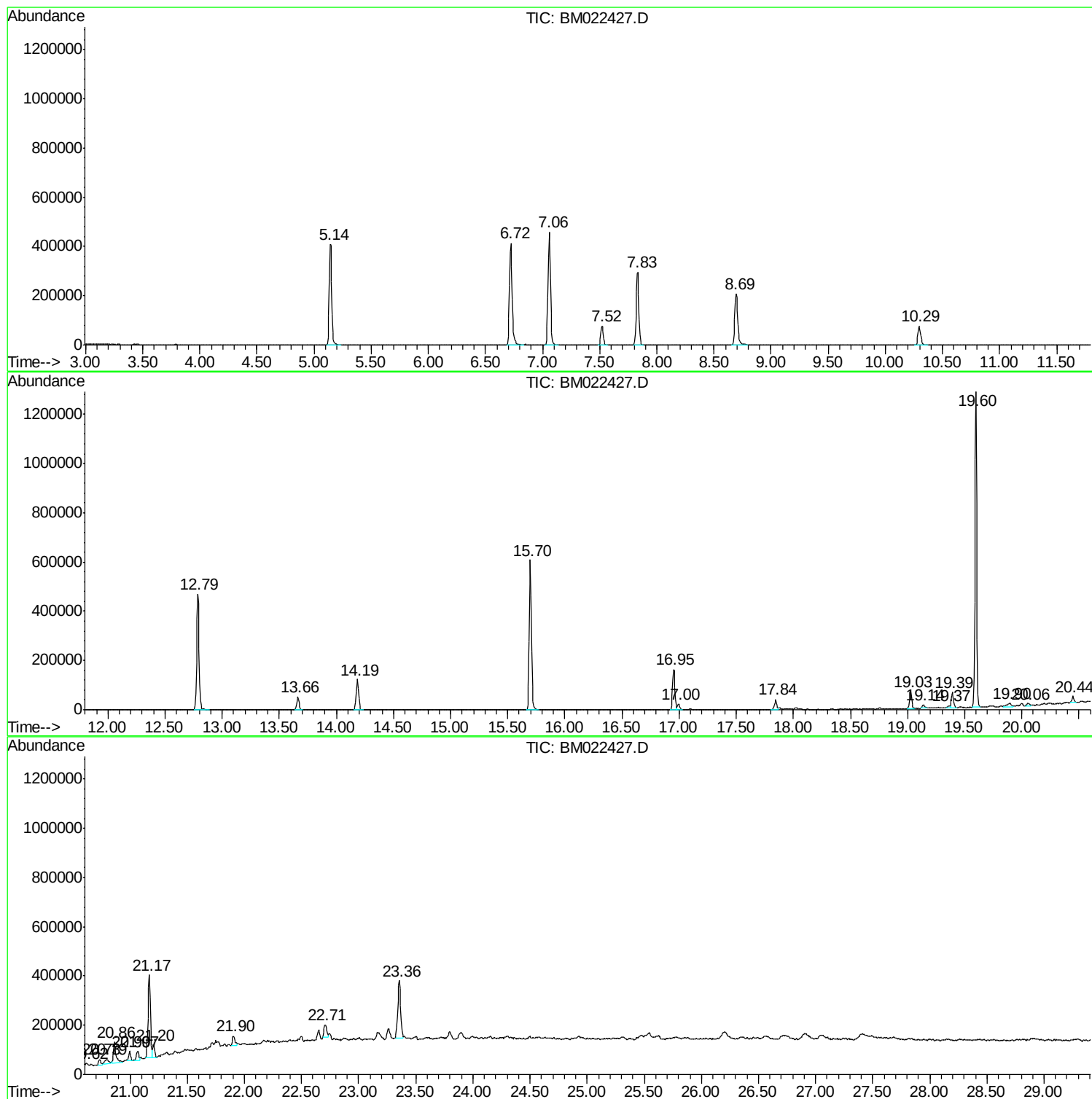
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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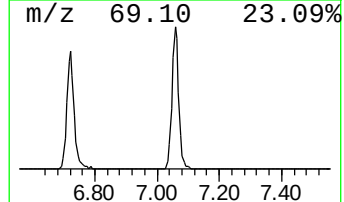
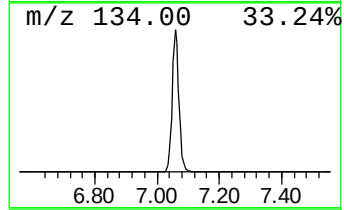
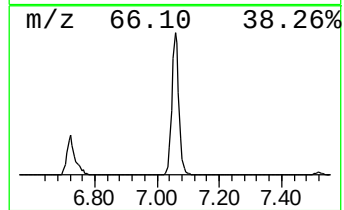
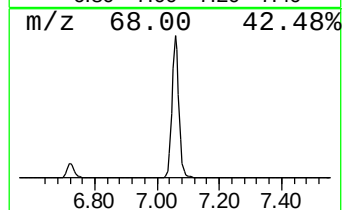
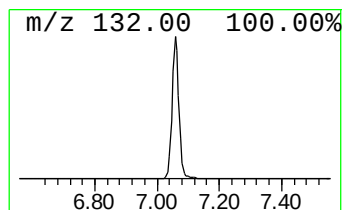
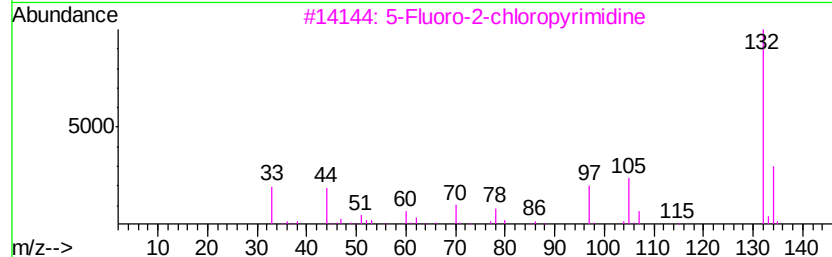
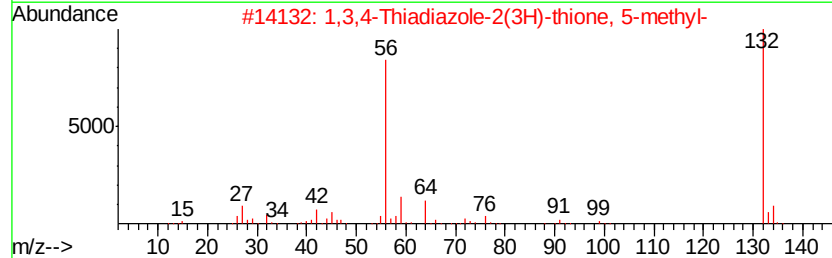
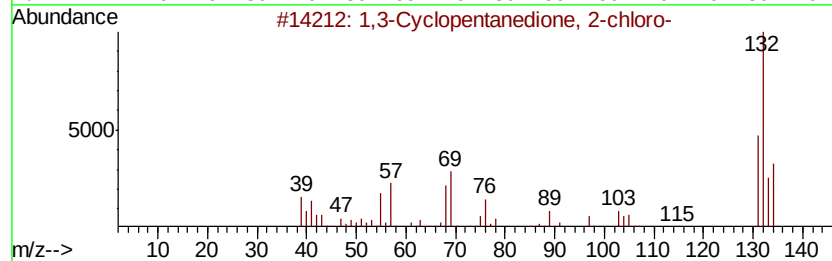
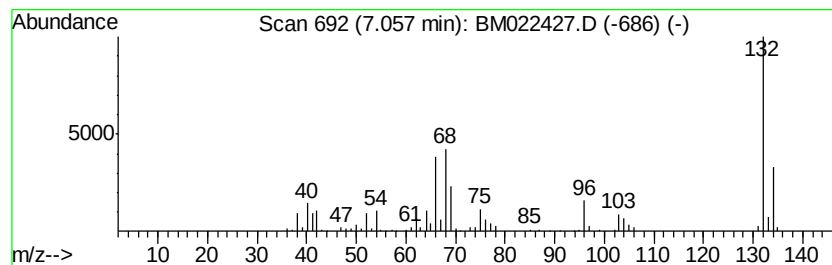
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	121.21 ng	710010	1,4-Dichlorobenzene-d4	7.52

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10



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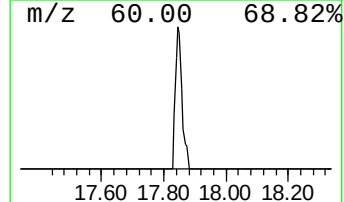
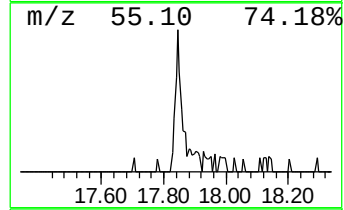
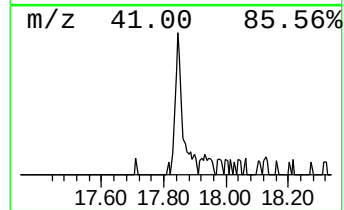
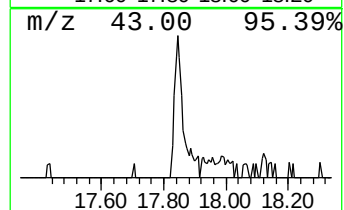
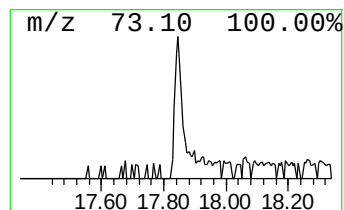
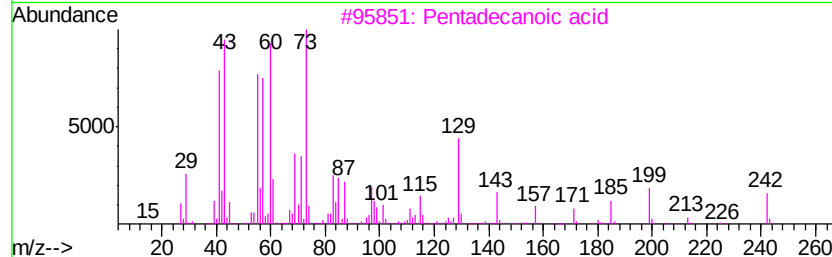
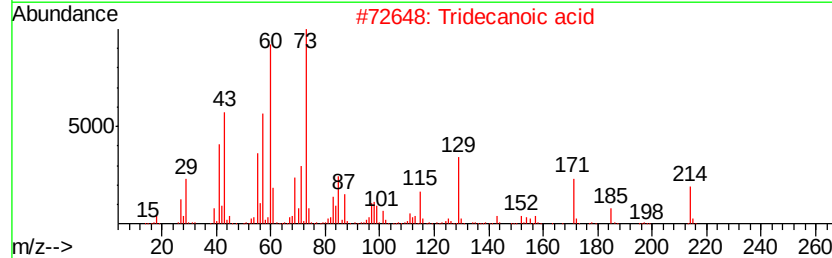
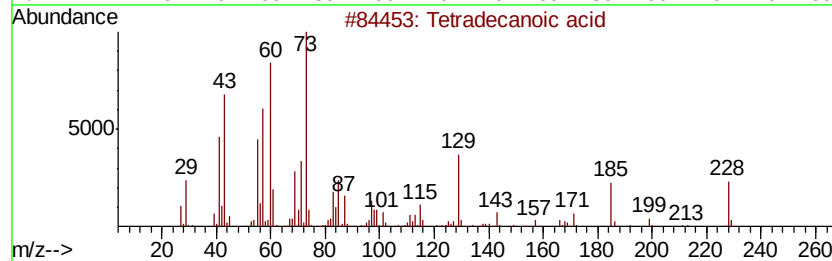
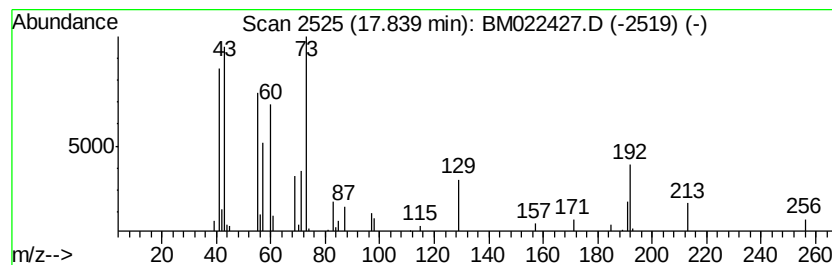
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082919.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.84	4.77 ng	55994	Phenanthrene-d10		16.95
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
2	Tridecanoic acid	214	C13H26O2	000638-53-9	50
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4	Undecanoic acid	186	C11H22O2	000112-37-8	43
5	Dodecanoic acid	200	C12H24O2	000143-07-7	43



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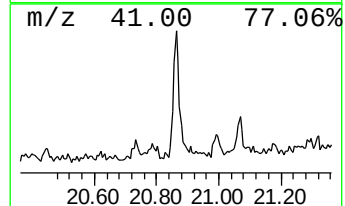
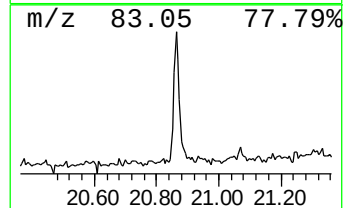
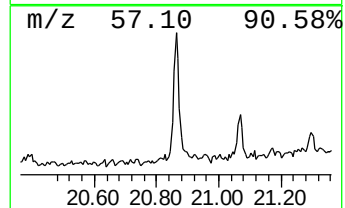
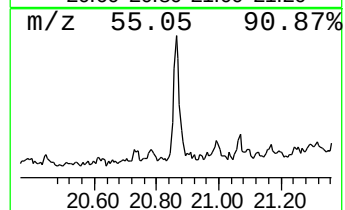
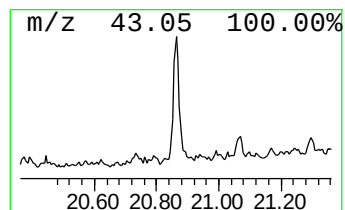
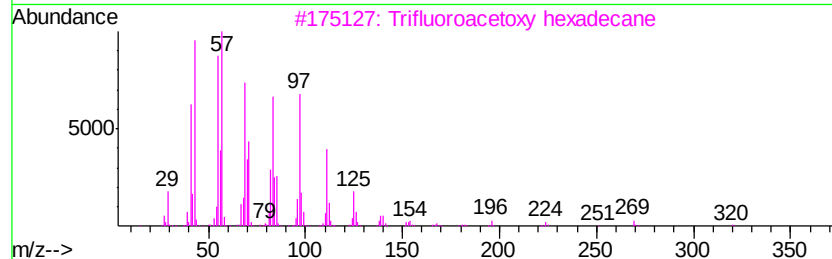
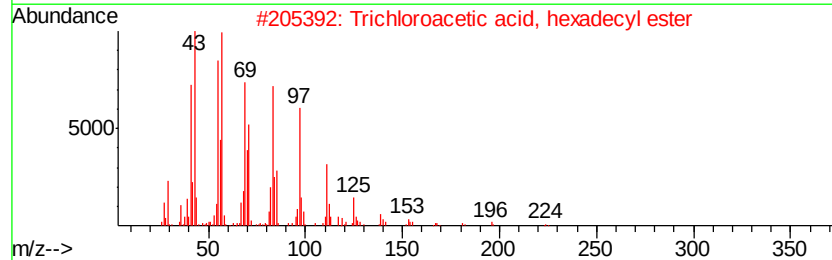
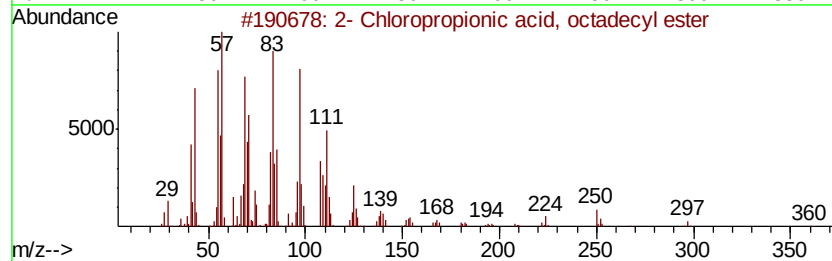
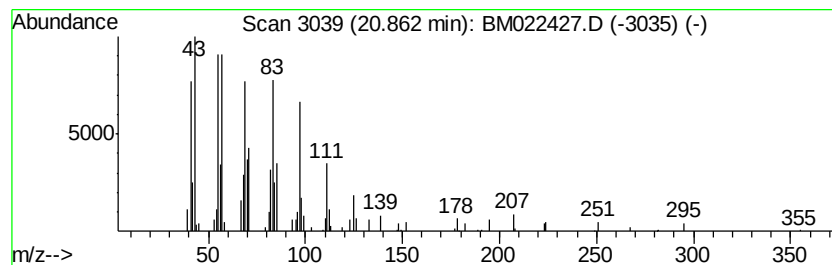
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2- Chloropropionic acid, oc... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.86	5.92 ng	139087	Chrysene-d12	21.17	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	91
4	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	90
5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	90



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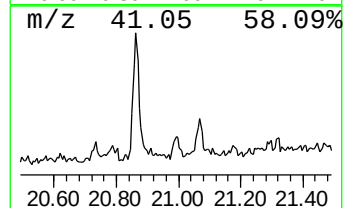
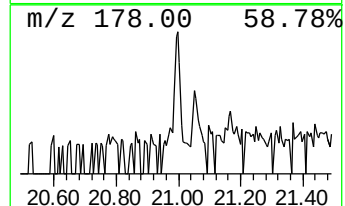
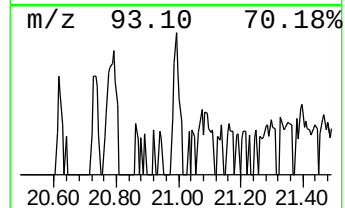
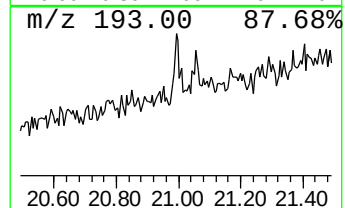
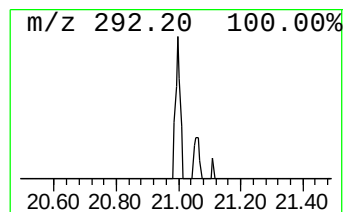
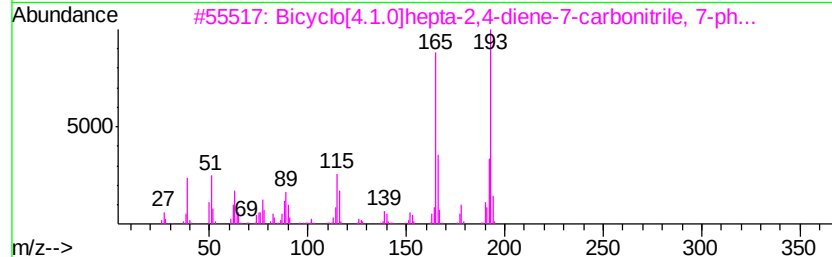
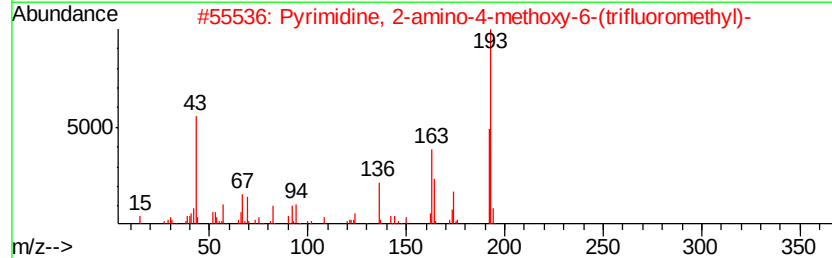
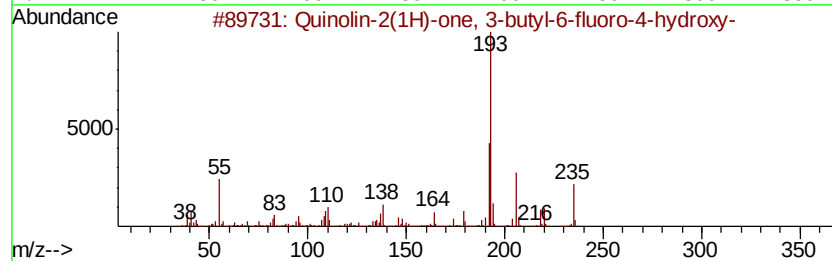
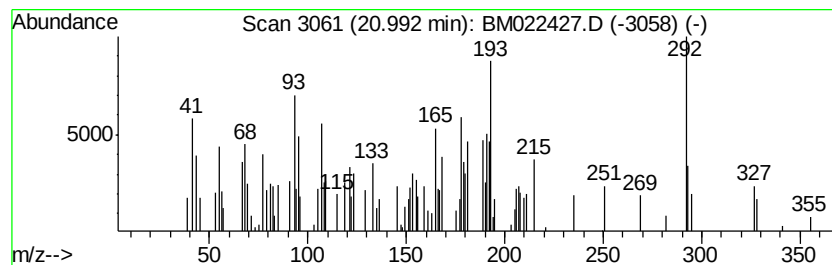
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown20.99 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.99	2.02 ng	47507	Chrysene-d12	21.17	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Quinolin-2(1H)-one, 3-butyl-6-fl...	235	C13H14FN02	279691-75-7	27
2	Pyrimidine, 2-amino-4-methoxy-6-...	193	C6H6F3N3O	016097-61-3	25
3	Bicyclo[4.1.0]hepta-2,4-diene-7-...	193	C14H11N	032777-15-4	18
4	1H-Pyrazole, 1-methyl-4-(4,4,5,5...	208	C10H17BN2O2	1000319-69-0	18
5	Methanimidamide, N,N-dimethyl-N'...	193	C9H11N3O2	002103-47-1	18



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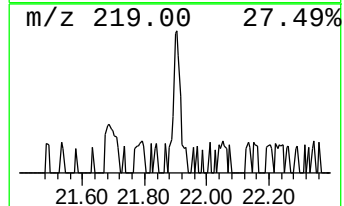
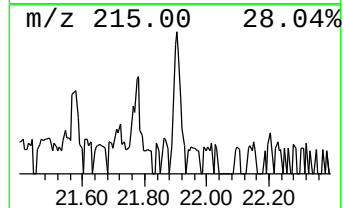
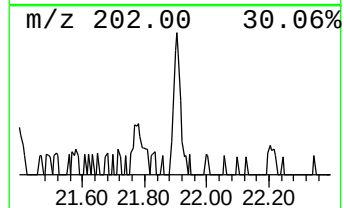
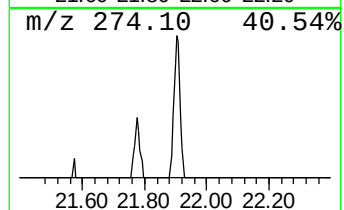
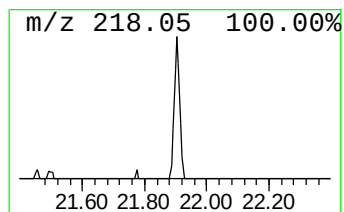
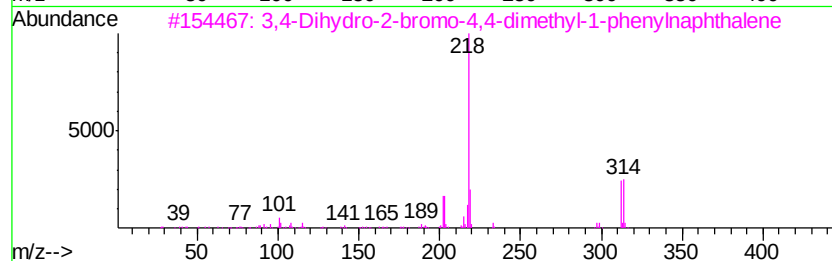
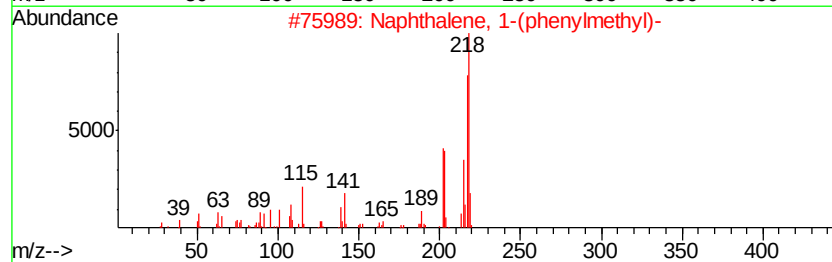
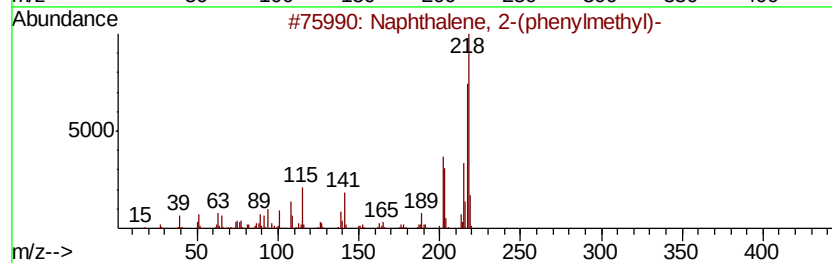
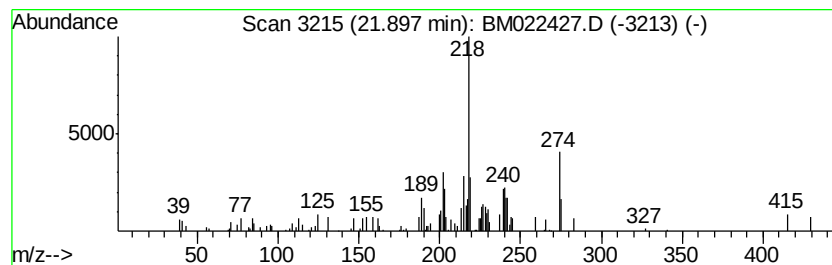
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082919.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown21.90 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.90	2.53 ng	59582	Chrysene-d12	21.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2-(phenylmethyl)-	218	C17H14	000613-59-2	38
2		Naphthalene, 1-(phenylmethyl)-	218	C17H14	000611-45-0	38
3		3,4-Dihydro-2-bromo-4,4-dimethyl...	312	C18H17Br	071161-44-9	35
4		Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	35
5		Tetrachloro-o-benzoquinone	244	C6Cl4O2	002435-53-2	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM082919\
Data File : BM022427.D
Acq On : 30 Aug 2019 02:51
Operator : HP/JU
Sample : K4514-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S301A-J-2.0-2.5-082319

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.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
unknown7.06	7.06	121.2	ng	710010	1	7.52	117152	20.0
Tetradecanoic acid	17.84	4.8	ng	55994	4	16.95	234556	20.0
2- Chloropropioni...	20.86	5.9	ng	139087	5	21.17	470224	20.0
unknown20.99	20.99	2.0	ng	47507	5	21.17	470224	20.0
unknown21.90	21.90	2.5	ng	59582	5	21.17	470224	20.0