

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
 Data File : BG059774.D
 Acq On : 20 Nov 2023 18:27
 Operator : MA/JU
 Sample : 05311-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-1

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_G\Methods\8270-BG111623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059774.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.826	406	415	423	rBV	381014	603290	27.29%	5.515%
2	7.453	684	692	700	rBV	464978	705842	31.93%	6.453%
3	8.329	834	841	848	rBV2	120084	205131	9.28%	1.875%
4	9.527	1036	1045	1055	rVB2	253687	463841	20.98%	4.240%
5	11.178	1320	1326	1333	rVB	201423	354073	16.02%	3.237%
6	13.581	1728	1735	1741	rVB	869699	1325478	59.96%	12.117%
7	13.781	1765	1769	1775	rVB5	19505	38134	1.73%	0.349%
8	14.962	1964	1970	1976	rVB	332069	493817	22.34%	4.514%
9	16.443	2216	2222	2233	rBV	762068	1161365	52.54%	10.617%
10	17.712	2432	2438	2443	rBV	396474	597251	27.02%	5.460%
11	17.753	2443	2445	2450	rVB	46801	57456	2.60%	0.525%
12	18.522	2568	2576	2582	rBV5	52367	104415	4.72%	0.955%
13	18.622	2590	2593	2598	rVB4	21428	31885	1.44%	0.291%
14	18.758	2614	2616	2622	rBV7	22468	43776	1.98%	0.400%
15	19.463	2733	2736	2742	rVB7	44149	65678	2.97%	0.600%
16	19.745	2778	2784	2788	rVV	169687	241008	10.90%	2.203%
17	19.886	2804	2808	2813	rBV8	18581	45768	2.07%	0.418%
18	19.991	2824	2826	2832	rVB7	17997	25753	1.17%	0.235%
19	20.068	2835	2839	2842	rVV5	29660	44564	2.02%	0.407%
20	20.109	2842	2846	2851	rVB	188005	261959	11.85%	2.395%
21	20.285	2870	2876	2882	rBV	1797624	2210467	100.00%	20.207%
22	20.420	2894	2899	2906	rBV	27440	76121	3.44%	0.696%
23	20.585	2926	2927	2931	rVB4	32169	24634	1.11%	0.225%
24	21.572	3092	3095	3101	rVB6	93109	145149	6.57%	1.327%
25	21.619	3101	3103	3109	rBV7	19826	29984	1.36%	0.274%
26	22.036	3166	3174	3180	rBV3	298474	661247	29.91%	6.045%
27	22.089	3180	3183	3188	rVB	77741	114499	5.18%	1.047%
28	24.216	3540	3545	3547	rBV6	20768	33622	1.52%	0.307%
29	24.457	3580	3586	3592	rBV3	50686	123436	5.58%	1.128%
30	25.279	3724	3726	3730	rVB4	29622	30063	1.36%	0.275%
31	25.444	3748	3754	3759	rBV6	37369	83601	3.78%	0.764%
32	25.614	3775	3783	3793	rVB2	161756	483395	21.87%	4.419%
33	31.507	4782	4786	4789	rBV6	14921	26185	1.18%	0.239%
34	32.224	4907	4908	4911	rBV3	28578	26024	1.18%	0.238%

Sum of corrected areas: 10938911

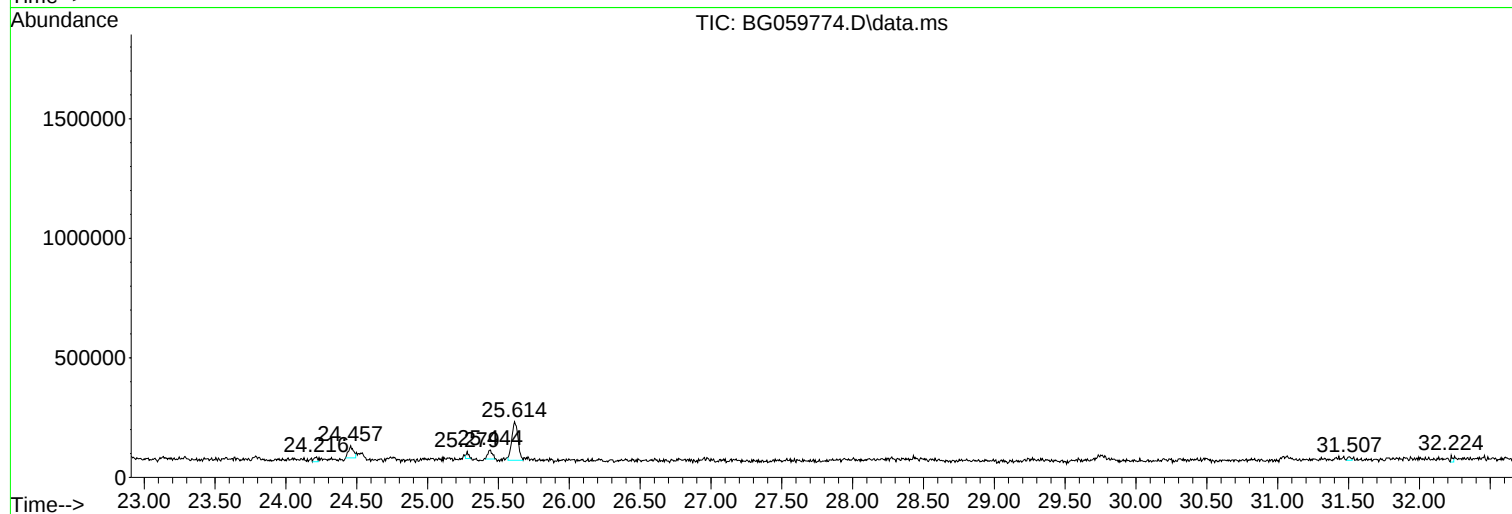
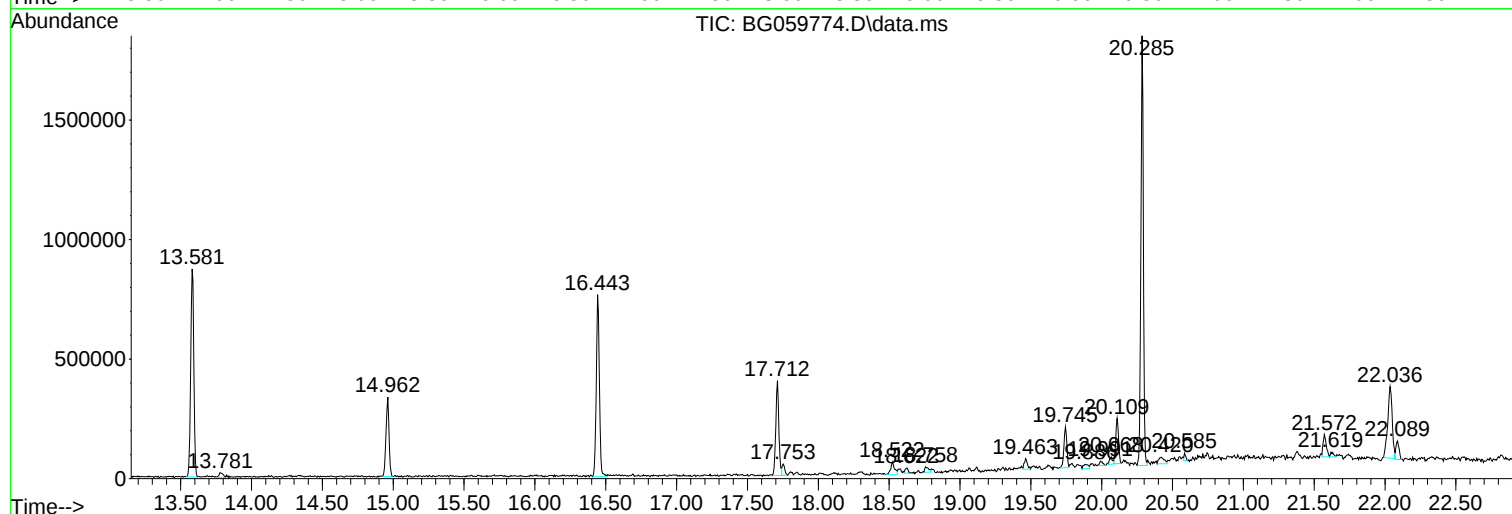
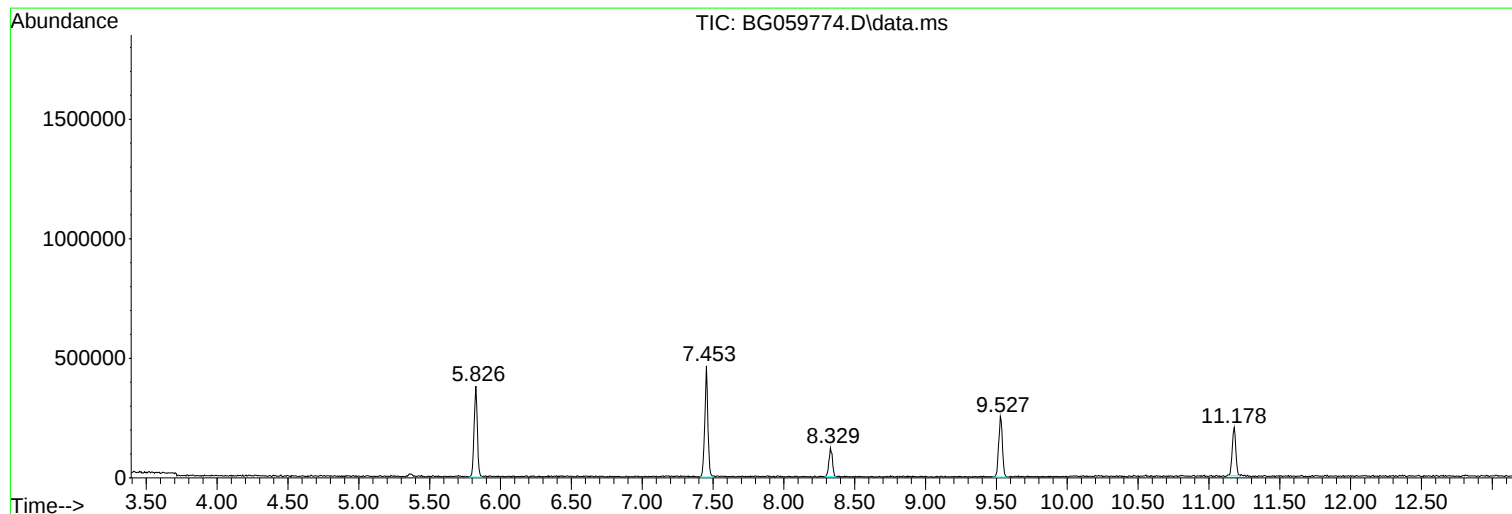
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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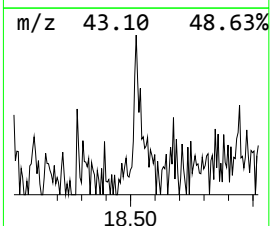
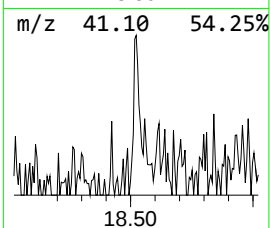
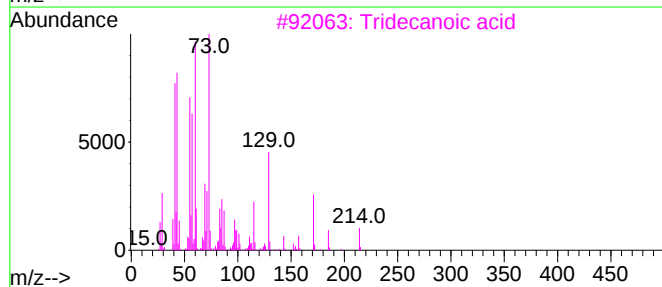
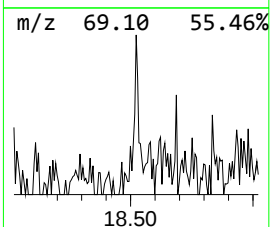
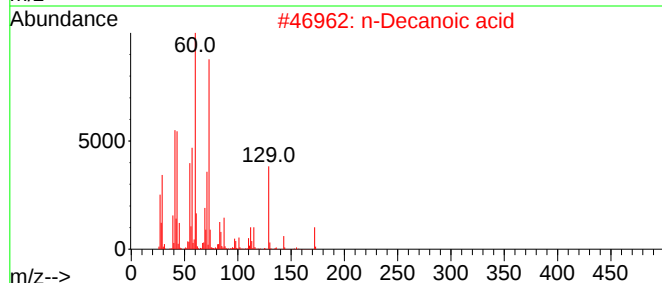
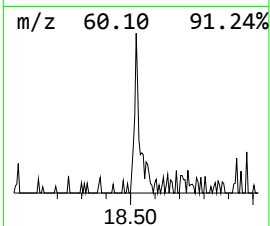
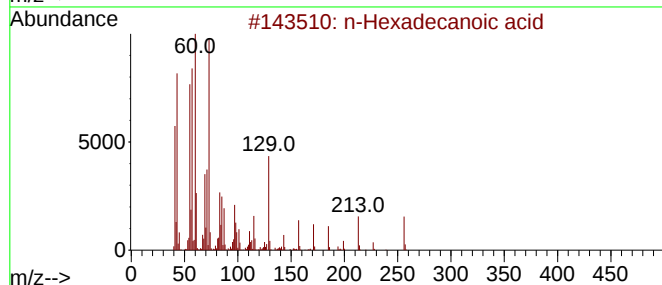
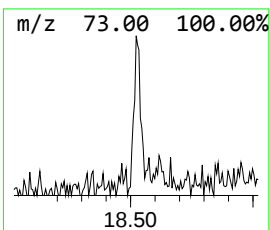
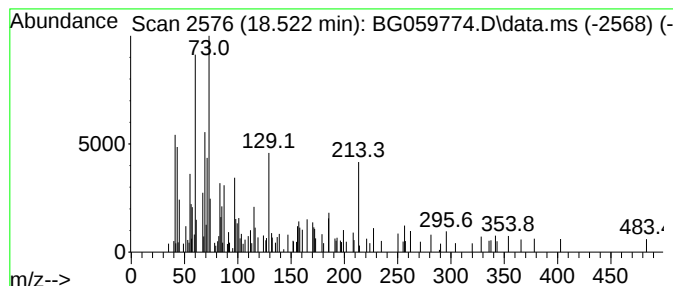
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.523	3.50 ng	104415	Phenanthrene-d10	17.712

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
2			n-Decanoic acid	172	C10H20O2	000334-48-5	50
3			Tridecanoic acid	214	C13H26O2	000638-53-9	49
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	47
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	43



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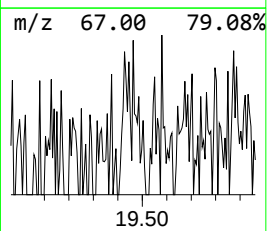
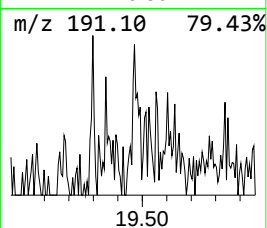
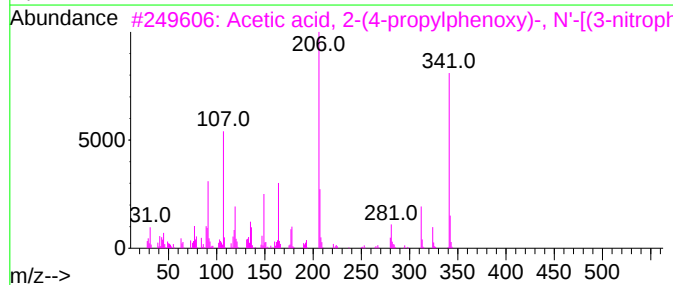
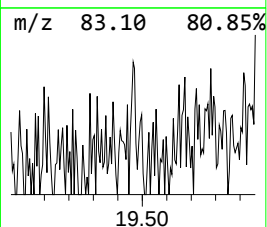
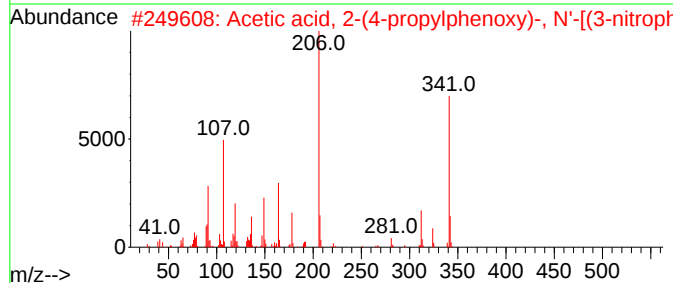
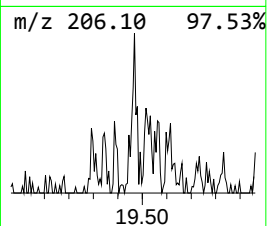
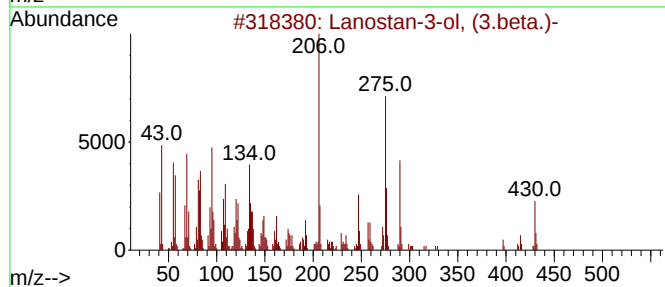
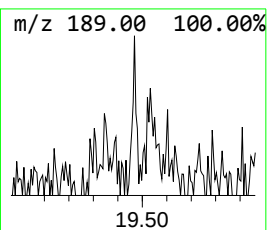
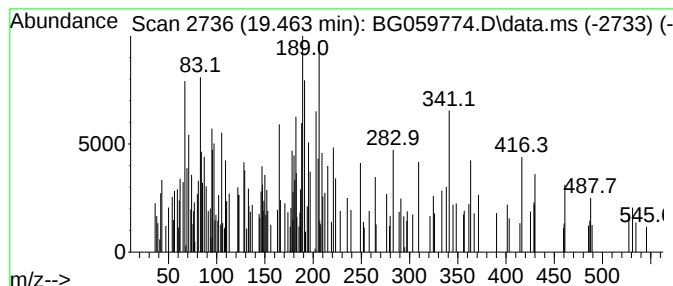
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown19.463 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.463	2.20 ng	65678	Phenanthrene-d10	17.712

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lanostan-3-ol, (3.beta.)-	430	C30H54O	004581-87-7	22
2			Acetic acid, 2-(4-propylphenoxy)...	341	C18H19N3O4	1000319-38-7	14
3			Acetic acid, 2-(4-propylphenoxy)...	341	C18H19N3O4	1000319-38-6	14
4			4-(2,4-Dinitrophenylazo)-N-(2,2,...	419	C15H10F5N5O4	1010224-92-9	8
5			1-(4-Nitrophenyl)-4-(3,4,5-trime...	401	C20H23N3O6	349116-90-1	2



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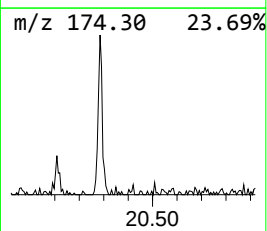
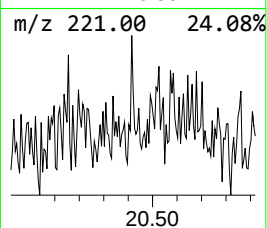
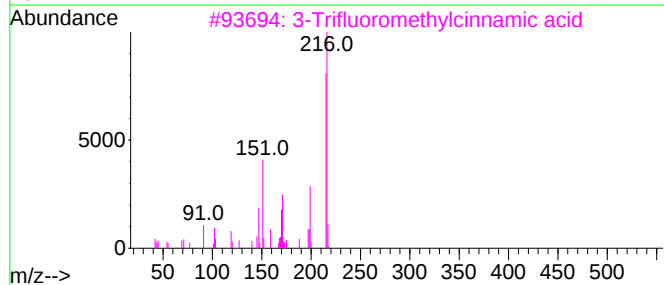
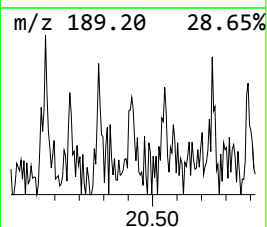
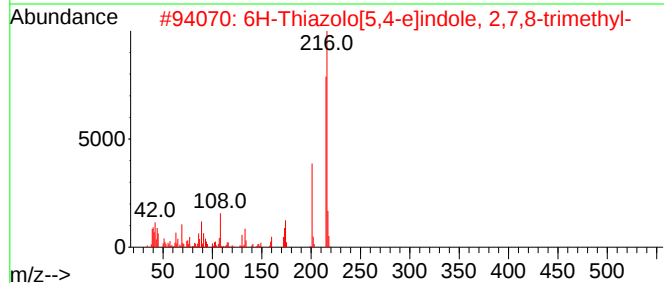
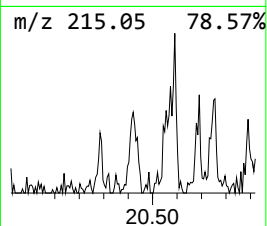
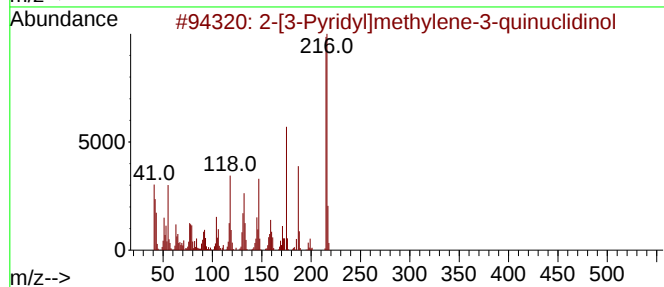
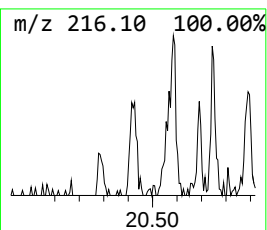
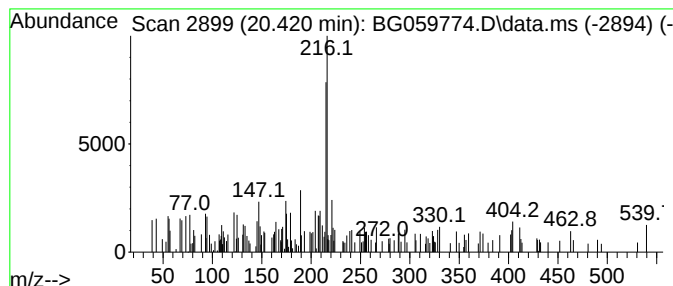
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-[3-Pyridyl]methylene-3-qu... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.420	2.30 ng	76121	Chrysene-d12	22.036

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[3-Pyridyl]methylene-3-quinucl...	216	C13H16N2O	273748-56-4	62		
2	6H-Thiazolo[5,4-e]indole, 2,7,8-...	216	C12H12N2S	1000338-32-0	62		
3	3-Trifluoromethylcinnamic acid	216	C10H7F3O2	000779-89-5	58		
4	Benzoic acid, 3-(3,5-dimethyl-1-...	216	C12H12N2O2	312531-88-7	58		
5	4H-Thiazolo[5,4-b]indole, 2,5,7-...	216	C12H12N2S	1010304-43-7	43		



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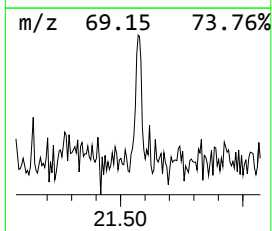
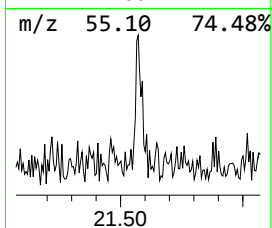
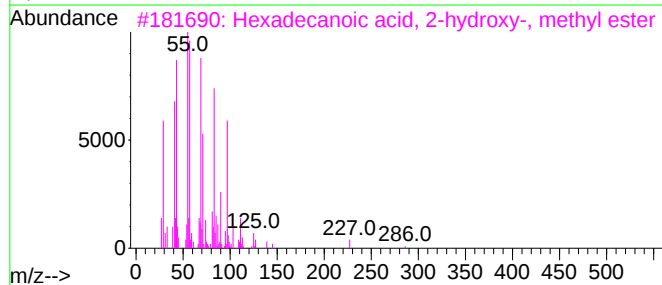
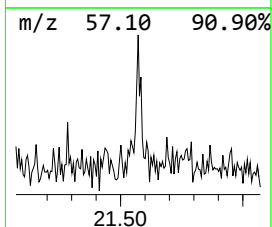
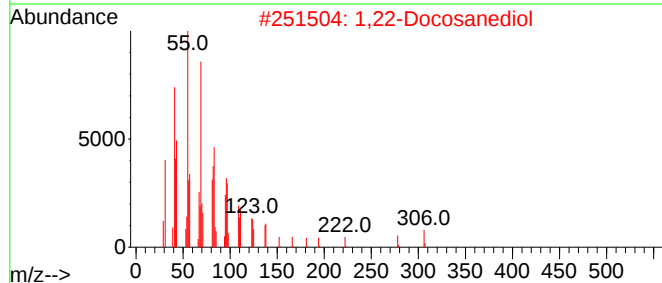
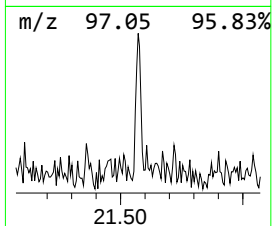
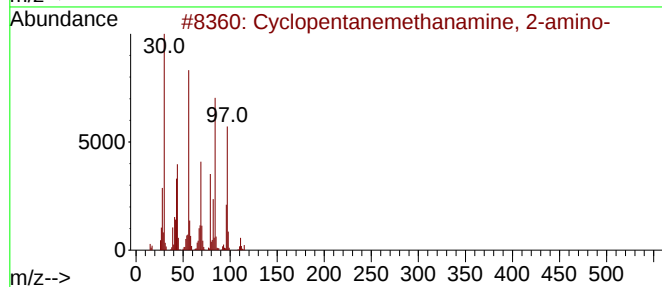
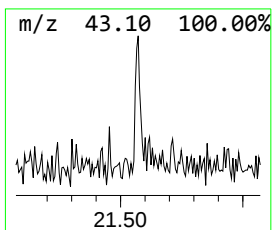
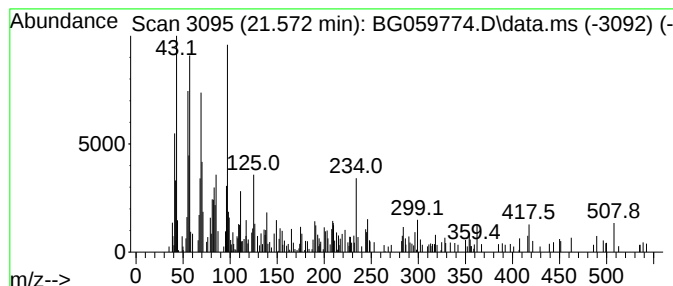
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Peak Number 4 unknown21.572 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.572	4.39 ng	145149	Chrysene-d12	22.036

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanemethanamine, 2-amino-	114	C6H14N2	021544-02-5	42
2			1,22-Docosanediol	342	C22H46O2	022513-81-1	38
3			Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	32
4			Methyl 2-hydroxydodecanoate	230	C13H26O3	051067-85-7	32
5			Iron, monocarbonyl-1,5-cycloocta...	390	C19H26FeO5	1000152-15-0	12



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.523	3.5	ng	104415	4	17.712	597251	20.0
unknown19.463	19.463	2.2	ng	65678	4	17.712	597251	20.0
2-[3-Pyridyl]me...	20.420	2.3	ng	76121	5	22.036	661247	20.0
unknown21.572	21.572	4.4	ng	145149	5	22.036	661247	20.0