

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
 Data File : BG059836.D
 Acq On : 23 Nov 2023 3:10
 Operator : MA/JU
 Sample : 05445-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SOIL-1-1115

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: BG059836.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.406	168	173	174	rBV5	10305	13179	1.04%	0.160%
2	4.829	239	245	247	rBV6	7779	12966	1.02%	0.157%
3	4.900	255	257	261	rBV2	13465	17901	1.41%	0.217%
4	5.822	407	414	424	rBV	402930	670494	52.92%	8.138%
5	7.450	683	691	702	rBV2	304773	543329	42.89%	6.595%
6	8.331	833	841	847	rBV2	100554	180180	14.22%	2.187%
7	9.530	1038	1045	1053	rVB2	213910	363171	28.67%	4.408%
8	11.181	1319	1326	1332	rBV	148968	281011	22.18%	3.411%
9	13.584	1729	1735	1742	rVB2	583350	885382	69.89%	10.746%
10	13.707	1750	1756	1762	rVB8	8750	15989	1.26%	0.194%
11	13.783	1763	1769	1773	rBV4	16659	24933	1.97%	0.303%
12	13.883	1784	1786	1791	rVB3	11253	12943	1.02%	0.157%
13	14.347	1858	1865	1870	rVB7	14948	26459	2.09%	0.321%
14	14.653	1913	1917	1922	rBV7	10052	14622	1.15%	0.177%
15	14.753	1927	1934	1937	rBV8	7882	19878	1.57%	0.241%
16	14.959	1963	1969	1977	rBV2	267140	434139	34.27%	5.269%
17	16.375	2207	2210	2214	rVB6	13718	15370	1.21%	0.187%
18	16.445	2215	2222	2229	rVB2	557241	850465	67.13%	10.323%
19	16.598	2243	2248	2250	rBV5	19078	28017	2.21%	0.340%
20	16.862	2288	2293	2295	rBV6	8054	15235	1.20%	0.185%
21	17.068	2325	2328	2331	rVB5	12330	18925	1.49%	0.230%
22	17.162	2338	2344	2346	rBV6	10798	14619	1.15%	0.177%
23	17.215	2349	2353	2355	rBV5	8647	14736	1.16%	0.179%
24	17.420	2383	2388	2391	rBV6	11063	20328	1.60%	0.247%
25	17.714	2431	2438	2444	rBV	343331	550079	43.42%	6.677%
26	17.767	2444	2447	2450	rVB5	14989	16306	1.29%	0.198%
27	18.243	2526	2528	2530	rBV3	12751	13449	1.06%	0.163%
28	18.372	2546	2550	2551	rBV4	10953	14212	1.12%	0.172%
29	18.525	2572	2576	2583	rBV3	122550	161318	12.73%	1.958%
30	18.701	2604	2606	2610	rBV5	16889	15857	1.25%	0.192%
31	19.759	2781	2786	2787	rVV5	28260	43237	3.41%	0.525%
32	19.782	2787	2790	2795	rVB7	42891	62479	4.93%	0.758%
33	20.047	2833	2835	2836	rBV2	16148	13832	1.09%	0.168%
34	20.111	2842	2846	2850	rVB4	30304	40862	3.23%	0.496%
35	20.288	2871	2876	2881	rBV	1012867	1266898	100.00%	15.377%
36	21.574	3091	3095	3102	rVB9	58692	106902	8.44%	1.298%

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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 >

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37	21.786	3129	3131	3134	rVB4	24407	23920	1.89%	0.290%
38	21.944	3156	3158	3161	rVB4	45174	42139	3.33%	0.511%
39	22.038	3168	3174	3180	rVB2	270741	493628	38.96%	5.991%
40	22.438	3237	3242	3243	rVB5	20500	30224	2.39%	0.367%
41	22.550	3258	3261	3262	rBV3	34498	27179	2.15%	0.330%
42	23.108	3354	3356	3358	rBV3	14640	19802	1.56%	0.240%
43	23.149	3361	3363	3365	rVB3	17814	13881	1.10%	0.168%
44	23.454	3410	3415	3417	rBV6	31597	45358	3.58%	0.551%
45	24.453	3581	3585	3586	rBV4	26630	28168	2.22%	0.342%
46	24.935	3663	3667	3668	rVB4	13780	14302	1.13%	0.174%
47	25.623	3775	3784	3795	rVB	168084	498008	39.31%	6.045%
48	25.846	3817	3822	3831	rVB	37884	93912	7.41%	1.140%
49	26.568	3944	3945	3948	rBV3	12352	12705	1.00%	0.154%
50	27.420	4088	4090	4093	rBV4	10621	13090	1.03%	0.159%
51	27.485	4099	4101	4104	rVV3	15493	21404	1.69%	0.260%
52	28.372	4248	4252	4253	rBV4	14789	12857	1.01%	0.156%
53	30.294	4576	4579	4582	rBV5	14196	15923	1.26%	0.193%
54	32.462	4946	4948	4951	rVB3	15483	13629	1.08%	0.165%
55	32.497	4951	4954	4957	rBV4	11692	19095	1.51%	0.232%

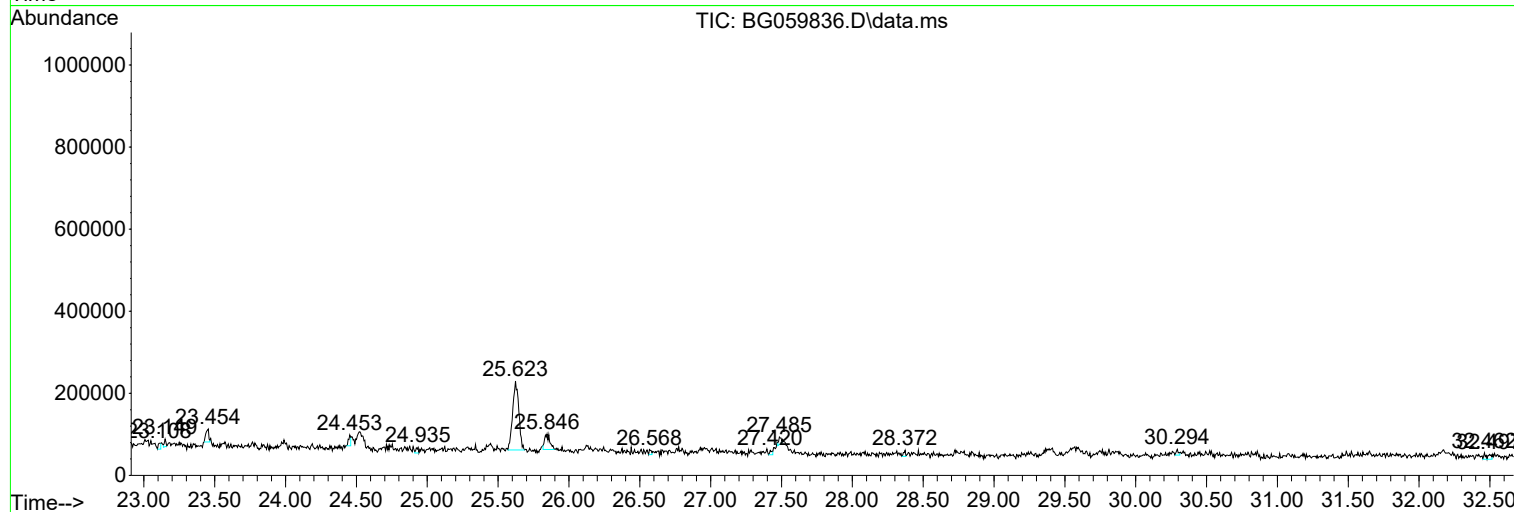
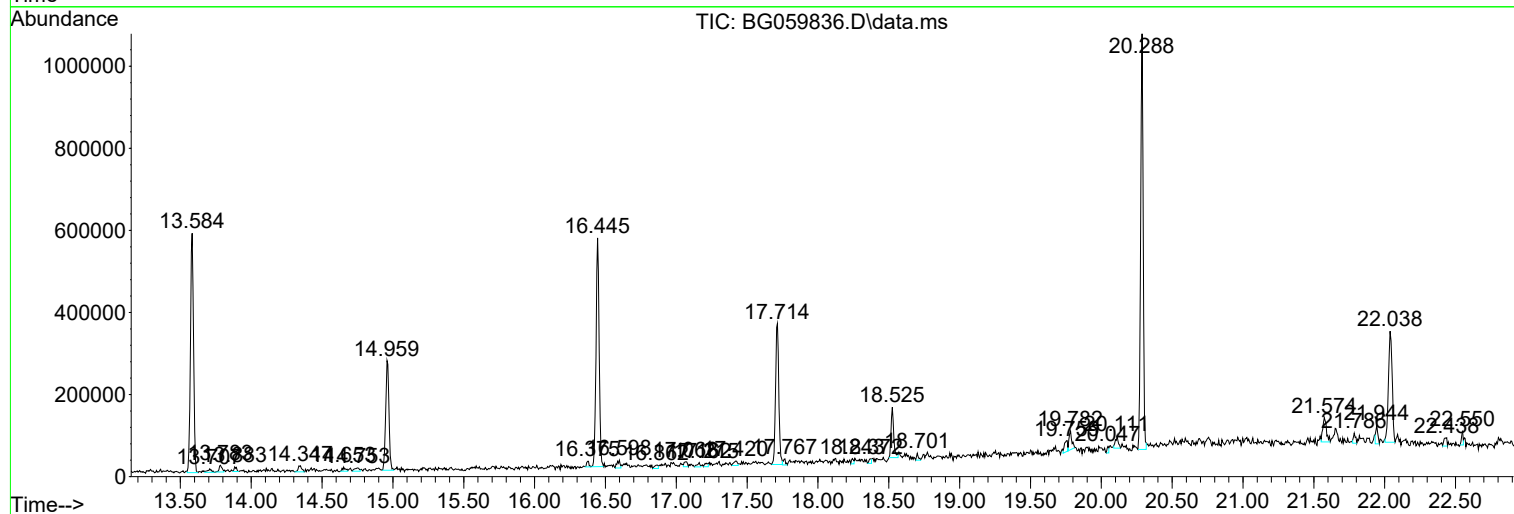
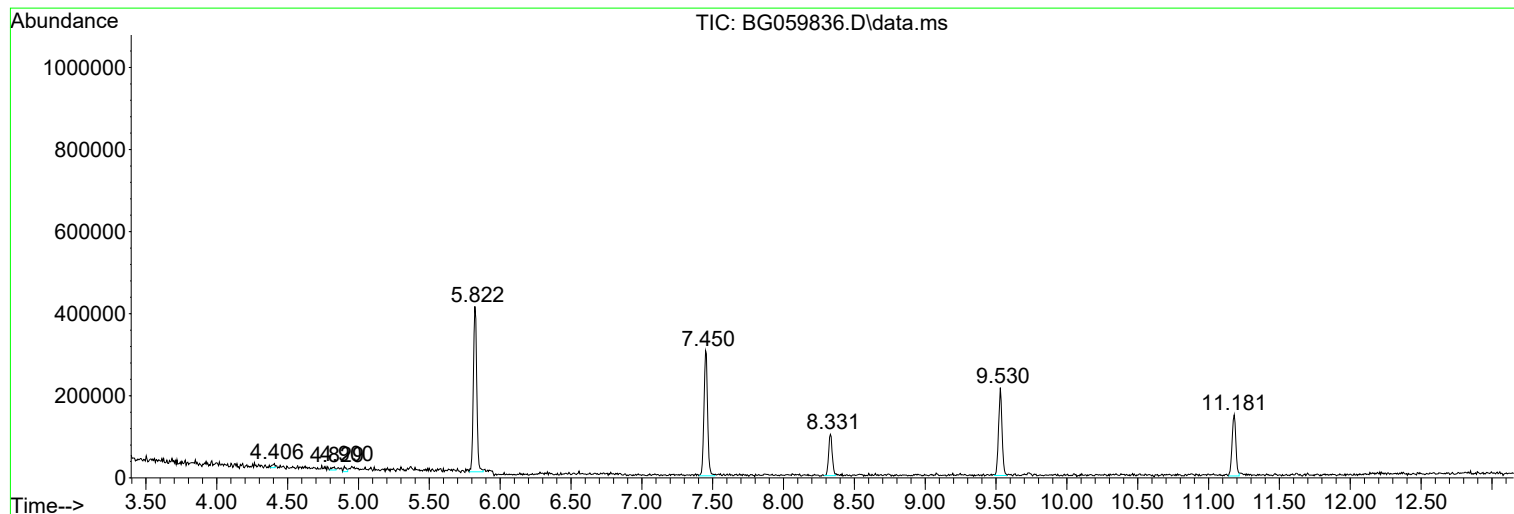
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 18 Sample Multiplier: 1

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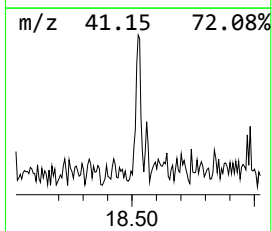
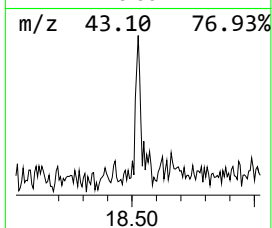
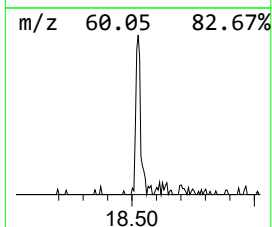
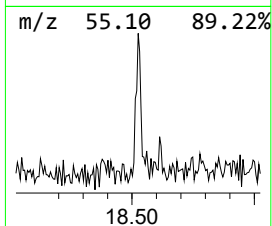
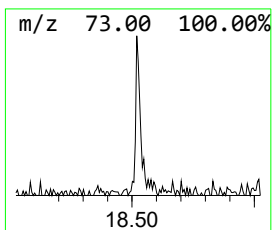
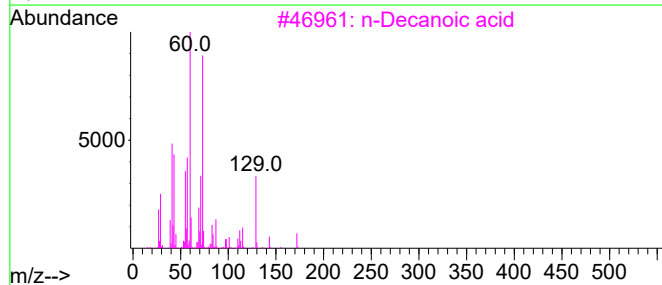
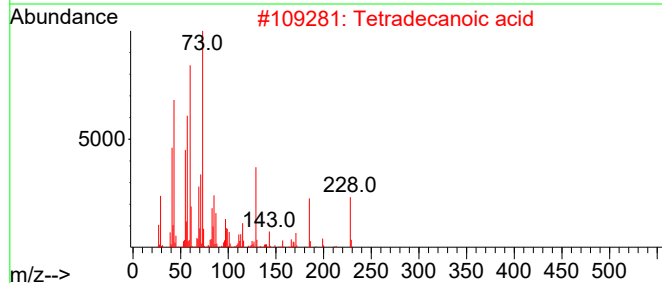
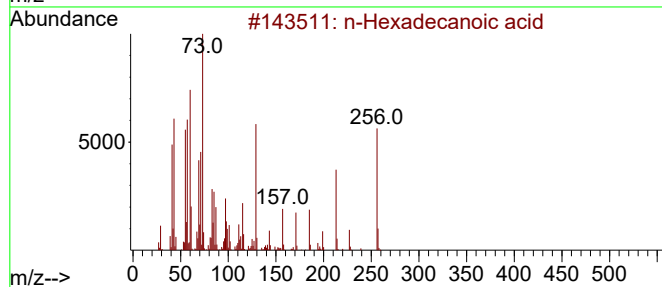
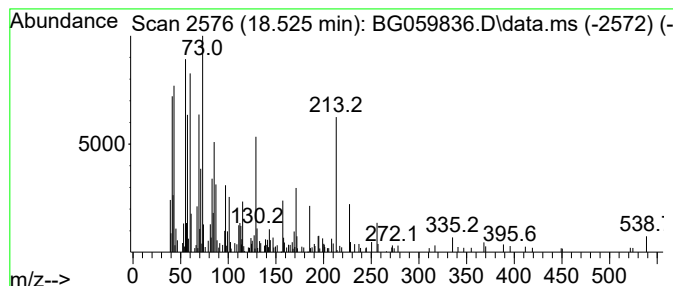
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.525	5.87 ng	161318	Phenanthrene-d10	17.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3			n-Decanoic acid	172	C10H20O2	000334-48-5	50
4			Dodecanoic acid	200	C12H24O2	000143-07-7	50
5			Undecanoic acid	186	C11H22O2	000112-37-8	49



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ALS Vial : 18 Sample Multiplier: 1

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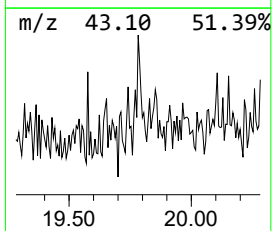
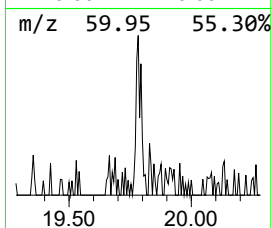
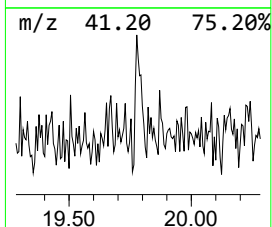
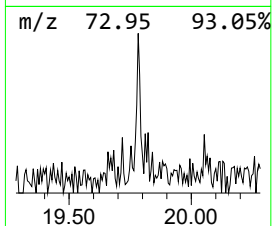
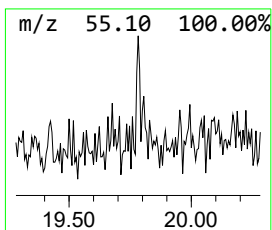
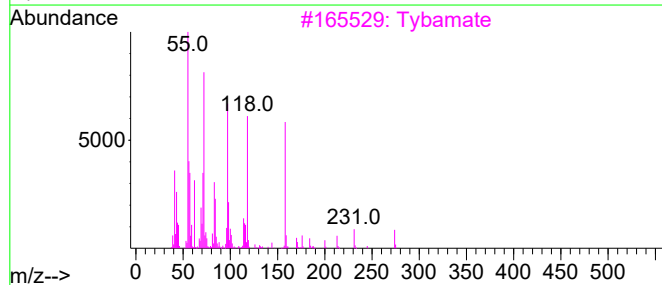
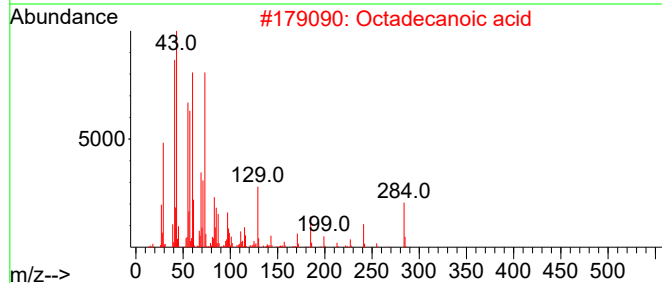
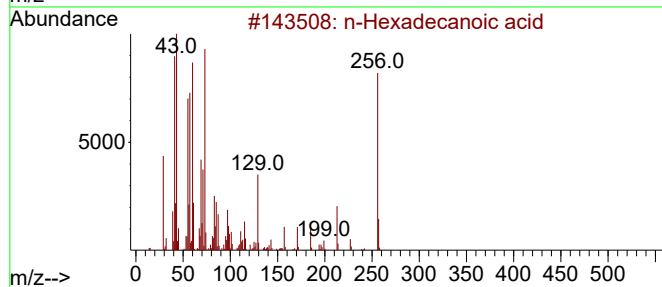
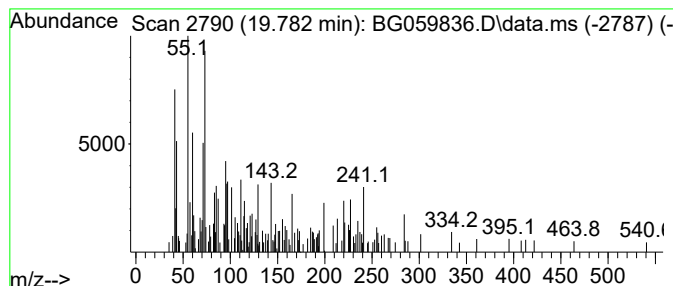
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown19.782 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.782	2.27 ng	62479	Phenanthrene-d10	17.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	25
2			Octadecanoic acid	284	C18H36O2	000057-11-4	15
3			Tybamate	274	C13H26N2O4	004268-36-4	11
4			1-(4-Methoxybenzyl)biguanidine	221	C10H15N5O	038164-13-5	11
5			n-Decanoic acid	172	C10H20O2	000334-48-5	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
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Misc :
ALS Vial : 18 Sample Multiplier: 1

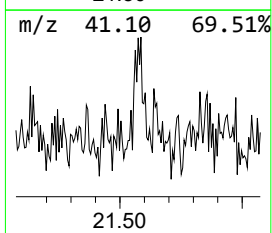
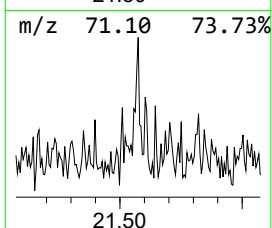
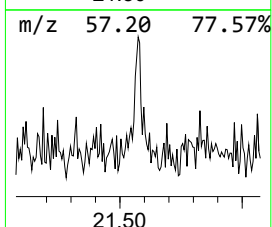
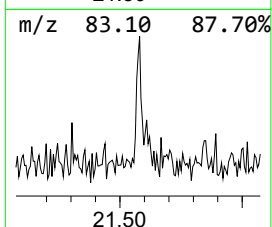
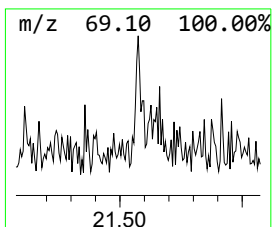
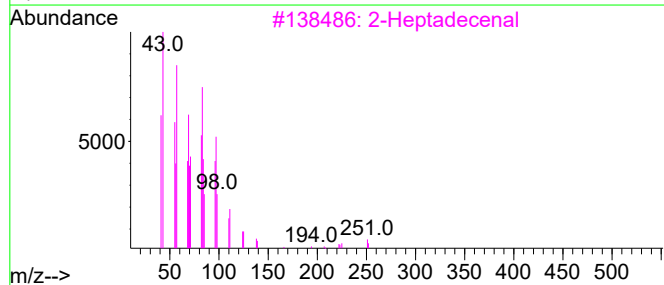
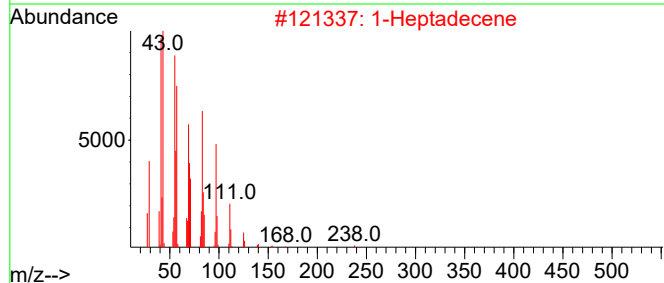
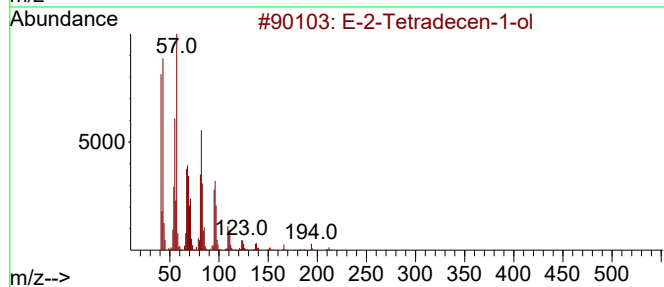
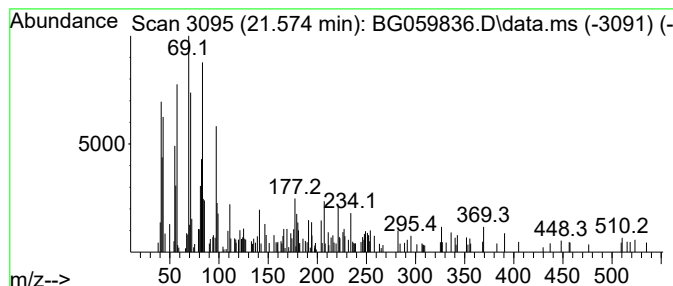
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 E-2-Tetradecen-1-ol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.574	4.33 ng	106902	Chrysene-d12	22.044	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-2-Tetradecen-1-ol	212	C14H28O	1000130-83-7	64
2	1-Heptadecene	238	C17H34	006765-39-5	49
3	2-Heptadecenal	252	C17H32O	1000143-48-6	43
4	5-Octen-2-one, 3,6-dimethyl-	154	C10H18O	064165-21-5	27
5	2,2-dimethylbutyric Acid, 2,2,2-...	198	C8H13F3O2	1000376-55-7	22



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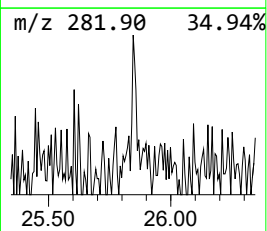
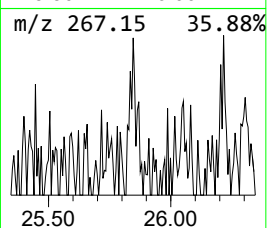
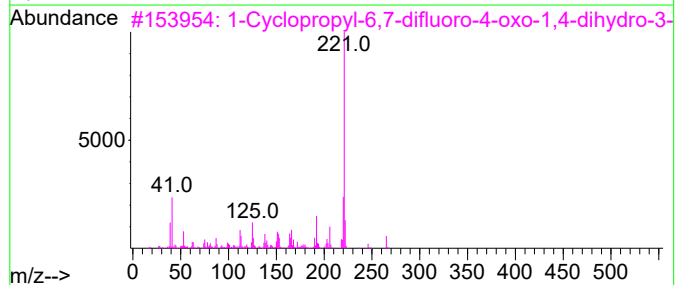
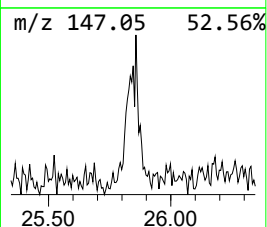
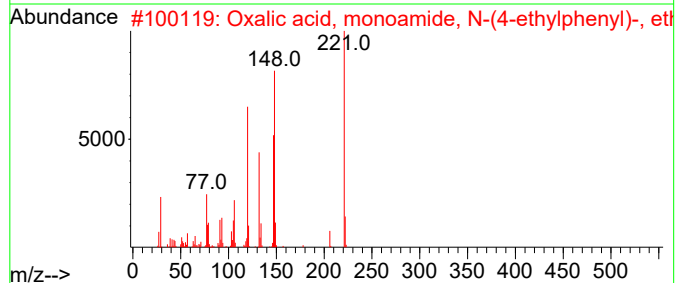
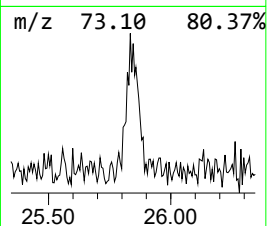
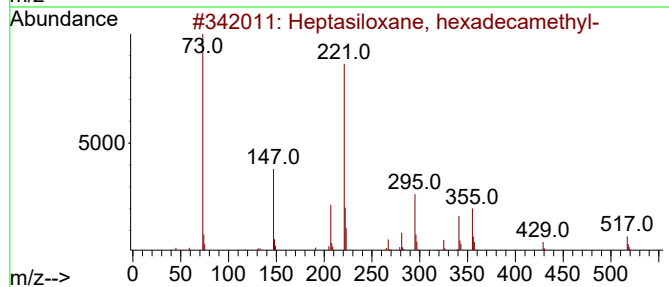
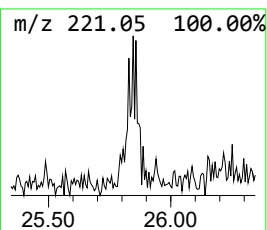
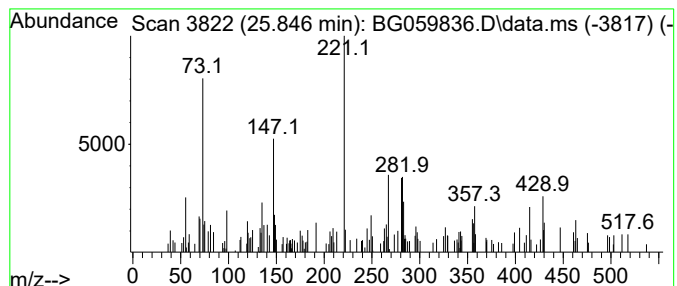
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown25.846 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.846	3.77 ng	93912	Perylene-d12	25.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	43
2			Oxalic acid, monoamide, N-(4-eth...	221	C12H15NO3	1000309-57-9	38
3			1-Cyclopropyl-6,7-difluoro-4-oxo...	265	C13H9F2NO3	1000496-58-9	35
4			2-Amino-4-(4-nitrophenyl)thiazole	221	C9H7N3O2S	002104-09-8	35
5			1-Oxo-6,7-dimethoxy-1,2,3,4-tetr...	221	C12H15NO3	052401-41-9	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.525	5.9	ng	161318	4	17.714	550079	20.0
unknown19.782	19.782	2.3	ng	62479	4	17.714	550079	20.0
E-2-Tetradecen-...	21.574	4.3	ng	106902	5	22.044	493628	20.0
unknown25.846	25.846	3.8	ng	93912	6	25.622	498008	20.0