

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
 Data File : BM042443.D
 Acq On : 25 Oct 2023 18:26
 Operator : MA/JU
 Sample : 05001-01 2X
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 486-WC-COMP

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-BM102123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042443.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	315	320	328	rBV	181486	248970	8.48%	0.757%
2	5.516	390	396	405	rBV	1104534	1581289	53.88%	4.807%
3	7.140	665	672	682	rBV	1105748	1767526	60.23%	5.373%
4	7.216	682	685	694	rVB	23818	41785	1.42%	0.127%
5	7.993	810	817	827	rVB	638517	988490	33.68%	3.005%
6	9.187	1009	1020	1029	rBV	659458	1086513	37.02%	3.303%
7	9.651	1095	1099	1105	rVB	24364	37595	1.28%	0.114%
8	10.810	1288	1296	1304	rBV	839057	1413716	48.17%	4.297%
9	13.257	1706	1712	1724	rVB	1533490	2158662	73.56%	6.562%
10	13.480	1742	1750	1754	rBV3	17073	32671	1.11%	0.099%
11	14.633	1938	1946	1953	rBV	1234030	1798878	61.30%	5.468%
12	15.680	2116	2124	2129	rBV	24135	41965	1.43%	0.128%
13	16.127	2193	2200	2210	rBV2	1185911	1833339	62.47%	5.573%
14	16.621	2280	2284	2285	rBV2	24907	29914	1.02%	0.091%
15	16.668	2289	2292	2299	rVB	49426	72823	2.48%	0.221%
16	17.386	2405	2414	2418	rBV	1561494	2173264	74.06%	6.606%
17	17.427	2418	2421	2428	rVV	369910	474486	16.17%	1.442%
18	17.515	2431	2436	2447	rVB	69518	128604	4.38%	0.391%
19	17.627	2451	2455	2461	rVB2	69252	91213	3.11%	0.277%
20	17.810	2477	2486	2489	rBV3	22232	43919	1.50%	0.134%
21	17.868	2493	2496	2500	rBV	24327	30616	1.04%	0.093%
22	18.110	2532	2537	2542	rBV3	40330	67685	2.31%	0.206%
23	18.233	2552	2558	2567	rBV	1163886	1702909	58.03%	5.176%
24	18.457	2591	2596	2599	rBV3	47092	68921	2.35%	0.210%
25	18.757	2643	2647	2650	rBV	35233	47434	1.62%	0.144%
26	19.168	2712	2717	2719	rBV2	128960	167189	5.70%	0.508%
27	19.368	2748	2751	2752	rBV	34267	34948	1.19%	0.106%
28	19.409	2752	2758	2760	rVV	245118	399131	13.60%	1.213%
29	19.439	2760	2763	2770	rVV	598489	797192	27.17%	2.423%
30	19.509	2770	2775	2792	rVV	882296	1302983	44.40%	3.961%
31	19.762	2815	2818	2821	rBV2	70592	103907	3.54%	0.316%
32	19.804	2821	2825	2832	rVB	436849	572577	19.51%	1.741%
33	19.998	2852	2858	2867	rBV	2310903	2934595	100.00%	8.920%
34	20.721	2978	2981	2983	rBV2	52950	53897	1.84%	0.164%
35	21.098	3042	3045	3051	rBV6	101298	151507	5.16%	0.461%
36	21.227	3063	3067	3074	rVB3	421525	599357	20.42%	1.822%

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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-BM102123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.562	3118	3124	3129	rBV	1897441	2810778	95.78%	8.544%
38	21.603	3129	3131	3135	rVB	183369	184730	6.29%	0.562%
39	22.074	3208	3211	3215	rBV	184642	203040	6.92%	0.617%
40	23.168	3393	3397	3407	rVB	421535	700642	23.88%	2.130%
41	24.027	3537	3543	3550	rVB	1041170	2103458	71.68%	6.394%
42	24.533	3624	3629	3638	rVB	372698	800711	27.29%	2.434%
43	24.650	3643	3649	3661	rVB	386353	1013375	34.53%	3.080%

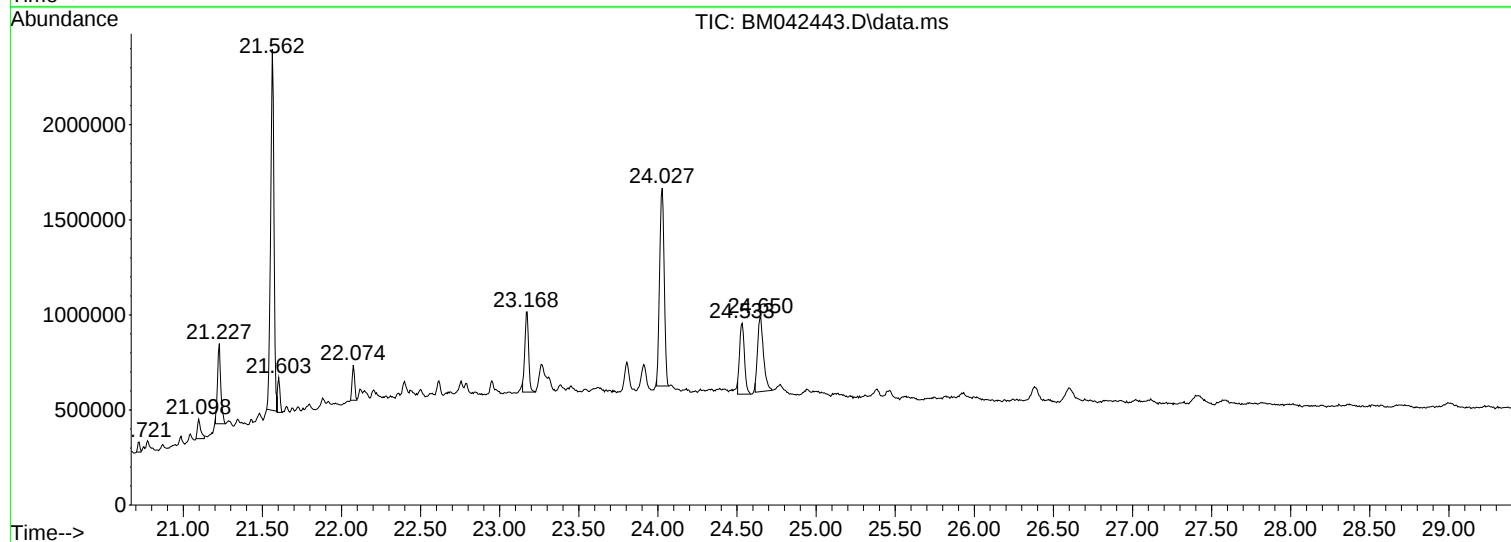
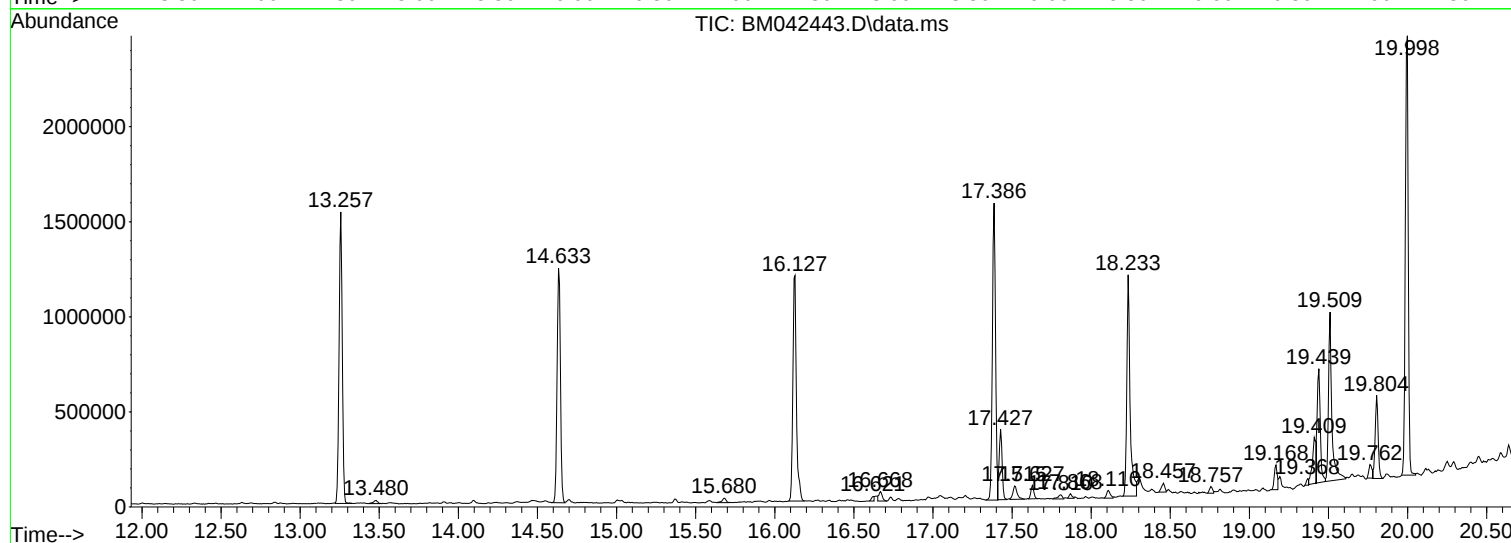
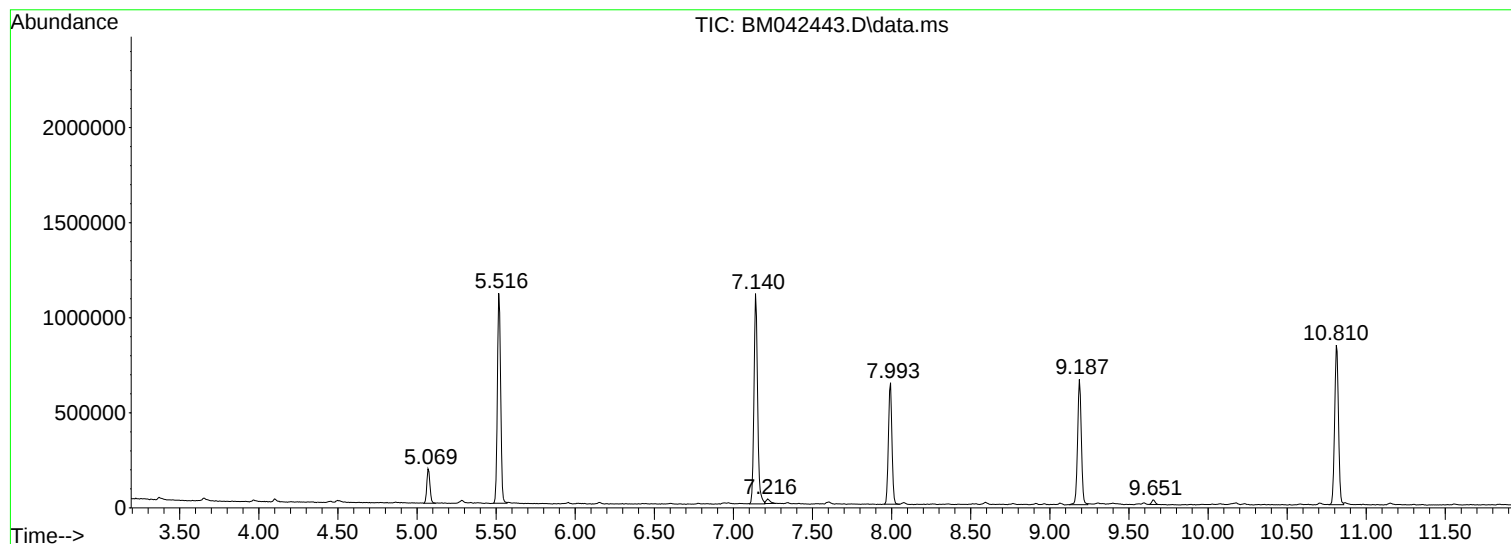
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Quant Title :

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



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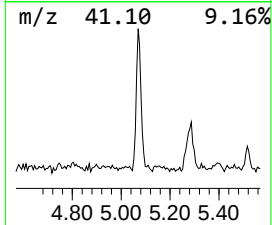
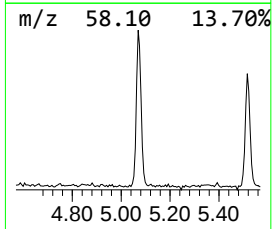
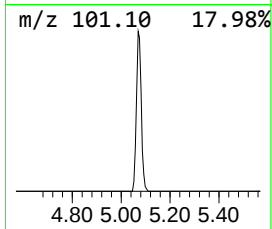
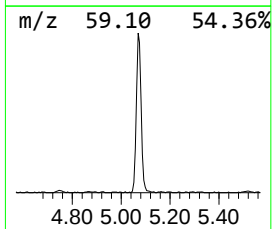
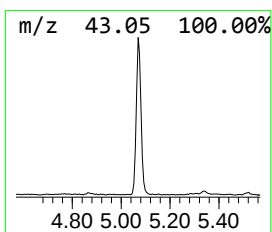
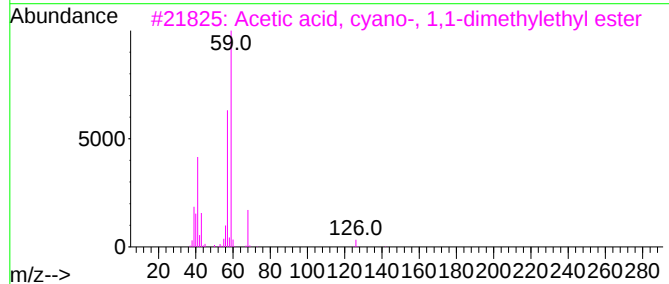
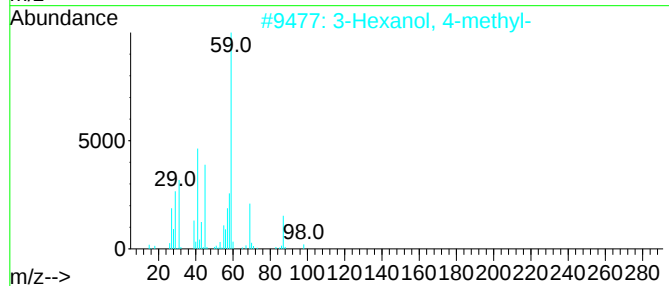
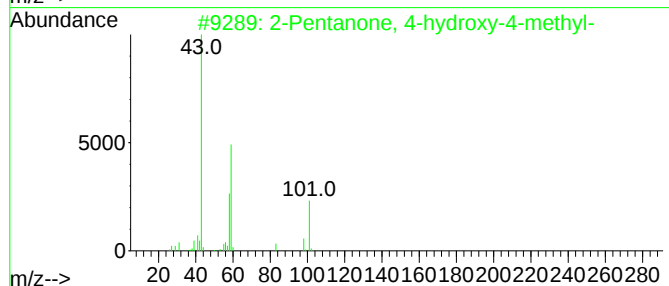
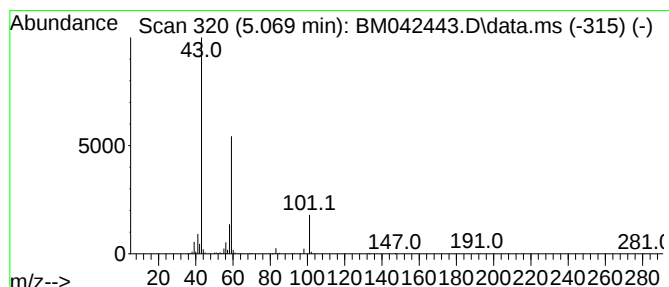
Instrument :
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Quant Title :

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.069	5.04 ng	248970	1,4-Dichlorobenzene-d4	7.993	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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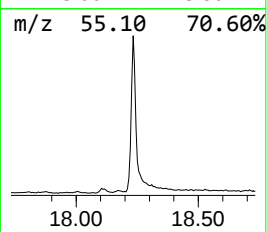
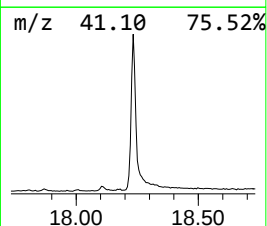
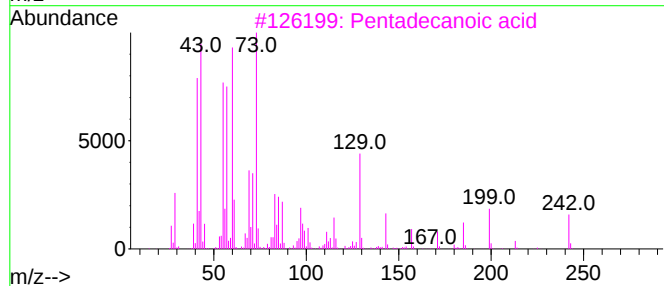
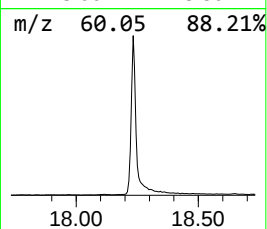
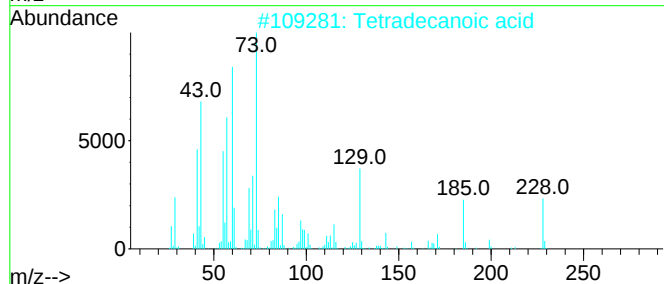
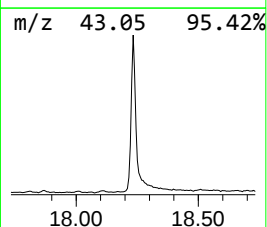
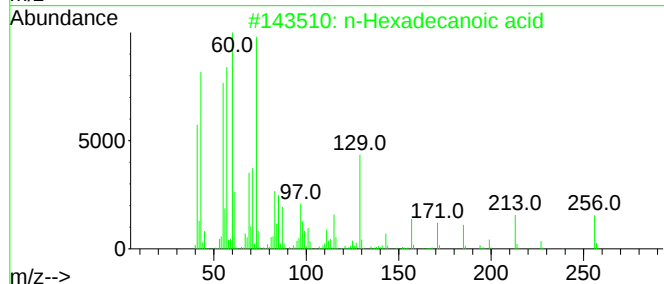
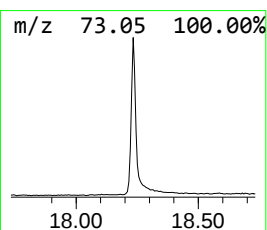
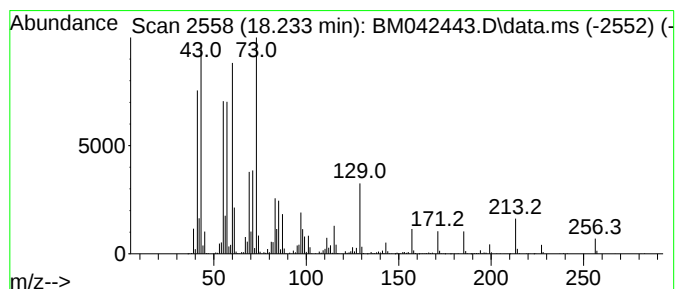
Quant Title :

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	15.67 ng	1702910	Phenanthrene-d10	17.386

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tridecanoic acid	214	C13H26O2	000638-53-9	87
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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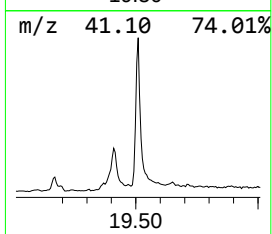
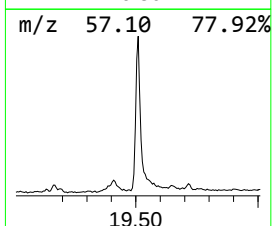
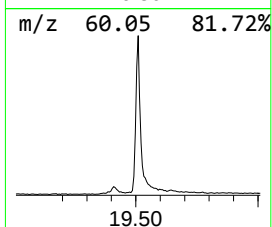
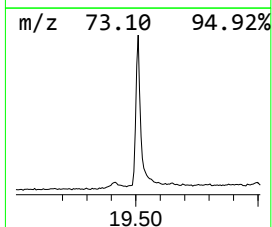
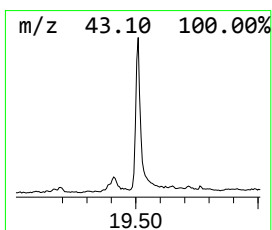
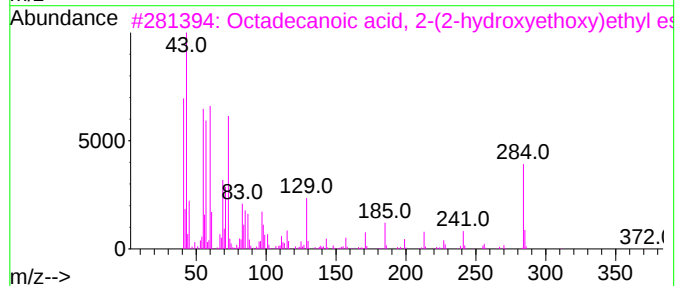
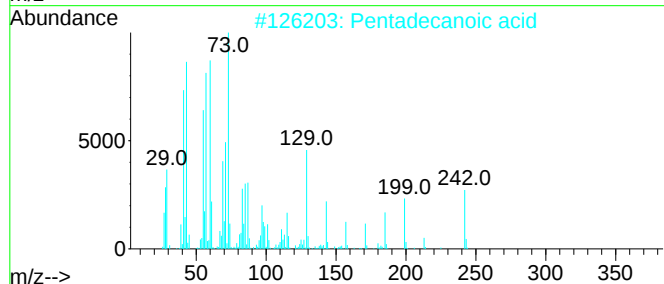
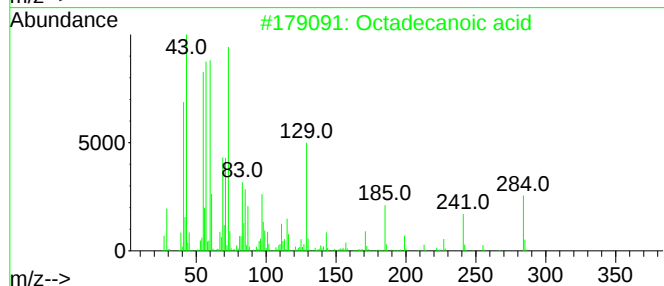
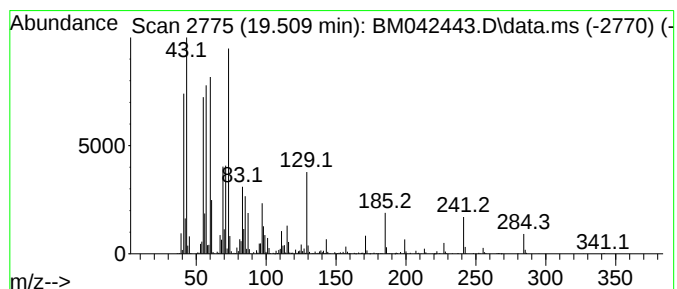
Quant Title :

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

Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.509	9.27 ng	1302980	Chrysene-d12	21.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



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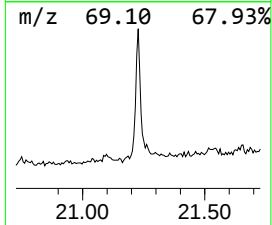
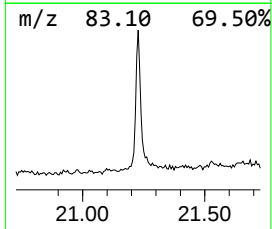
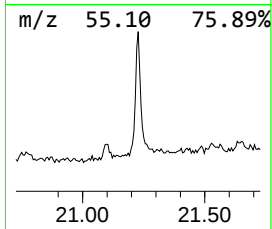
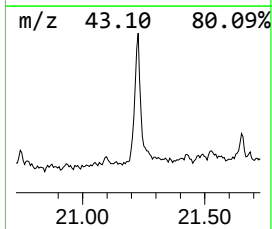
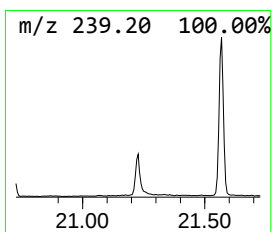
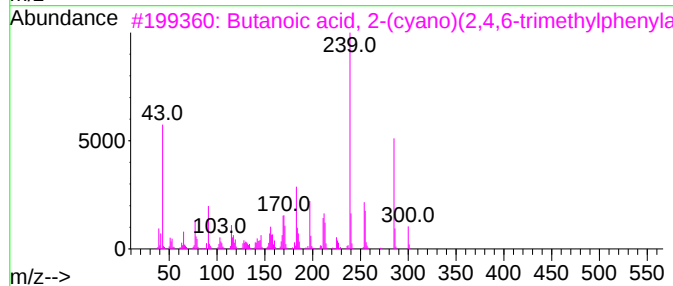
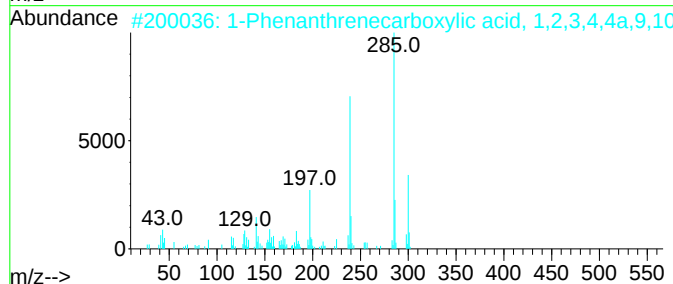
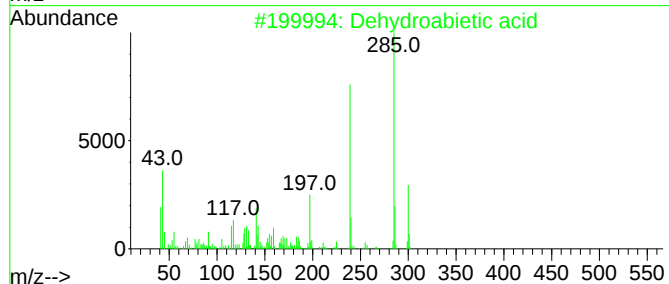
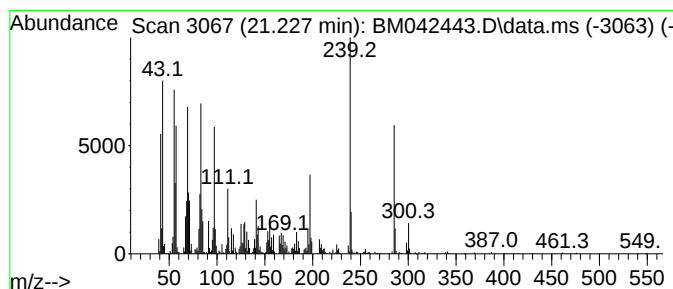
Quant Title :

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

Peak Number 4 Dehydroabietic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	4.26 ng	599357	Chrysene-d12	21.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dehydroabietic acid	300	C20H28O2	001740-19-8	92
2			1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	83
3			Butanoic acid, 2-(cyano)(2,4,6-t...	300	C17H20N2O3	1000267-71-7	58
4			3-Quinolinecarboxylic acid, 4-hy...	285	C13H10F3NO3	023851-84-5	45
5			Ethyl 4-hydroxy-6-(trifluorometh...	285	C13H10F3NO3	026893-12-9	43



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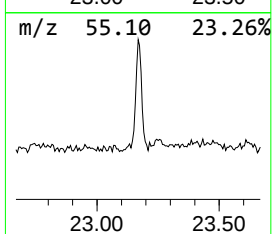
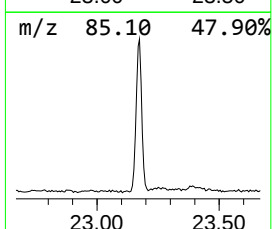
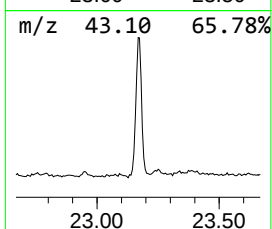
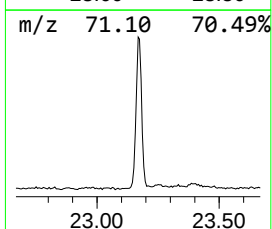
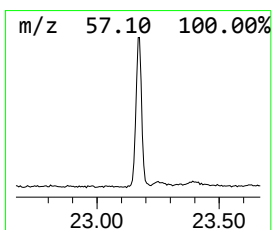
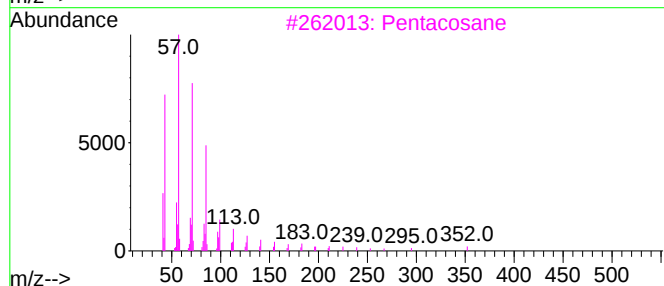
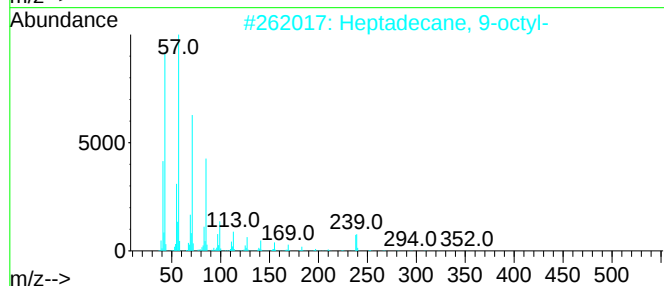
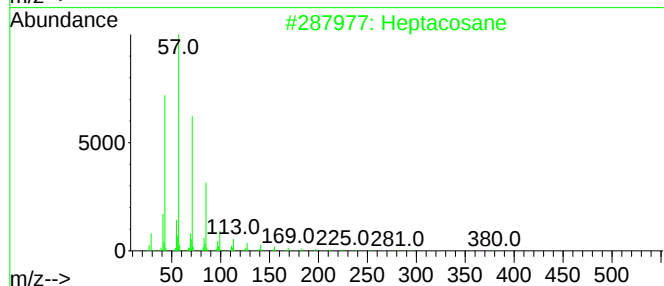
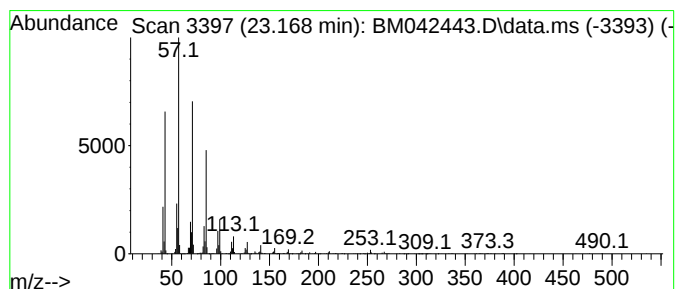
Quant Title :

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

Peak Number 5 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.168	6.66 ng	700642	Perylene-d12	24.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	96
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
3			Pentacosane	352	C25H52	000629-99-2	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042443.D
Acq On : 25 Oct 2023 18:26
Operator : MA/JU
Sample : 05001-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
486-WC-COMP

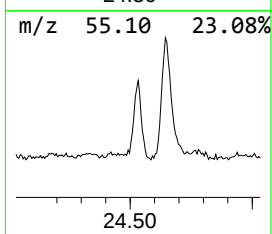
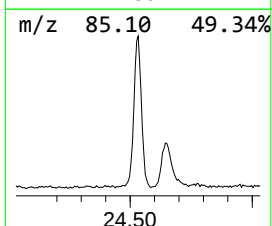
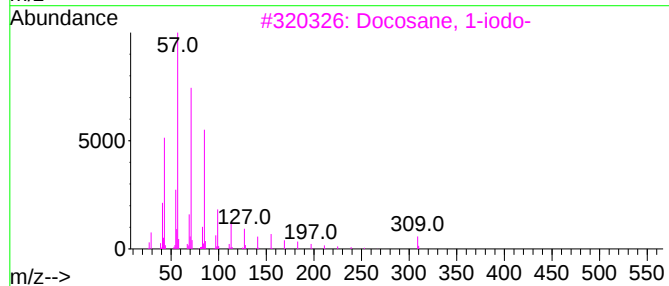
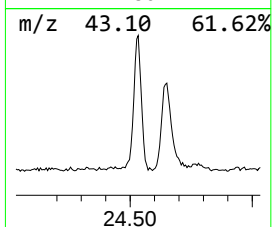
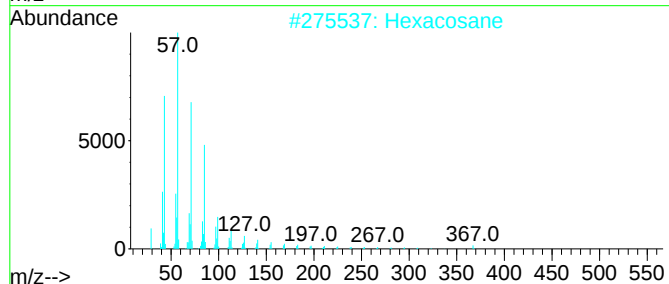
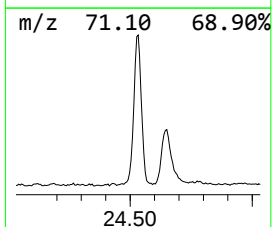
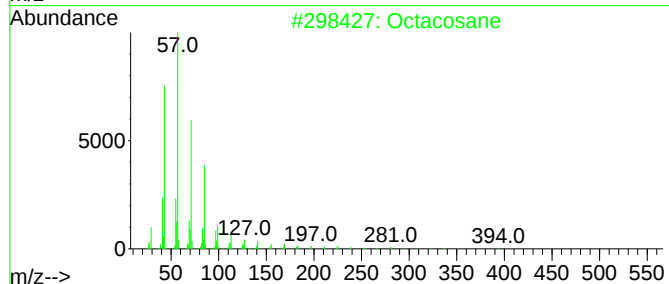
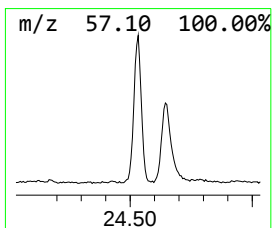
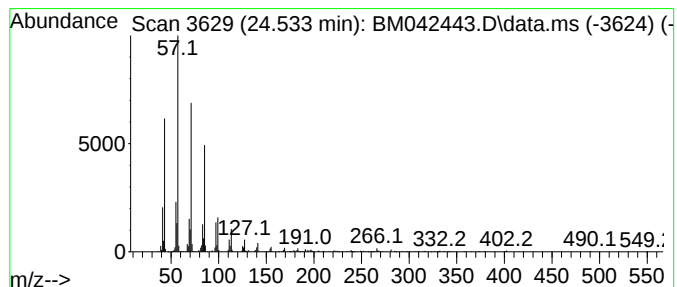
Quant Title :

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

Peak Number 6 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.533	7.61 ng	800711	Perylene-d12	24.027

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	87
2		Hexacosane	366	C26H54	000630-01-3	87
3		Docosane, 1-iodo-	436	C22H45I	1000406-31-9	86
4		Heneicosane	296	C21H44	000629-94-7	86
5		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042443.D
Acq On : 25 Oct 2023 18:26
Operator : MA/JU
Sample : 05001-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
486-WC-COMP

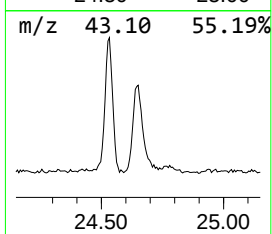
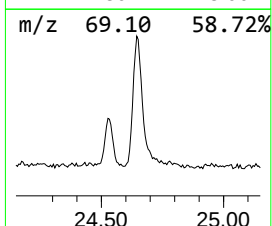
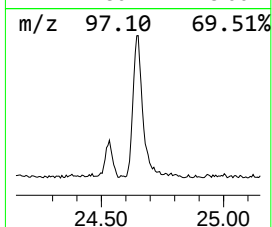
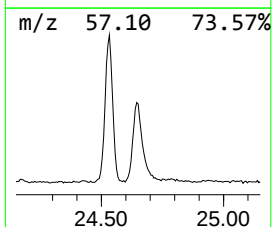
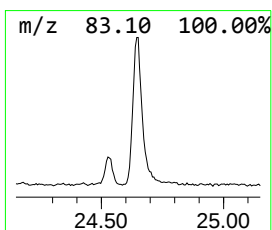
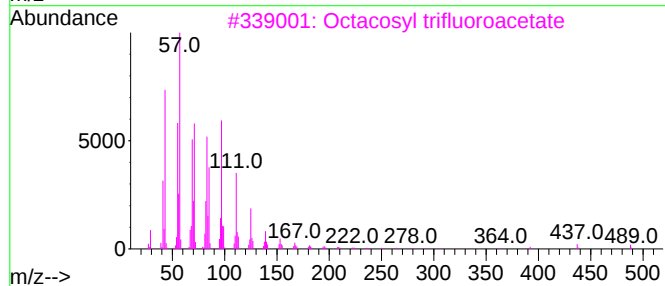
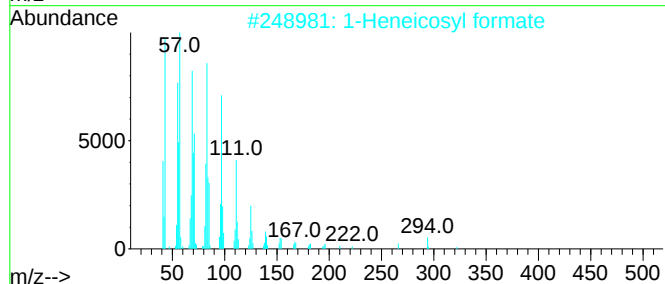
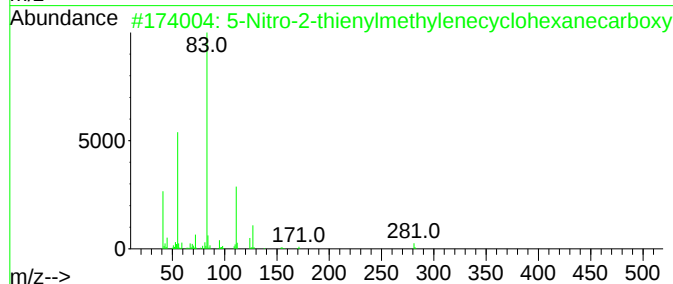
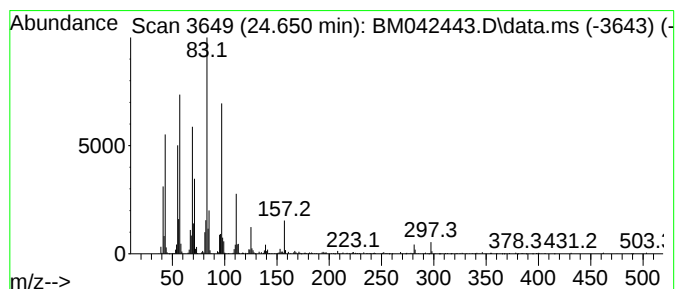
Quant Title :

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

Peak Number 7 unknown24.650 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.650	9.64 ng	1013380	Perylene-d12	24.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Nitro-2-thienylmethylenecyclohexanecarboxy	281	C12H15N3O3S	042826-29-9	45
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	42
3			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	41
4			Triacontan-15-ol	438	C30H62O	031849-26-0	38
5			Octacosyl pentafluoropropionate	556	C31H57F5O2	1000351-88-9	38



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Data File : BM042443.D
Acq On : 25 Oct 2023 18:26
Operator : MA/JU
Sample : 05001-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
486-WC-COMP

Quant Title :

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.069	5.0	ng	248970	1	7.993	988490	20.0
n-Hexadecanoic ...	18.233	15.7	ng	1702910	4	17.386	2173260	20.0
Octadecanoic acid	19.509	9.3	ng	1302980	5	21.562	2810780	20.0
Dehydroabietic ...	21.227	4.3	ng	599357	5	21.562	2810780	20.0
Heptacosane	23.168	6.7	ng	700642	6	24.027	2103460	20.0
Octacosane	24.533	7.6	ng	800711	6	24.027	2103460	20.0
unknown24.650	24.650	9.6	ng	1013380	6	24.027	2103460	20.0