

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021623\
 Data File : BM038769.D
 Acq On : 16 Feb 2023 22:34
 Operator : CG/JU
 Sample : 01552-15
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-04-4.0-6.0

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-BM020123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038769.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.993	299	307	319	rVB	278625	391647	12.71%	1.851%
2	5.469	380	388	399	rBV	888587	1253593	40.69%	5.924%
3	7.093	657	664	675	rBV	853977	1301169	42.23%	6.149%
4	7.910	797	803	810	rBV	256737	402151	13.05%	1.901%
5	9.092	997	1004	1014	rBV	515857	813957	26.42%	3.847%
6	10.728	1275	1282	1290	rBV	326979	545004	17.69%	2.576%
7	13.186	1693	1700	1707	rBV	1616731	2186604	70.97%	10.334%
8	14.557	1927	1933	1940	rBV	511794	755637	24.53%	3.571%
9	15.921	2158	2165	2173	rVB	31558	51387	1.67%	0.243%
10	16.051	2181	2187	2199	rBV	1391649	1803412	58.54%	8.523%
11	17.304	2394	2400	2404	rBV	630496	855495	27.77%	4.043%
12	17.345	2404	2407	2413	rVB	259791	331713	10.77%	1.568%
13	17.433	2414	2422	2428	rBV	64120	104207	3.38%	0.492%
14	17.715	2462	2470	2478	rBV2	19408	39736	1.29%	0.188%
15	18.192	2543	2551	2554	rBV2	211470	322305	10.46%	1.523%
16	18.227	2554	2557	2564	rVV	70897	114510	3.72%	0.541%
17	18.309	2567	2571	2576	rVV	26712	45803	1.49%	0.216%
18	18.374	2576	2582	2586	rVV3	78268	141216	4.58%	0.667%
19	18.409	2586	2588	2593	rVB2	29252	37532	1.22%	0.177%
20	18.680	2629	2634	2638	rBV	33500	50477	1.64%	0.239%
21	18.727	2638	2642	2648	rVB2	29836	44727	1.45%	0.211%
22	19.092	2700	2704	2708	rBV3	28775	49654	1.61%	0.235%
23	19.239	2724	2729	2734	rBV3	26442	55889	1.81%	0.264%
24	19.356	2744	2749	2756	rVB	786505	1013626	32.90%	4.790%
25	19.462	2763	2767	2772	rBV3	89297	125104	4.06%	0.591%
26	19.692	2801	2806	2808	rBV2	134780	217935	7.07%	1.030%
27	19.721	2808	2811	2818	rVV	690500	854974	27.75%	4.041%
28	19.792	2820	2823	2828	rVB2	35653	48966	1.59%	0.231%
29	19.921	2839	2845	2850	rBV	2895213	3080903	100.00%	14.560%
30	20.039	2861	2865	2873	rBV5	35866	93796	3.04%	0.443%
31	20.215	2892	2895	2900	rVB2	106295	132776	4.31%	0.627%
32	20.315	2908	2912	2915	rBV	75768	94334	3.06%	0.446%
33	21.168	3054	3057	3061	rBV2	185160	244590	7.94%	1.156%
34	21.480	3103	3110	3113	rBV2	719376	1345051	43.66%	6.357%
35	21.515	3113	3116	3122	rVB	346839	428419	13.91%	2.025%
36	23.139	3388	3392	3405	rVB2	275675	817872	26.55%	3.865%

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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-BM020123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.762	3494	3498	3504	rVB	228944	374210	12.15%	1.768%
38	23.868	3511	3516	3521	rVB	331752	589478	19.13%	2.786%

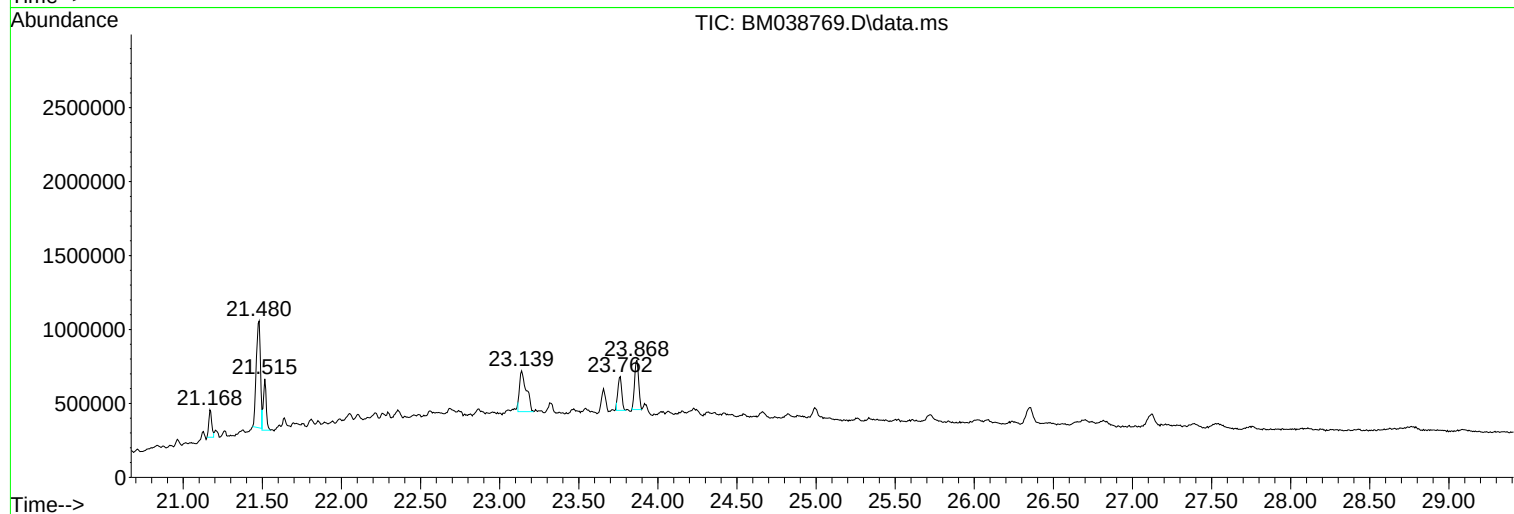
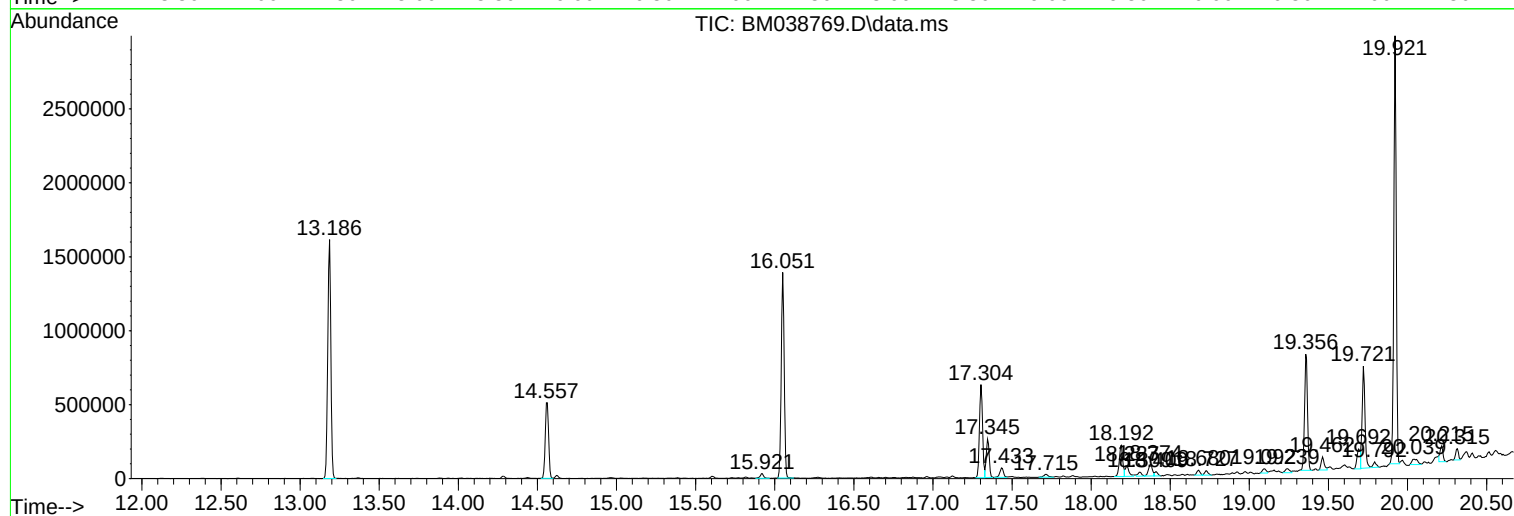
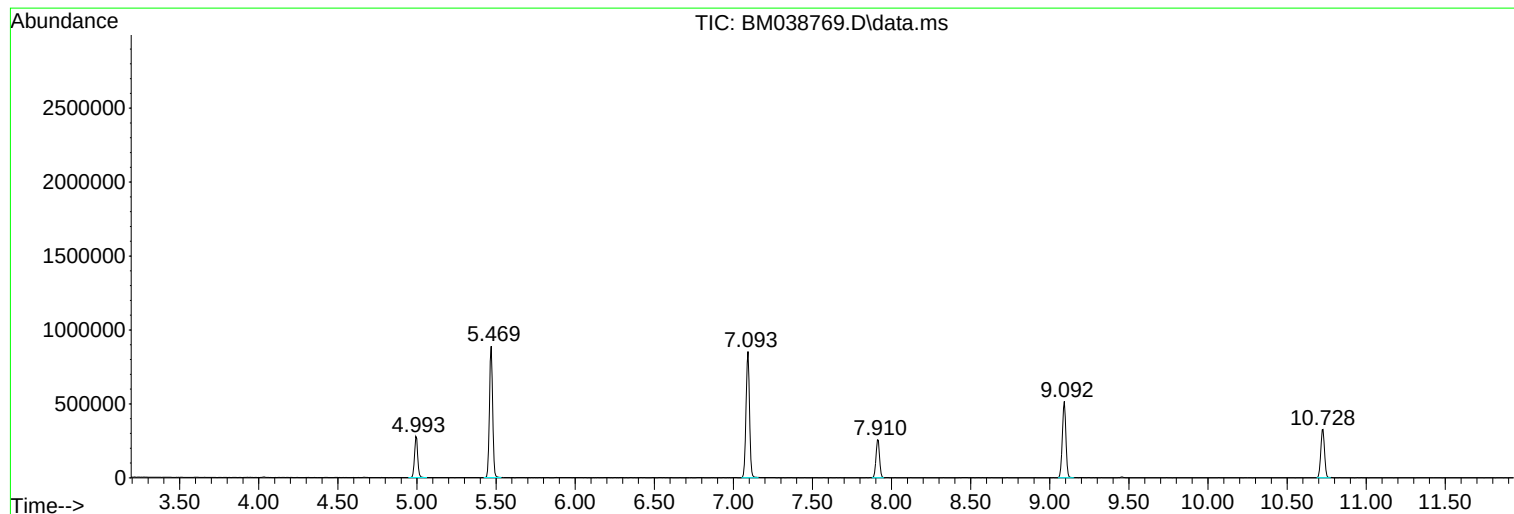
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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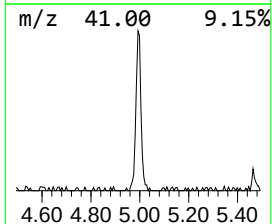
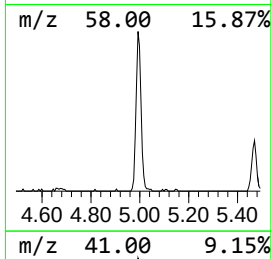
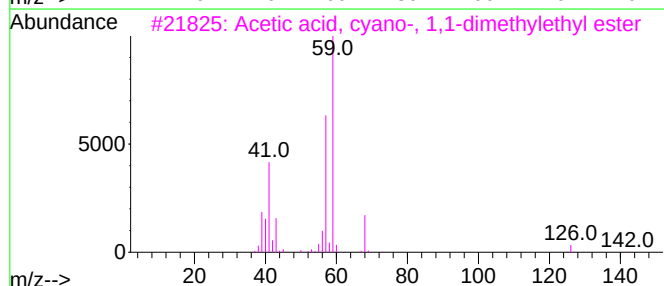
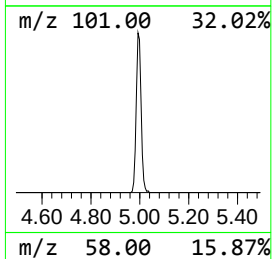
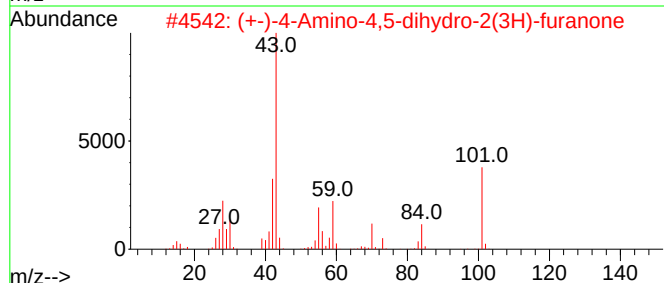
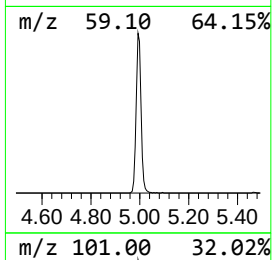
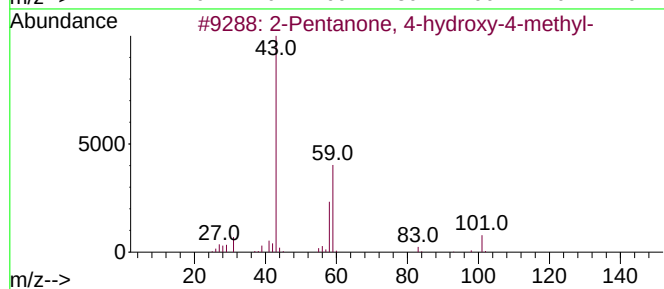
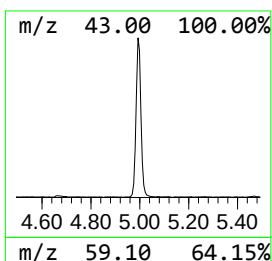
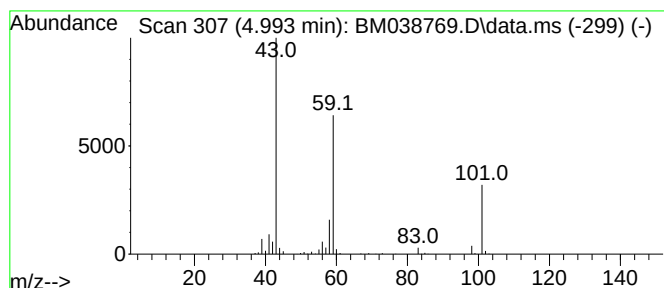
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.993	19.48 ng	391647	1,4-Dichlorobenzene-d4	7.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	40
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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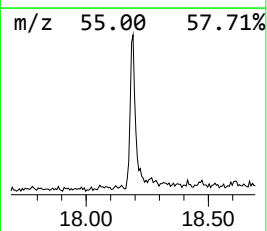
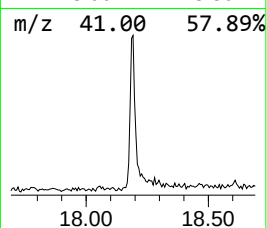
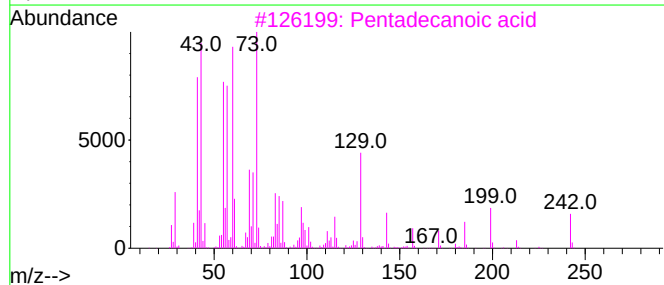
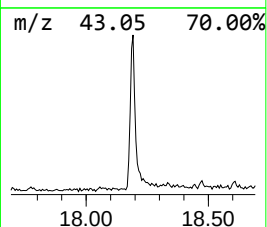
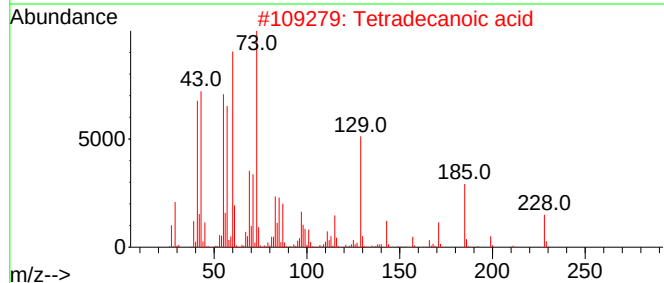
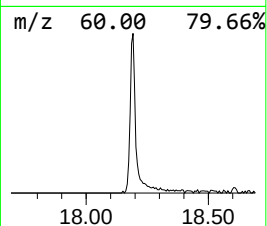
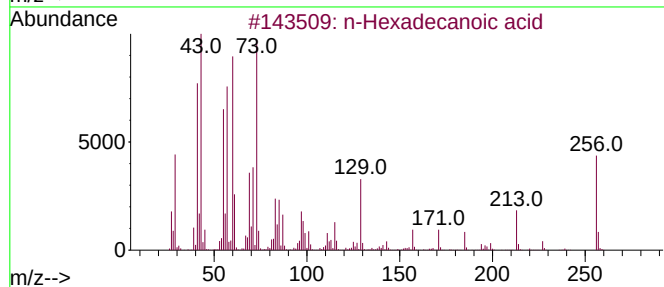
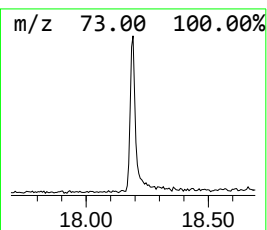
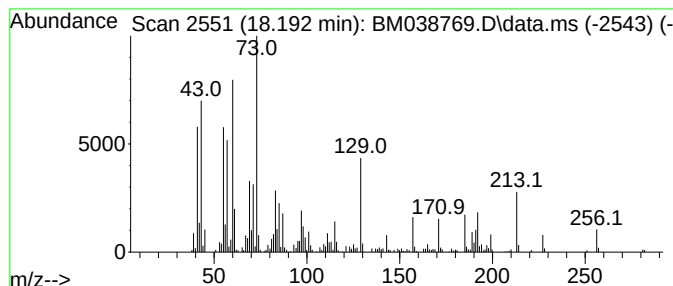
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	7.53 ng	322305	Phenanthrene-d10	17.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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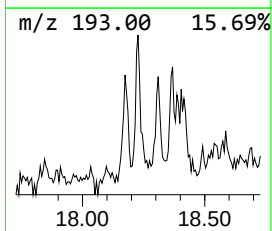
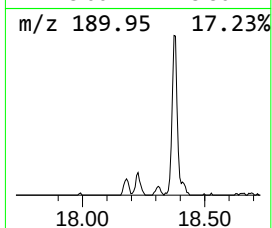
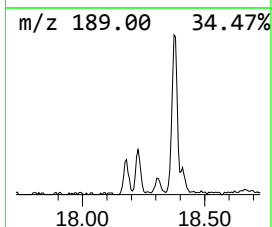
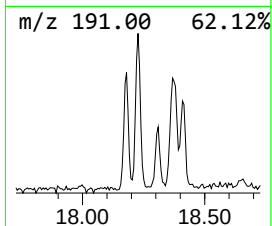
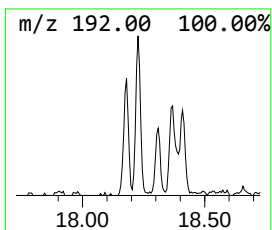
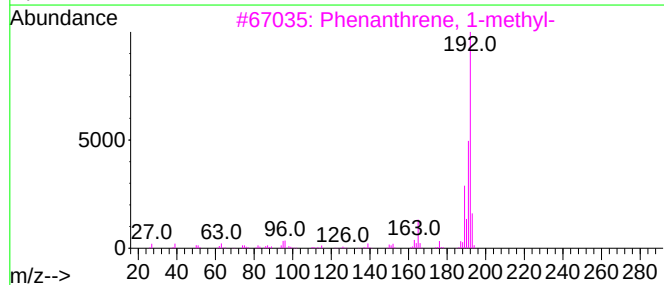
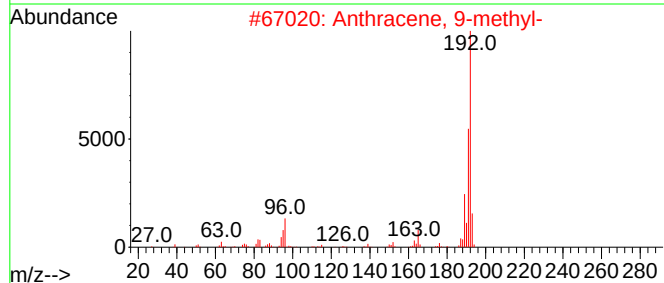
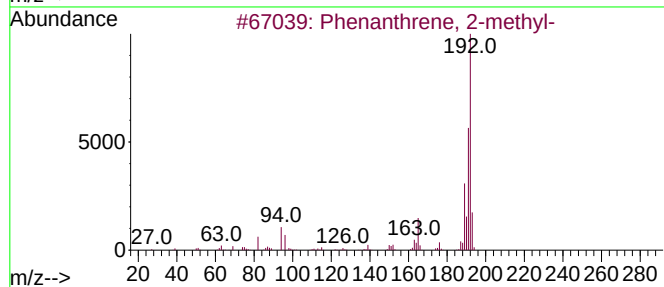
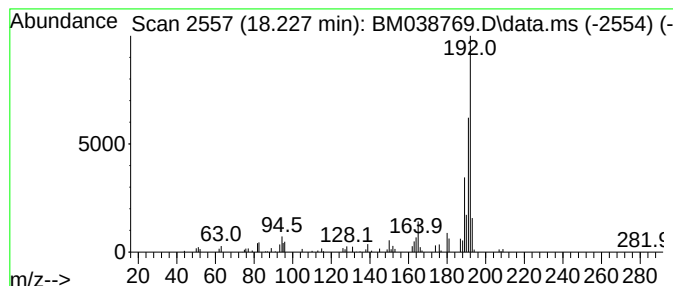
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.227	2.68 ng	114510	Phenanthrene-d10	17.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
2			Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	89
5			Anthracene, 2-methyl-	192	C15H12	000613-12-7	81



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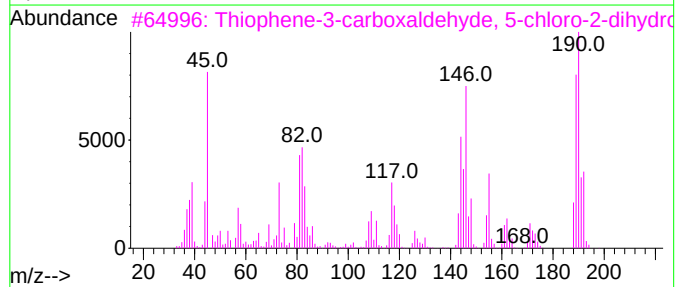
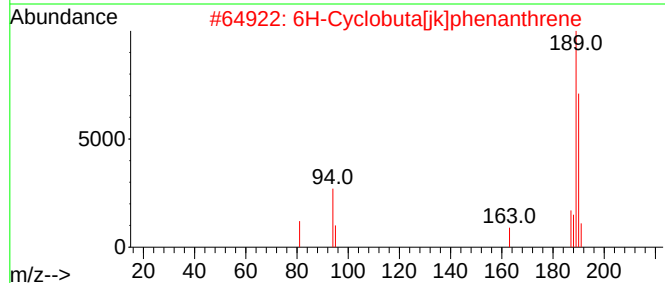
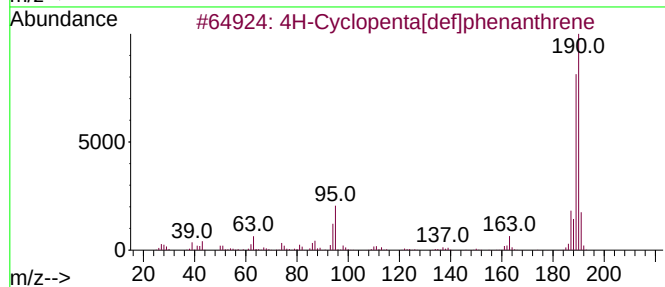
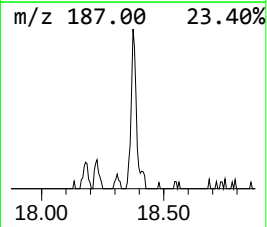
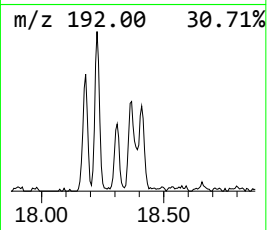
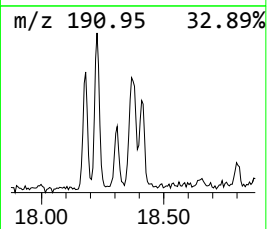
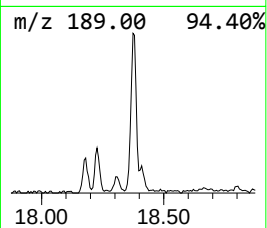
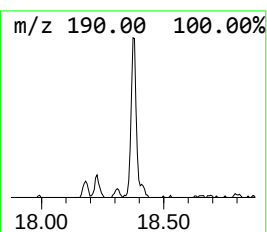
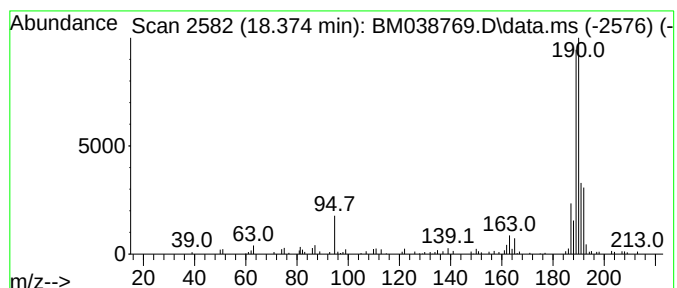
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.374	3.30 ng	141216	Phenanthrene-d10	17.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	56
3			Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
4			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
5			Megastigmatrienone	190	C13H18O	038818-55-2	22



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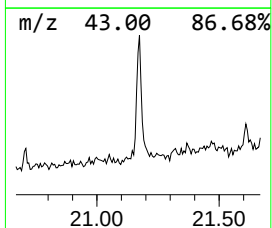
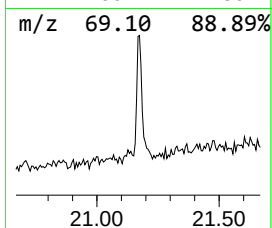
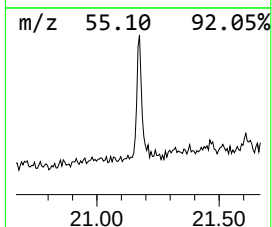
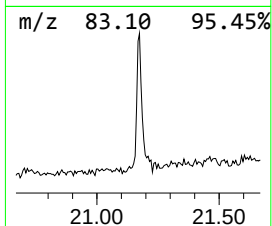
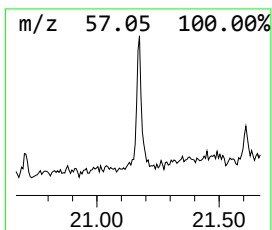
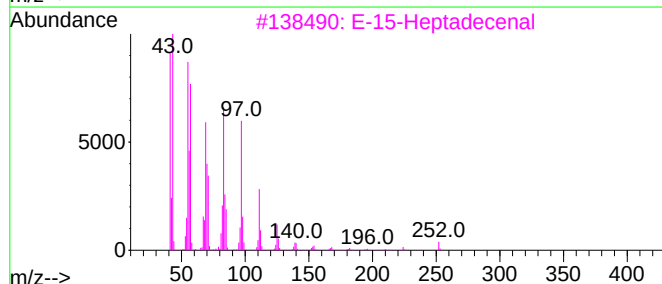
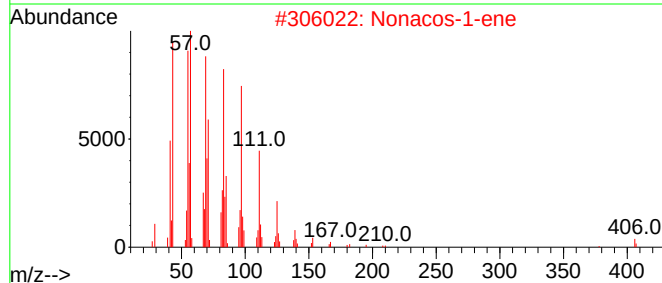
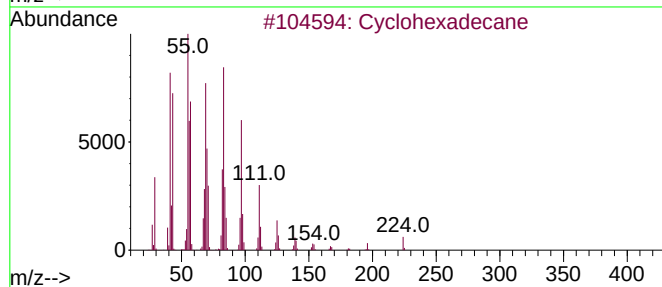
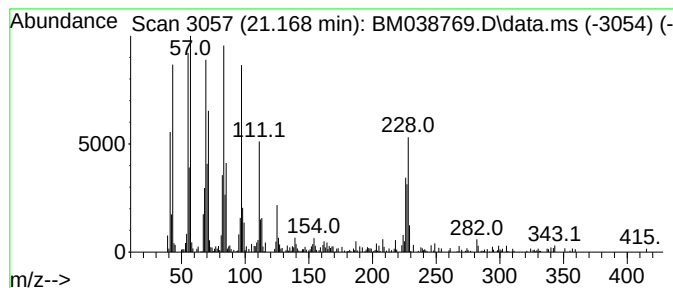
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.168	3.64 ng	244590	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	92
2			Nonacos-1-ene	406	C29H58	018835-35-3	90
3			E-15-Heptadecenal	252	C17H32O	1000130-97-9	90
4			Heptacos-1-ene	378	C27H54	015306-27-1	90
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021623\
Data File : BM038769.D
Acq On : 16 Feb 2023 22:34
Operator : CG/JU
Sample : 01552-15
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-04-4.0-6.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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-...	4.993	19.5	ng	391647	1	7.916	402151	20.0
n-Hexadecanoic ...	18.192	7.5	ng	322305	4	17.304	855495	20.0
Phenanthrene, 2...	18.227	2.7	ng	114510	4	17.304	855495	20.0
4H-Cyclopenta[d...	18.374	3.3	ng	141216	4	17.304	855495	20.0
Cyclohexadecane	21.168	3.6	ng	244590	5	21.480	1345050	20.0