

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080223\
 Data File : BM041246.D
 Acq On : 02 Aug 2023 15:53
 Operator : MA/JU
 Sample : 03810-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-P7A

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-BM072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041246.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	364	371	390	rBV	2044742	2966422	48.70%	6.177%
2	6.981	637	645	660	rBV	2114032	3335451	54.76%	6.946%
3	7.798	776	784	792	rBV	752183	1177651	19.33%	2.452%
4	8.975	976	984	995	rBV	1307139	2126564	34.91%	4.429%
5	10.604	1254	1261	1269	rBV	1076316	1749288	28.72%	3.643%
6	13.080	1674	1682	1695	rBV	3526471	4980524	81.77%	10.372%
7	14.463	1906	1917	1924	rBV	1757865	2493290	40.93%	5.192%
8	15.962	2163	2172	2190	rBV	3039761	4394329	72.14%	9.151%
9	16.627	2281	2285	2291	rBV5	47952	92615	1.52%	0.193%
10	17.121	2364	2369	2375	rBV2	54147	96716	1.59%	0.201%
11	17.221	2381	2386	2391	rBV	2097486	2866824	47.06%	5.970%
12	17.262	2391	2393	2398	rVB	113029	136241	2.24%	0.284%
13	17.356	2404	2409	2413	rVB	44005	65143	1.07%	0.136%
14	18.009	2516	2520	2525	rBV3	43214	69927	1.15%	0.146%
15	18.062	2525	2529	2534	rBV	423255	620084	10.18%	1.291%
16	18.127	2534	2540	2550	rVB2	1498524	2275515	37.36%	4.739%
17	18.233	2555	2558	2564	rVV	64412	104462	1.71%	0.218%
18	18.292	2564	2568	2573	rVV2	134398	246783	4.05%	0.514%
19	18.339	2573	2576	2581	rVB	81118	111350	1.83%	0.232%
20	18.421	2585	2590	2594	rBV5	63564	113867	1.87%	0.237%
21	18.662	2628	2631	2639	rVB6	43920	74472	1.22%	0.155%
22	19.027	2688	2693	2698	rBV	175019	323710	5.31%	0.674%
23	19.086	2698	2703	2706	rVV3	53831	110818	1.82%	0.231%
24	19.174	2712	2718	2724	rBV4	92183	218287	3.58%	0.455%
25	19.239	2727	2729	2731	rVV	60638	68108	1.12%	0.142%
26	19.292	2734	2738	2746	rVB	612272	940815	15.45%	1.959%
27	19.403	2753	2757	2767	rBV2	525574	773514	12.70%	1.611%
28	19.627	2791	2795	2796	rBV2	112435	139344	2.29%	0.290%
29	19.656	2796	2800	2808	rVB	736237	1053854	17.30%	2.195%
30	19.733	2809	2813	2817	rVB2	82442	124387	2.04%	0.259%
31	19.862	2829	2835	2840	rBV	5025343	6091257	100.00%	12.685%
32	19.980	2852	2855	2865	rVB3	100759	220646	3.62%	0.459%
33	20.309	2908	2911	2914	rBV	148884	210880	3.46%	0.439%
34	20.450	2932	2935	2939	rVB	184888	228453	3.75%	0.476%
35	20.497	2940	2943	2947	rVB	125799	143275	2.35%	0.298%
36	20.656	2968	2970	2974	rVB	122775	139418	2.29%	0.290%

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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-BM072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.127	3047	3050	3058	rVB3	940136	1356915	22.28%	2.826%
38	21.427	3095	3101	3105	rBV2	1895174	2889707	47.44%	6.018%
39	21.462	3105	3107	3114	rVB	374333	426141	7.00%	0.887%
40	22.050	3204	3207	3214	rVB	365685	513447	8.43%	1.069%
41	23.797	3499	3504	3511	rVB	1076693	1949430	32.00%	4.060%

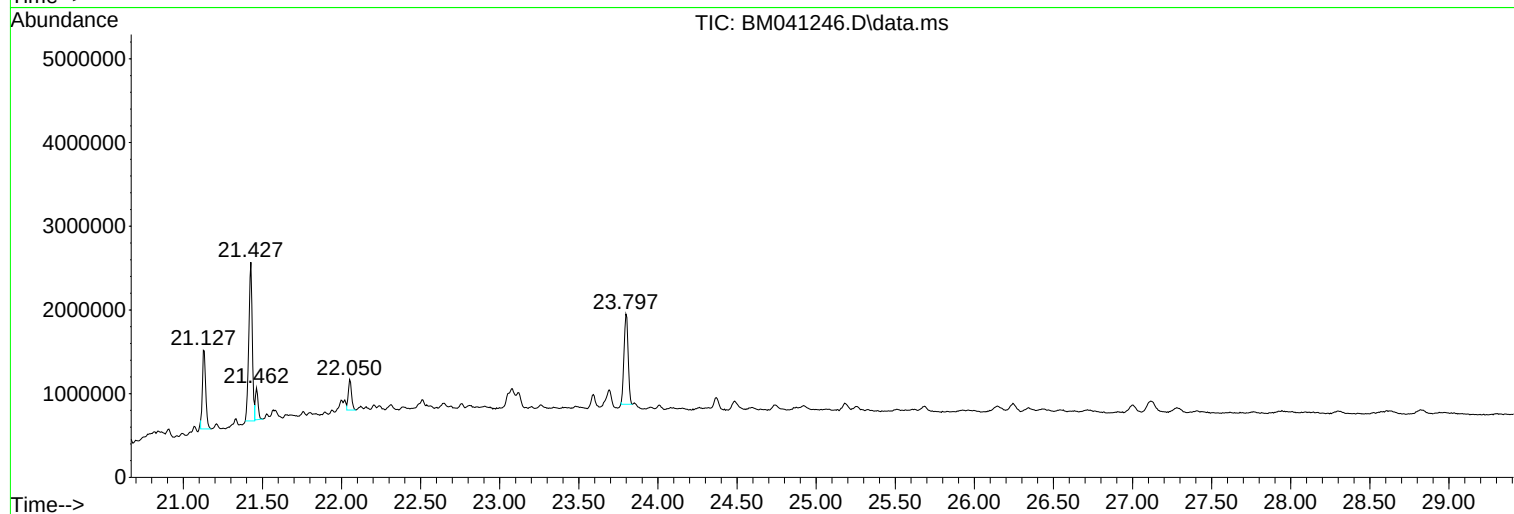
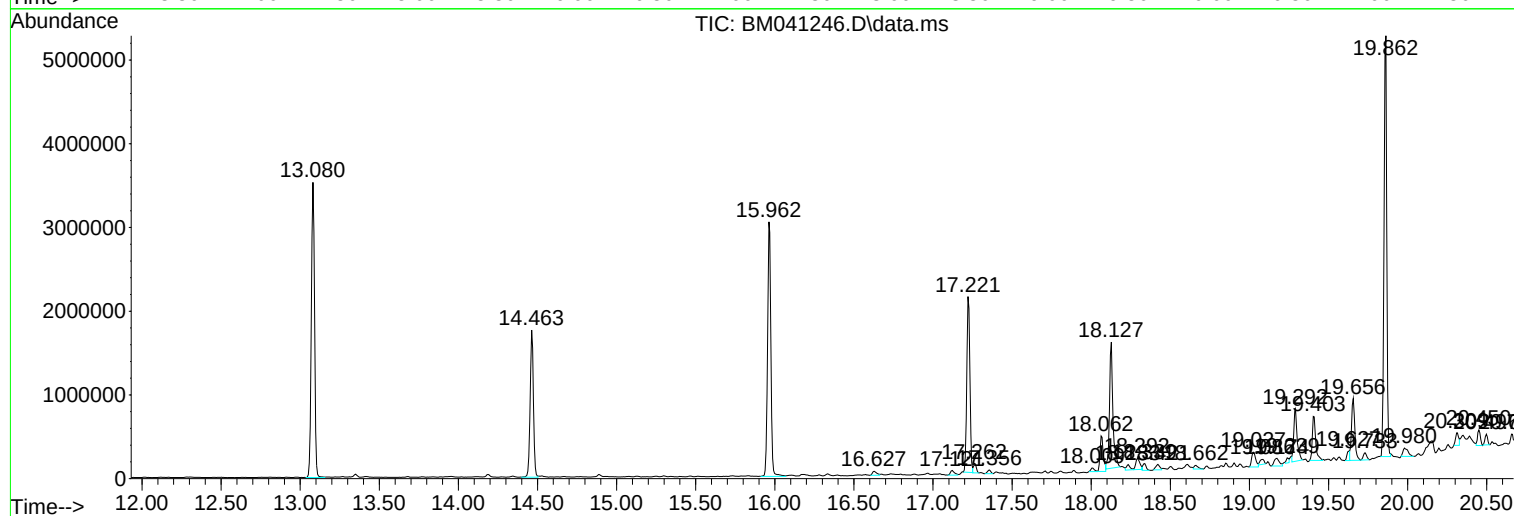
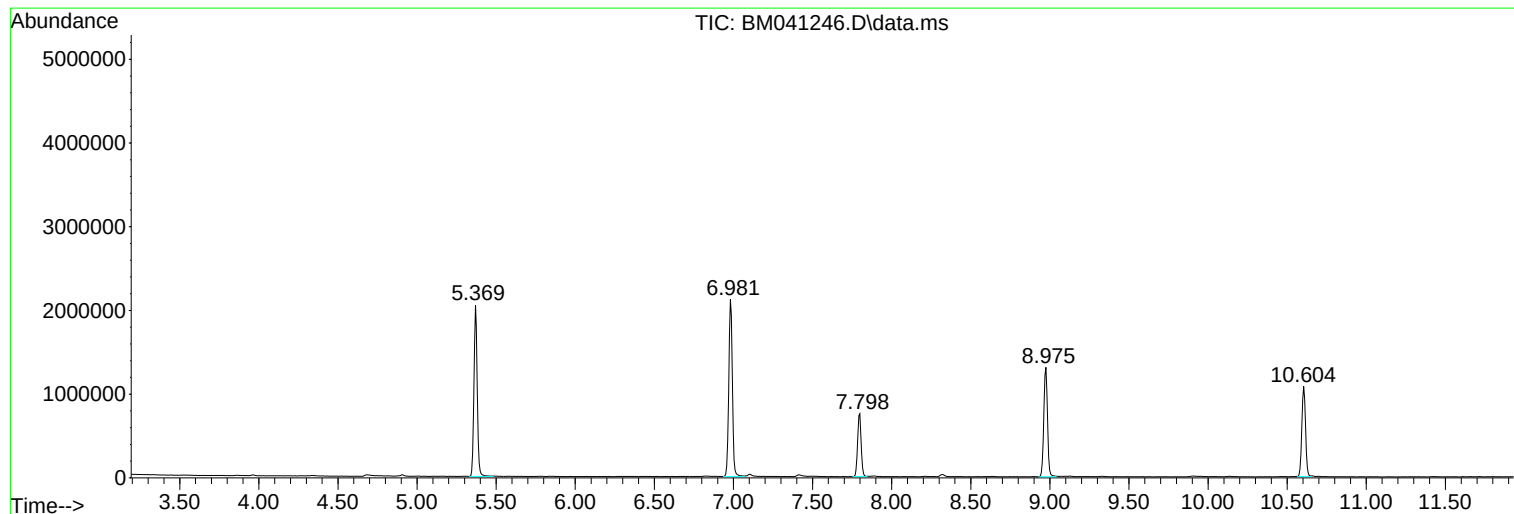
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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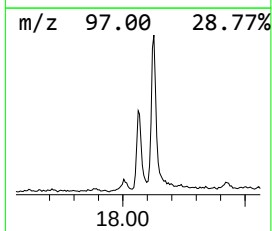
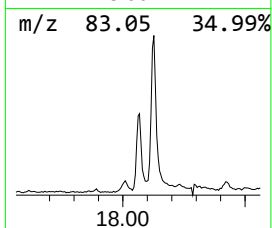
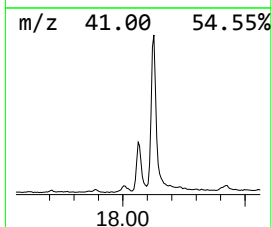
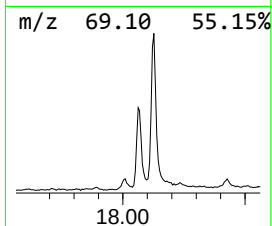
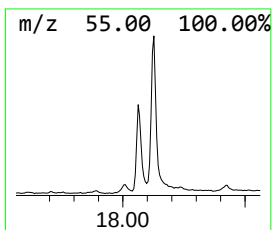
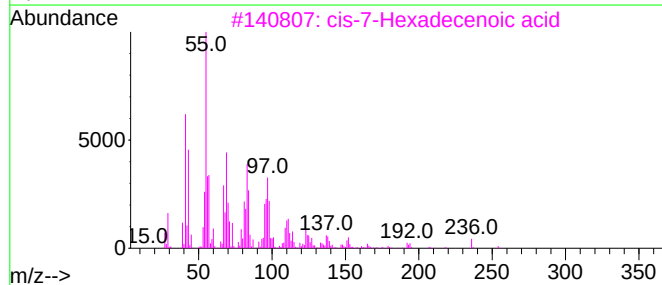
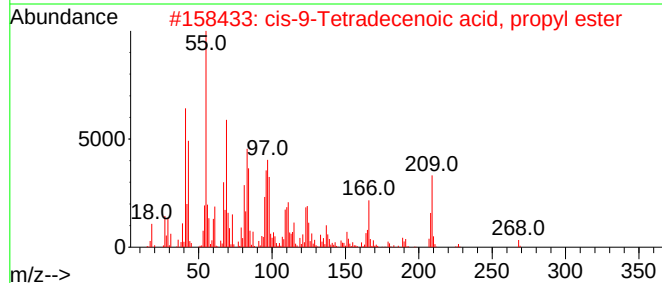
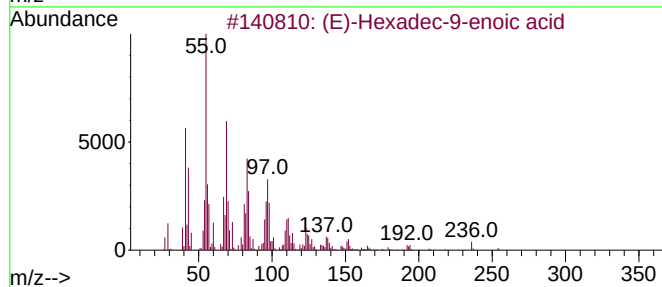
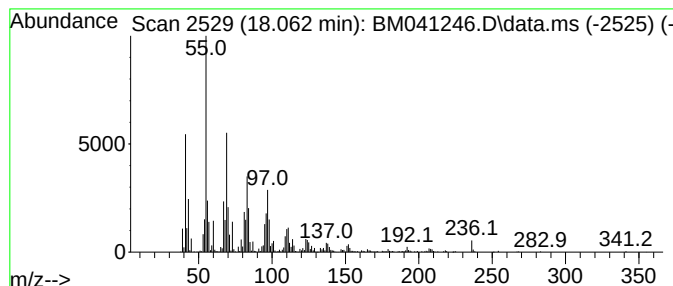
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (E)-Hexadec-9-enoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.062	4.33 ng	620084	Phenanthrene-d10	17.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	98
2			cis-9-Tetradecenoic acid, propyl...	268	C17H32O2	1000405-14-2	94
3			cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	93
4			Palmitoleic acid	254	C16H30O2	000373-49-9	91
5			cis-Vaccenic acid	282	C18H34O2	000506-17-2	91



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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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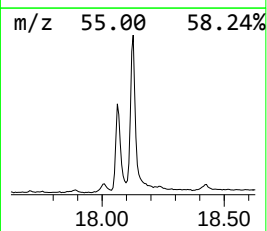
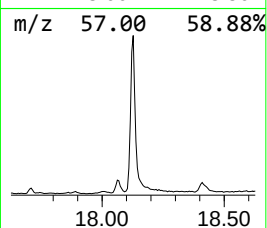
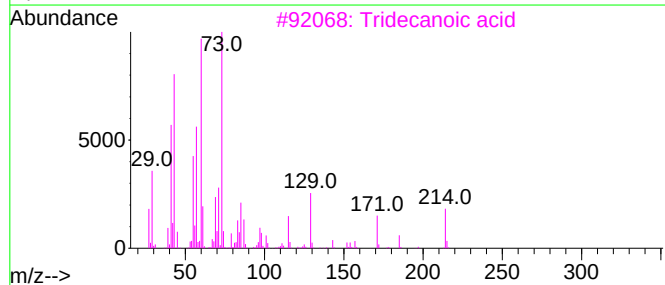
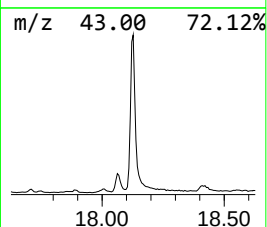
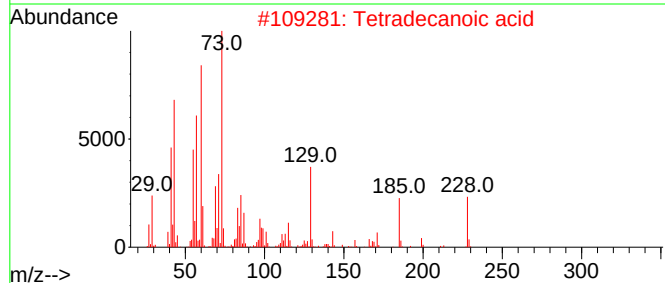
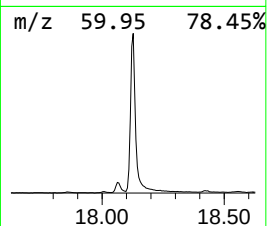
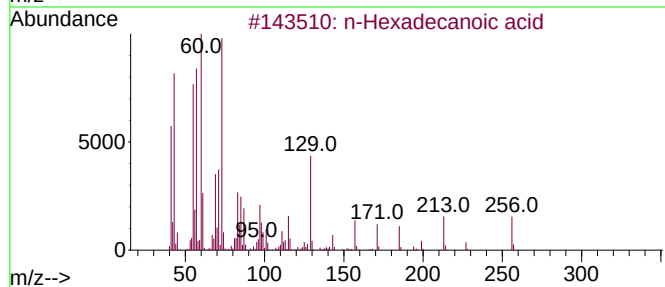
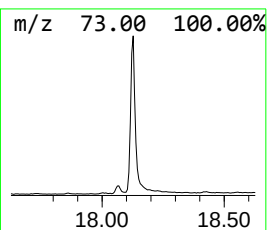
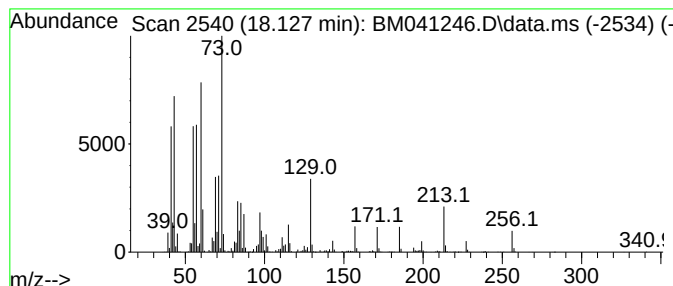
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
18.127	15.87 ng	2275520	Phenanthrene-d10	17.221

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			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	47



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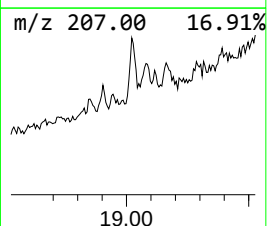
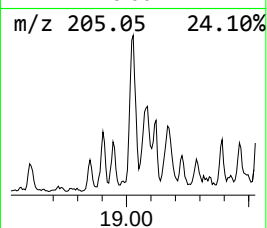
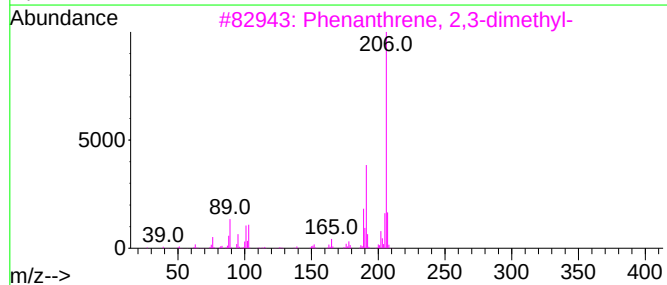
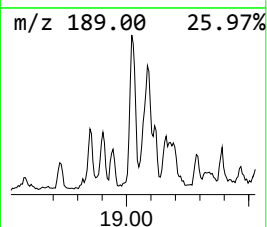
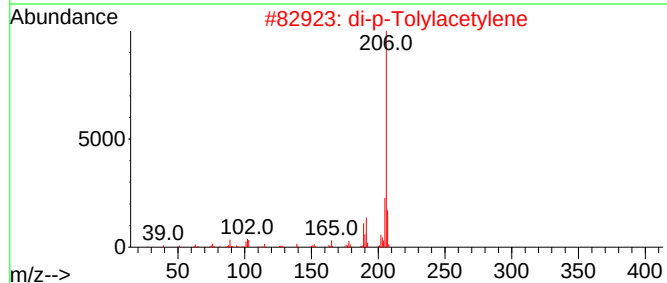
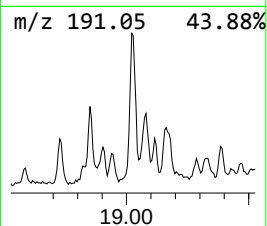
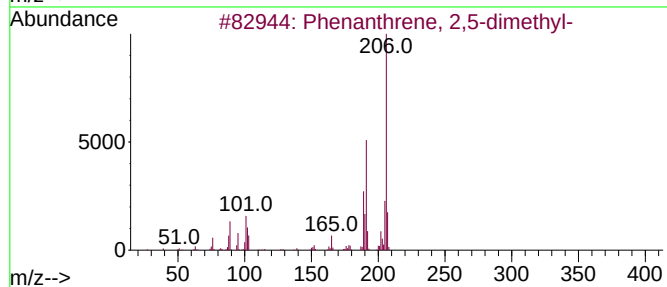
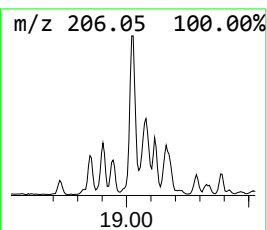
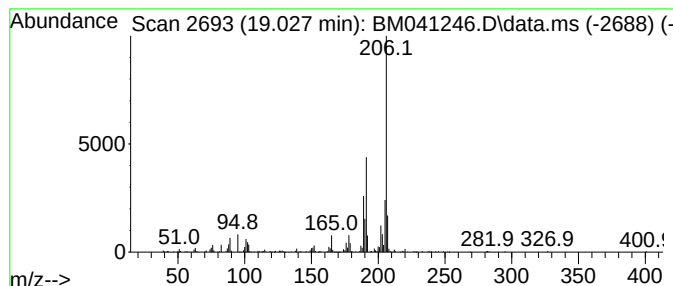
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Phenanthrene, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.027	2.26 ng	323710	Phenanthrene-d10	17.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	97
2			di-p-Tolylacetylene	206	C16H14	002789-88-0	93
3			Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	93
4			9,10-Dimethylantracene	206	C16H14	000781-43-1	91
5			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	90



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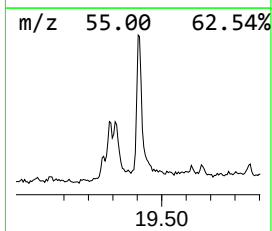
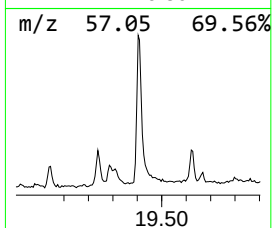
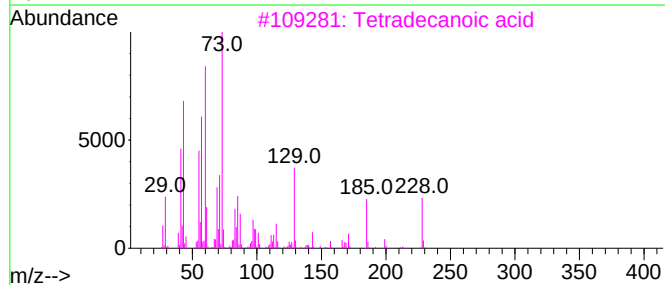
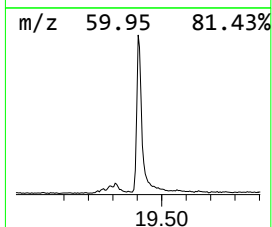
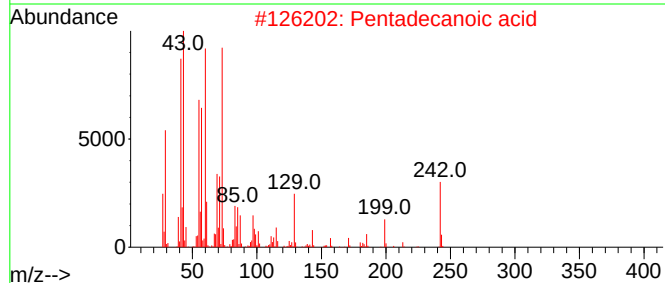
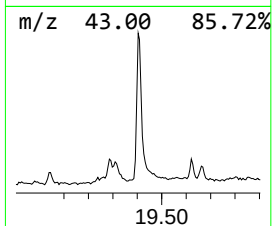
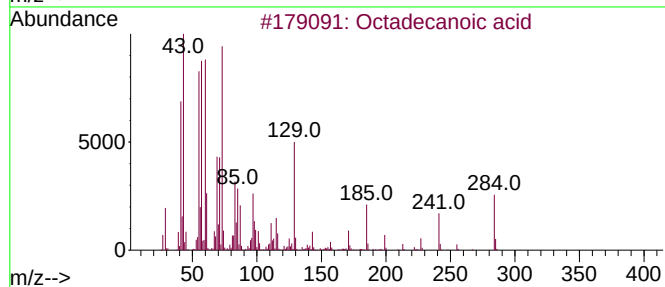
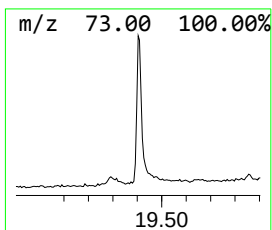
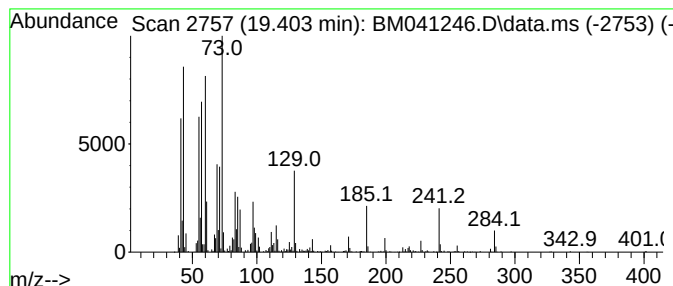
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.403	5.35 ng	773514	Chrysene-d12	21.427

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	35
5			Octadecane	254	C18H38	000593-45-3	25



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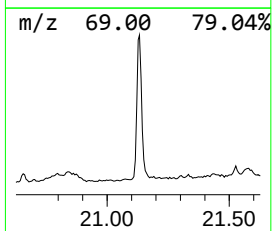
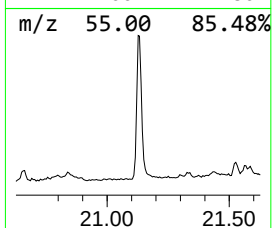
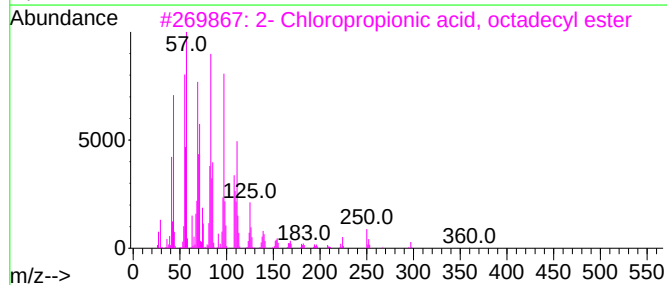
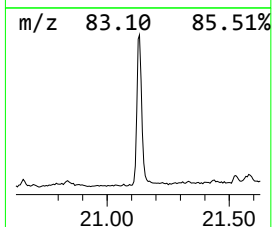
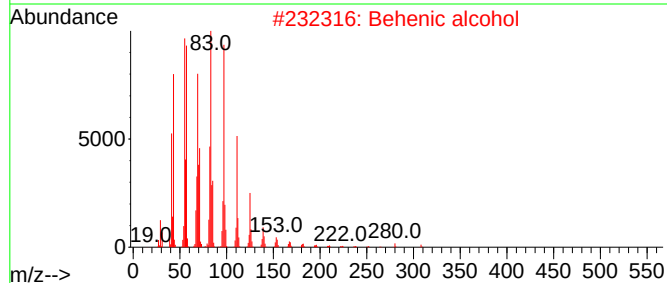
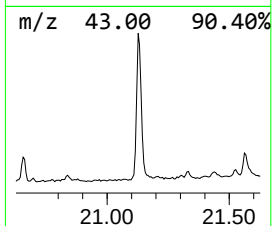
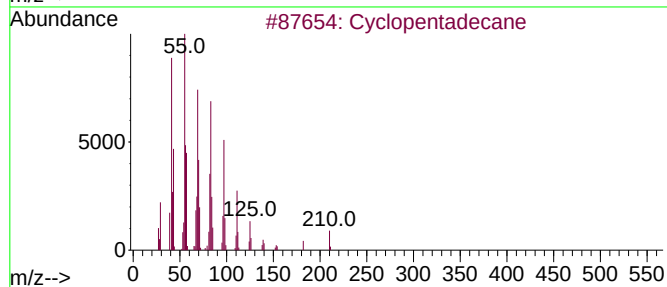
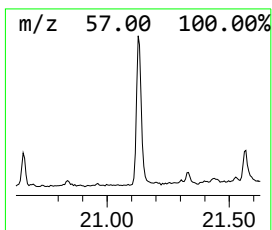
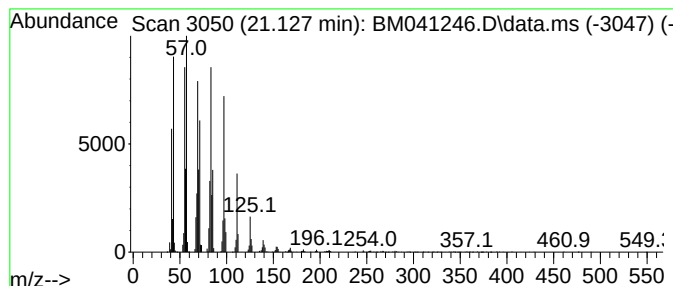
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	9.39 ng	1356920	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	96
2			Behenic alcohol	326	C22H46O	000661-19-8	91
3			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			1-Tetracosene	336	C24H48	010192-32-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080223\
Data File : BM041246.D
Acq On : 02 Aug 2023 15:53
Operator : MA/JU
Sample : 03810-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P7A

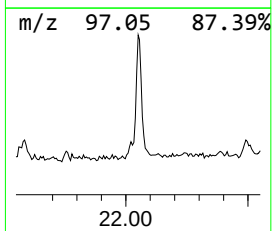
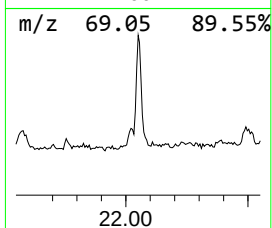
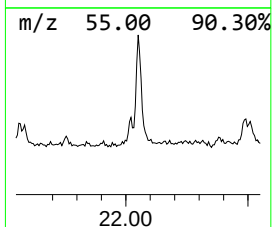
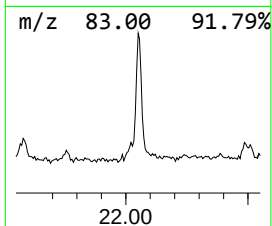
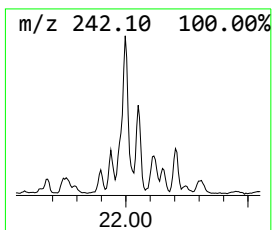
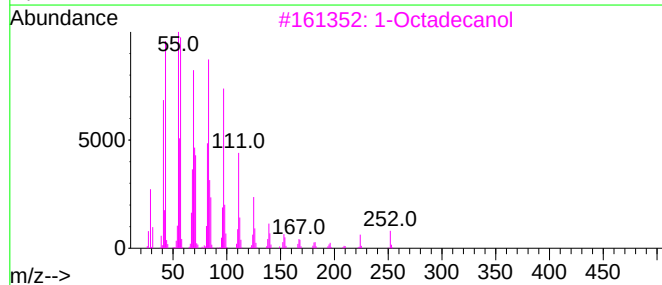
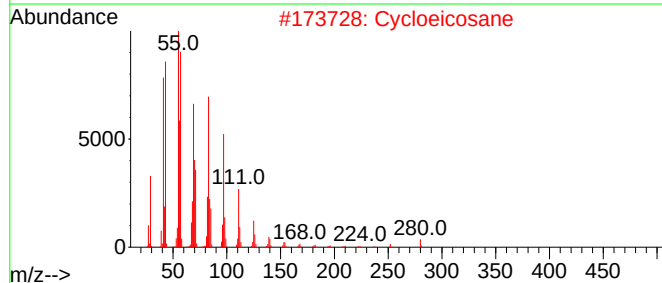
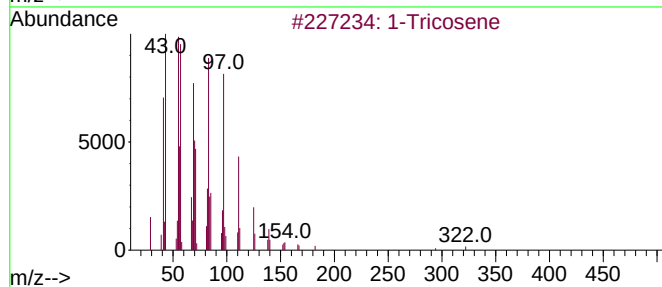
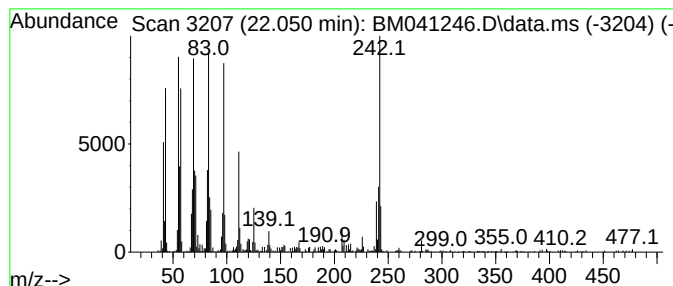
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Tricosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.050	3.55 ng	513447	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tricosene	322	C23H46	018835-32-0	87
2			Cycloeicosane	280	C20H40	000296-56-0	80
3			1-Octadecanol	270	C18H38O	000112-92-5	78
4			Behenic alcohol	326	C22H46O	000661-19-8	70
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080223\
Data File : BM041246.D
Acq On : 02 Aug 2023 15:53
Operator : MA/JU
Sample : 03810-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P7A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(E)-Hexadec-9-e...	18.062	4.3	ng	620084	4	17.221	2866820	20.0
n-Hexadecanoic ...	18.127	15.9	ng	2275520	4	17.221	2866820	20.0
Phenanthrene, 2...	19.027	2.3	ng	323710	4	17.221	2866820	20.0
Octadecanoic acid	19.403	5.3	ng	773514	5	21.427	2889710	20.0
Cyclopentadecane	21.127	9.4	ng	1356920	5	21.427	2889710	20.0
1-Tricosene	22.050	3.5	ng	513447	5	21.427	2889710	20.0