

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080822\
 Data File : BM036159.D
 Acq On : 09 Aug 2022 00:17
 Operator : CG/JU
 Sample : N3962-19
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RVE-204

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-BM080122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036159.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.946	308	316	321	rBV	218174	305363	2.62%	0.335%
2	5.434	392	399	411	rBV	4456437	6378446	54.82%	6.992%
3	7.051	667	674	691	rBV	4188071	6488532	55.77%	7.113%
4	7.845	802	809	817	rBV	1016186	1573160	13.52%	1.725%
5	9.016	1001	1008	1028	rBV	2572277	4176416	35.90%	4.578%
6	9.945	1158	1166	1172	rBV	54057	123408	1.06%	0.135%
7	10.651	1275	1286	1292	rBV	1262824	2134914	18.35%	2.340%
8	12.322	1564	1570	1581	rBV2	51634	131108	1.13%	0.144%
9	13.116	1696	1705	1717	rBV	6100582	9107265	78.28%	9.984%
10	14.486	1931	1938	1944	rBV	1758103	2571675	22.10%	2.819%
11	15.974	2181	2191	2198	rBV	4665338	6693176	57.53%	7.337%
12	17.227	2395	2404	2408	rBV	2057331	2902120	24.94%	3.181%
13	17.268	2408	2411	2416	rVB	547426	688976	5.92%	0.755%
14	17.357	2423	2426	2431	rVB	111435	147311	1.27%	0.161%
15	18.127	2549	2557	2566	rBV2	497577	927967	7.98%	1.017%
16	18.298	2581	2586	2590	rBV3	104406	189319	1.63%	0.208%
17	18.598	2633	2637	2642	rBV2	69015	120958	1.04%	0.133%
18	19.286	2748	2754	2761	rBV	1605448	2240602	19.26%	2.456%
19	19.645	2806	2815	2824	rBV	1599407	2566392	22.06%	2.813%
20	19.756	2831	2834	2839	rVB	168320	193145	1.66%	0.212%
21	19.851	2844	2850	2855	rBV	9648644	11634450	100.00%	12.754%
22	19.968	2866	2870	2877	rBV3	112923	254351	2.19%	0.279%
23	20.139	2889	2899	2906	rBV2	455337	1001514	8.61%	1.098%
24	20.239	2913	2916	2919	rBV	154528	194901	1.68%	0.214%
25	20.339	2930	2933	2937	rBV2	108398	129589	1.11%	0.142%
26	20.445	2947	2951	2954	rBV2	161004	269727	2.32%	0.296%
27	20.486	2955	2958	2962	rVB2	174430	224734	1.93%	0.246%
28	20.833	3014	3017	3021	rBV3	220367	275700	2.37%	0.302%
29	20.886	3024	3026	3033	rVB	206827	265501	2.28%	0.291%
30	21.121	3059	3066	3073	rBV5	1715517	2565323	22.05%	2.812%
31	21.297	3093	3096	3098	rBV2	179023	182076	1.56%	0.200%
32	21.403	3108	3114	3118	rBV2	2966989	5151540	44.28%	5.647%
33	21.445	3118	3121	3129	rVB	1383230	1710071	14.70%	1.875%
34	21.562	3138	3141	3148	rVB2	256386	344665	2.96%	0.378%
35	22.033	3214	3221	3227	rBV3	851174	1554825	13.36%	1.704%
36	23.044	3387	3393	3398	rBV2	2128149	4402927	37.84%	4.827%

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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-BM080122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.091	3398	3401	3410	rVB2	1448888	2458162	21.13%	2.695%
38	23.556	3475	3480	3487	rVB	885291	1607533	13.82%	1.762%
39	23.656	3492	3497	3504	rVB	1341166	2486064	21.37%	2.725%
40	23.762	3510	3515	3520	rBV2	1510535	2598266	22.33%	2.848%
41	24.362	3612	3617	3625	rVB	1063221	2250620	19.34%	2.467%

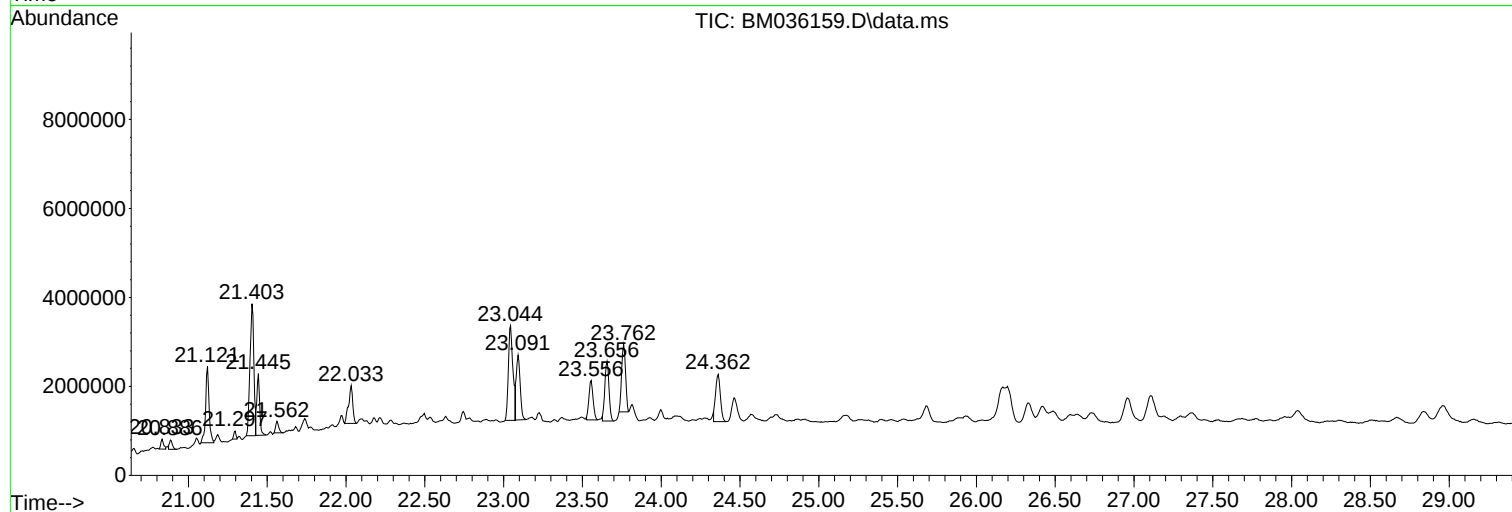
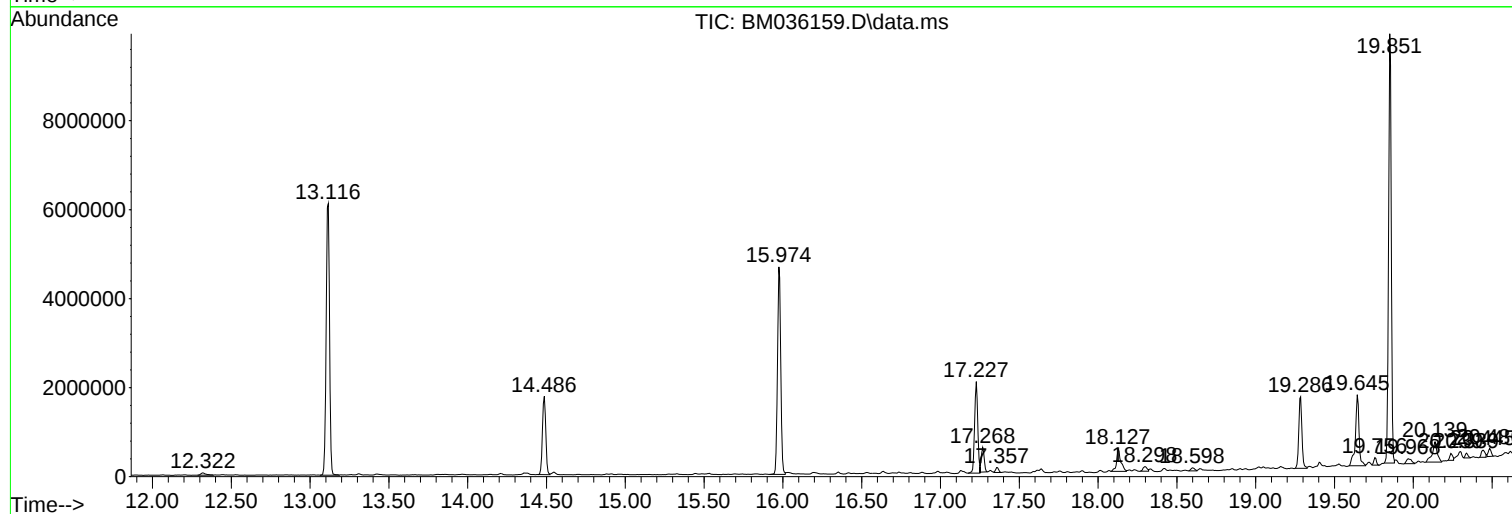
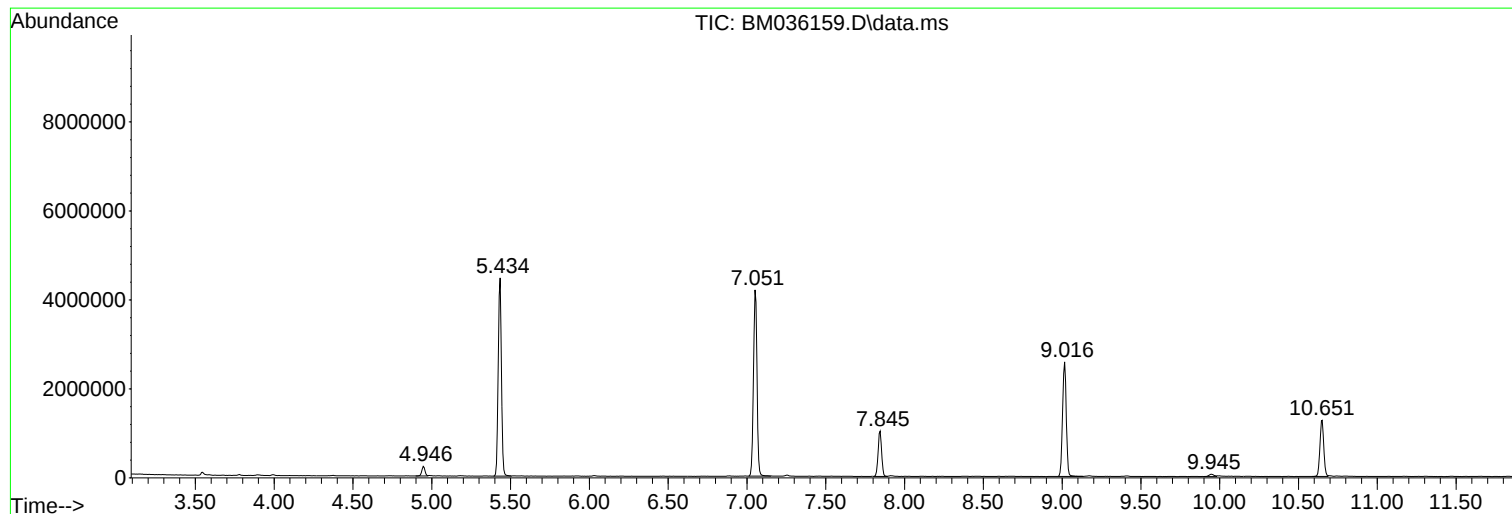
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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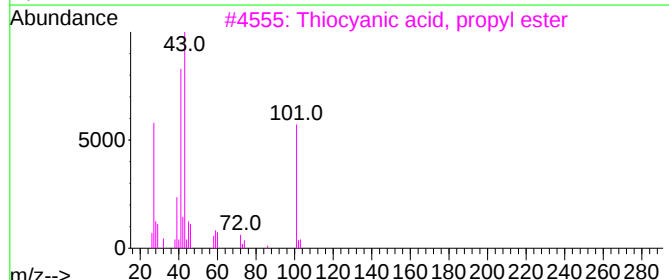
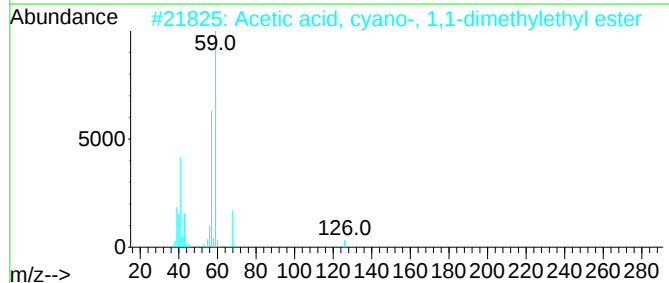
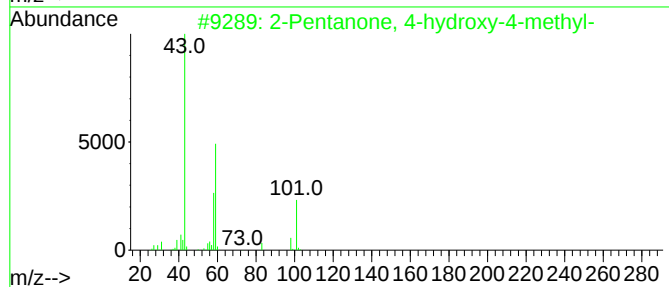
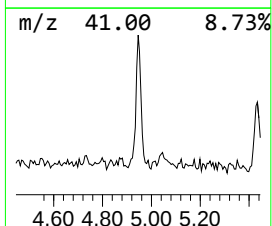
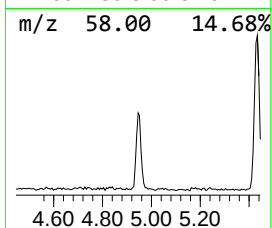
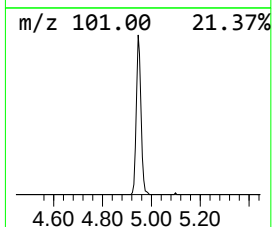
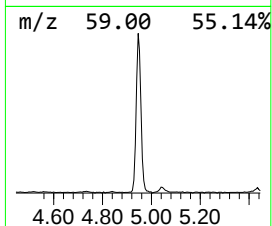
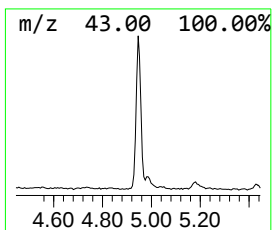
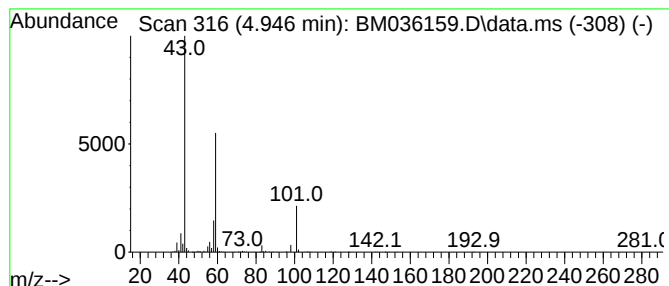
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.946	3.88 ng	305363	1,4-Dichlorobenzene-d4	7.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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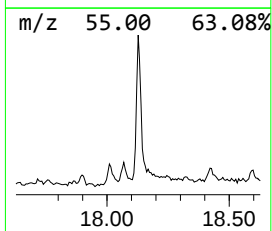
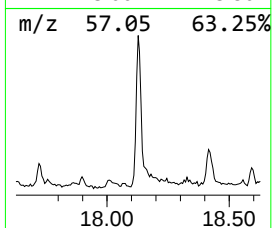
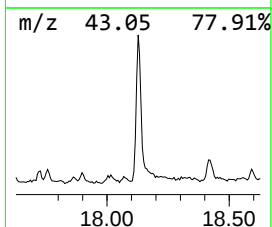
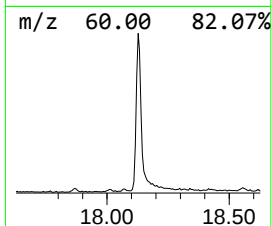
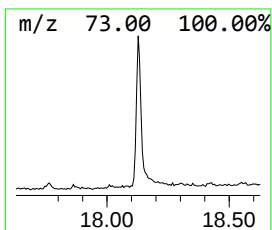
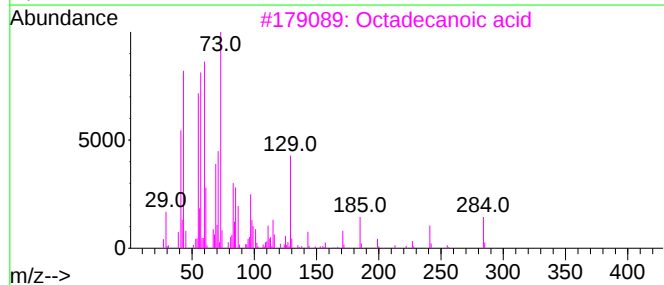
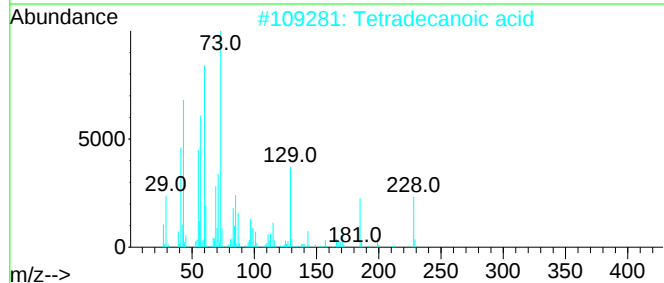
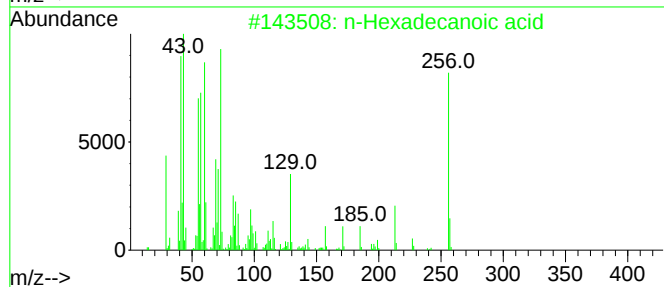
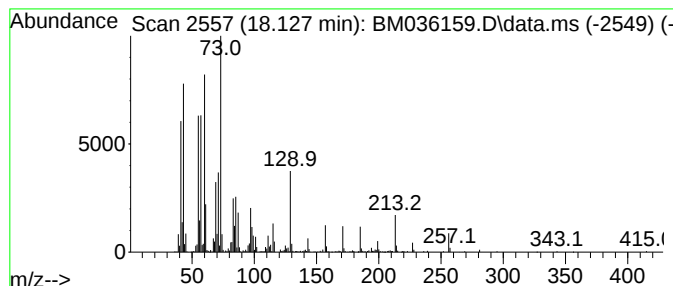
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	6.40 ng	927967	Phenanthrene-d10	17.227

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			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Tridecanoic acid	214	C13H26O2	000638-53-9	90



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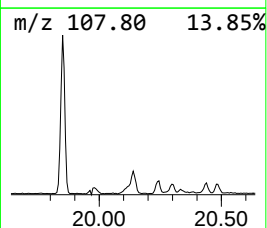
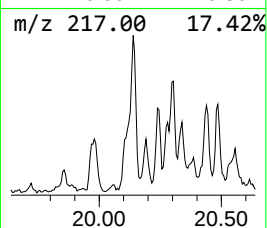
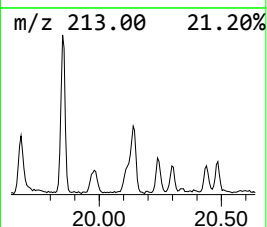
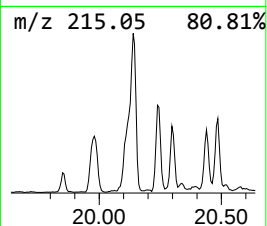
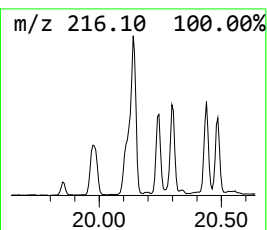
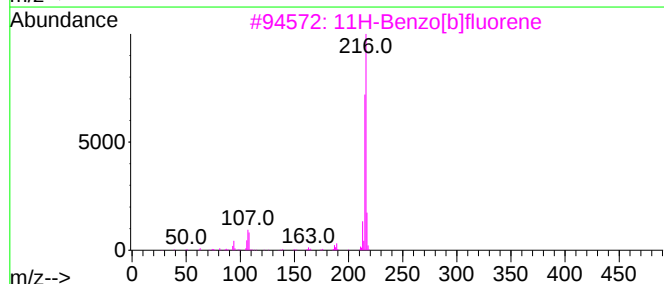
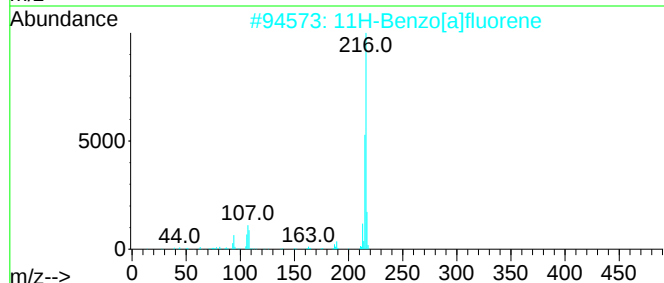
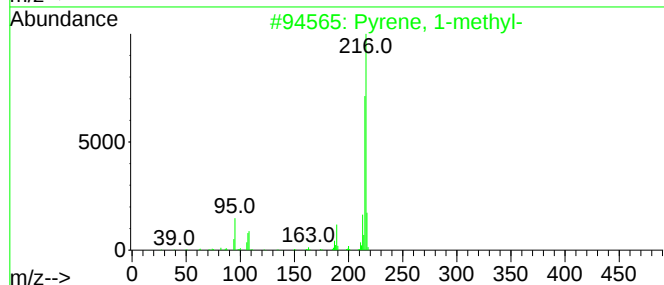
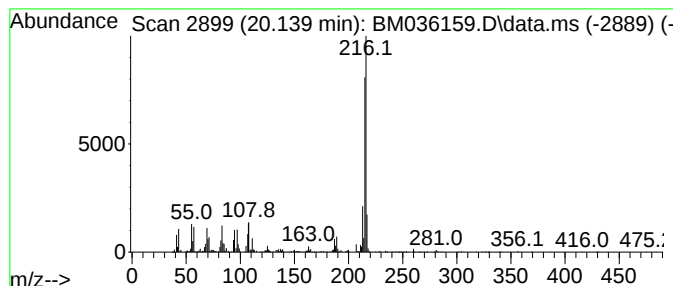
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pyrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.139	3.89 ng	1001510	Chrysene-d12	21.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	89
5			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74



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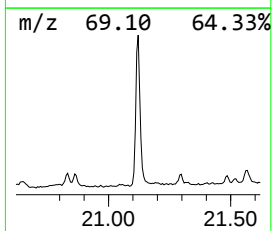
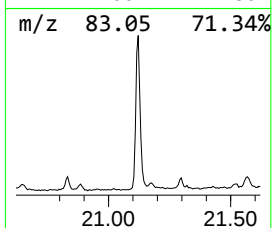
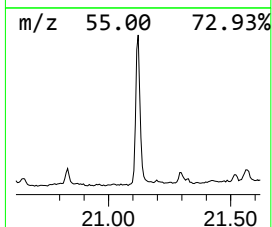
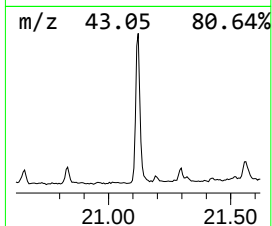
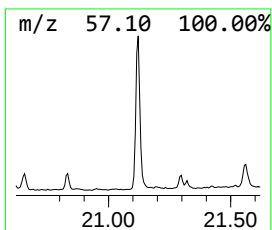
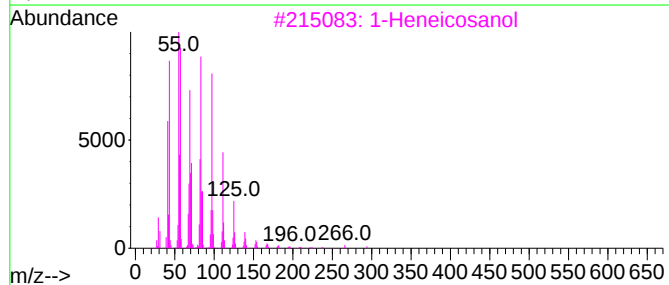
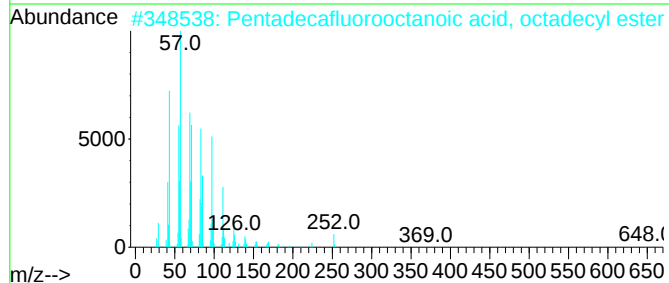
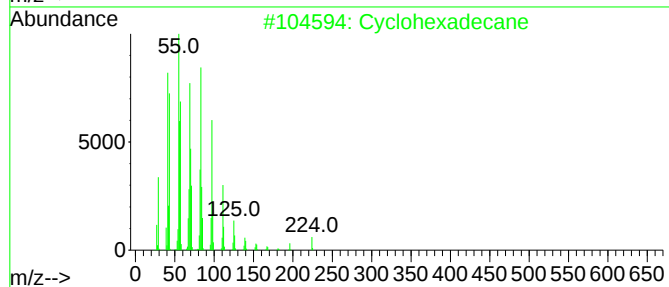
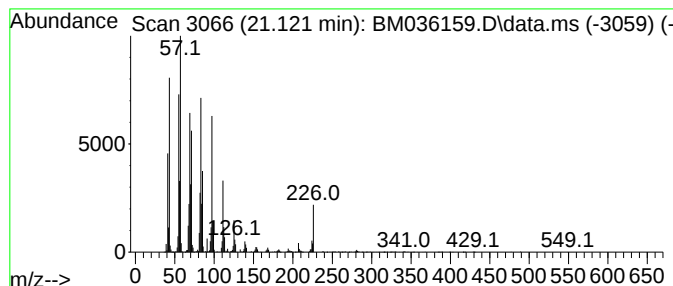
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.121	9.96 ng	2565320	Chrysene-d12	21.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			1-Hexacosene	364	C26H52	018835-33-1	91
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



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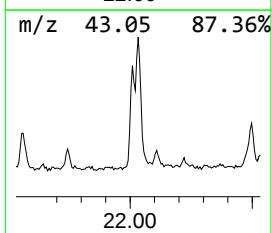
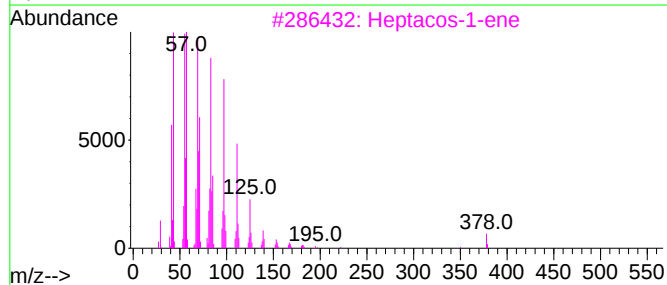
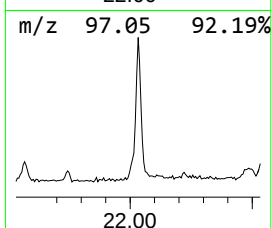
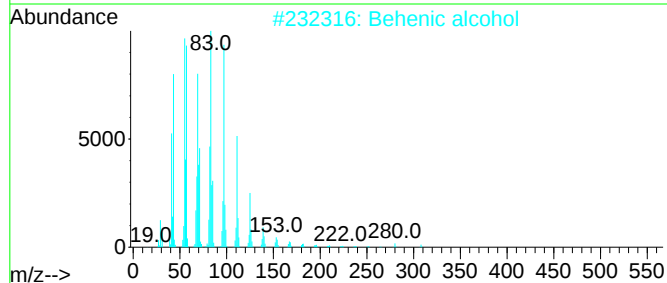
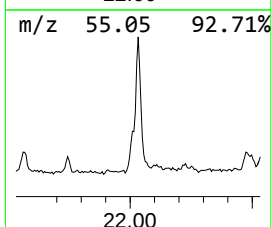
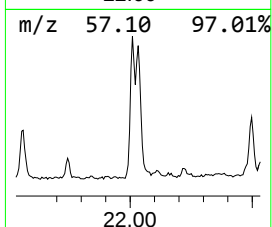
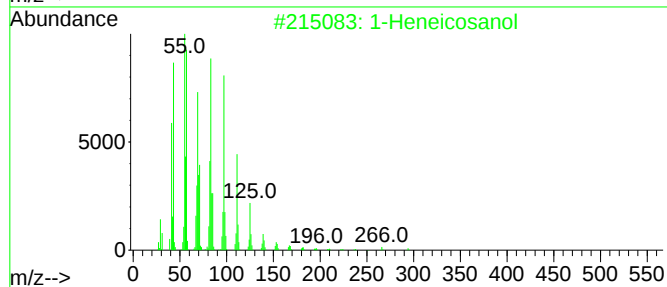
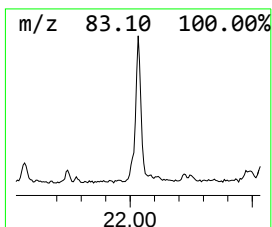
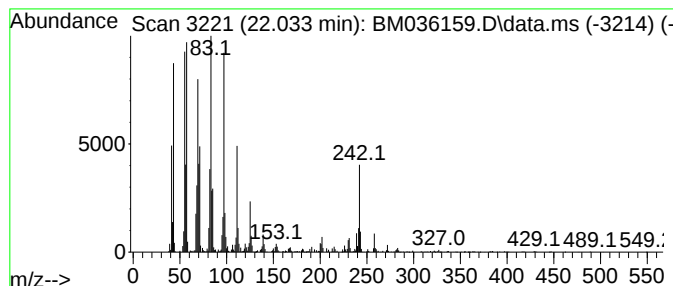
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.033	6.04 ng	1554830	Chrysene-d12	21.403

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	93
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		Heptacos-1-ene	378	C27H54	015306-27-1	91
4		Pentacos-1-ene	350	C25H50	016980-85-1	91
5		1-Tetracosene	336	C24H48	010192-32-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080822\
Data File : BM036159.D
Acq On : 09 Aug 2022 00:17
Operator : CG/JU
Sample : N3962-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-204

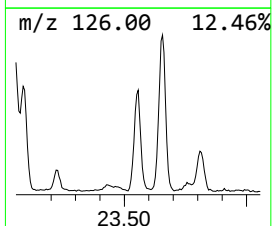
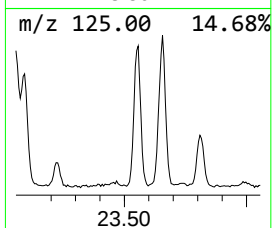
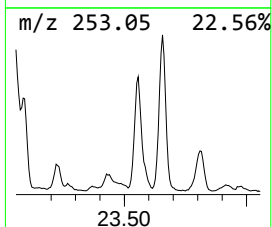
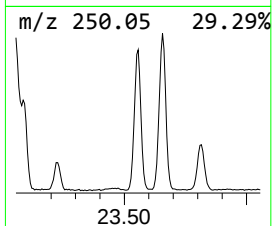
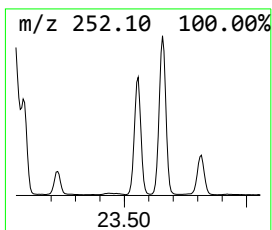
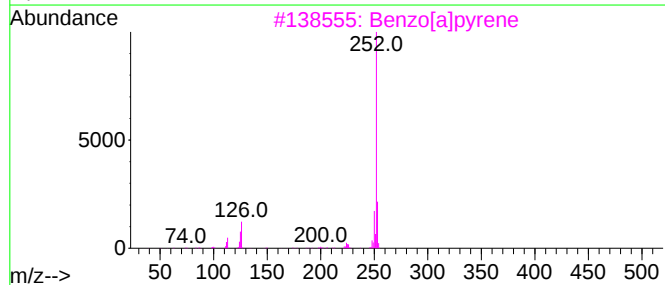
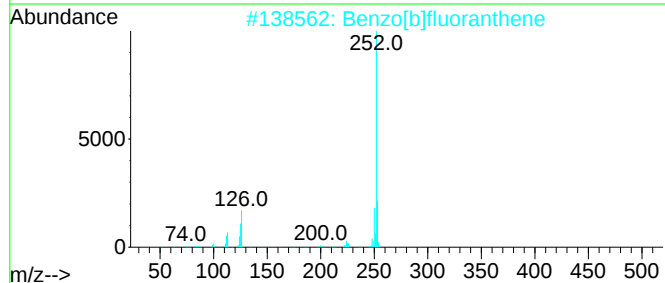
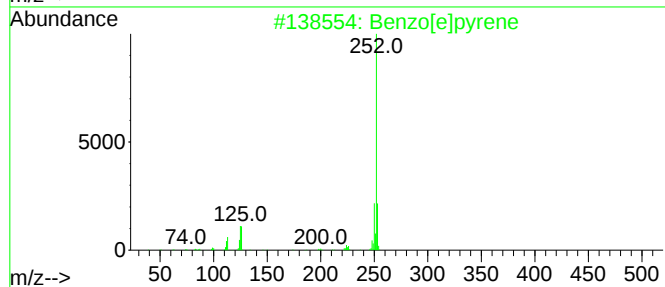
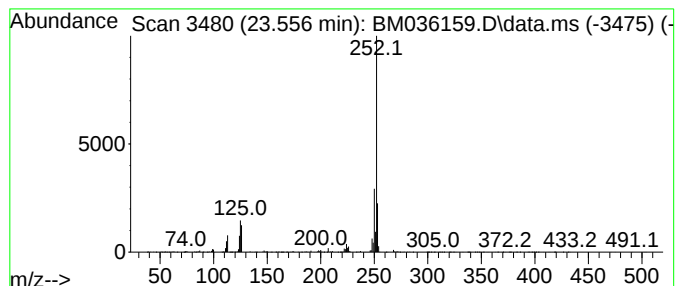
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.556	12.37 ng	1607530	Perylene-d12	23.762

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
3			Benzo[a]pyrene	252	C20H12	000050-32-8	98
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080822\
Data File : BM036159.D
Acq On : 09 Aug 2022 00:17
Operator : CG/JU
Sample : N3962-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

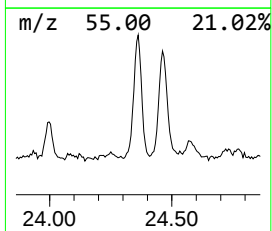
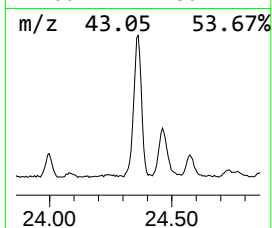
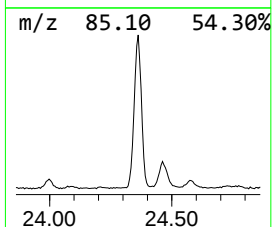
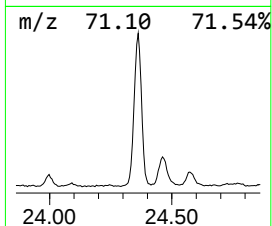
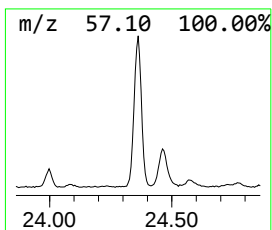
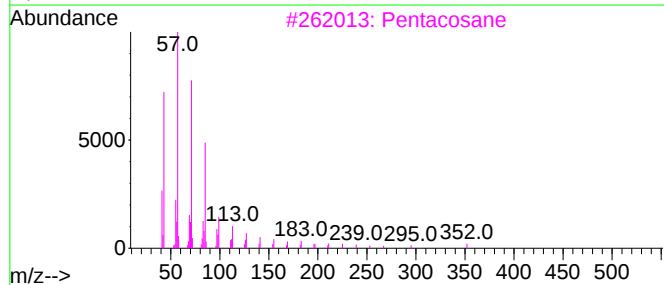
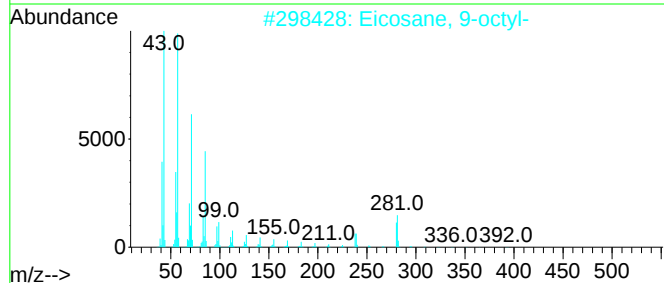
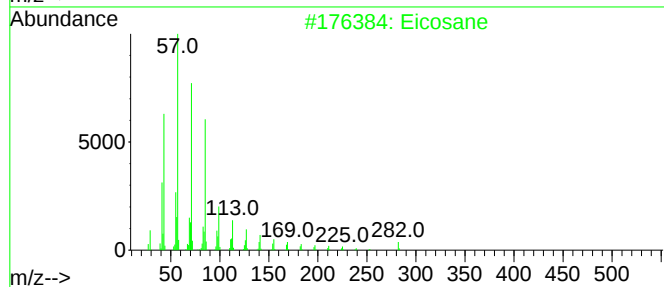
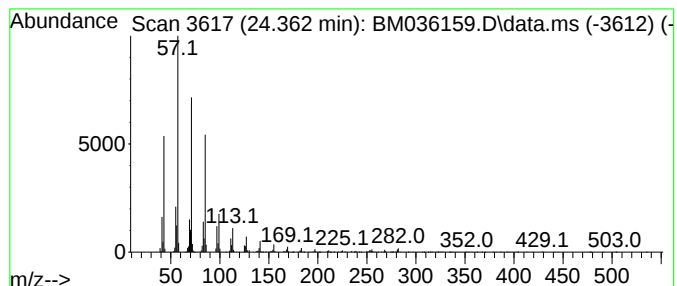
Instrument :
BNA_M
ClientSampleId :
RVE-204

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.362	17.32 ng	2250620	Perylene-d12	23.762	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Eicosane, 9-octyl-	394	C28H58	013475-77-9	93
3	Pentacosane	352	C25H52	000629-99-2	93
4	Heneicosane	296	C21H44	000629-94-7	90
5	Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080822\
Data File : BM036159.D
Acq On : 09 Aug 2022 00:17
Operator : CG/JU
Sample : N3962-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-204

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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-...	4.946	3.9	ng	305363	1	7.845	1573160	20.0
n-Hexadecanoic ...	18.127	6.4	ng	927967	4	17.227	2902120	20.0
Pyrene, 1-methyl-	20.139	3.9	ng	1001510	5	21.403	5151540	20.0
Cyclohexadecane	21.121	10.0	ng	2565320	5	21.403	5151540	20.0
1-Heneicosanol	22.033	6.0	ng	1554830	5	21.403	5151540	20.0
Benzo[e]pyrene	23.556	12.4	ng	1607530	6	23.762	2598270	20.0
Eicosane	24.362	17.3	ng	2250620	6	23.762	2598270	20.0