

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
 Data File : BM039986.D
 Acq On : 24 May 2023 16:22
 Operator : CG/JU
 Sample : 02888-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MID2-44(10-11)

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-BM052323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039986.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.093	301	307	317	rVB	332831	459025	3.61%	0.614%
2	5.563	380	387	396	rBV	5616491	7784741	61.24%	10.405%
3	7.169	652	660	672	rBV	4933936	7544071	59.35%	10.083%
4	8.016	795	804	812	rBV	1344313	2050759	16.13%	2.741%
5	9.181	994	1002	1012	rBV	2865916	4588287	36.09%	6.133%
6	10.834	1275	1283	1289	rBV	1630675	2699826	21.24%	3.609%
7	13.280	1691	1699	1707	rBV	7400581	10247766	80.62%	13.697%
8	14.651	1925	1932	1949	rBV	2055426	2926142	23.02%	3.911%
9	16.004	2153	2162	2168	rBV	435184	596869	4.70%	0.798%
10	16.133	2177	2184	2192	rBV	5075075	6738621	53.01%	9.007%
11	17.392	2392	2398	2404	rBV	2141012	2953266	23.23%	3.947%
12	18.286	2544	2550	2559	rBV	494837	786433	6.19%	1.051%
13	19.445	2743	2747	2762	rVB2	418415	680414	5.35%	0.909%
14	19.562	2762	2767	2782	rBV	380638	596649	4.69%	0.797%
15	19.809	2801	2809	2820	rVB2	106848	256200	2.02%	0.342%
16	20.009	2838	2843	2853	rBV	10551516	12711879	100.00%	16.991%
17	20.633	2945	2949	2954	rBV3	104287	178515	1.40%	0.239%
18	20.704	2954	2961	2970	rVV	1789068	2249982	17.70%	3.007%
19	20.815	2976	2980	2985	rVB2	92328	145352	1.14%	0.194%
20	21.280	3054	3059	3069	rBV	448191	643108	5.06%	0.860%
21	21.486	3090	3094	3099	rBV	356711	404109	3.18%	0.540%
22	21.574	3102	3109	3113	rVV	2447659	3363611	26.46%	4.496%
23	21.609	3113	3115	3121	rVB	229419	278999	2.19%	0.373%
24	22.709	3298	3302	3309	rBV2	261997	402531	3.17%	0.538%
25	23.280	3394	3399	3403	rBV2	183034	348360	2.74%	0.466%
26	24.027	3519	3526	3537	rVB	1563998	3180963	25.02%	4.252%

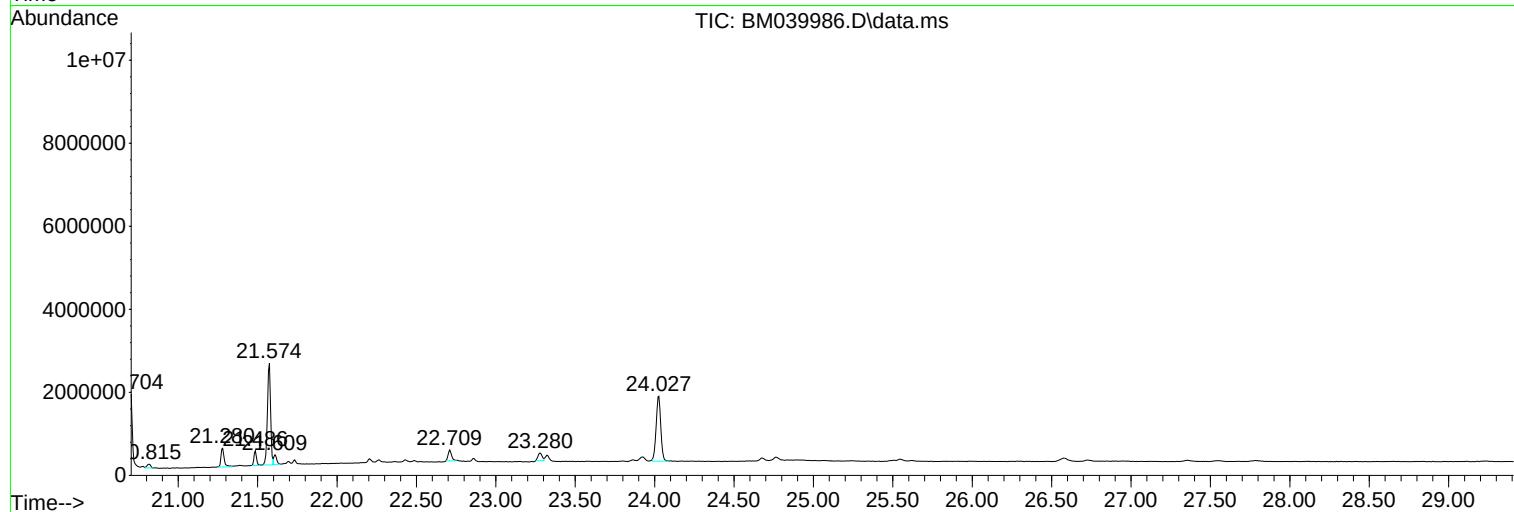
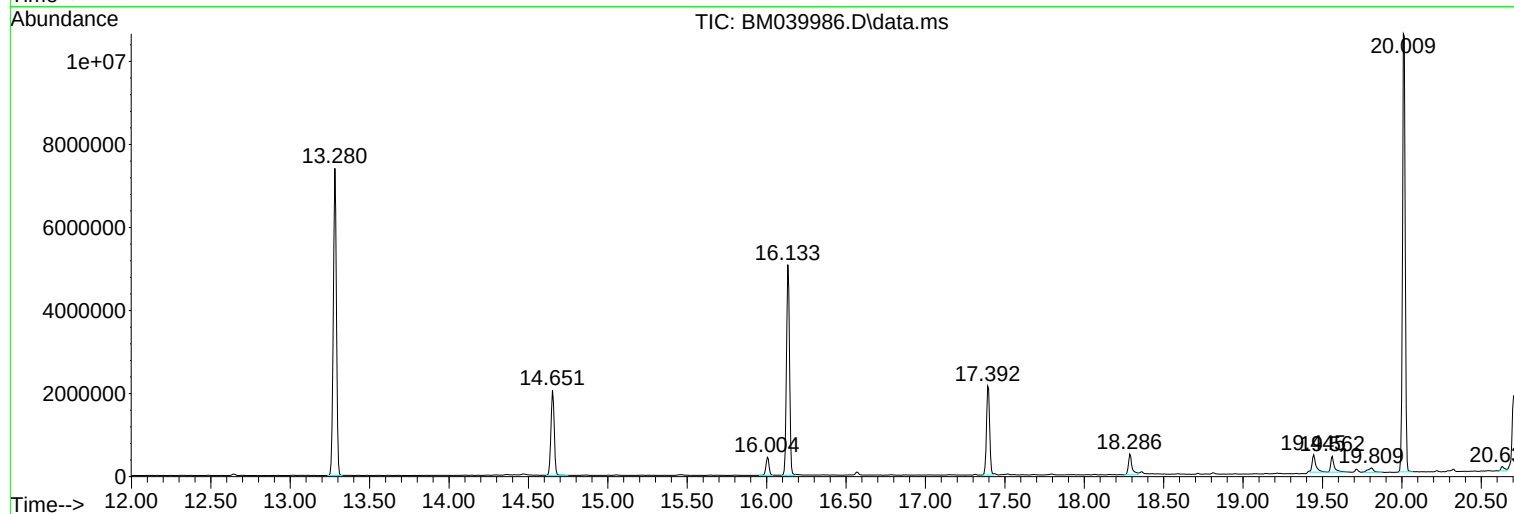
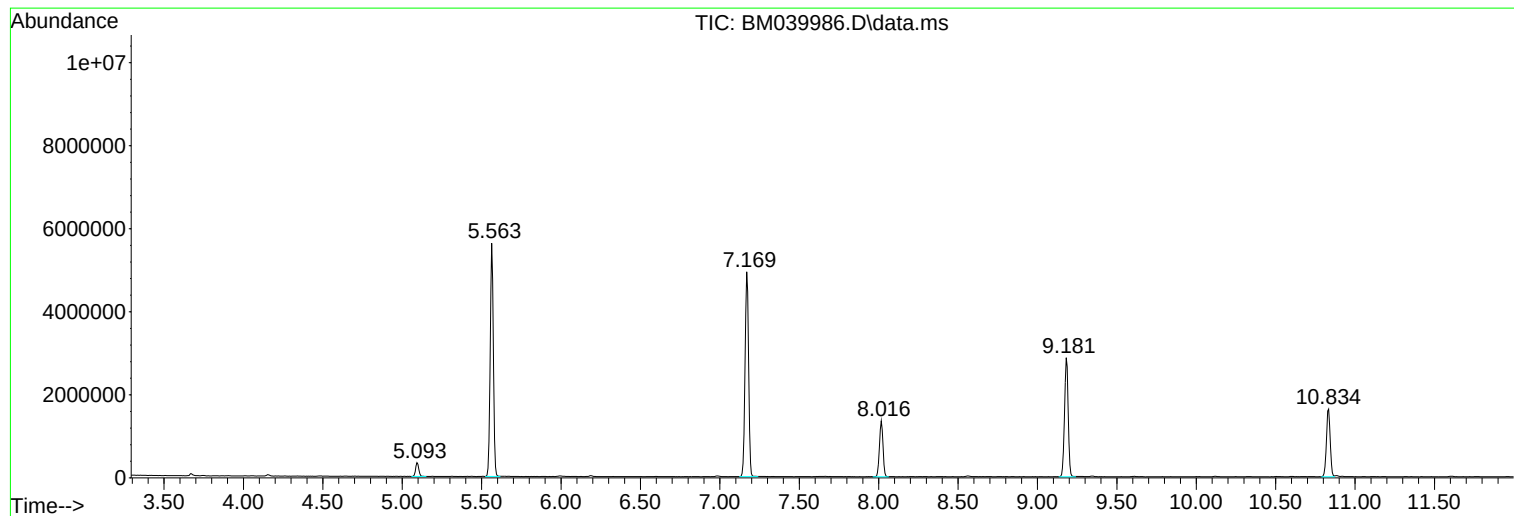
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ClientSampleId :
MID2-44(10-11)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.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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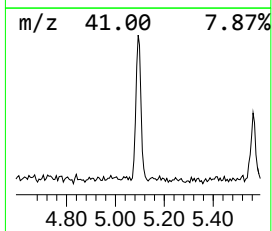
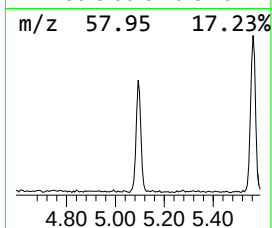
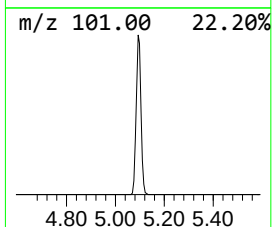
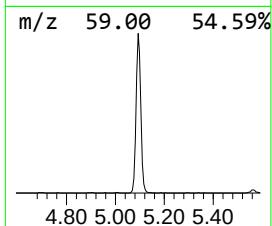
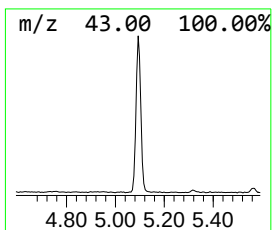
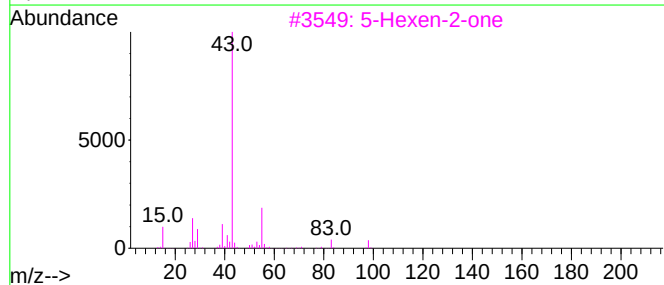
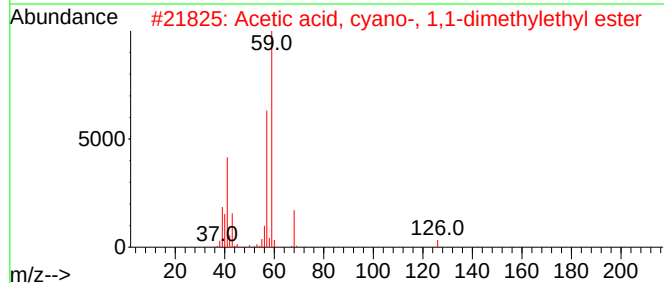
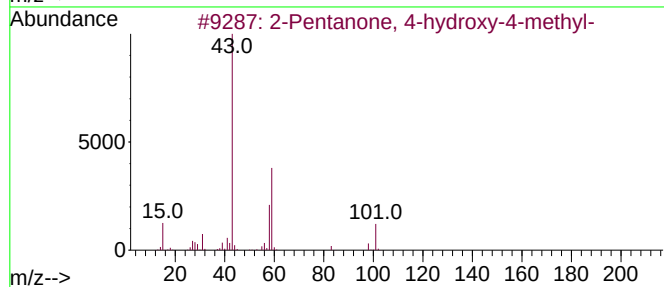
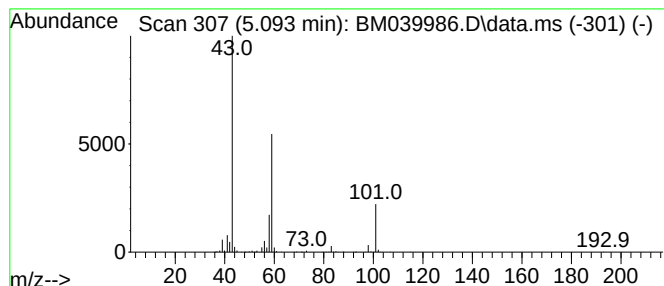
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	4.48 ng	459025	1,4-Dichlorobenzene-d4	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
4	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9	
5	Hexanamide	115	C6H13NO	000628-02-4	9	



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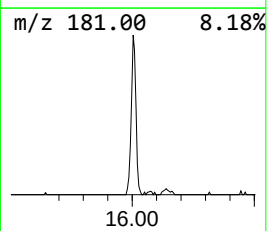
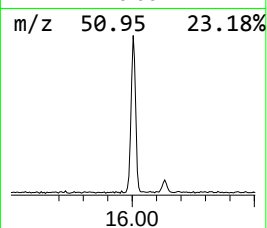
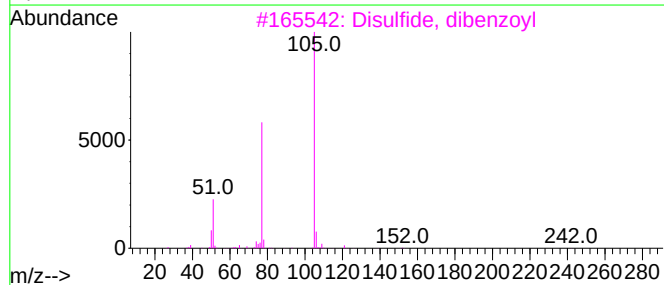
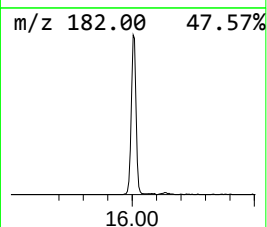
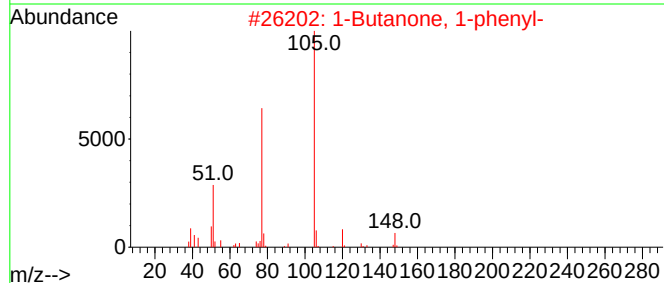
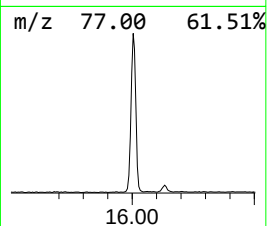
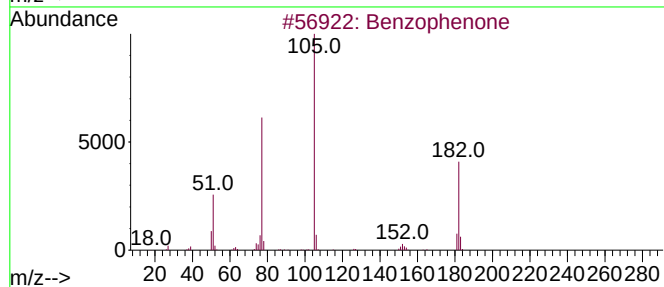
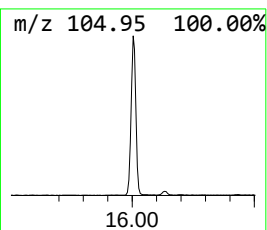
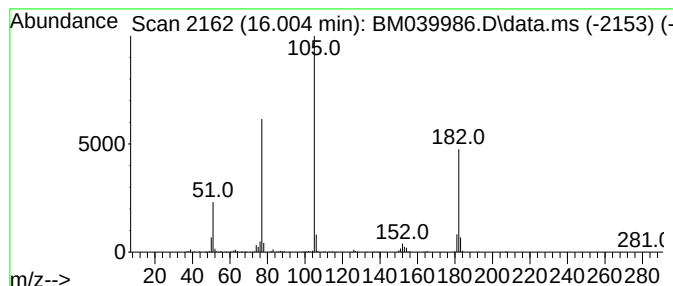
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.004	4.08 ng	596869	Acenaphthene-d10	14.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47
3			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47



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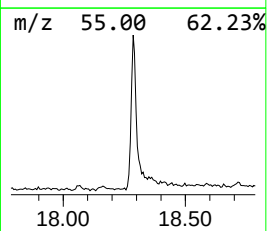
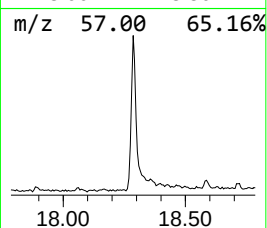
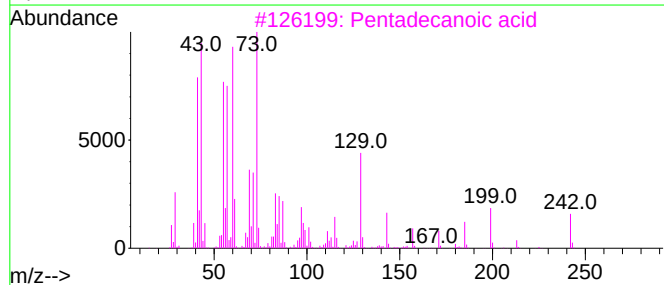
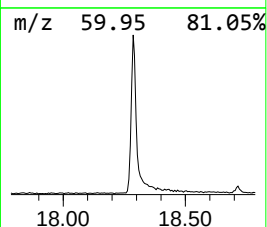
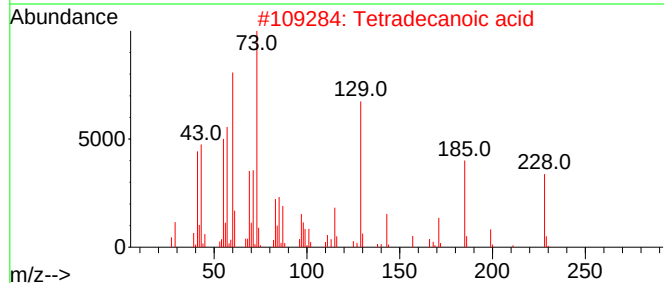
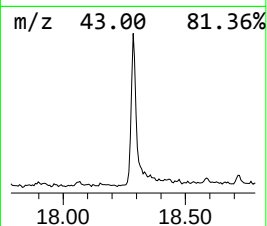
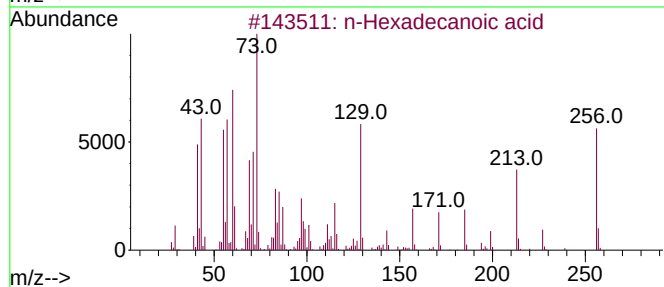
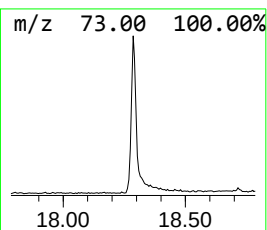
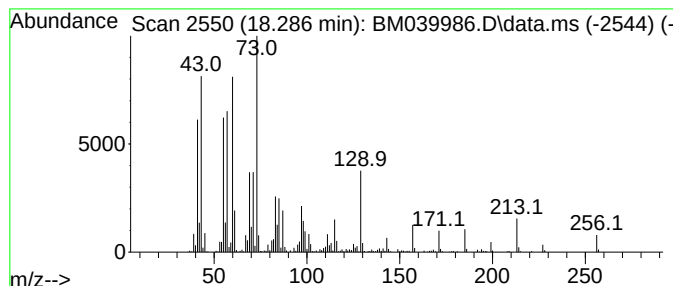
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	5.33 ng	786433	Phenanthrene-d10	17.392

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			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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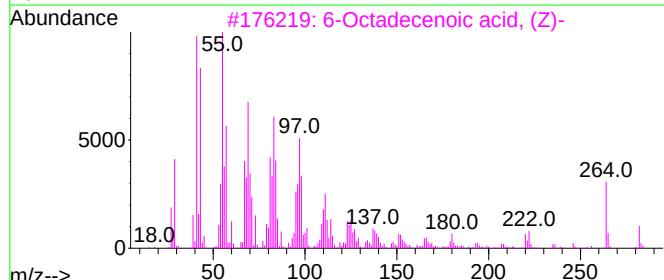
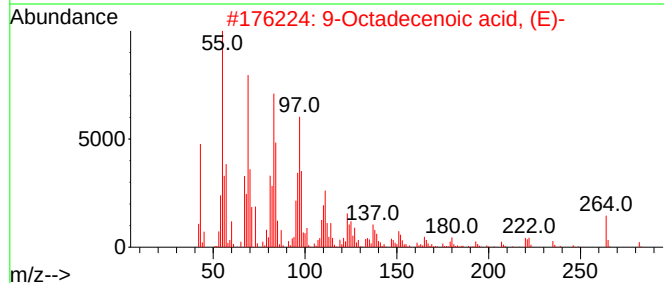
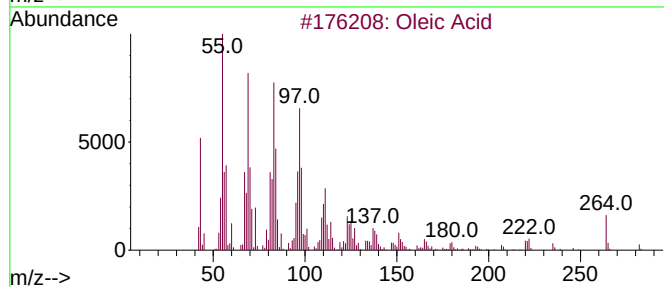
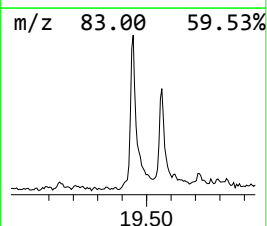
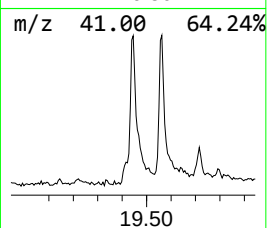
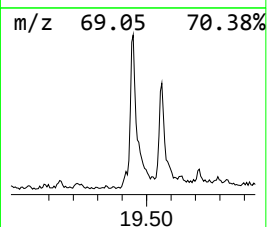
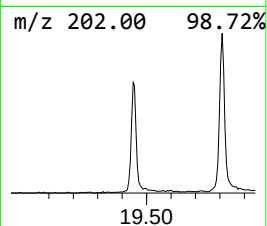
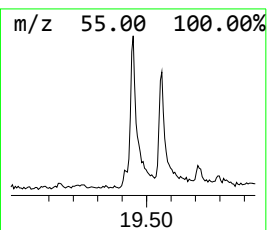
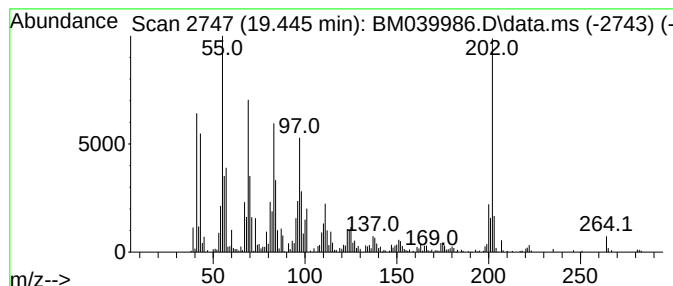
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Oleic Acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	4.61 ng	680414	Phenanthrene-d10	17.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oleic Acid	282	C18H34O2	000112-80-1	97
2			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	96
3			6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	76
4			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	74
5			9-Octadecenoic acid	282	C18H34O2	002027-47-6	70



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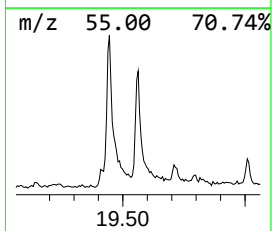
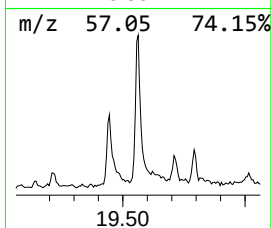
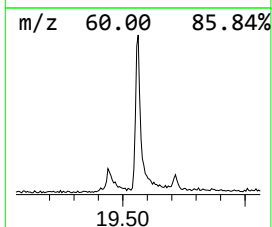
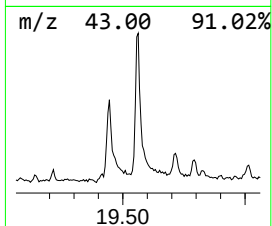
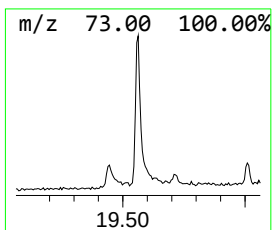
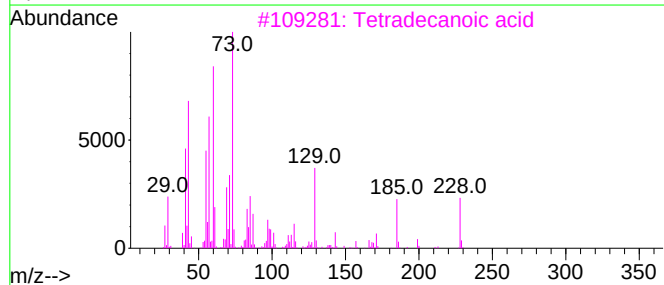
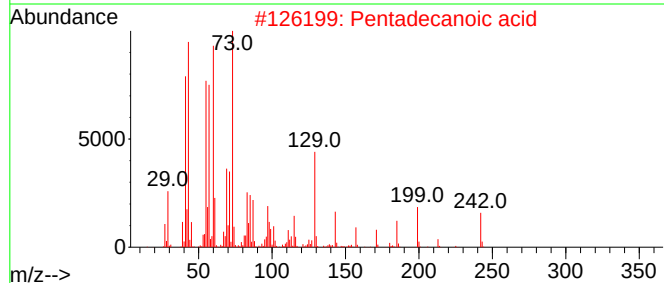
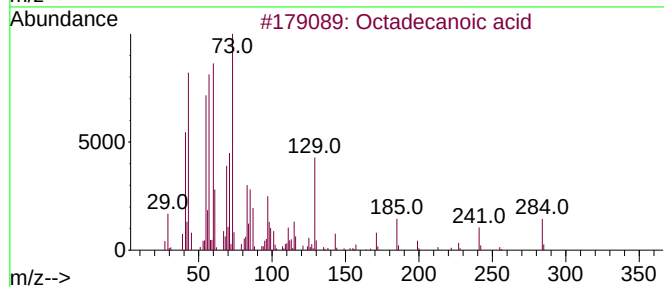
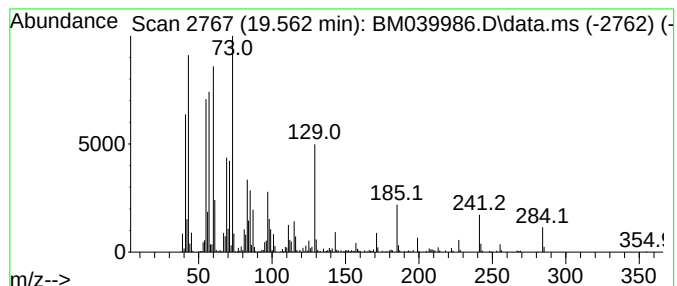
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.562	3.55 ng	596649	Chrysene-d12	21.574

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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



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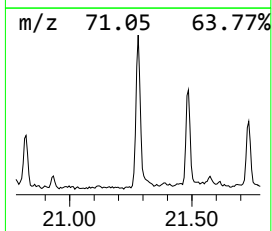
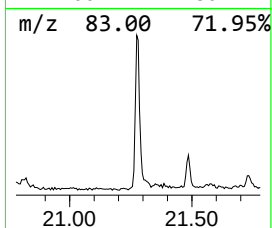
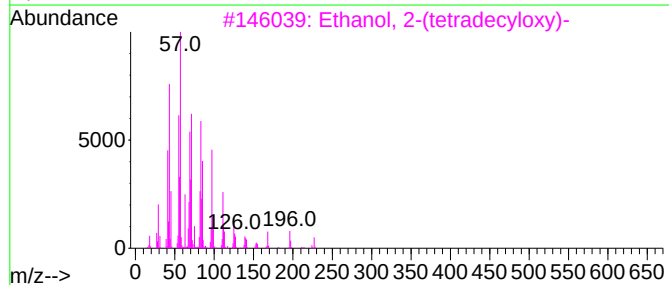
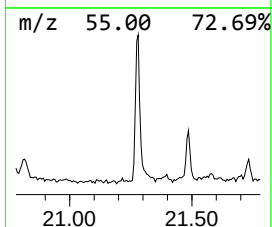
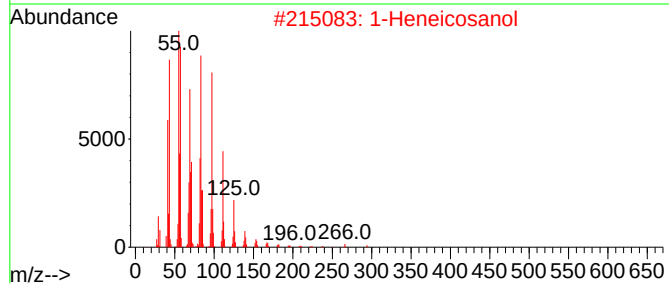
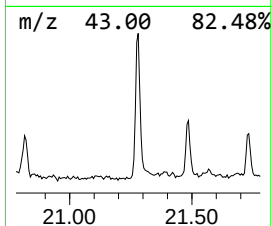
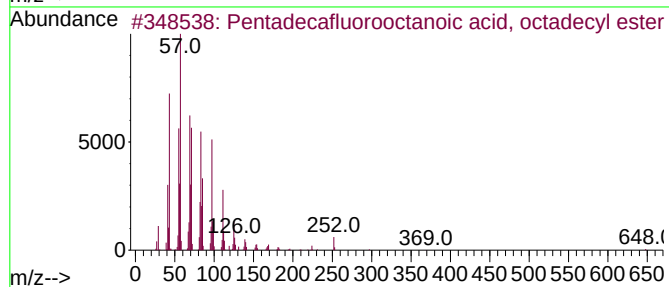
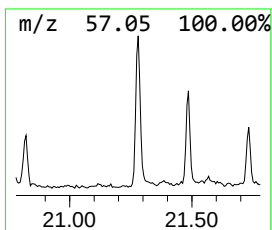
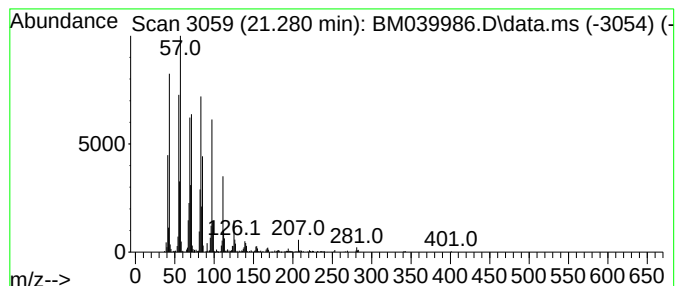
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BNA_M
ClientSampleId :
MID2-44(10-11)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.280	3.82 ng	643108	Chrysene-d12		21.574	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...		666	C26H37F15O2	1000406-04-8	95
2	1-Heneicosanol		312	C21H44O	015594-90-8	93
3	Ethanol, 2-(tetradecyloxy)-		258	C16H34O2	002136-70-1	91
4	Nonadecyl pentafluoropropionate		430	C22H39F5O2	1000351-88-8	91
5	Octacosanol		410	C28H58O	000557-61-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039986.D
Acq On : 24 May 2023 16:22
Operator : CG/JU
Sample : 02888-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MID2-44(10-11)

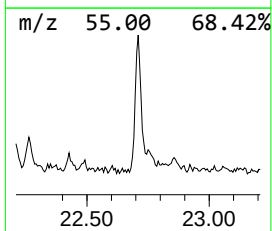
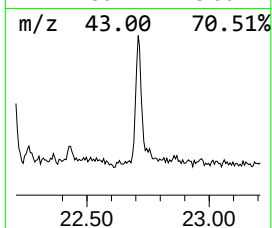
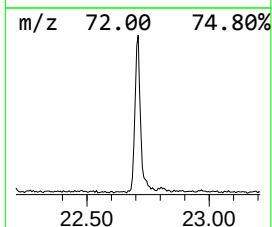
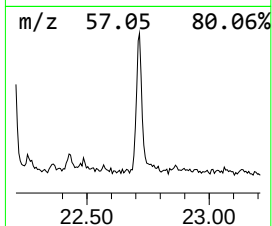
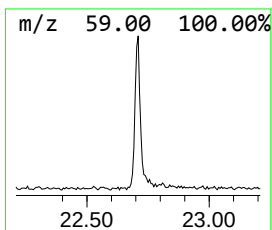
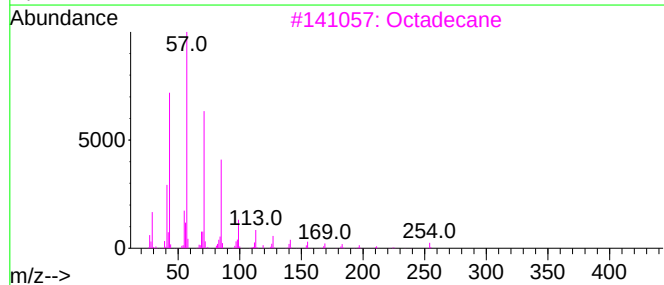
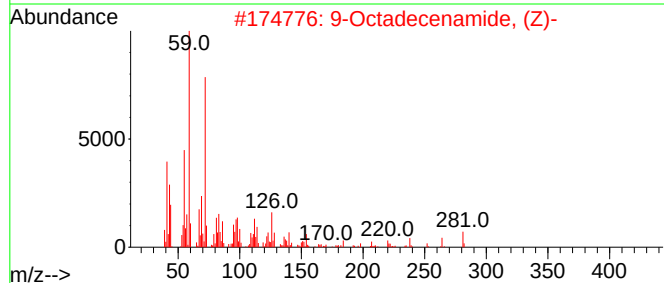
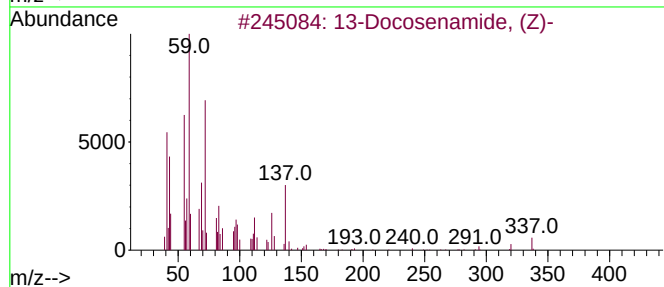
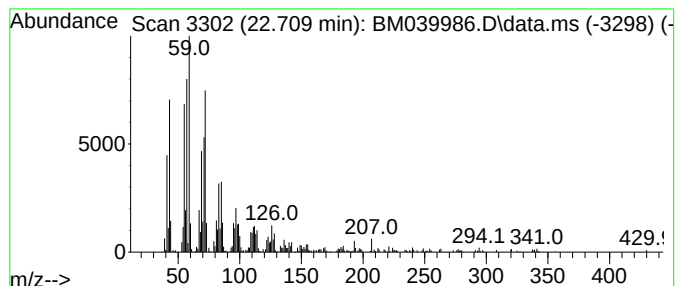
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.709	2.39 ng	402531	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	62
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
3			Octadecane	254	C18H38	000593-45-3	56
4			Carbonic acid, eicosyl prop-1-en...	382	C24H46O3	1000383-10-8	41
5			1-Propene, 2-methyl-3-propoxy-	114	C7H14O	053897-29-3	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039986.D
Acq On : 24 May 2023 16:22
Operator : CG/JU
Sample : 02888-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MID2-44(10-11)

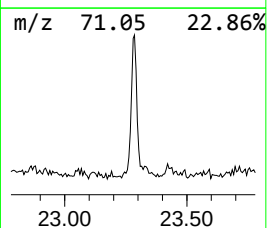
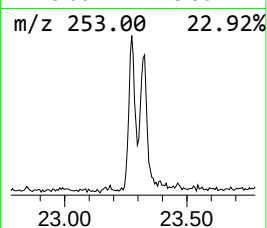
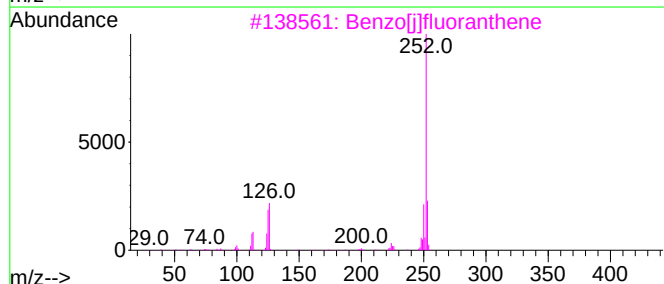
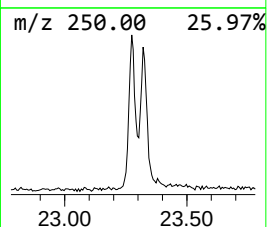
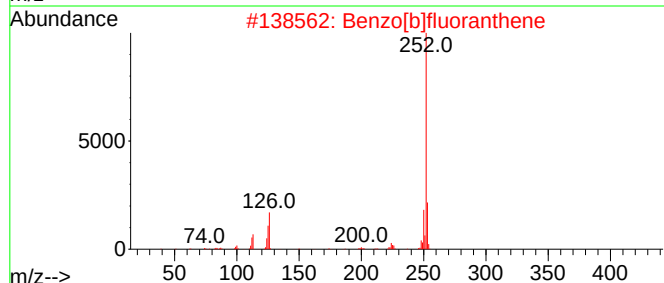
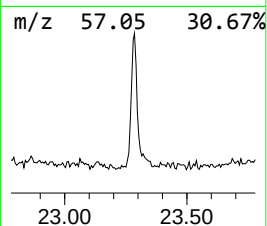
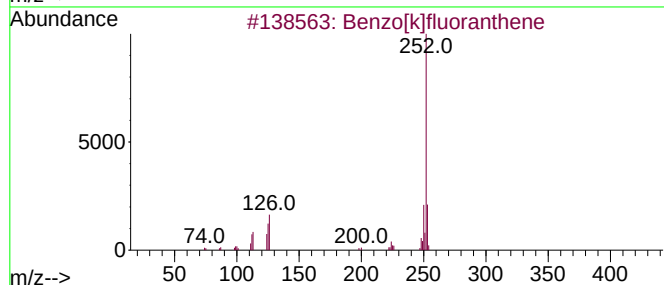
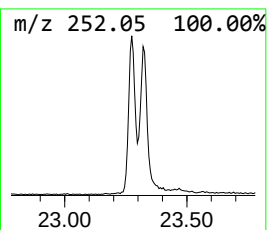
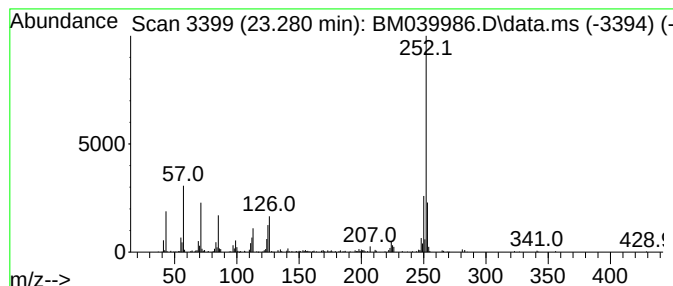
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[j]fluoranthene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.280	2.19 ng	348360	Perylene-d12	24.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
4			Benzo[a]pyrene	252	C20H12	000050-32-8	94
5			Benzo[e]pyrene	252	C20H12	000192-97-2	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039986.D
Acq On : 24 May 2023 16:22
Operator : CG/JU
Sample : 02888-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MID2-44(10-11)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.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
2-Pentanone, 4-...	5.093	4.5	ng	459025	1	8.016	2050760	20.0
Benzophenone	16.004	4.1	ng	596869	3	14.651	2926140	20.0
n-Hexadecanoic ...	18.286	5.3	ng	786433	4	17.392	2953270	20.0
Oleic Acid	19.445	4.6	ng	680414	4	17.392	2953270	20.0
Octadecanoic acid	19.562	3.5	ng	596649	5	21.574	3363610	20.0
Pentadecafluoro...	21.280	3.8	ng	643108	5	21.574	3363610	20.0
13-Docosenamide...	22.709	2.4	ng	402531	5	21.574	3363610	20.0
Benzo[j]fluoran...	23.280	2.2	ng	348360	6	24.027	3180960	20.0