

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041223\
 Data File : BM039404.D
 Acq On : 12 Apr 2023 15:27
 Operator : CG/JU
 Sample : 02292-09
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 IDW-SO-G3-041123

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-BM032923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039404.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.951	294	300	310	rVB	398834	560717	6.02%	0.824%
2	5.445	377	384	407	rBV	3296014	5089339	54.66%	7.482%
3	7.069	653	660	680	rBV	3068220	5086432	54.62%	7.478%
4	7.857	788	794	807	rBV	739017	1189321	12.77%	1.749%
5	9.033	986	994	1009	rBV	1763115	3099606	33.29%	4.557%
6	10.669	1264	1272	1285	rBV	900214	1588054	17.05%	2.335%
7	13.133	1685	1691	1709	rBV	4220247	6604414	70.93%	9.710%
8	14.515	1919	1926	1939	rBV	1290456	1953062	20.97%	2.871%
9	14.945	1993	1999	2009	rBV	91631	173735	1.87%	0.255%
10	15.880	2153	2158	2163	rVB	179577	255367	2.74%	0.375%
11	16.009	2174	2180	2202	rBV	3301708	4998516	53.68%	7.349%
12	16.674	2288	2293	2300	rBV	106123	203002	2.18%	0.298%
13	17.262	2387	2393	2408	rBV	1533458	2231222	23.96%	3.280%
14	18.045	2522	2526	2533	rBV7	46366	93211	1.00%	0.137%
15	18.174	2540	2548	2563	rBV	3956057	6451990	69.29%	9.486%
16	18.309	2565	2571	2590	rVB2	280205	968751	10.40%	1.424%
17	18.839	2658	2661	2671	rVB5	51971	97613	1.05%	0.144%
18	19.303	2736	2740	2742	rBV2	147711	204527	2.20%	0.301%
19	19.415	2753	2759	2761	rBV	505618	910639	9.78%	1.339%
20	19.445	2761	2764	2784	rVB	2570427	3903719	41.92%	5.739%
21	19.892	2835	2840	2853	rBV	7160865	9311705	100.00%	13.690%
22	20.197	2889	2892	2901	rVB4	106624	164911	1.77%	0.242%
23	20.292	2902	2908	2919	rVV	687387	1457348	15.65%	2.143%
24	21.021	3027	3032	3040	rBV	806532	1378155	14.80%	2.026%
25	21.156	3051	3055	3068	rBV	901575	1453175	15.61%	2.136%
26	21.456	3101	3106	3120	rBV	2009464	2800350	30.07%	4.117%
27	21.674	3138	3143	3158	rBV	741824	1382653	14.85%	2.033%
28	22.368	3257	3261	3270	rVB	547529	917052	9.85%	1.348%
29	22.556	3290	3293	3301	rVB	307400	424191	4.56%	0.624%
30	23.844	3506	3512	3528	rVB2	1397032	3065928	32.93%	4.507%

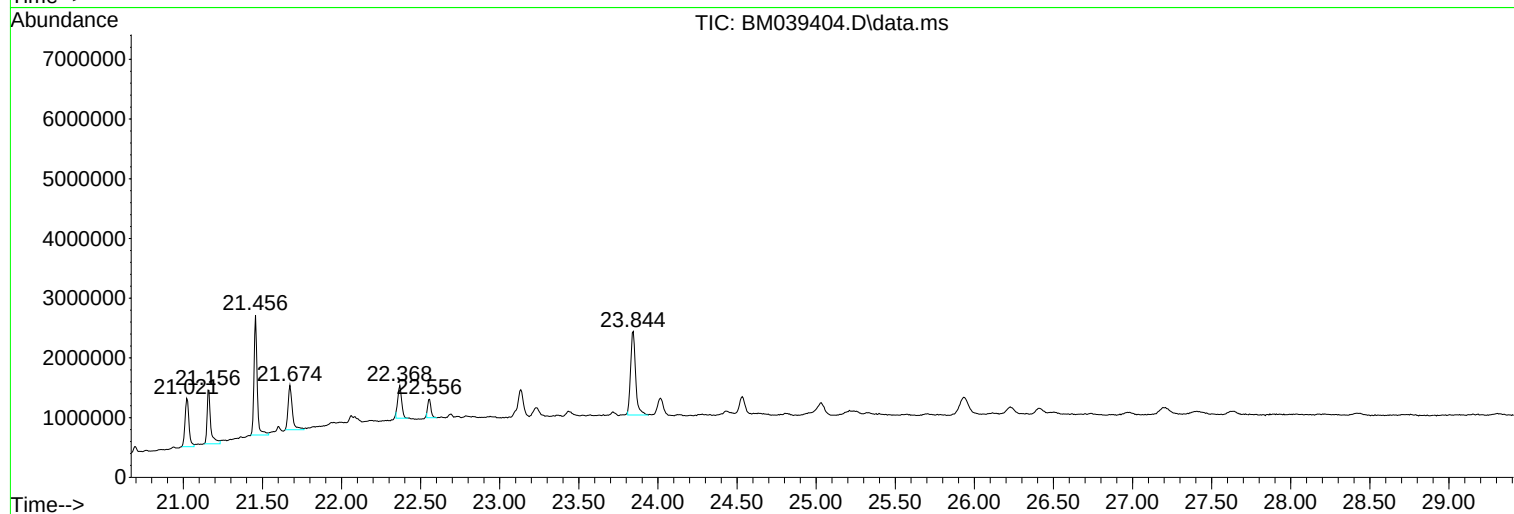
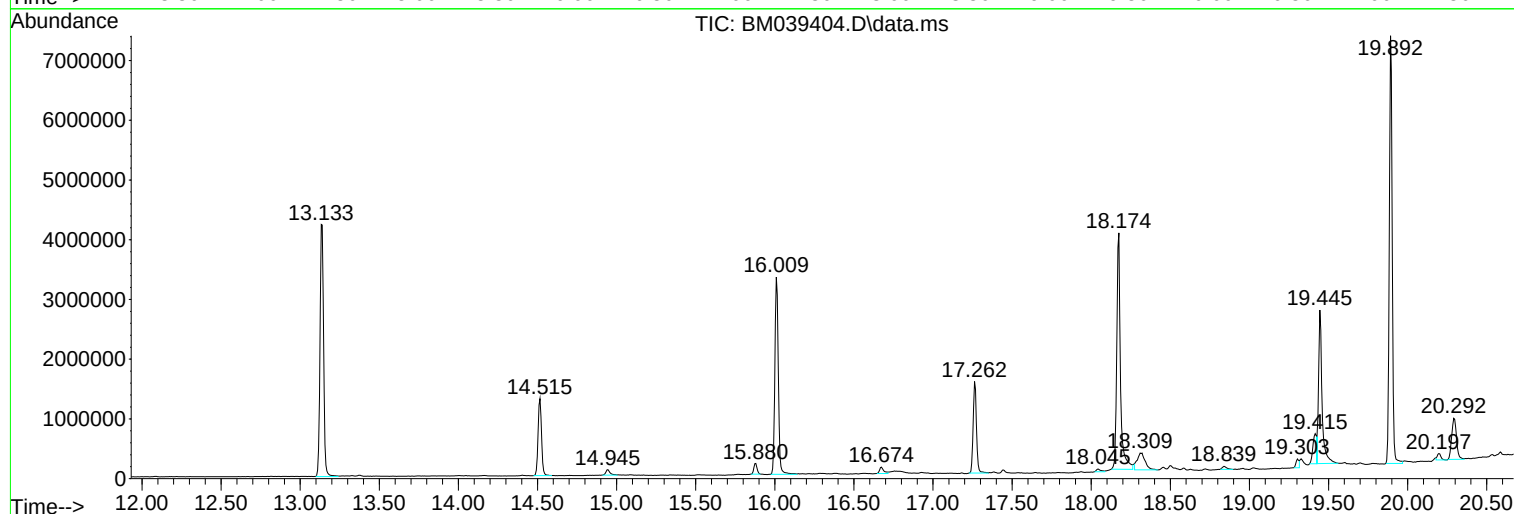
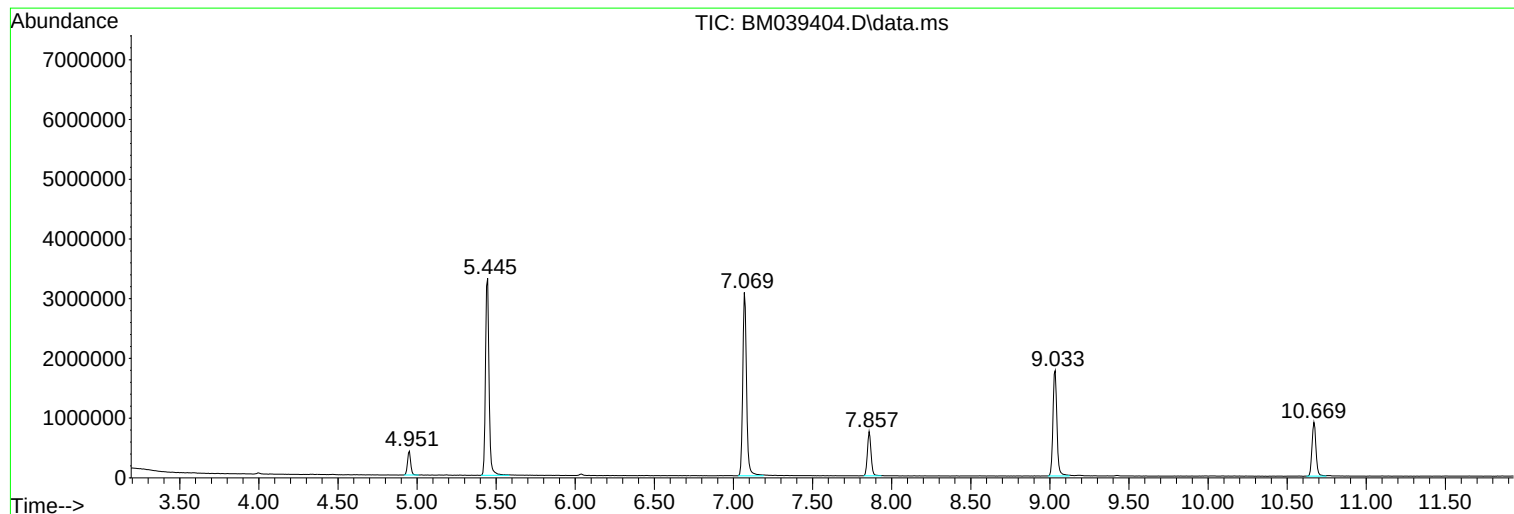
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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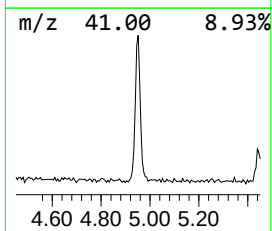
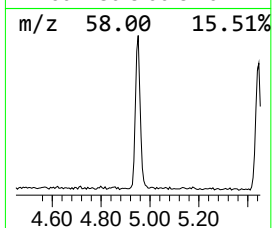
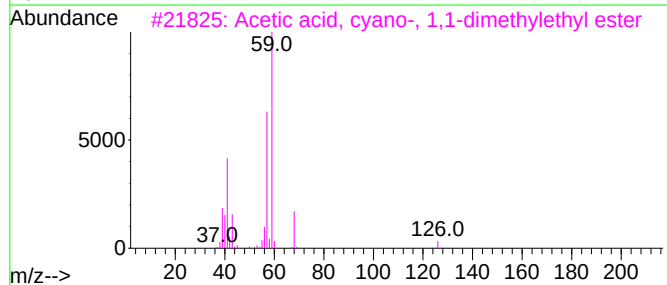
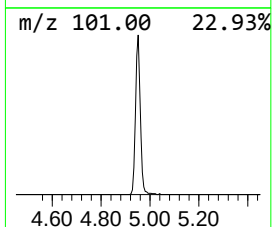
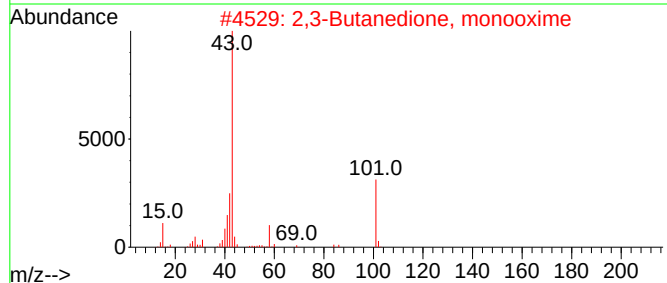
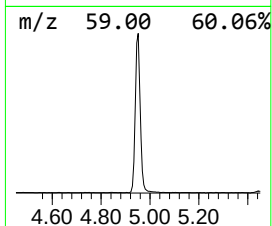
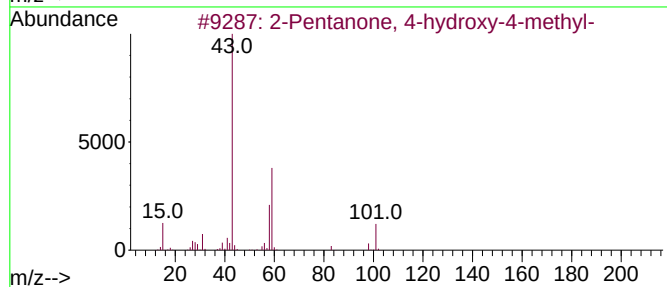
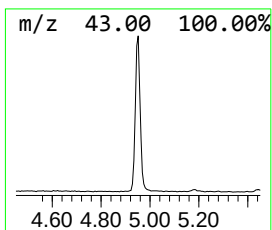
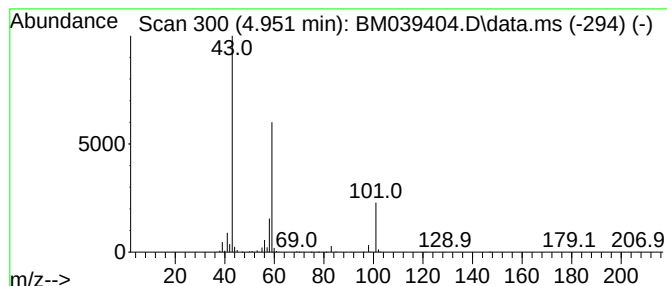
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.951	9.43 ng	560717	1,4-Dichlorobenzene-d4	7.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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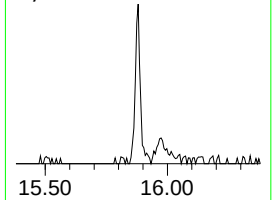
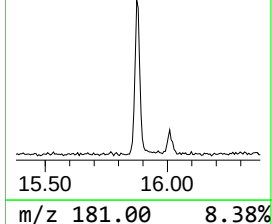
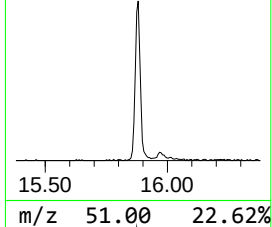
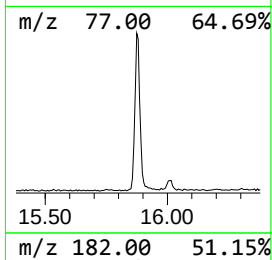
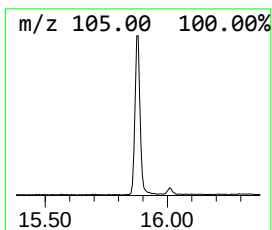
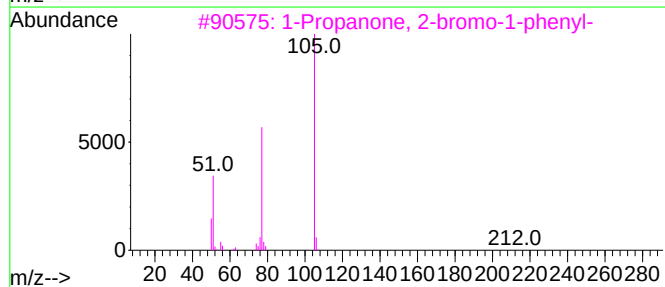
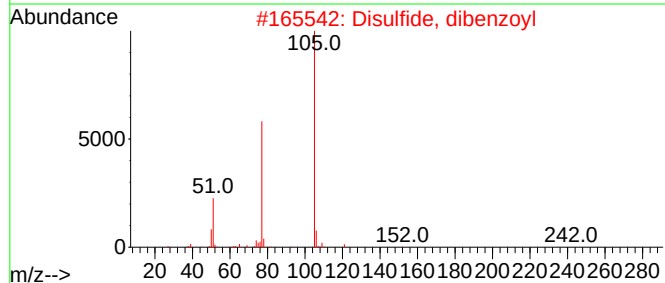
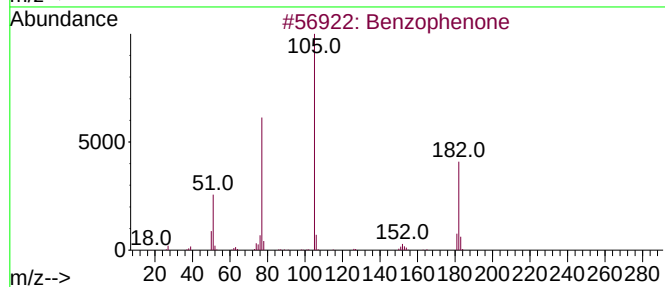
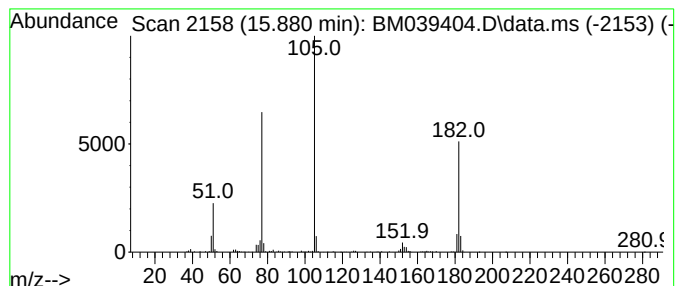
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.880	2.62 ng	255367	Acenaphthene-d10	14.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47
5			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47



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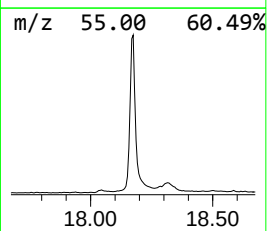
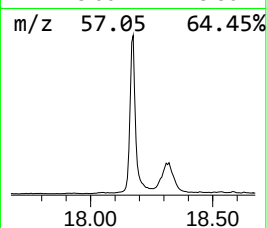
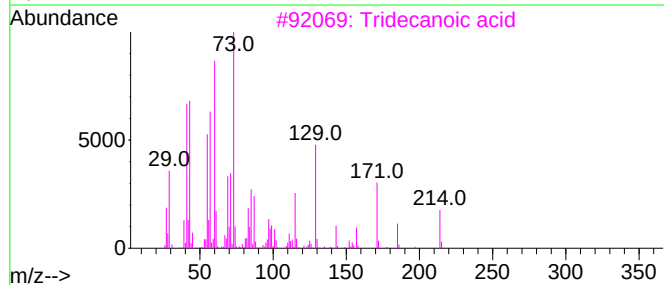
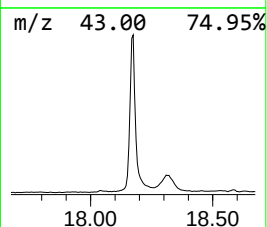
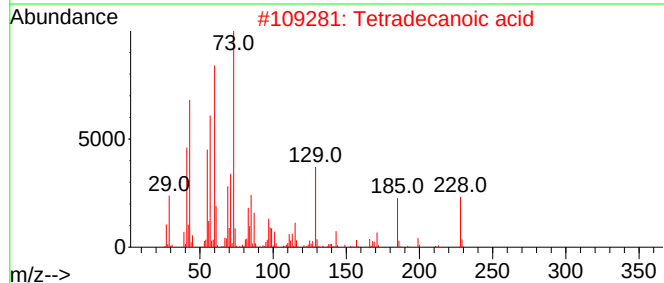
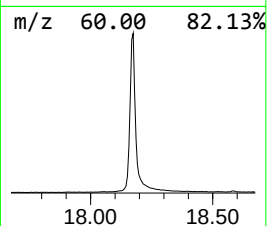
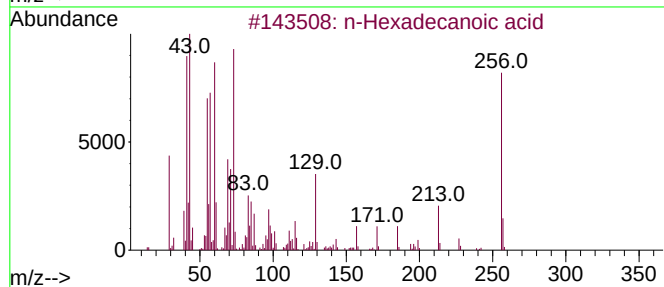
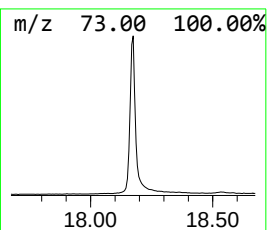
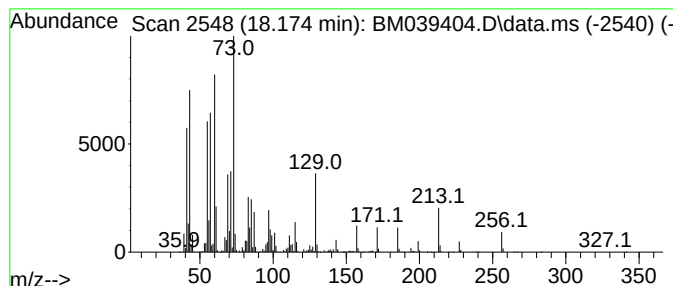
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.174	57.83 ng	6451990	Phenanthrene-d10		17.262	
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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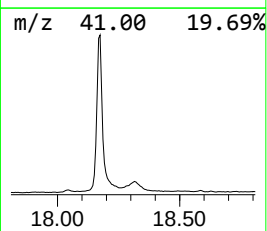
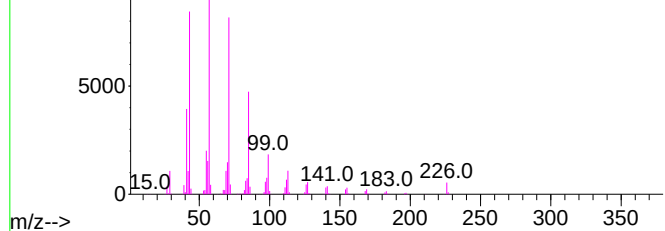
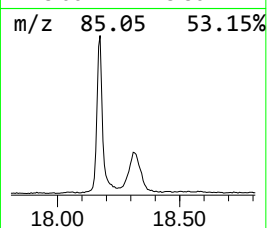
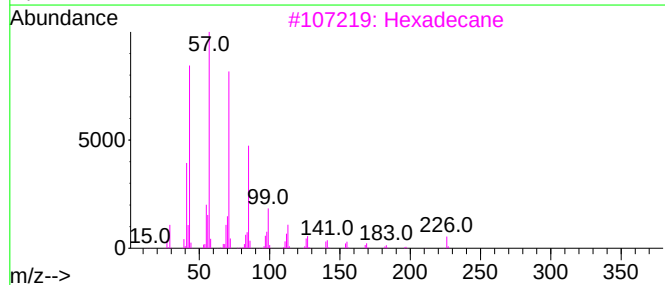
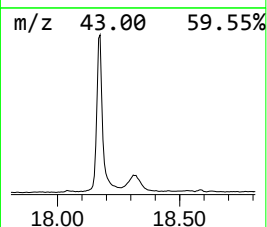
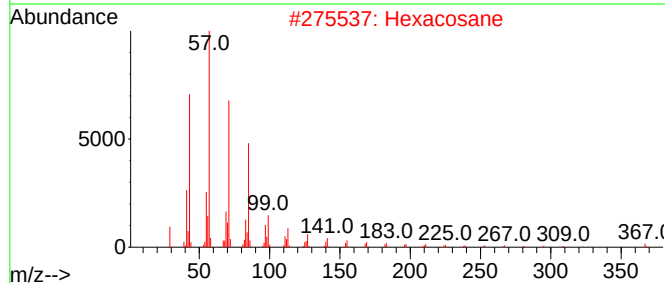
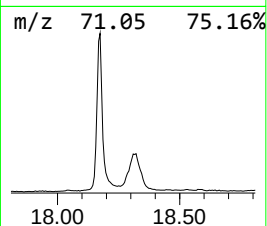
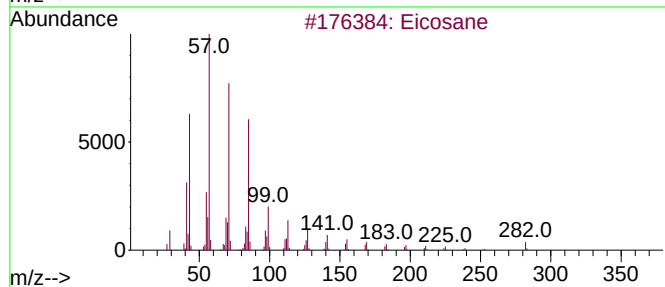
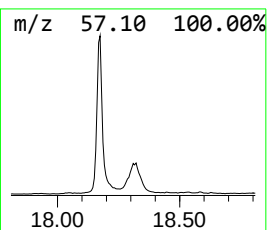
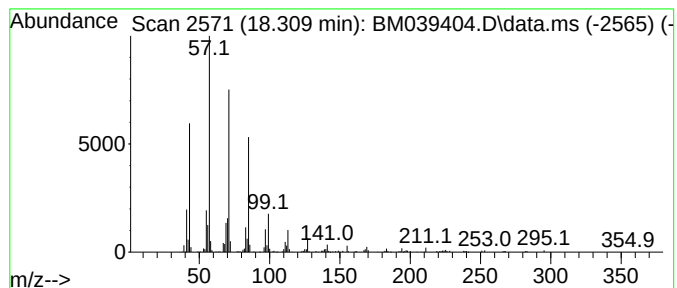
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Peak Number 4 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.309	8.68 ng	968751	Phenanthrene-d10	17.262

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Hexacosane	366	C26H54	000630-01-3	91
3			Hexadecane	226	C16H34	000544-76-3	91
4			Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90



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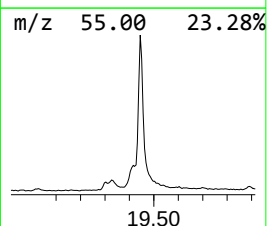
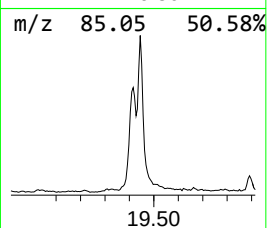
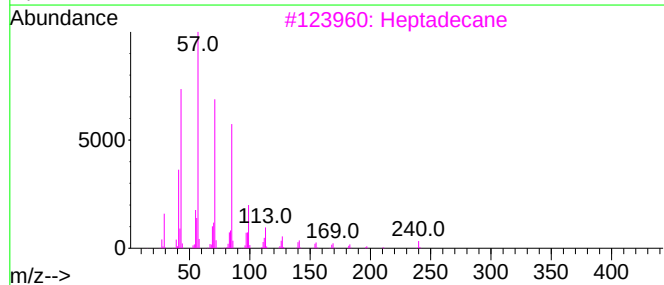
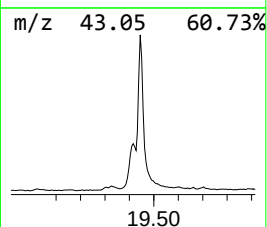
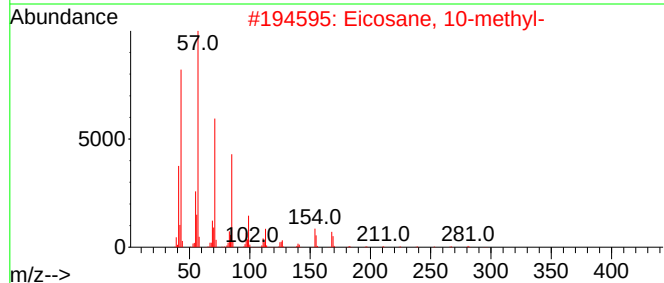
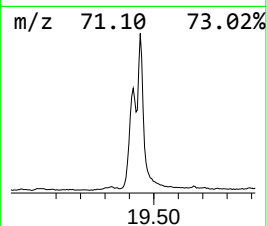
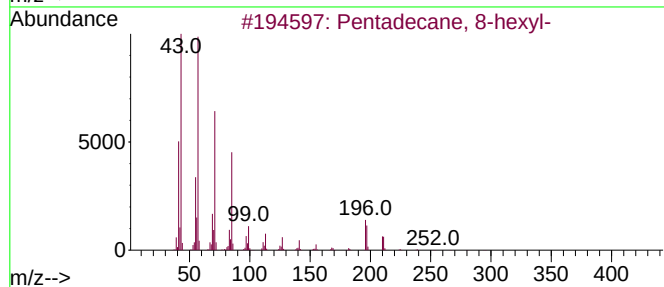
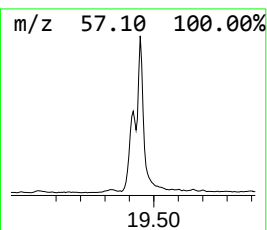
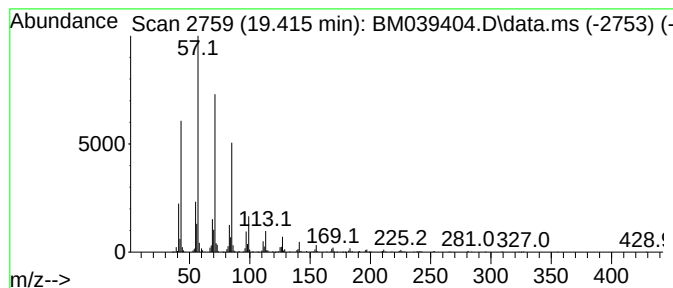
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Peak Number 5 Pentadecane, 8-hexyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.415	6.50 ng	910639	Chrysene-d12	21.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2			Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
3			Heptadecane	240	C17H36	000629-78-7	93
4			Heneicosane	296	C21H44	000629-94-7	91
5			Hexacosane	366	C26H54	000630-01-3	91



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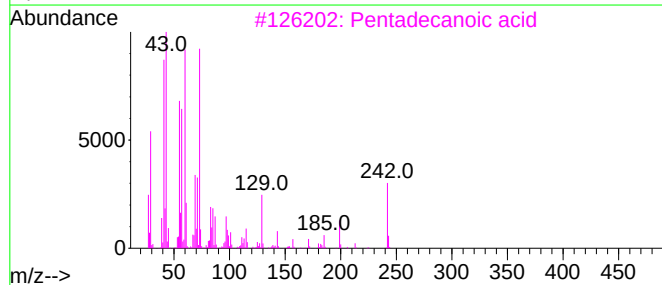
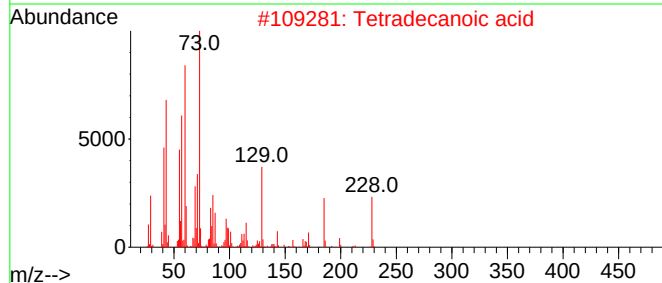
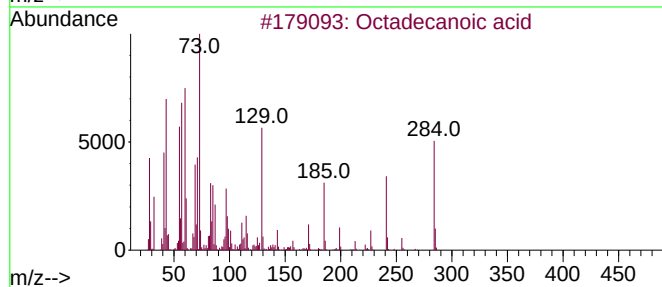
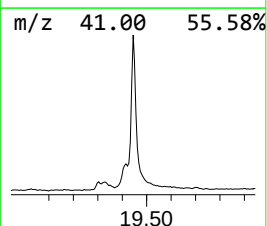
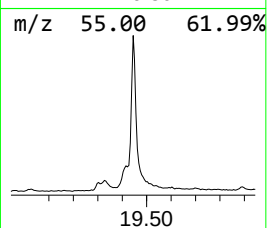
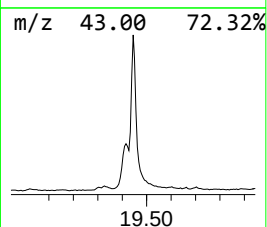
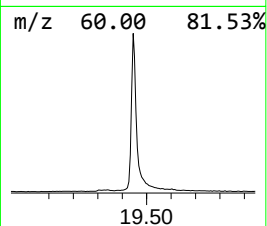
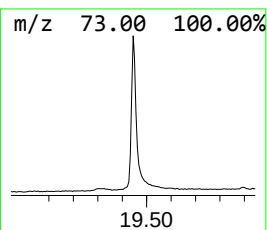
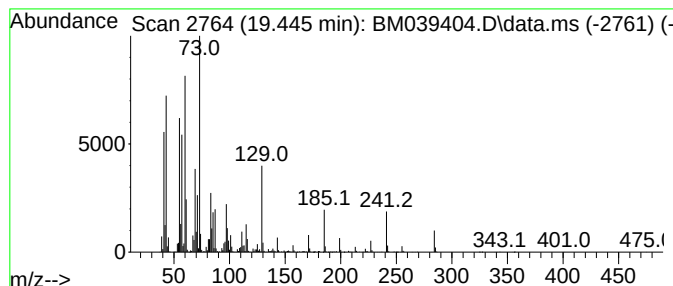
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	27.88 ng	3903720	Chrysene-d12	21.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4			Tridecanoic acid	214	C13H26O2	000638-53-9	62
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041223\
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Acq On : 12 Apr 2023 15:27
Operator : CG/JU
Sample : 02292-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
IDW-SO-G3-041123

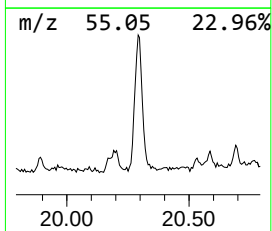
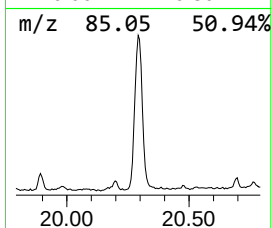
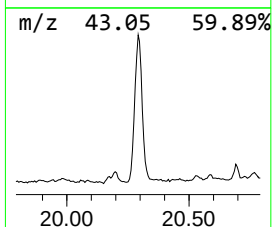
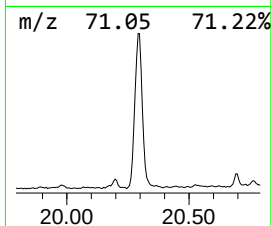
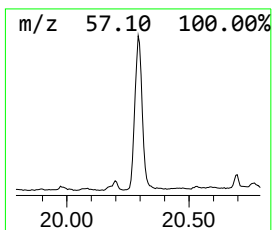
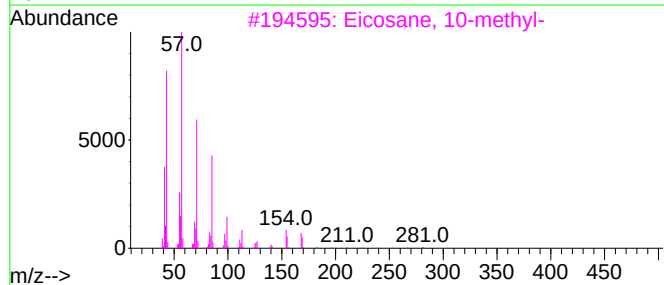
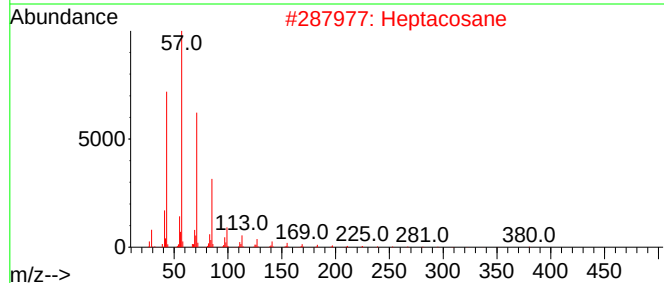
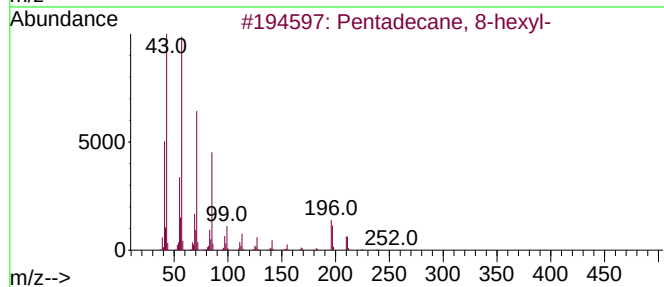
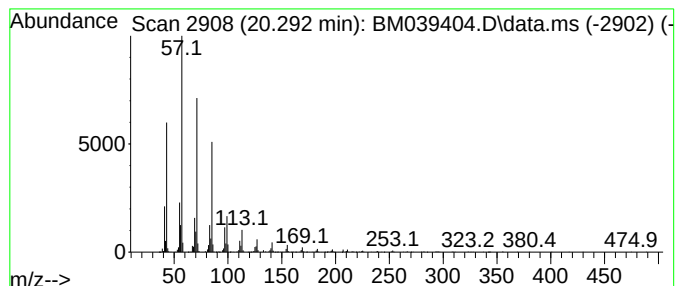
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.291	10.41 ng	1457350	Chrysene-d12	21.456

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2		Heptacosane	380	C27H56	000593-49-7	93
3		Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
4		Heneicosane	296	C21H44	000629-94-7	91
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041223\
Data File : BM039404.D
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Instrument :
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ClientSampleId :
IDW-SO-G3-041123

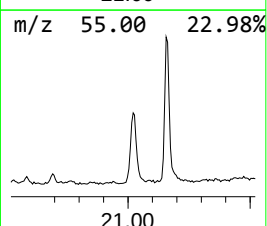
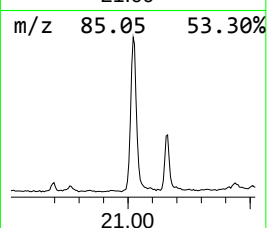
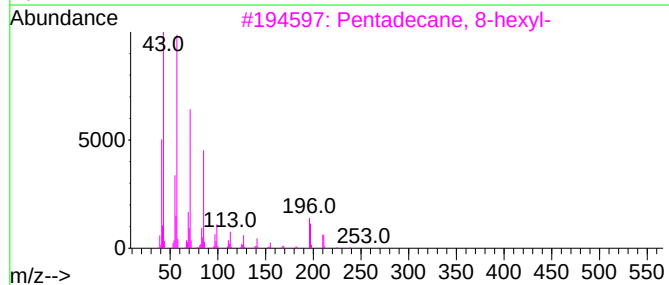
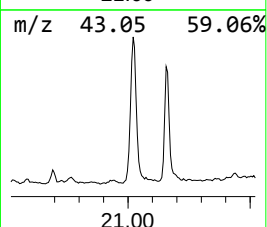
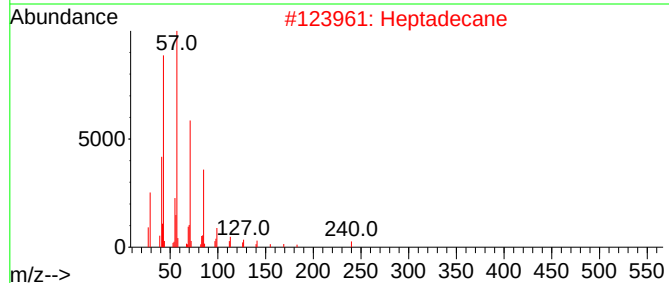
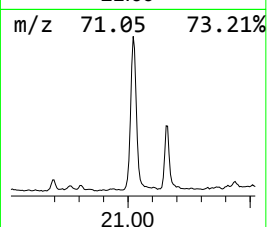
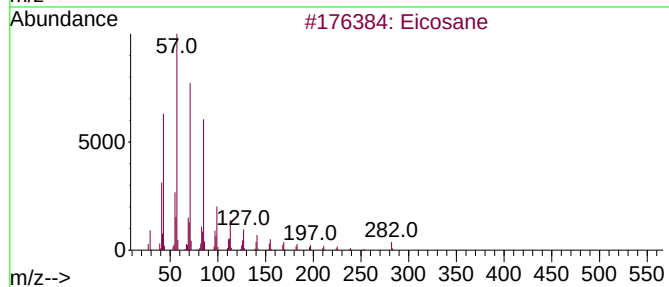
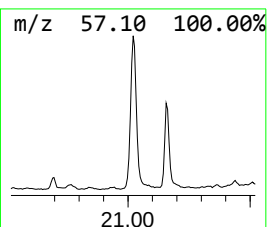
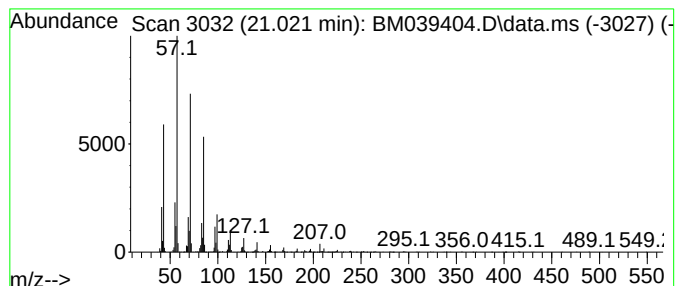
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.021	9.84 ng	1378160	Chrysene-d12	21.456

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	97
2		Heptadecane	240	C17H36	000629-78-7	94
3		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
4		Hexadecane, 5-butyl-	282	C20H42	006912-07-8	93
5		Eicosane, 10-methyl-	296	C21H44	054833-23-7	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041223\
Data File : BM039404.D
Acq On : 12 Apr 2023 15:27
Operator : CG/JU
Sample : 02292-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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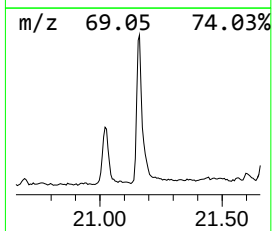
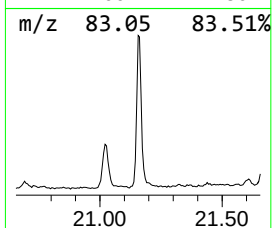
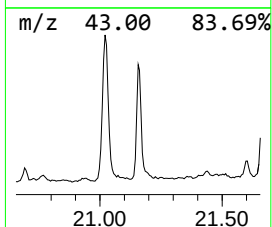
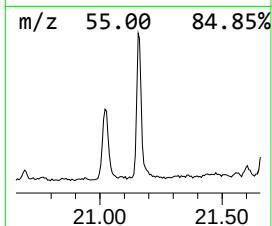
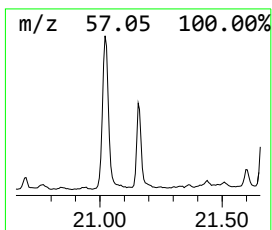
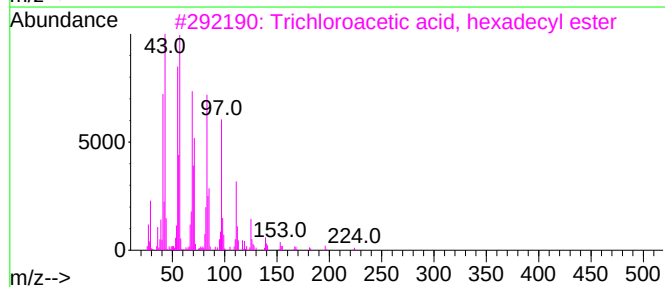
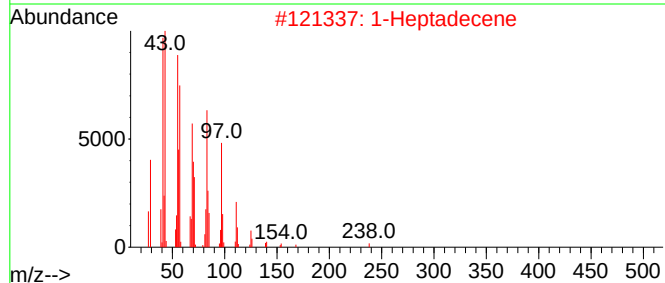
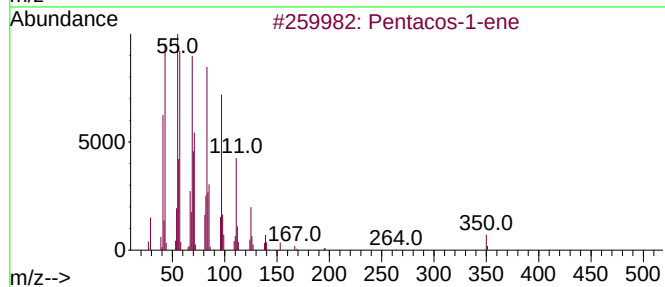
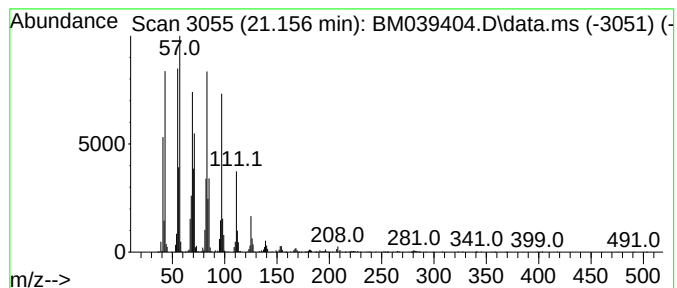
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacos-1-ene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.156	10.38 ng	1453180	Chrysene-d12	21.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacos-1-ene	350	C25H50	016980-85-1	94
2			1-Heptadecene	238	C17H34	006765-39-5	92
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
5			1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041223\
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Acq On : 12 Apr 2023 15:27
Operator : CG/JU
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Instrument :
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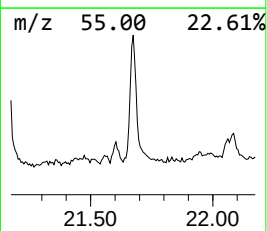
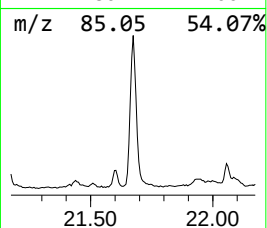
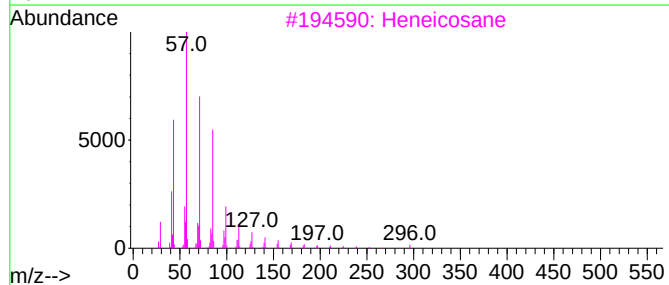
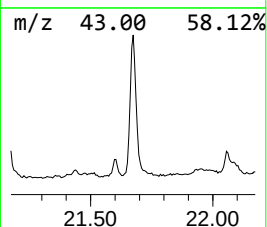
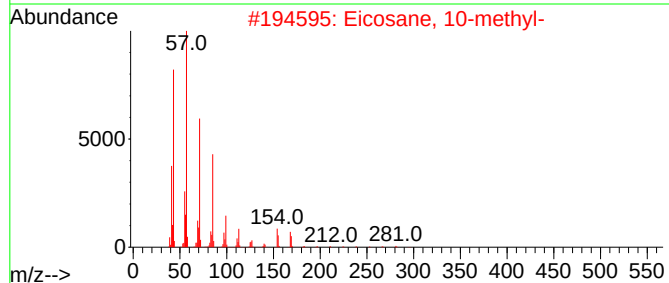
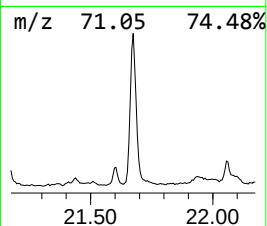
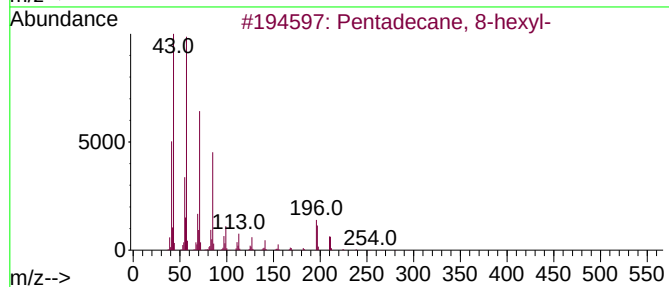
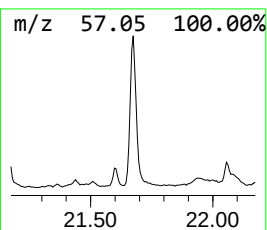
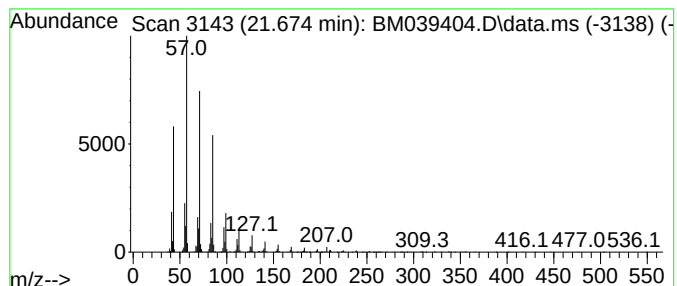
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane, 10-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.674	9.87 ng	1382650	Chrysene-d12	21.456

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2		Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041223\
Data File : BM039404.D
Acq On : 12 Apr 2023 15:27
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ALS Vial : 4 Sample Multiplier: 1

Instrument :
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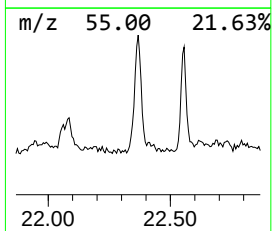
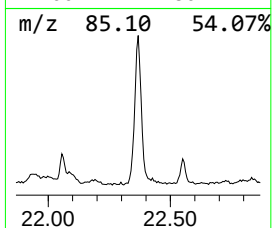
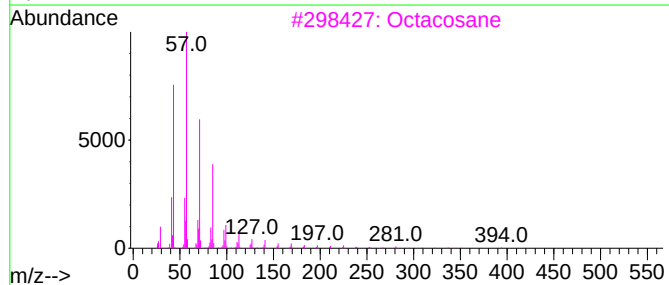
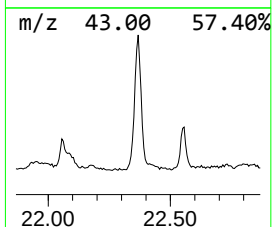
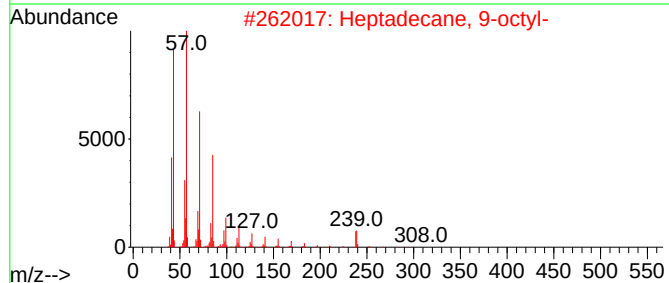
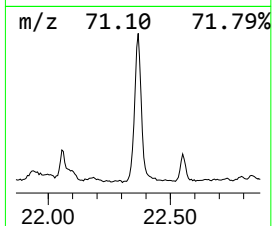
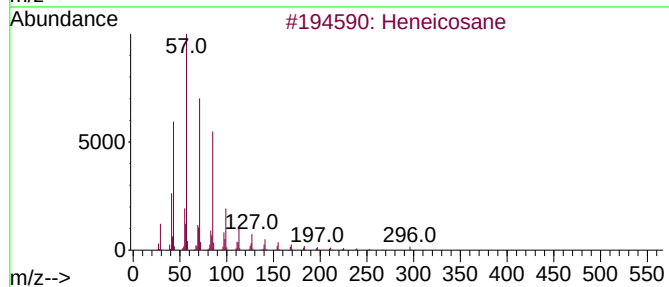
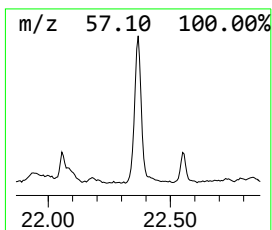
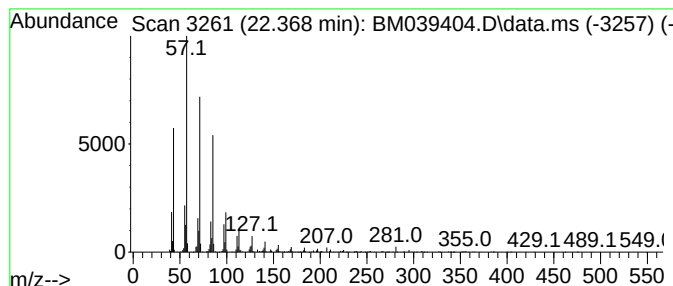
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.368	6.55 ng	917052	Chrysene-d12	21.456

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	96
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
3		Octacosane	394	C28H58	000630-02-4	91
4		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041223\
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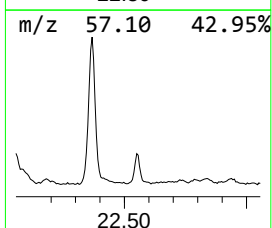
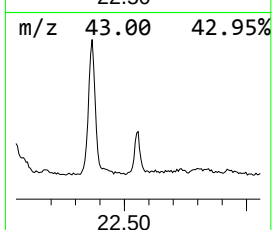
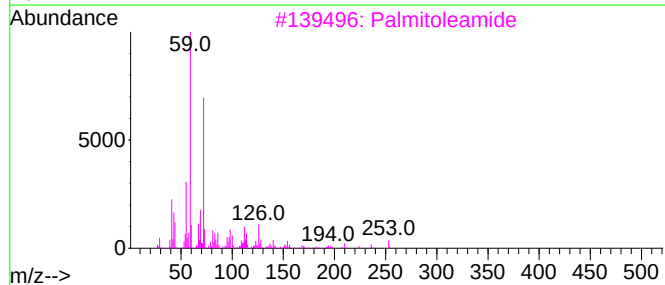
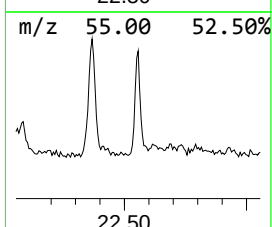
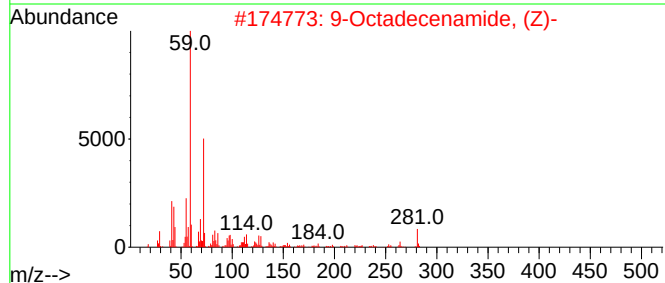
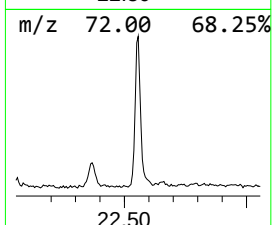
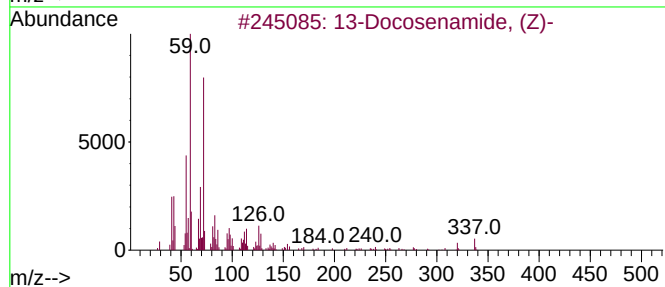
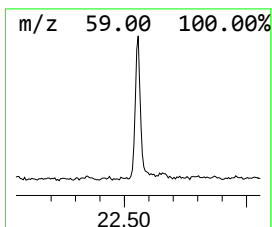
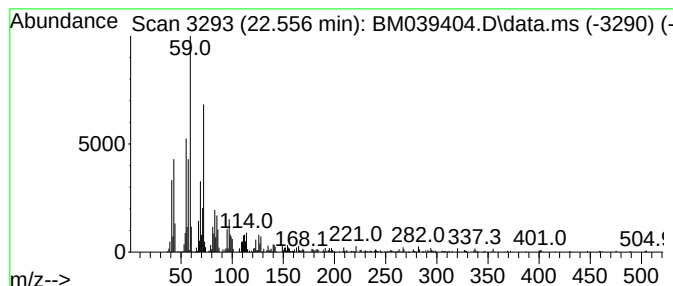
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 13-Docosenamide, (Z)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.556	3.03 ng	424191	Chrysene-d12		21.456	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-		337	C22H43NO	000112-84-5	89
2	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	64
3	Palmitoleamide		253	C16H31NO	106010-22-4	52
4	Benzeneethanamine, 2-fluoro-.bet...		229	C11H16FN03	061338-98-5	49
5	2,2-Dimethyl-tetrahydro-[1,3]dio...		190	C8H14O5	1000194-40-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041223\
Data File : BM039404.D
Acq On : 12 Apr 2023 15:27
Operator : CG/JU
Sample : 02292-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IDW-SO-G3-041123

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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-...	4.951	9.4	ng	560717	1	7.857	1189320	20.0
Benzophenone	15.880	2.6	ng	255367	3	14.515	1953060	20.0
n-Hexadecanoic ...	18.174	57.8	ng	6451990	4	17.262	2231220	20.0
Eicosane	18.309	8.7	ng	968751	4	17.262	2231220	20.0
Pentadecane, 8-...	19.415	6.5	ng	910639	5	21.456	2800350	20.0
Octadecanoic acid	19.445	27.9	ng	3903720	5	21.456	2800350	20.0
Heptacosane	20.291	10.4	ng	1457350	5	21.456	2800350	20.0
Heptadecane	21.021	9.8	ng	1378160	5	21.456	2800350	20.0
Pentacos-1-ene	21.156	10.4	ng	1453180	5	21.456	2800350	20.0
Eicosane, 10-me...	21.674	9.9	ng	1382650	5	21.456	2800350	20.0
Heneicosane	22.368	6.5	ng	917052	5	21.456	2800350	20.0
13-Docosenamide...	22.556	3.0	ng	424191	5	21.456	2800350	20.0