

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
 Data File : BG061088.D
 Acq On : 2 May 2024 11:17
 Operator : MA/JU
 Sample : P2330-09
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C-2(0.5-1.5)

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_G\Methods\8270-BG043024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061088.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	23	28	36	rBV	22080	37616	2.30%	0.424%
2	3.675	112	117	127	rVB	14846	23169	1.42%	0.261%
3	5.525	425	432	442	rBV	359483	567935	34.70%	6.399%
4	7.106	693	701	712	rBV	383475	655297	40.04%	7.383%
5	7.934	834	842	849	rBV	117805	192298	11.75%	2.167%
6	9.086	1029	1038	1047	rVB	245521	433411	26.48%	4.883%
7	10.725	1310	1317	1324	rBV	144921	257001	15.70%	2.896%
8	13.181	1729	1735	1742	rBV	691522	1084350	66.25%	12.217%
9	14.562	1963	1970	1977	rBV	248190	374391	22.88%	4.218%
10	16.048	2217	2223	2233	rBV	634993	965242	58.98%	10.875%
11	17.306	2431	2437	2442	rBV	305479	441827	27.00%	4.978%
12	17.347	2442	2444	2452	rVB2	15858	20639	1.26%	0.233%
13	18.205	2584	2590	2602	rBV	121703	182273	11.14%	2.054%
14	19.280	2769	2773	2780	rVB5	16468	32854	2.01%	0.370%
15	19.362	2780	2787	2793	rBV	60006	91186	5.57%	1.027%
16	19.480	2801	2807	2817	rBV2	57594	101773	6.22%	1.147%
17	19.644	2831	2835	2840	rVB6	13976	24328	1.49%	0.274%
18	19.721	2840	2848	2855	rBV	49015	86688	5.30%	0.977%
19	19.926	2877	2883	2889	rBV	1328479	1636679	100.00%	18.440%
20	20.149	2916	2921	2928	rBV2	33473	74206	4.53%	0.836%
21	20.314	2945	2949	2954	rBV2	10023	19754	1.21%	0.223%
22	20.890	3042	3047	3053	rBV2	48955	81431	4.98%	0.917%
23	21.242	3102	3107	3114	rBV6	37499	89814	5.49%	1.012%
24	21.565	3155	3162	3167	rBV2	294497	524819	32.07%	5.913%
25	21.659	3173	3178	3184	rVB2	38505	73973	4.52%	0.833%
26	22.370	3295	3299	3302	rBV4	20608	36483	2.23%	0.411%
27	22.523	3320	3325	3330	rBV2	35306	75973	4.64%	0.856%
28	22.570	3330	3333	3343	rVB3	38075	79615	4.86%	0.897%
29	23.510	3488	3493	3501	rVB4	21890	50966	3.11%	0.574%
30	23.828	3542	3547	3556	rVB2	37660	89824	5.49%	1.012%
31	24.679	3684	3692	3703	rBV	152268	469765	28.70%	5.293%

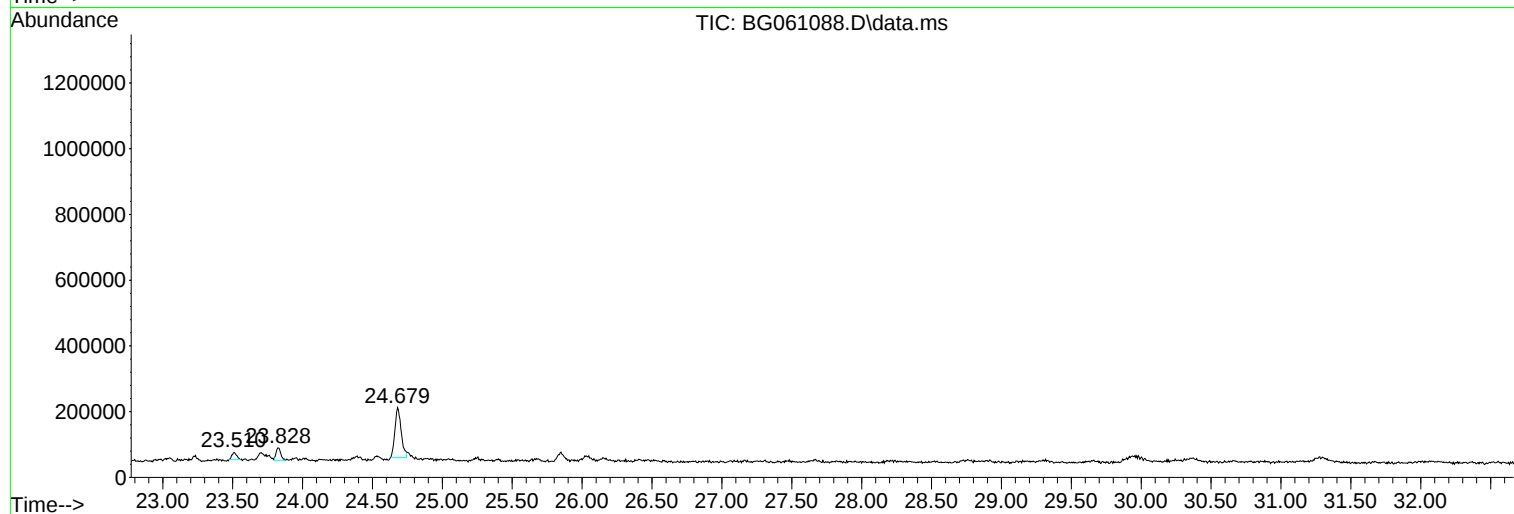
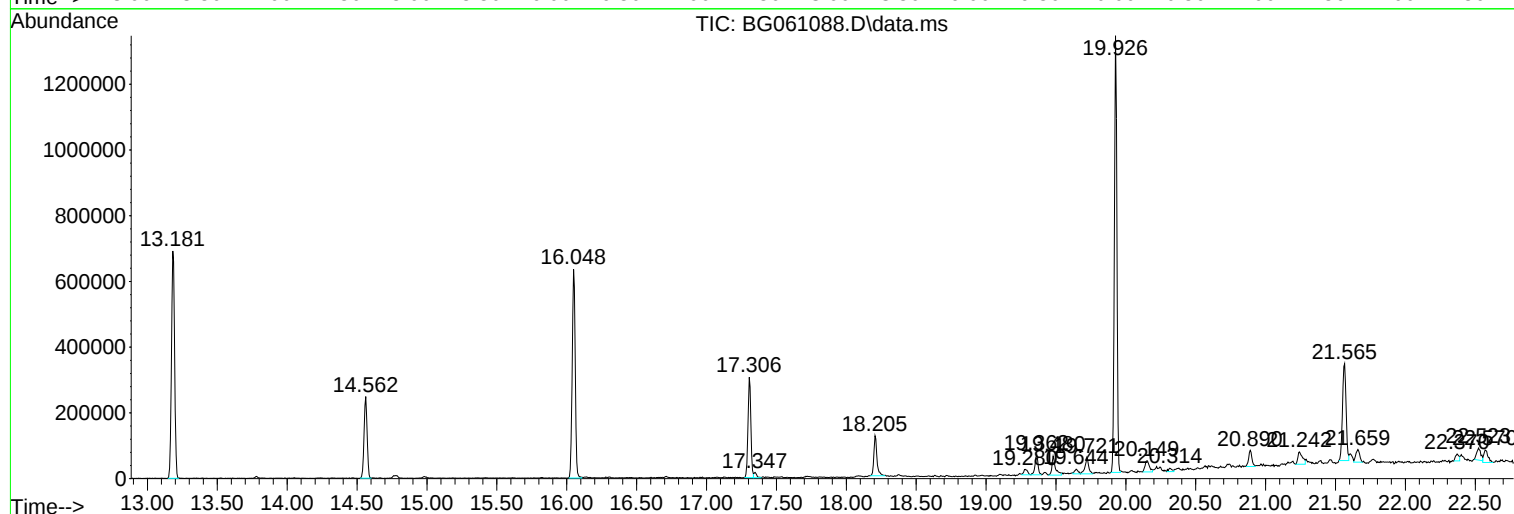
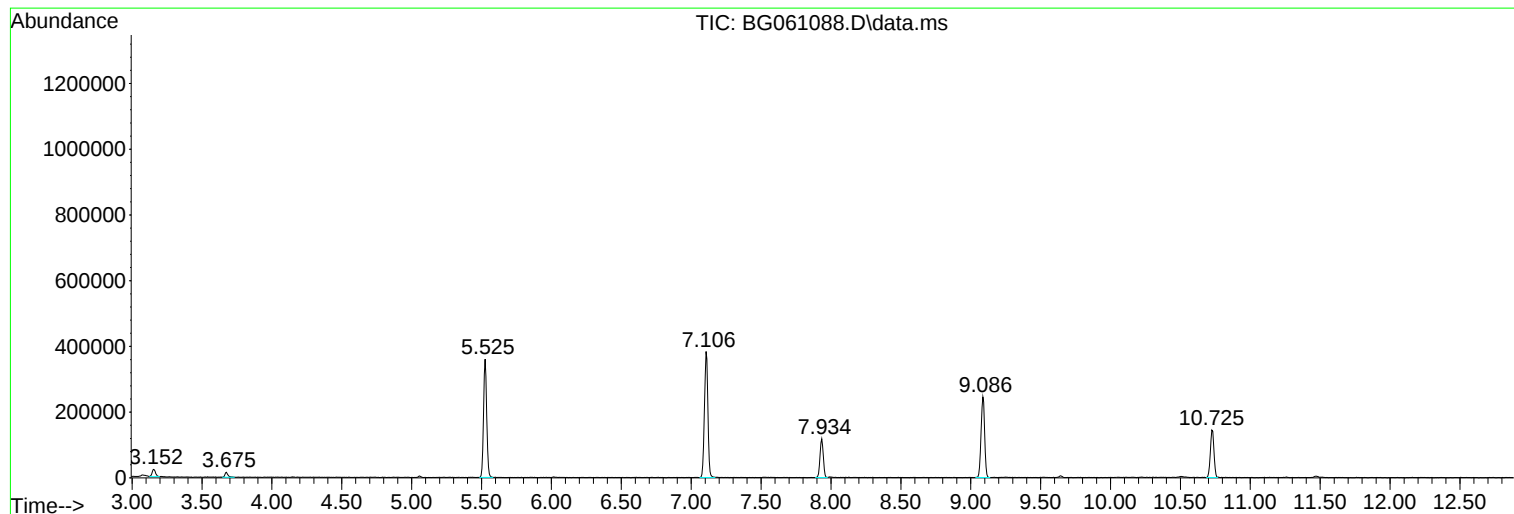
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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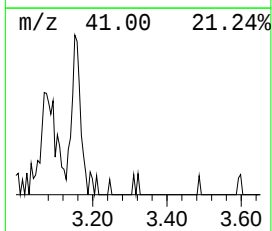
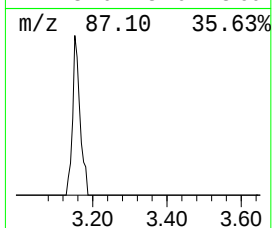
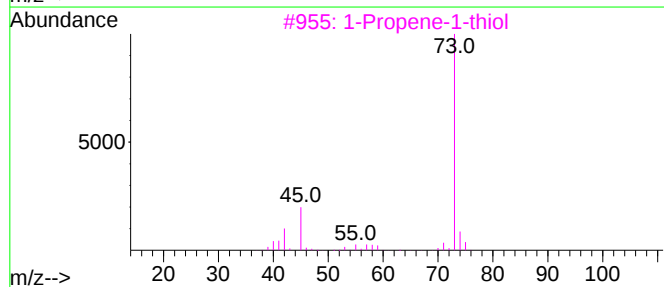
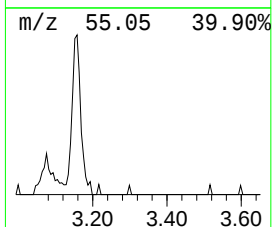
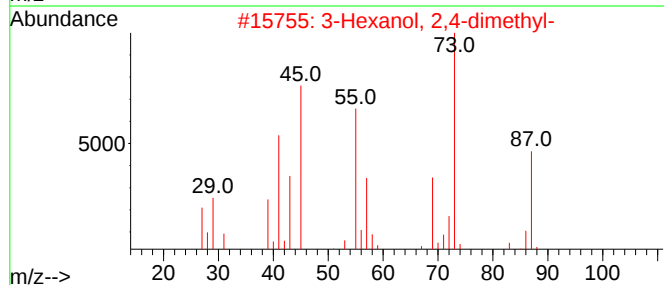
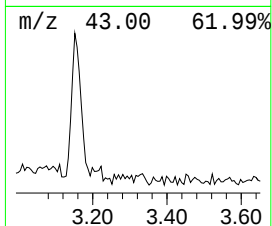
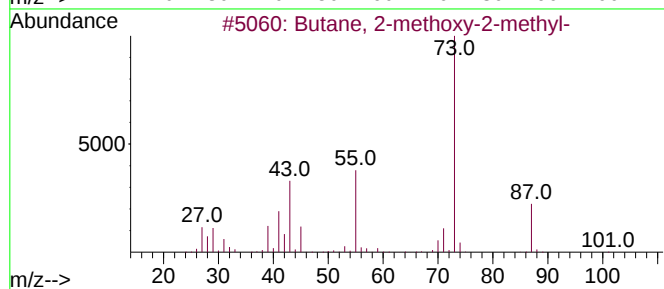
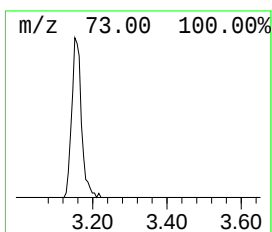
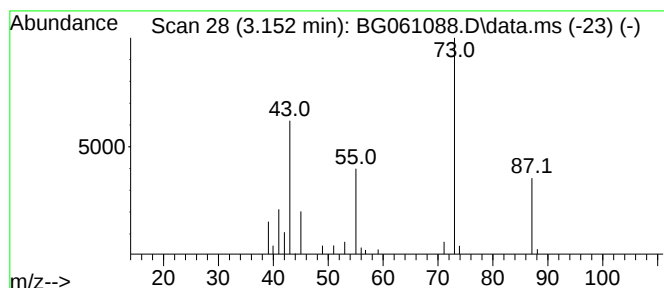
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	3.91 ng	37616	1,4-Dichlorobenzene-d4	7.934

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2		3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	40
3		1-Propene-1-thiol	74	C3H6S	000925-89-3	37
4		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
5		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25



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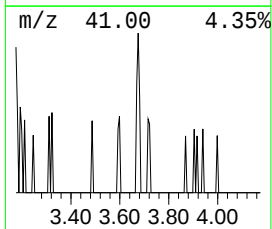
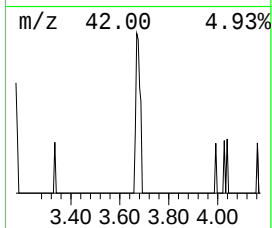
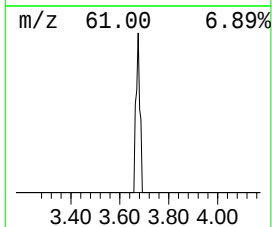
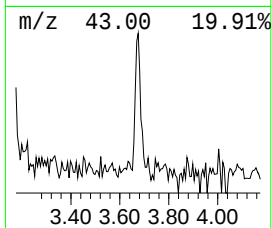
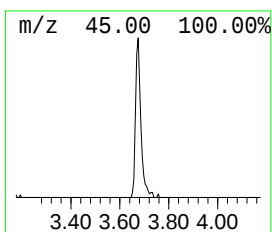
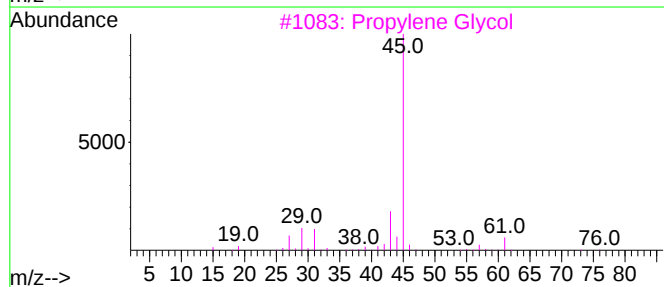
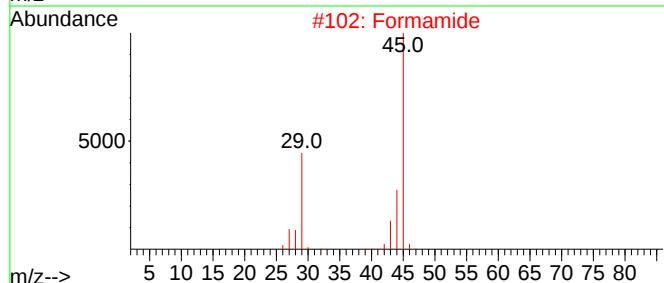
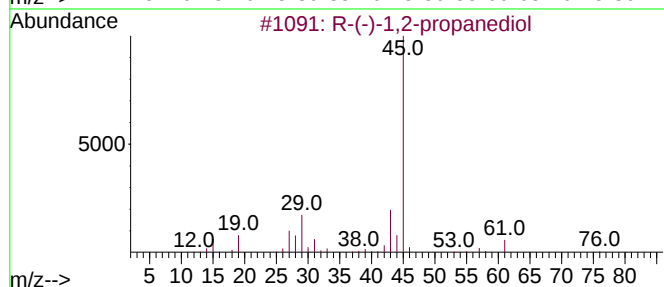
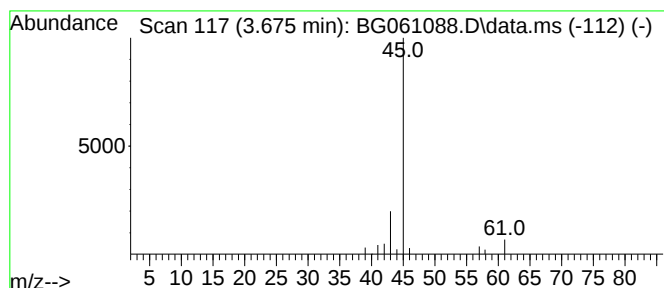
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown3.675 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.675	2.41 ng	23169	1,4-Dichlorobenzene-d4	7.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	9
2	Formamide			45	CH3NO	000075-12-7	5
3	Propylene Glycol			76	C3H8O2	000057-55-6	4
4	Thiirane			60	C2H4S	000420-12-2	4
5	Isopropyl Alcohol			60	C3H8O	000067-63-0	4



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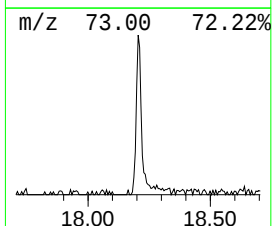
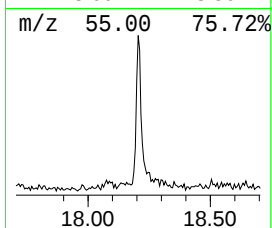
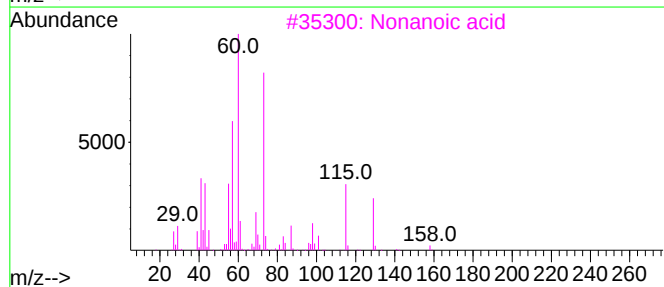
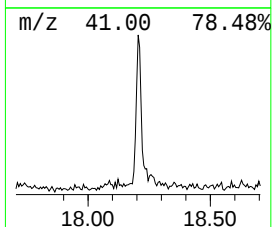
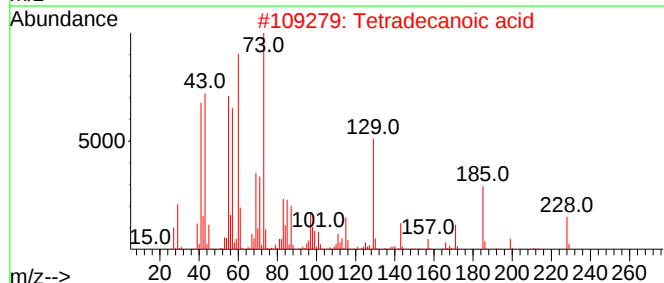
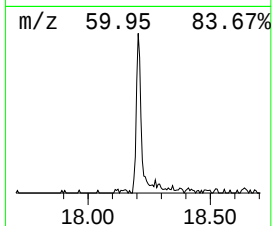
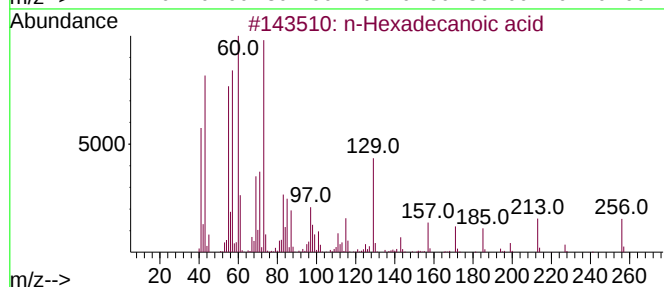
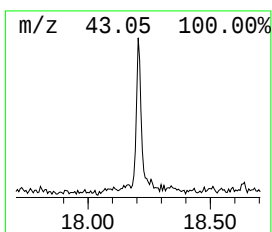
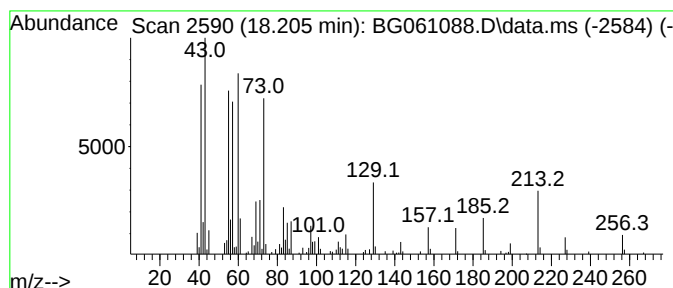
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.205	8.25 ng	182273	Phenanthrene-d10	17.306

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3			Nonanoic acid	158	C9H18O2	000112-05-0	53
4			n-Decanoic acid	172	C10H20O2	000334-48-5	53
5			Tridecanoic acid	214	C13H26O2	000638-53-9	52



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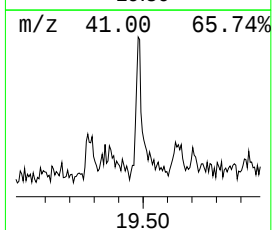
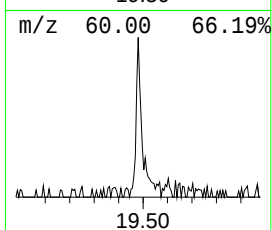
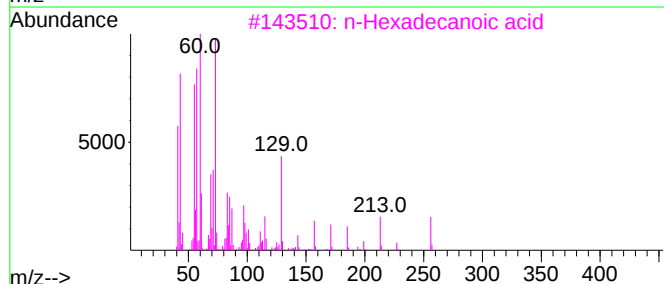
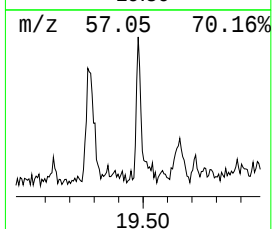
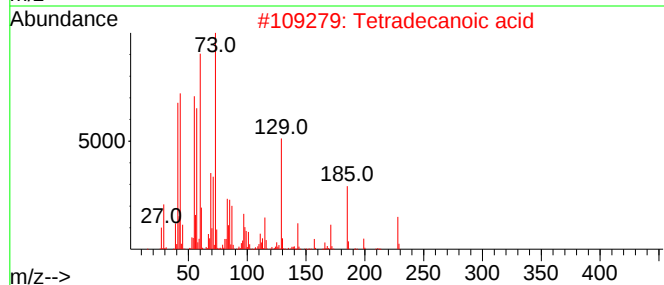
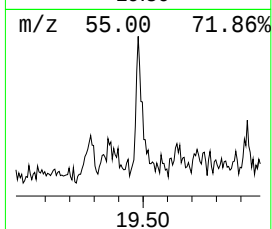
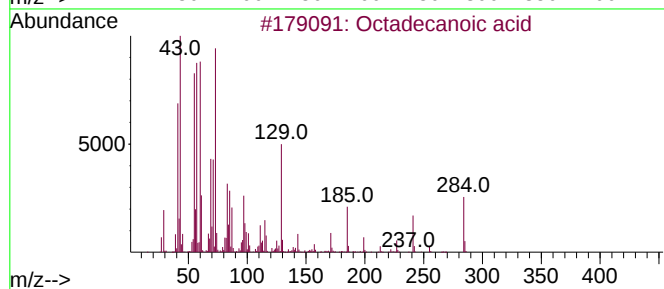
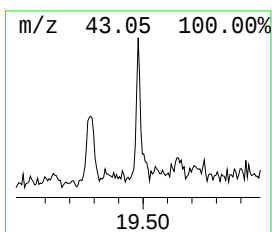
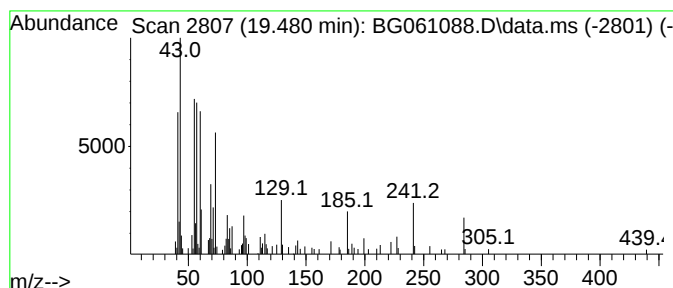
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.480	3.88 ng	101773	Chrysene-d12	21.566

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
4			Undecanoic acid	186	C11H22O2	000112-37-8	46
5			Tridecanoic acid	214	C13H26O2	000638-53-9	43



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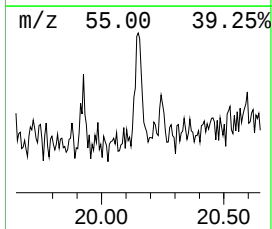
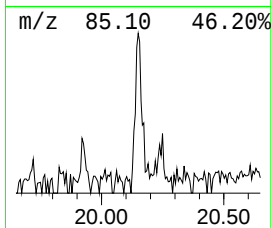
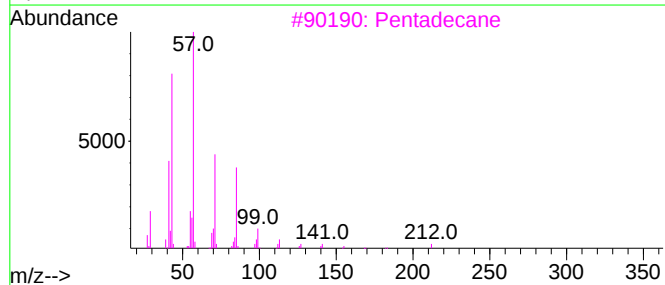
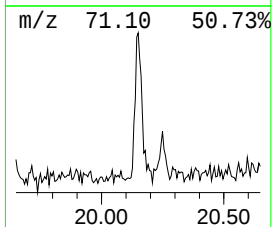
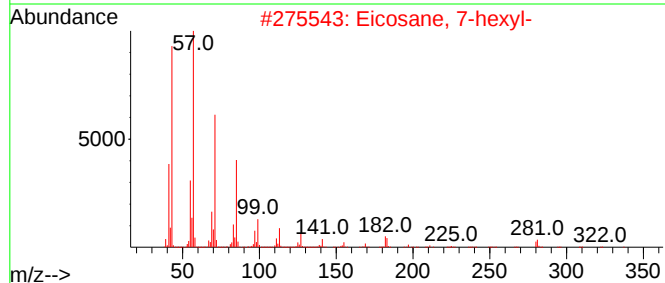
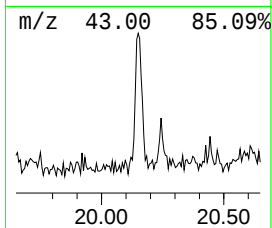
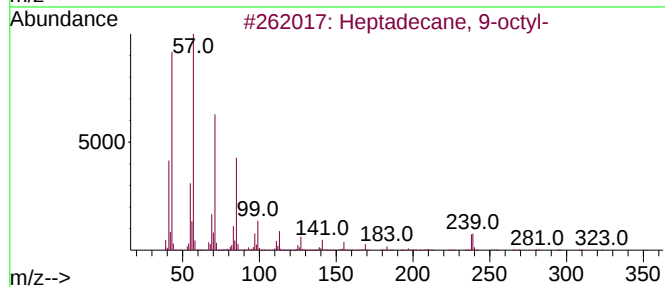
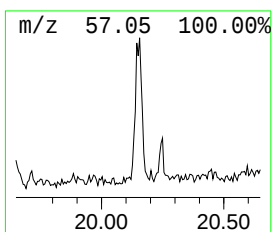
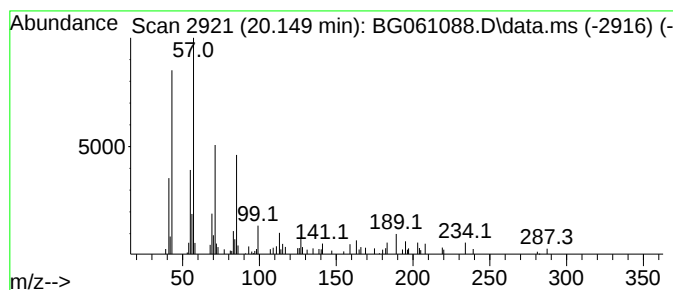
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.150	2.83 ng	74206	Chrysene-d12	21.566

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	74
2			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	72
3			Pentadecane	212	C15H32	000629-62-9	72
4			Octacosane	394	C28H58	000630-02-4	72
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	72



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C-2(0.5-1.5)

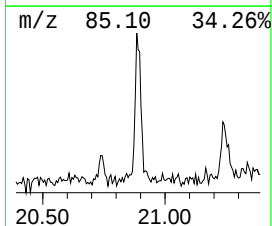
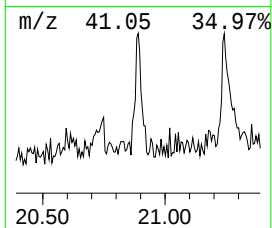
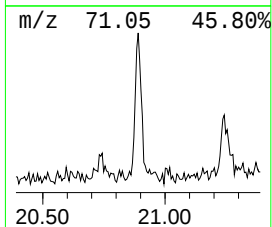
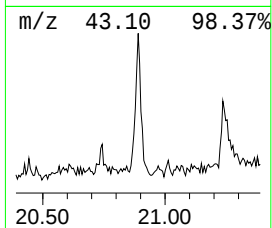
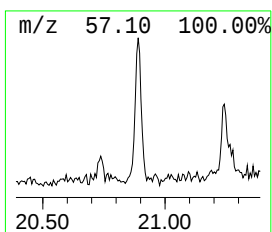
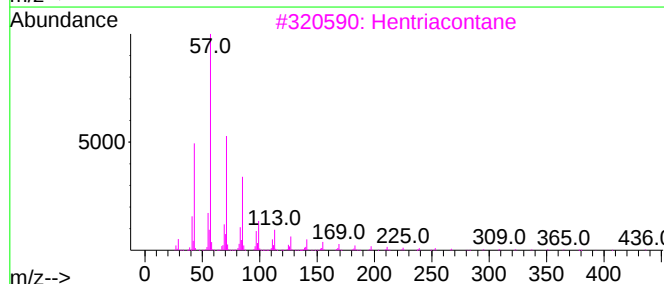
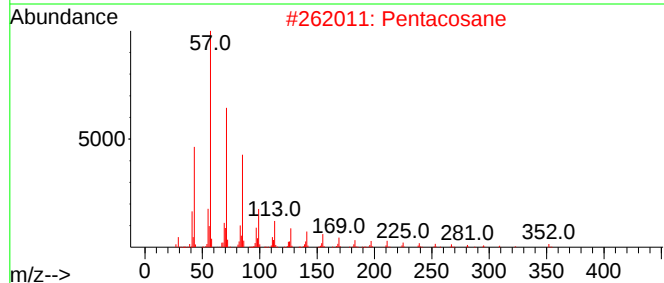
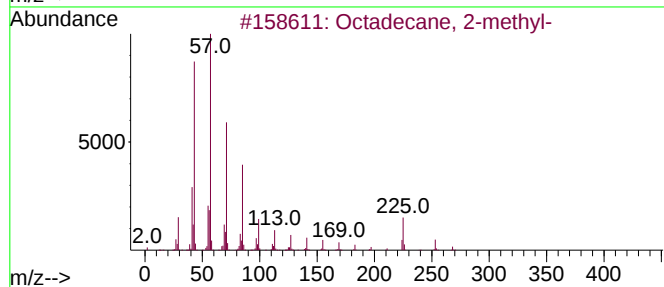
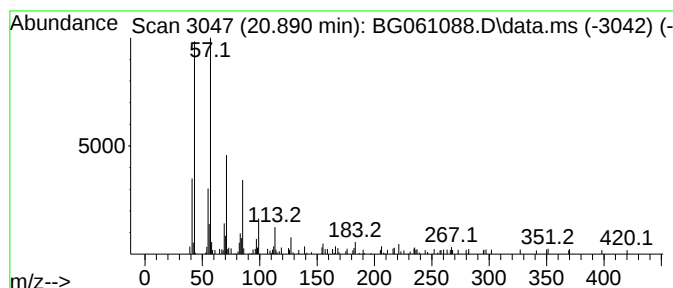
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.890	3.10 ng	81431	Chrysene-d12	21.566

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane, 2-methyl-	268	C19H40	001560-88-9	87
2		Pentacosane	352	C25H52	000629-99-2	83
3		Hentriacontane	437	C31H64	000630-04-6	80
4		Docosane, 7-hexyl-	394	C28H58	055373-86-9	80
5		Heptacosane	380	C27H56	000593-49-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061088.D
Acq On : 2 May 2024 11:17
Operator : MA/JU
Sample : P2330-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C-2(0.5-1.5)

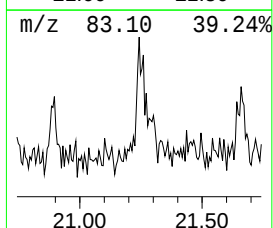
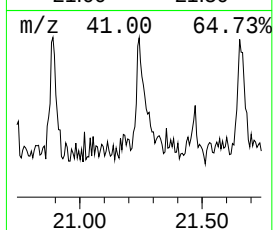
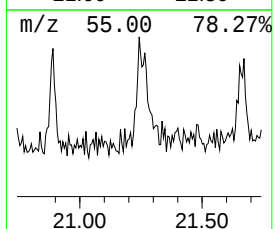
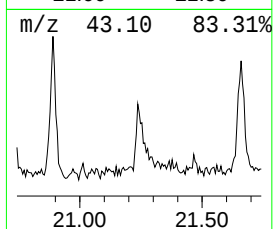
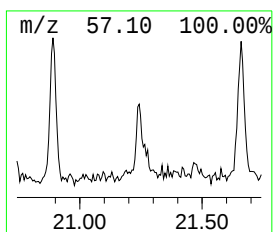
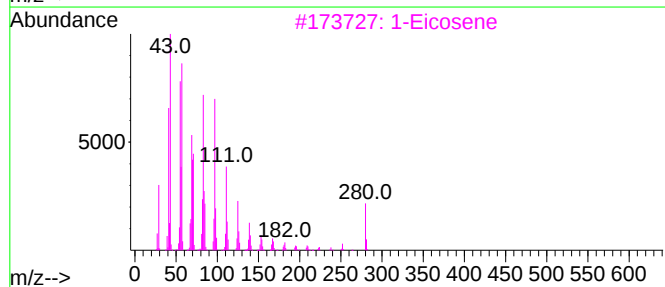
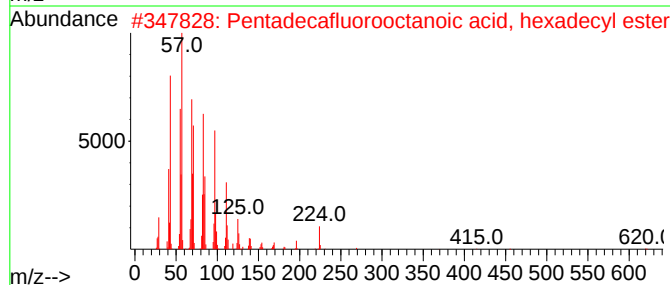
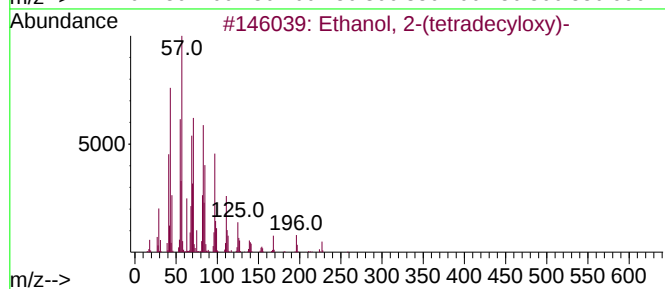
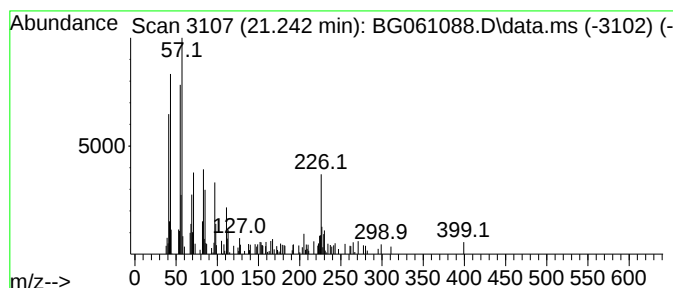
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.242	3.42 ng	89814	Chrysene-d12		21.566	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-		258	C16H34O2	002136-70-1	52
2	Pentadecafluorooctanoic acid, he...		638	C24H33F15O2	1000406-04-6	50
3	1-Eicosene		280	C20H40	003452-07-1	49
4	Docosyl isobutyl ether		382	C26H54O	1000406-33-1	47
5	Isobutyl tetracosyl ether		410	C28H58O	1000406-33-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061088.D
Acq On : 2 May 2024 11:17
Operator : MA/JU
Sample : P2330-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C-2(0.5-1.5)

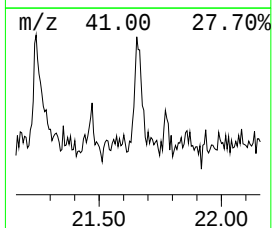
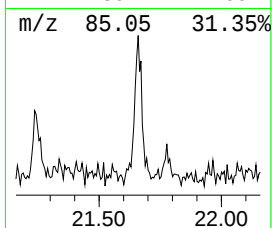
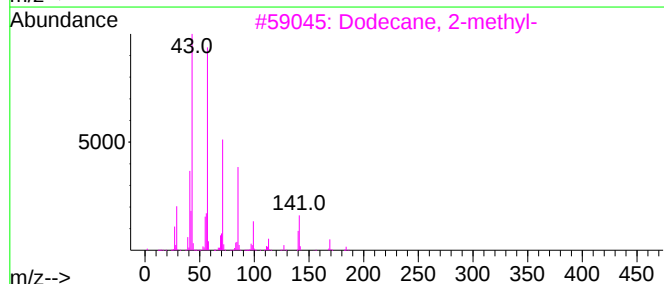
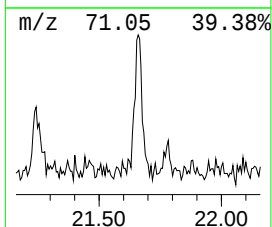
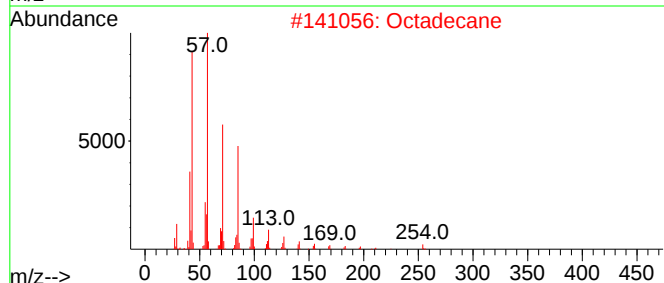
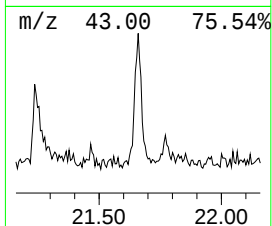
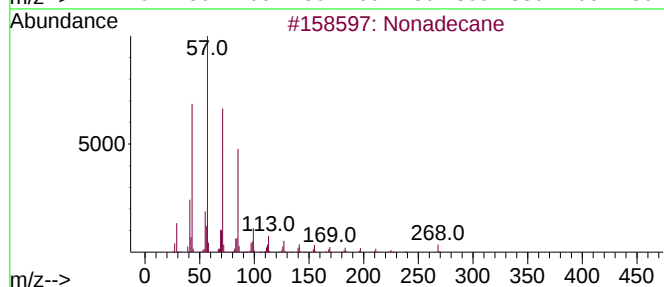
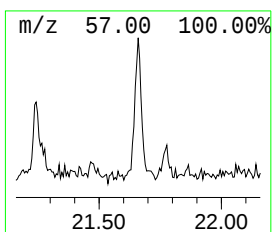
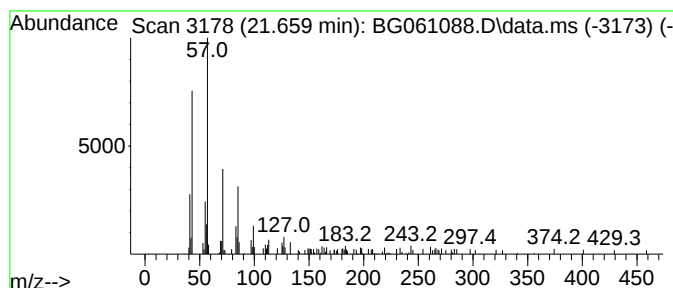
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.660	2.82 ng	73973	Chrysene-d12	21.566

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	89
2		Octadecane	254	C18H38	000593-45-3	76
3		Dodecane, 2-methyl-	184	C13H28	001560-97-0	74
4		Tetradecane	198	C14H30	000629-59-4	70
5		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061088.D
Acq On : 2 May 2024 11:17
Operator : MA/JU
Sample : P2330-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C-2(0.5-1.5)

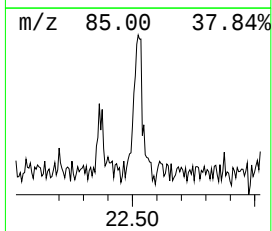
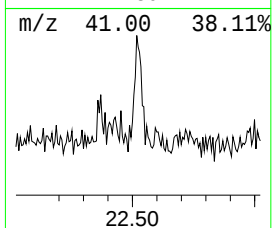
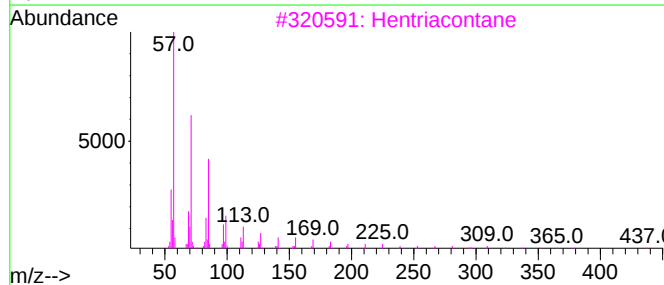
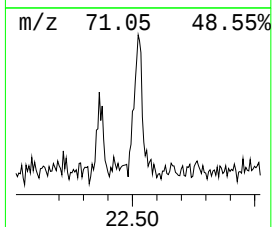
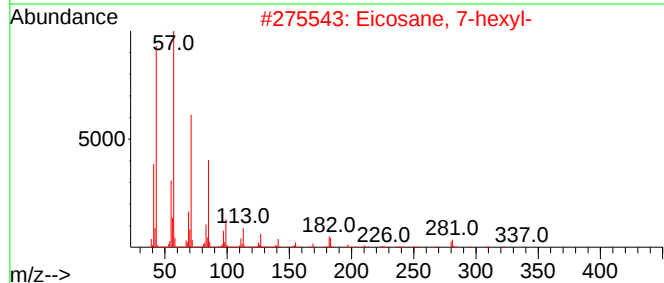
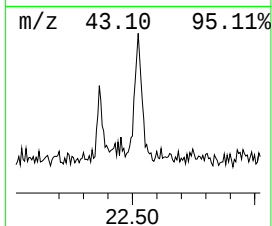
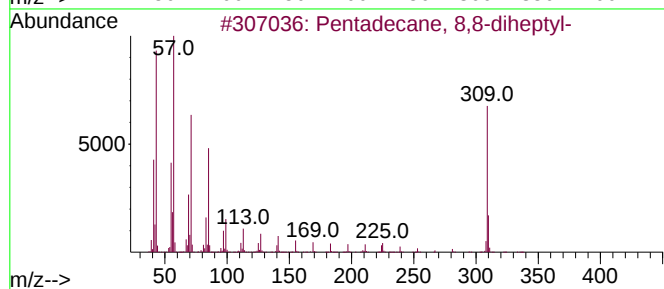
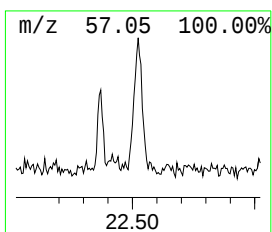
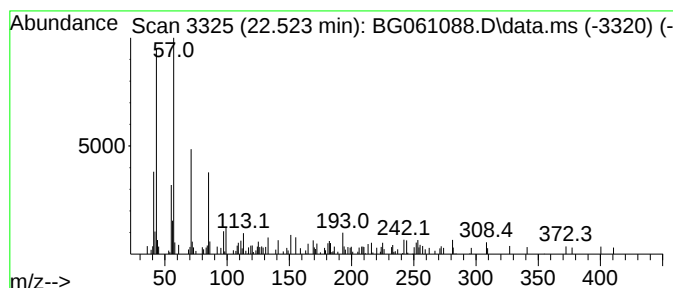
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane, 8,8-diheptyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.523	2.90 ng	75973	Chrysene-d12	21.566

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 8,8-diheptyl-	408	C29H60	055268-72-9	70
2			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	58
3			Hentriacontane	437	C31H64	000630-04-6	58
4			Dodecane, 2-methyl-	184	C13H28	001560-97-0	53
5			Octadecane	254	C18H38	000593-45-3	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061088.D
Acq On : 2 May 2024 11:17
Operator : MA/JU
Sample : P2330-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

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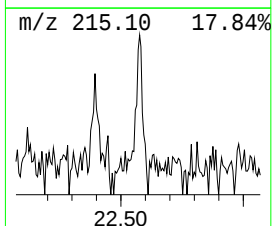
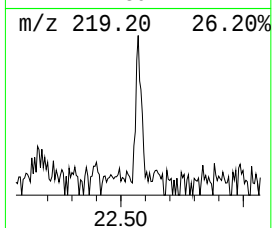
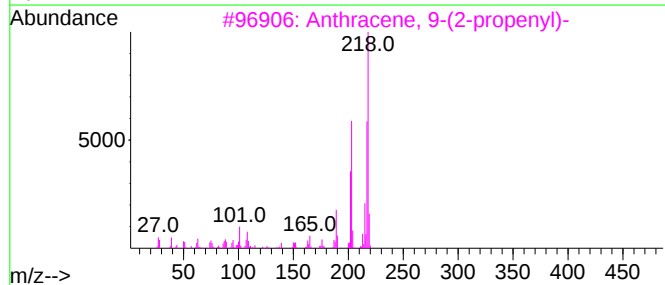
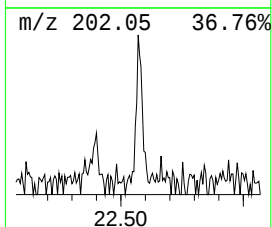
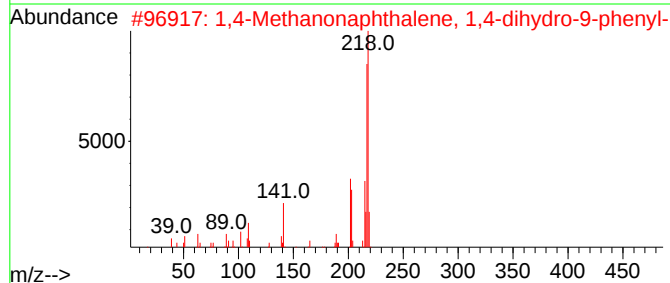
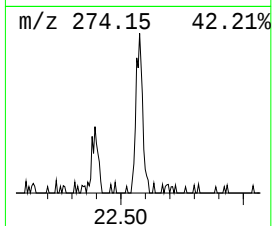
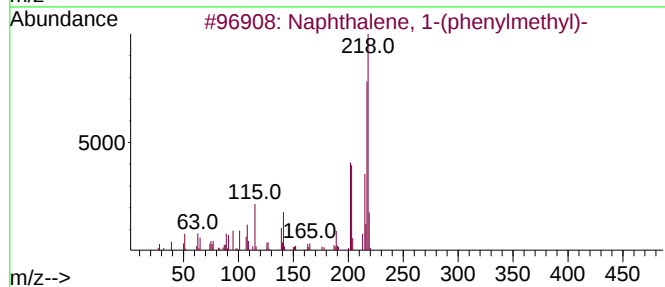
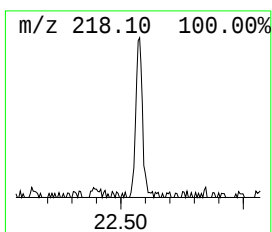
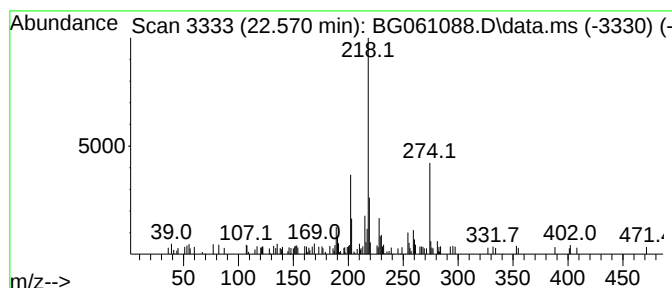
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown22.750 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.570	3.03 ng	79615	Chrysene-d12	21.566

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1-(phenylmethyl)-	218	C17H14	000611-45-0	47
2		1,4-Methanonaphthalene, 1,4-dihy...	218	C17H14	055028-73-4	47
3		Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	46
4		2-Amino-1,2,3,4-tetrahydronaphth...	335	C17H29N02Si2	1000501-34-0	43
5		1,4-Naphthoquinone, 2-ethyl-5,8-...	218	C12H10O4	015012-53-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061088.D
Acq On : 2 May 2024 11:17
Operator : MA/JU
Sample : P2330-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

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ClientSampleId :
C-2(0.5-1.5)

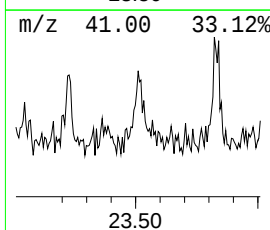
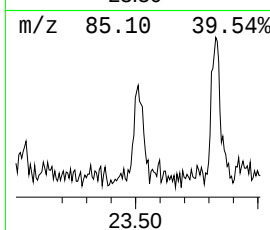
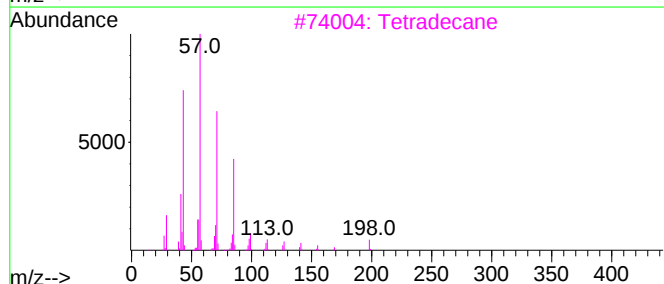
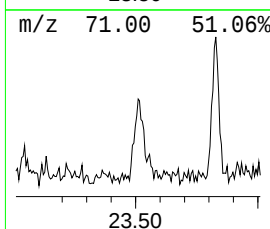
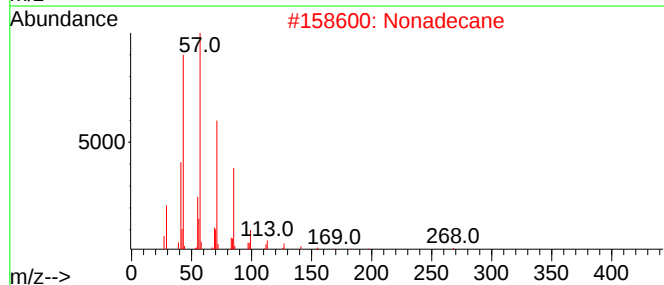
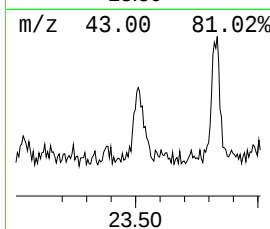
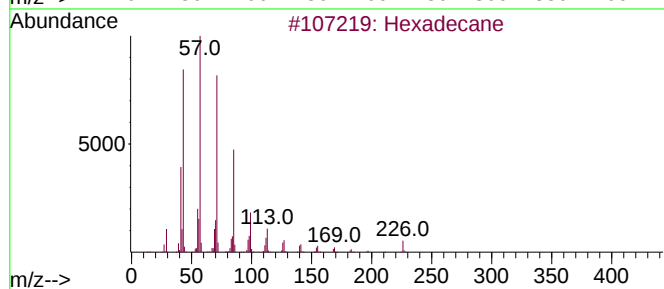
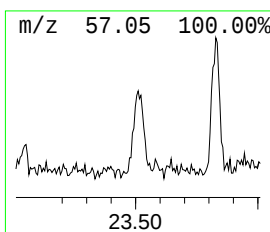
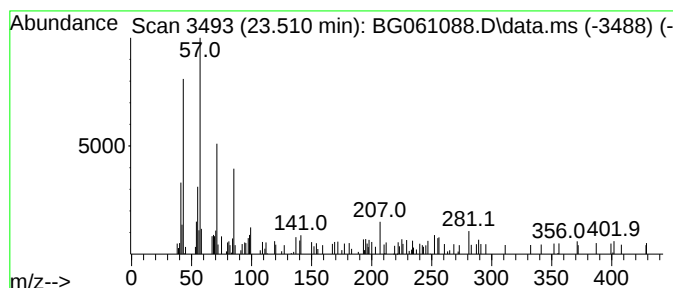
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.510	2.17 ng	50966	Perylene-d12	24.680

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane	226	C16H34	000544-76-3	95
2		Nonadecane	268	C19H40	000629-92-5	92
3		Tetradecane	198	C14H30	000629-59-4	91
4		Heptadecane	240	C17H36	000629-78-7	90
5		Pentadecane	212	C15H32	000629-62-9	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061088.D
Acq On : 2 May 2024 11:17
Operator : MA/JU
Sample : P2330-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C-2(0.5-1.5)

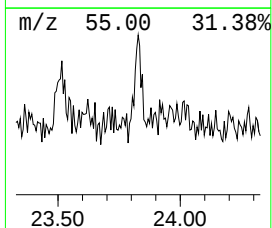
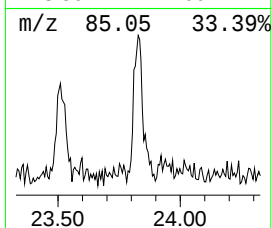
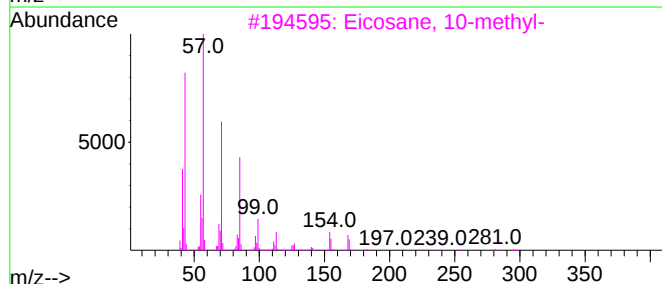
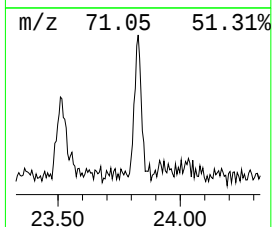
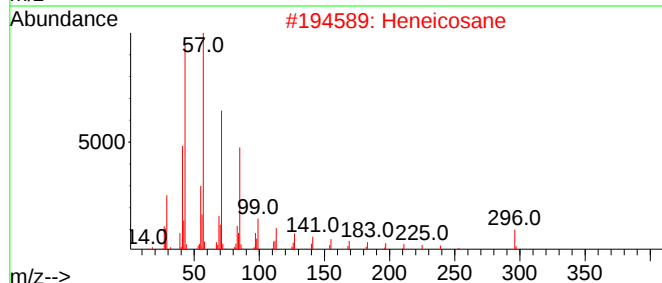
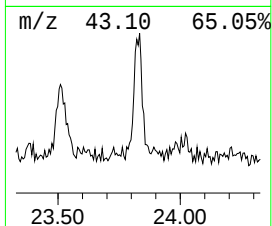
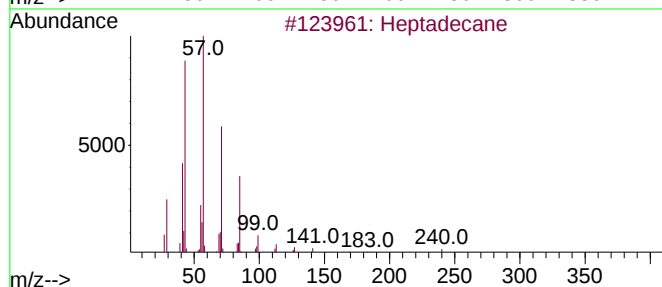
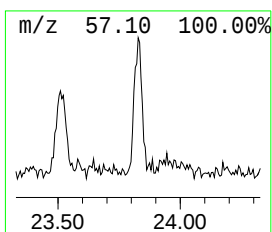
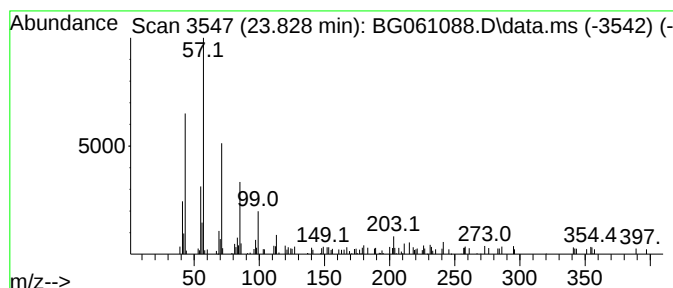
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.828	3.82 ng	89824	Perylene-d12	24.680

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	96
2		Heneicosane	296	C21H44	000629-94-7	58
3		Eicosane, 10-methyl-	296	C21H44	054833-23-7	58
4		Heptacosane	380	C27H56	000593-49-7	52
5		Nonadecane	268	C19H40	000629-92-5	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061088.D
Acq On : 2 May 2024 11:17
Operator : MA/JU
Sample : P2330-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C-2(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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
Butane, 2-metho...	3.152	3.9	ng	37616	1	7.934	192298	20.0
unknown3.675	3.675	2.4	ng	23169	1	7.934	192298	20.0
n-Hexadecanoic ...	18.205	8.3	ng	182273	4	17.306	441827	20.0
Octadecanoic acid	19.480	3.9	ng	101773	5	21.566	524819	20.0
Heptadecane, 9-...	20.150	2.8	ng	74206	5	21.566	524819	20.0
Octadecane, 2-m...	20.890	3.1	ng	81431	5	21.566	524819	20.0
Ethanol, 2-(tet...	21.242	3.4	ng	89814	5	21.566	524819	20.0
Nonadecane	21.660	2.8	ng	73973	5	21.566	524819	20.0
Pentadecane, 8,...	22.523	2.9	ng	75973	5	21.566	524819	20.0
unknown22.750	22.570	3.0	ng	79615	5	21.566	524819	20.0
Hexadecane	23.510	2.2	ng	50966	6	24.680	469765	20.0
Heptadecane	23.828	3.8	ng	89824	6	24.680	469765	20.0