

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
 Data File : BG061113.D
 Acq On : 3 May 2024 19:35
 Operator : MA/JU
 Sample : P2355-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 VB16173

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: BG061113.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	43	rVB	180030	309744	13.12%	2.433%
2	5.526	424	432	443	rVB	423615	673450	28.52%	5.290%
3	7.112	692	702	711	rBV	481127	816706	34.58%	6.416%
4	7.935	835	842	848	rBV	120208	195007	8.26%	1.532%
5	8.699	964	972	980	rBV	122129	202598	8.58%	1.592%
6	9.092	1031	1039	1048	rVB	295076	518637	21.96%	4.074%
7	10.731	1310	1318	1324	rBV	149305	268227	11.36%	2.107%
8	13.187	1728	1736	1742	rBV	721564	1104299	46.76%	8.675%
9	14.562	1958	1970	1978	rBV	243053	386523	16.37%	3.036%
10	14.985	2033	2042	2054	rBV3	23569	41777	1.77%	0.328%
11	15.279	2084	2092	2097	rBV4	14569	23742	1.01%	0.187%
12	16.055	2217	2224	2231	rBV	765386	1155872	48.95%	9.080%
13	16.719	2332	2337	2346	rBV	133181	196533	8.32%	1.544%
14	17.312	2428	2438	2442	rVV	296896	451116	19.10%	3.544%
15	17.353	2442	2445	2450	rVB	45315	64310	2.72%	0.505%
16	17.488	2464	2468	2475	rBV4	20834	29636	1.25%	0.233%
17	18.099	2566	2572	2577	rBV7	11206	23887	1.01%	0.188%
18	18.234	2586	2595	2607	rBV	1385551	2361566	100.00%	18.552%
19	19.368	2779	2788	2792	rBV	257313	465568	19.71%	3.657%
20	19.410	2792	2795	2803	rVV2	126644	231620	9.81%	1.820%
21	19.492	2805	2809	2818	rVB	299210	400770	16.97%	3.148%
22	19.727	2841	2849	2860	rVB	91133	178136	7.54%	1.399%
23	19.932	2878	2884	2889	rVV	1160895	1476472	62.52%	11.599%
24	21.243	3103	3107	3111	rBV2	50771	69070	2.92%	0.543%
25	21.472	3142	3146	3150	rVB	97826	134967	5.72%	1.060%
26	21.572	3156	3163	3168	rBV	282883	536154	22.70%	4.212%
27	23.834	3543	3548	3556	rVB2	72766	146880	6.22%	1.154%
28	24.692	3688	3694	3701	rBV2	93595	266296	11.28%	2.092%

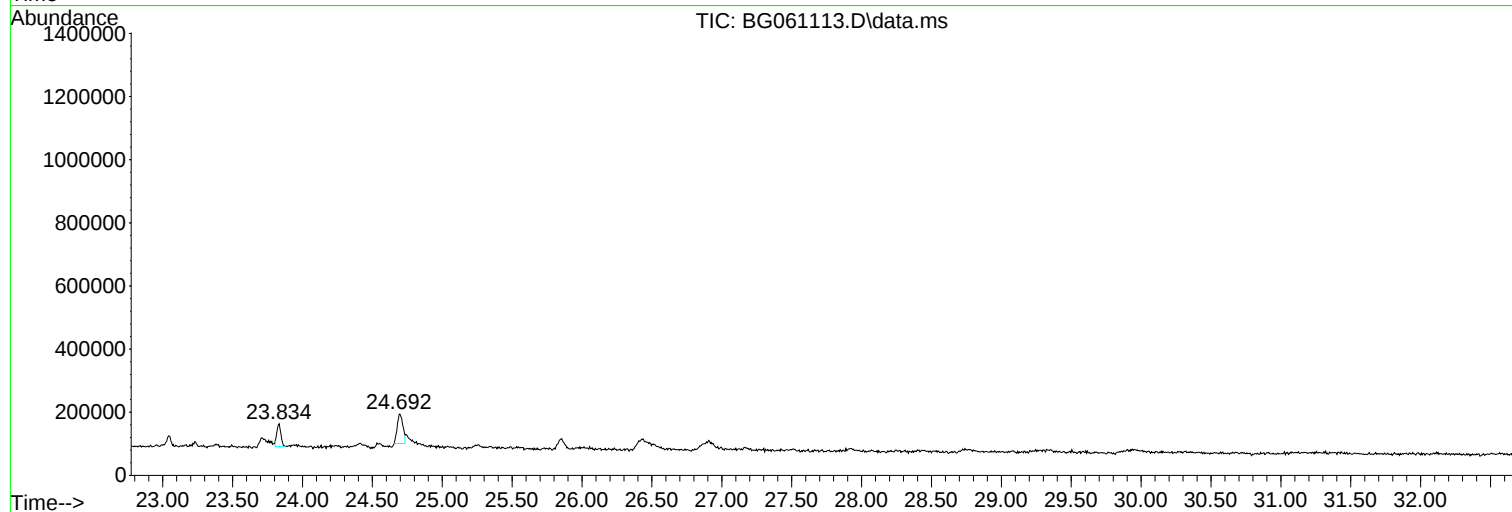
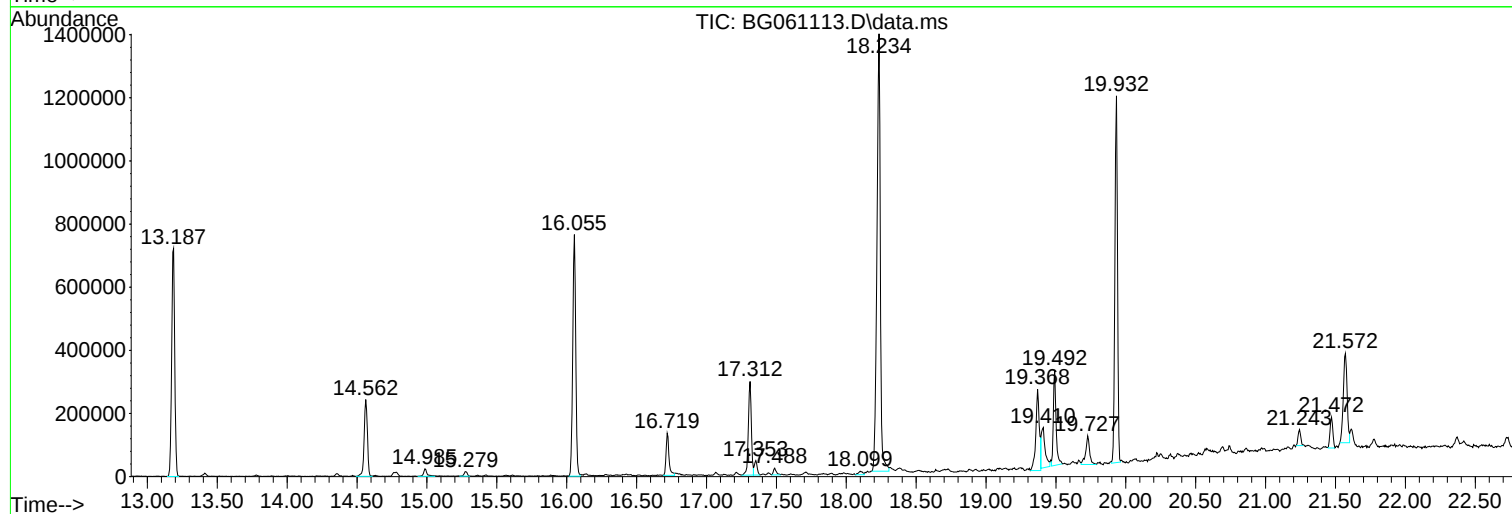
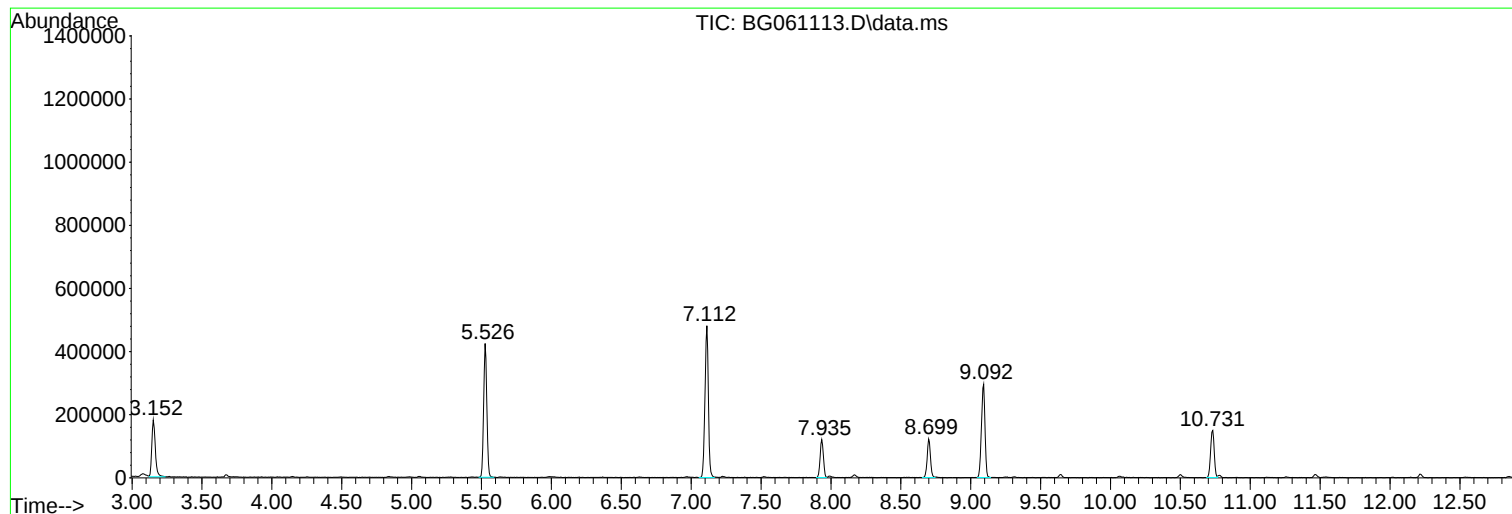
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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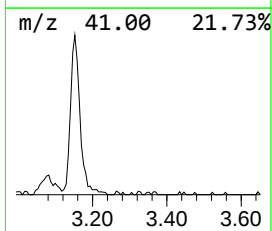
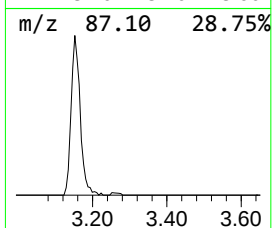
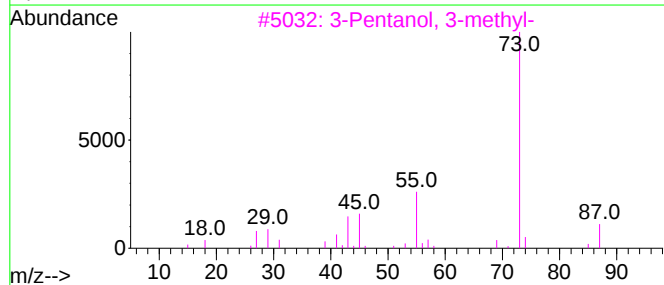
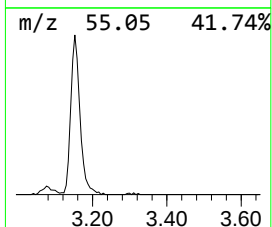
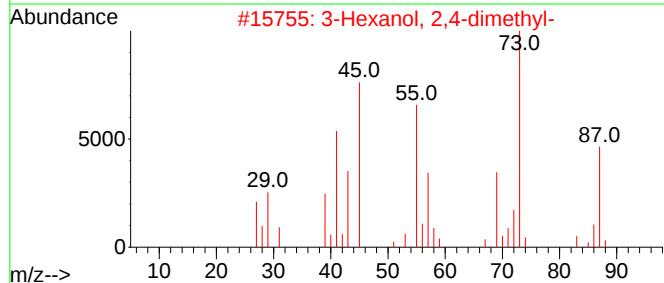
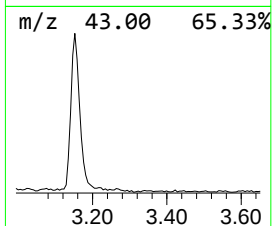
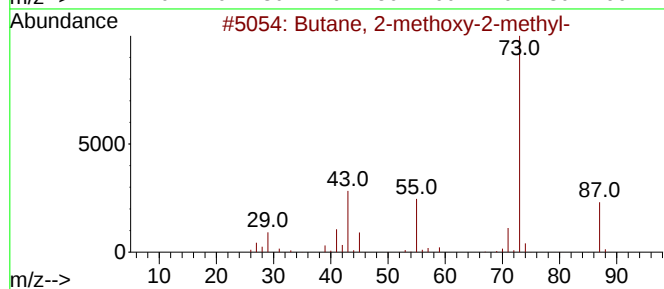
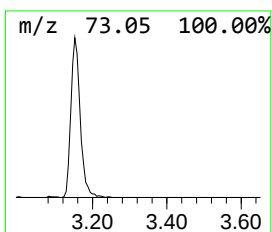
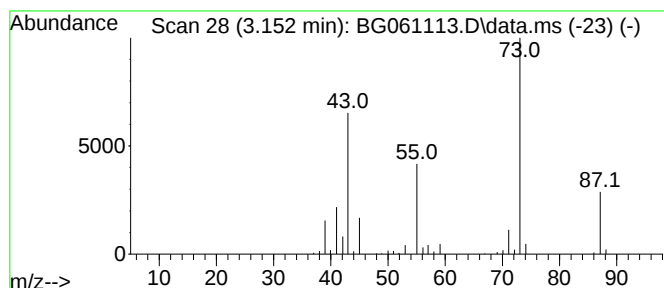
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	31.77 ng	309744	1,4-Dichlorobenzene-d4	7.935

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	39
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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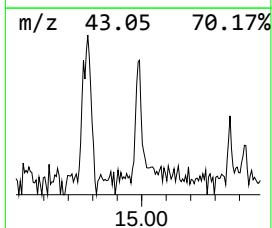
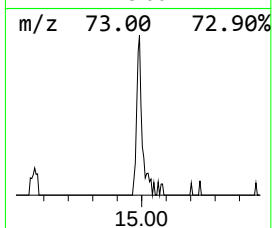
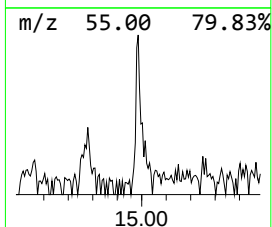
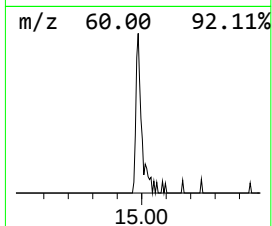
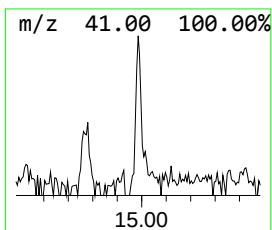
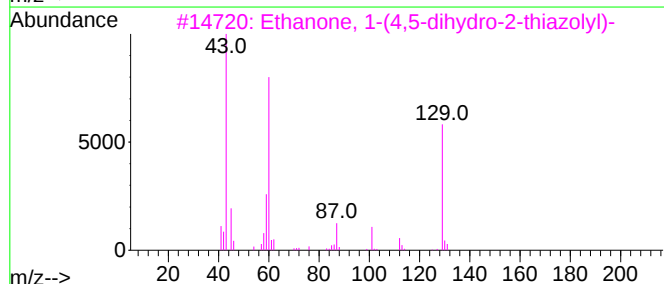
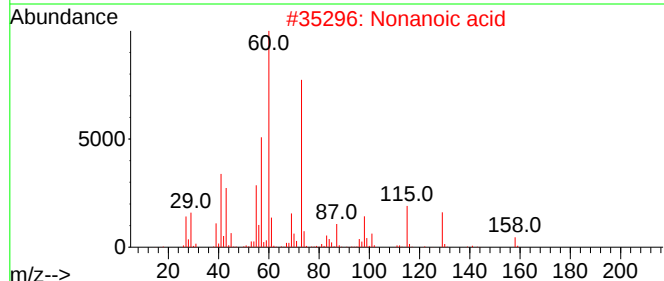
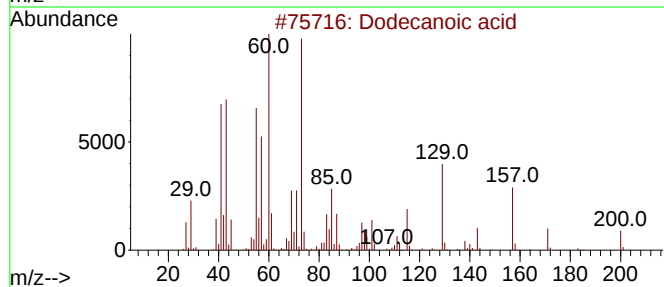
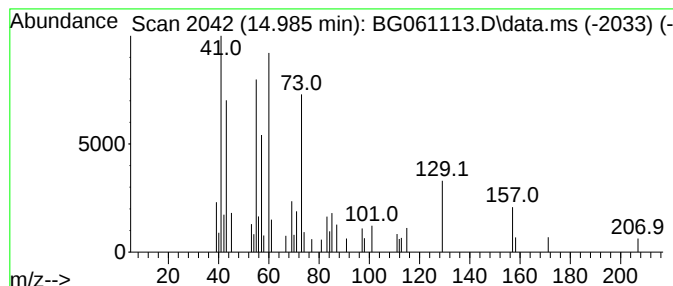
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Dodecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.985	2.16 ng	41777	Acenaphthene-d10	14.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	68
2			Nonanoic acid	158	C9H18O2	000112-05-0	58
3			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	52
4			Octanoic acid	144	C8H16O2	000124-07-2	50
5			Undecanoic acid	186	C11H22O2	000112-37-8	50



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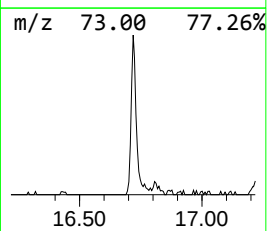
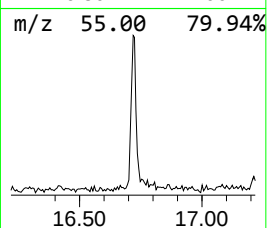
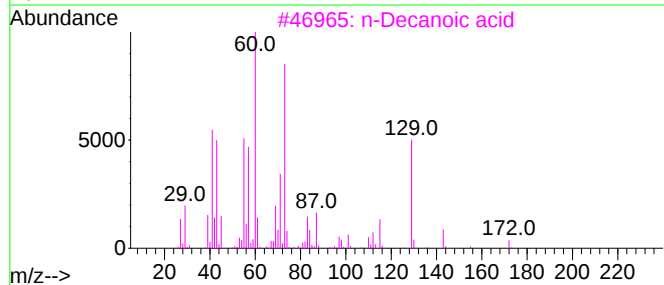
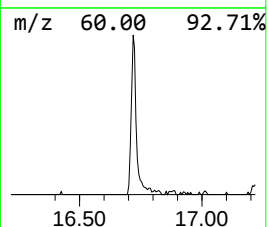
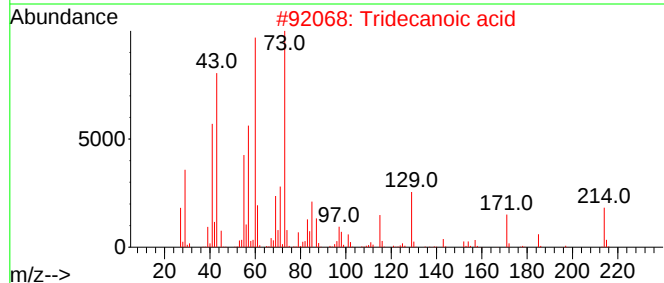
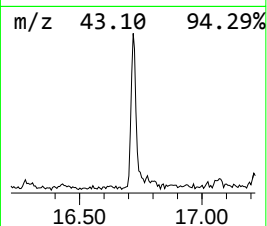
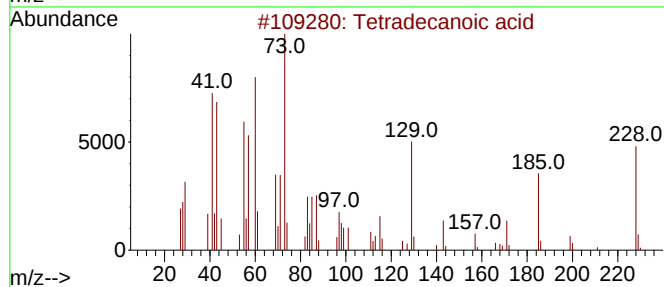
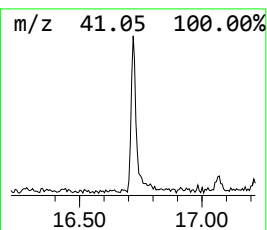
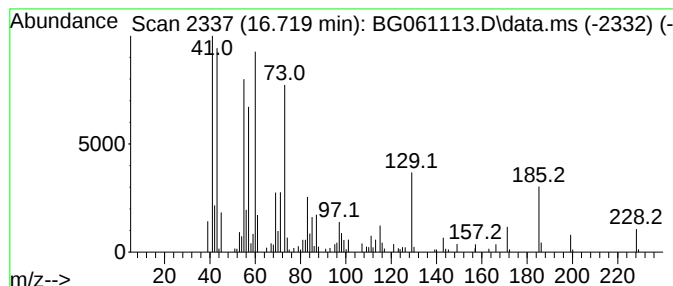
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.719	8.71 ng	196533	Phenanthrene-d10	17.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	72
3			n-Decanoic acid	172	C10H20O2	000334-48-5	64
4			Undecanoic acid	186	C11H22O2	000112-37-8	59
5			11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	50



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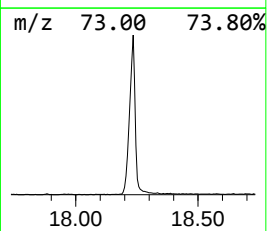
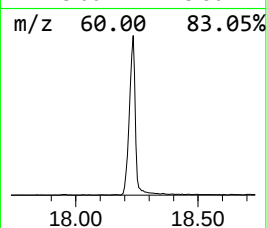
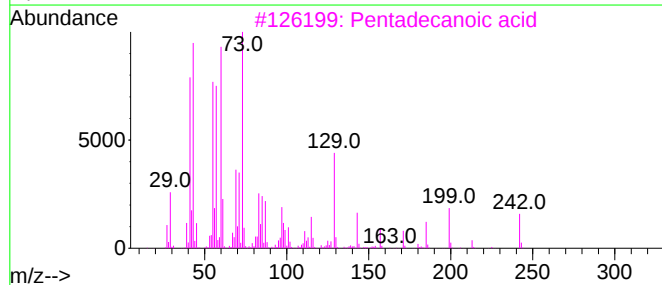
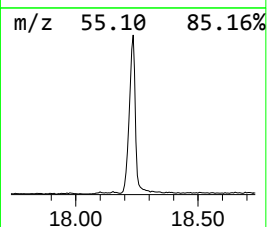
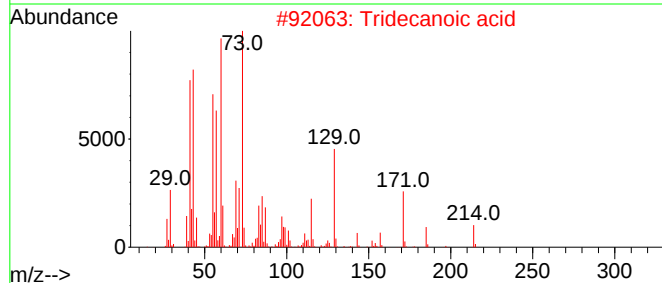
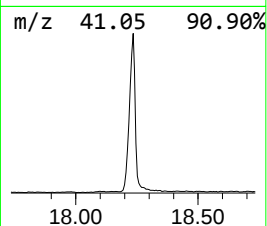
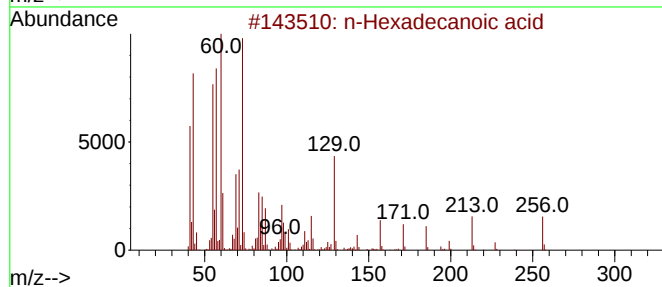
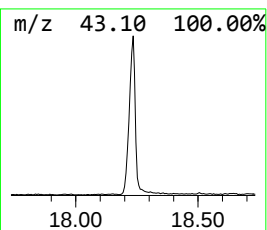
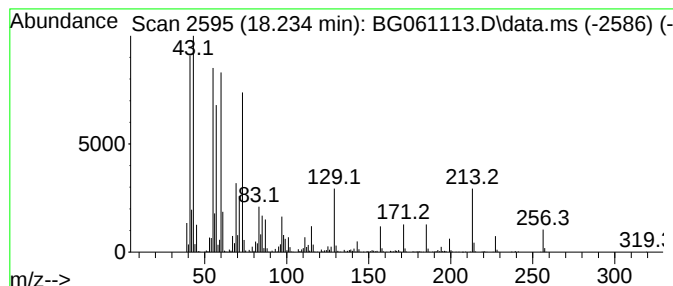
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.234	104.70 ng	2361570	Phenanthrene-d10	17.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	96
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			Dodecanoic acid	200	C12H24O2	000143-07-7	50



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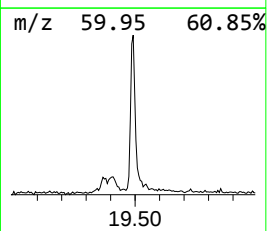
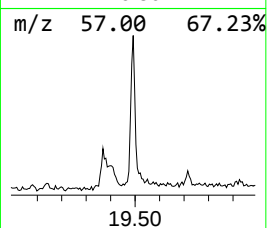
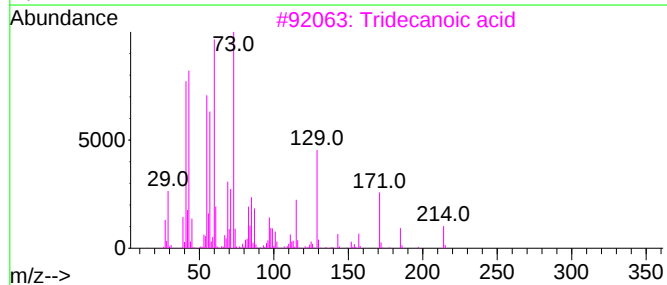
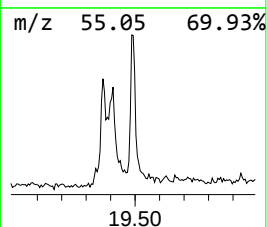
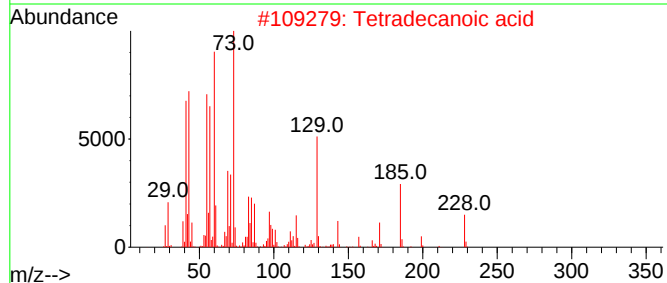
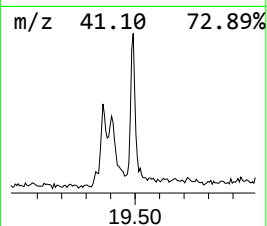
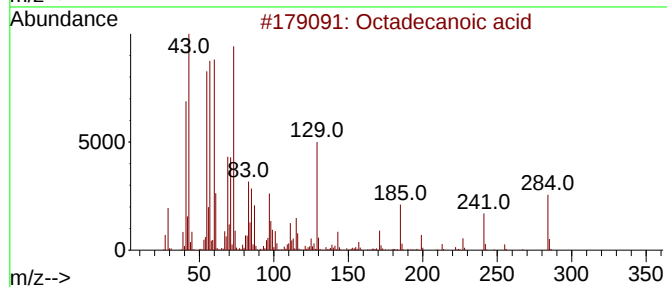
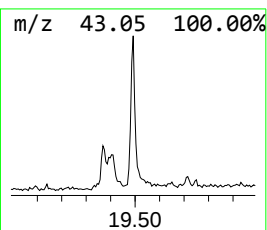
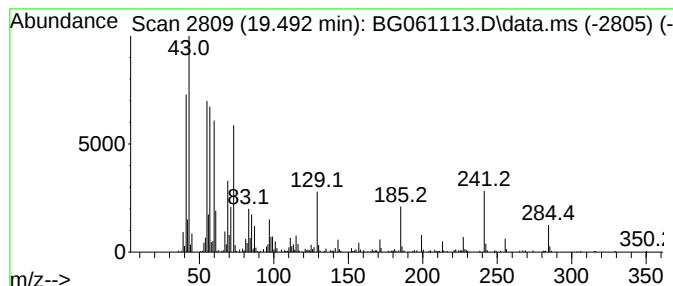
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.492	14.95 ng	400770	Chrysene-d12	21.572

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	52
3			Tridecanoic acid	214	C13H26O2	000638-53-9	49
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5			Dodecanoic acid	200	C12H24O2	000143-07-7	46



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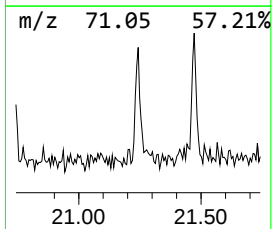
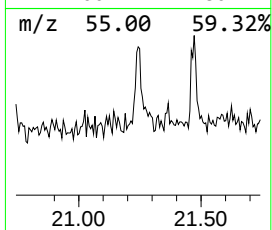
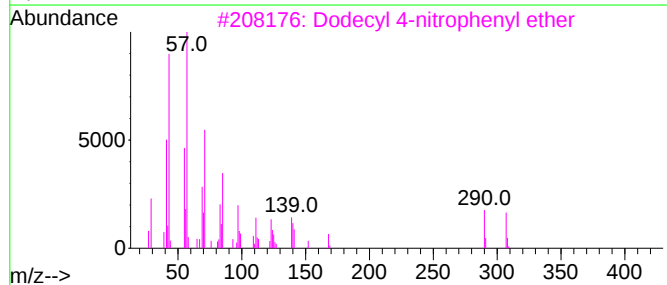
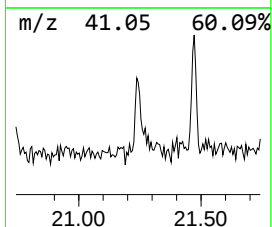
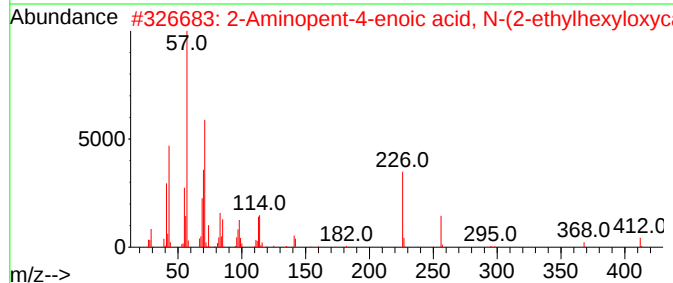
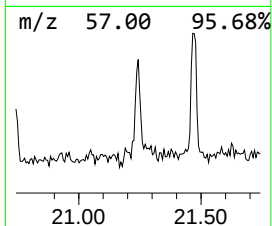
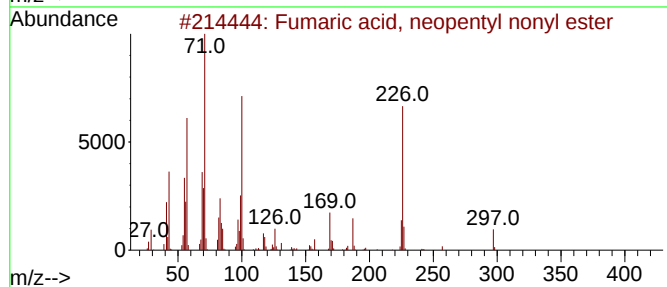
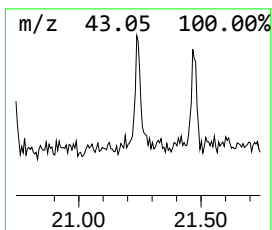
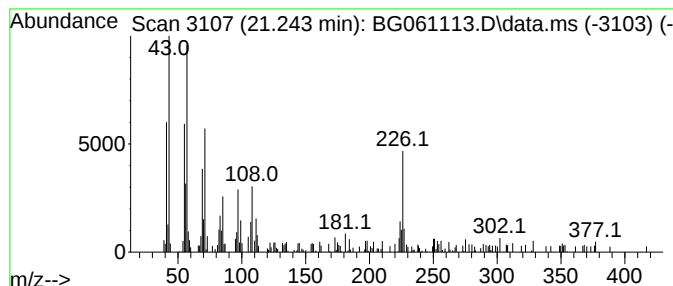
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown21.243 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.243	2.58 ng	69070	Chrysene-d12	21.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fumaric acid, neopentyl nonyl ester	312	C18H32O4	1000339-24-7	43
2			2-Aminopent-4-enoic acid, N-(2-e...	453	C27H51NO4	1000393-16-8	43
3			Dodecyl 4-nitrophenyl ether	307	C18H29NO3	065039-18-1	30
4			Tetracosane	338	C24H50	000646-31-1	27
5			15-Methylnonacosane	422	C30H62	065820-60-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061113.D
Acq On : 3 May 2024 19:35
Operator : MA/JU
Sample : P2355-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VB16173

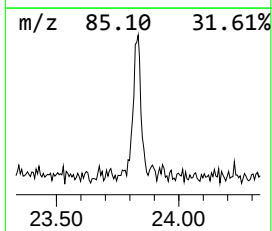
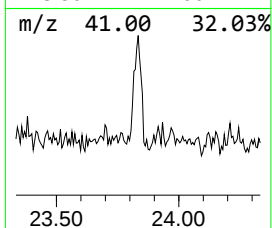
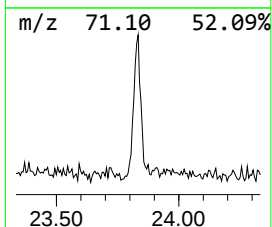
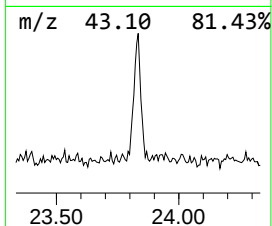
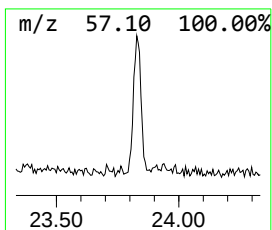
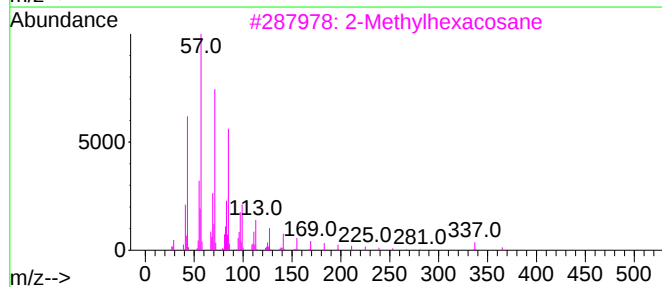
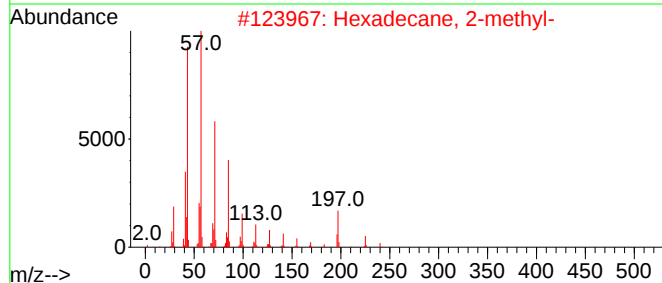
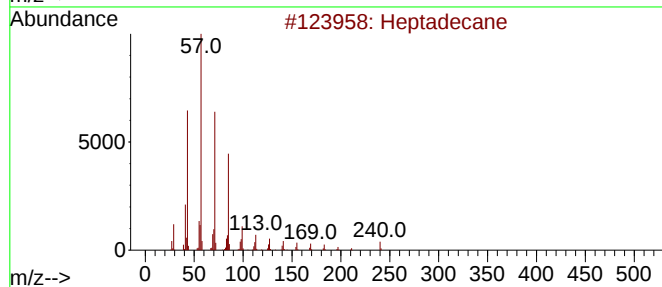
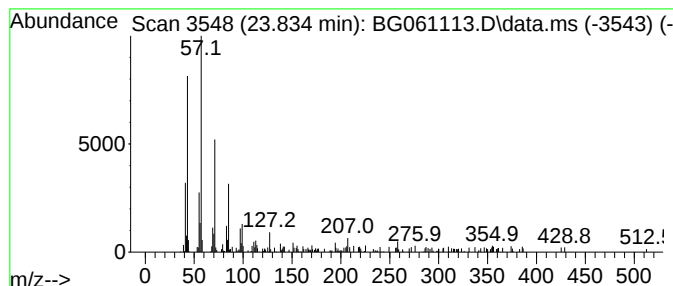
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.834	11.03 ng	146880	Perylene-d12	24.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	95
2			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	72
3			2-Methylhexacosane	380	C27H56	001561-02-0	72
4			Eicosane, 10-methyl-	296	C21H44	054833-23-7	70
5			Hexacosane	366	C26H54	000630-01-3	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061113.D
Acq On : 3 May 2024 19:35
Operator : MA/JU
Sample : P2355-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VB16173

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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
Butane, 2-metho...	3.152	31.8	ng	309744	1	7.935	195007	20.0
Dodecanoic acid	14.985	2.2	ng	41777	3	14.562	386523	20.0
Tetradecanoic acid	16.719	8.7	ng	196533	4	17.312	451116	20.0
n-Hexadecanoic ...	18.234	104.7	ng	2361570	4	17.312	451116	20.0
Octadecanoic acid	19.492	14.9	ng	400770	5	21.572	536154	20.0
unknown21.243	21.243	2.6	ng	69070	5	21.572	536154	20.0
Heptadecane	23.834	11.0	ng	146880	6	24.698	266296	20.0