

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
 Data File : BG060763.D
 Acq On : 3 Apr 2024 15:27
 Operator : MA/JU
 Sample : P1956-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RBR200010

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-BG032924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060763.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.099	14	19	27	rBV4	37554	100062	2.39%	0.442%
2	3.182	27	33	48	rVB	450735	933906	22.28%	4.125%
3	3.693	115	120	130	rBV	47977	78232	1.87%	0.346%
4	5.544	427	435	444	rBV	1209276	1995918	47.62%	8.817%
5	7.118	695	703	713	rVB	1062312	1780422	42.48%	7.865%
6	7.958	838	846	853	rBV	276664	459267	10.96%	2.029%
7	9.110	1031	1042	1049	rBV	634674	1117599	26.66%	4.937%
8	10.755	1312	1322	1329	rBV	345869	625695	14.93%	2.764%
9	13.211	1732	1740	1754	rVB	1604810	2470872	58.95%	10.915%
10	14.586	1965	1974	1982	rBV	558015	874564	20.87%	3.863%
11	14.815	2004	2013	2017	rBV5	19415	46777	1.12%	0.207%
12	16.072	2220	2227	2236	rBV	1361166	2104300	50.20%	9.296%
13	17.330	2435	2441	2446	rBV	736985	1116202	26.63%	4.931%
14	17.371	2446	2448	2454	rVB	41694	55651	1.33%	0.246%
15	18.246	2592	2597	2606	rBV	316571	453023	10.81%	2.001%
16	19.386	2785	2791	2797	rBV	165205	257382	6.14%	1.137%
17	19.521	2809	2814	2820	rBV	167925	233787	5.58%	1.033%
18	19.745	2848	2852	2857	rVB	186138	265577	6.34%	1.173%
19	19.956	2882	2888	2899	rVB	3131812	4191472	100.00%	18.515%
20	20.074	2904	2908	2913	rBV5	23072	51129	1.22%	0.226%
21	20.209	2927	2931	2933	rBV5	30514	46334	1.11%	0.205%
22	20.738	3018	3021	3026	rBV	135982	149823	3.57%	0.662%
23	21.278	3109	3113	3119	rBV3	149833	249989	5.96%	1.104%
24	21.595	3160	3167	3172	rBV2	803260	1412068	33.69%	6.238%
25	22.806	3368	3373	3379	rBV2	174217	287160	6.85%	1.268%
26	24.739	3693	3702	3714	rBV	460143	1280559	30.55%	5.657%

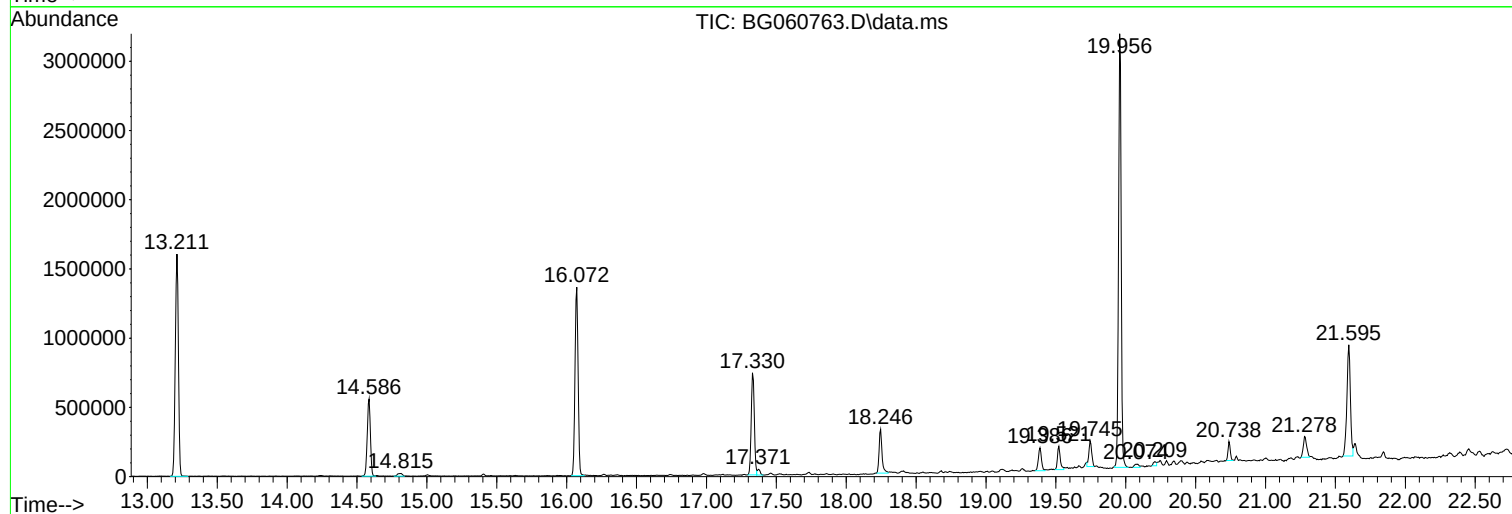
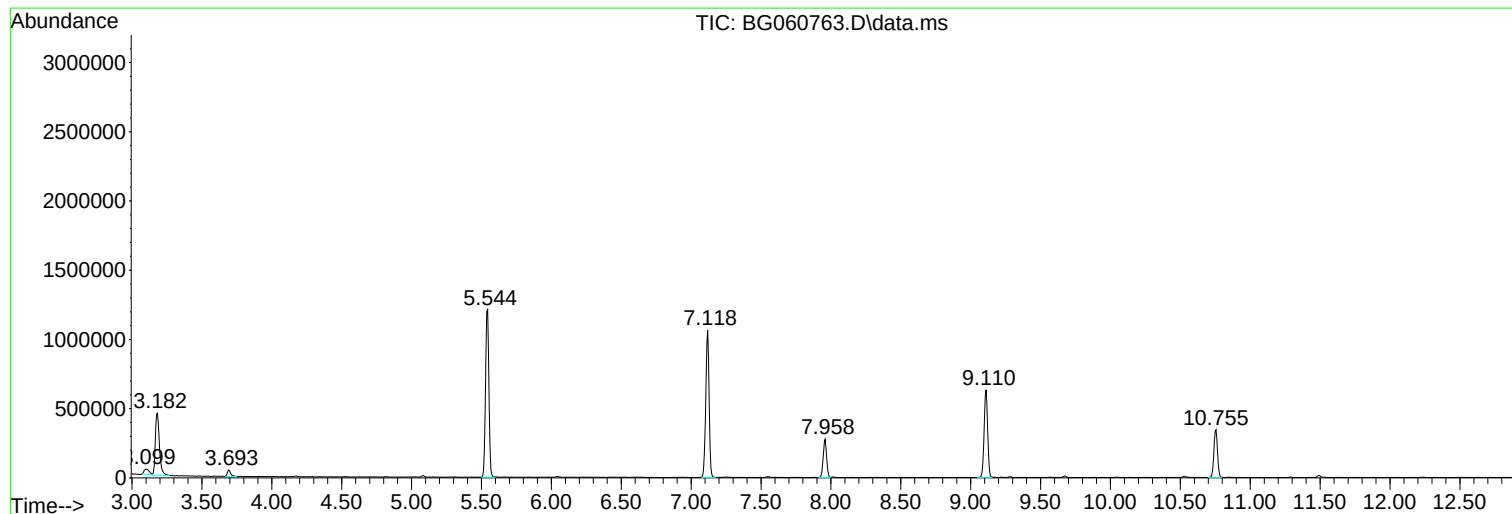
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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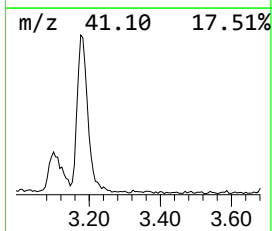
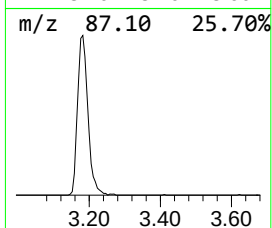
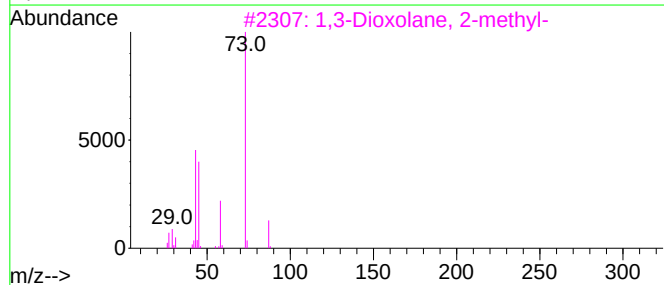
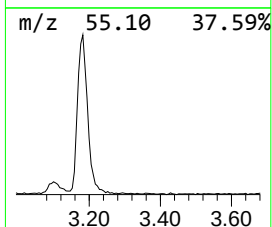
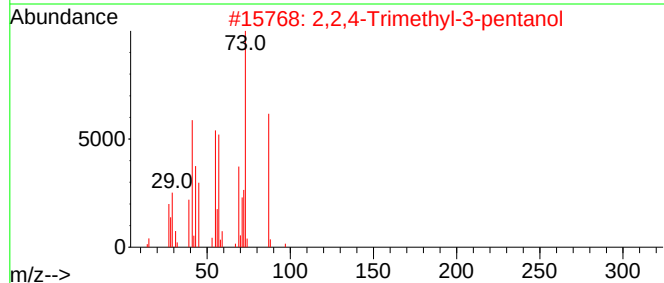
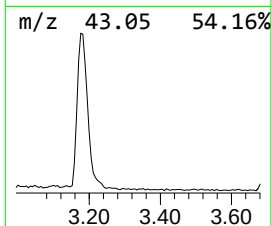
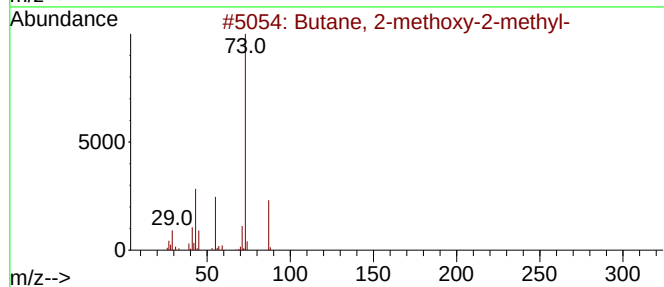
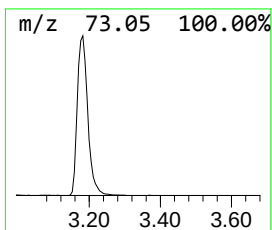
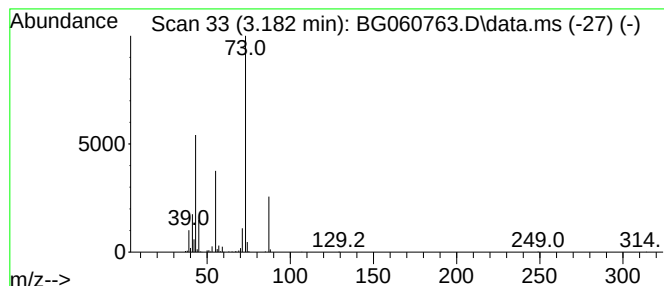
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.182	40.67 ng	933906	1,4-Dichlorobenzene-d4	7.958

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Butanoic acid, 2-hydroxy-2-methyl-	132	C6H12O3	032793-34-3	25
5			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	25



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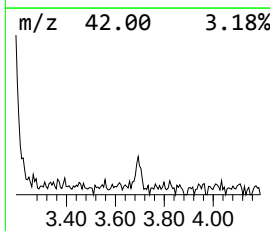
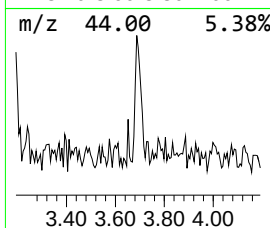
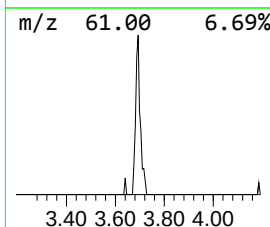
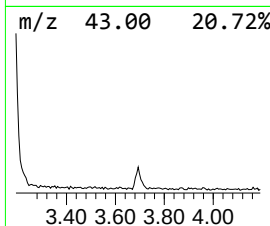
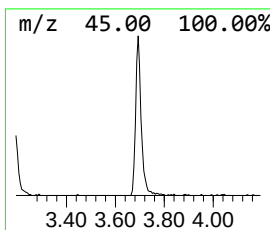
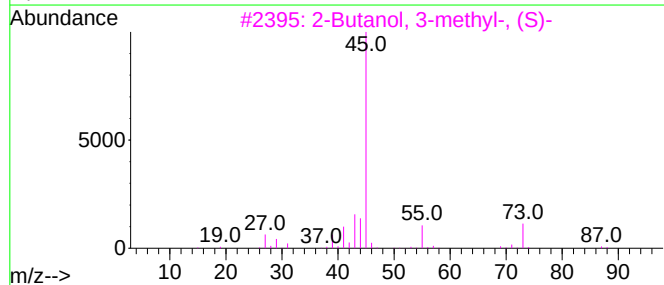
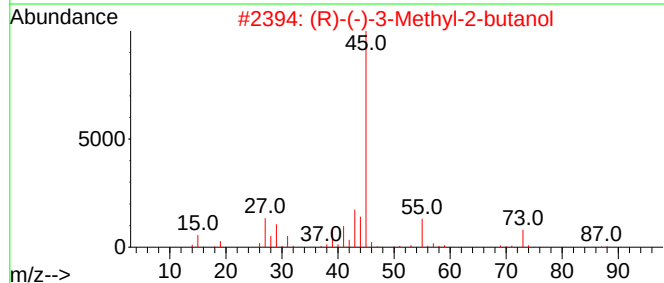
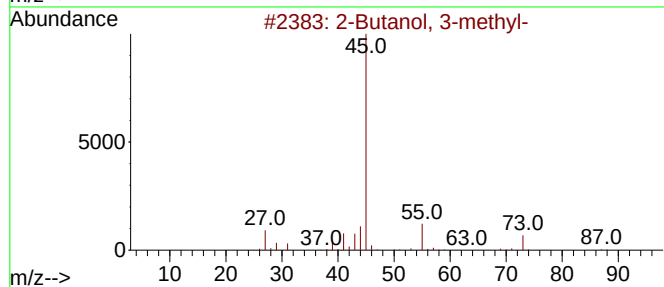
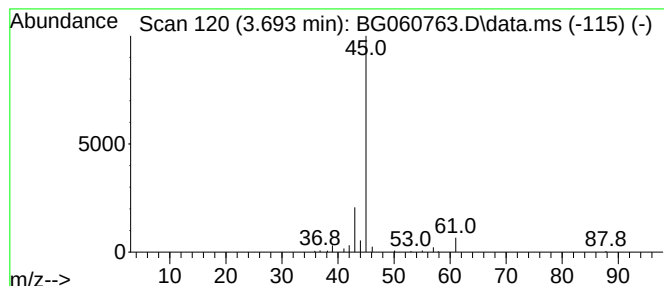
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown3.693 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.693	3.41 ng	78232	1,4-Dichlorobenzene-d4	7.958

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 3-methyl-			88	C5H12O	000598-75-4	9
2	(R)-(-)-3-Methyl-2-butanol			88	C5H12O	001572-93-6	9
3	2-Butanol, 3-methyl-, (S)-			88	C5H12O	001517-66-4	9
4	2-Pentanol, 4-methyl-			102	C6H14O	000108-11-2	9
5	2-Heptanol, (S)-			116	C7H16O	006033-23-4	9



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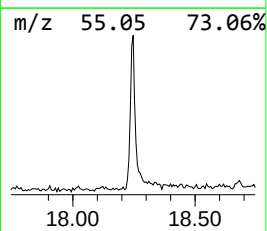
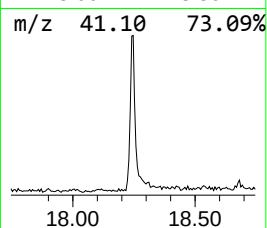
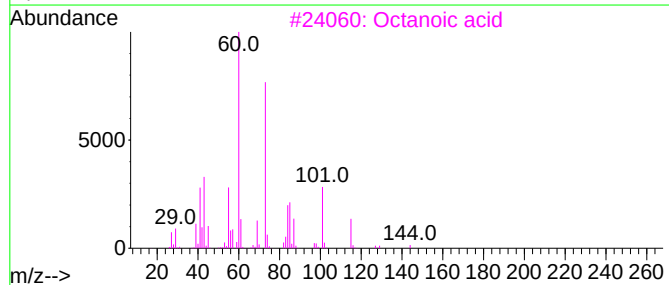
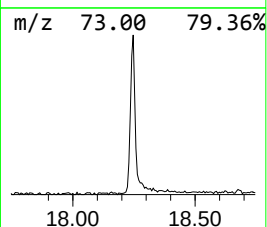
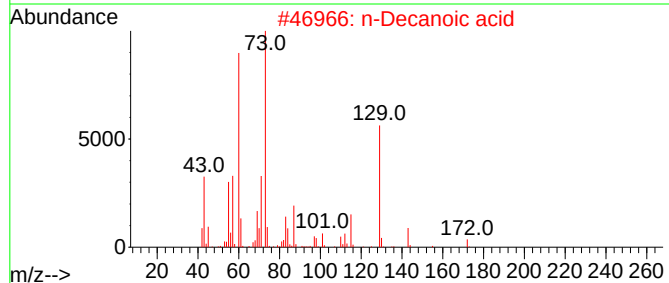
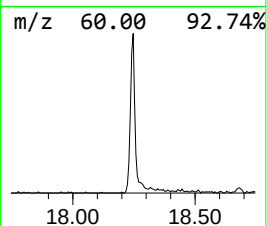
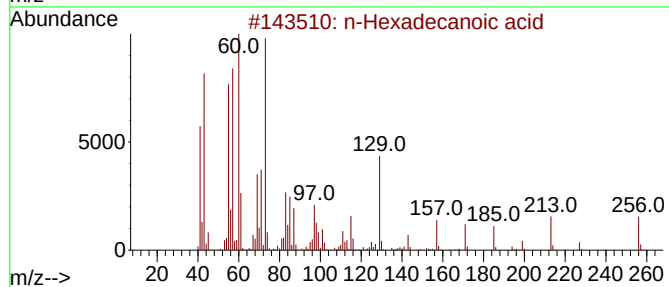
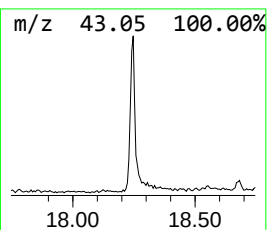
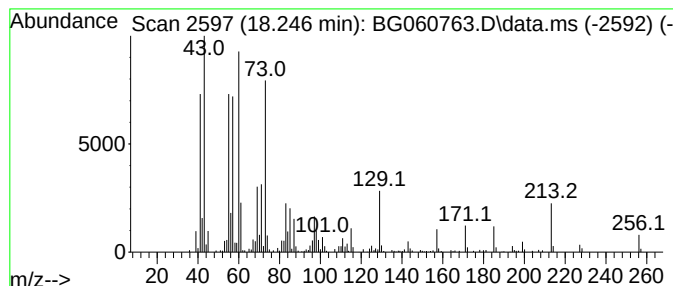
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.246	8.12 ng	453023	Phenanthrene-d10	17.330

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		n-Decanoic acid	172	C10H20O2	000334-48-5	60
3		Octanoic acid	144	C8H16O2	000124-07-2	60
4		Tridecanoic acid	214	C13H26O2	000638-53-9	59
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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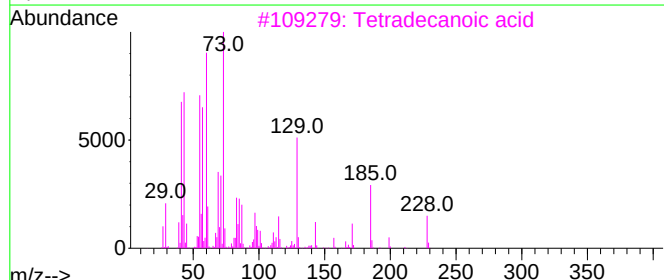
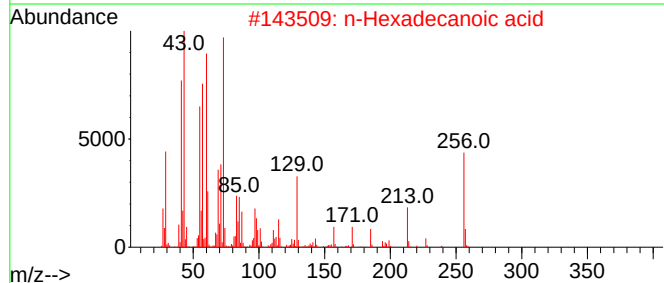
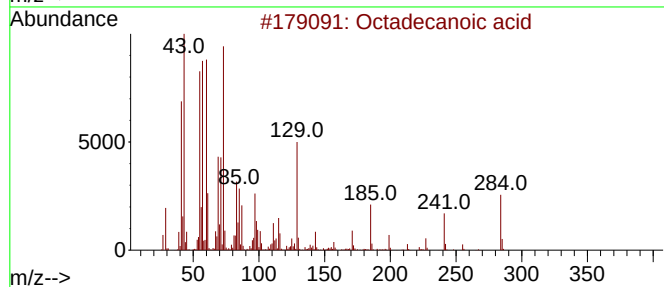
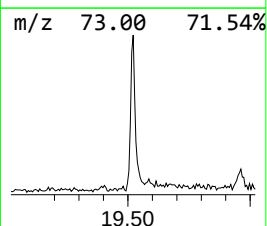
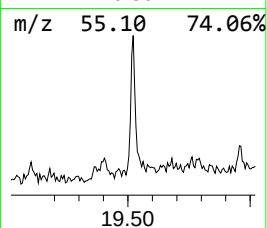
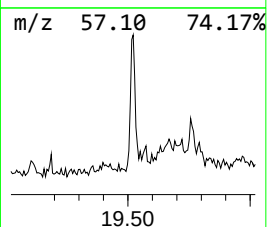
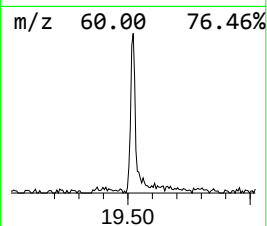
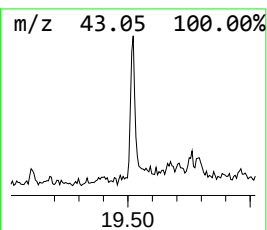
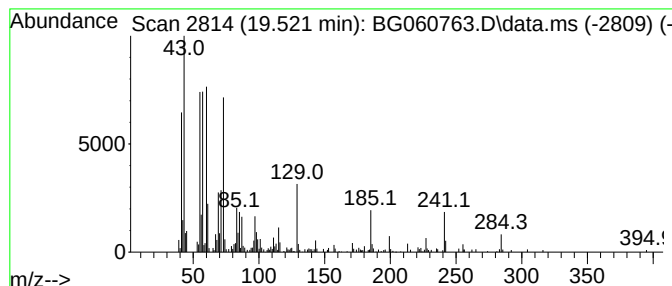
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Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.521	3.31 ng	233787	Chrysene-d12	21.595

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	59
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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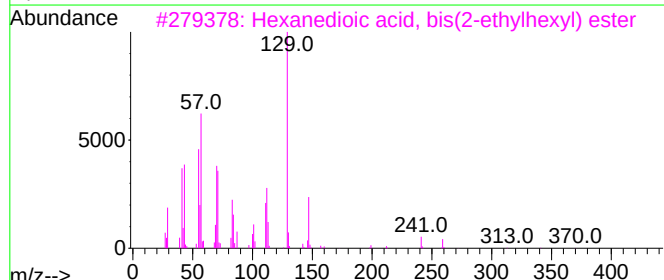
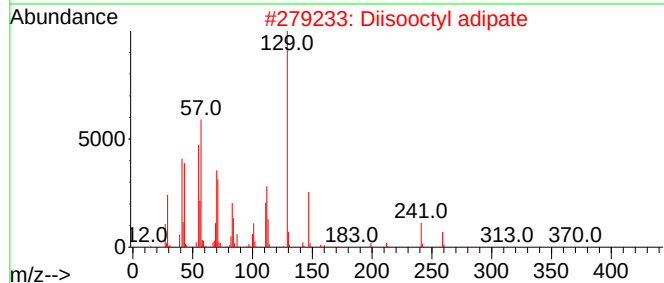
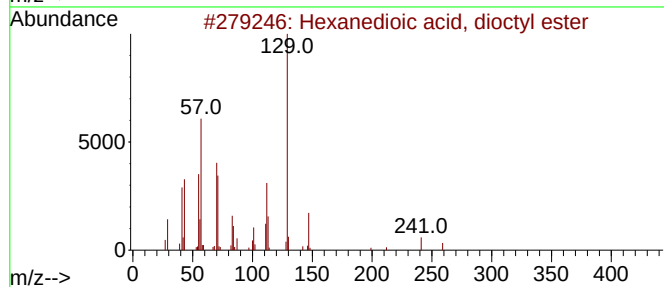
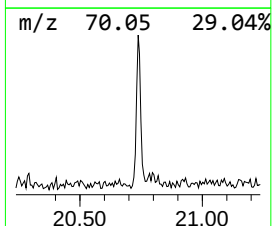
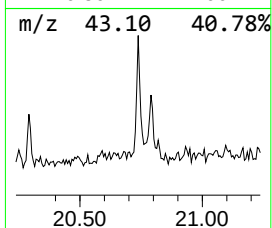
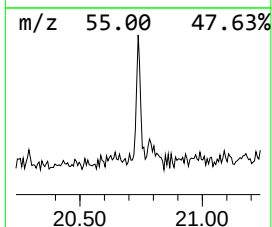
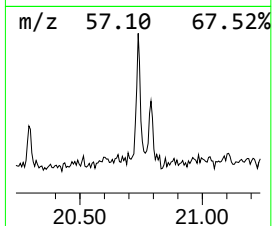
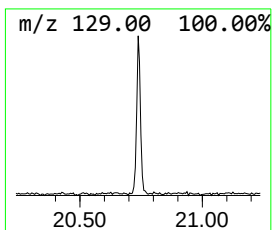
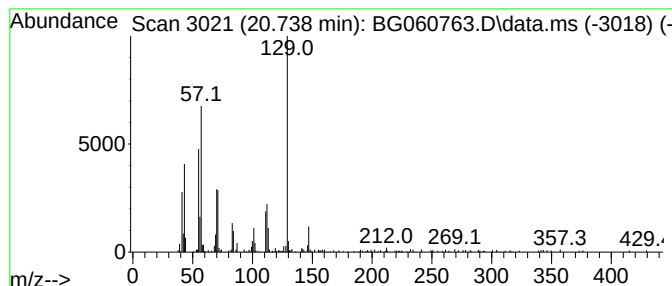
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Peak Number 6 Hexanedioic acid, dioctyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.738	2.12 ng	149823	Chrysene-d12	21.595

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	91
2			Diisooctyl adipate	370	C22H42O4	001330-86-5	78
3			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	72
4			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	58
5			Adipic acid, decyl 3-hexyl ester	370	C22H42O4	1000353-62-9	47



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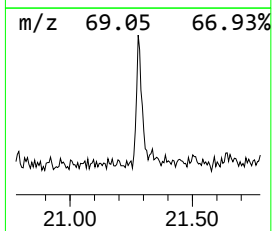
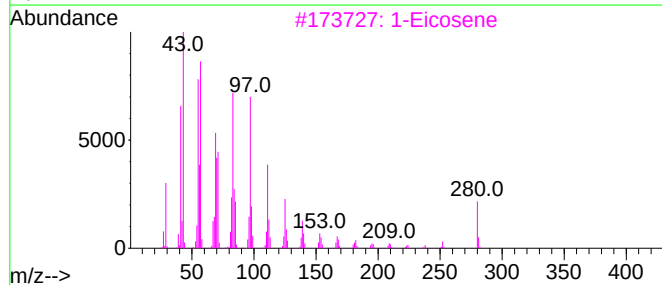
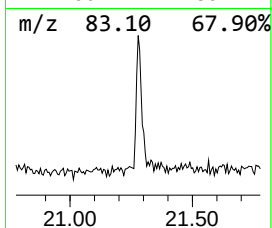
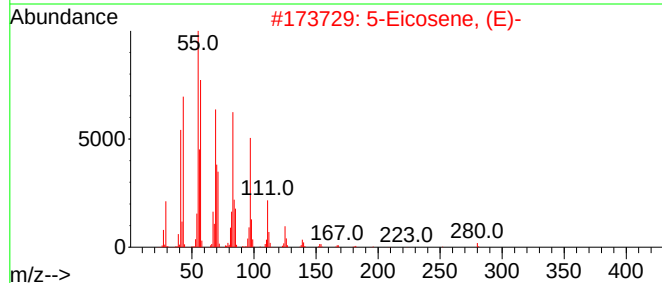
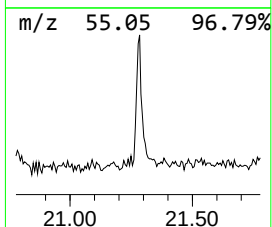
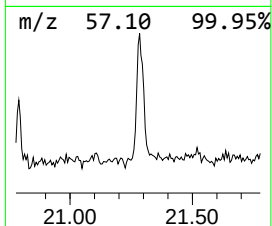
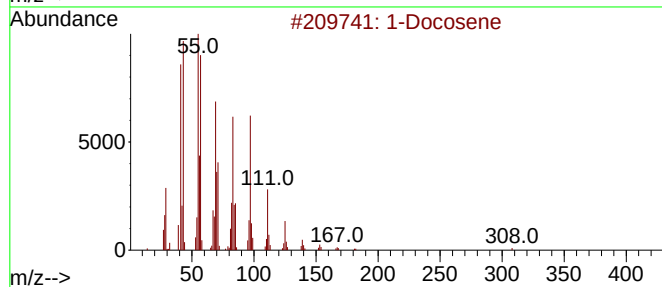
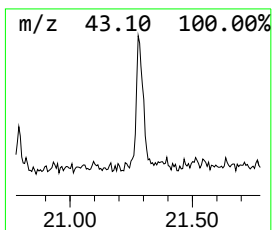
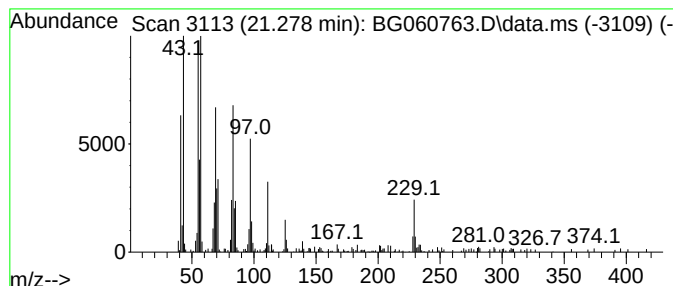
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.278	3.54 ng	249989	Chrysene-d12	21.595

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	95
2	5-Eicosene, (E)-			280	C20H40	074685-30-6	94
3	1-Eicosene			280	C20H40	003452-07-1	93
4	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	91
5	Henicos-1-ene			294	C21H42	001599-68-4	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
Data File : BG060763.D
Acq On : 3 Apr 2024 15:27
Operator : MA/JU
Sample : P1956-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200010

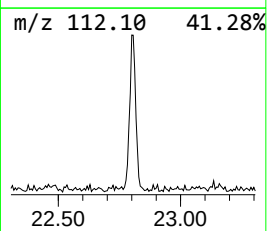
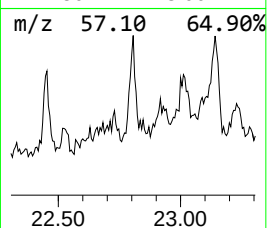
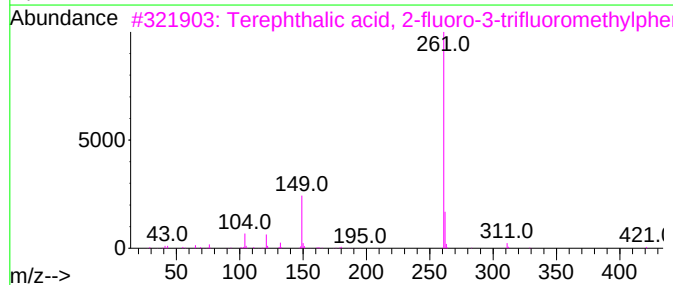
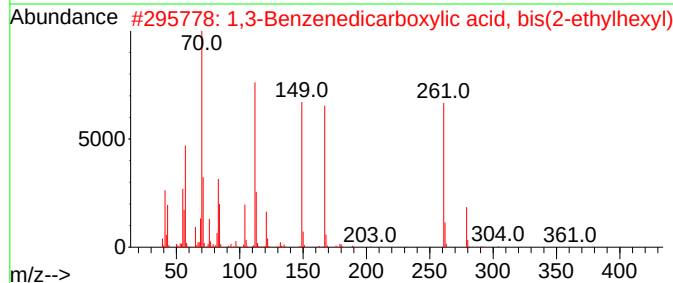
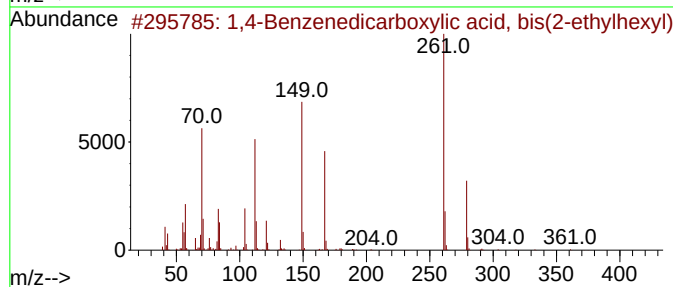
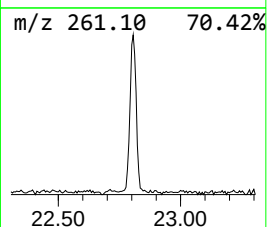
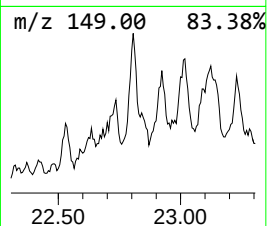
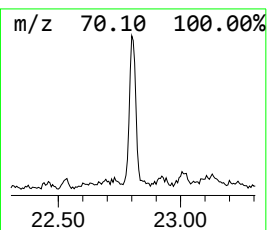
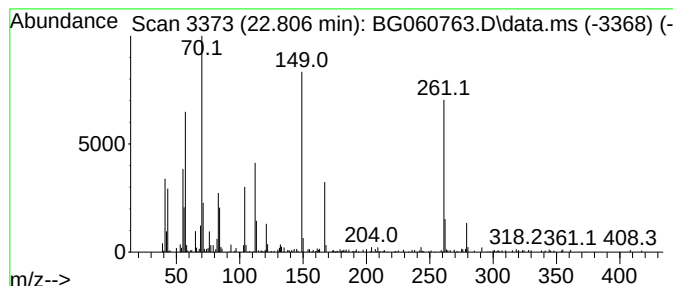
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.806	4.07 ng	287160	Chrysene-d12	21.595

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	53
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	46
3			Terephthalic acid, 2-fluoro-3-tr...	440	C23H24F4O4	1010415-81-5	35
4			Phthalic acid, oct-3-yl pentyl e...	348	C21H32O4	1000377-71-4	27
5			Terephthalic acid, 3-hexyl octyl...	362	C22H34O4	1000356-23-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
Data File : BG060763.D
Acq On : 3 Apr 2024 15:27
Operator : MA/JU
Sample : P1956-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200010

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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...	3.182	40.7	ng	933906	1	7.958	459267	20.0
unknown3.693	3.693	3.4	ng	78232	1	7.958	459267	20.0
n-Hexadecanoic ...	18.246	8.1	ng	453023	4	17.330	1116200	20.0
Octadecanoic acid	19.521	3.3	ng	233787	5	21.595	1412070	20.0
Hexanedioic aci...	20.738	2.1	ng	149823	5	21.595	1412070	20.0
1-Docosene	21.278	3.5	ng	249989	5	21.595	1412070	20.0
1,4-Benzenedica...	22.806	4.1	ng	287160	5	21.595	1412070	20.0