

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040524\
Data File : BG060794.D
Acq On : 5 Apr 2024 13:40
Operator : MA/JU
Sample : P1996-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP1

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: BG060794.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.096	13	18	26	rVV3	31141	78045	2.06%	0.405%
2	3.178	26	32	45	rVB	281562	483867	12.80%	2.513%
3	3.689	115	119	128	rVB	26666	41458	1.10%	0.215%
4	5.540	425	434	446	rBV	859773	1362318	36.03%	7.075%
5	7.115	693	702	713	rBV	946384	1567733	41.46%	8.142%
6	7.955	837	845	852	rBV	217666	352684	9.33%	1.832%
7	9.107	1033	1041	1050	rBV	533682	938791	24.83%	4.876%
8	10.752	1312	1321	1331	rBV	268371	473336	12.52%	2.458%
9	13.208	1732	1739	1753	rBV	1348324	2097878	55.48%	10.895%
10	14.583	1962	1973	1980	rBV	475206	722400	19.11%	3.752%
11	14.812	2001	2012	2020	rBV	295888	671591	17.76%	3.488%
12	16.069	2219	2226	2235	rBV	1357621	2064926	54.61%	10.724%
13	17.332	2434	2441	2448	rBV	663123	986918	26.10%	5.126%
14	18.114	2568	2574	2580	rBV5	22345	40497	1.07%	0.210%
15	18.243	2591	2596	2612	rBV	297485	462878	12.24%	2.404%
16	19.101	2738	2742	2747	rBV2	36090	44870	1.19%	0.233%
17	19.518	2808	2813	2818	rBV	63285	89452	2.37%	0.465%
18	19.959	2882	2888	2894	rBV	2777432	3781102	100.00%	19.637%
19	21.275	3108	3112	3121	rBV2	186946	322388	8.53%	1.674%
20	21.592	3160	3166	3175	rBV2	658666	1079465	28.55%	5.606%
21	22.450	3308	3312	3320	rVB2	41996	69970	1.85%	0.363%
22	23.319	3454	3460	3468	rVB	170048	321900	8.51%	1.672%
23	24.735	3691	3701	3713	rBV2	428055	1200320	31.75%	6.234%

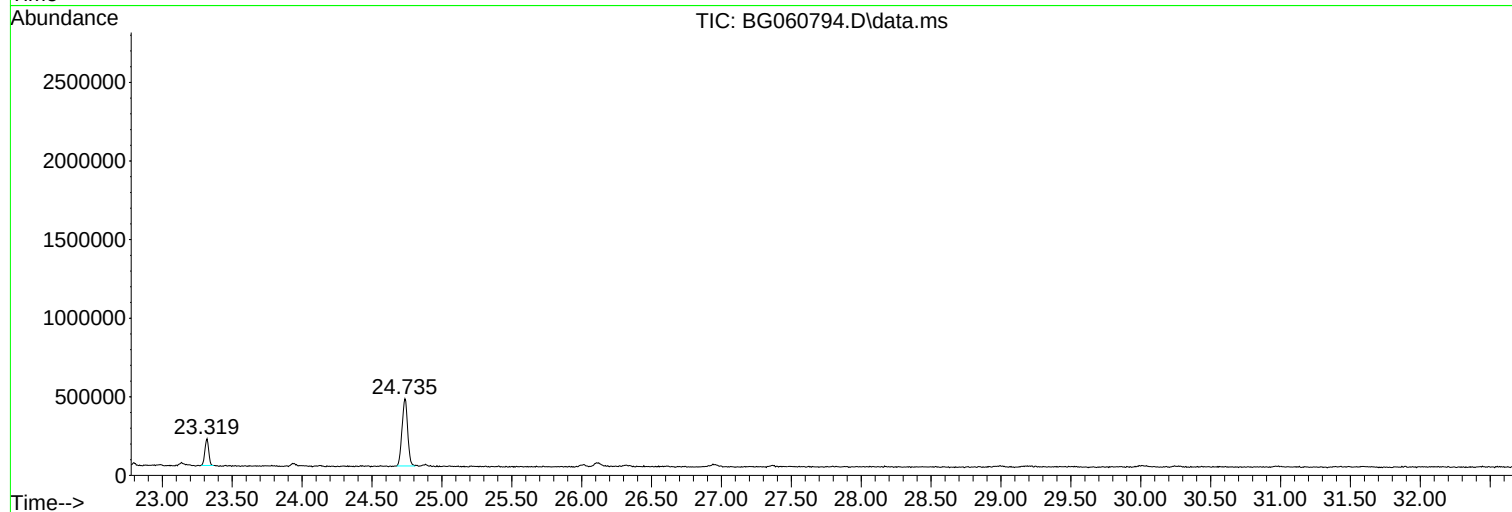
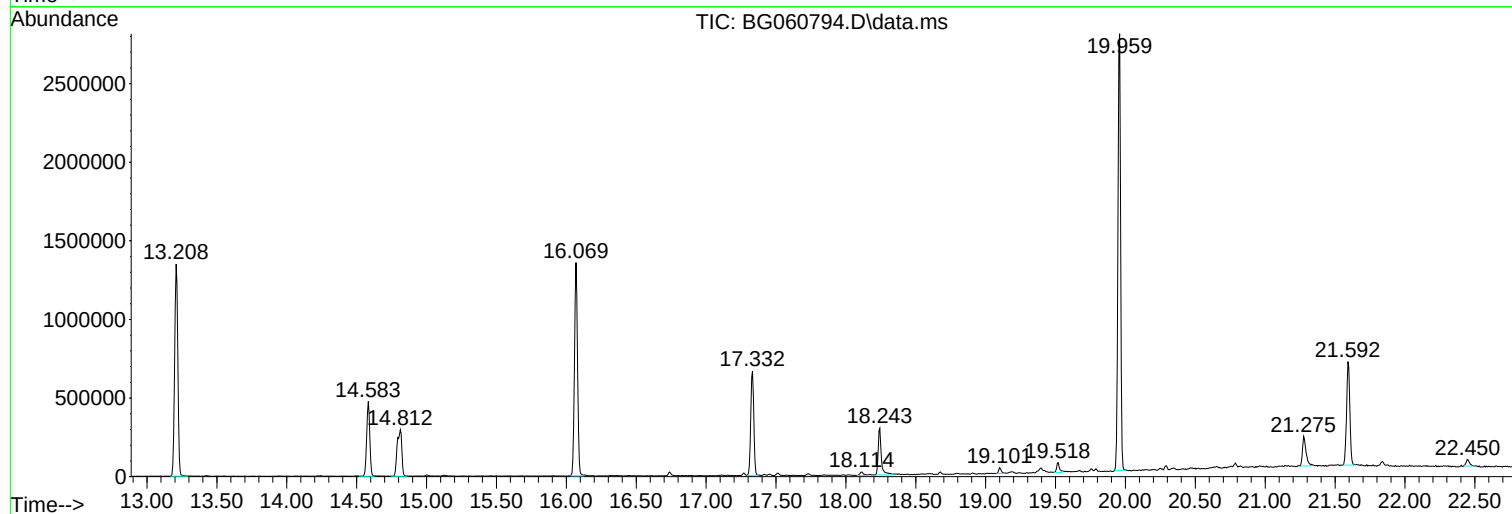
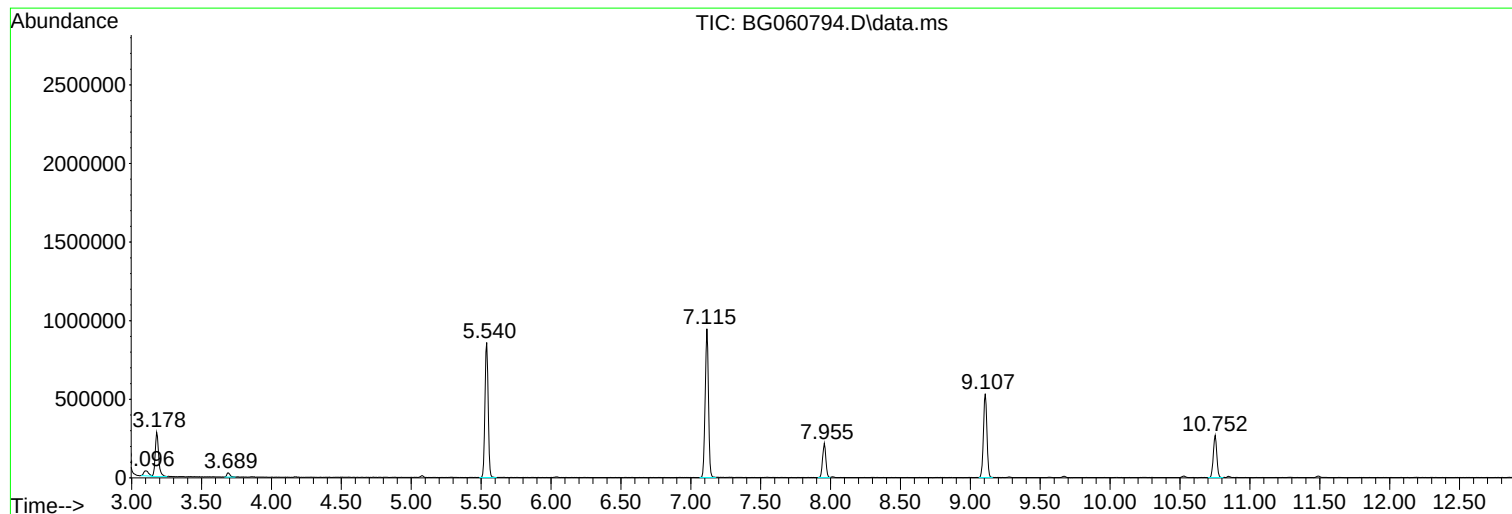
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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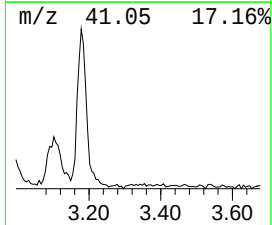
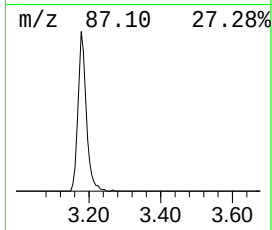
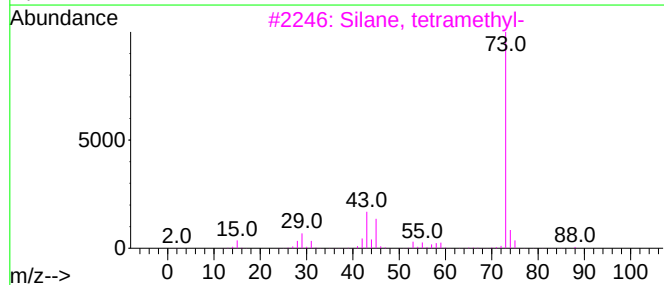
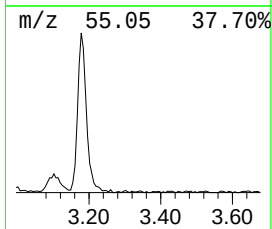
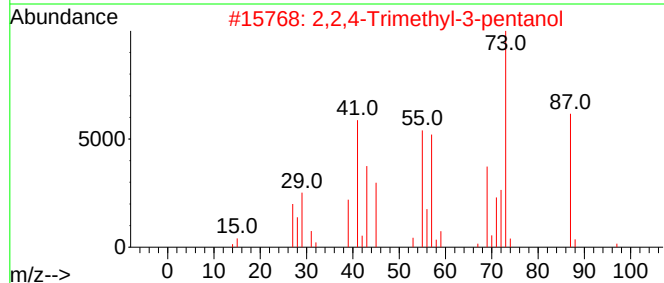
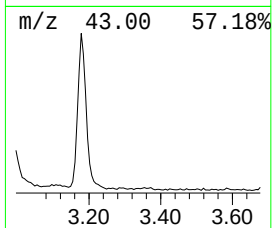
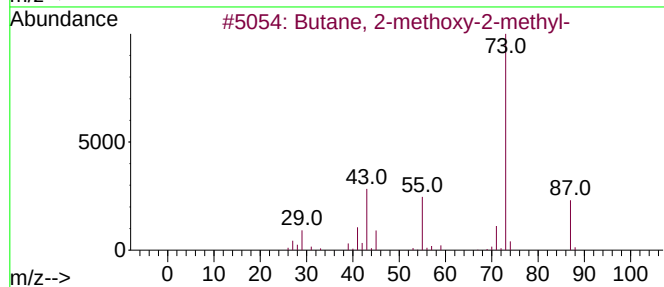
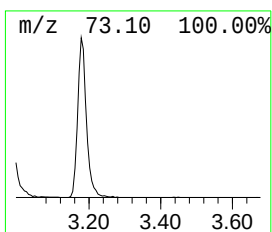
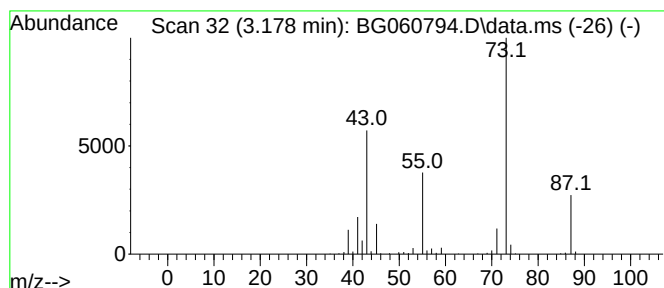
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.178	27.44 ng	483867	1,4-Dichlorobenzene-d4	7.955

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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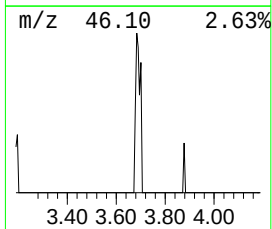
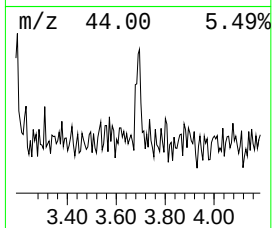
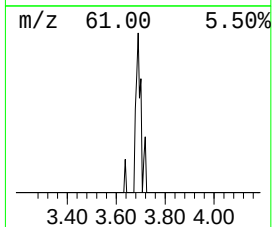
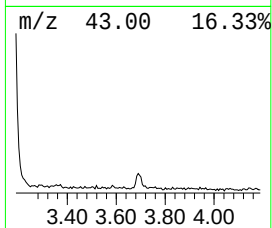
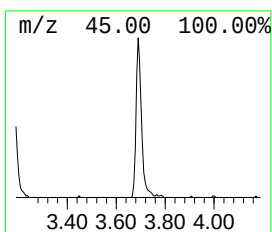
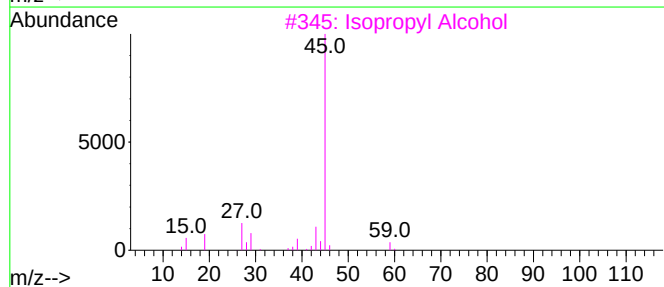
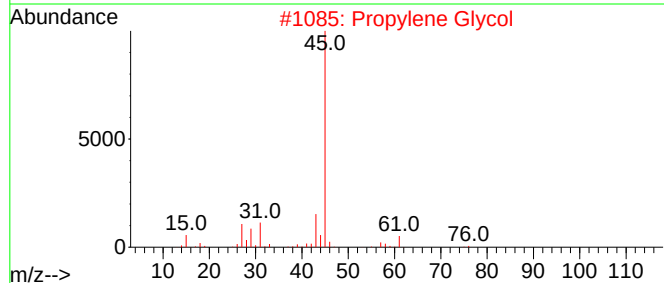
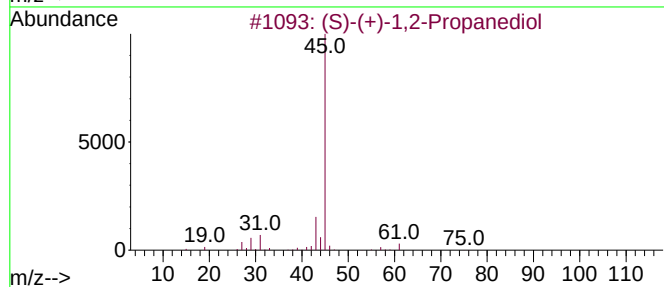
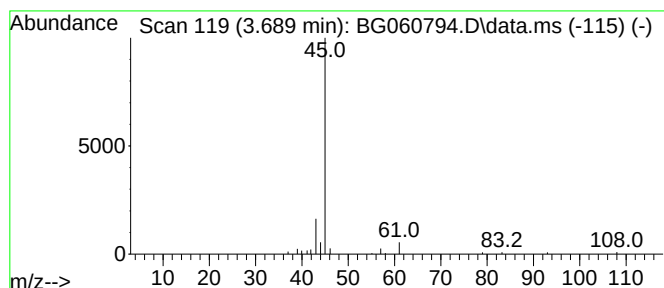
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TIC Integration Parameters: LSCINT.P

Peak Number 3 (S)-(+)-1,2-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.689	2.35 ng	41458	1,4-Dichlorobenzene-d4	7.955

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2		Propylene Glycol	76	C3H8O2	000057-55-6	9
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4		Ethane, 1,1-diethoxy-	118	C6H14O2	000105-57-7	9
5		Hydrazine, propyl-	74	C3H10N2	005039-61-2	9



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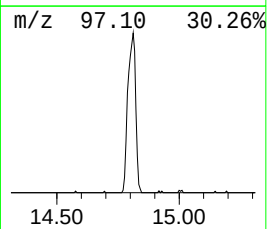
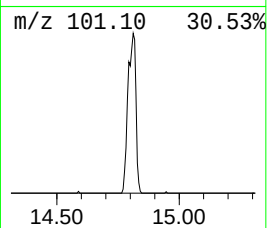
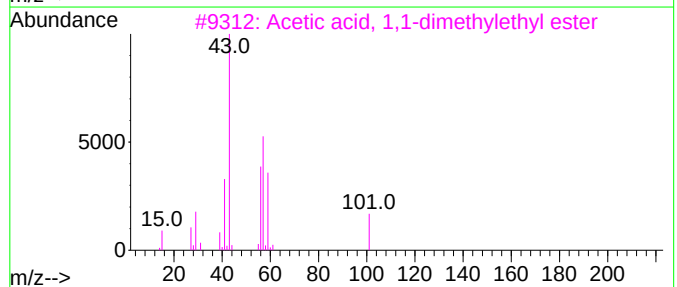
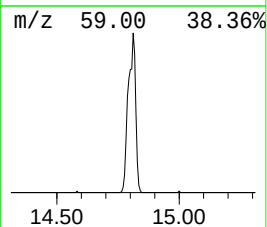
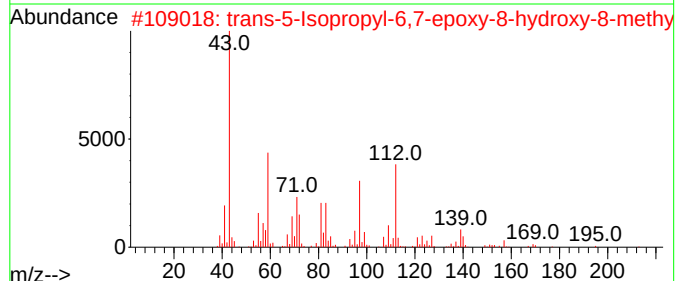
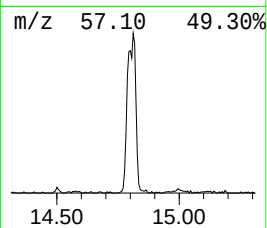
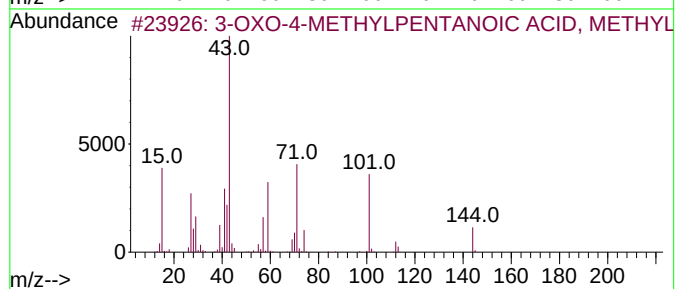
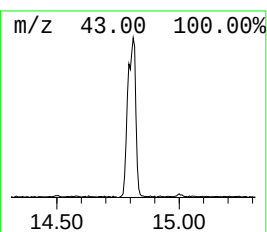
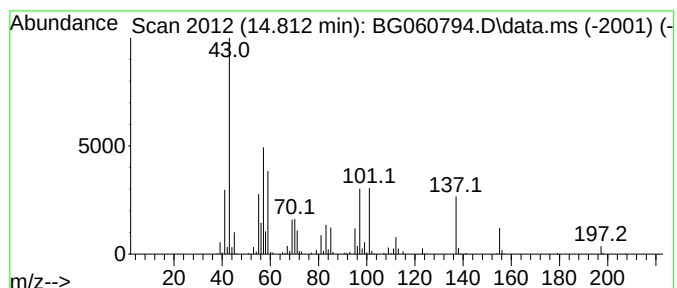
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Peak Number 4 unknown14.812 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.812	18.59 ng	671591	Acenaphthene-d10	14.583

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	25
2			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	20
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	16
4			Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	14
5			2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	14



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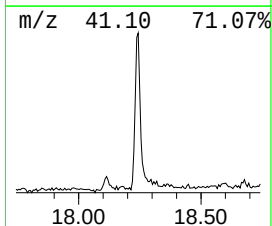
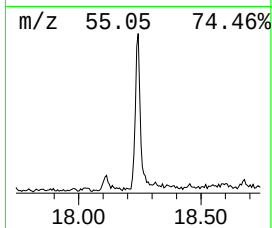
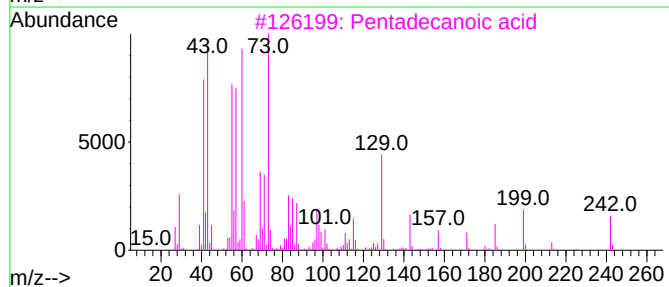
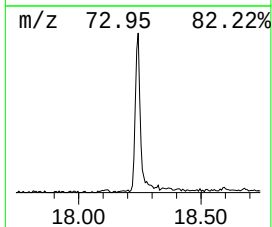
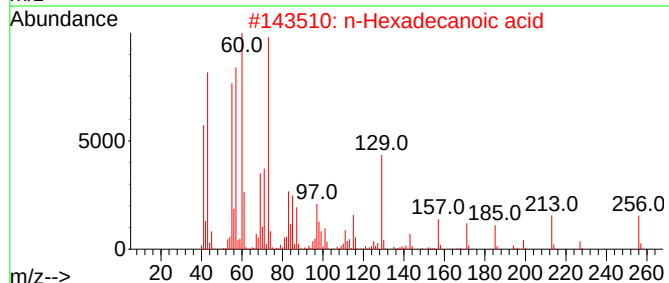
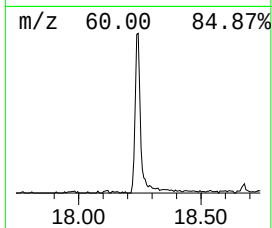
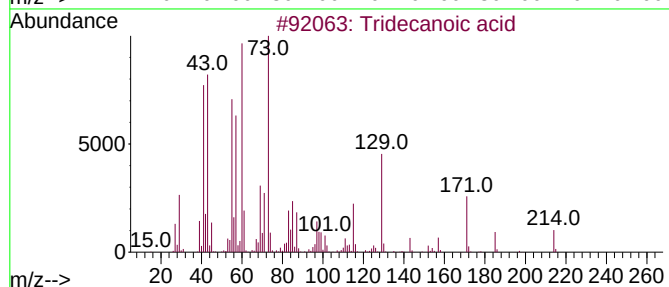
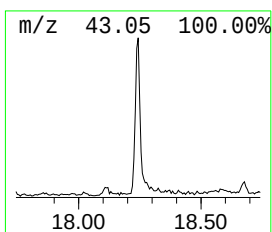
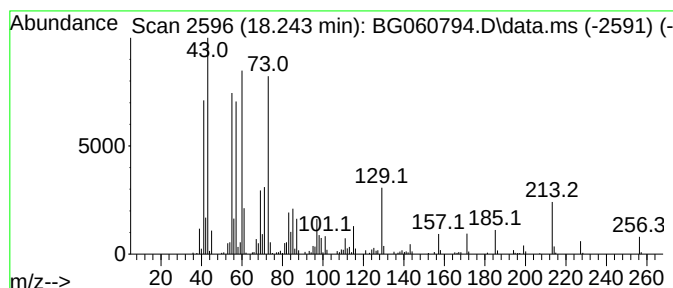
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Peak Number 5 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.243	9.38 ng	462878	Phenanthrene-d10	17.332

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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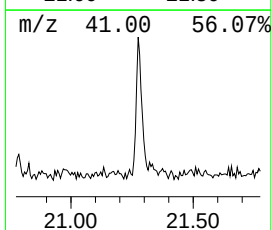
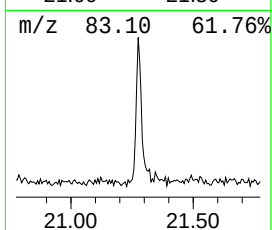
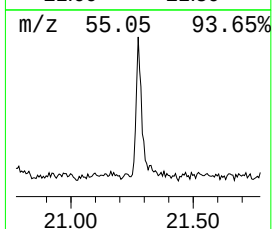
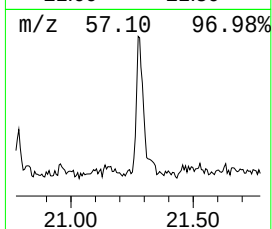
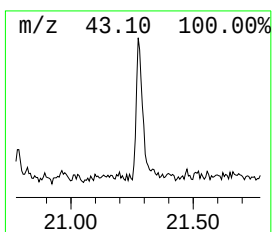
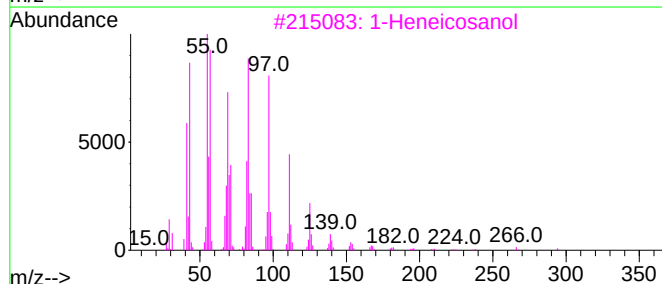
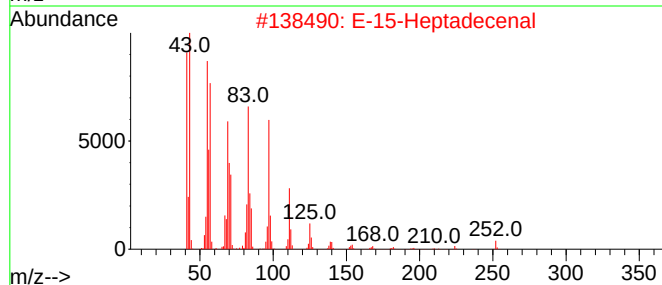
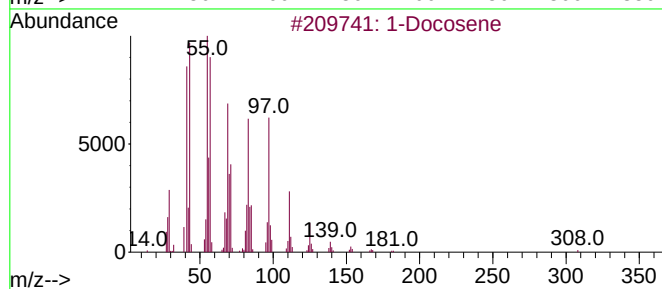
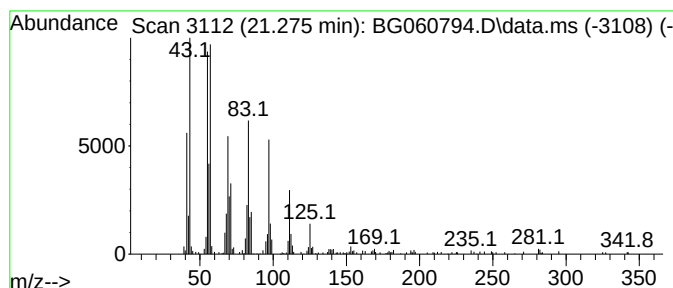
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Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.275	5.97 ng	322388	Chrysene-d12	21.592

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	94
2	E-15-Heptadecenal		252	C17H32O	1000130-97-9	94
3	1-Heneicosanol		312	C21H44O	015594-90-8	91
4	1-Hexadecanol		242	C16H34O	036653-82-4	91
5	Trichloroacetic acid, pentadecyl...		372	C17H31Cl3O2	074339-53-0	91



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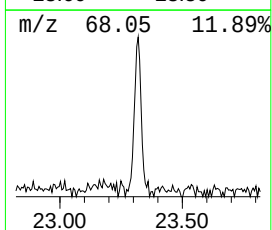
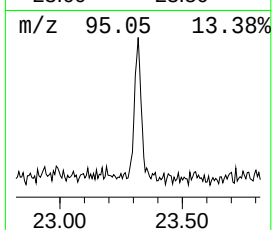
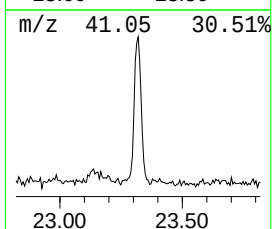
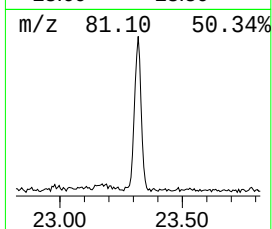
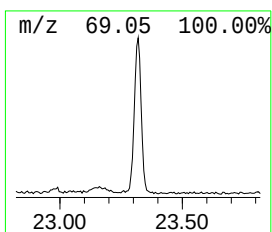
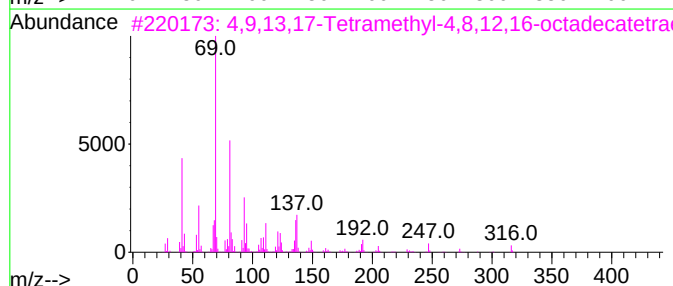
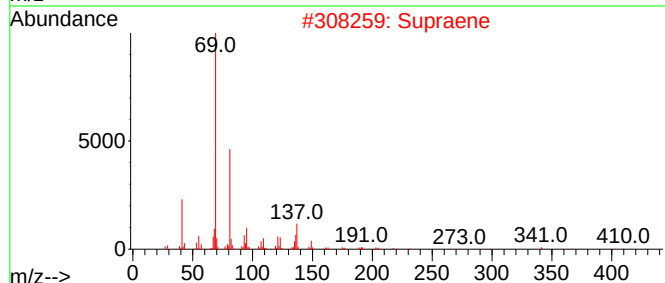
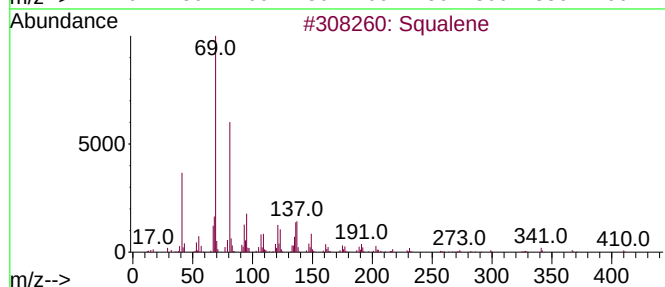
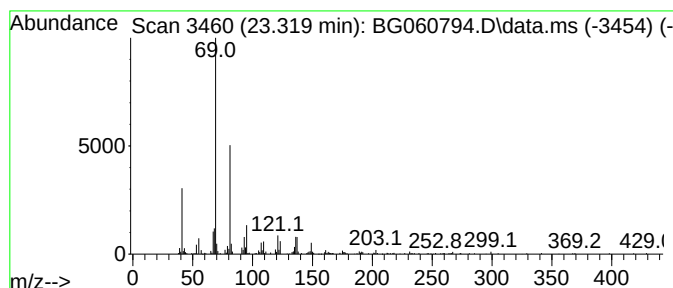
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.319	5.36 ng	321900	Perylene-d12	24.735

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			Supraene	410	C30H50	007683-64-9	87
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
4			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58
5			2,6-Octadiene, 2,7-dimethyl-	138	C10H18	016736-42-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040524\
Data File : BG060794.D
Acq On : 5 Apr 2024 13:40
Operator : MA/JU
Sample : P1996-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.178	27.4	ng	483867	1	7.955	352684	20.0
(S)-(+)-1,2-Pro...	3.689	2.4	ng	41458	1	7.955	352684	20.0
unknown14.812	14.812	18.6	ng	671591	3	14.583	722400	20.0
Tridecanoic acid	18.243	9.4	ng	462878	4	17.332	986918	20.0
1-Docosene	21.275	6.0	ng	322388	5	21.592	1079470	20.0
Squalene	23.319	5.4	ng	321900	6	24.735	1200320	20.0