

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040424\
 Data File : BG060773.D
 Acq On : 4 Apr 2024 11:13
 Operator : MA/JU
 Sample : PB159958BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB159958BL

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: BG060773.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	14	18	29	rVB2	35222	71659	1.06%	0.275%
2	5.076	350	355	364	rBV	59002	89913	1.33%	0.345%
3	5.540	426	434	445	rBV	1151925	1790747	26.56%	6.864%
4	7.121	695	703	713	rBV	1198627	1982389	29.40%	7.599%
5	7.961	838	846	852	rVB	208165	344852	5.11%	1.322%
6	9.113	1033	1042	1050	rBV	702910	1224814	18.17%	4.695%
7	10.758	1310	1322	1331	rBV	288235	504685	7.49%	1.935%
8	13.214	1733	1740	1750	rBV	1881024	2881261	42.73%	11.044%
9	14.589	1965	1974	1986	rBV2	522837	804007	11.92%	3.082%
10	16.075	2219	2227	2240	rBV	1901106	2864540	42.48%	10.980%
11	17.338	2434	2442	2448	rBV	812146	1242043	18.42%	4.761%
12	19.442	2795	2800	2804	rBV	55045	67604	1.00%	0.259%
13	19.677	2835	2840	2845	rBV	157124	202337	3.00%	0.776%
14	19.965	2881	2889	2897	rBV	4891308	6742507	100.00%	25.845%
15	20.723	3014	3018	3023	rBV	143837	173566	2.57%	0.665%
16	21.598	3161	3167	3179	rVB	981884	1577282	23.39%	6.046%
17	23.143	3426	3430	3438	rVB2	84531	161158	2.39%	0.618%
18	23.948	3562	3567	3576	rVB	116940	242654	3.60%	0.930%
19	24.747	3693	3703	3715	rVB	578930	1646302	24.42%	6.311%
20	24.900	3722	3729	3737	rVB2	135336	337674	5.01%	1.294%
21	26.034	3913	3922	3933	rVB2	117560	375743	5.57%	1.440%
22	27.385	4143	4152	4166	rVB3	113772	415830	6.17%	1.594%
23	29.031	4421	4432	4445	rVB4	83617	344620	5.11%	1.321%

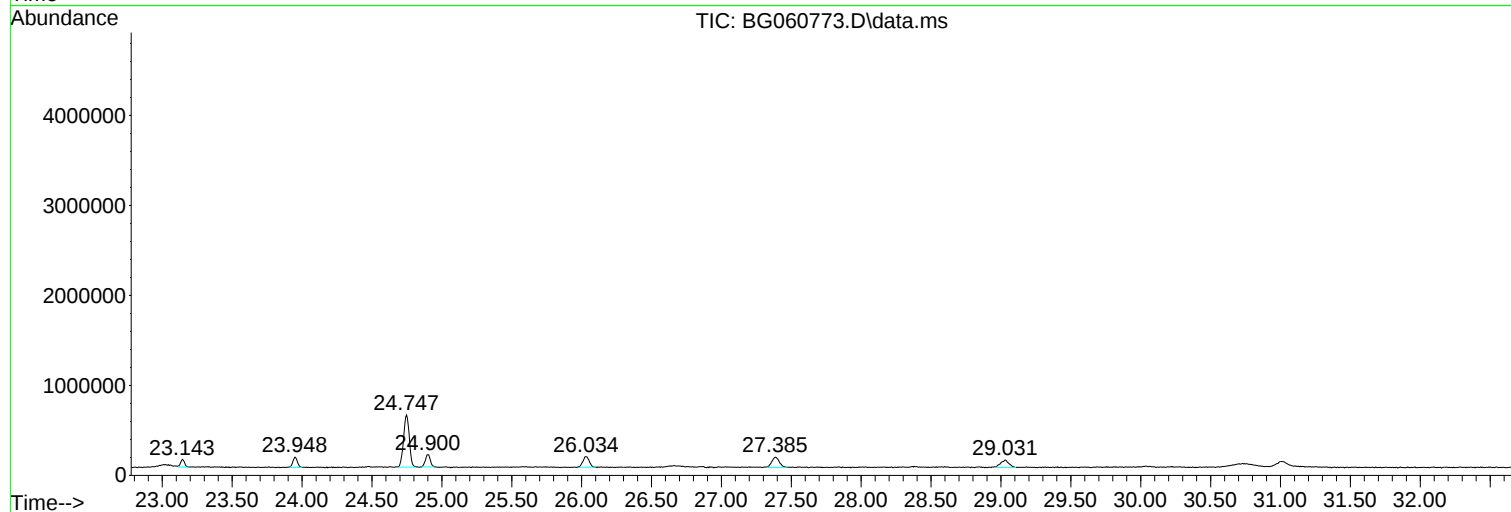
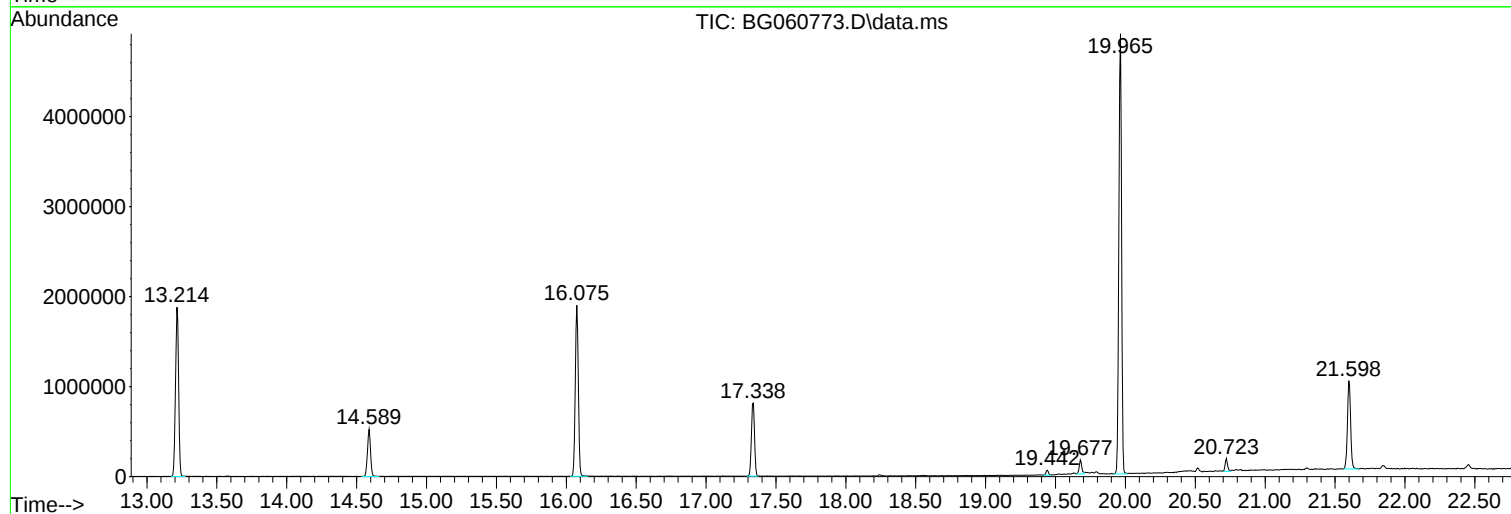
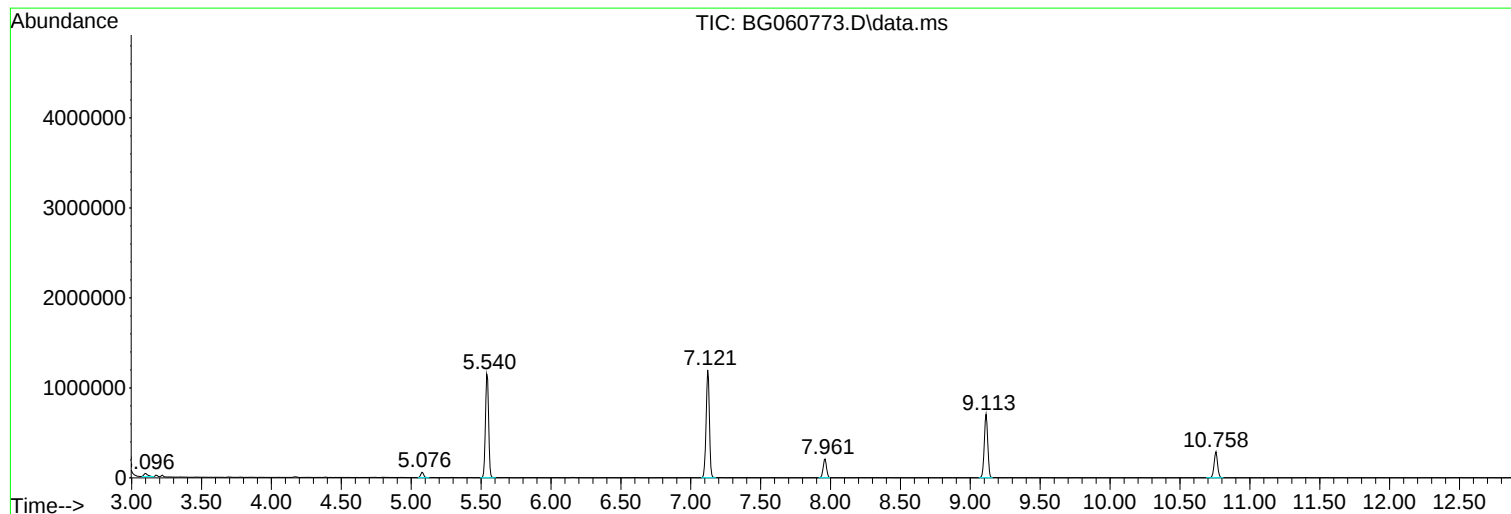
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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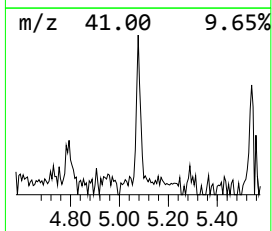
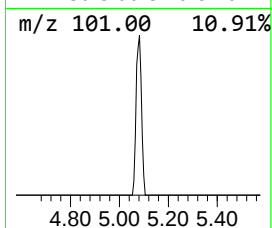
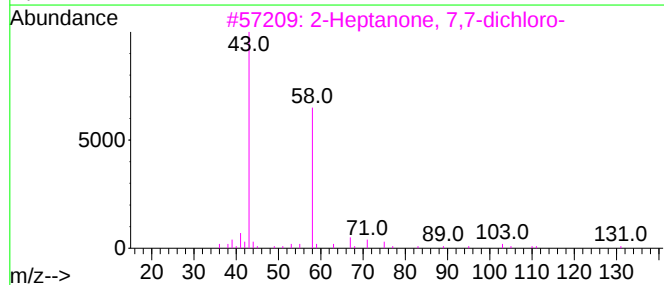
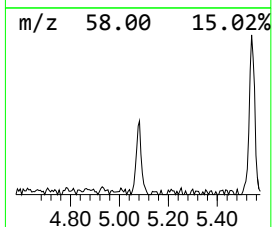
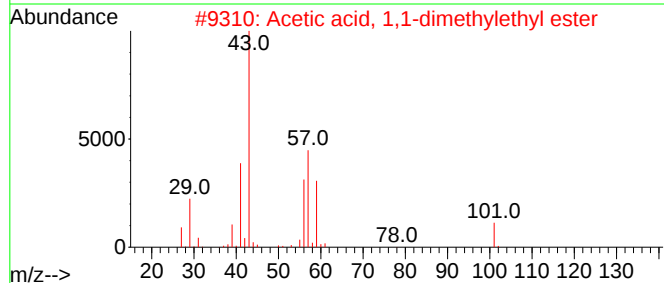
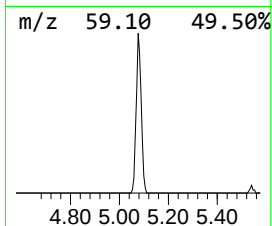
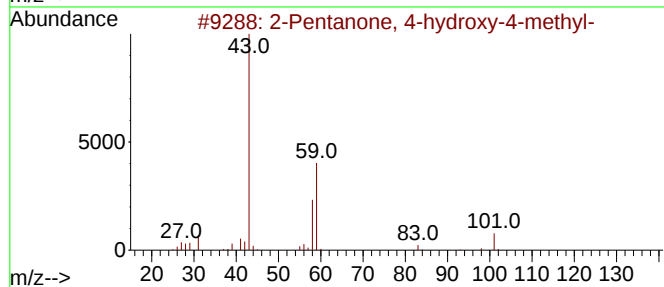
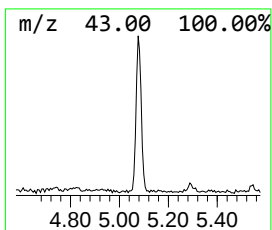
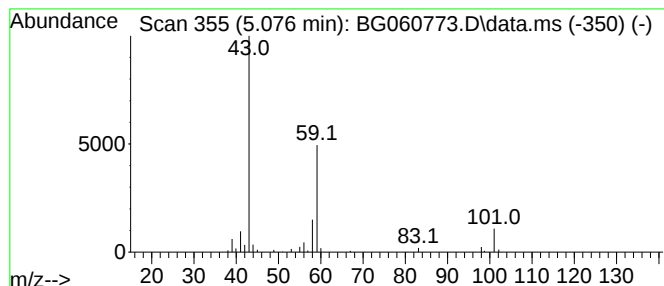
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.076	5.21 ng	89913	1,4-Dichlorobenzene-d4	7.961

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28	
3	2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	12	
4	Propylamine	59	C3H9N	000107-10-8	9	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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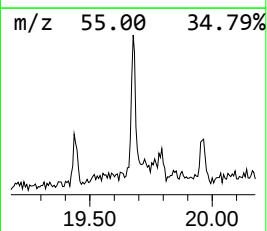
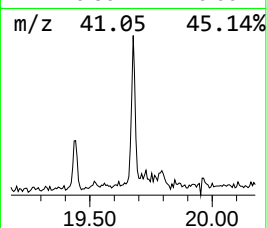
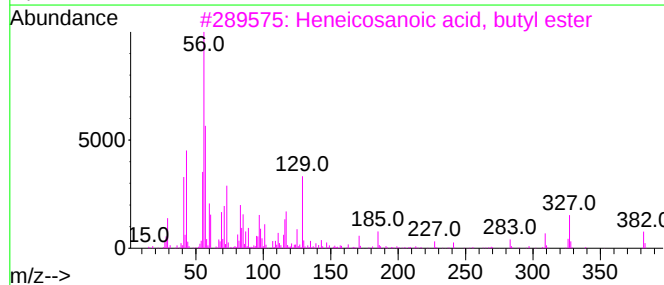
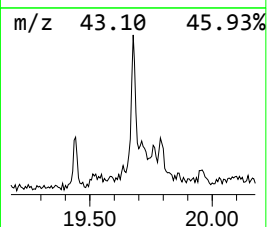
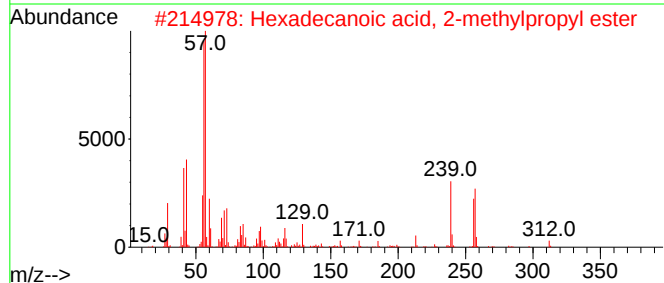
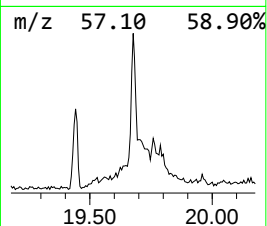
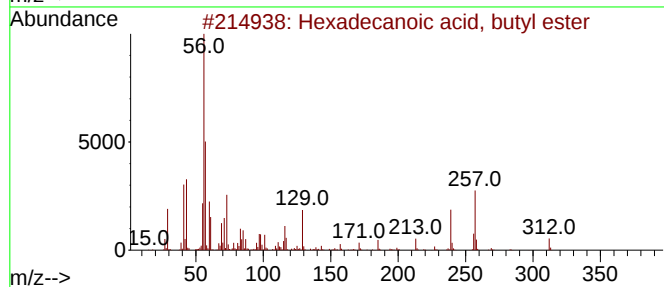
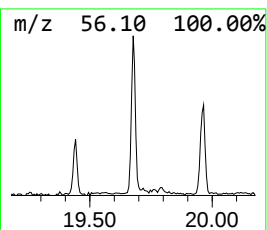
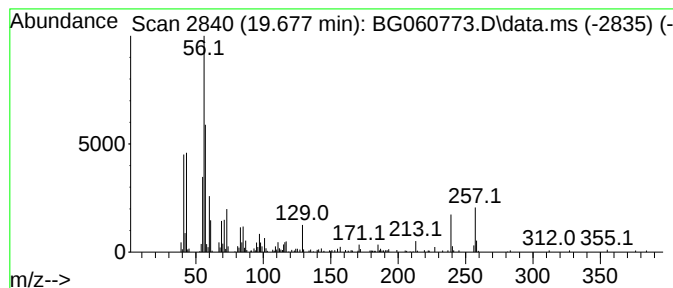
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Peak Number 3 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.677	2.57 ng	202337	Chrysene-d12	21.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	87
3			Heneicosanoic acid, butyl ester	382	C25H50O2	1000405-18-0	59
4			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43



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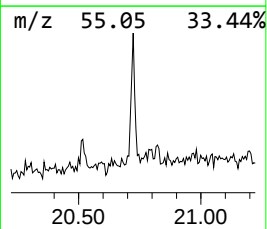
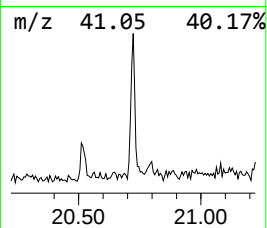
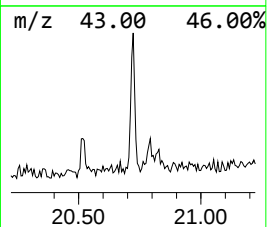
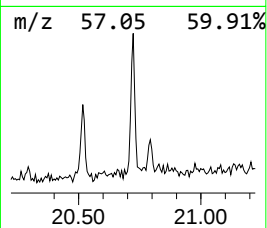
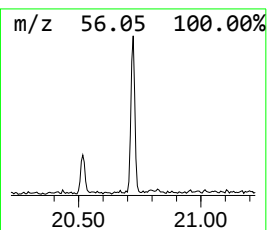
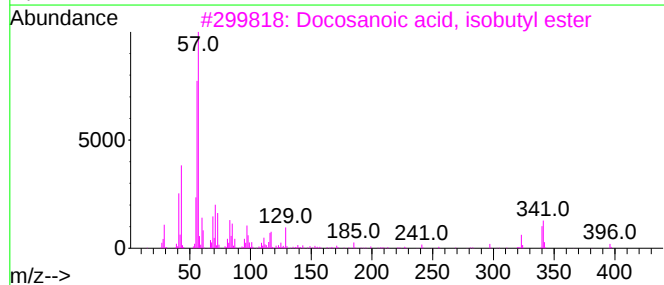
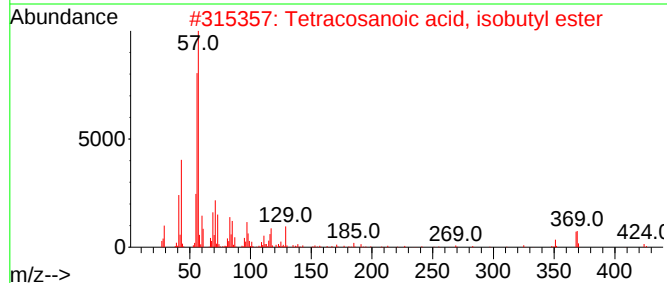
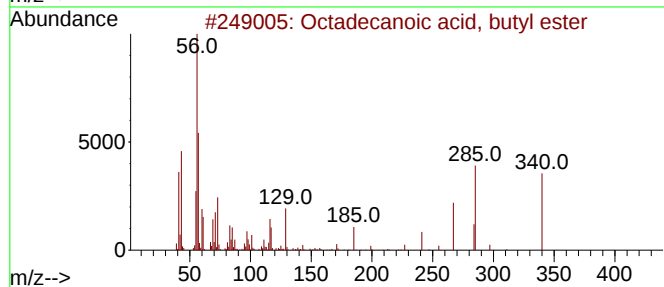
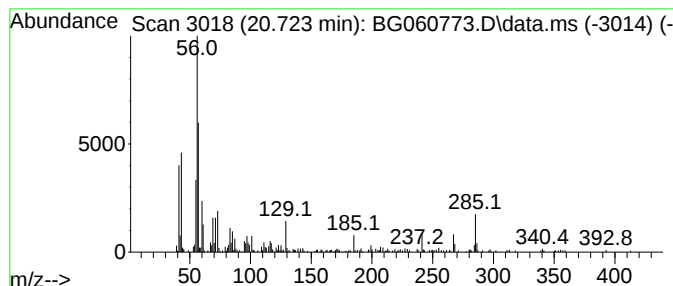
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.723	2.20 ng	173566	Chrysene-d12	21.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	64
2			Tetracosanoic acid, isobutyl ester	424	C28H56O2	1010405-17-3	50
3			Docosanoic acid, isobutyl ester	396	C26H52O2	1000405-17-1	38
4			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
5			Docosanoic acid, butyl ester	396	C26H52O2	026718-96-7	38



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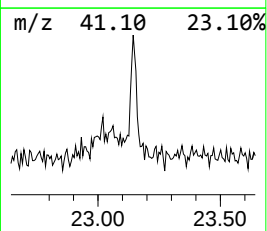
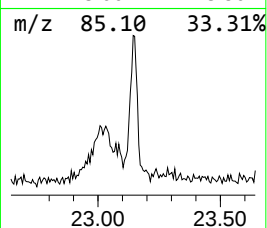
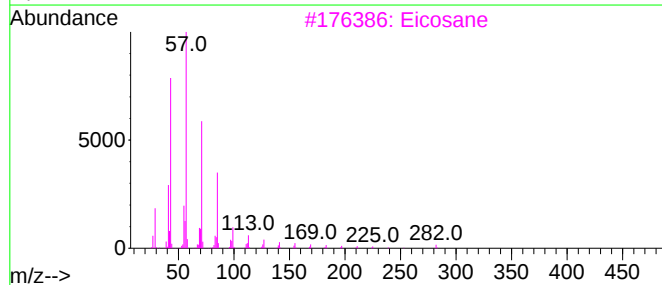
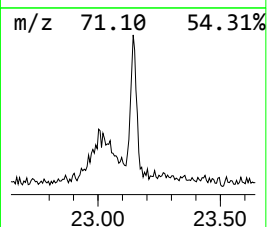
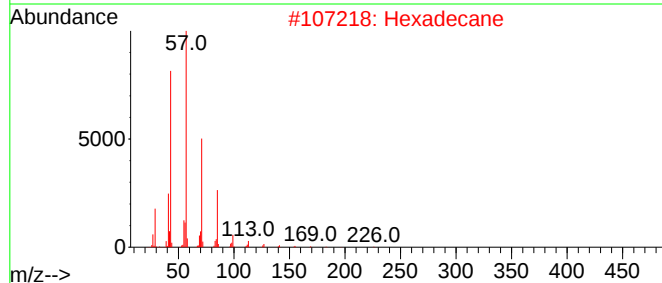
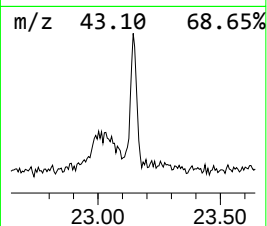
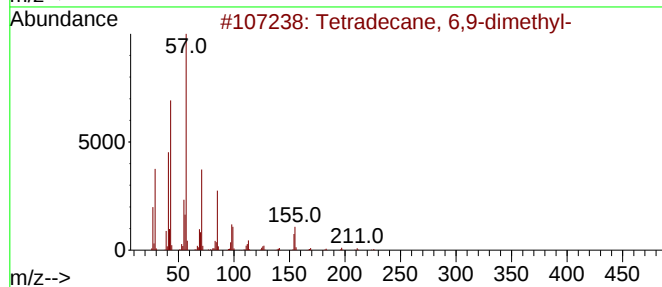
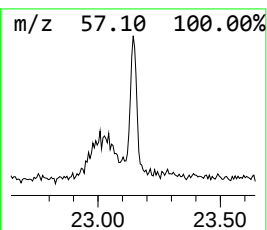
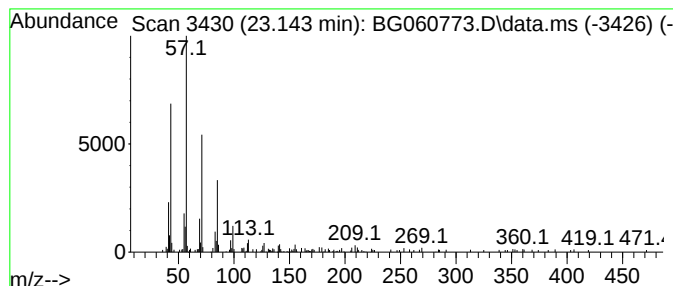
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Peak Number 5 Tetradecane, 6,9-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.143	2.04 ng	161158	Chrysene-d12	21.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 6,9-dimethyl-	226	C16H34	055045-13-1	87
2			Hexadecane	226	C16H34	000544-76-3	87
3			Eicosane	282	C20H42	000112-95-8	83
4			Tridecane, 7-hexyl-	268	C19H40	007225-66-3	80
5			Heptadecane	240	C17H36	000629-78-7	80



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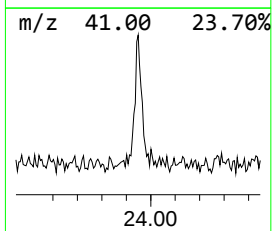
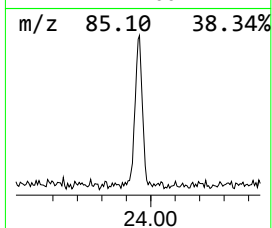
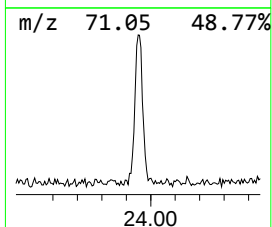
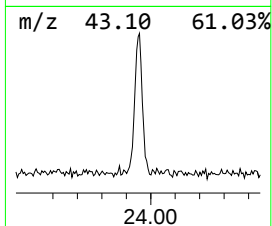
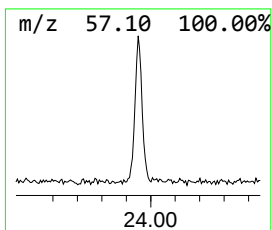
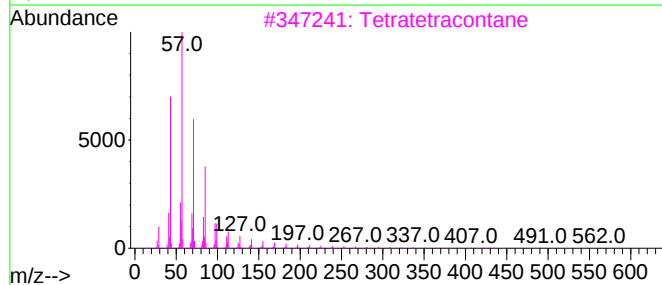
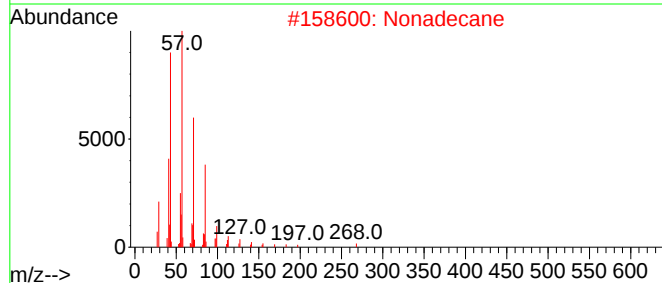
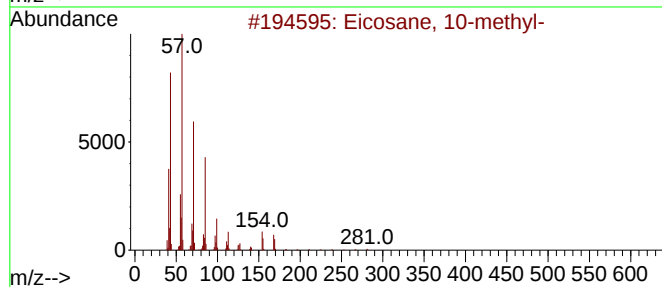
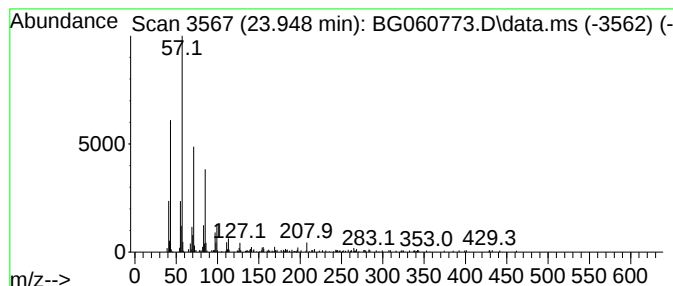
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Peak Number 6 Eicosane, 10-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.948	2.95 ng	242654	Perylene-d12	24.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
2			Nonadecane	268	C19H40	000629-92-5	90
3			Tetratetracontane	619	C44H90	007098-22-8	87
4			Tricosane, 2-methyl-	338	C24H50	001928-30-9	87
5			Tetracosane	338	C24H50	000646-31-1	83



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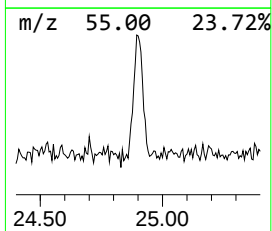
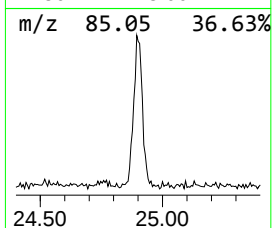
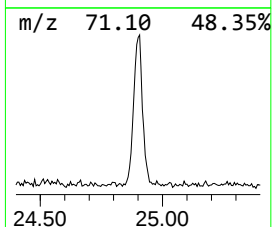
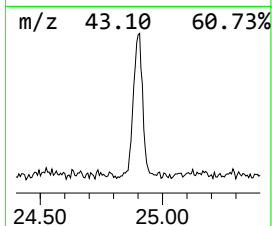
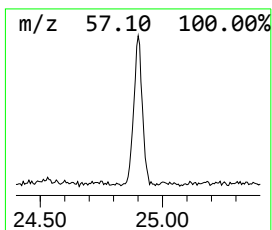
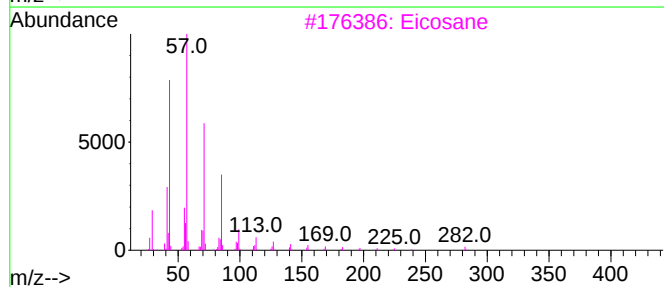
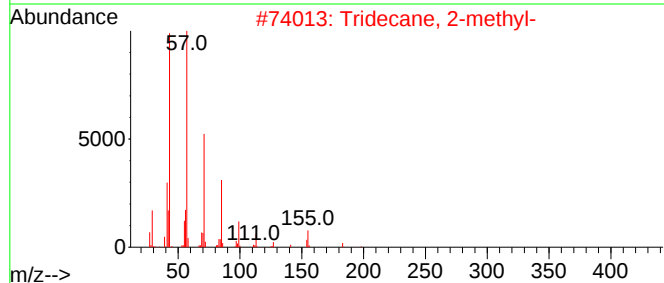
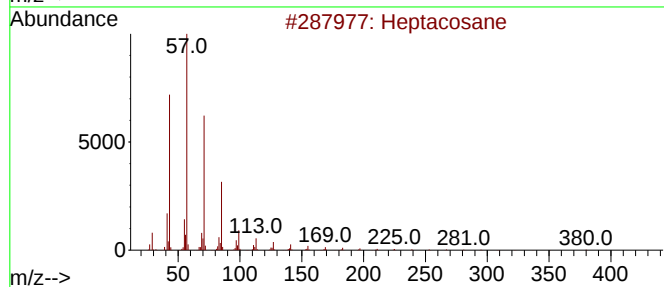
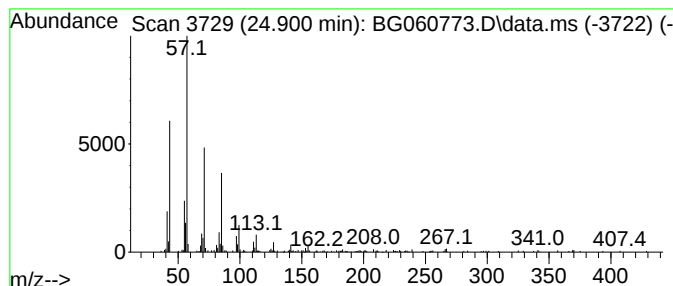
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.900	4.10 ng	337674	Perylene-d12	24.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	87
2			Tridecane, 2-methyl-	198	C14H30	001560-96-9	87
3			Eicosane	282	C20H42	000112-95-8	87
4			Hentriacontane	437	C31H64	000630-04-6	87
5			Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040424\
Data File : BG060773.D
Acq On : 4 Apr 2024 11:13
Operator : MA/JU
Sample : PB159958BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB159958BL

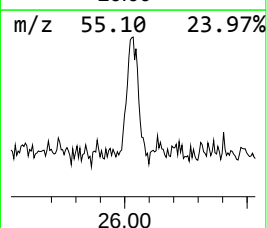
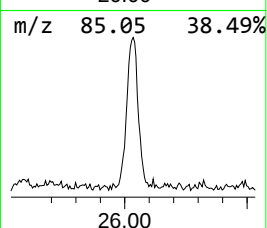
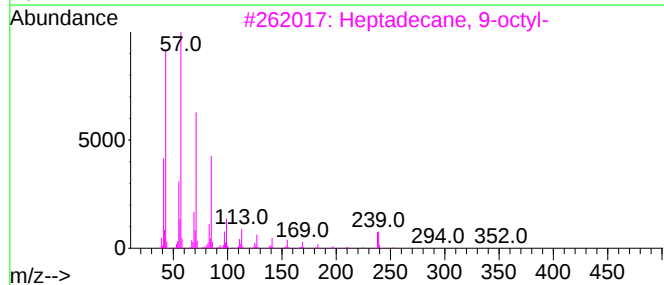
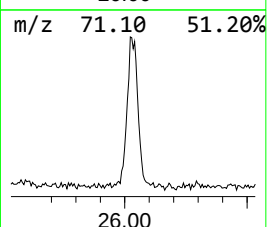
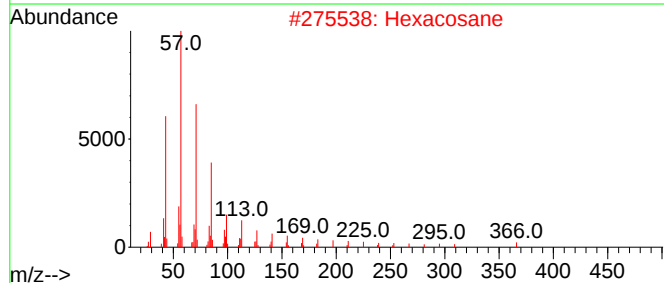
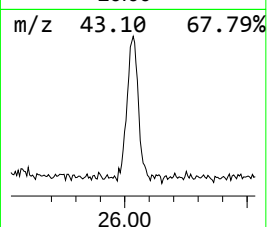
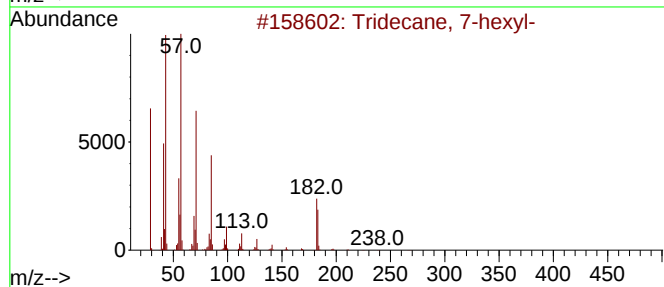
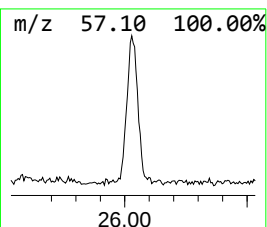
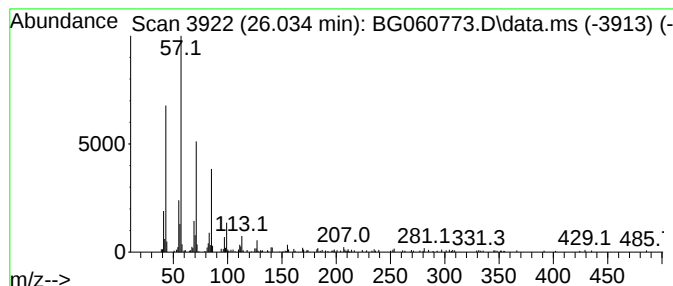
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecane, 7-hexyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.034	4.56 ng	375743	Perylene-d12	24.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 7-hexyl-	268	C19H40	007225-66-3	93
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4			Heptacosane	380	C27H56	000593-49-7	83
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040424\
Data File : BG060773.D
Acq On : 4 Apr 2024 11:13
Operator : MA/JU
Sample : PB159958BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

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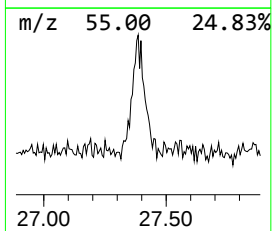
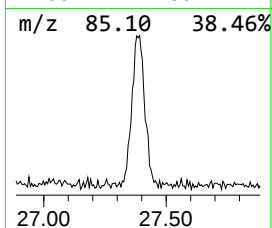
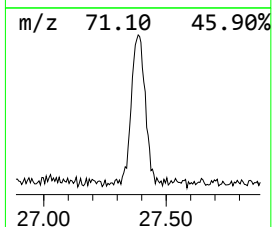
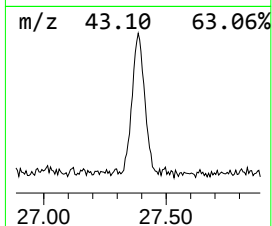
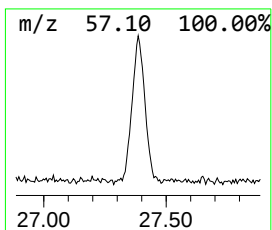
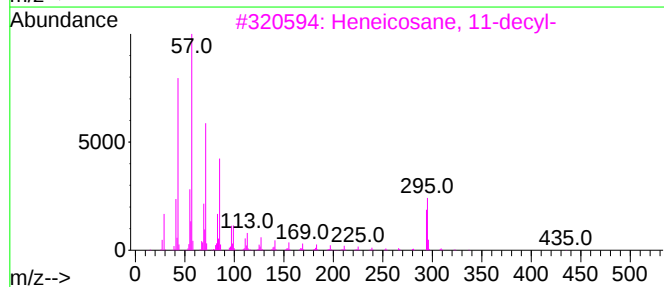
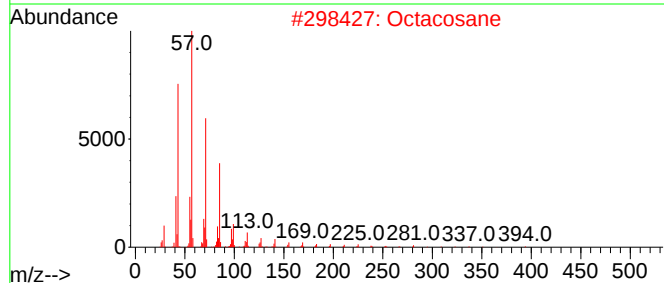
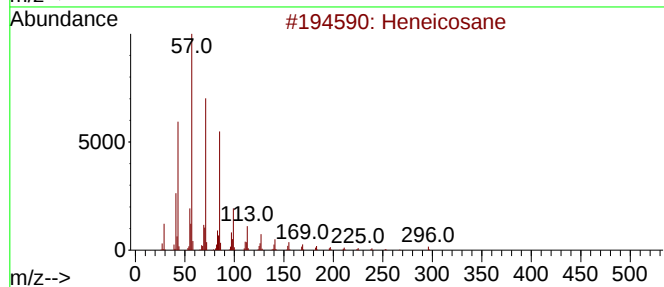
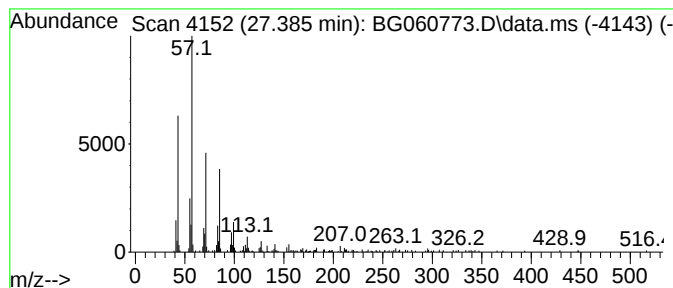
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.386	5.05 ng	415830	Perylene-d12	24.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	95
2			Octacosane	394	C28H58	000630-02-4	90
3			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87
4			Tetracosane	338	C24H50	000646-31-1	87
5			Hexatriacontane	507	C36H74	000630-06-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040424\
Data File : BG060773.D
Acq On : 4 Apr 2024 11:13
Operator : MA/JU
Sample : PB159958BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB159958BL

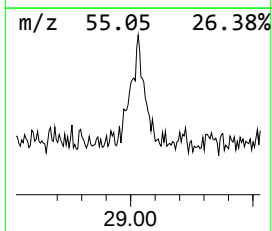
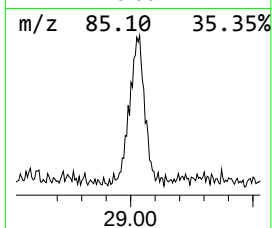
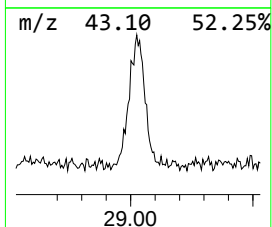
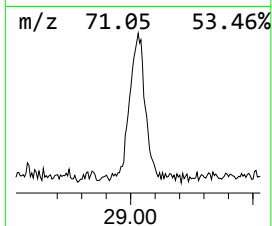
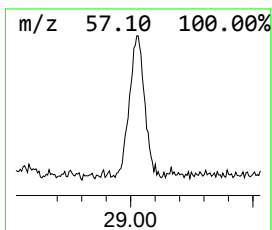
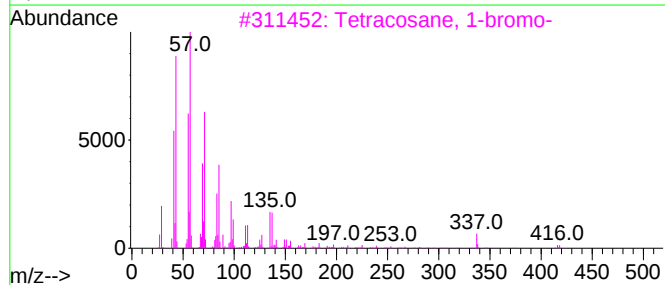
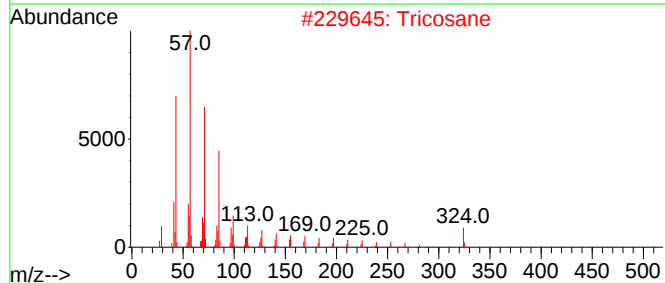
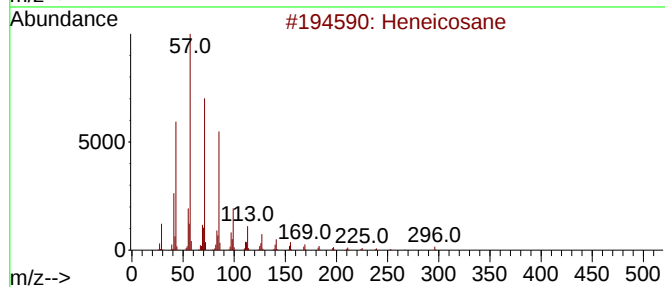
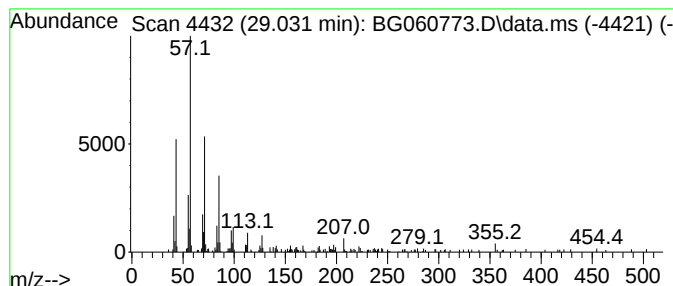
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tricosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.031	4.19 ng	344620	Perylene-d12	24.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	97
2			Tricosane	324	C23H48	000638-67-5	89
3			Tetracosane, 1-bromo-	416	C24H49Br	006946-24-3	81
4			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	76
5			Hentriacontane	437	C31H64	000630-04-6	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040424\
Data File : BG060773.D
Acq On : 4 Apr 2024 11:13
Operator : MA/JU
Sample : PB159958BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB159958BL

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
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Hexadecanoic ac...	19.677	2.6	ng	202337	5	21.598	1577280	20.0
Octadecanoic ac...	20.723	2.2	ng	173566	5	21.598	1577280	20.0
Tetradecane, 6,...	23.143	2.0	ng	161158	5	21.598	1577280	20.0
Eicosane, 10-me...	23.948	3.0	ng	242654	6	24.747	1646300	20.0
Heptacosane	24.900	4.1	ng	337674	6	24.747	1646300	20.0
Tridecane, 7-he...	26.034	4.6	ng	375743	6	24.747	1646300	20.0
Heneicosane	27.386	5.0	ng	415830	6	24.747	1646300	20.0
Tricosane	29.031	4.2	ng	344620	6	24.747	1646300	20.0