

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
 Data File : BG057792.D
 Acq On : 21 Jun 2023 20:07
 Operator : CG/JU
 Sample : 03074-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GP-01

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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057792.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.494	402	409	419	rVB	646117	981023	35.14%	7.181%
2	7.080	671	679	688	rBV	639895	1085631	38.89%	7.946%
3	7.920	816	822	828	rBV	120508	195894	7.02%	1.434%
4	9.084	1010	1020	1031	rBV	369205	642477	23.02%	4.703%
5	10.723	1292	1299	1307	rBV	179078	311576	11.16%	2.281%
6	13.179	1710	1717	1729	rBV	975248	1514016	54.24%	11.082%
7	14.554	1945	1951	1958	rVB	298321	466167	16.70%	3.412%
8	15.911	2177	2182	2189	rBV	97730	134427	4.82%	0.984%
9	16.040	2197	2204	2212	rBV	906711	1395887	50.01%	10.217%
10	17.297	2412	2418	2426	rBV	459340	676727	24.24%	4.953%
11	18.190	2564	2570	2585	rBV2	93733	160721	5.76%	1.176%
12	19.377	2767	2772	2776	rVB	61114	74472	2.67%	0.545%
13	19.465	2783	2787	2793	rBV3	25304	43889	1.57%	0.321%
14	19.612	2807	2812	2817	rBV	141570	151094	5.41%	1.106%
15	19.730	2828	2832	2836	rVB	29614	38497	1.38%	0.282%
16	19.918	2858	2864	2870	rBV	2144099	2791387	100.00%	20.432%
17	20.447	2951	2954	2958	rVB	40771	44812	1.61%	0.328%
18	20.652	2985	2989	2993	rBV	111460	118898	4.26%	0.870%
19	20.717	2996	3000	3003	rVB	31415	36685	1.31%	0.269%
20	21.169	3071	3077	3080	rBV	52741	104713	3.75%	0.766%
21	21.205	3080	3083	3092	rVV3	177477	376602	13.49%	2.757%
22	21.287	3092	3097	3106	rVB	216929	317450	11.37%	2.324%
23	21.551	3135	3142	3149	rBV	483988	759483	27.21%	5.559%
24	21.751	3172	3176	3181	rVB	51885	68390	2.45%	0.501%
25	22.344	3273	3277	3288	rVB2	43134	86826	3.11%	0.636%
26	23.026	3389	3393	3399	rVB	33301	54737	1.96%	0.401%
27	23.819	3522	3528	3534	rBV2	28258	59984	2.15%	0.439%
28	24.701	3669	3678	3693	rVB2	301727	900993	32.28%	6.595%
29	25.975	3889	3895	3903	rVB6	26630	68628	2.46%	0.502%

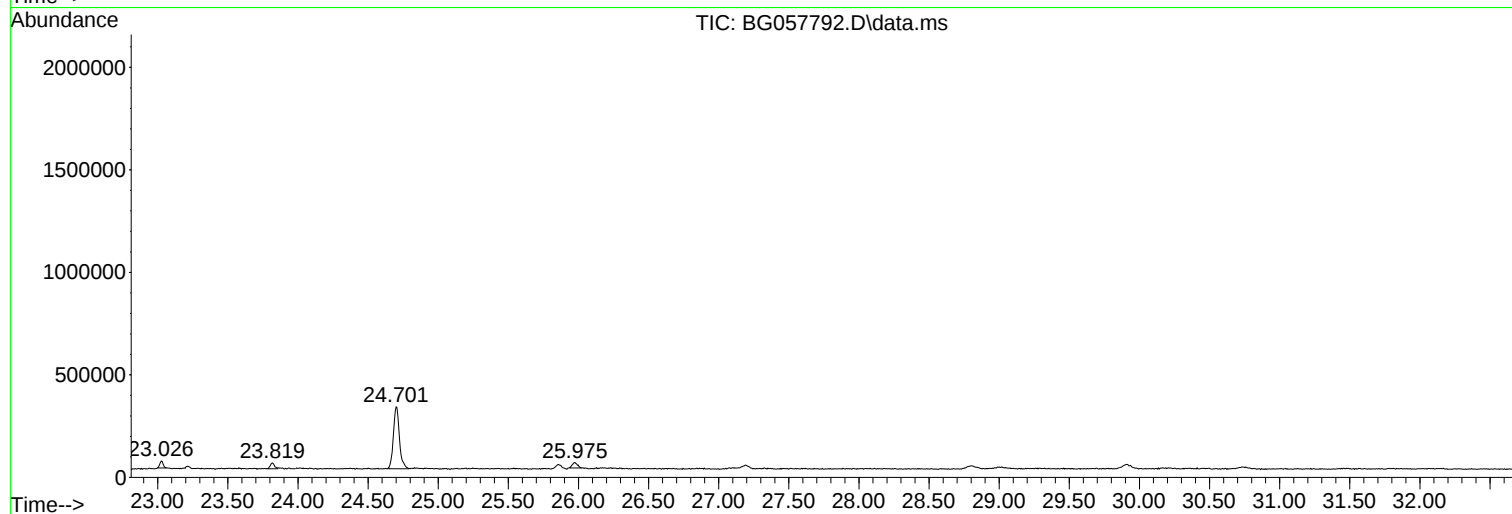
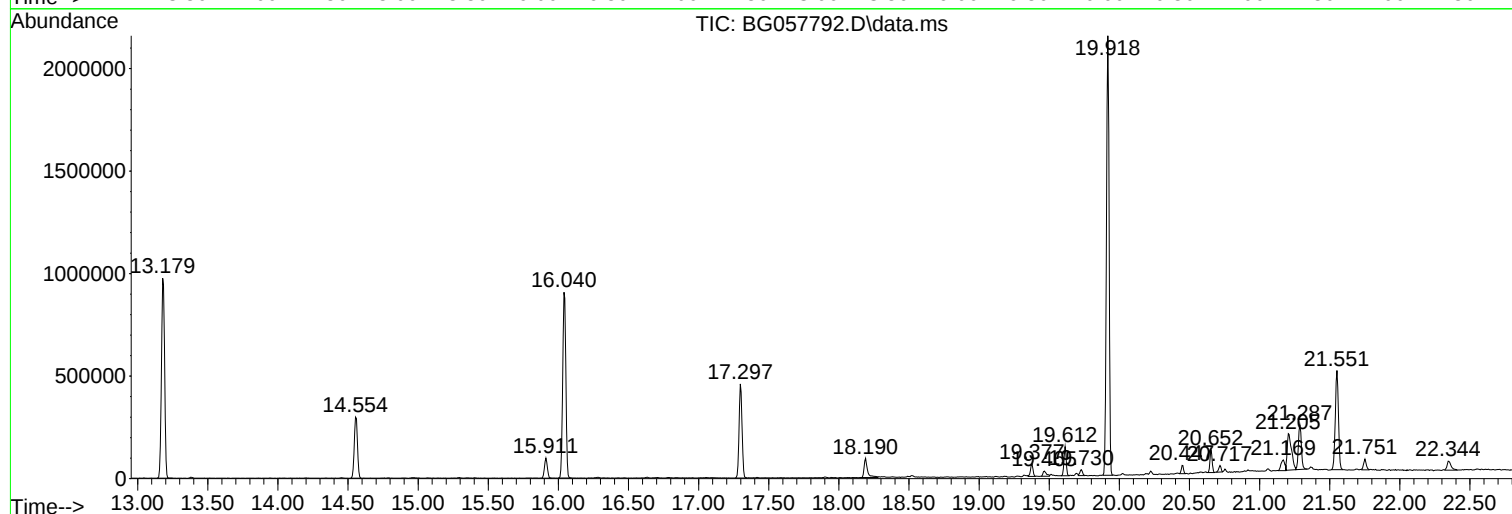
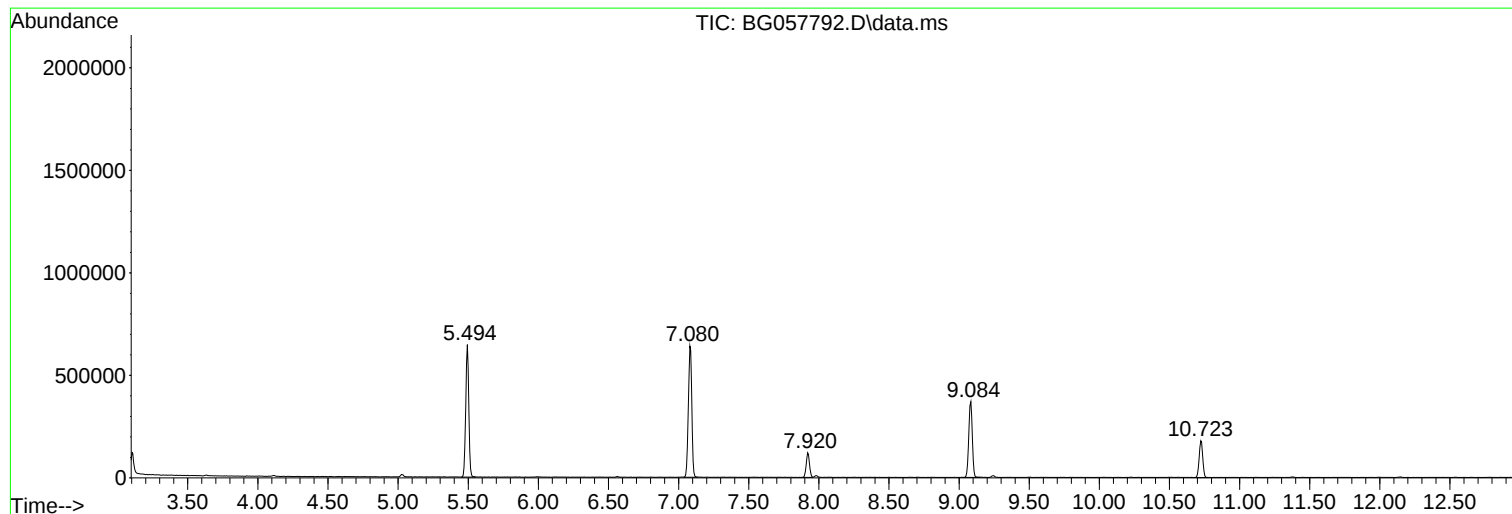
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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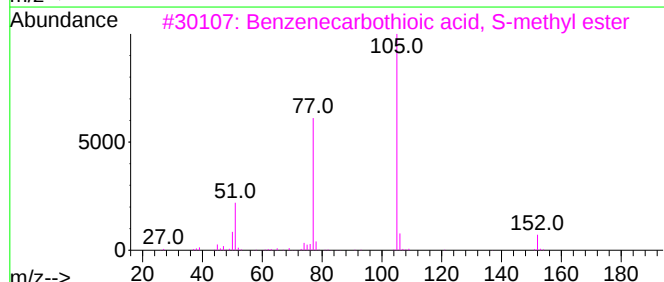
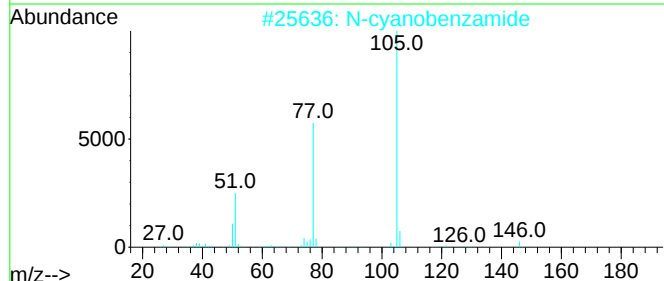
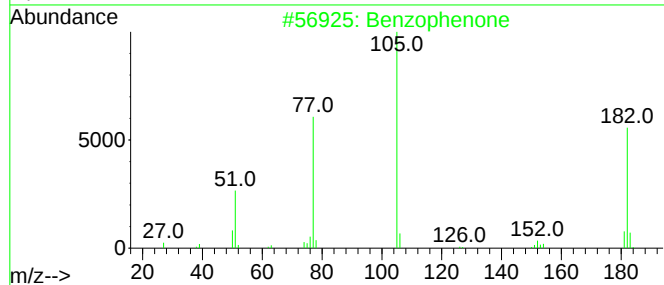
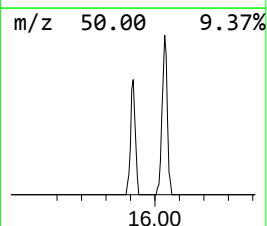
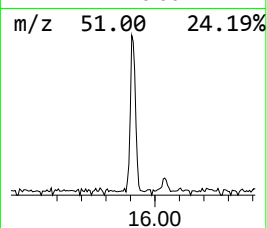
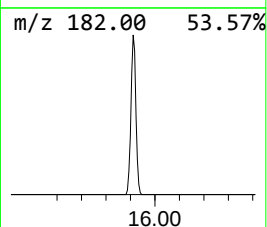
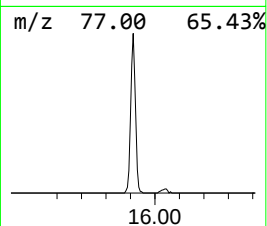
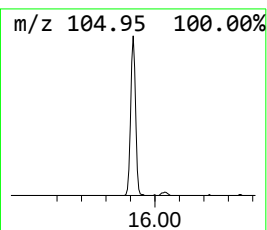
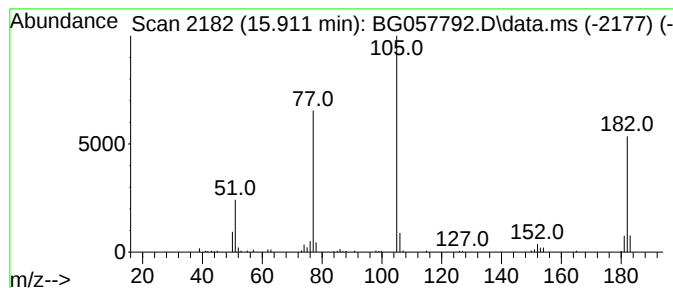
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.911	5.77 ng	134427	Acenaphthene-d10	14.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-cyanobenzamide	146	C8H6N2O	015150-25-1	50
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50



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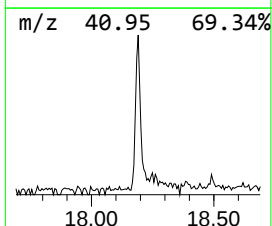
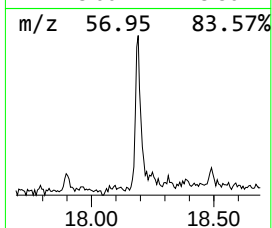
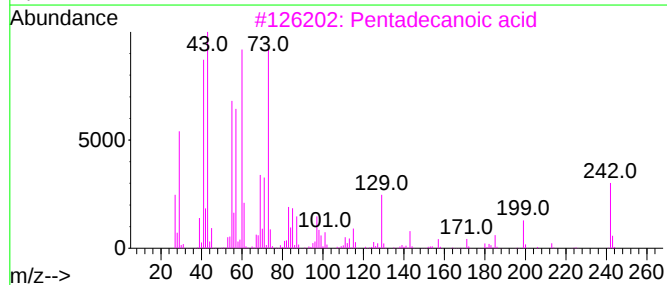
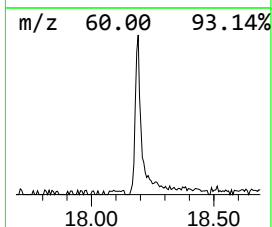
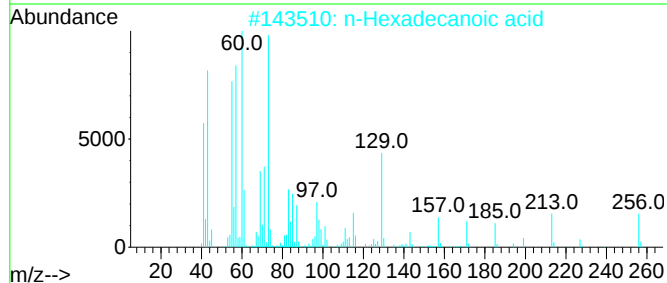
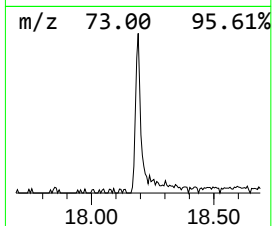
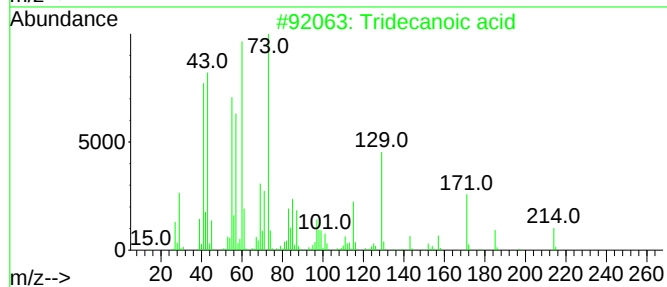
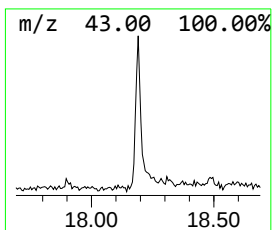
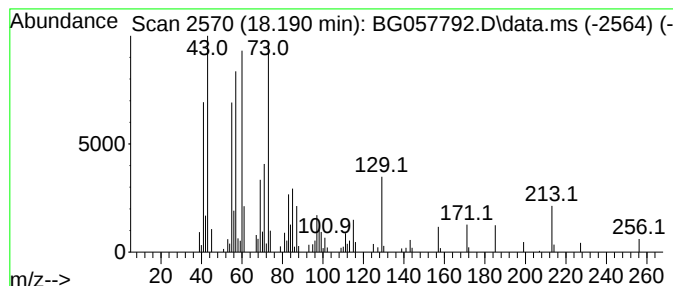
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Peak Number 2 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.191	4.75 ng	160721	Phenanthrene-d10	17.297

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	90
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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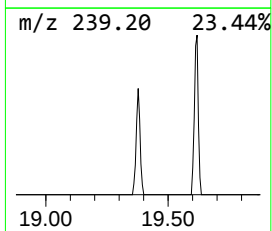
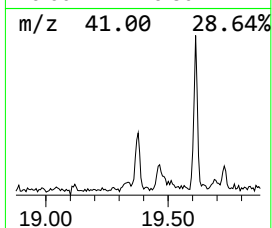
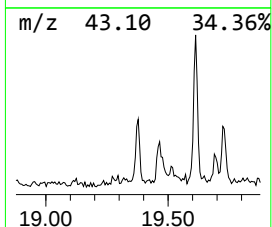
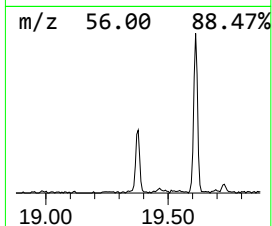
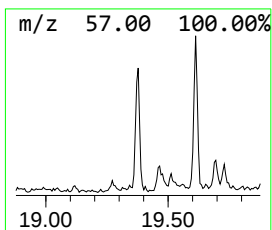
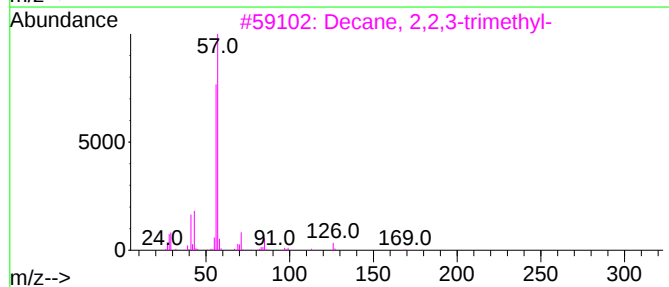
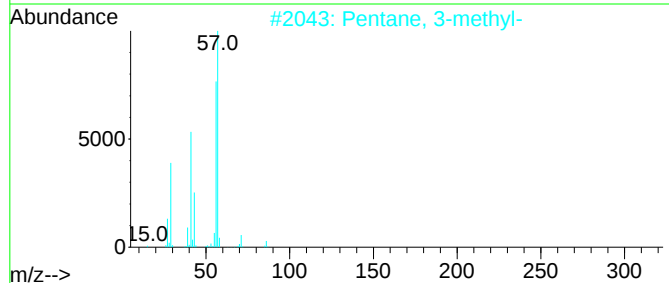
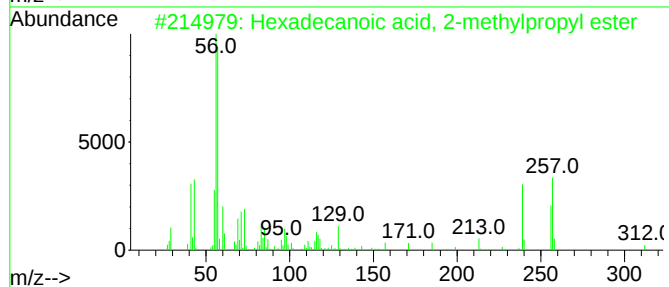
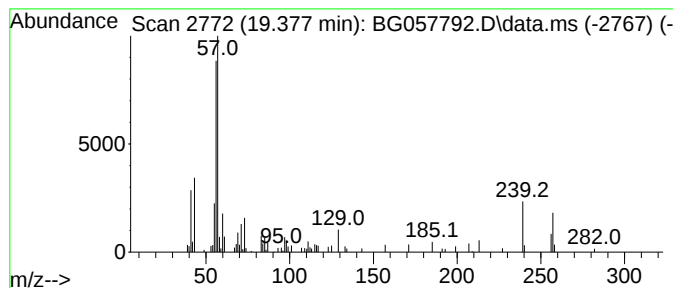
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Peak Number 3 Hexadecanoic acid, 2-methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.377	2.20 ng	74472	Phenanthrene-d10	17.297

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	72
2			Pentane, 3-methyl-	86	C6H14	000096-14-0	46
3			Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	43
4			Nonane, 2,2,3-trimethyl-	170	C12H26	055499-04-2	43
5			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43



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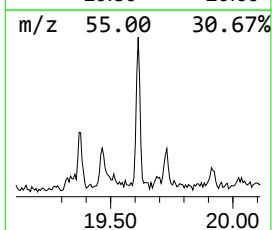
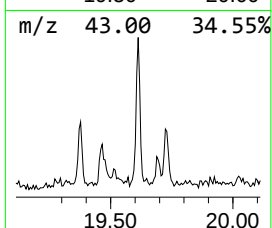
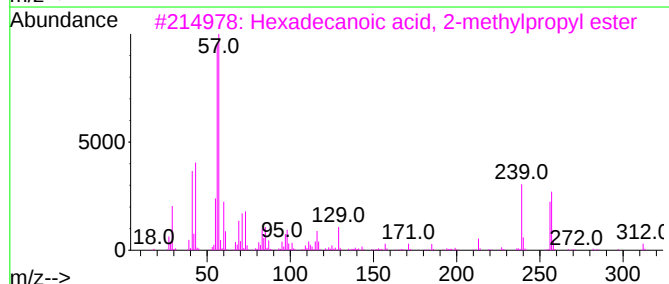
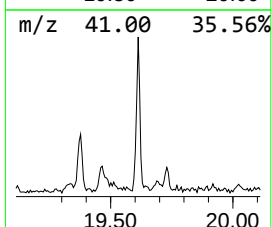
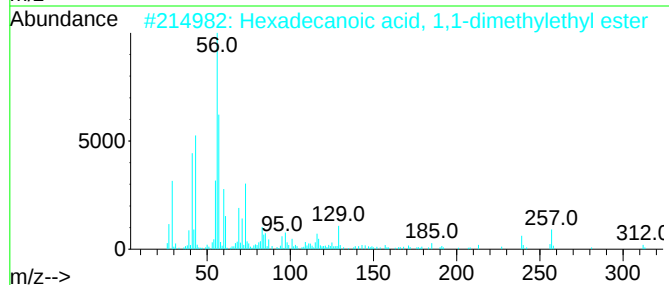
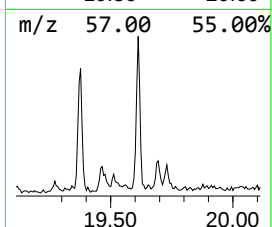
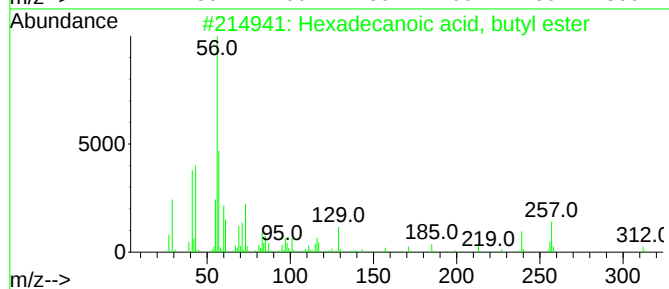
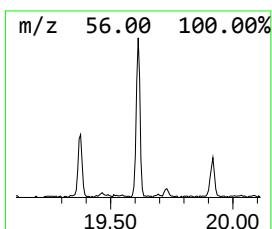
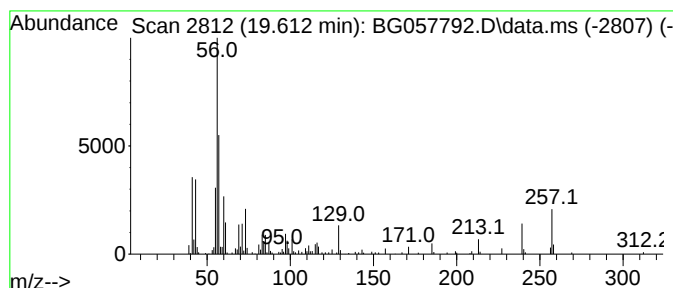
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.612	3.98 ng	151094	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	38
4			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38



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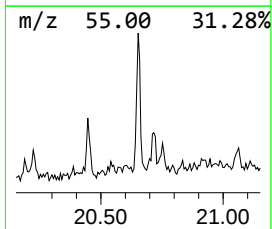
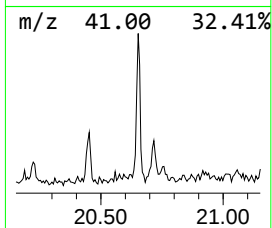
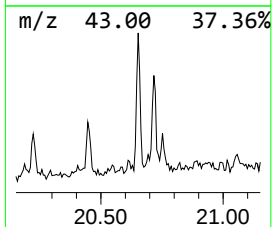
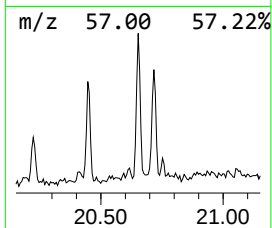
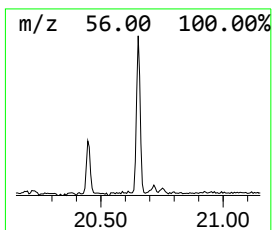
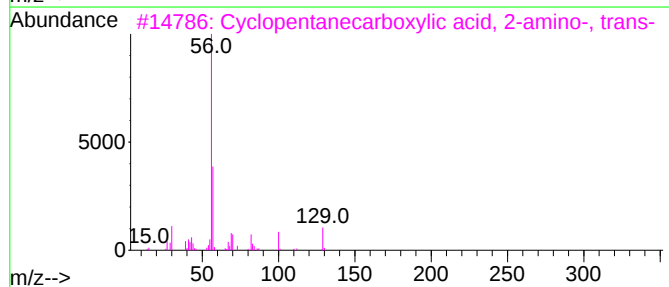
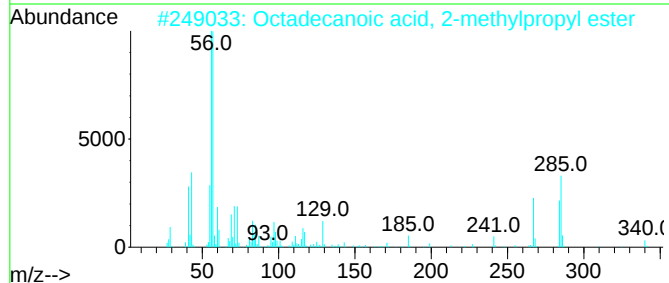
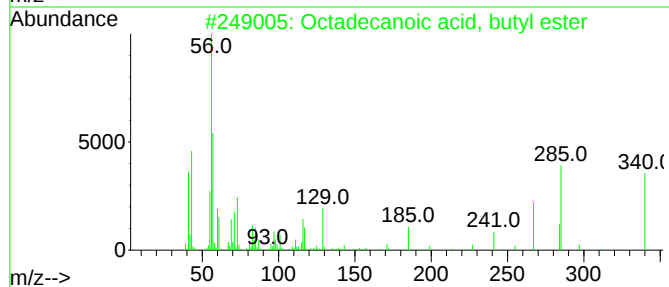
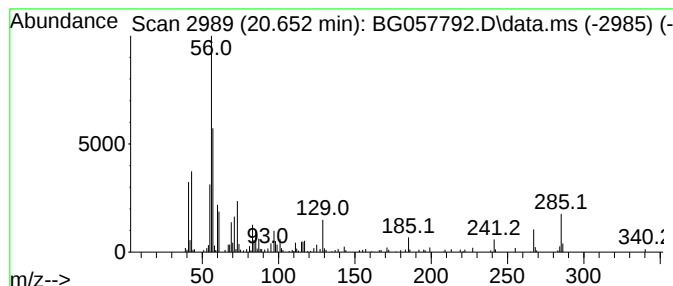
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.652	3.13 ng	118898	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2			Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	70
3			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
4			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
5			Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37



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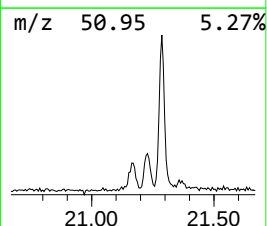
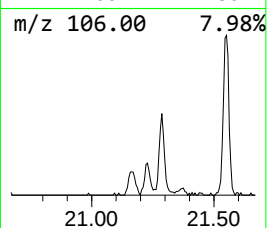
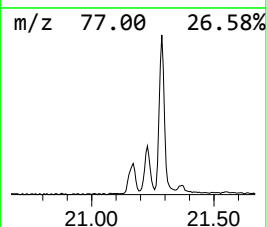
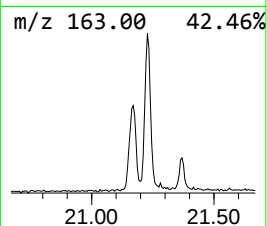
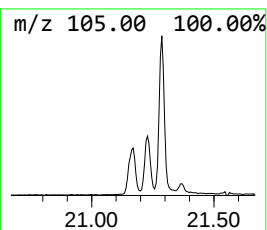
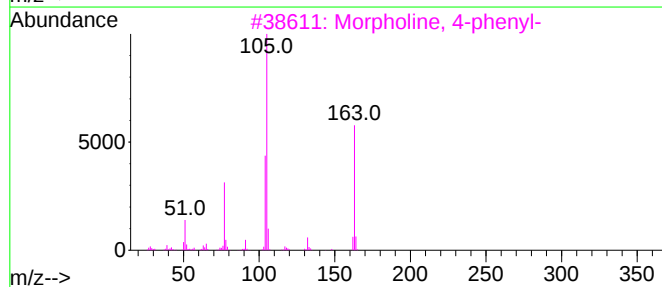
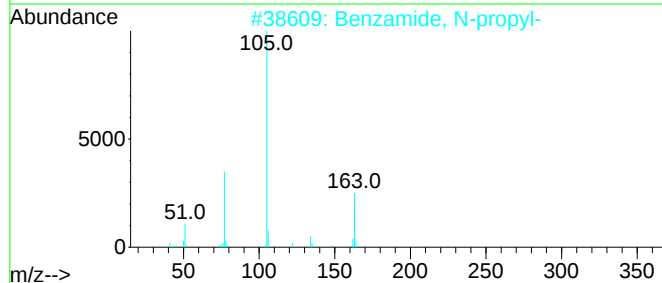
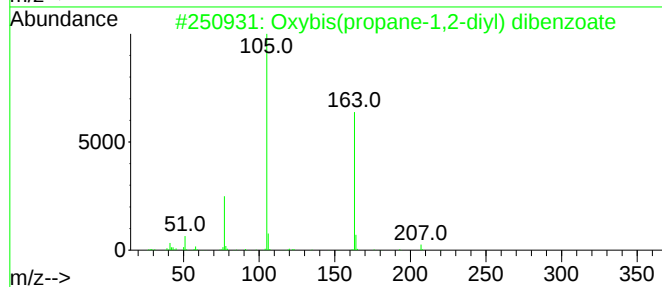
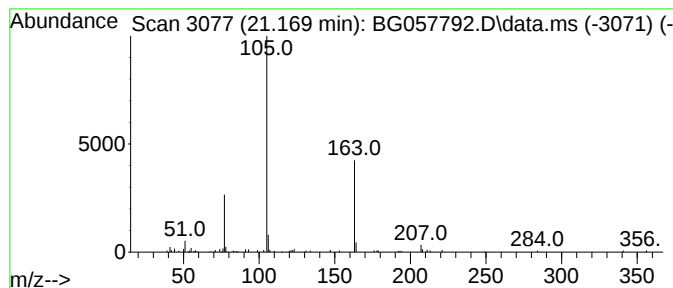
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Oxybis(propene-1,2-diyl) di... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.169	2.76 ng	104713	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	72
2			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
3			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	52
4			N-(6-Methoxy-1,3-benzothiazol-2(...	284	C15H12N2O2S	035353-26-5	35
5			Imidazole, 2-fluoro-1-tribenzoyl...	530	C29H23FN2O7	1000129-58-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057792.D
Acq On : 21 Jun 2023 20:07
Operator : CG/JU
Sample : 03074-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GP-01

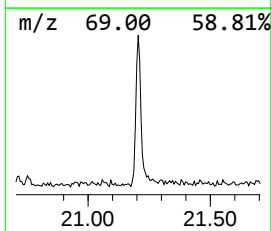
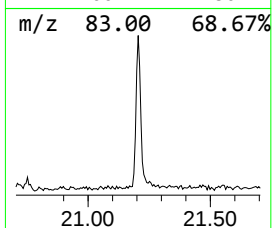
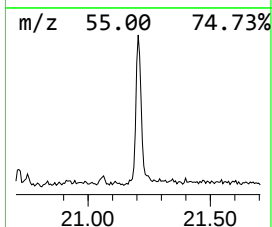
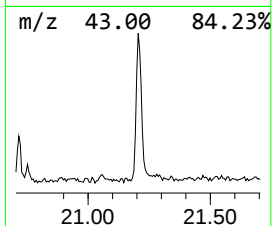
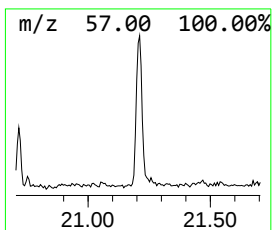
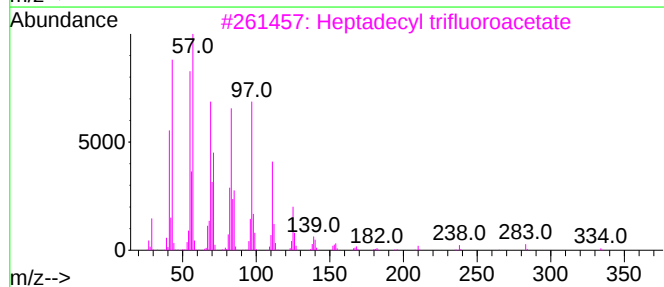
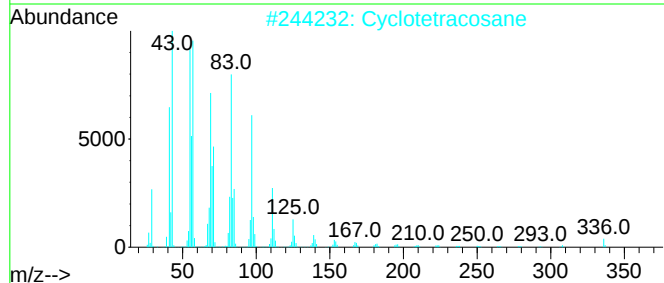
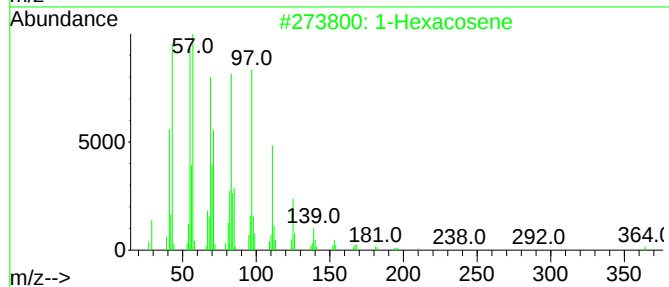
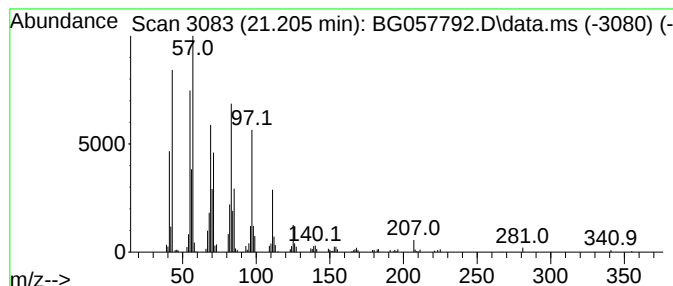
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Hexacosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.205	9.92 ng	376602	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosene	364	C26H52	018835-33-1	94
2			Cyclotetracosane	336	C24H48	000297-03-0	94
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057792.D
Acq On : 21 Jun 2023 20:07
Operator : CG/JU
Sample : 03074-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

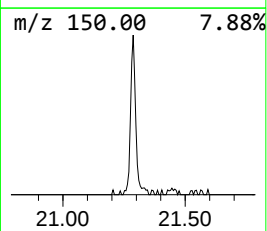
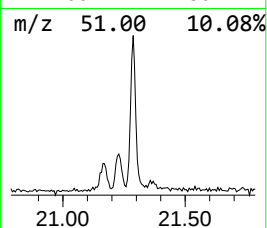
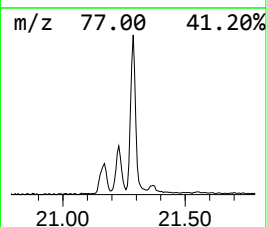
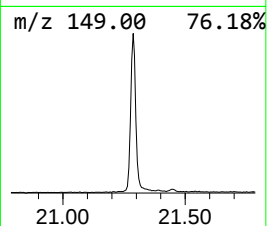
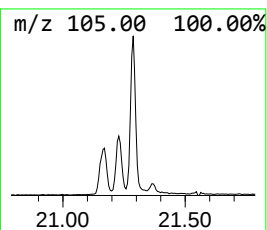
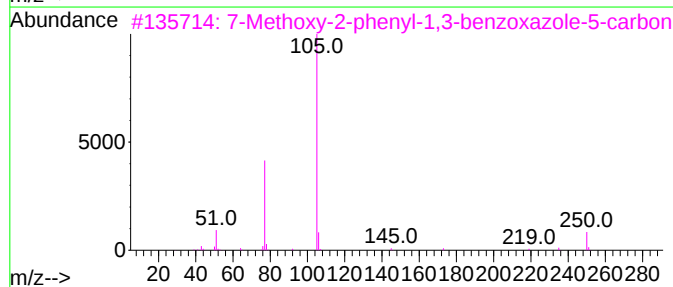
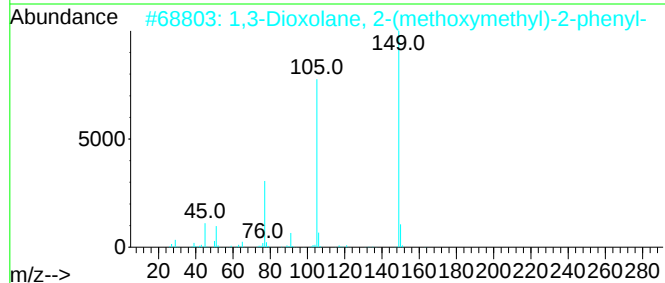
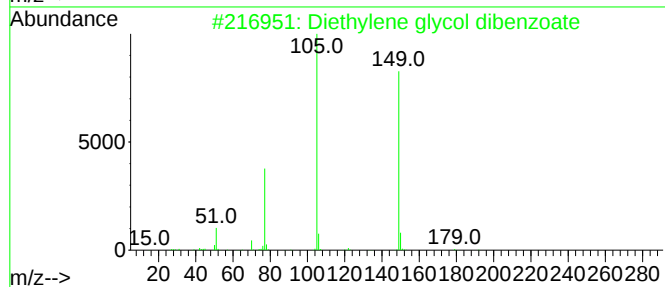
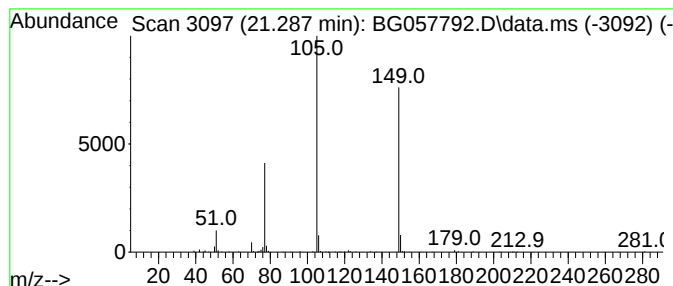
Instrument :
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ClientSampleId :
GP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.287	8.36 ng	317450	Chrysene-d12	21.551	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
3	7-Methoxy-2-phenyl-1,3-benzoxazo...	250	C15H10N2O2	1000436-00-1	35
4	Vinyl benzoate	148	C9H8O2	000769-78-8	35
5	N-(Methoxymethyl)benzamide	165	C9H11NO2	013156-28-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057792.D
Acq On : 21 Jun 2023 20:07
Operator : CG/JU
Sample : 03074-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GP-01

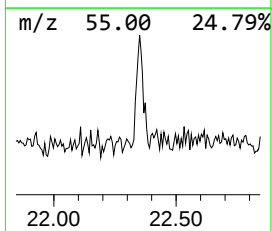
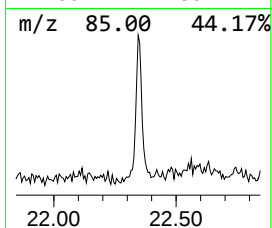
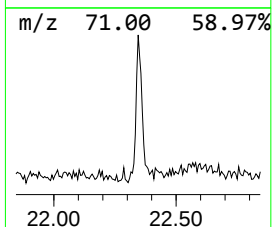
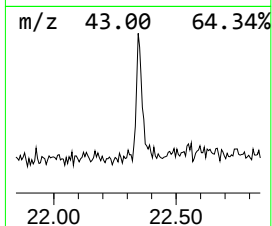
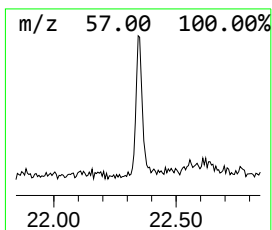
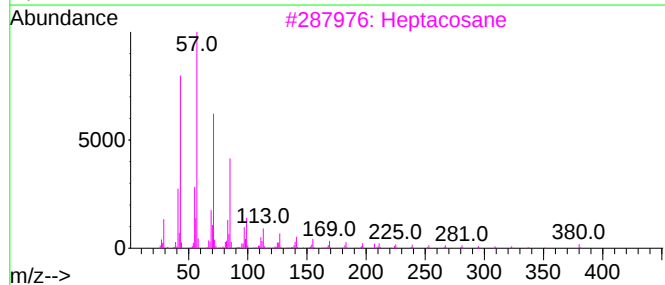
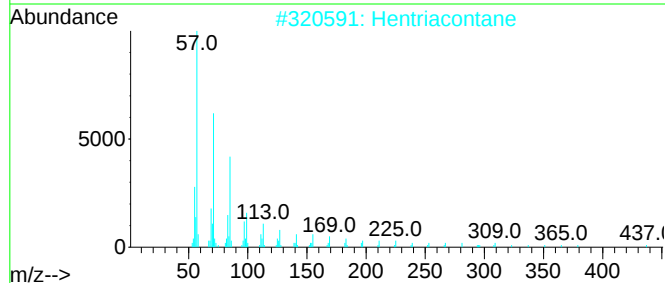
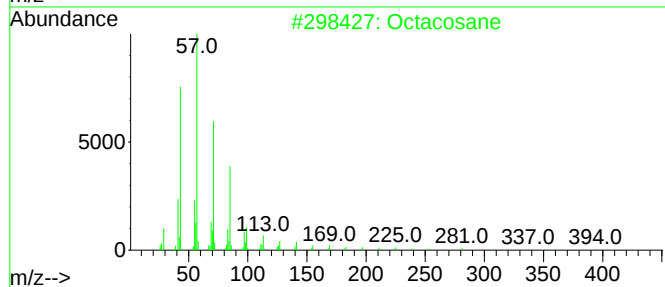
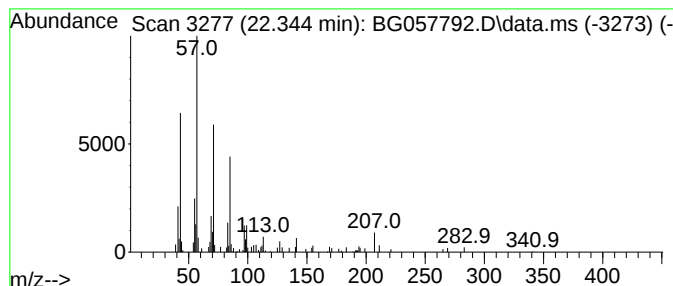
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.345	2.29 ng	86826	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Hentriacontane	437	C31H64	000630-04-6	87
3			Heptacosane	380	C27H56	000593-49-7	87
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5			Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057792.D
Acq On : 21 Jun 2023 20:07
Operator : CG/JU
Sample : 03074-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.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
Benzophenone	15.911	5.8	ng	134427	3	14.554	466167	20.0
Tridecanoic acid	18.191	4.8	ng	160721	4	17.297	676727	20.0
Hexadecanoic ac...	19.377	2.2	ng	74472	4	17.297	676727	20.0
Hexadecanoic ac...	19.612	4.0	ng	151094	5	21.551	759483	20.0
Octadecanoic ac...	20.652	3.1	ng	118898	5	21.551	759483	20.0
Oxybis(propane-...	21.169	2.8	ng	104713	5	21.551	759483	20.0
1-Hexacosene	21.205	9.9	ng	376602	5	21.551	759483	20.0
Diethylene glyc...	21.287	8.4	ng	317450	5	21.551	759483	20.0
Octacosane	22.345	2.3	ng	86826	5	21.551	759483	20.0