

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
 Data File : BG060080.D
 Acq On : 19 Dec 2023 00:19
 Operator : MA/JU
 Sample : 05791-10
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-1B-A-J

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-BG121323.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060080.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.141	4	9	26	rVB	300439	761971	10.45%	2.706%
2	5.527	408	415	424	rVB	428127	727113	9.97%	2.582%
3	7.107	678	684	692	rBV	283934	495249	6.79%	1.759%
4	7.953	819	828	834	rBV	318945	535441	7.34%	1.902%
5	9.117	1018	1026	1034	rBV	806650	1394594	19.12%	4.953%
6	10.762	1294	1306	1314	rBV	382500	779592	10.69%	2.769%
7	13.218	1716	1724	1731	rVB	2452126	3779945	51.83%	13.424%
8	14.593	1949	1958	1968	rVB2	649338	1185754	16.26%	4.211%
9	16.079	2204	2211	2217	rBV	2099958	3081849	42.26%	10.945%
10	16.872	2342	2346	2354	rBV	253250	355821	4.88%	1.264%
11	17.342	2420	2426	2432	rBV	832792	1239349	16.99%	4.401%
12	18.006	2533	2539	2546	rBV4	115233	197948	2.71%	0.703%
13	18.130	2555	2560	2568	rBV2	159410	225288	3.09%	0.800%
14	18.229	2573	2577	2583	rBV	347874	458454	6.29%	1.628%
15	18.329	2589	2594	2601	rBV2	213900	511483	7.01%	1.816%
16	18.993	2703	2707	2710	rBV2	129037	201192	2.76%	0.714%
17	19.164	2732	2736	2740	rBV	240583	375382	5.15%	1.333%
18	19.381	2770	2773	2783	rBV2	306821	785470	10.77%	2.789%
19	19.510	2790	2795	2798	rBV3	497720	812703	11.14%	2.886%
20	19.739	2832	2834	2838	rBV	258942	319614	4.38%	1.135%
21	19.963	2865	2872	2879	rBV	5142393	7292832	100.00%	25.899%
22	20.280	2922	2926	2929	rBV	614014	977314	13.40%	3.471%
23	20.456	2953	2956	2962	rBV4	812000	1664109	22.82%	5.910%

Sum of corrected areas: 28158467

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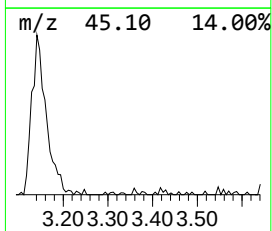
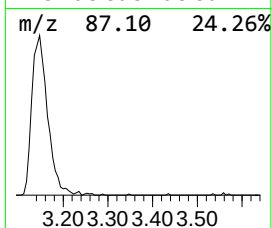
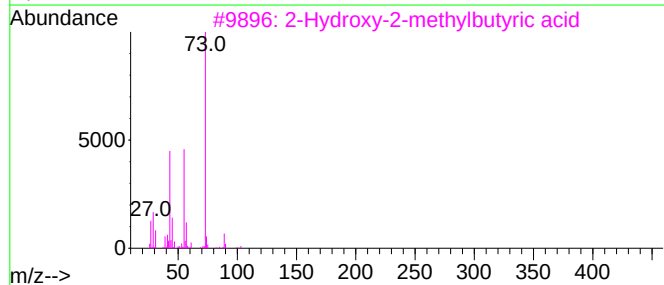
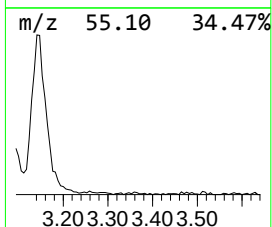
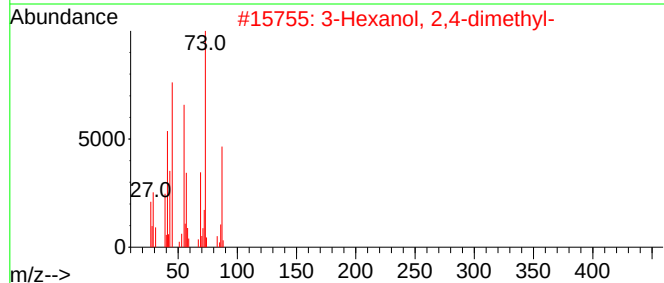
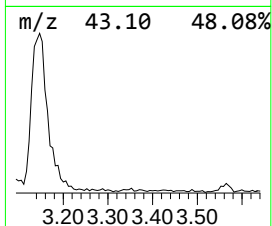
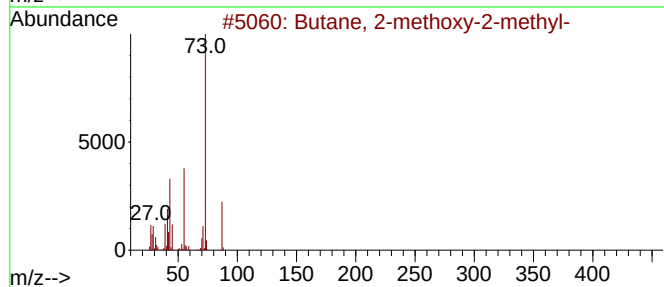
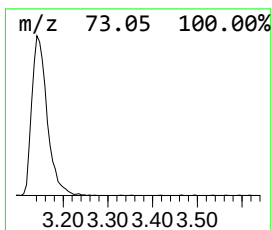
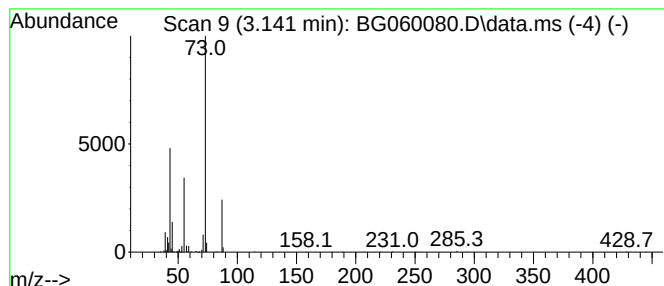
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.141	28.46 ng	761971	1,4-Dichlorobenzene-d4	7.953

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	50
3			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	9



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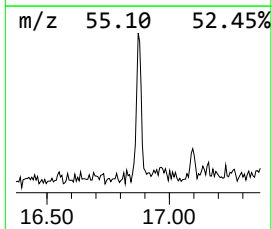
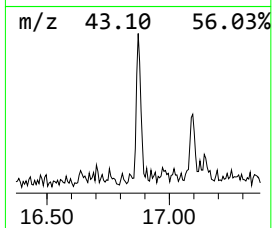
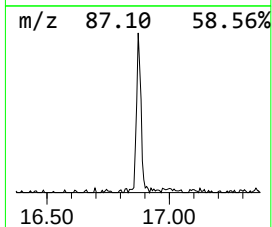
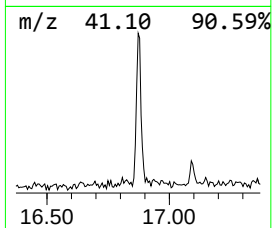
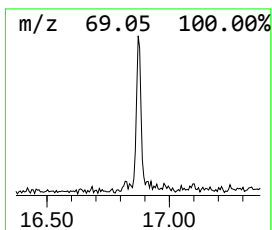
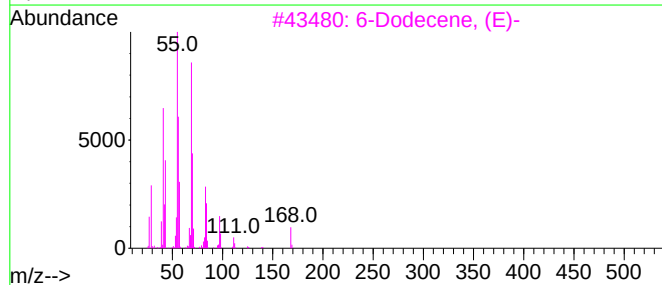
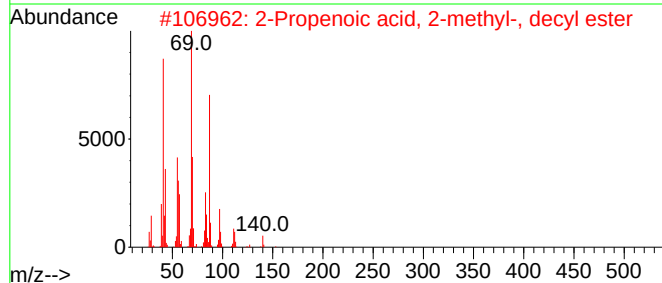
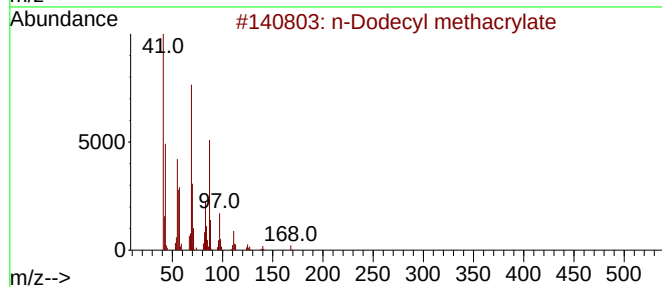
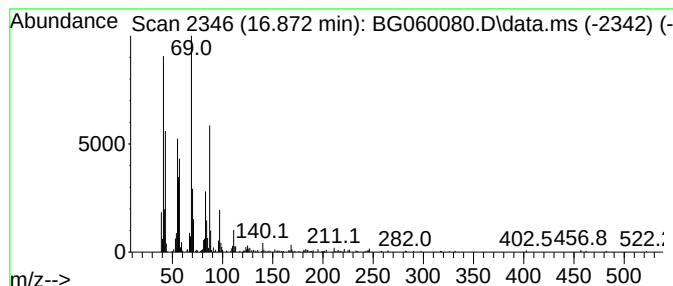
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Dodecyl methacrylate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.872	5.74 ng	355821	Phenanthrene-d10	17.342

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	91
2		2-Propenoic acid, 2-methyl-, dec...	226	C14H26O2	003179-47-3	87
3		6-Dodecene, (E)-	168	C12H24	007206-17-9	52
4		1-Hexene, 3,3,5-trimethyl-	126	C9H18	013427-43-5	43
5		Cyclododecane	168	C12H24	000294-62-2	38



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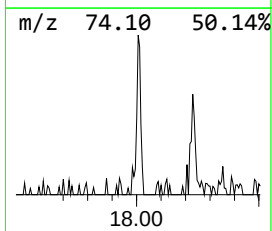
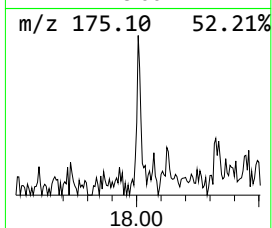
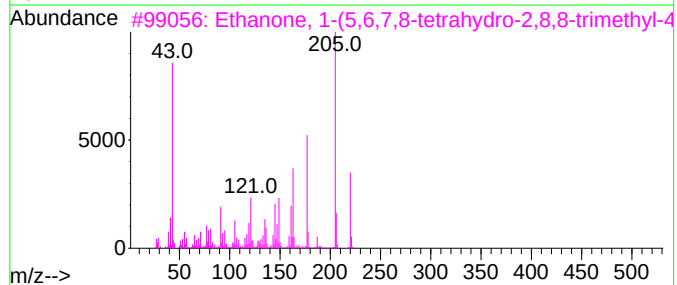
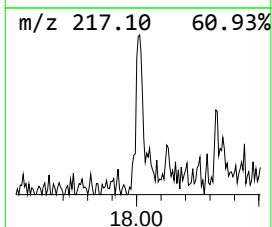
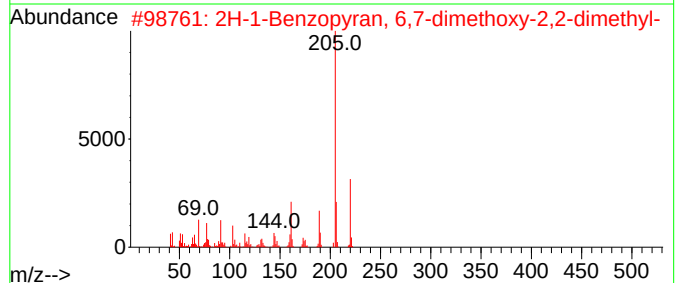
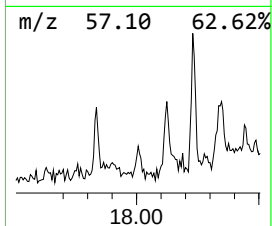
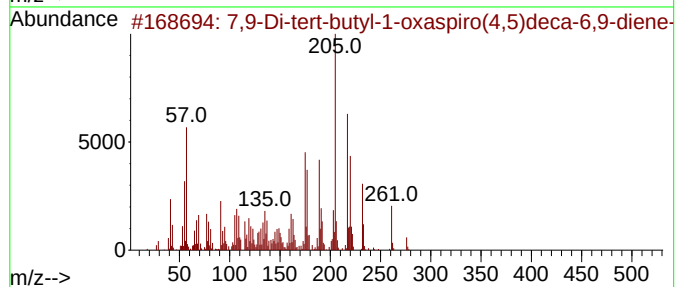
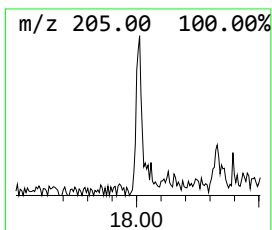
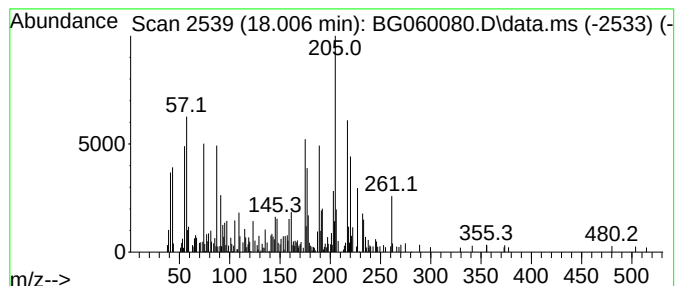
Instrument :
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Peak Number 3 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.006	3.19 ng	197948	Phenanthrene-d10	17.342	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	87
2	2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	42
3	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	41
4	5-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-92-1	38
5	9-Ethyl-10-methylanthracene	220	C17H16	019713-49-6	38



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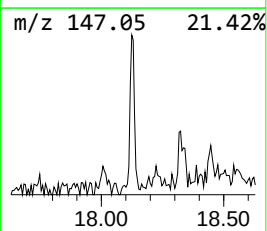
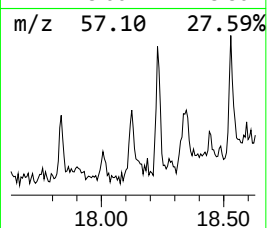
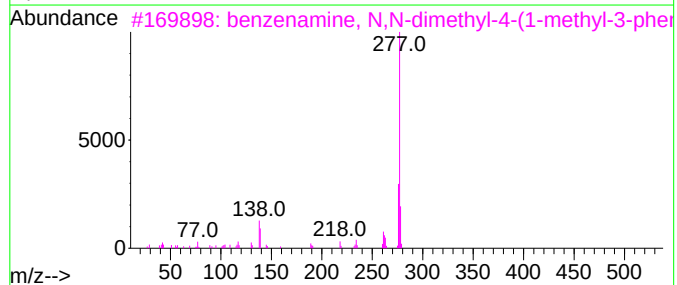
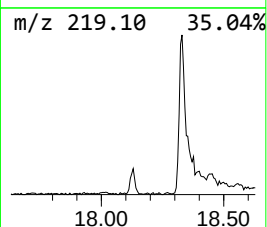
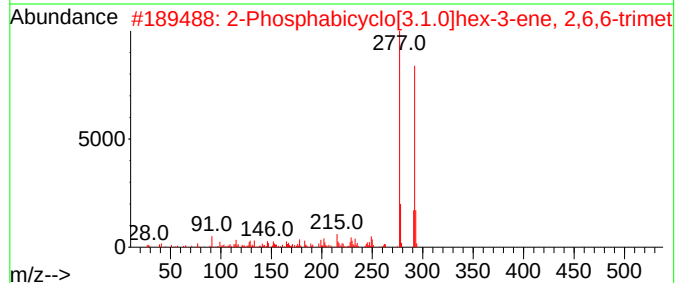
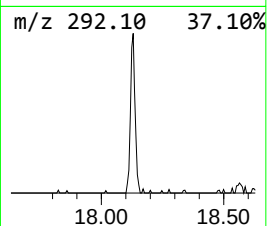
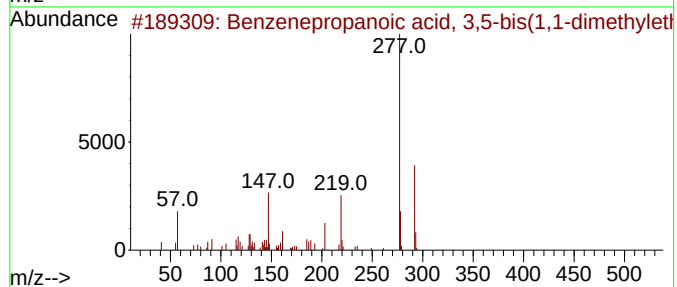
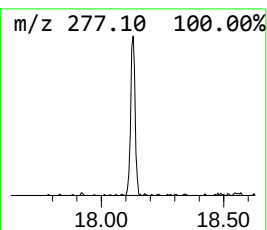
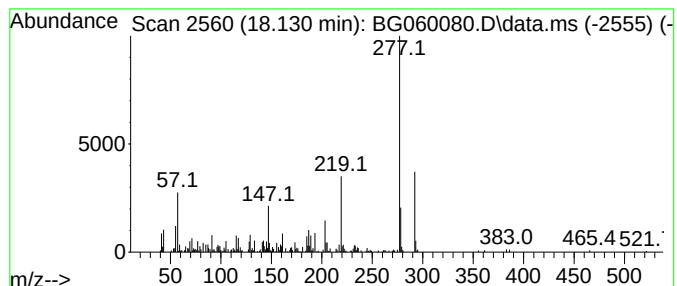
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzenepropanoic acid, 3,5-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.130	3.64 ng	225288	Phenanthrene-d10	17.342

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenepropanoic acid, 3,5-bis(1...	292	C18H28O3	006386-38-5	93
2			2-Phosphabicyclo[3.1.0]hex-3-ene...	292	C20H21P	1000161-75-2	50
3			benzenamine, N,N-dimethyl-4-(1-m...	277	C18H19N3	1000397-11-0	43
4			Lysicamine monophenol	277	C17H11NO3	052410-28-3	43
5			Ethanone, 1-(5,7,8-trimethoxy-2,...	292	C16H20O5	000482-07-5	40



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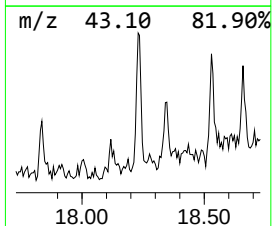
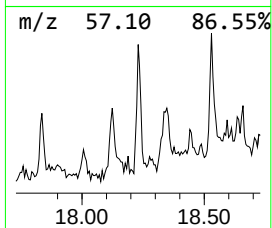
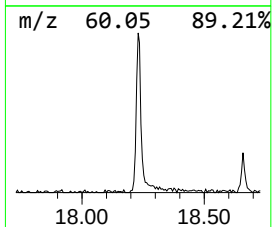
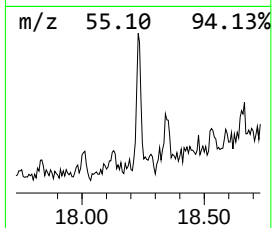
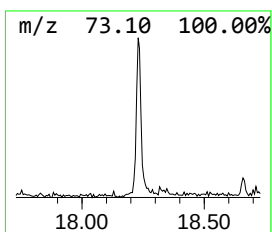
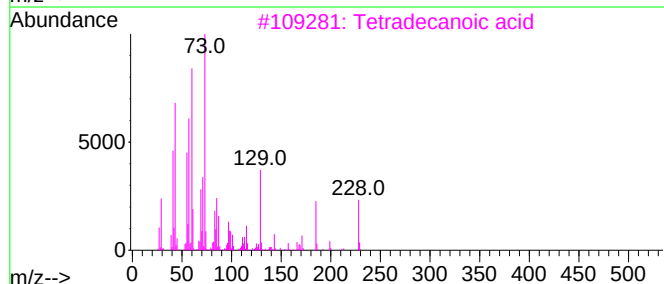
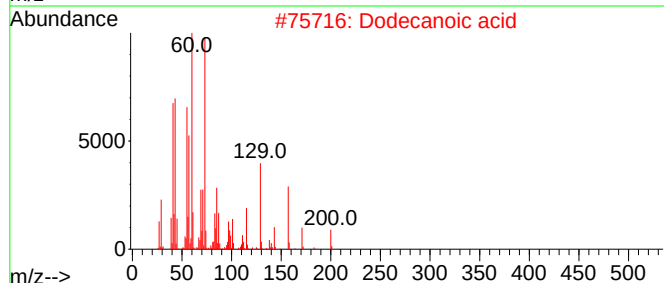
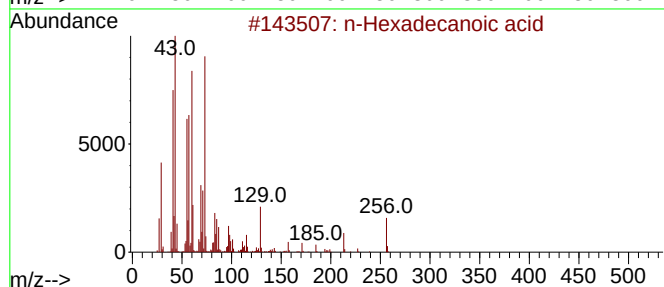
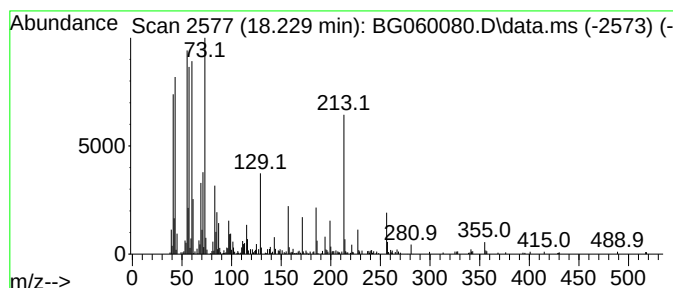
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.230	7.40 ng	458454	Phenanthrene-d10	17.342	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Dodecanoic acid	200	C12H24O2	000143-07-7	60
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50



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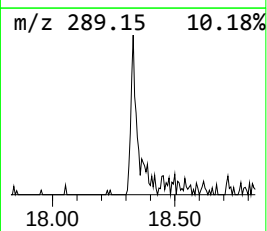
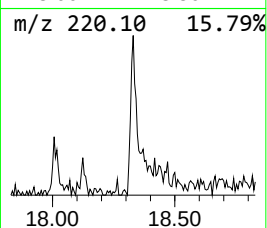
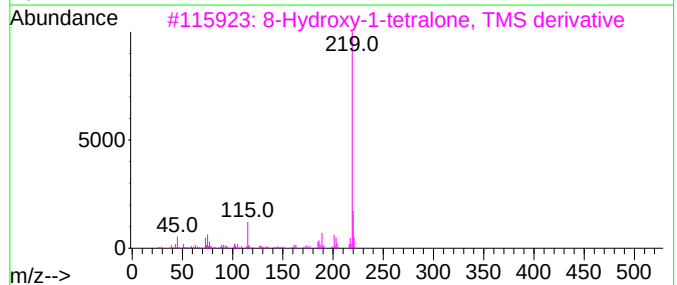
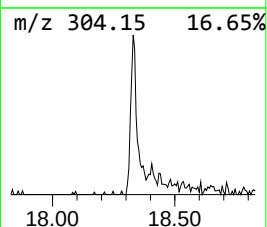
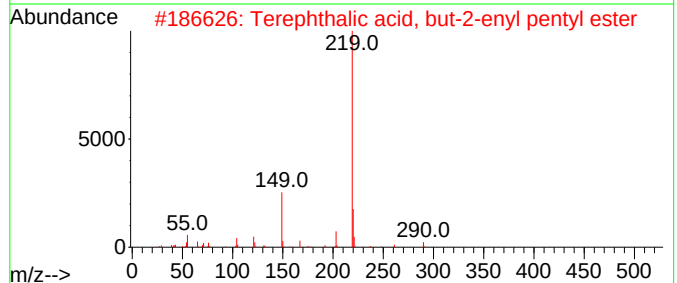
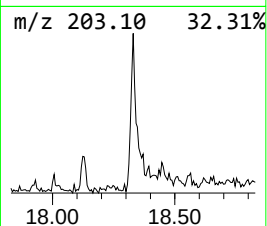
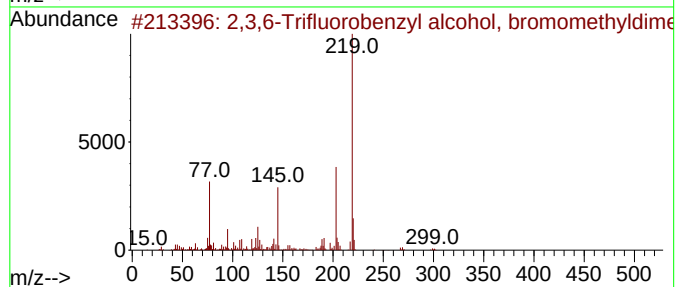
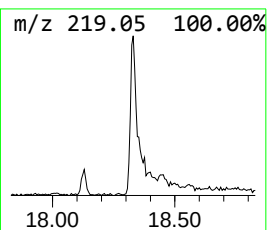
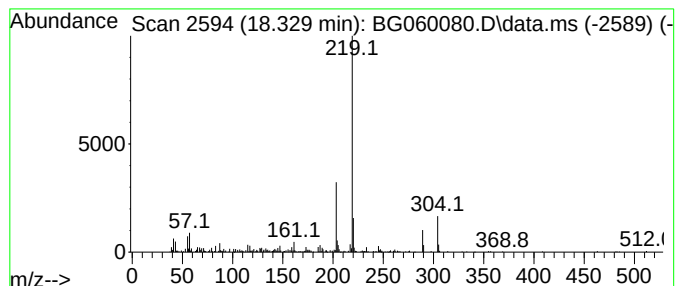
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 2,3,6-Trifluorobenzyl alcoh... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.329	8.25 ng	511483	Phenanthrene-d10	17.342

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,3,6-Trifluorobenzyl alcohol, b...	312	C10H12BrF3OSi	1000376-06-3	59
2		Terephthalic acid, but-2-enyl pe...	290	C17H22O4	1000356-31-2	52
3		8-Hydroxy-1-tetralone, TMS deriv...	234	C13H18O2Si	1000161-48-8	50
4		Terephthalic acid, 4-bromophenyl...	390	C19H19BrO4	1000323-68-0	50
5		Quinoline, 2-(3-tolyl)-	219	C16H13N	024641-30-3	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
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Acq On : 19 Dec 2023 00:19
Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

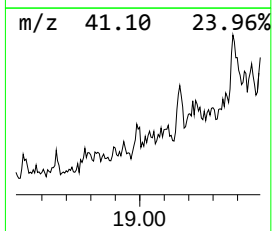
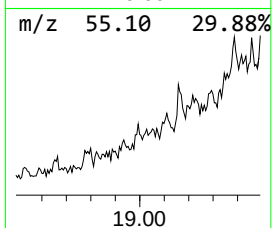
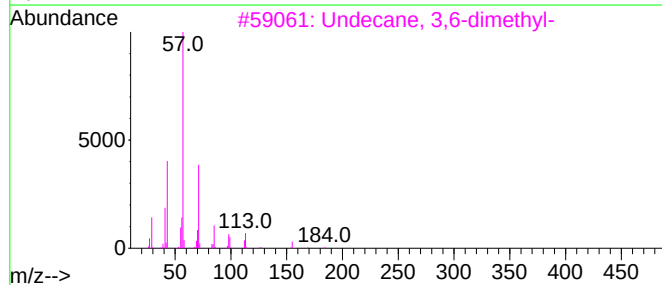
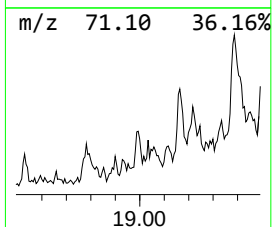
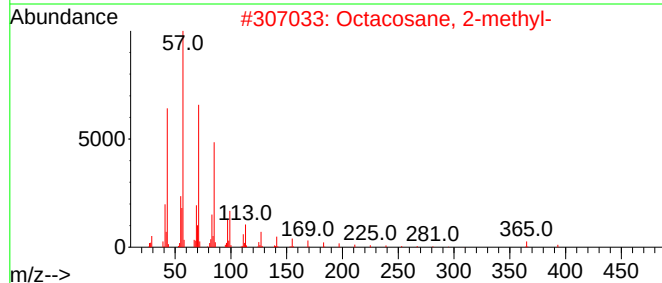
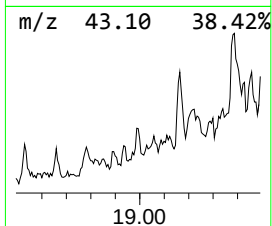
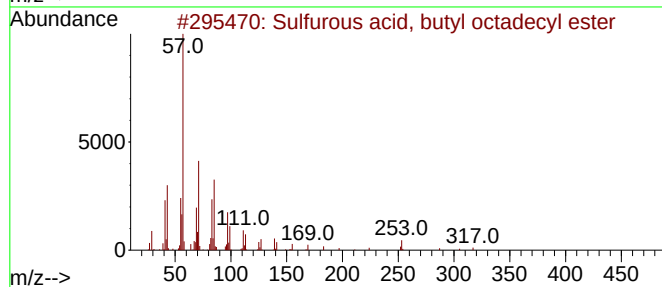
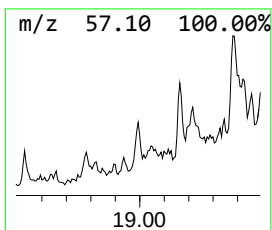
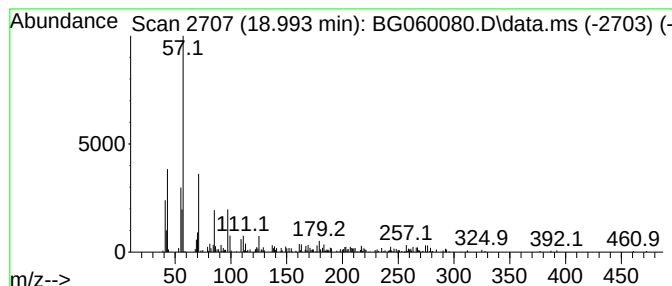
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, butyl octadecyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.993	3.25 ng	201192	Phenanthrene-d10	17.342	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	59
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	53
3	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	50
4	Decane, 2,6,6-trimethyl-	184	C13H28	062108-24-1	47
5	Nonadecane	268	C19H40	000629-92-5	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
Data File : BG060080.D
Acq On : 19 Dec 2023 00:19
Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

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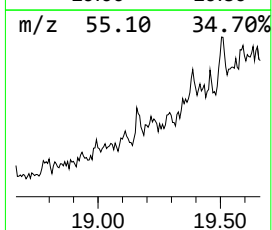
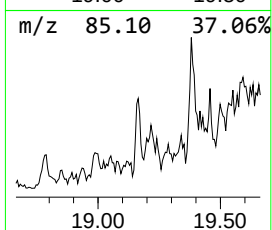
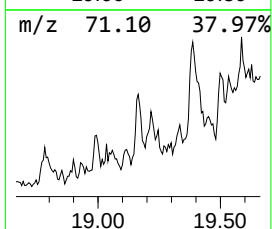
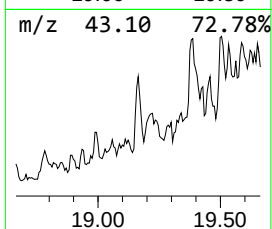
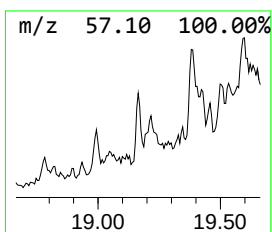
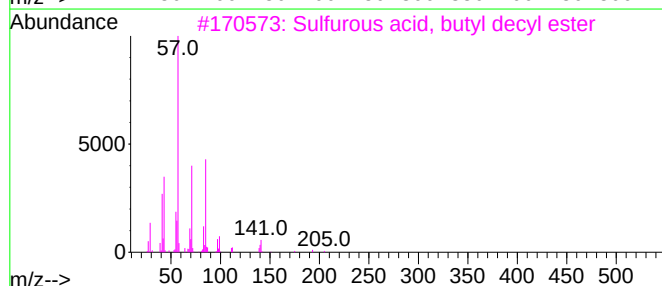
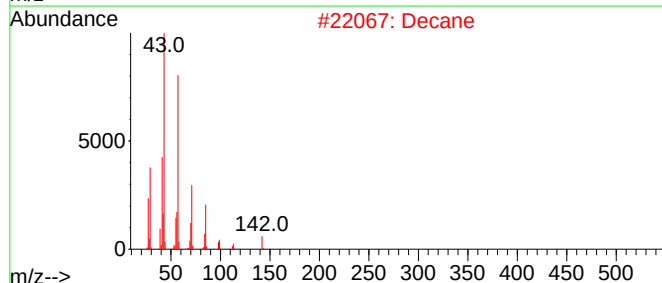
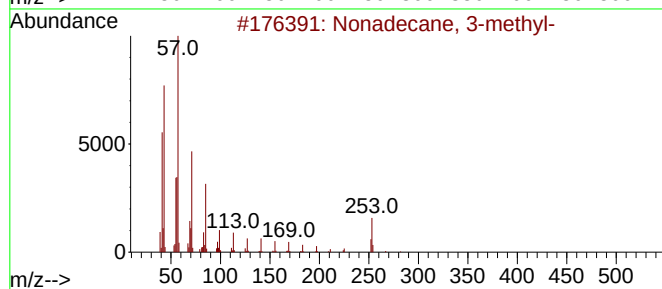
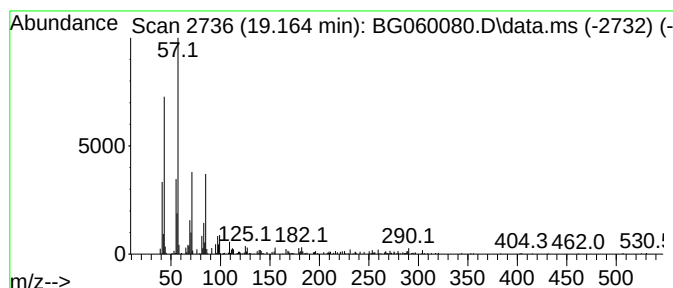
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.164	6.06 ng	375382	Phenanthrene-d10	17.342

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 3-methyl-	282	C20H42	006418-45-7	89
2			Decane	142	C10H22	000124-18-5	68
3			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	64
4			Tetradecane, 6,9-dimethyl-	226	C16H34	055045-13-1	64
5			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
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Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

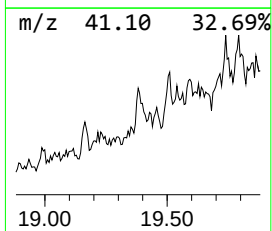
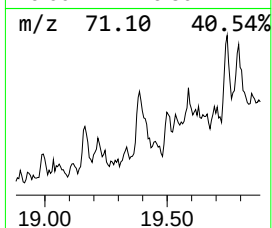
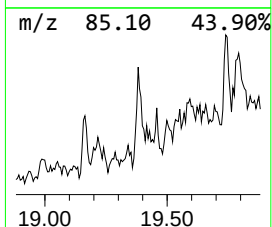
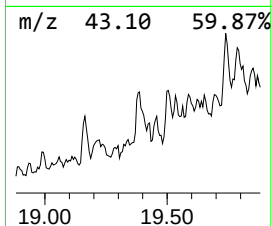
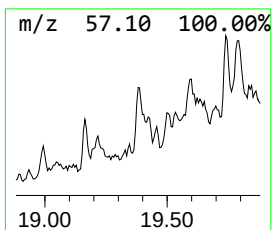
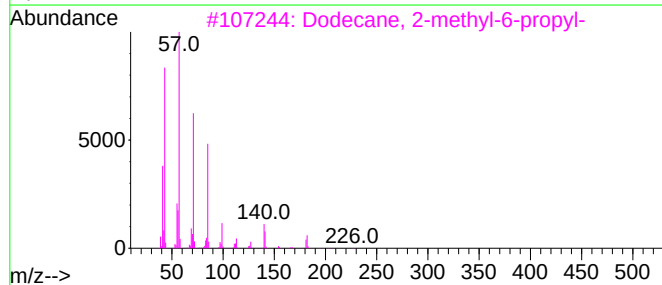
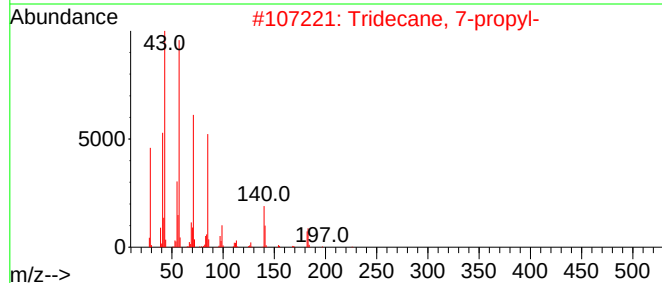
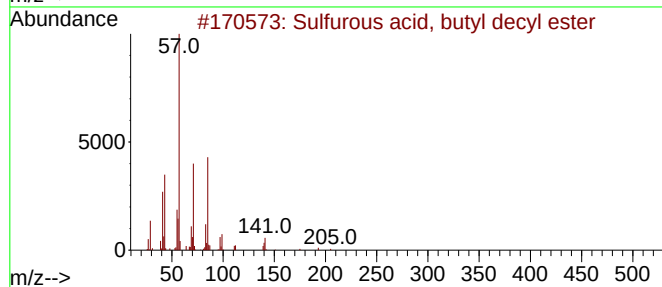
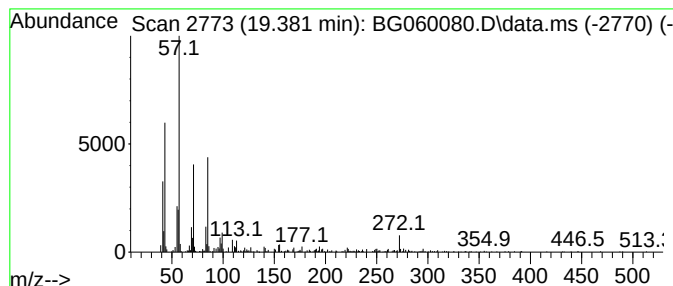
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Sulfurous acid, butyl decyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.381	12.68 ng	785470	Phenanthrene-d10		17.342	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl decyl ester		278	C14H30O3S	1000309-17-7	86
2	Tridecane, 7-propyl-		226	C16H34	055045-09-5	86
3	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	68
4	Hexane, 2,3,4-trimethyl-		128	C9H20	000921-47-1	64
5	1-Iodoundecane		282	C11H23I	004282-44-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
Data File : BG060080.D
Acq On : 19 Dec 2023 00:19
Operator : MA/JU
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Misc :
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Instrument :
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ClientSampleId :
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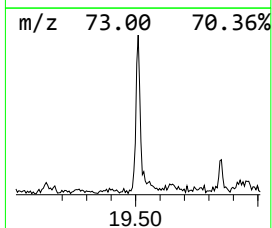
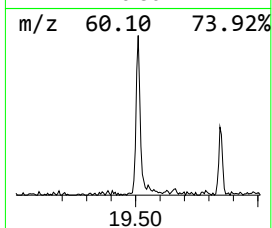
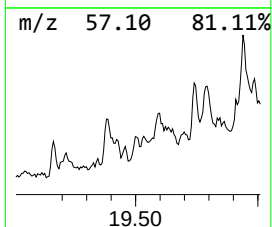
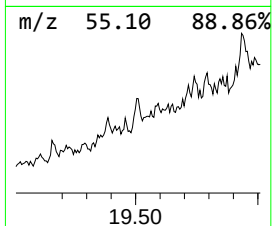
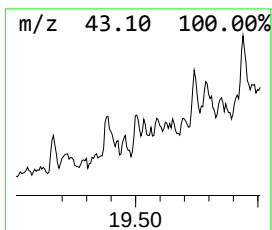
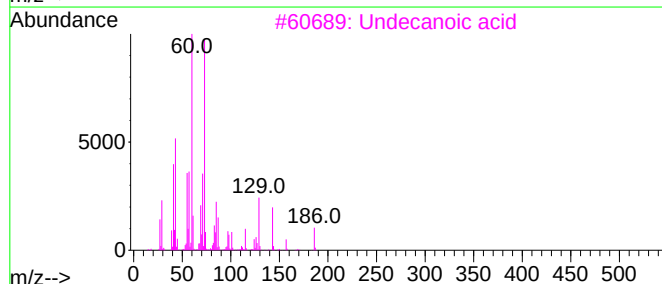
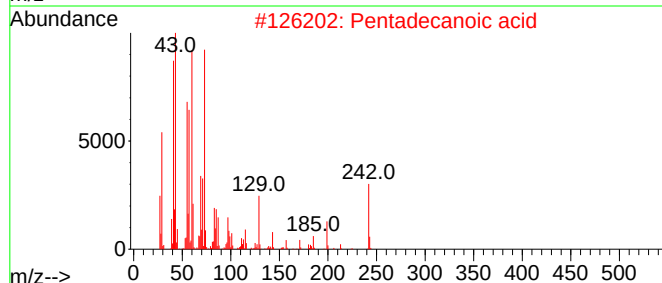
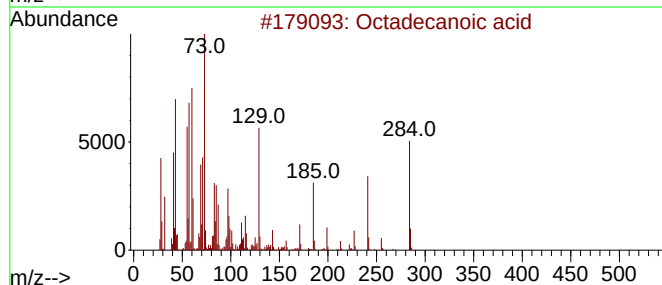
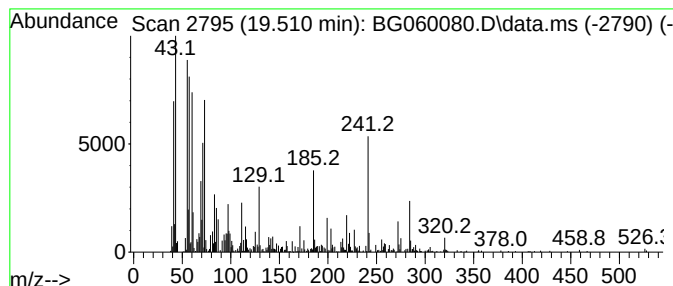
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.510	9.77 ng	812703	Chrysene-d12	21.620

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	38
3	Undecanoic acid	186	C11H22O2	000112-37-8	38
4	Nonanoic acid	158	C9H18O2	000112-05-0	38
5	n-Decanoic acid	172	C10H20O2	000334-48-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
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Instrument :
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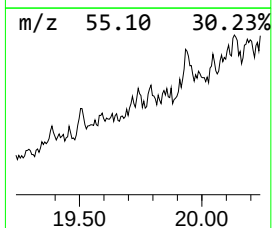
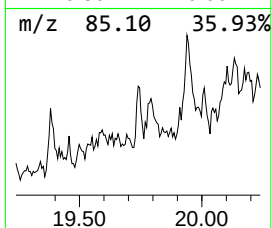
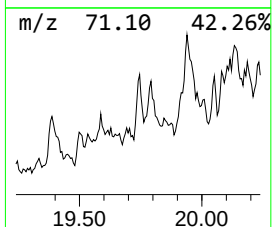
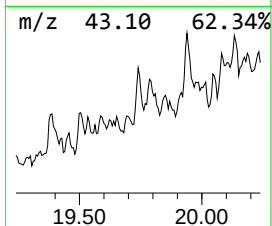
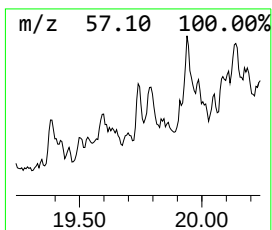
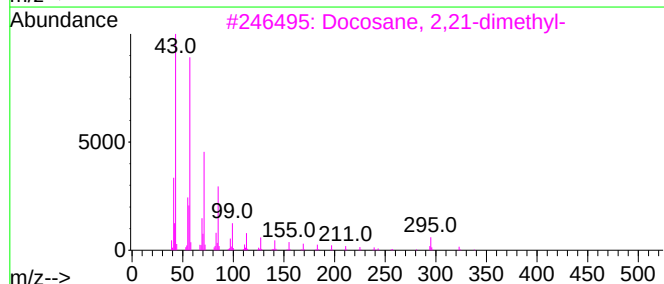
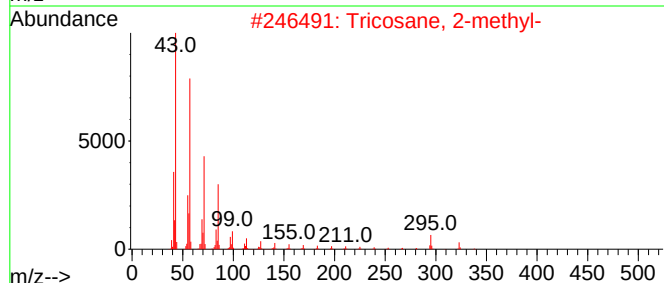
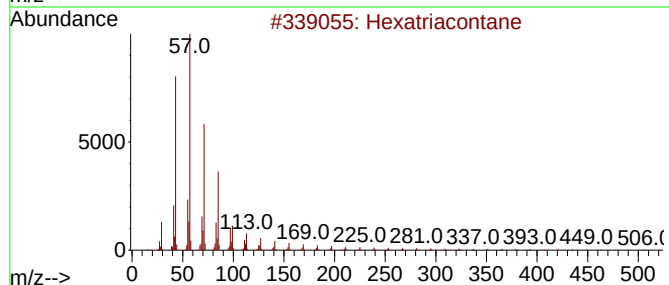
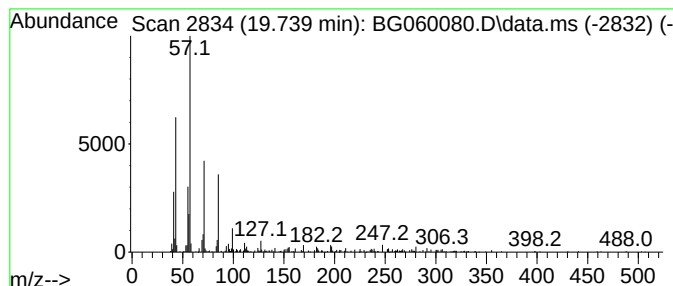
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Hexatriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.740	3.84 ng	319614	Chrysene-d12	21.620

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexatriacontane	507	C36H74	000630-06-8	87
2		Tricosane, 2-methyl-	338	C24H50	001928-30-9	83
3		Docosane, 2,21-dimethyl-	338	C24H50	077536-31-3	83
4		Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	80
5		Pentadecane	212	C15H32	000629-62-9	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
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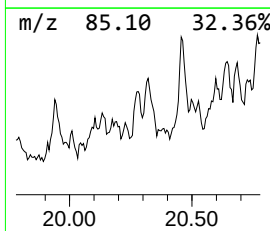
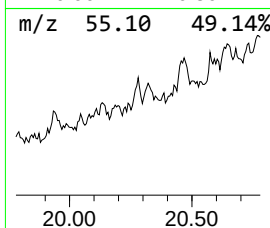
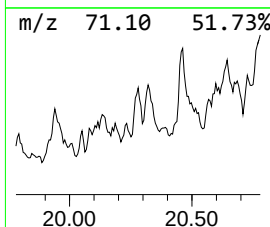
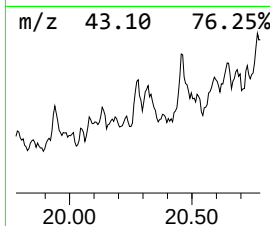
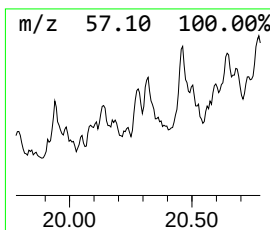
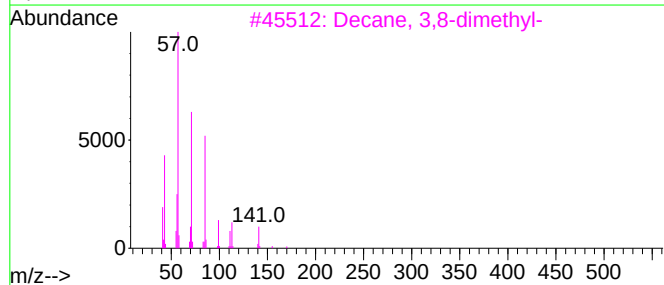
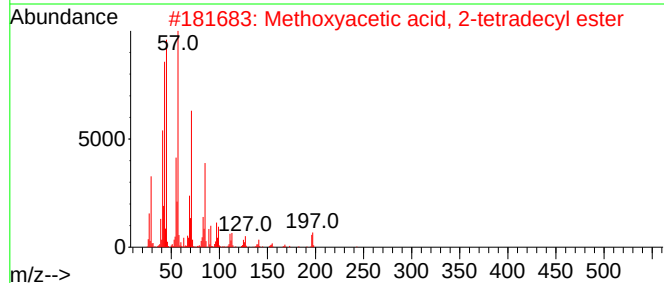
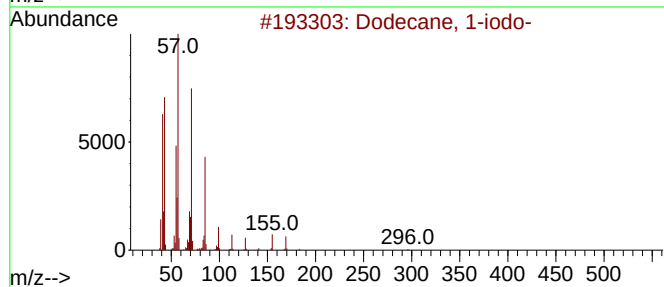
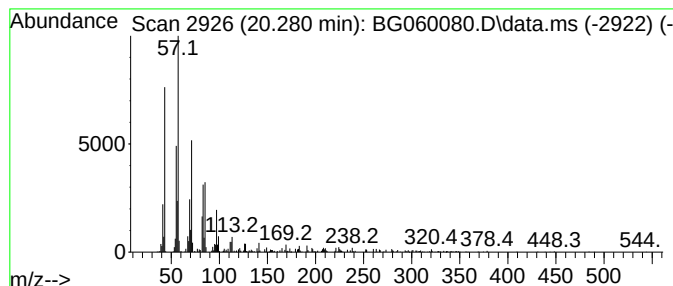
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Dodecane, 1-iodo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.280	11.75 ng	977314	Chrysene-d12	21.620

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
2			Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	64
3			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64
4			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	58
5			Tritetracontane	605	C43H88	007098-21-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
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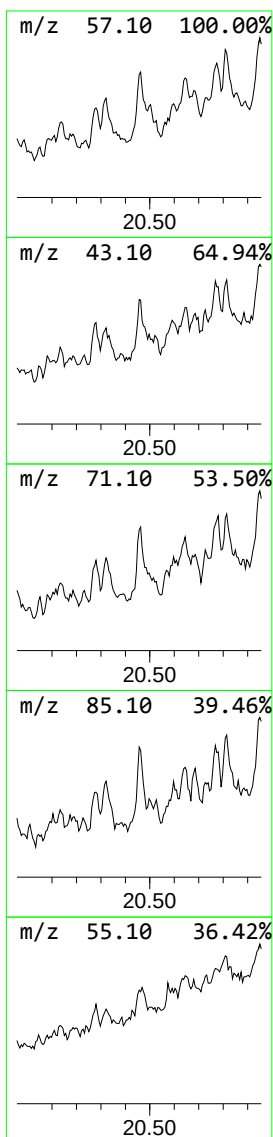
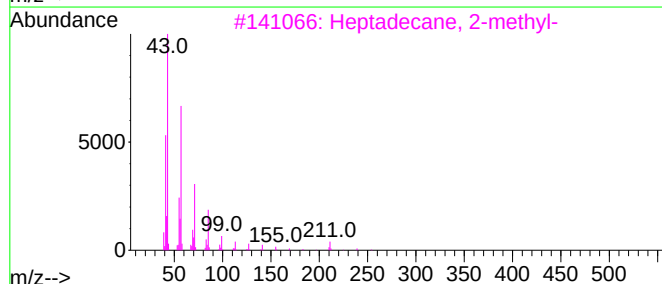
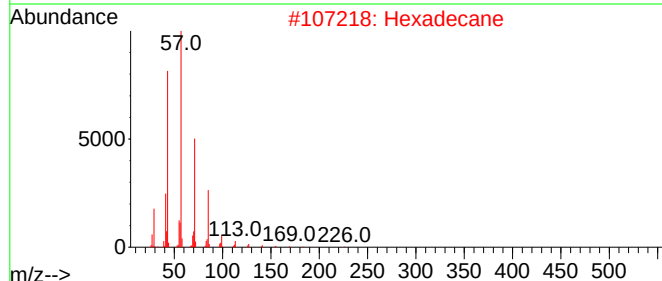
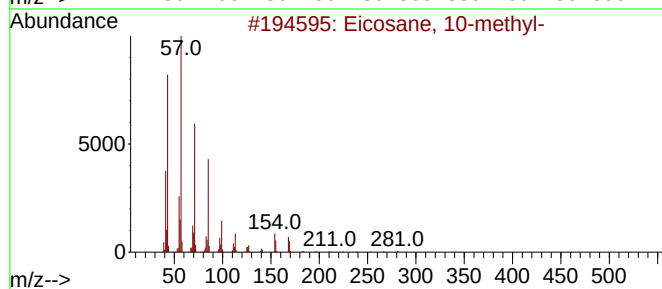
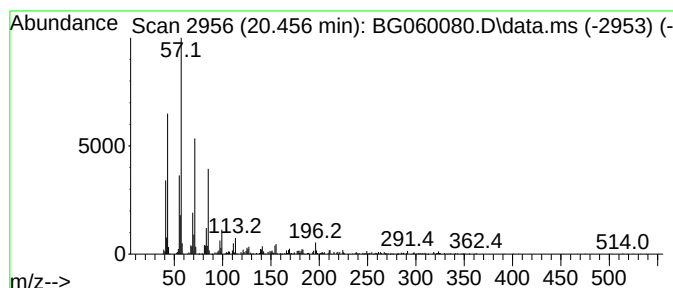
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Eicosane, 10-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.456	20.00 ng	1664110	Chrysene-d12	21.620	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
2	Hexadecane	226	C16H34	000544-76-3	87
3	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
Data File : BG060080.D
Acq On : 19 Dec 2023 00:19
Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-A-J

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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...	3.141	28.5	ng	761971	1	7.953	535441	20.0
n-Dodecyl metha...	16.872	5.7	ng	355821	4	17.342	1239350	20.0
7,9-Di-tert-but...	18.006	3.2	ng	197948	4	17.342	1239350	20.0
Benzenepropanoi...	18.130	3.6	ng	225288	4	17.342	1239350	20.0
n-Hexadecanoic ...	18.230	7.4	ng	458454	4	17.342	1239350	20.0
2,3,6-Trifluoro...	18.329	8.3	ng	511483	4	17.342	1239350	20.0
Sulfurous acid,...	18.993	3.3	ng	201192	4	17.342	1239350	20.0
Nonadecane, 3-m...	19.164	6.1	ng	375382	4	17.342	1239350	20.0
Sulfurous acid,...	19.381	12.7	ng	785470	4	17.342	1239350	20.0
Octadecanoic acid	19.510	9.8	ng	812703	5	21.620	1664110	20.0
Hexatriacontane	19.740	3.8	ng	319614	5	21.620	1664110	20.0
Dodecane, 1-iodo-	20.280	11.8	ng	977314	5	21.620	1664110	20.0
Eicosane, 10-me...	20.456	20.0	ng	1664110	5	21.620	1664110	20.0