

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
 Data File : BG059843.D
 Acq On : 23 Nov 2023 8:35
 Operator : MA/JU
 Sample : 05294-05
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WT-5

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-BG111623.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059843.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.822	407	414	423	rVB	445138	718437	25.65%	3.462%
2	7.456	684	692	702	rBV	513175	904202	32.29%	4.357%
3	8.331	832	841	848	rBV2	142898	251232	8.97%	1.211%
4	9.530	1038	1045	1054	rVB2	358245	640659	22.88%	3.087%
5	11.175	1319	1325	1334	rVB	180739	350128	12.50%	1.687%
6	13.584	1727	1735	1742	rBV	1291707	1957131	69.89%	9.430%
7	13.784	1761	1769	1776	rBV4	44395	82122	2.93%	0.396%
8	14.959	1964	1969	1977	rVB	328673	520991	18.60%	2.510%
9	16.445	2216	2222	2231	rVB2	1086222	1598827	57.09%	7.704%
10	17.708	2432	2437	2443	rBV	404698	635341	22.69%	3.061%
11	18.525	2571	2576	2583	rBV3	263386	378467	13.51%	1.824%
12	19.459	2733	2735	2739	rBV5	32145	29039	1.04%	0.140%
13	19.788	2787	2791	2794	rBV4	132077	165295	5.90%	0.796%
14	20.288	2871	2876	2881	rBV	2350779	2800467	100.00%	13.494%
15	21.099	3012	3014	3017	rVB4	88074	87484	3.12%	0.422%
16	21.786	3127	3131	3137	rVB3	207750	347417	12.41%	1.674%
17	22.039	3170	3174	3180	rVB2	304574	520482	18.59%	2.508%
18	22.550	3256	3261	3269	rVB	411302	741036	26.46%	3.571%
19	23.449	3407	3414	3424	rVB	551113	1207398	43.11%	5.818%
20	24.524	3590	3597	3608	rVB2	610473	1641883	58.63%	7.911%
21	25.623	3782	3784	3795	rVB3	189912	446572	15.95%	2.152%
22	25.840	3812	3821	3834	rBV4	563292	1792002	63.99%	8.635%
23	27.491	4091	4102	4115	rBV3	454463	1828289	65.29%	8.809%
24	29.559	4441	4454	4456	rBV4	296481	898269	32.08%	4.328%
25	32.162	4889	4897	4898	rBV7	111286	210548	7.52%	1.015%

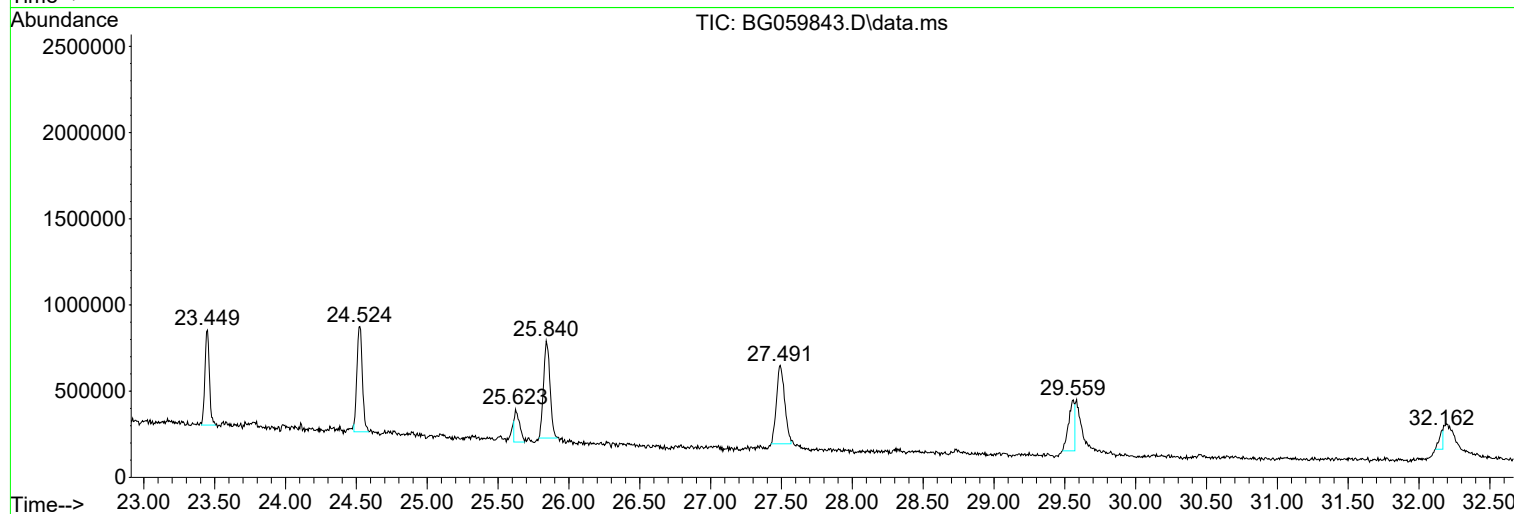
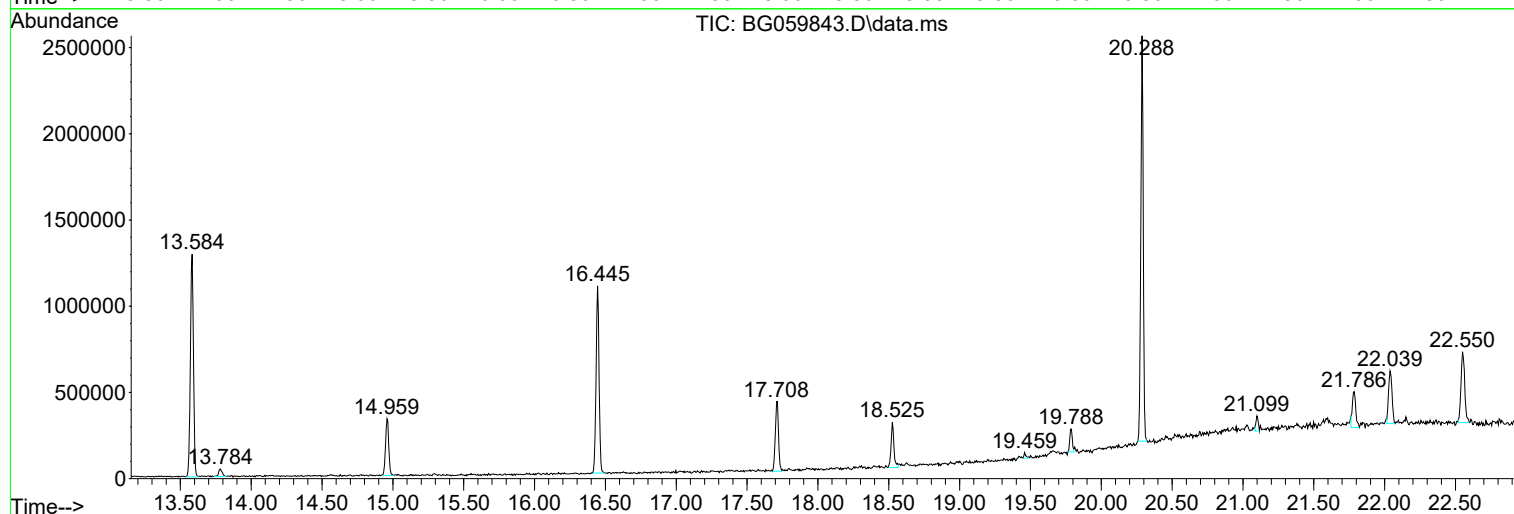
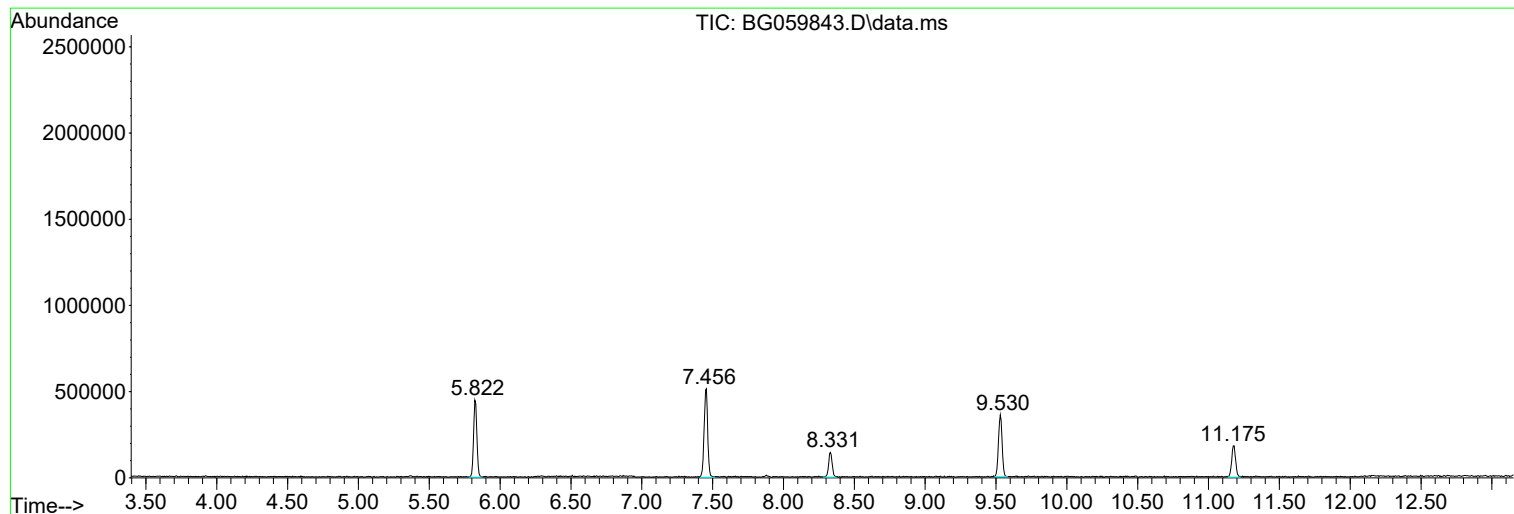
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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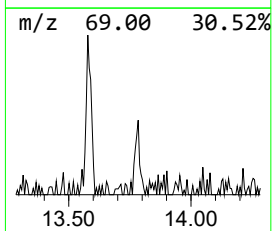
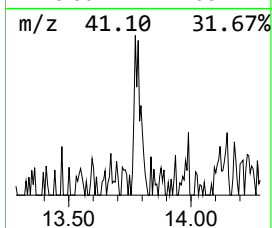
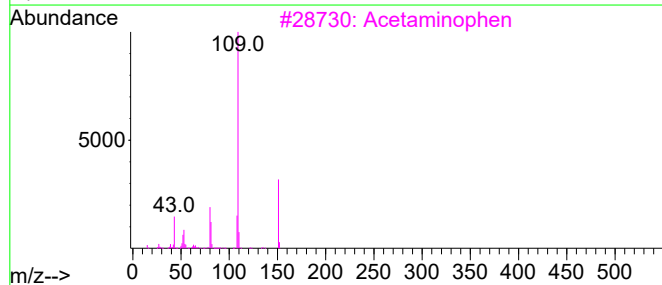
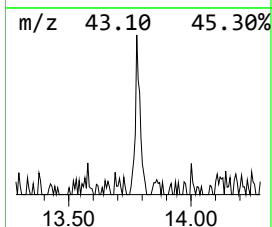
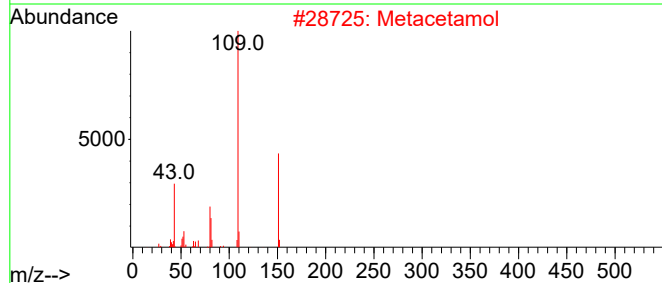
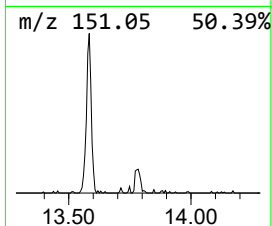
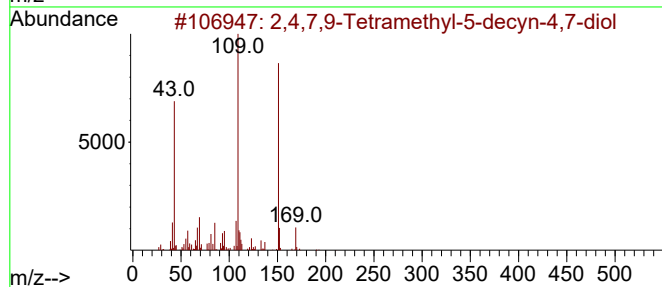
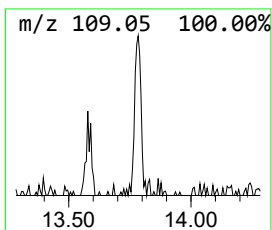
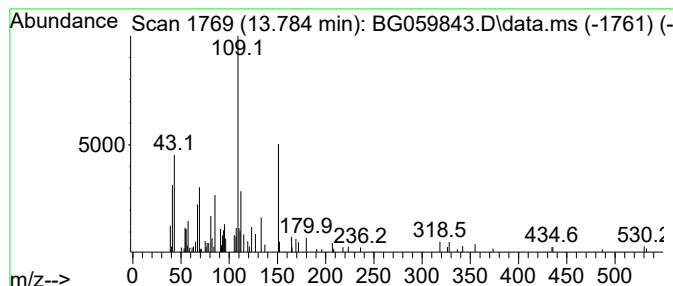
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.784	3.15 ng	82122	Acenaphthene-d10		14.959	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	64
2	Metacetamol		151	C8H9NO2	000621-42-1	49
3	Acetaminophen		151	C8H9NO2	000103-90-2	47
4	N-(4-tert-Butoxyphenyl)acetamide		207	C12H17NO2	002109-73-1	47
5	3,4-Pyridinediamine		109	C5H7N3	000054-96-6	30



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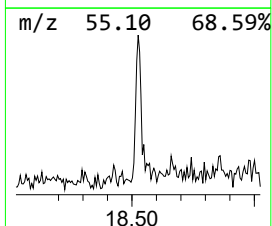
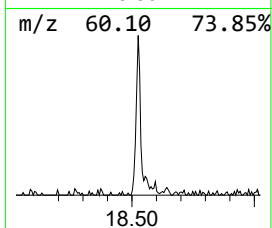
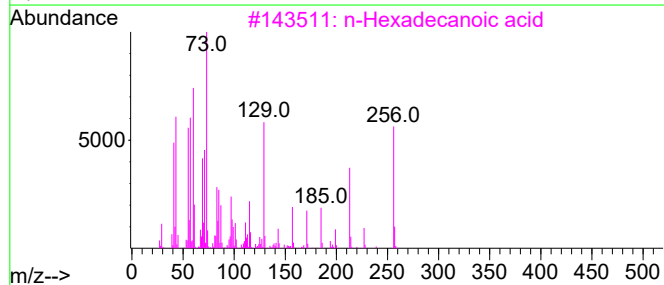
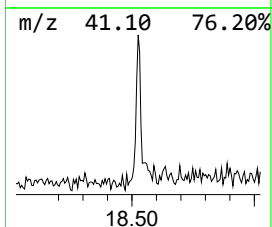
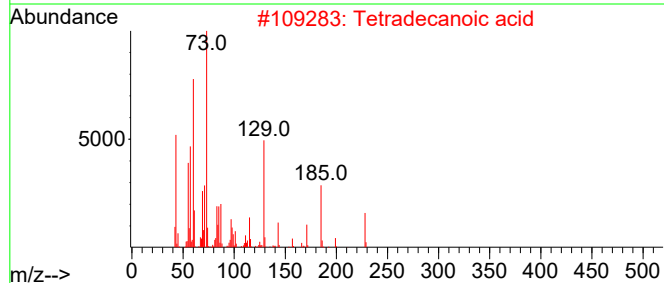
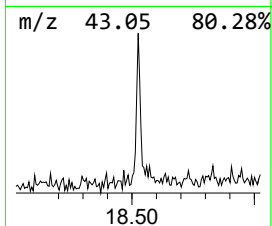
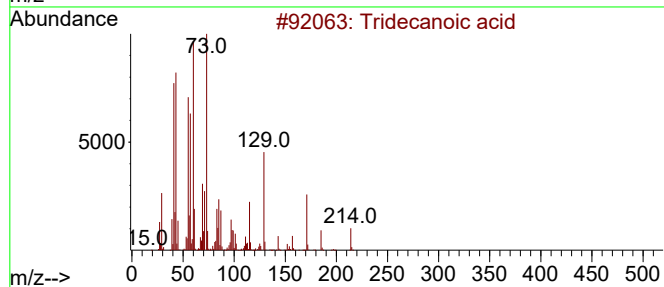
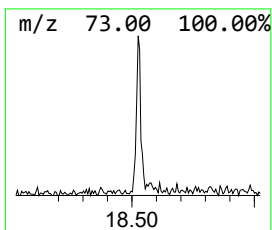
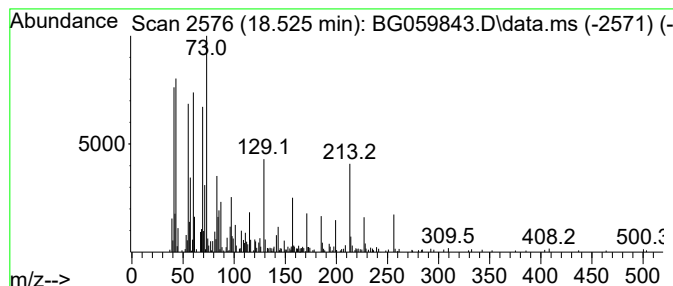
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Tridecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.525	11.91 ng	378467	Phenanthrene-d10	17.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	93
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5			Dodecanoic acid	200	C12H24O2	000143-07-7	62



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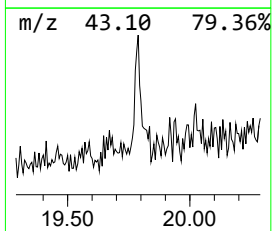
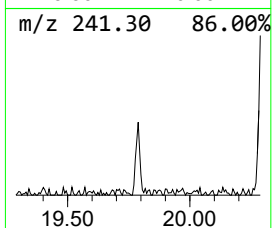
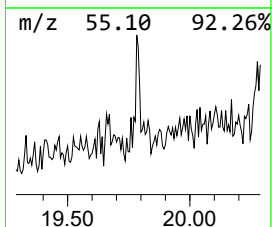
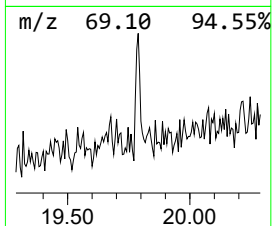
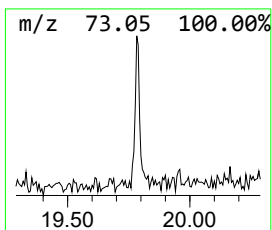
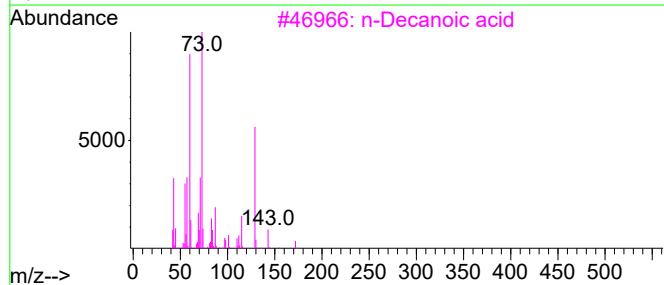
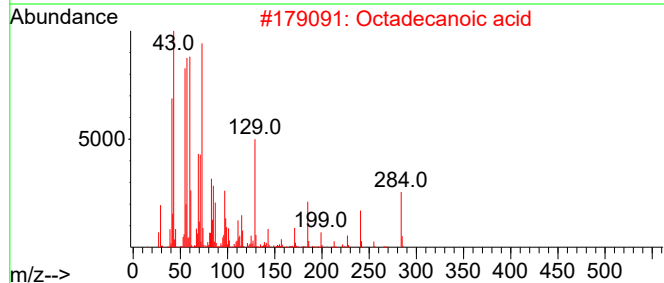
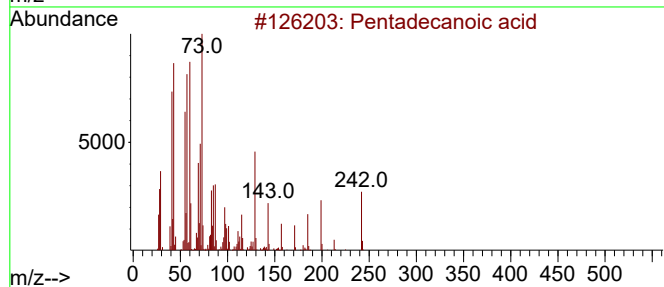
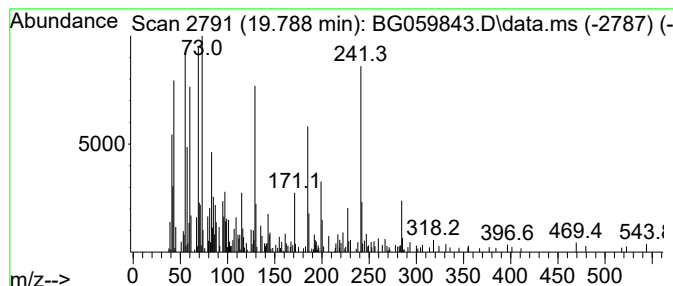
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown19.788 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.788	5.20 ng	165295	Phenanthrene-d10	17.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	43
2			Octadecanoic acid	284	C18H36O2	000057-11-4	42
3			n-Decanoic acid	172	C10H20O2	000334-48-5	42
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	35
5			Undecanoic acid	186	C11H22O2	000112-37-8	18



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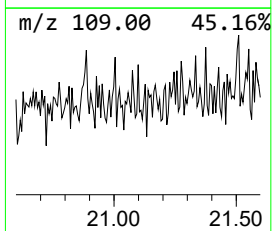
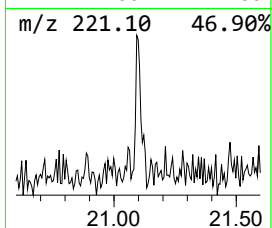
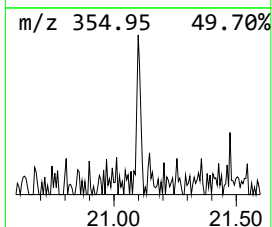
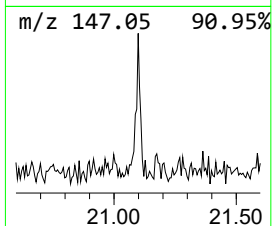
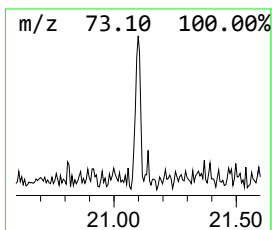
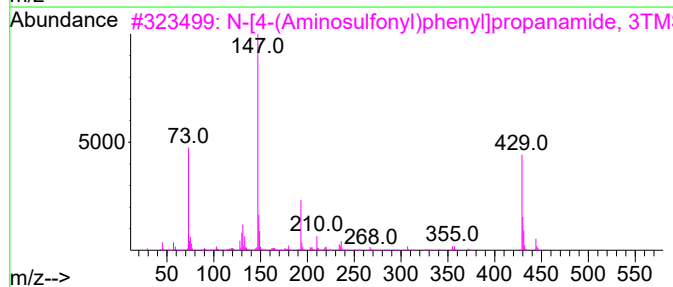
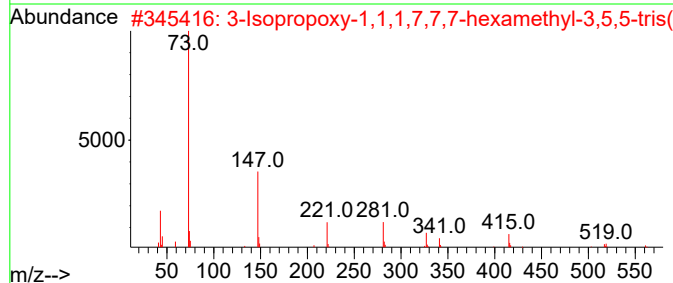
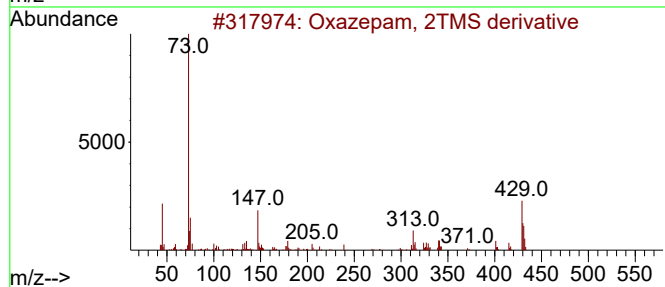
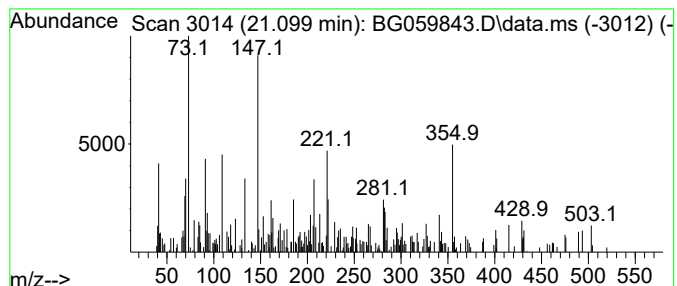
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Peak Number 4 unknown21.099 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.099	3.36 ng	87484	Chrysene-d12	22.039	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazepam, 2TMS derivative	430	C21H27ClN2O2Si2	055319-93-2	42
2	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	35
3	N-[4-(Aminosulfonyl)phenyl]propa...	444	C18H36N2O3SSi3	1000500-82-8	32
4	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	32
5	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27



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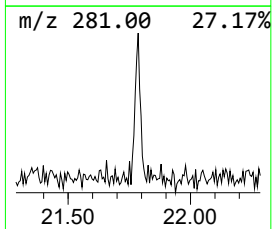
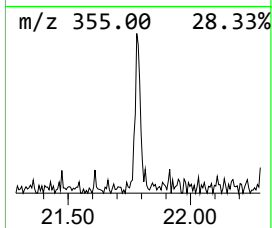
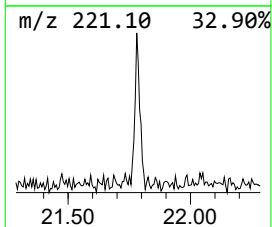
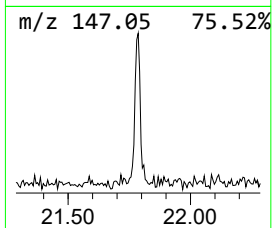
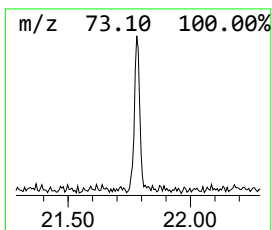
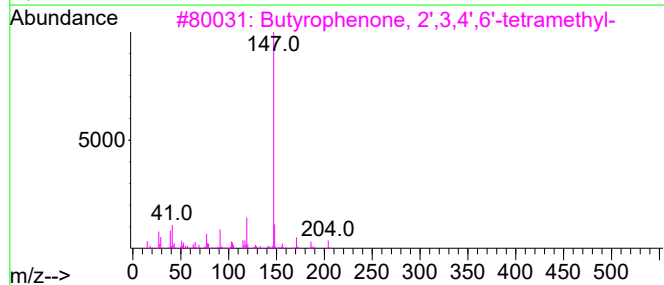
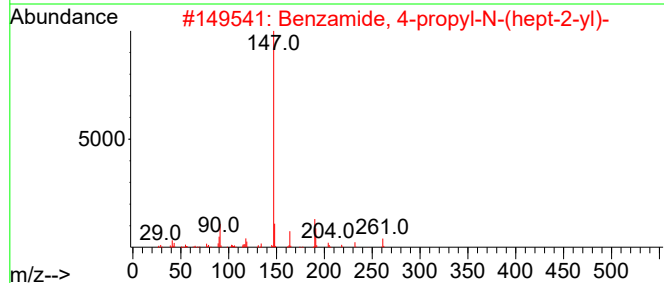
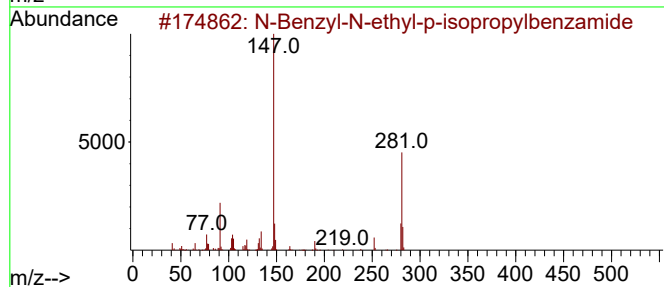
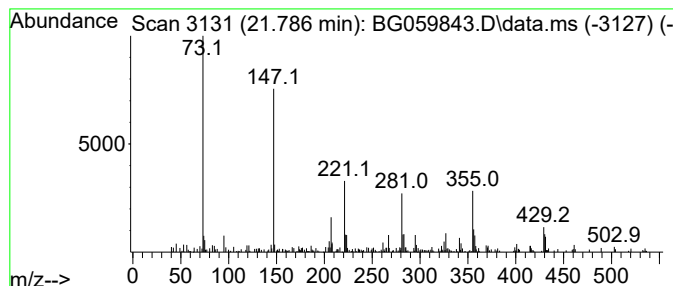
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Peak Number 5 N-Benzyl-N-ethyl-p-isopropyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.786	13.35 ng	347417	Chrysene-d12	22.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	52
2			Benzamide, 4-propyl-N-(hept-2-yl)-	261	C17H27NO	1000439-17-0	37
3			Butyrophenone, 2',3,4',6'-tetram...	204	C14H20O	005344-18-3	37
4			4-Pentamethyldisilyloxyhexadecane	372	C21H48OSi2	1000216-95-2	37
5			Butanedioic acid, 2TMS derivative	262	C10H22O4Si2	040309-57-7	37



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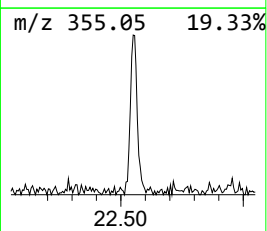
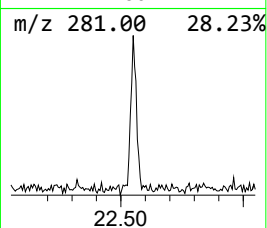
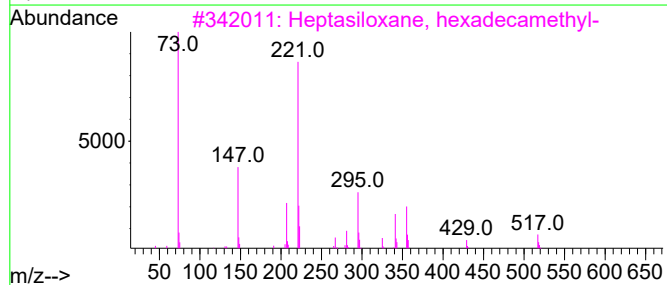
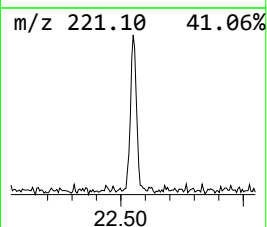
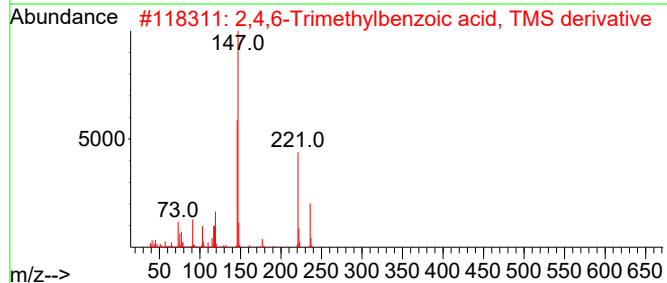
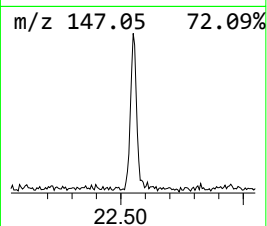
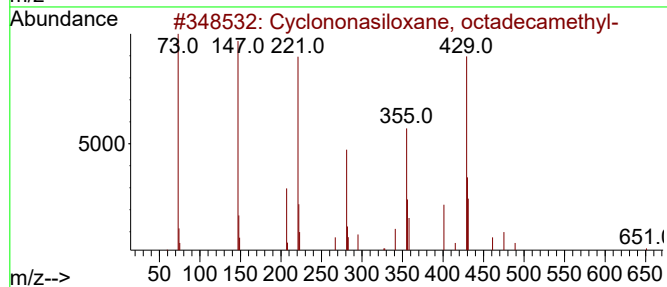
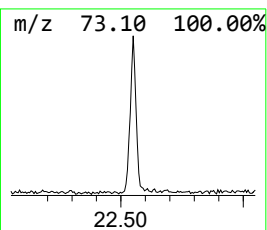
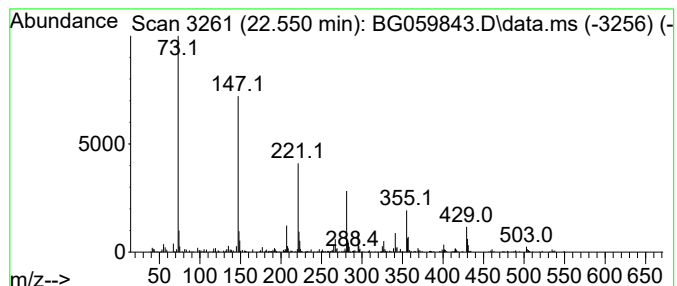
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclononasiloxane, octadeca... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.550	28.48 ng	741036	Chrysene-d12	22.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
2			2,4,6-Trimethylbenzoic acid, TMS...	236	C13H20O2Si	070079-88-8	37
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	30
4			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	28
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
Data File : BG059843.D
Acq On : 23 Nov 2023 8:35
Operator : MA/JU
Sample : 05294-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WT-5

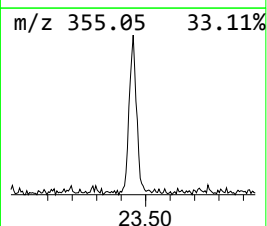
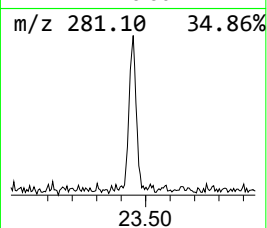
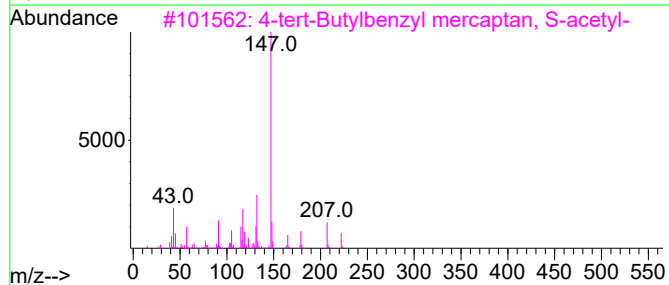
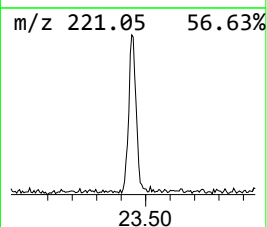
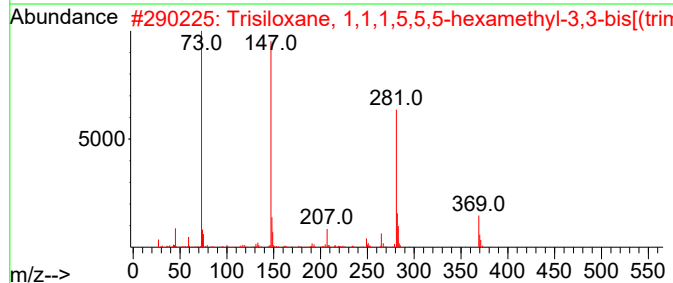
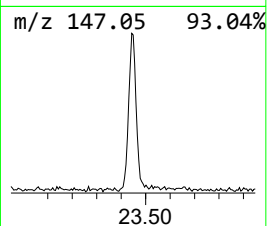
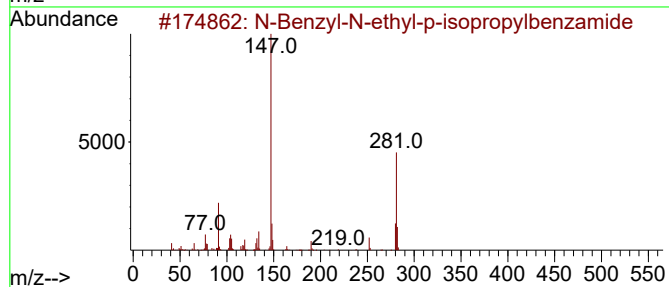
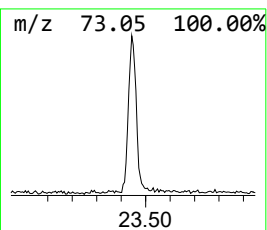
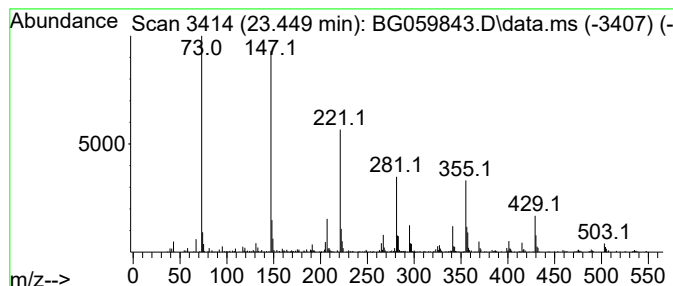
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown23.449 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.449	46.40 ng	1207400	Chrysene-d12	22.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	43
2			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	32
3			4-tert-Butylbenzyl mercaptan, S-...	222	C13H18OS	362528-98-1	27
4			1,3-Dimethyl-5-pentamethyldisily...	258	C13H30OSi2	1000216-94-7	27
5			4-(3-Aminophenoxy)phthalic acid,...	489	C23H35NO5Si3	1000468-77-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
Data File : BG059843.D
Acq On : 23 Nov 2023 8:35
Operator : MA/JU
Sample : 05294-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WT-5

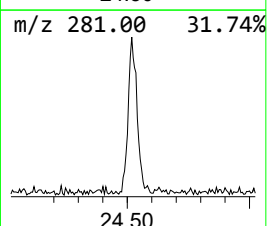
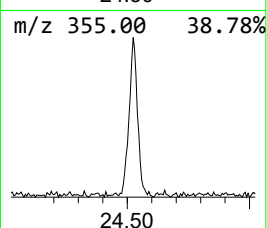
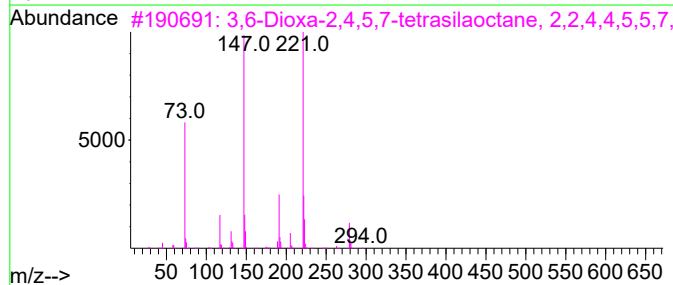
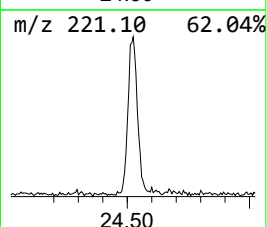
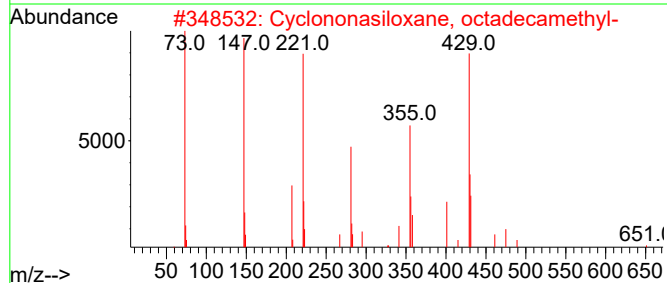
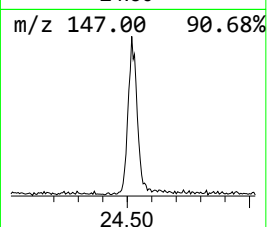
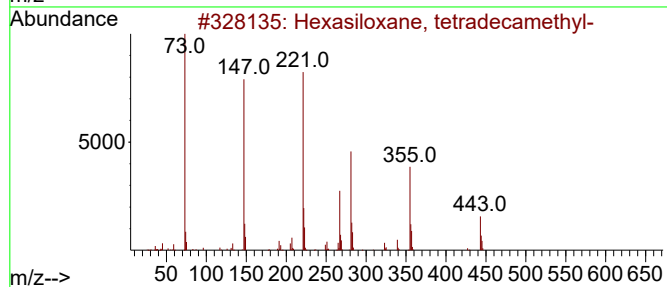
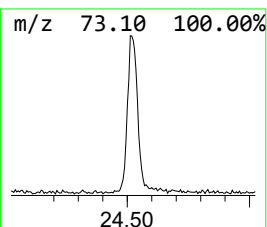
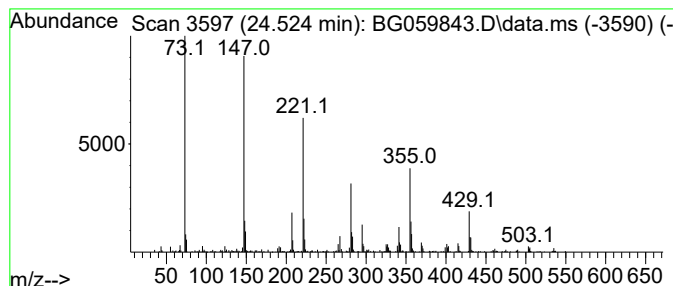
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexasiloxane, tetradecamethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.524	73.53 ng	1641880	Perylene-d12	25.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	64
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	58
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
4			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	35
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
Data File : BG059843.D
Acq On : 23 Nov 2023 8:35
Operator : MA/JU
Sample : 05294-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WT-5

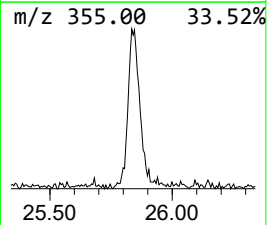
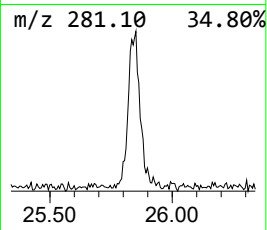
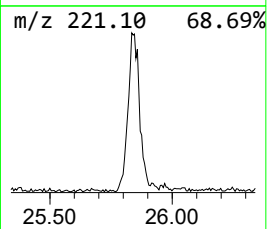
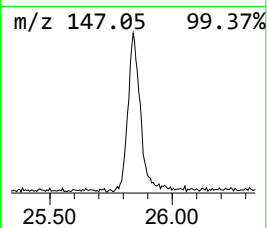
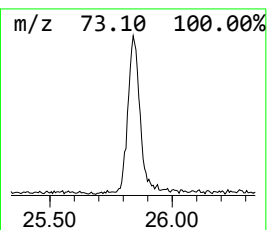
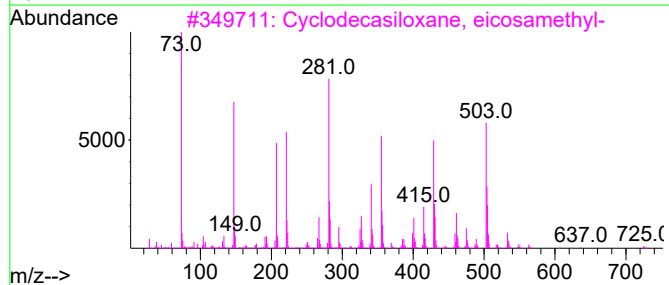
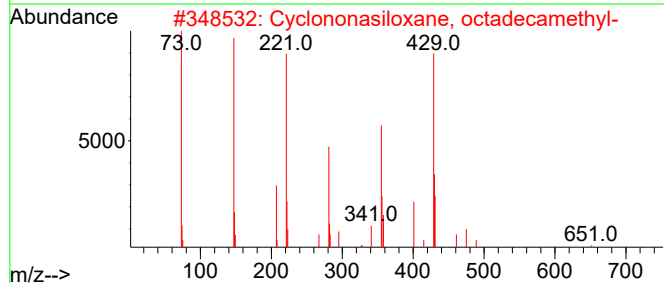
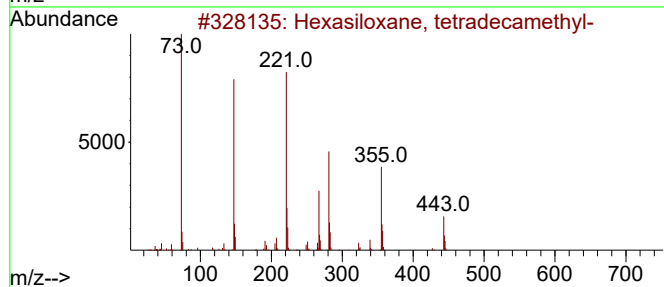
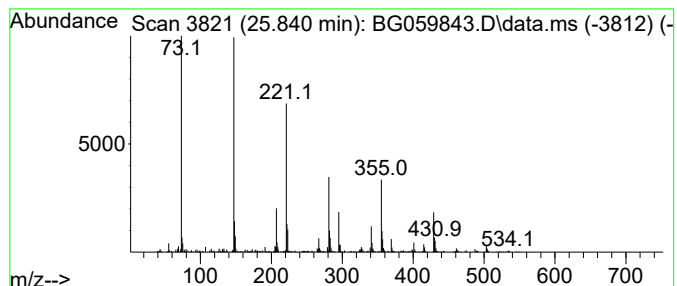
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown25.840 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.840	80.26 ng	1792000	Perylene-d12	25.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	53
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	47
3			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	41
4			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	32
5			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
Data File : BG059843.D
Acq On : 23 Nov 2023 8:35
Operator : MA/JU
Sample : 05294-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WT-5

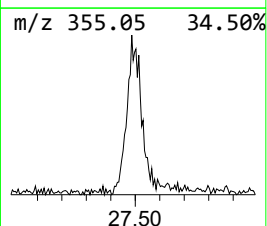
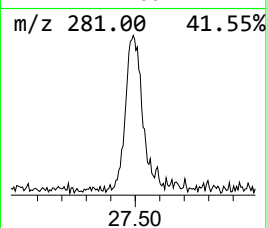
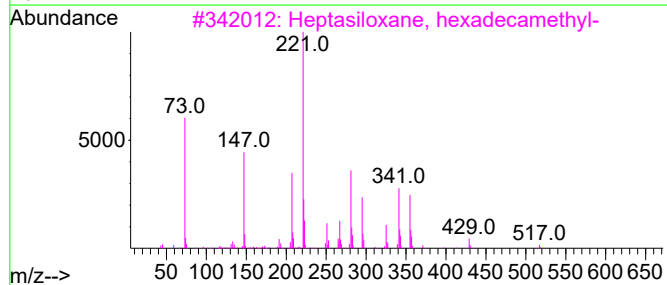
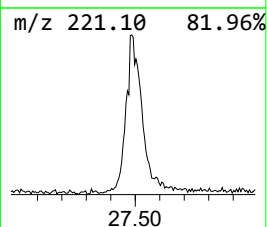
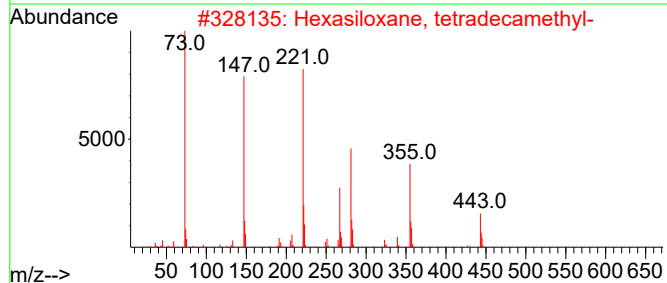
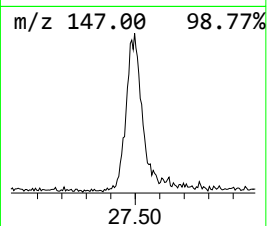
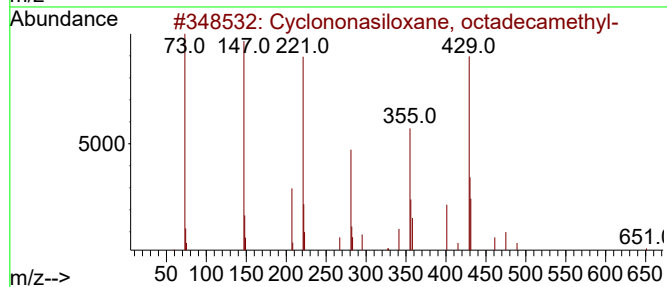
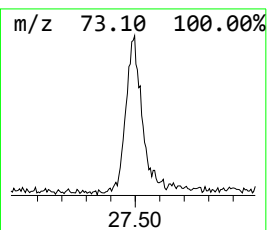
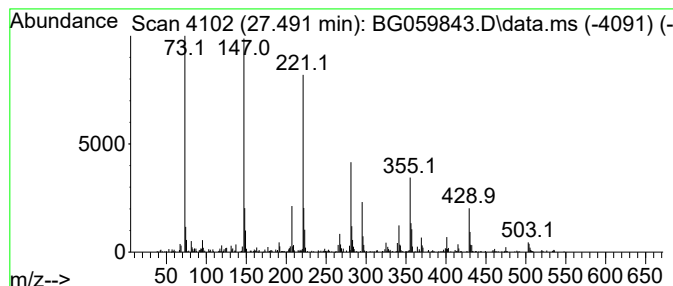
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptasiloxane, hexadecamethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.491	81.88 ng	1828290	Perylene-d12	25.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	78
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	64
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27
5			7-Methylimidazo[1,2-a]pyrimidin-...	221	C10H15N3OSi	1010468-48-3	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
Data File : BG059843.D
Acq On : 23 Nov 2023 8:35
Operator : MA/JU
Sample : 05294-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WT-5

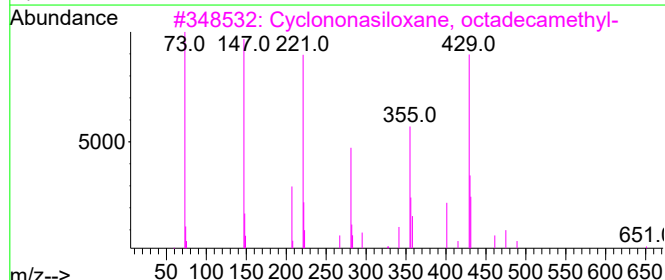
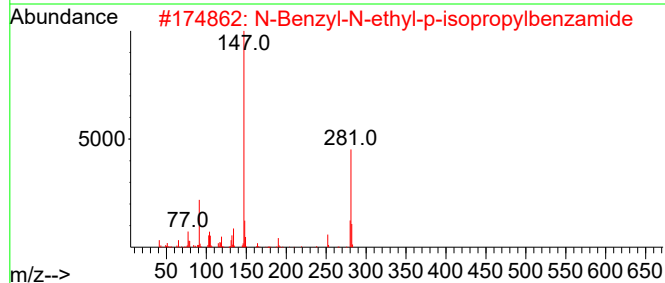
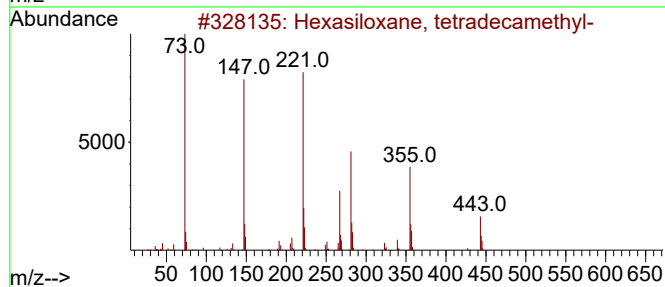
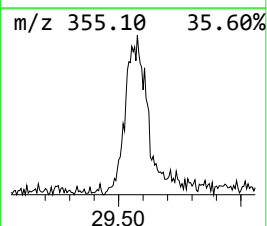
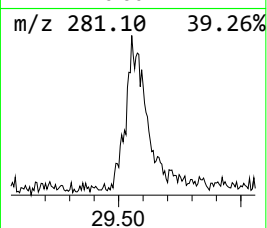
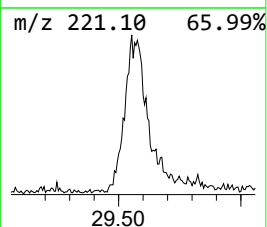
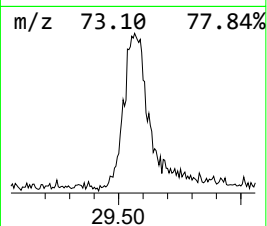
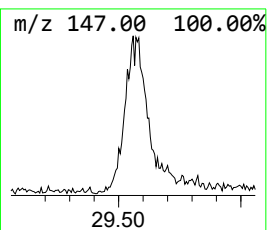
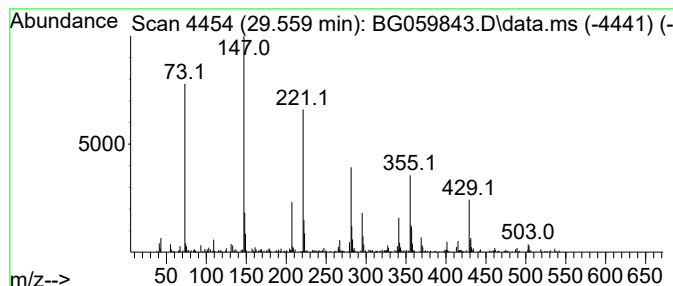
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown29.559 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.559	40.23 ng	898269	Perylene-d12	25.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	50
2			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	43
3			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	40
4			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	37
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
Data File : BG059843.D
Acq On : 23 Nov 2023 8:35
Operator : MA/JU
Sample : 05294-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

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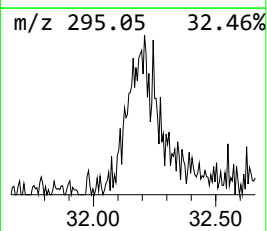
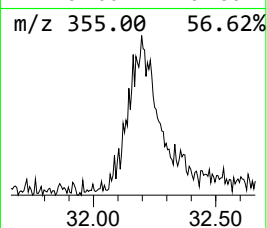
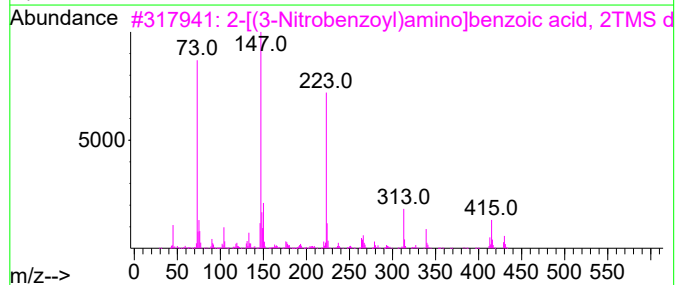
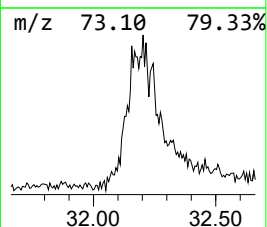
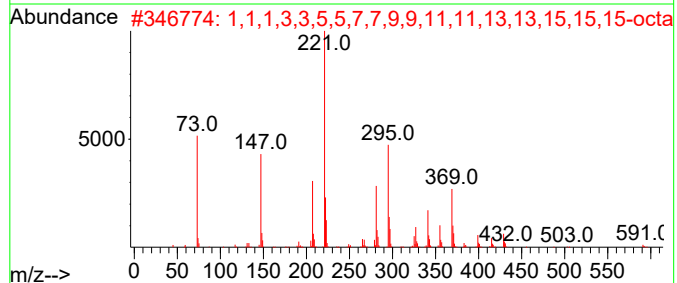
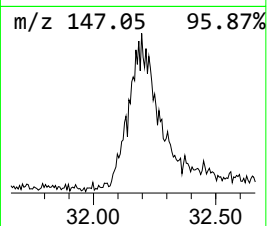
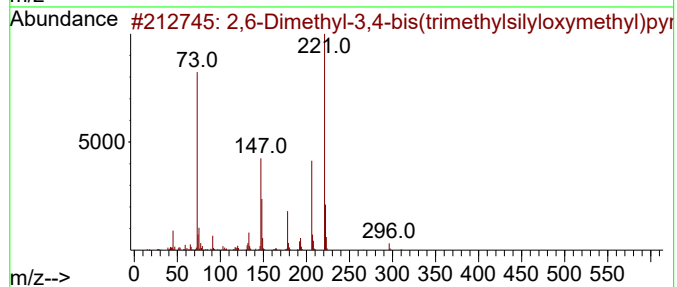
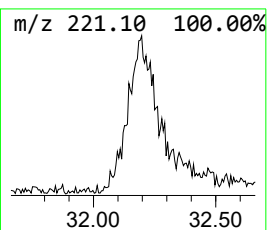
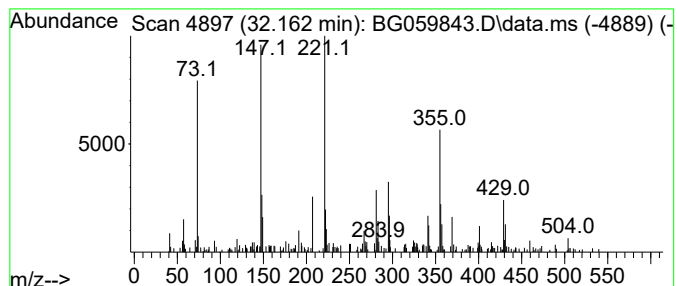
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown32.162 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
32.162	9.43 ng	210548	Perylene-d12	25.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dimethyl-3,4-bis(trimethylsi...	311	C15H29NO2Si2	1000079-52-1	27		
2	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	22		
3	2-[(3-Nitrobenzoyl)amino]benzoic...	430	C20H26N2O5Si2	1000474-80-8	15		
4	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	14		
5	4-Fluoro-5-(4-morpholinyl)-1,2-b...	355	C16H30FN3OSi2	1000479-80-2	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
Data File : BG059843.D
Acq On : 23 Nov 2023 8:35
Operator : MA/JU
Sample : 05294-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WT-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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
2,4,7,9-Tetrame...	13.784	3.1	ng	82122	3	14.959	520991	20.0
Tridecanoic acid	18.525	11.9	ng	378467	4	17.714	635341	20.0
unknown19.788	19.788	5.2	ng	165295	4	17.714	635341	20.0
unknown21.099	21.099	3.4	ng	87484	5	22.039	520482	20.0
N-Benzyl-N-ethy...	21.786	13.4	ng	347417	5	22.039	520482	20.0
Cyclononasiloxa...	22.550	28.5	ng	741036	5	22.039	520482	20.0
unknown23.449	23.449	46.4	ng	1207400	5	22.039	520482	20.0
Hexasiloxane, t...	24.524	73.5	ng	1641880	6	25.623	446572	20.0
unknown25.840	25.840	80.3	ng	1792000	6	25.623	446572	20.0
Heptasiloxane, ...	27.491	81.9	ng	1828290	6	25.623	446572	20.0
unknown29.559	29.559	40.2	ng	898269	6	25.623	446572	20.0
unknown32.162	32.162	9.4	ng	210548	6	25.623	446572	20.0