LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030725\
Data File : BG064062.D
Acq On : 7 Mar 2025 17:00
Operator : RC/JU
Sample : Q1494-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PURGE-WATER

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-BG030525.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG064062.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.449	395	402	412	rBV	381862	581023	17.56%	3.434%
2	7.024	663	670	681	rBV	258765	411721	12.44%	2.434%
3	7.864	806	813	820	rBV	143582	235042	7.10%	1.389%
4	9.016	1001	1009	1017	rBV	511641	874901	26.44%	5.171%
5	10.649	1280	1287	1296	rVB	193575	338215	10.22%	1.999%
6	13.117	1698	1707	1713	rBV	1230711	1905718	57.60%	11.265%
7	13.393	1748	1754	1760	rBV	40855	63740	1.93%	0.377%
8	13.693	1797	1805	1810	rBV	94301	134210	4.06%	0.793%
9	14.486	1933	1940	1947	rBV	334817	504991	15.26%	2.985%
10	15.843	2166	2171	2180	rBV	40900	62127	1.88%	0.367%
11	15.972	2186	2193	2202	rBV	1064500	1608628	48.62%	9.509%
12	17.230	2400	2407	2413	rBV2	409314	629258	19.02%	3.720%
13	17.917	2518	2524	2530	rBV	830618	1024945	30.98%	6.058%
14	18.135	2557	2561	2565	rBV3	31040	42686	1.29%	0.252%
15	19.057	2712	2718	2720	rBV	1180088	1381289	41.75%	8.165%
16	19.086	2720	2723	2734	rVB2	788250	1045835	31.61%	6.182%
17	19.222	2741	2746	2751	rBV	333329	393892	11.90%	2.328%
18	19.850	2847	2853	2863	rBV	2424606	3308683	100.00%	19.557%
19	21.460	3121	3127	3136	rBV2	461502	716842	21.67%	4.237%
20	21.542	3137	3141	3146	rVB5	22104	39361	1.19%	0.233%
21	22.265	3258	3264	3271	rBV4	38065	69142	2.09%	0.409%
22	23.099	3400	3406	3412	rBV4	56587	113662	3.44%	0.672%
23	24.092	3566	3575	3583	rBV4	62608	158073	4.78%	0.934%
24	24.474	3631	3640	3652	rBV	261758	708027	21.40%	4.185%
25	25.314	3774	3783	3794	rBV3	56164	164325	4.97%	0.971%
26	26.842	4031	4043	4058	rVB7	50574	193263	5.84%	1.142%
27	28.763	4356	4370	4383	rBV10	33142	166256	5.02%	0.983%
28	31.155	4765	4777	4778	rBV8	19008	41912	1.27%	0.248%

Sum of corrected areas: 16917767

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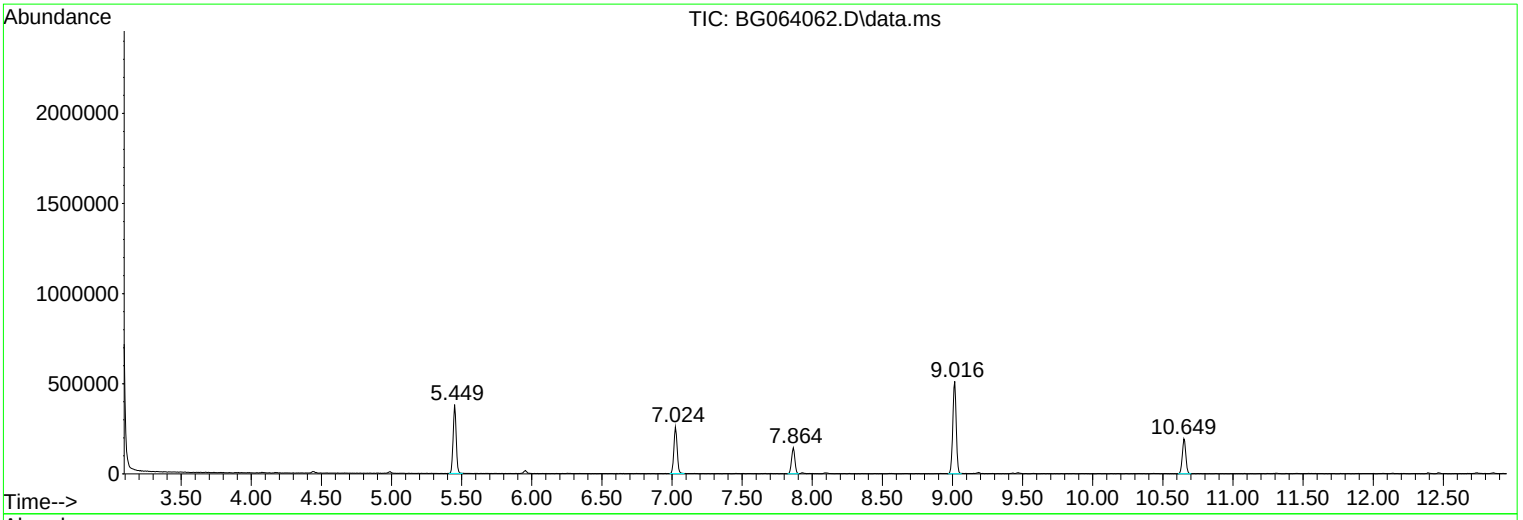
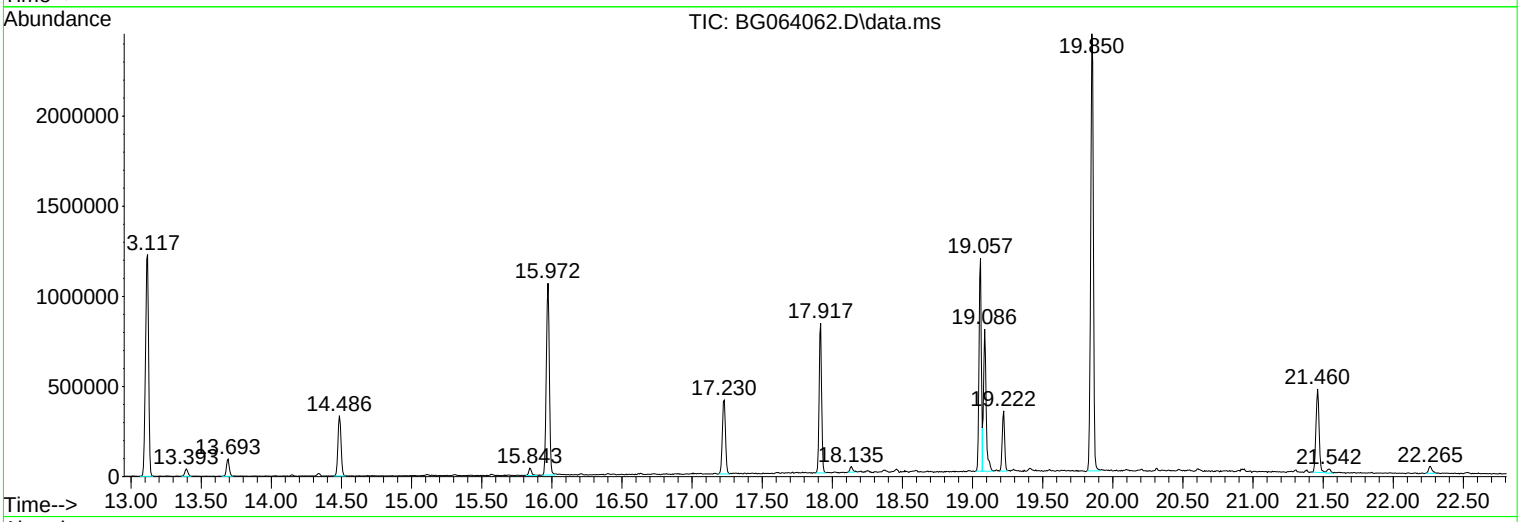
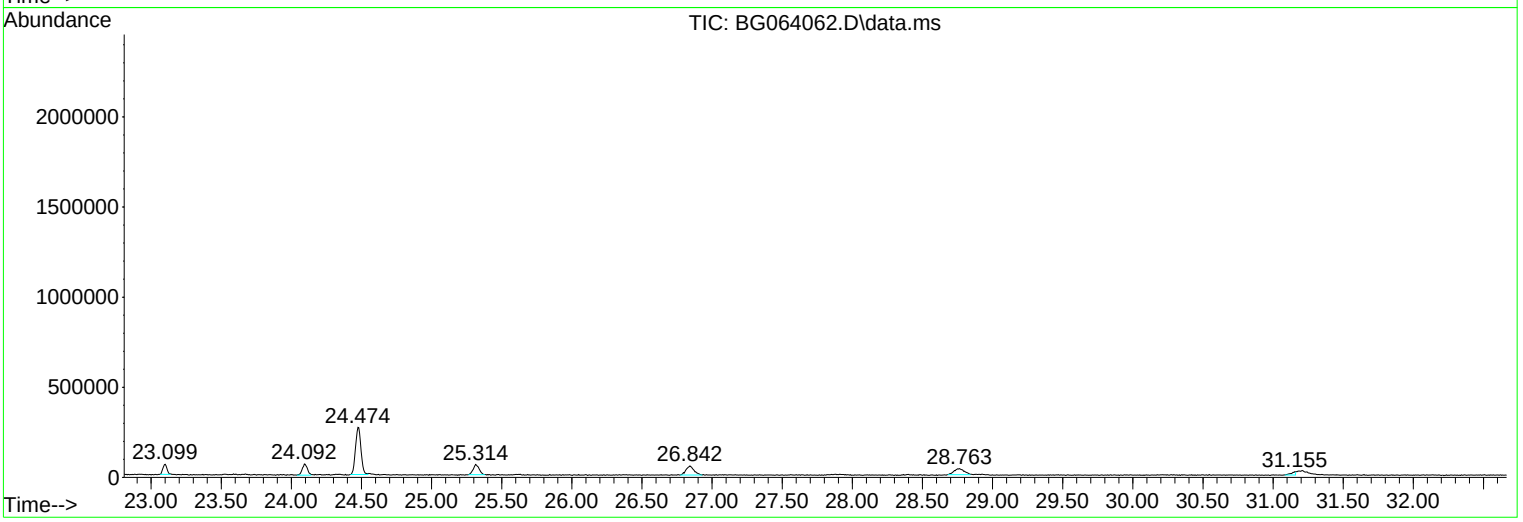
Instrument :
BNA_G
ClientSampleId :
PURGE-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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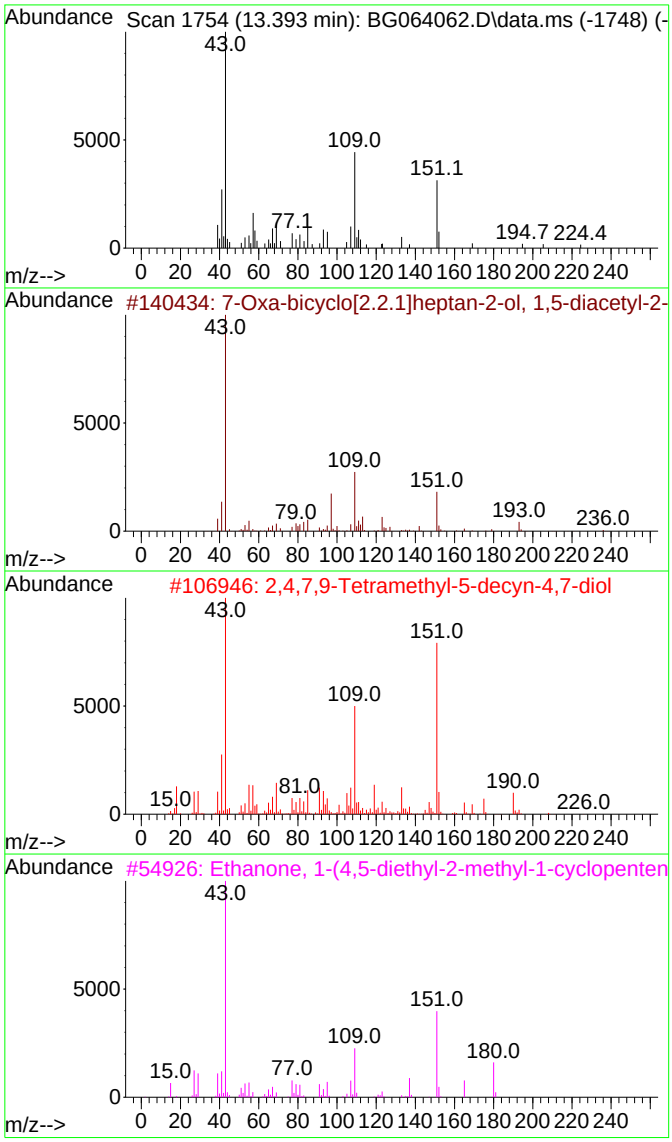
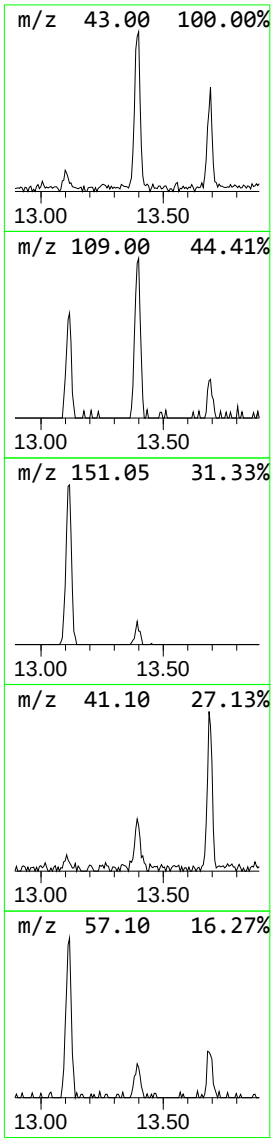
****
Peak Number 1 7-Oxa-bicyclo[2.2.1]heptan-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.393	2.52 ng	63740	Acenaphthene-d10	14.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Oxa-bicyclo[2.2.1]heptan-2-ol,...	254	C14H22O4	329362-13-2	64
2	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	56
3	Ethanone, 1-(4,5-diethyl-2-methy...	180	C12H20O	062338-24-3	40
4	4-(1,5-Dihydroxy-2,6,6-trimethyl...	224	C13H20O3	1000191-85-2	32
5	Sobrerol 8-acetate	212	C12H20O3	093133-02-9	17





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Sample : Q1494-01
Misc :
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Instrument :
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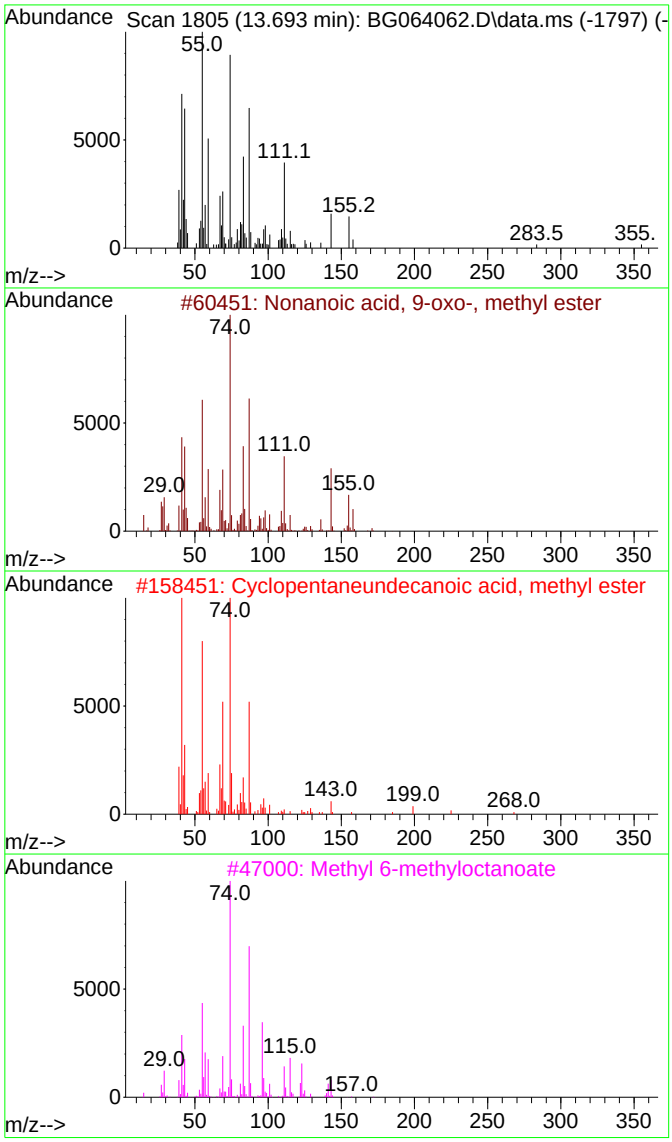
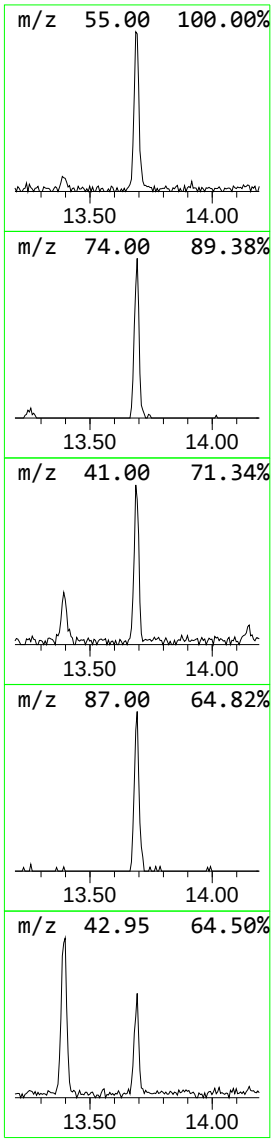
****
Peak Number 2 Nonanoic acid, 9-oxo-, meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.693	5.32 ng	134210	Acenaphthene-d10	14.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid, 9-oxo-, methyl ester	186	C10H18O3	001931-63-1	64
2	Cyclopentaneundecanoic acid, met...	268	C17H32O2	025779-85-5	47
3	Methyl 6-methyloctanoate	172	C10H20O2	005129-62-4	43
4	Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	35
5	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	35





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Sample : Q1494-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
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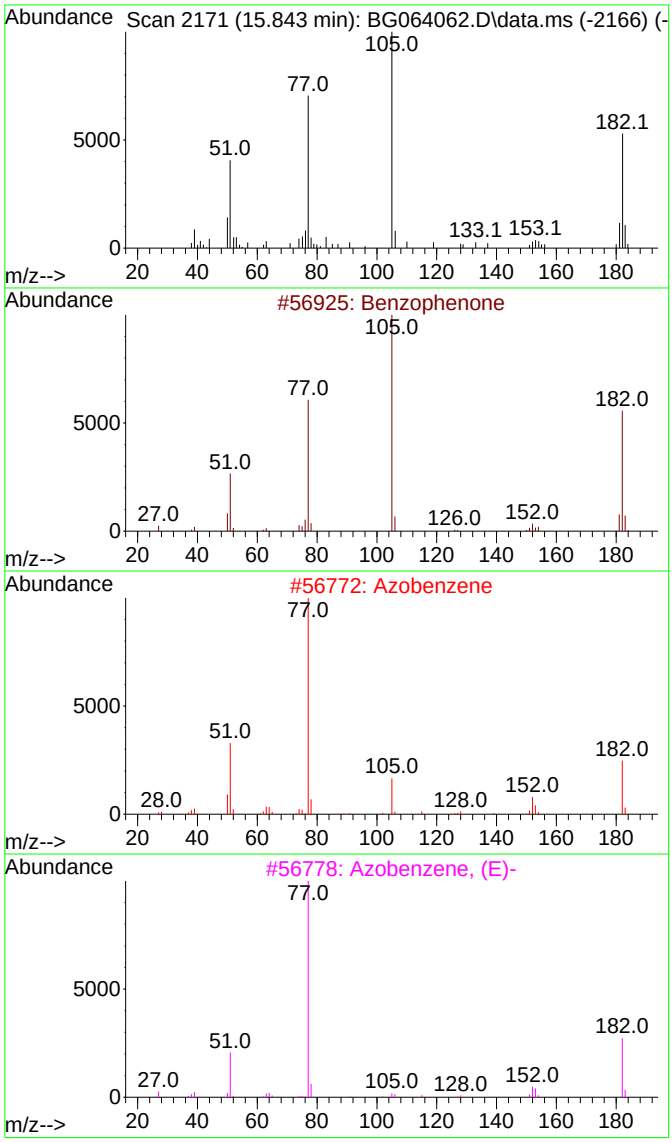
TIC Integration Parameters: LSCINT.P

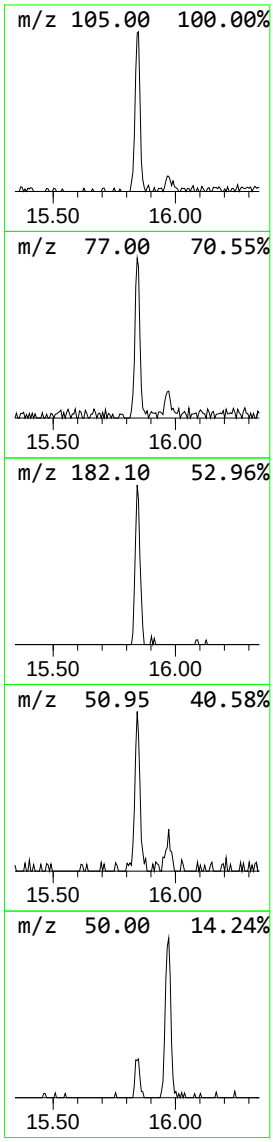
****

Peak Number 3 Benzophenone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.843	2.46 ng	62127	Acenaphthene-d10	14.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	Azobenzene	182	C12H10N2	000103-33-3	72
3	Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
4	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	53
5	1,2(4H)-Oxazine-3-ol, 5,6-dihydr...	219	C11H9NO4	1000253-25-6	47





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PURGE-WATER

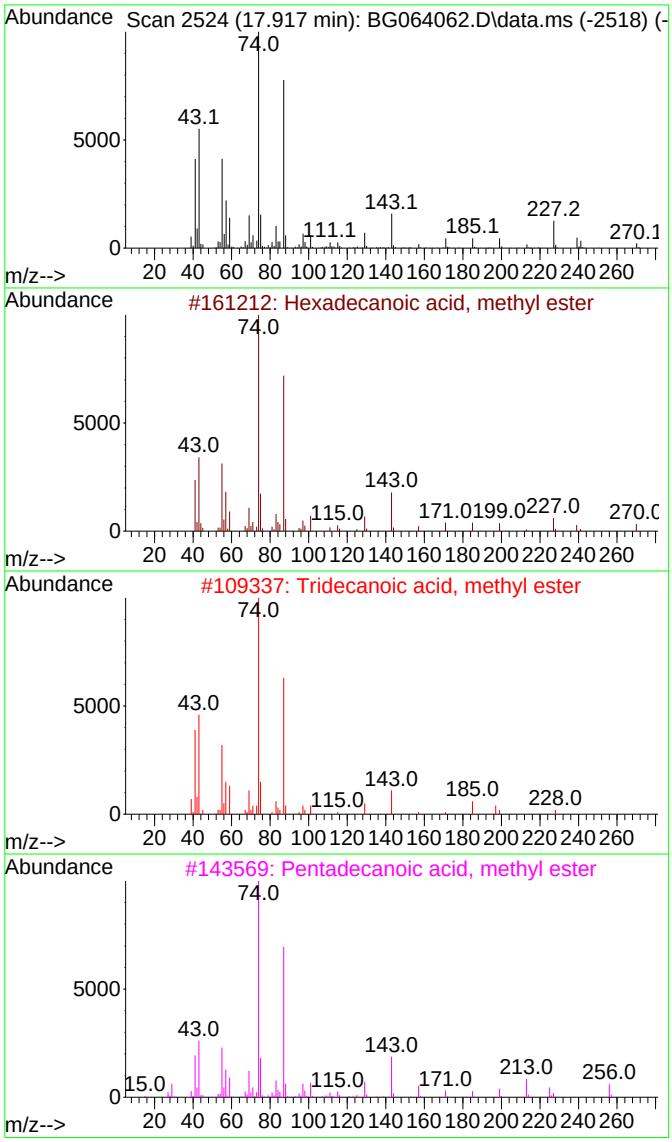
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

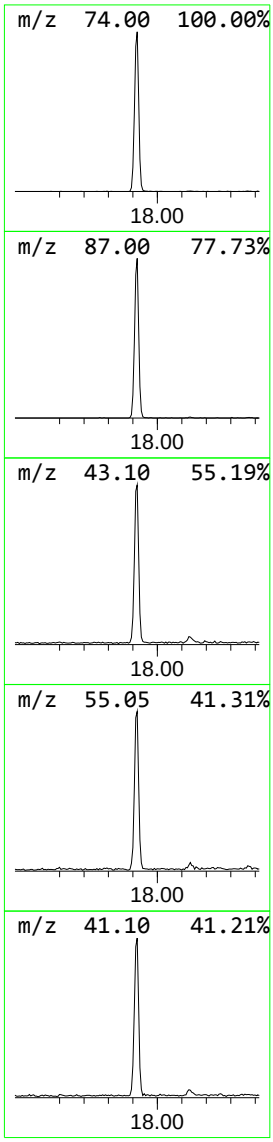
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.917	32.58 ng	1024950	Phenanthrene-d10	17.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80
5	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	80





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Sample : Q1494-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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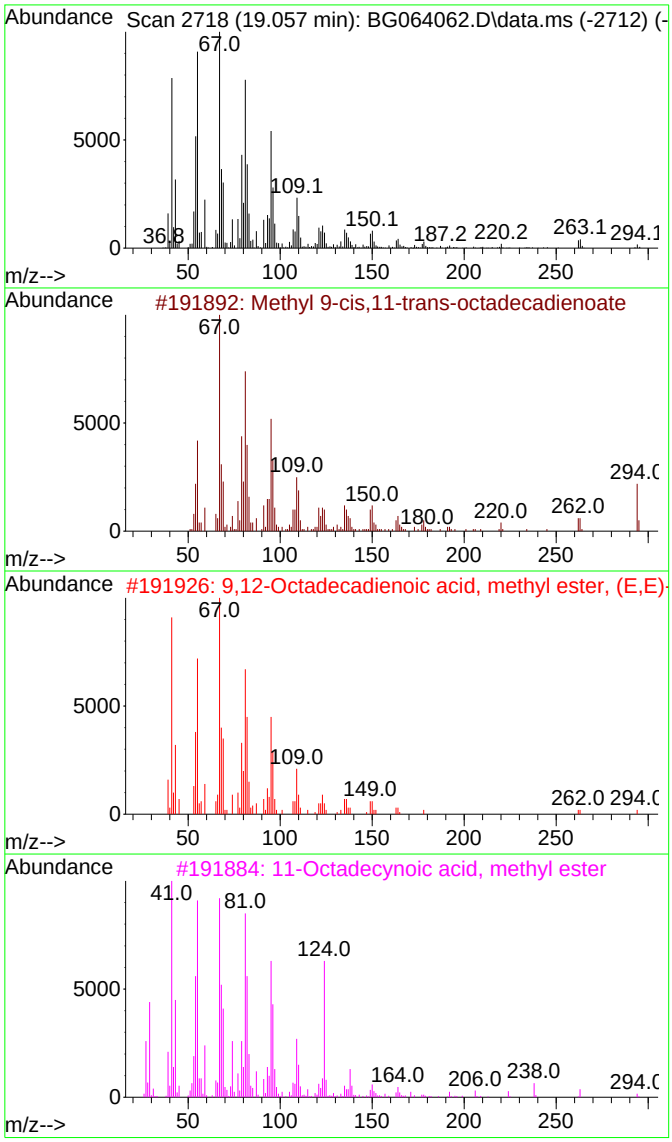
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

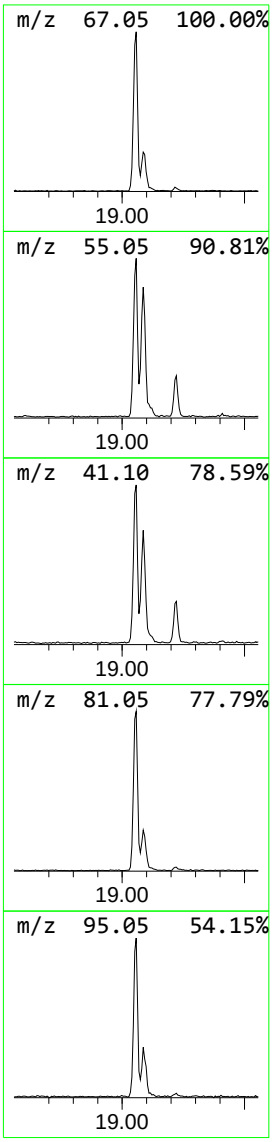
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Methyl 9-cis,11-trans-octad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.057	43.90 ng	1381290	Phenanthrene-d10	17.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
3	11-Octadecynoic acid, methyl ester	294	C19H34O2	026543-37-3	94
4	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	90
5	Linoelaidic acid	280	C18H32O2	000506-21-8	90





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
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TIC Library : C:\Database\NIST20.L
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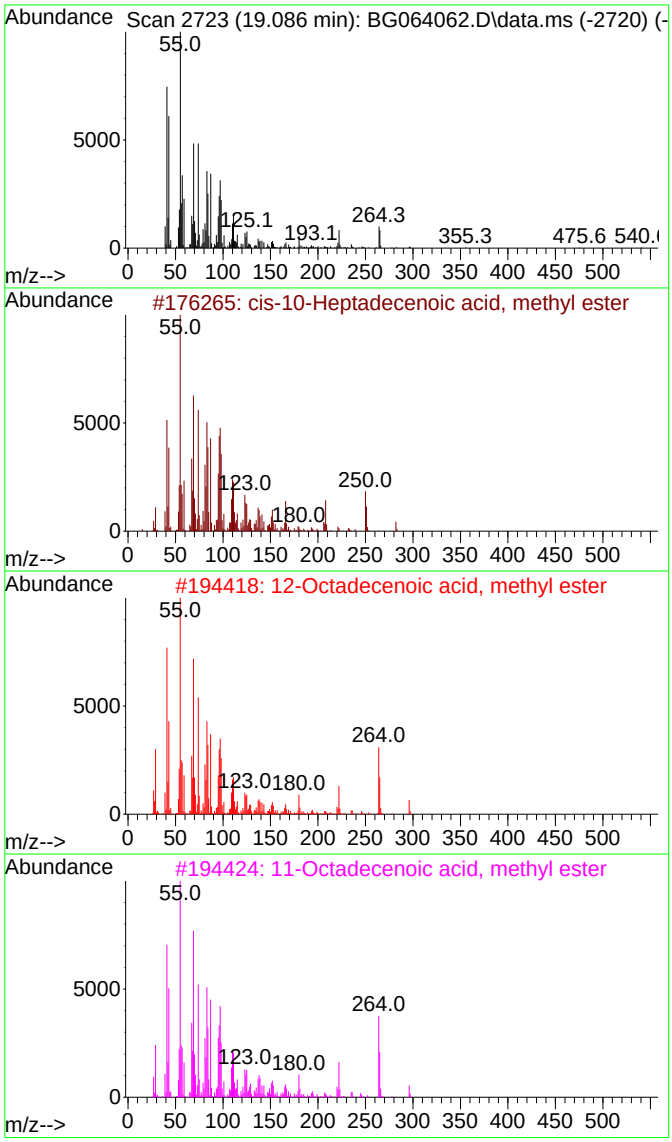
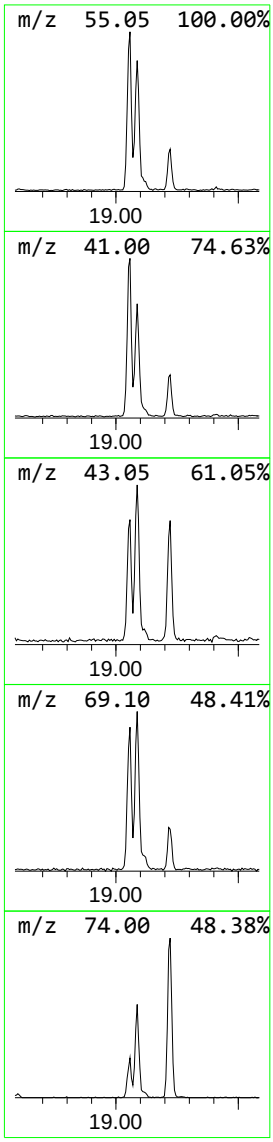
****
Peak Number 6 cis-10-Heptadecenoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.086	33.24 ng	1045840	Phenanthrene-d10	17.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	97
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	93
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	93
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91





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TIC Library : C:\Database\NIST20.L
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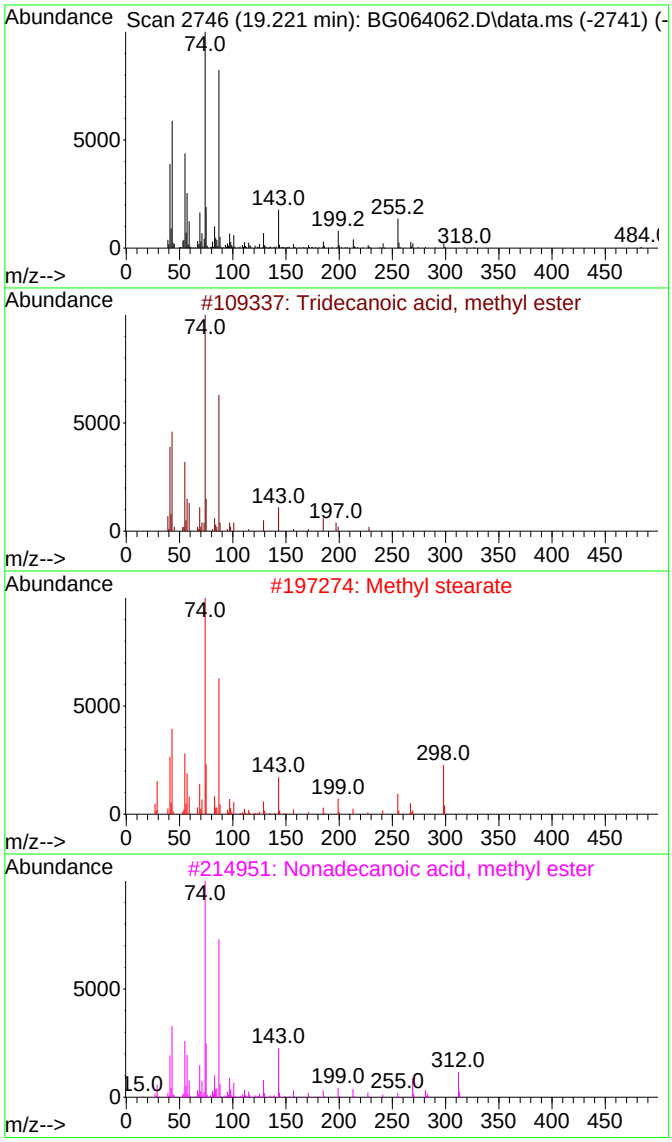
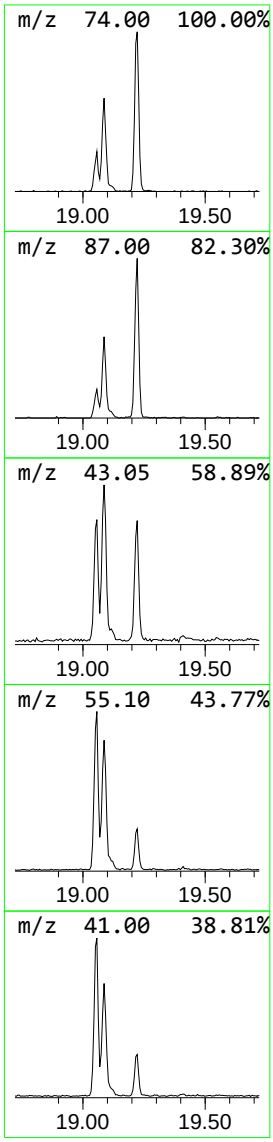
****
Peak Number 7 Tridecanoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.221	12.52 ng	393892	Phenanthrene-d10	17.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
2	Methyl stearate	298	C19H38O2	000112-61-8	91
3	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	90
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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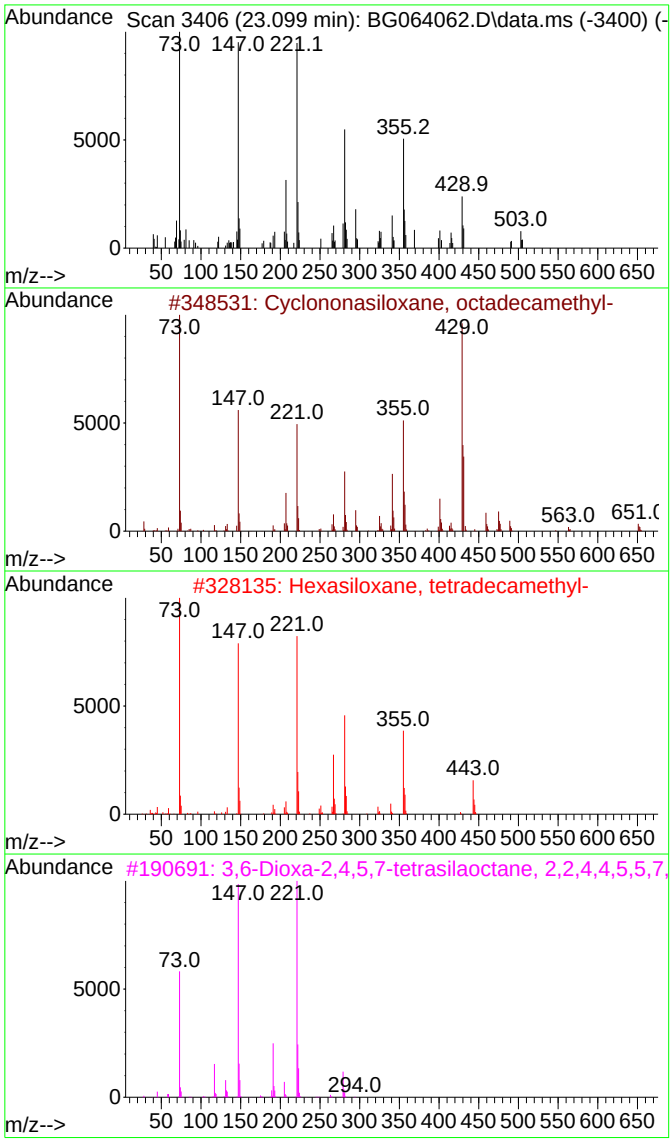
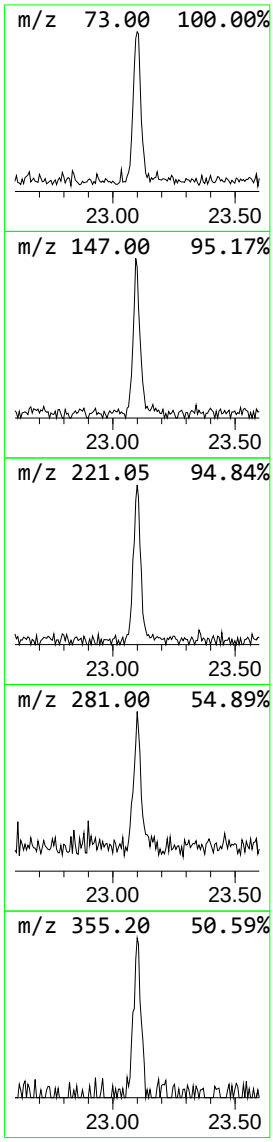
****
Peak Number 8 Cyclononasiloxane, octadeca... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.099	3.21 ng	113662	Perylene-d12	24.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	90
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
4	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27
5	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27





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Sample : Q1494-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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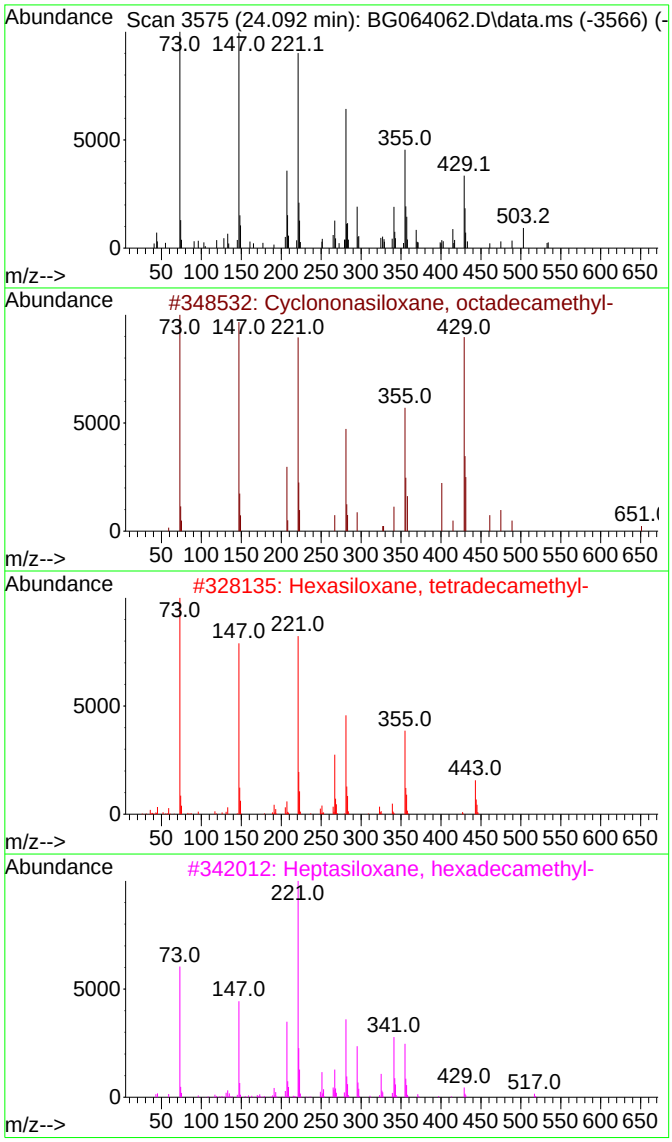
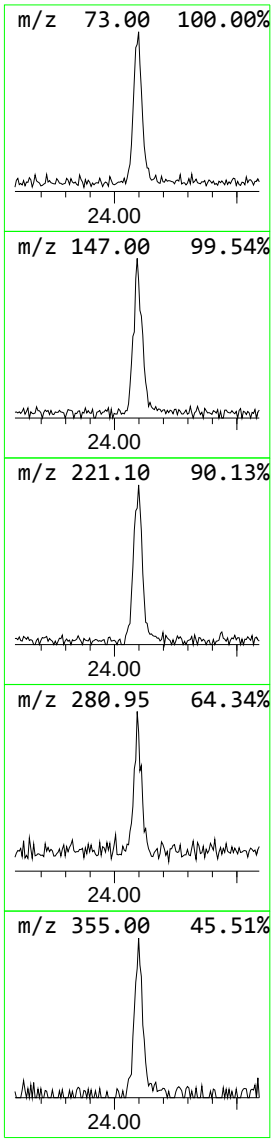
****
Peak Number 9 Hexasiloxane, tetradecamethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.092	4.47 ng	158073	Perylene-d12	24.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	58
3	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	43
4	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	35
5	Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	22





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Data File : BG064062.D
Acq On : 7 Mar 2025 17:00
Operator : RC/JU
Sample : Q1494-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PURGE-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.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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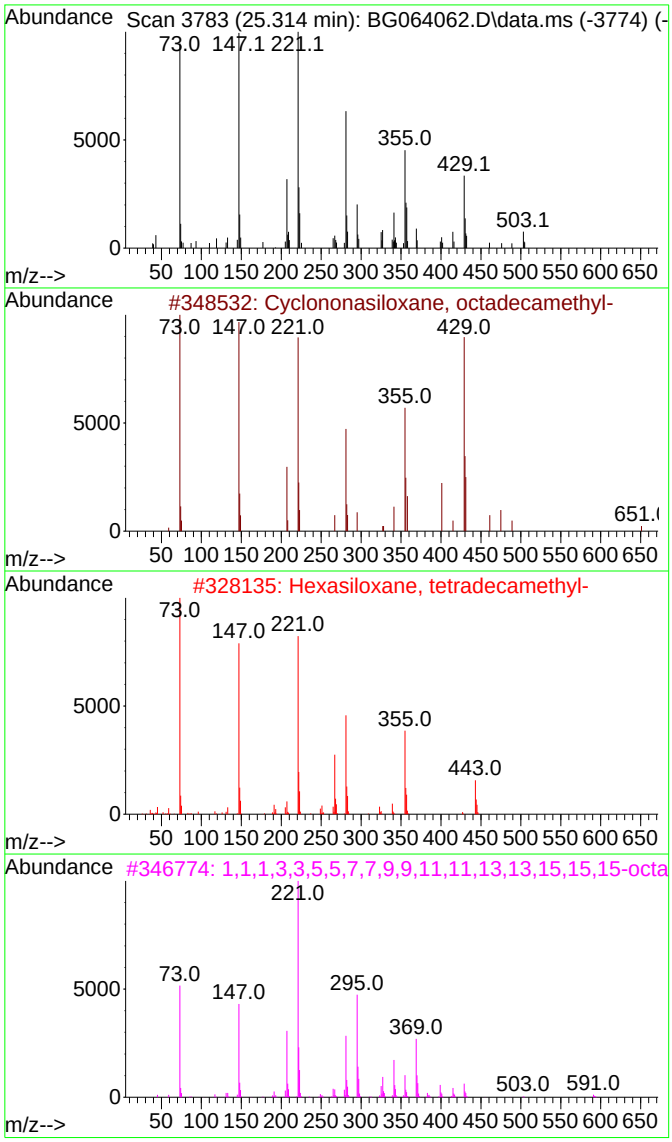
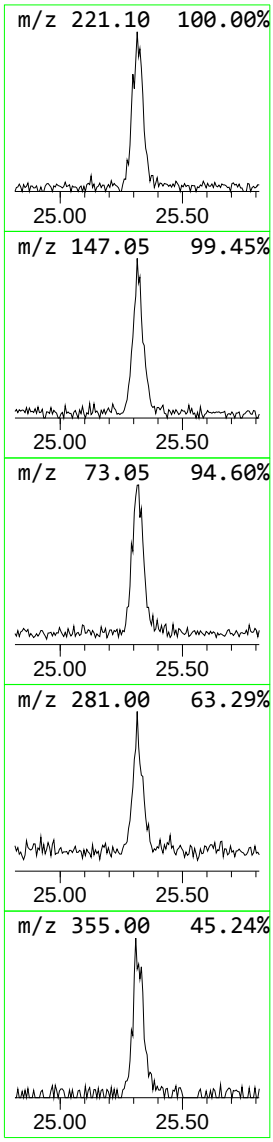
Peak Number 10 25.314 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.314	4.64 ng	164325	Perylene-d12	24.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	80
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
3	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	43
4	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	43
5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030725\
Data File : BG064062.D
Acq On : 7 Mar 2025 17:00
Operator : RC/JU
Sample : Q1494-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PURGE-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.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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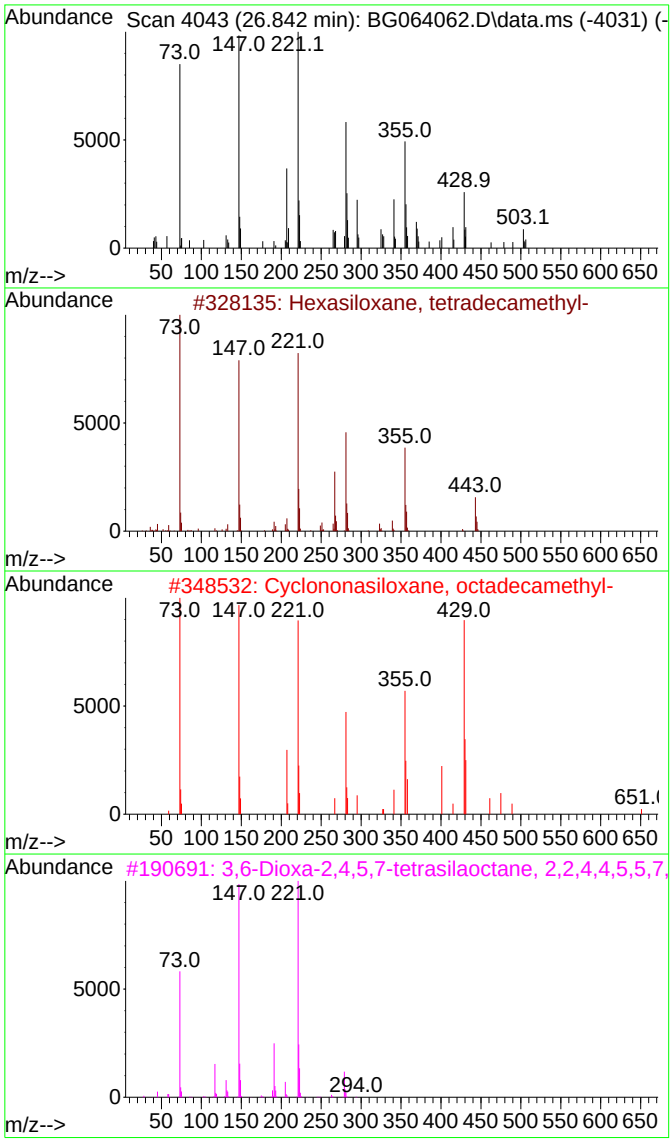
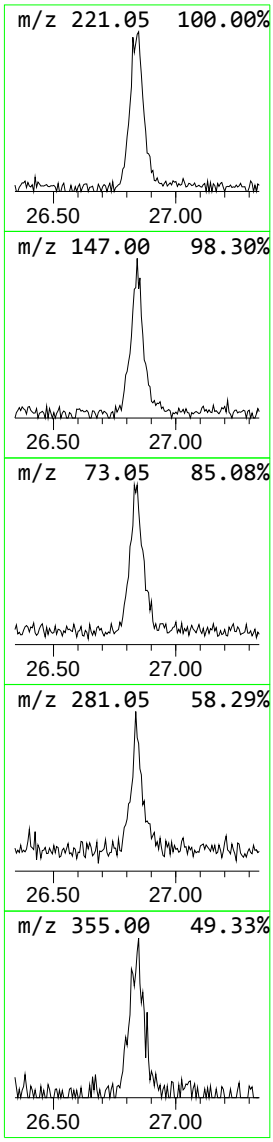
Peak Number 11 unknown26.842 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.842	5.46 ng	193263	Perylene-d12	24.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
2	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
4	Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	30
5	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030725\
Data File : BG064062.D
Acq On : 7 Mar 2025 17:00
Operator : RC/JU
Sample : Q1494-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PURGE-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.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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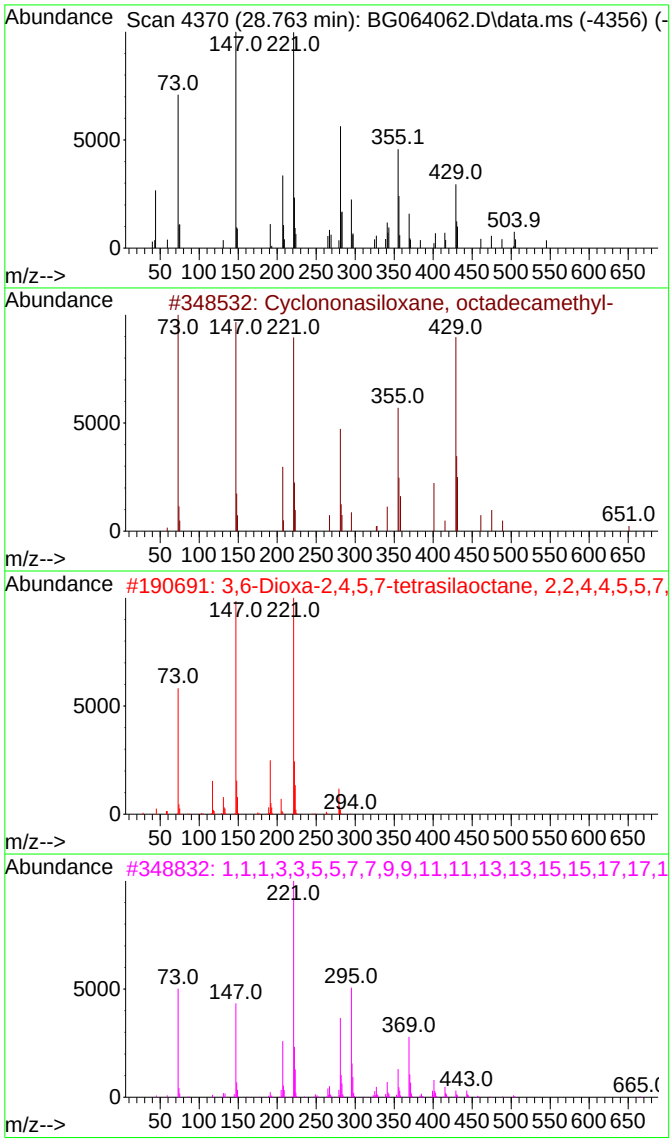
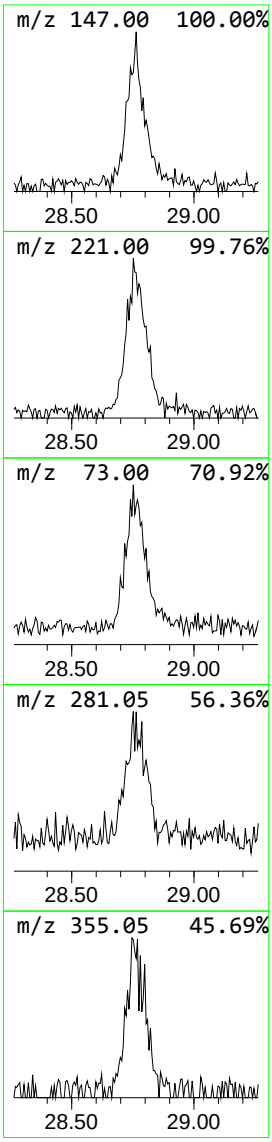
Peak Number 12 unknown28.763 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.763	4.70 ng	166256	Perylene-d12	24.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	91
2	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	43
3	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	680	C20H60O8Si9	002652-13-3	40
4	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
5	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030725\
Data File : BG064062.D
Acq On : 7 Mar 2025 17:00
Operator : RC/JU
Sample : Q1494-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PURGE-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
7-Oxa-bicyclo[2...	13.393	2.5	ng	63740	3	14.486	504991	20.0
Nonanoic acid, ...	13.693	5.3	ng	134210	3	14.486	504991	20.0
Benzophenone	15.843	2.5	ng	62127	3	14.486	504991	20.0
Hexadecanoic ac...	17.917	32.6	ng	1024950	4	17.230	629258	20.0
Methyl 9-cis,11...	19.057	43.9	ng	1381290	4	17.230	629258	20.0
cis-10-Heptadec...	19.086	33.2	ng	1045840	4	17.230	629258	20.0
Tridecanoic aci...	19.221	12.5	ng	393892	4	17.230	629258	20.0
Cyclononasiloxa...	23.099	3.2	ng	113662	6	24.480	708027	20.0
Hexasiloxane, t...	24.092	4.5	ng	158073	6	24.480	708027	20.0
25.314	25.314	4.6	ng	164325	6	24.480	708027	20.0
unknown26.842	26.842	5.5	ng	193263	6	24.480	708027	20.0
unknown28.763	28.763	4.7	ng	166256	6	24.480	708027	20.0