LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136532.D
Acq On : 13 Dec 2023 11:54
Operator : CG\JU
Sample : PB157507BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157507BL

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_F\Methods\8270-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136532.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	498	504	511	rBV	41282	56791	1.40%	0.257%
2	5.445	566	571	574	rBV	2755570	2595872	64.19%	11.734%
3	6.439	734	740	743	rBV	2467570	2546783	62.97%	11.512%
4	6.792	797	800	804	rBV	692961	559853	13.84%	2.531%
5	7.357	890	896	899	rBV	1735578	1684282	41.65%	7.614%
6	8.069	1013	1017	1021	rBV	832998	781234	19.32%	3.531%
7	9.151	1195	1201	1204	rBV	3988664	3592094	88.82%	16.238%
8	9.827	1311	1316	1319	rBV	1145309	943787	23.34%	4.266%
9	10.621	1446	1451	1454	rBV	2382587	2176912	53.83%	9.840%
10	11.321	1566	1570	1573	rBV	1227330	1020006	25.22%	4.611%
11	12.921	1837	1842	1845	rBV	4385242	4044136	100.00%	18.281%
12	13.974	2017	2021	2029	rBV	813351	768097	18.99%	3.472%
13	14.451	2095	2102	2106	rBV	64065	71775	1.77%	0.324%
14	14.839	2163	2168	2176	rBV2	72375	98478	2.44%	0.445%
15	15.274	2237	2242	2251	rBV	77285	125666	3.11%	0.568%
16	15.456	2267	2273	2286	rVB	458178	639650	15.82%	2.891%
17	15.786	2323	2329	2339	rBV2	76526	139281	3.44%	0.630%
18	16.403	2426	2434	2443	rBV2	48805	116871	2.89%	0.528%
19	17.145	2553	2560	2571	rVB3	33246	95076	2.35%	0.430%
20	18.056	2710	2715	2724	rVB6	21384	65504	1.62%	0.296%

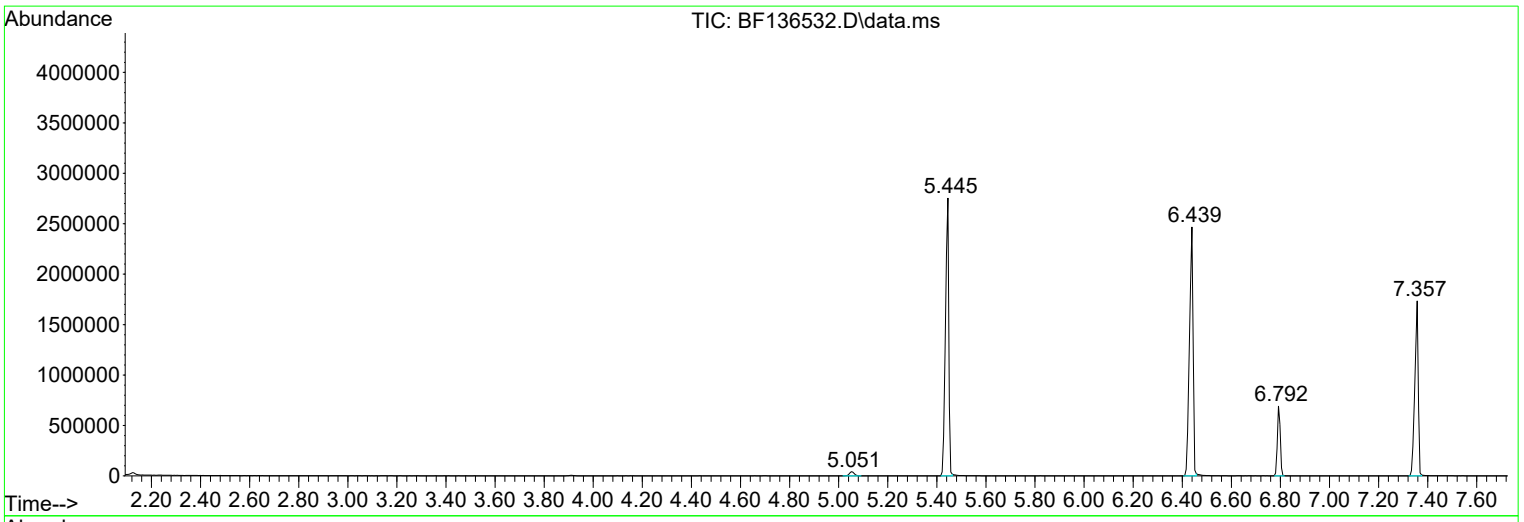
Sum of corrected areas: 22122148

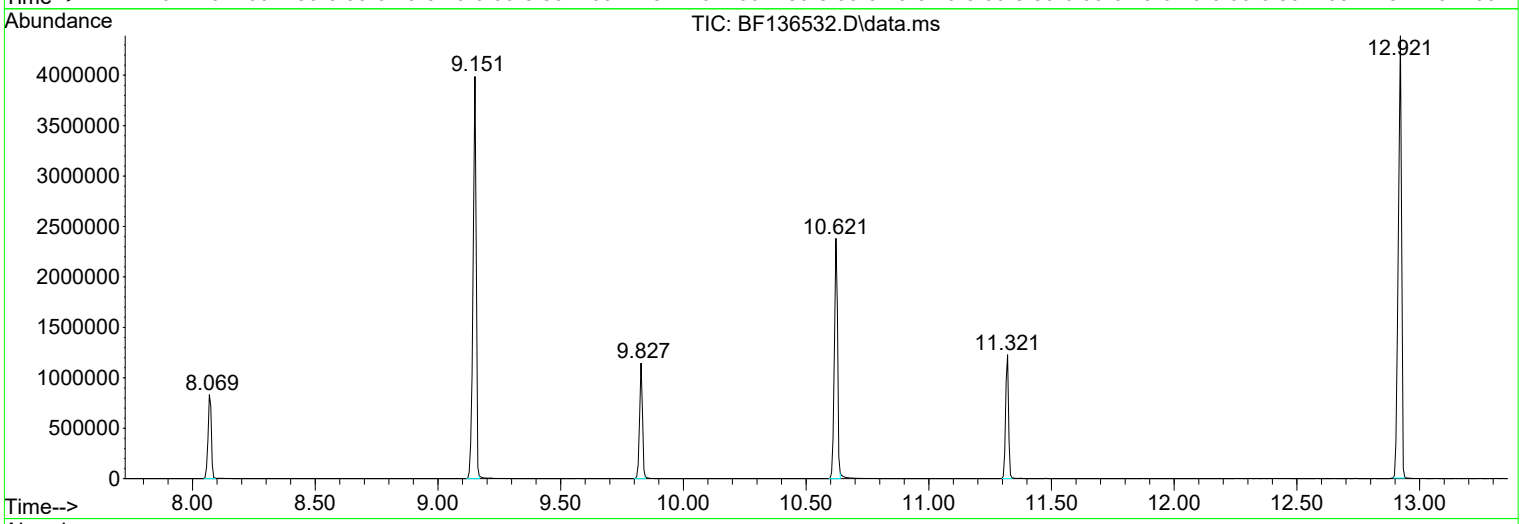
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136532.D
Acq On : 13 Dec 2023 11:54
Operator : CG\JU
Sample : PB157507BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

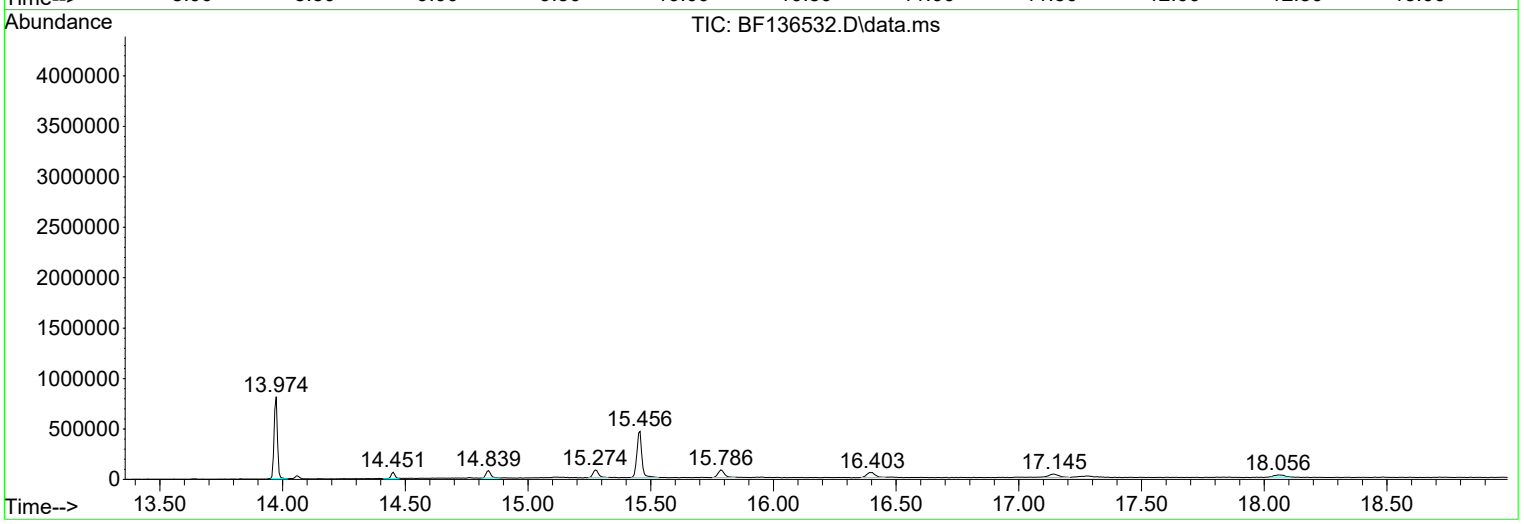
Instrument :
BNA_F
ClientSampleId :
PB157507BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136532.D
Acq On : 13 Dec 2023 11:54
Operator : CG\JU
Sample : PB157507BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157507BL

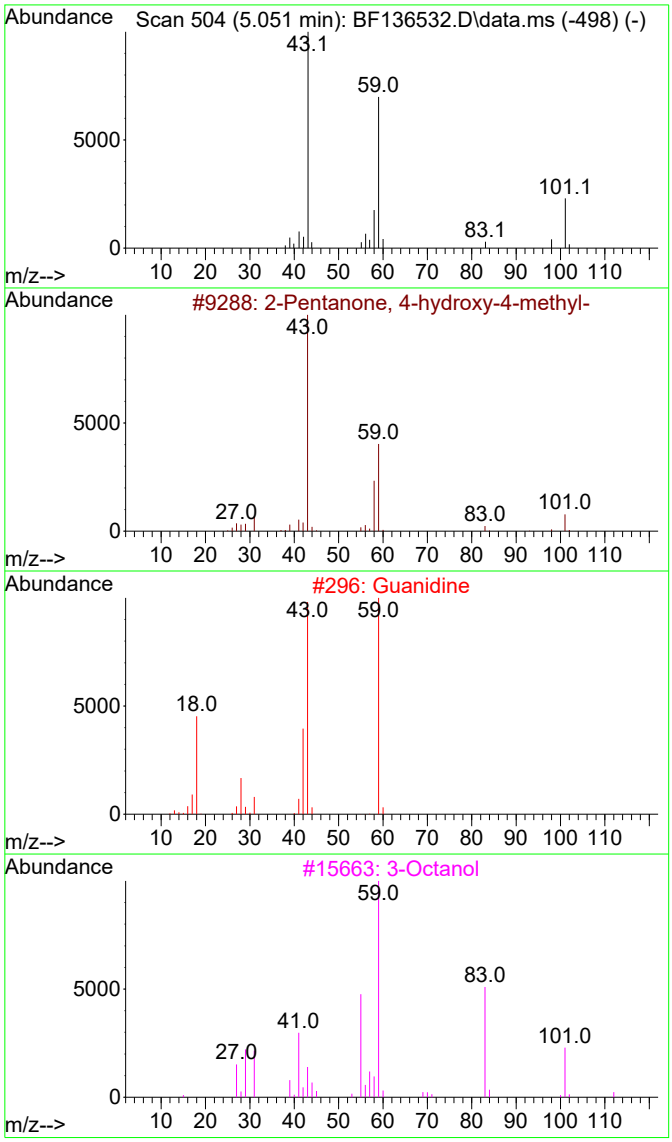
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

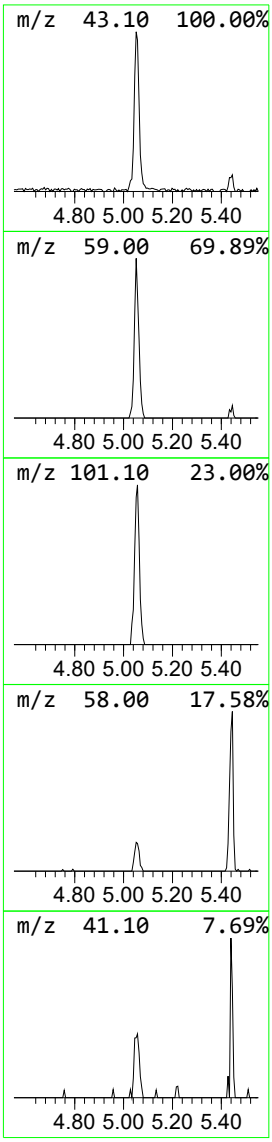
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	2.03 ng	56791	1,4-Dichlorobenzene-d4	6.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Guanidine	59	CH5N3	000113-00-8	43
3	3-Octanol	130	C8H18O	000589-98-0	36
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136532.D
Acq On : 13 Dec 2023 11:54
Operator : CG\JU
Sample : PB157507BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157507BL

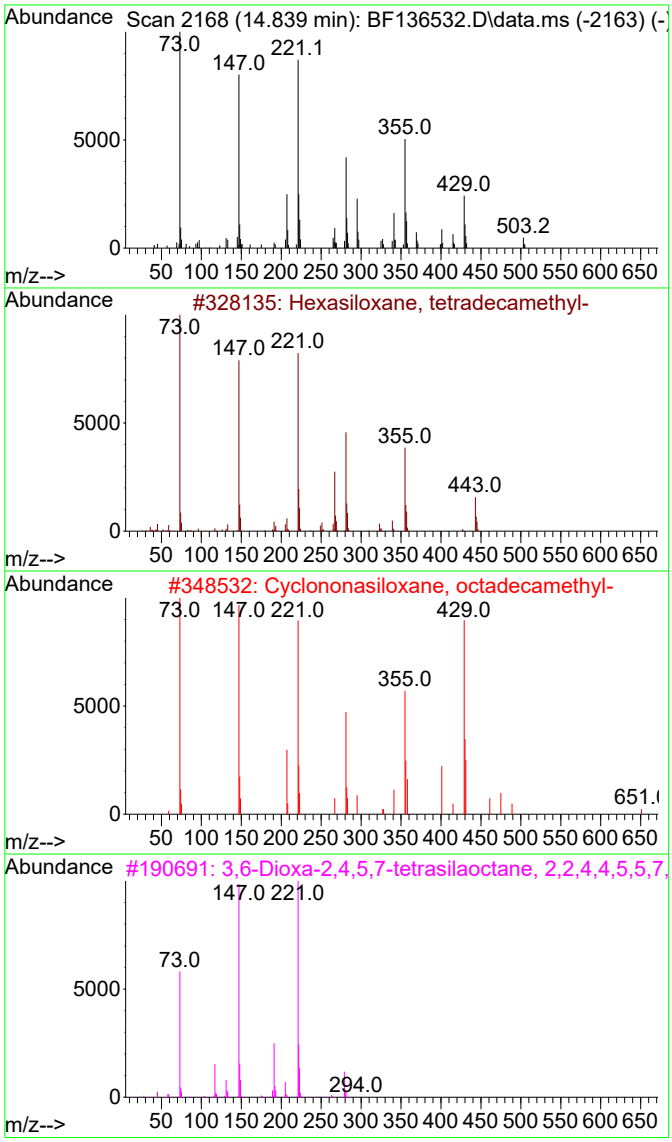
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

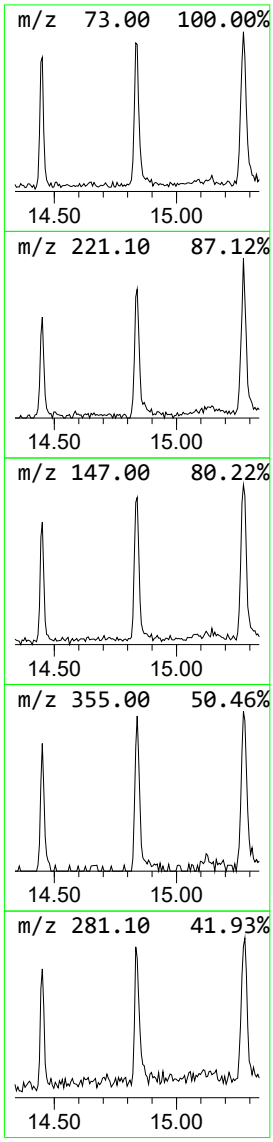
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexasiloxane, tetradecamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	3.08 ng	98478	Perylene-d12	15.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
2	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	52
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
4	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	35
5	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136532.D
Acq On : 13 Dec 2023 11:54
Operator : CG\JU
Sample : PB157507BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157507BL

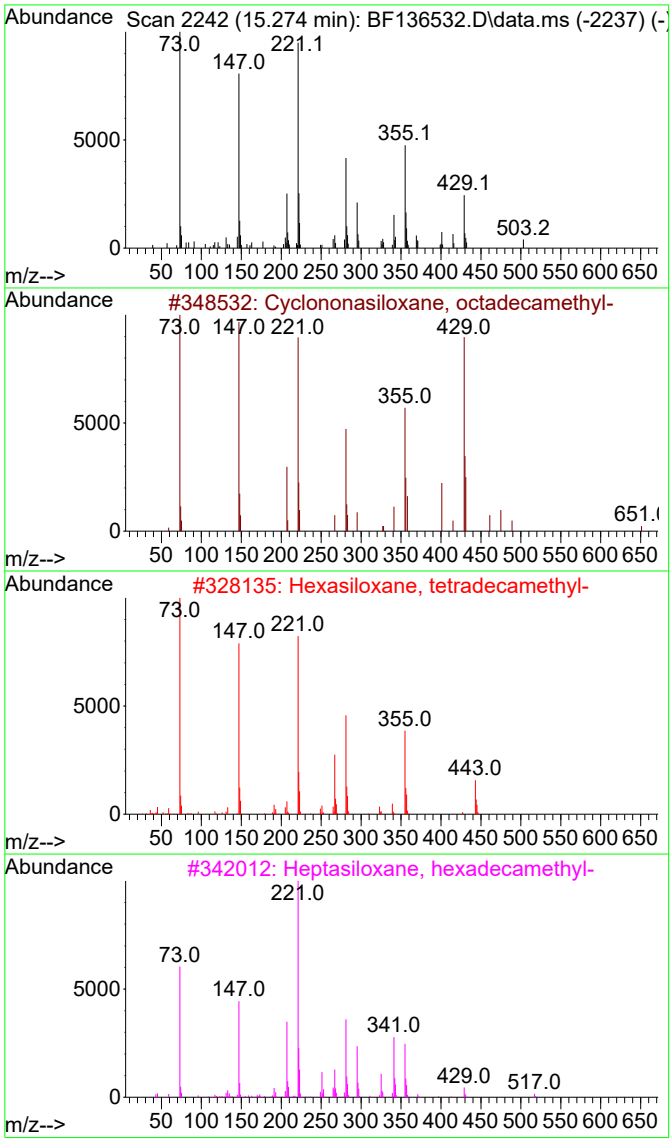
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

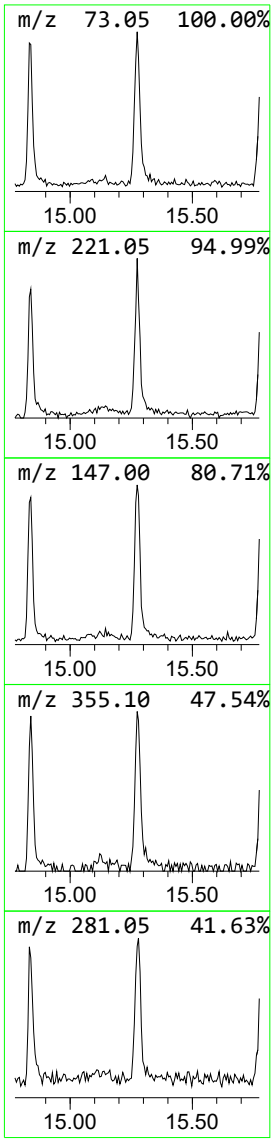
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclononasiloxane, octadeca... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.274	3.93 ng	125666	Perylene-d12	15.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	58
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	53
3	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	42
4	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	27
5	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136532.D
Acq On : 13 Dec 2023 11:54
Operator : CG\JU
Sample : PB157507BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157507BL

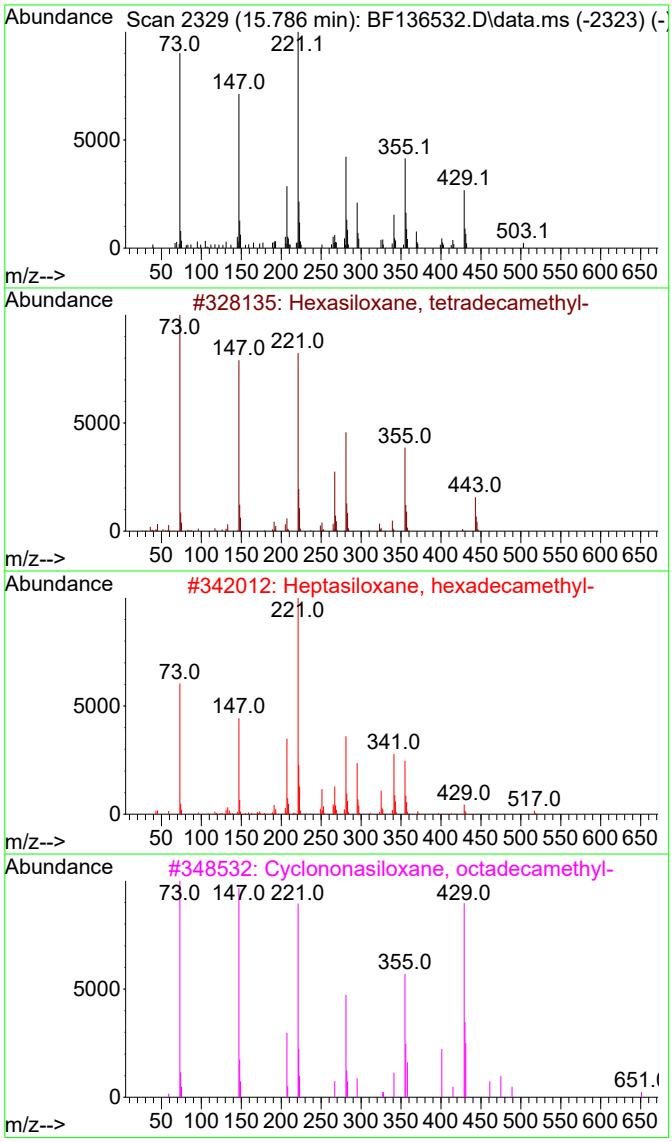
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

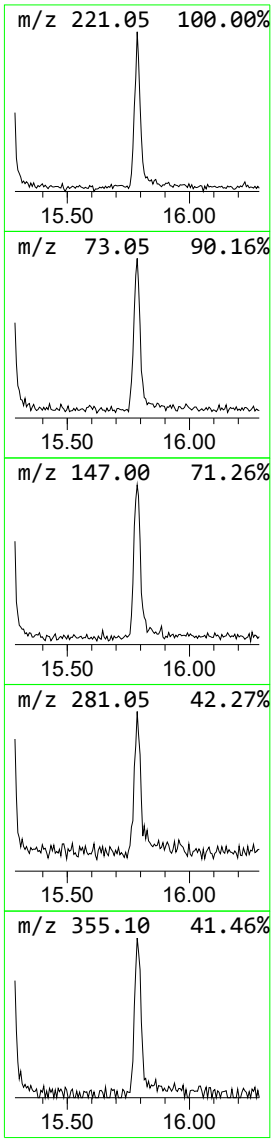
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Heptasiloxane, hexadecamethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	4.35 ng	139281	Perylene-d12	15.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
2	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	59
3	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	58
4	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
5	2-Methyl-6-tert-butylphenol, TMS...	236	C14H24OSi	1000467-04-9	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136532.D
Acq On : 13 Dec 2023 11:54
Operator : CG\JU
Sample : PB157507BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157507BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

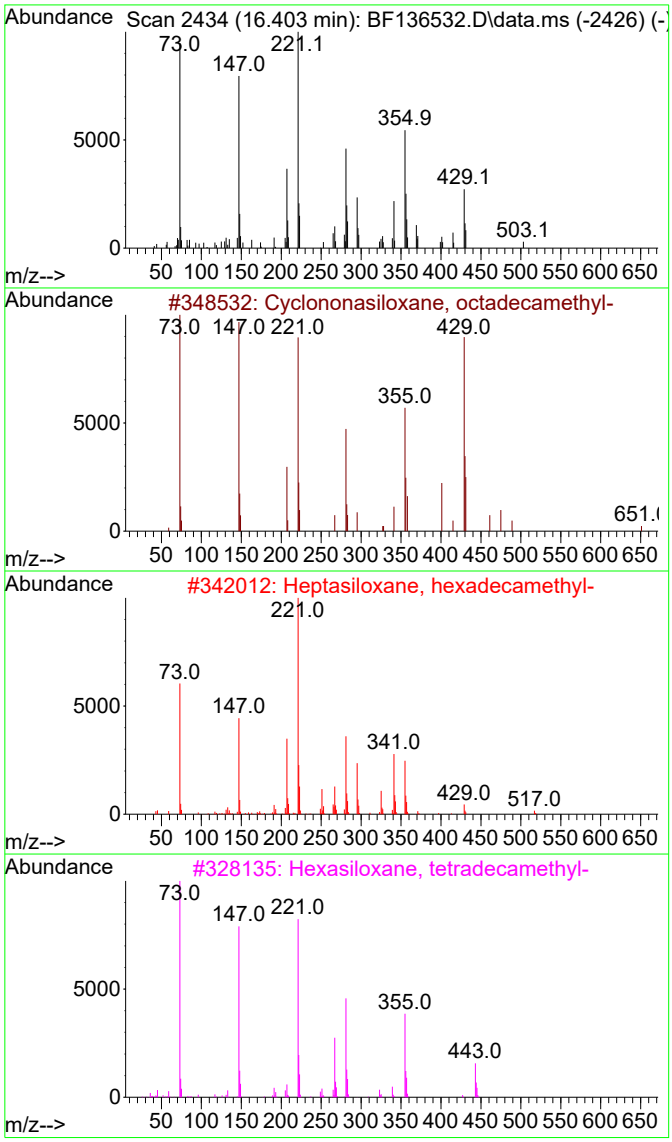
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

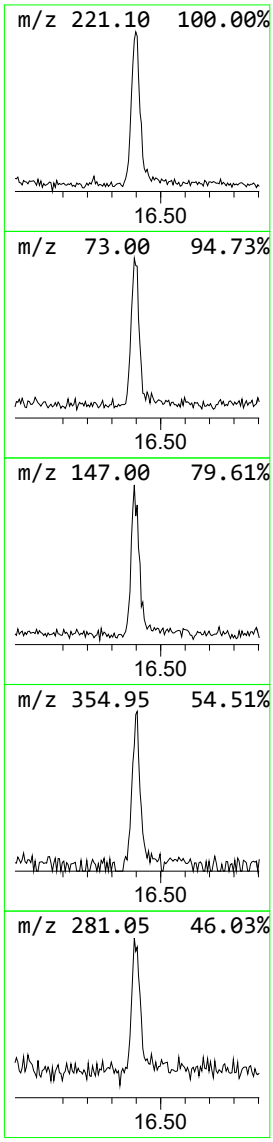
****

Peak Number 5 unknown16.403 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.403	3.65 ng	116871	Perylene-d12	15.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	64
2	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	43
3	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	40
4	3,4-Dihydroxyphenylglycol, 4TMS ...	458	C20H42O4Si4	056114-62-6	25
5	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136532.D
Acq On : 13 Dec 2023 11:54
Operator : CG\JU
Sample : PB157507BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157507BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

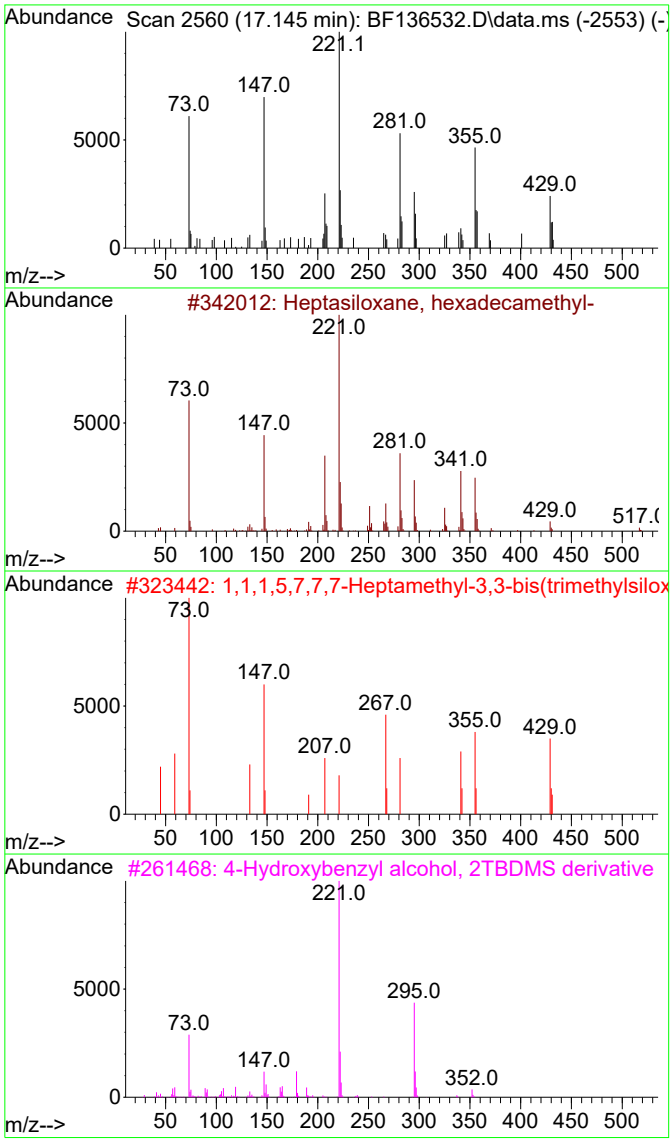
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

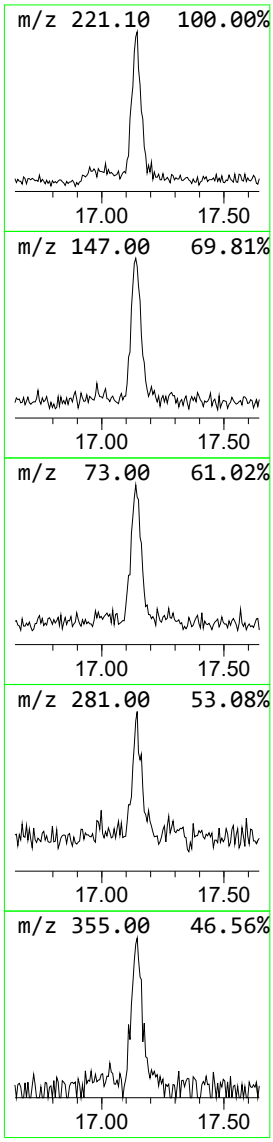
****

Peak Number 6 unknown17.145 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.145	2.97 ng	95076	Perylene-d12	15.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	50
2	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	32
3	4-Hydroxybenzyl alcohol, 2TBDMS ...	352	C19H36O2Si2	1000364-43-9	17
4	9H-carbazole, 3-ethenyl-9-ethyl-	221	C16H15N	1000400-80-8	10
5	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136532.D
Acq On : 13 Dec 2023 11:54
Operator : CG\JU
Sample : PB157507BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157507BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

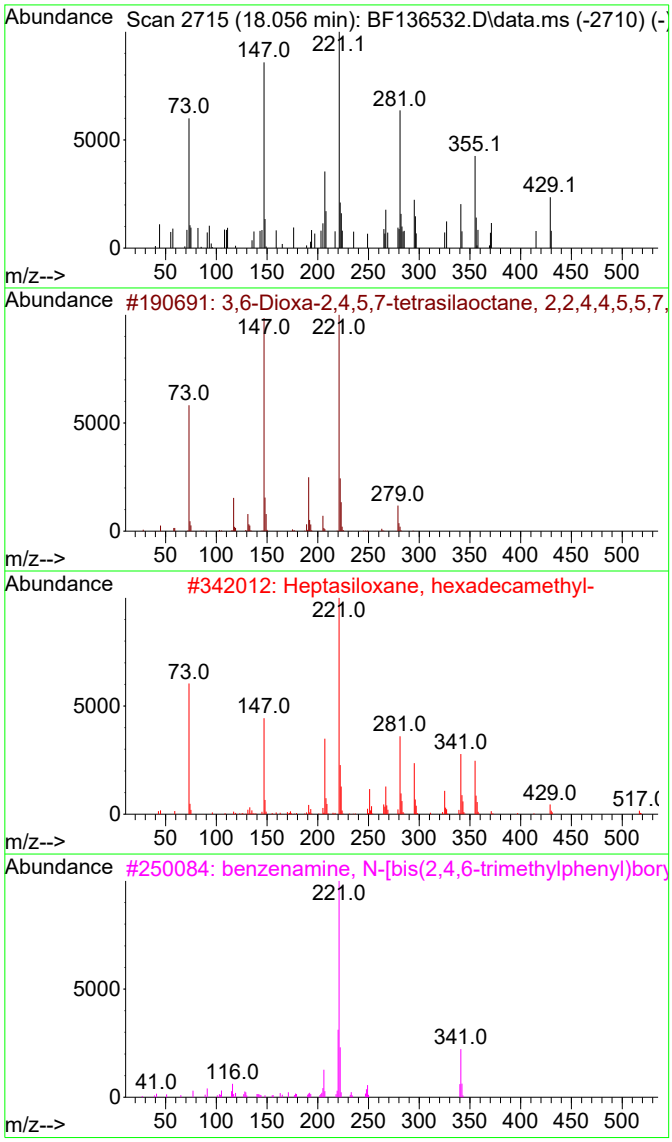
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

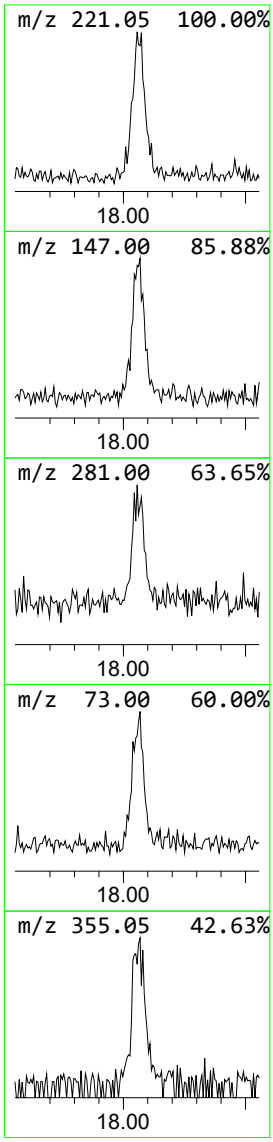
****

Peak Number 7 unknown18.056 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.056	2.05 ng	65504	Perylene-d12	15.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	43
2	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
3	benzenamine, N-[bis(2,4,6-trimet...	341	C24H28BN	1000398-20-2	22
4	Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	22
5	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136532.D
Acq On : 13 Dec 2023 11:54
Operator : CG\JU
Sample : PB157507BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157507BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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
2-Pentanone, 4-...	5.051	2.0	ng	56791	1	6.792	559853	20.0
Hexasiloxane, t...	14.839	3.1	ng	98478	6	15.456	639650	20.0
Cyclononasiloxa...	15.274	3.9	ng	125666	6	15.456	639650	20.0
Heptasiloxane, ...	15.786	4.3	ng	139281	6	15.456	639650	20.0
unknown16.403	16.403	3.6	ng	116871	6	15.456	639650	20.0
unknown17.145	17.145	3.0	ng	95076	6	15.456	639650	20.0
unknown18.056	18.056	2.0	ng	65504	6	15.456	639650	20.0