

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
 Data File : BF136829.D
 Acq On : 29 Dec 2023 15:10
 Operator : CG\JU
 Sample : 05975-09
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-GWDUP01-122023

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136829.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.893	130	137	144	rBV	29759	49461	2.08%	0.404%
2	3.522	238	244	252	rBV	122052	184573	7.75%	1.508%
3	3.869	294	303	310	rBV	33160	48387	2.03%	0.395%
4	4.416	388	396	399	rBV	1785005	2380418	100.00%	19.449%
5	4.669	431	439	444	rBV	788379	916223	38.49%	7.486%
6	5.010	494	497	504	rBV	39099	38117	1.60%	0.311%
7	5.275	539	542	546	rBV	77934	71182	2.99%	0.582%
8	6.110	681	684	689	rBV	30108	26562	1.12%	0.217%
9	6.404	730	734	738	rBV	1387793	1230085	51.68%	10.050%
10	6.440	738	740	750	rVB2	120614	200192	8.41%	1.636%
11	6.781	794	798	802	rBV	636784	481055	20.21%	3.930%
12	7.339	889	893	897	rBV	835922	795798	33.43%	6.502%
13	7.528	922	925	935	rBV	349135	370731	15.57%	3.029%
14	7.598	935	937	943	rVB	28840	27546	1.16%	0.225%
15	8.057	1011	1015	1018	rBV	787300	627504	26.36%	5.127%
16	8.575	1099	1103	1110	rBV	209820	177647	7.46%	1.451%
17	9.133	1194	1198	1201	rBV	1692118	1408221	59.16%	11.505%
18	9.304	1223	1227	1231	rBV5	14339	31939	1.34%	0.261%
19	9.492	1256	1259	1263	rVB	50321	45967	1.93%	0.376%
20	9.816	1310	1314	1325	rBV	442163	417377	17.53%	3.410%
21	11.122	1531	1536	1540	rBV2	19594	23806	1.00%	0.194%
22	11.310	1564	1568	1571	rBV	771764	686358	28.83%	5.608%
23	11.704	1631	1635	1641	rBV	39168	37058	1.56%	0.303%
24	12.904	1833	1839	1842	rBV	1796347	1495422	62.82%	12.218%
25	13.963	2015	2019	2025	rBV	383637	375446	15.77%	3.067%
26	14.433	2090	2099	2103	rBV9	11064	28388	1.19%	0.232%
27	15.457	2268	2273	2282	rVB9	29537	64131	2.69%	0.524%

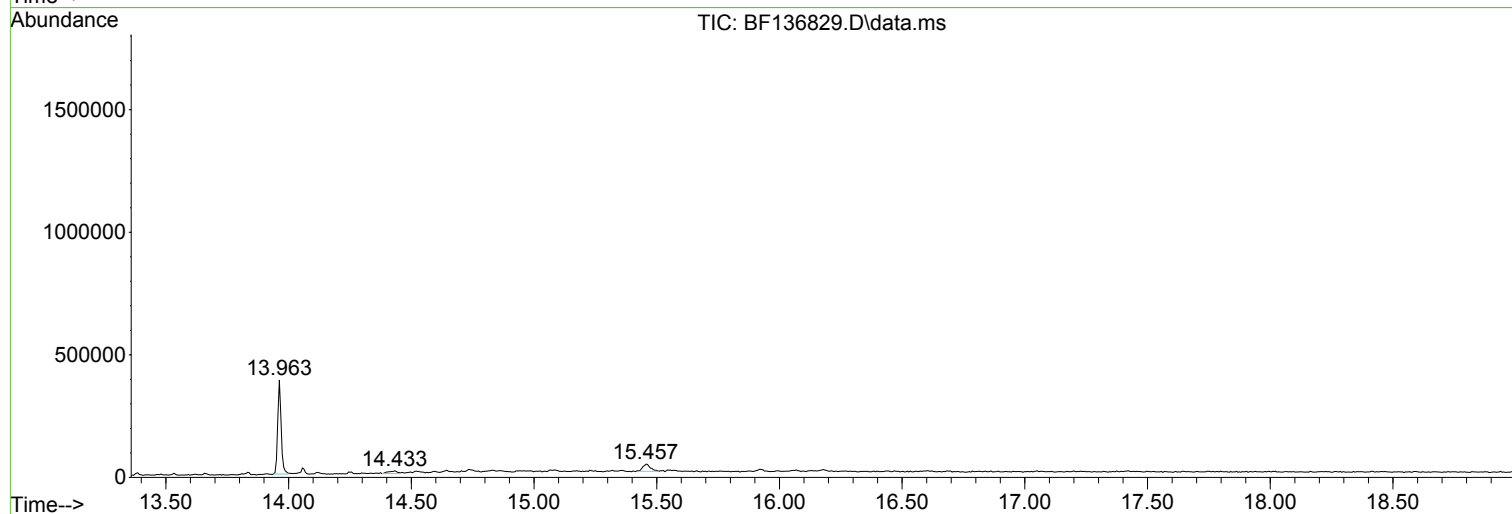
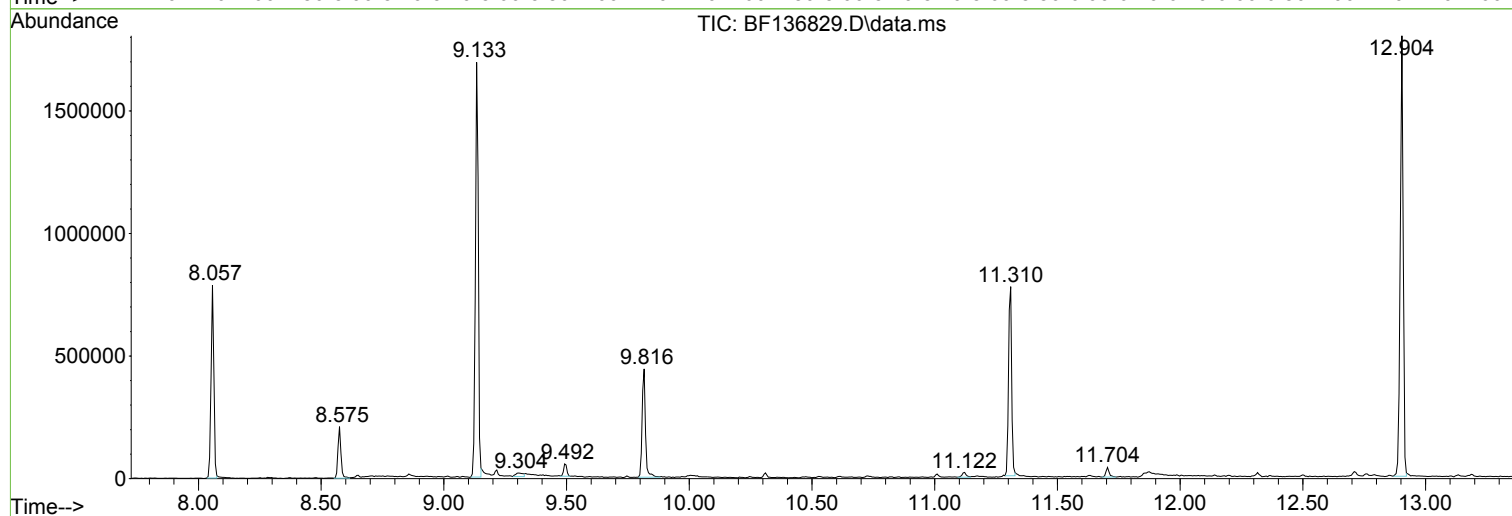
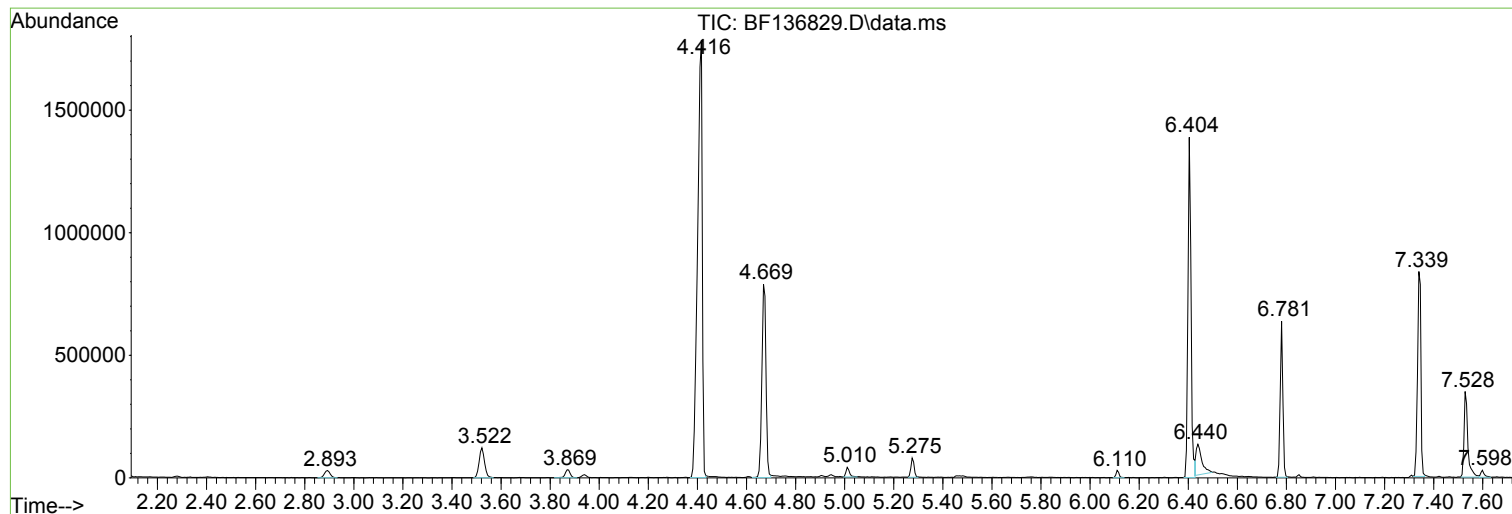
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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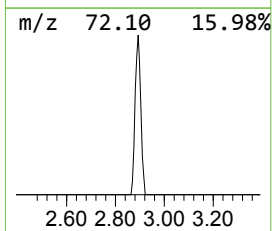
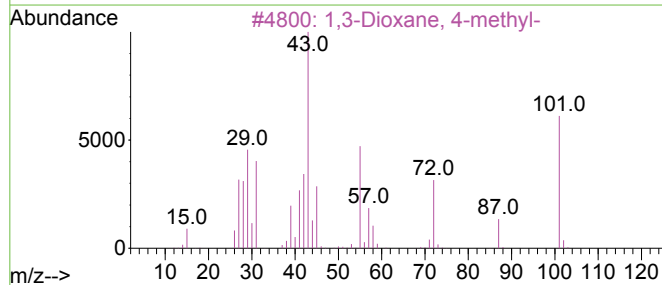
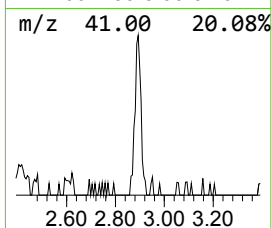
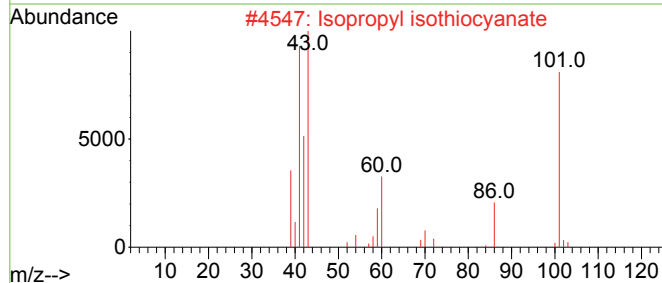
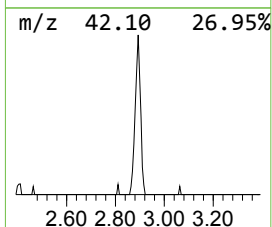
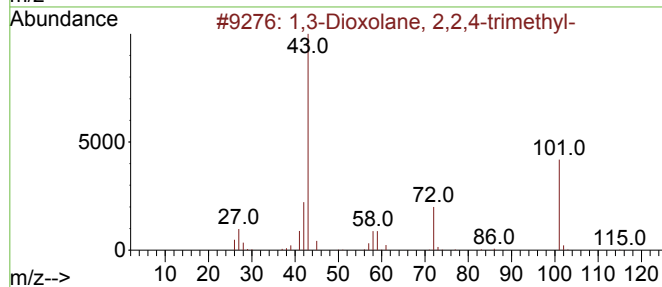
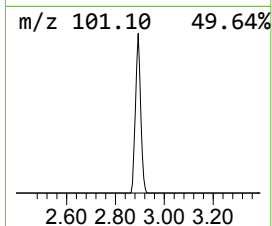
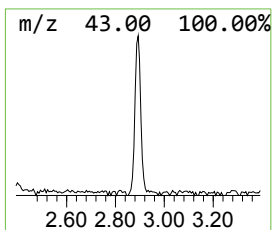
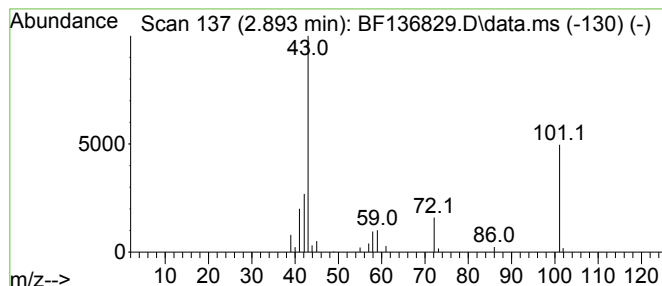
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.893	2.06 ng	49461	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	78
2		Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	42
3		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	38
4		Furazan-3-ol, 4-amino-	101	C2H3N3O2	159013-90-8	9
5		Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9



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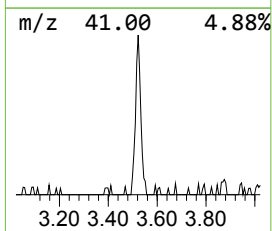
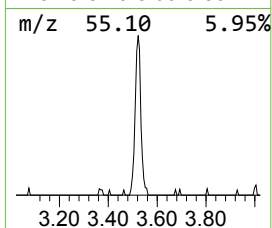
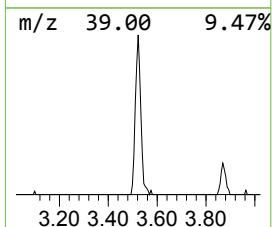
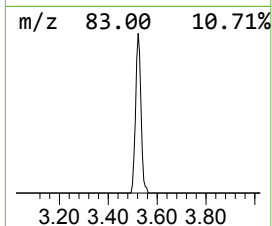
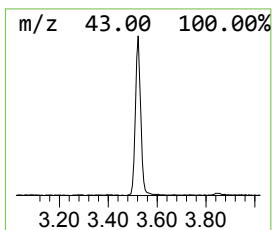
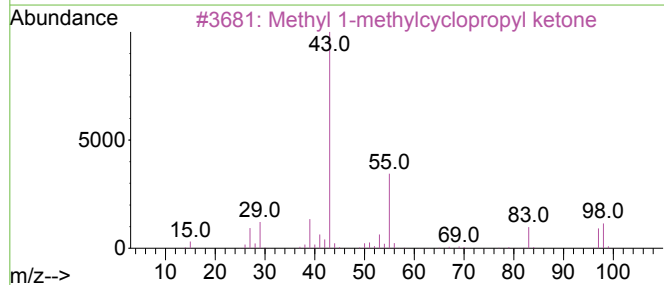
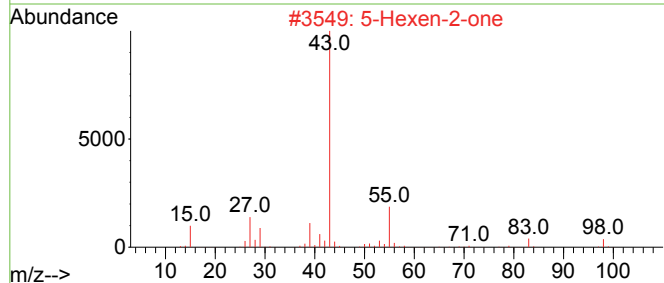
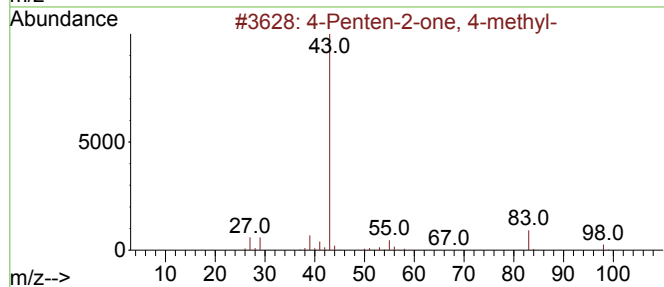
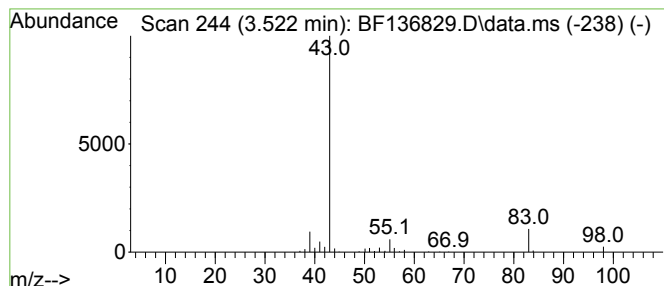
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.522	7.67 ng	184573	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2		5-Hexen-2-one	98	C6H10O	000109-49-9	27
3		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	10
4		2-Pentanone, 5-hydroxy-	102	C5H10O2	001071-73-4	9
5		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9



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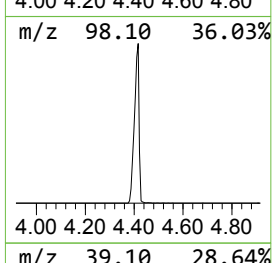
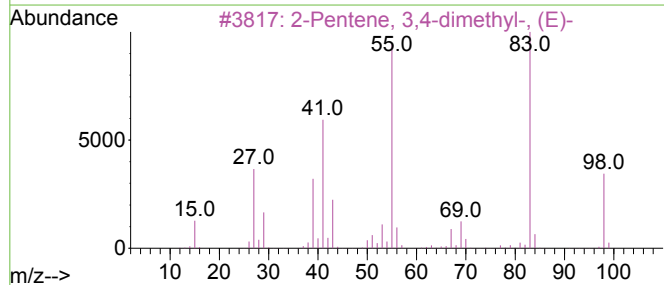
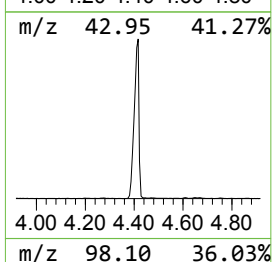
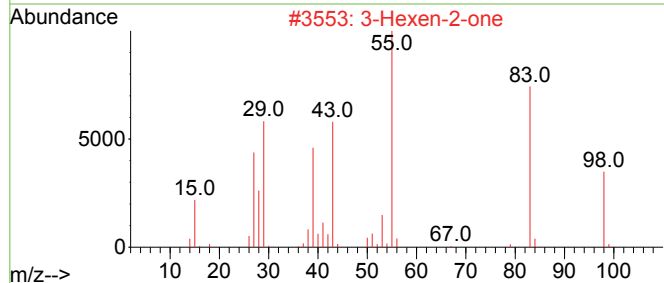
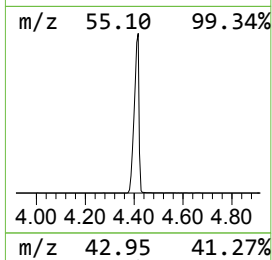
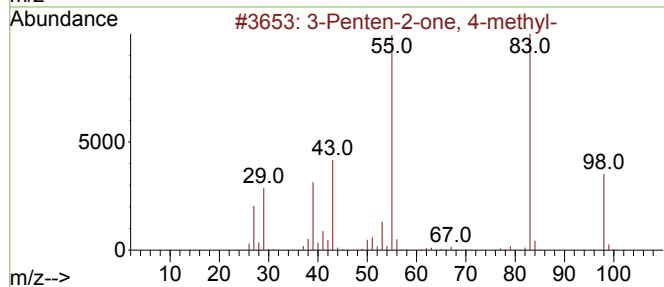
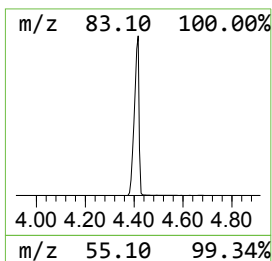
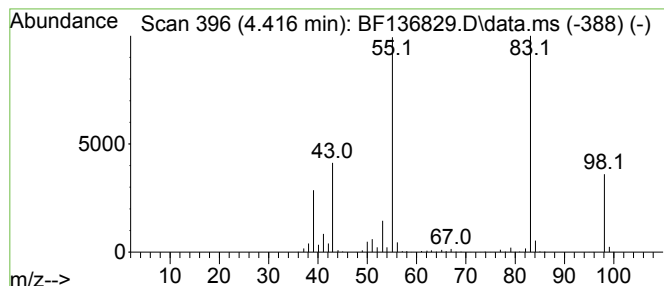
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.416	98.97 ng	2380420	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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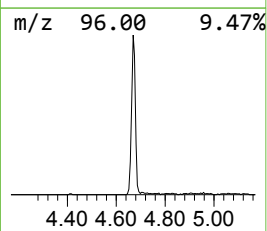
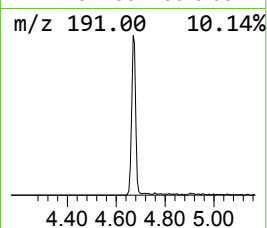
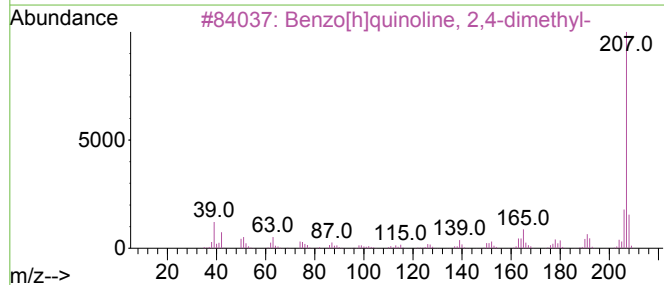
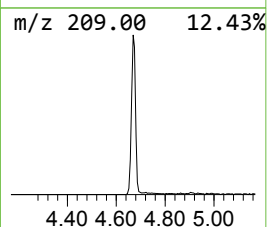
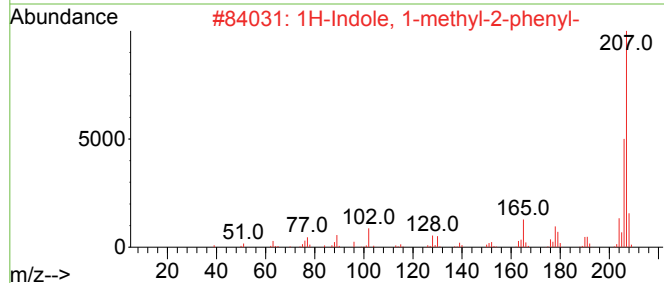
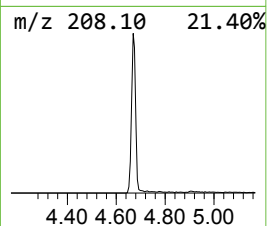
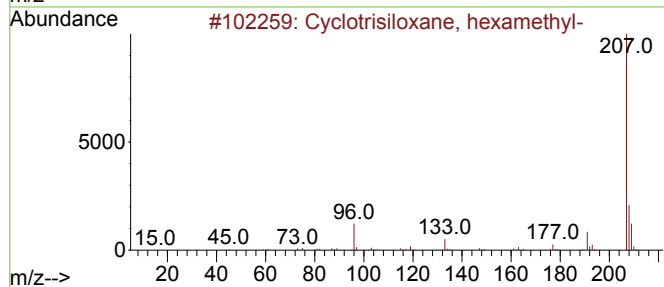
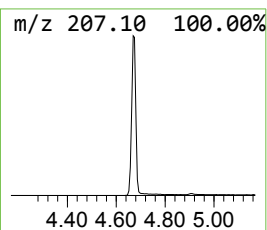
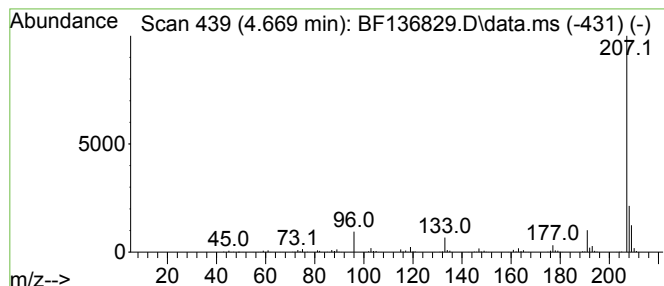
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclotrisiloxane, hexamethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.669	38.09 ng	916223	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	91
2			1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	39
3			Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	38
4			5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	38
5			4-tert-Octylphenol, TMS derivative	278	C17H30OSi	078721-87-6	38



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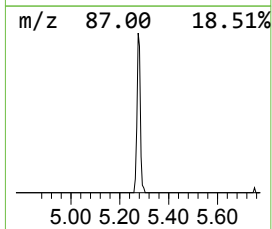
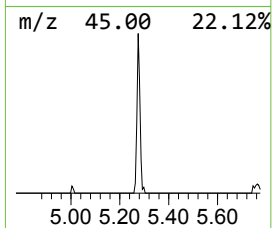
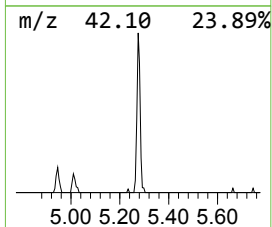
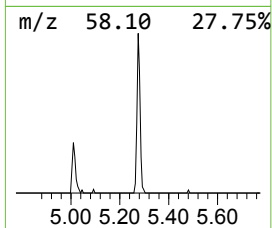
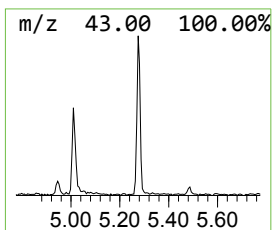
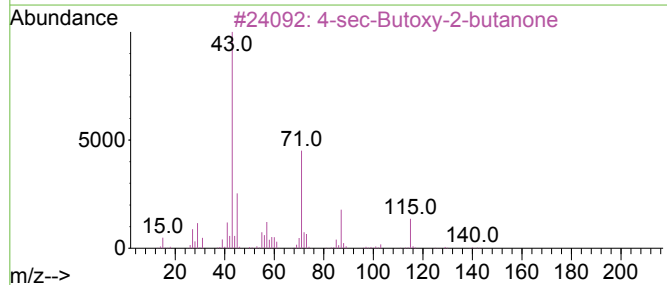
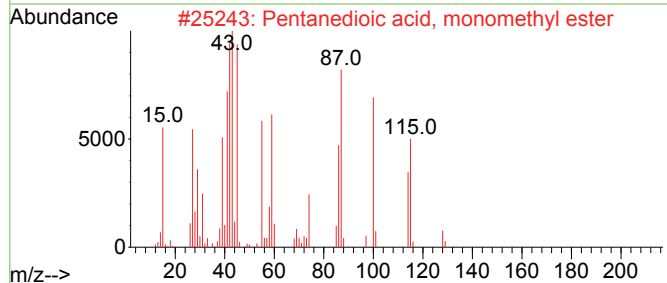
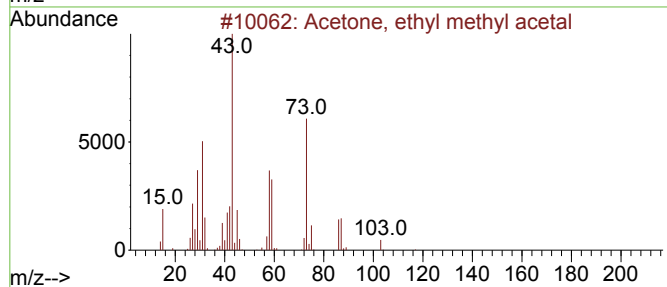
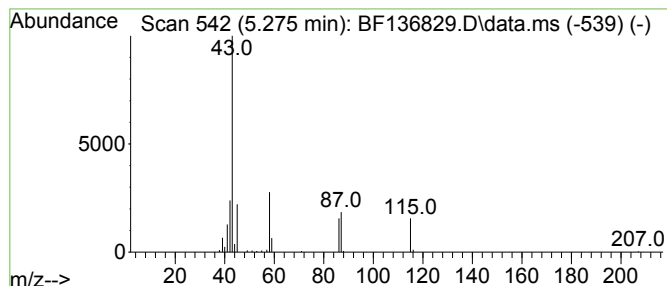
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 unknown5.275 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.275	2.96 ng	71182	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetone, ethyl methyl acetal	118	C6H14O2	029328-22-1	33
2			Pentanedioic acid, monomethyl ester	146	C6H10O4	001501-27-5	28
3			4-sec-Butoxy-2-butanone	144	C8H16O2	057545-63-8	25
4			Oxirane, trimethyl-	86	C5H10O	005076-19-7	23
5			2-Pentanone	86	C5H10O	000107-87-9	10



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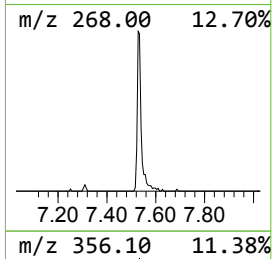
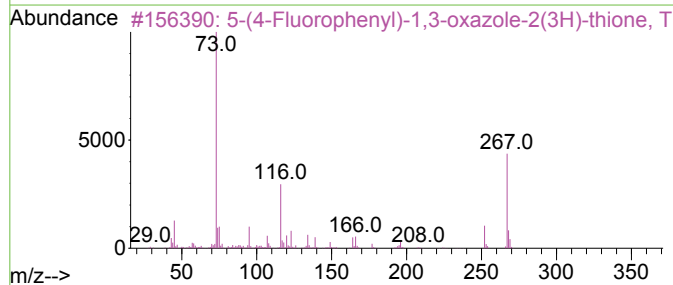
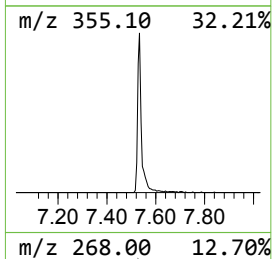
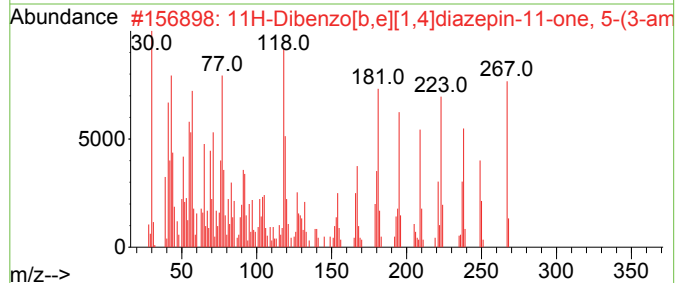
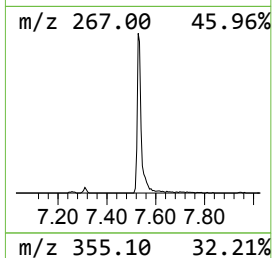
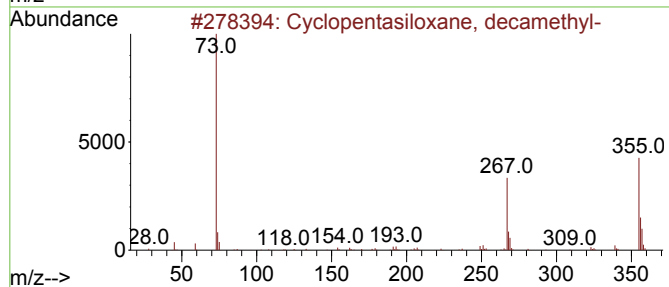
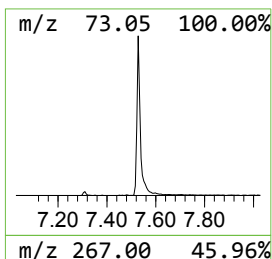
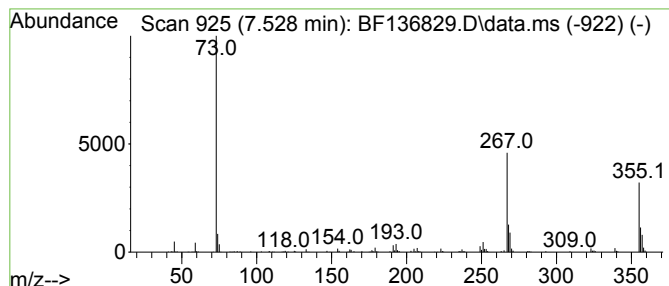
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclopentasiloxane, decamet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.528	11.82 ng	370731	Naphthalene-d8	8.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	76
2			11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	38
3			5-(4-Fluorophenyl)-1,3-oxazole-2...	267	C12H14FNOSi	1000497-07-6	38
4			2-[(3-Chloro-2-methylphenyl)amin...	357	C15H28ClN3OSi2	1000514-51-8	35
5			N-(Trifluoroacetyl)-O,O',O''-tri...	481	C19H34F3NO4Si3	1010072-26-3	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136829.D
Acq On : 29 Dec 2023 15:10
Operator : CG\JU
Sample : 05975-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-GWDUP01-122023

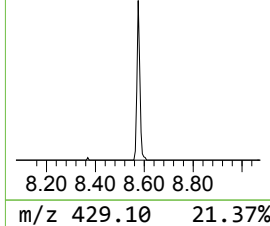
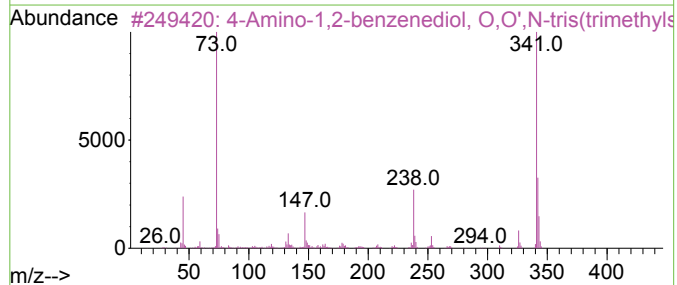
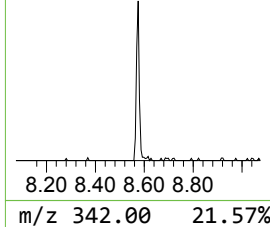
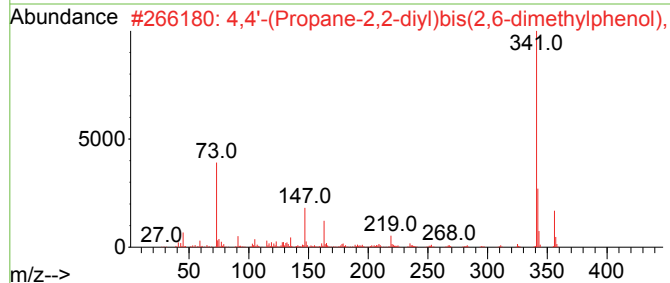
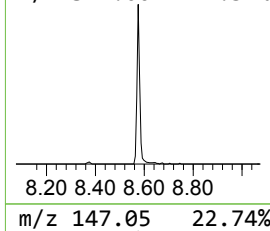
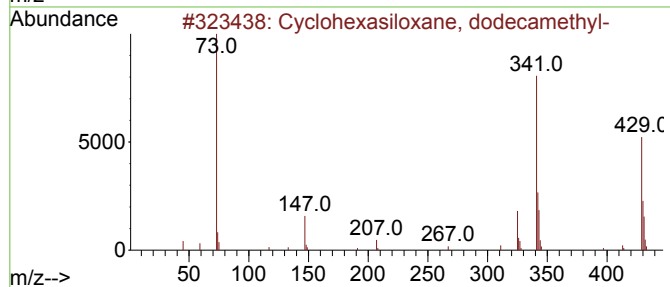
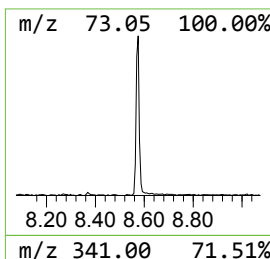
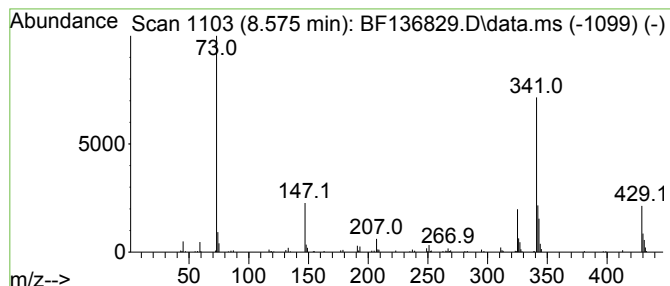
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexasiloxane, dodecane... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.575	5.66 ng	177647	Naphthalene-d8	8.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	90
2			4,4'-(Propane-2,2-diyl)bis(2,6-d...	356	C22H32O2Si	1000488-58-4	47
3			4-Amino-1,2-benzenediol, O,O',N...	341	C15H31NO2Si3	1000493-87-4	43
4			Phosphonoacetic Acid, 3TMS deriv...	356	C11H29O5PSi3	053044-27-2	42
5			Silane, methylvinyl(2,4-dimethyl...	456	C25H52O3Si2	1000417-01-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136829.D
Acq On : 29 Dec 2023 15:10
Operator : CG\JU
Sample : 05975-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

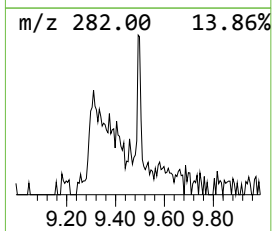
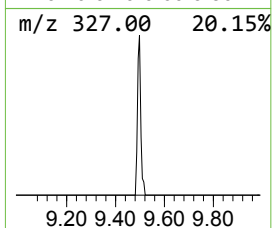
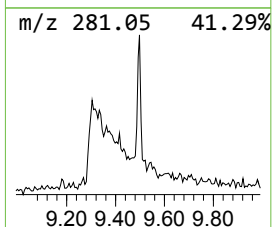
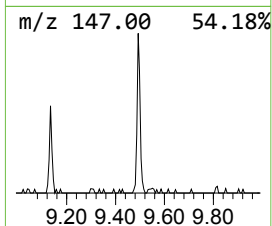
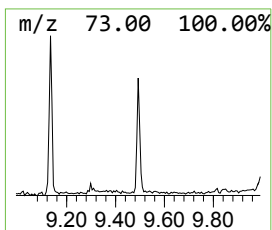
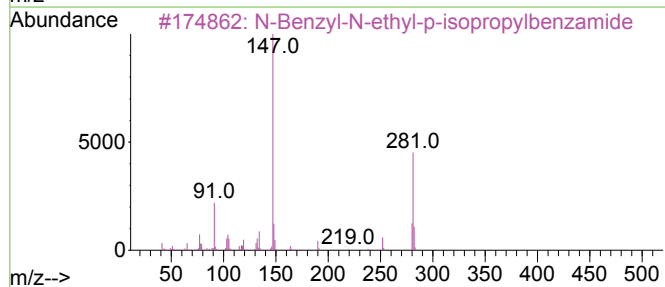
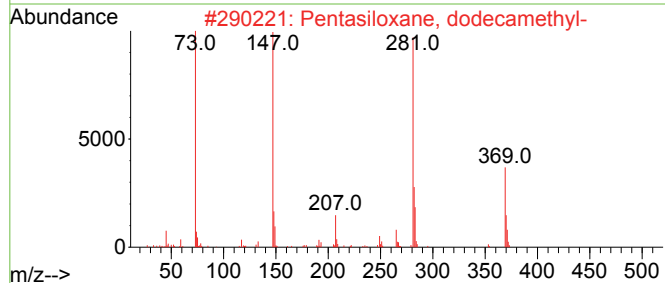
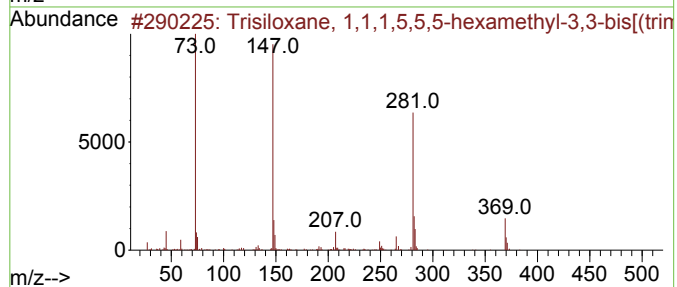
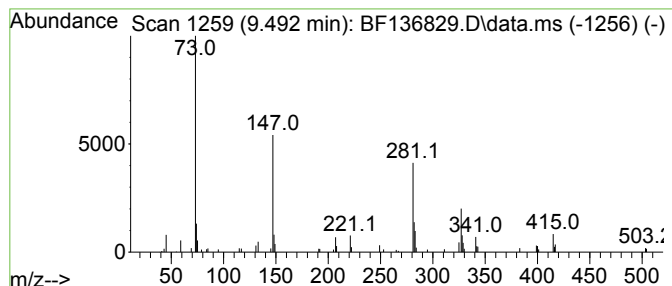
Instrument :
BNA_F
ClientSampleId :
RT-GWDUP01-122023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trisiloxane, 1,1,1,5,5,5-he... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.492	2.20 ng	45967	Acenaphthene-d10	9.816	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	52
2	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	50
3	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	47
4	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	38
5	8-Bromo-6-fluoro-4-hydroxyquinol...	429	C16H21BrFN03Si2	1000512-28-5	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136829.D
Acq On : 29 Dec 2023 15:10
Operator : CG\JU
Sample : 05975-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-GWDUP01-122023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
1,3-Dioxolane, ...	2.893	2.1	ng	49461	1	6.781	481055	20.0
4-Penten-2-one,...	3.522	7.7	ng	184573	1	6.781	481055	20.0
3-Penten-2-one,...	4.416	99.0	ng	2380420	1	6.781	481055	20.0
Cyclotrisiloxan...	4.669	38.1	ng	916223	1	6.781	481055	20.0
unknown5.275	5.275	3.0	ng	71182	1	6.781	481055	20.0
Cyclopentasilox...	7.528	11.8	ng	370731	2	8.057	627504	20.0
Cyclohexasiloxa...	8.575	5.7	ng	177647	2	8.057	627504	20.0
Trisiloxane, 1,...	9.492	2.2	ng	45967	3	9.816	417377	20.0