LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132706.D
Acq On : 08 Mar 2023 23:42
Operator : CG\JU
Sample : 01829-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-11-20230306

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-BF022223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132706.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.216	443	447	453	rVB	847727	898216	19.99%	4.494%
2	5.622	512	516	523	rBV	2160890	2096298	46.65%	10.489%
3	6.634	684	688	696	rBV	1976880	2135856	47.54%	10.687%
4	6.993	745	749	752	rBV	1022011	803786	17.89%	4.022%
5	7.551	841	844	848	rBV	1400515	1223886	27.24%	6.124%
6	8.157	943	947	953	rBV3	54749	128756	2.87%	0.644%
7	8.275	964	967	970	rBV	1012427	890680	19.82%	4.457%
8	8.351	977	980	988	rBV	495471	533576	11.88%	2.670%
9	8.810	1051	1058	1064	rBV4	148046	282011	6.28%	1.411%
10	9.051	1096	1099	1102	rBV	185890	202943	4.52%	1.015%
11	9.351	1147	1150	1153	rBV	2881564	2425484	53.98%	12.137%
12	9.381	1153	1155	1157	rVB	516839	392333	8.73%	1.963%
13	9.416	1158	1161	1163	rVV	571221	530821	11.81%	2.656%
14	9.463	1167	1169	1171	rBV2	391800	320301	7.13%	1.603%
15	9.622	1192	1196	1199	rVB	5165664	4493217	100.00%	22.483%
16	9.804	1225	1227	1230	rVB3	412187	310322	6.91%	1.553%
17	9.904	1241	1244	1247	rBV2	614246	685137	15.25%	3.428%
18	9.939	1247	1250	1253	rBV	1412700	1631320	36.31%	8.163%

Sum of corrected areas: 19984943

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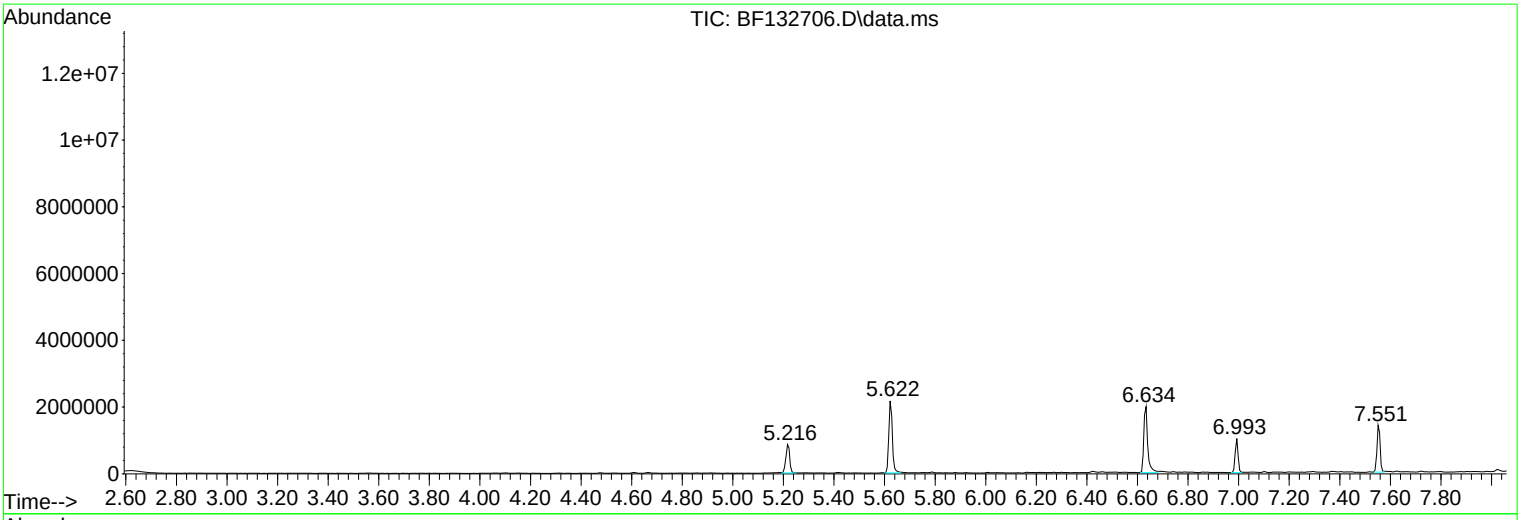
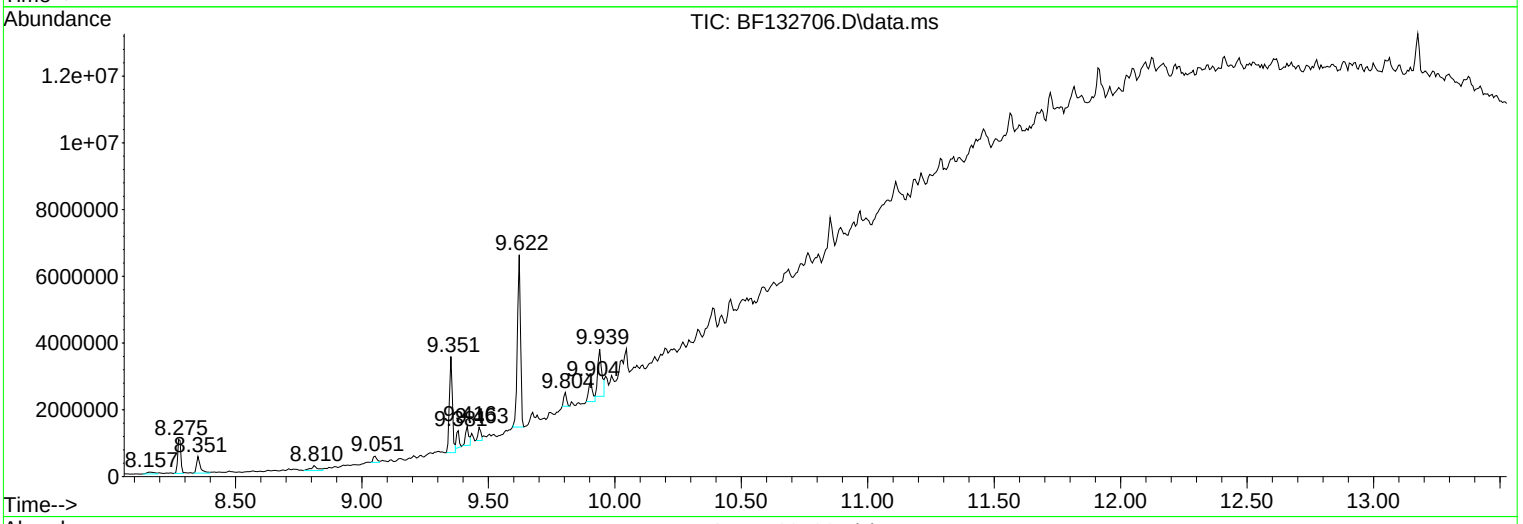
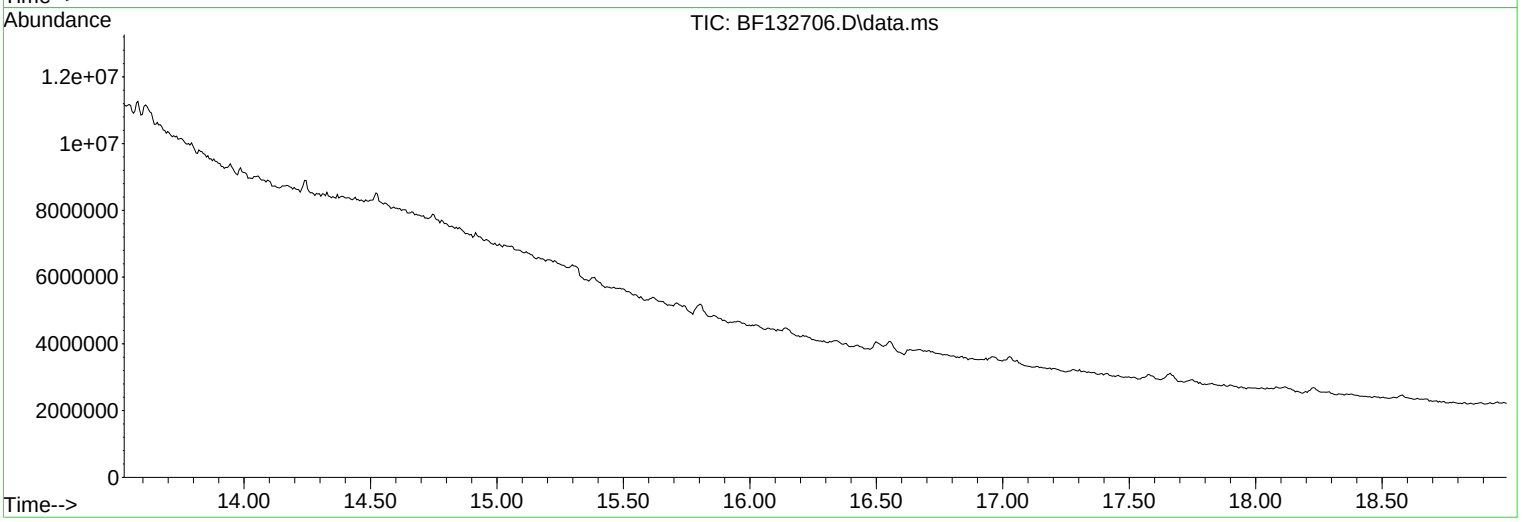
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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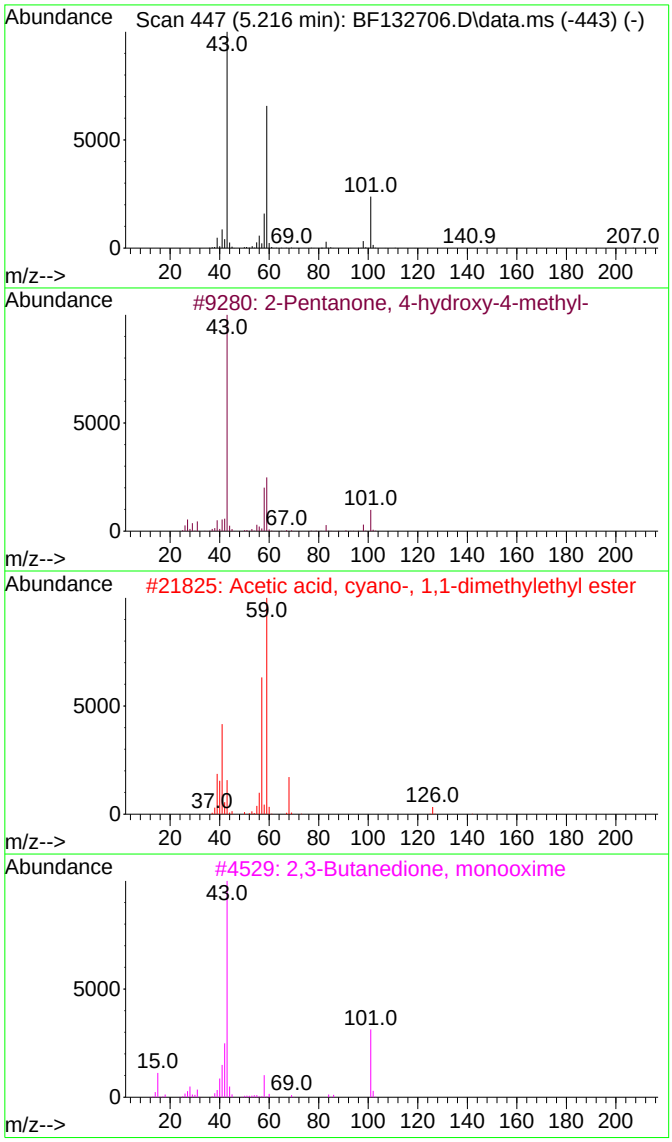
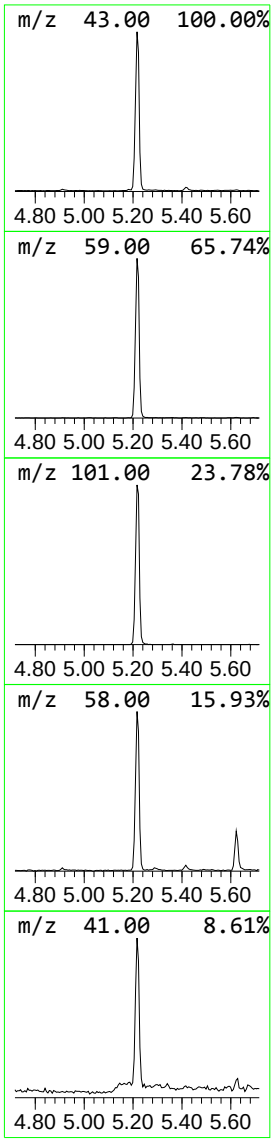
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.216	22.35 ng	898216	1,4-Dichlorobenzene-d4	6.993

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Guanidine	59	CH5N3	000113-00-8	9





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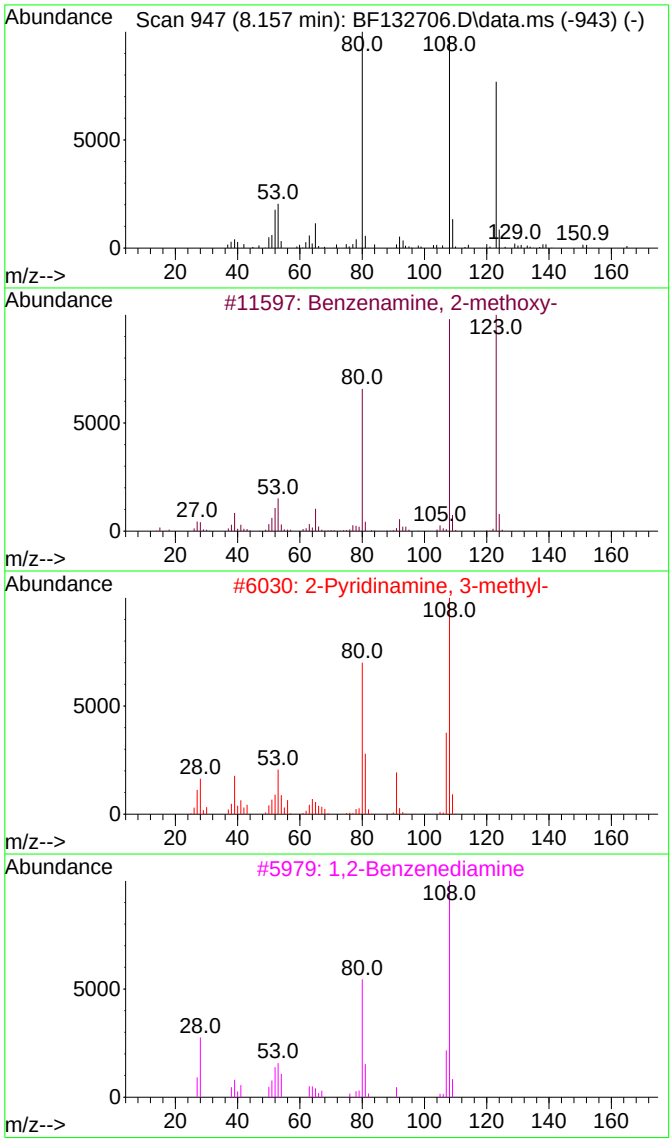
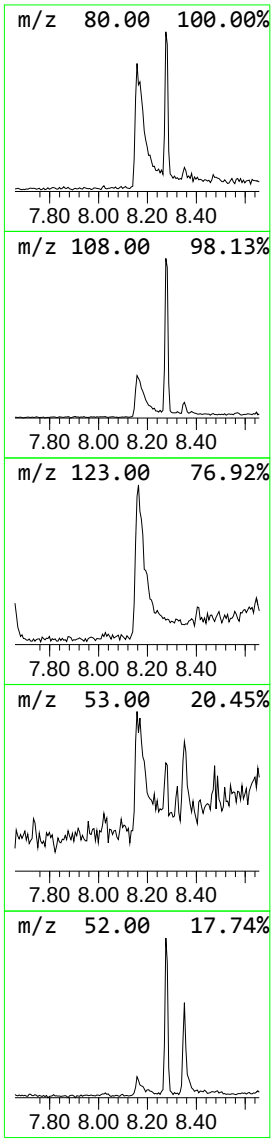
****

Peak Number 2 Benzenamine, 2-methoxy- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.157	2.89 ng	128756	Naphthalene-d8	8.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2-methoxy-	123	C7H9NO	000090-04-0	91
2	2-Pyridinamine, 3-methyl-	108	C6H8N2	001603-40-3	72
3	1,2-Benzenediamine	108	C6H8N2	000095-54-5	64
4	1,4-Benzenediamine	108	C6H8N2	000106-50-3	64
5	Pyrazinamide	123	C5H5N3O	000098-96-4	64





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Acq On : 08 Mar 2023 23:42
Operator : CG\JU
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Misc :
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Instrument :
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ClientSampleId :
SS-11-20230306

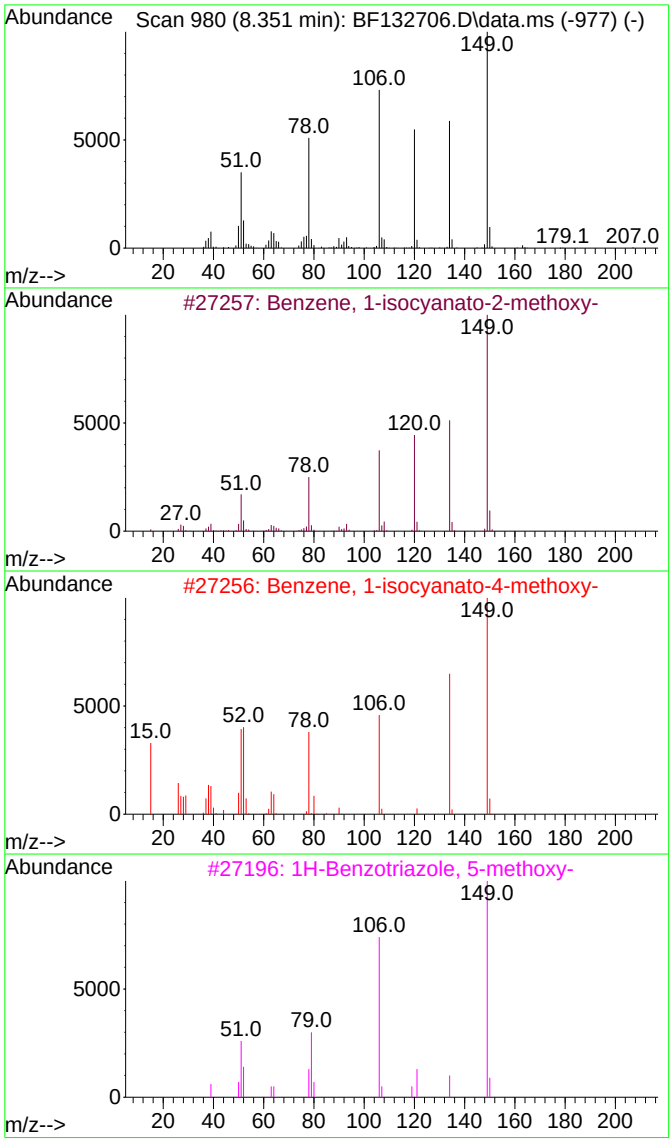
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

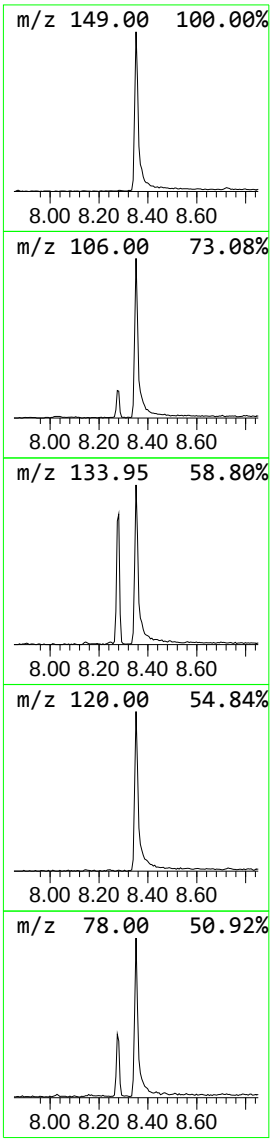
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-isocyanato-2-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.351	11.98 ng	533576	Naphthalene-d8	8.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-isocyanato-2-methoxy-	149	C8H7NO2	000700-87-8	94
2	Benzene, 1-isocyanato-4-methoxy-	149	C8H7NO2	005416-93-3	59
3	1H-Benzotriazole, 5-methoxy-	149	C7H7N3O	027799-91-3	53
4	Benzonitrile, 4-hydroxy-3-methoxy-	149	C8H7NO2	004421-08-3	43
5	Benzene, 1-isocyanato-3-methoxy-	149	C8H7NO2	018908-07-1	38





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

TIC Library : C:\Database\NIST20.L
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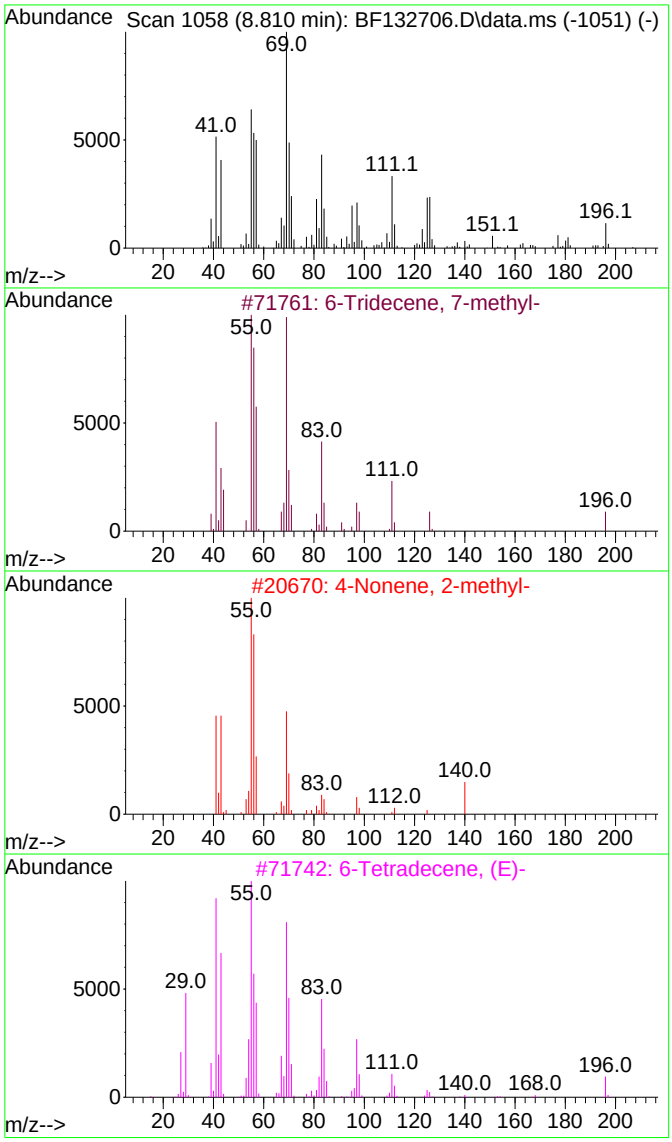
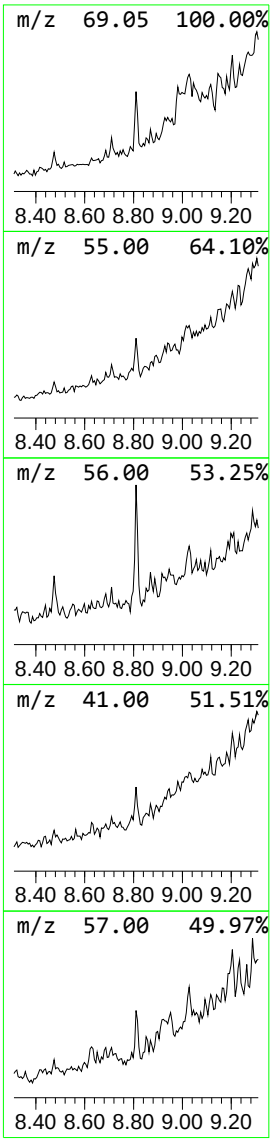
****

Peak Number 4 6-Tridecene, 7-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.810	6.33 ng	282011	Naphthalene-d8	8.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Tridecene, 7-methyl-	196	C14H28	024949-42-6	76
2	4-Nonene, 2-methyl-	140	C10H20	055724-84-0	64
3	6-Tetradecene, (E)-	196	C14H28	041446-64-4	60
4	Cyclopentane, propyl-	112	C8H16	002040-96-2	58
5	Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	58





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

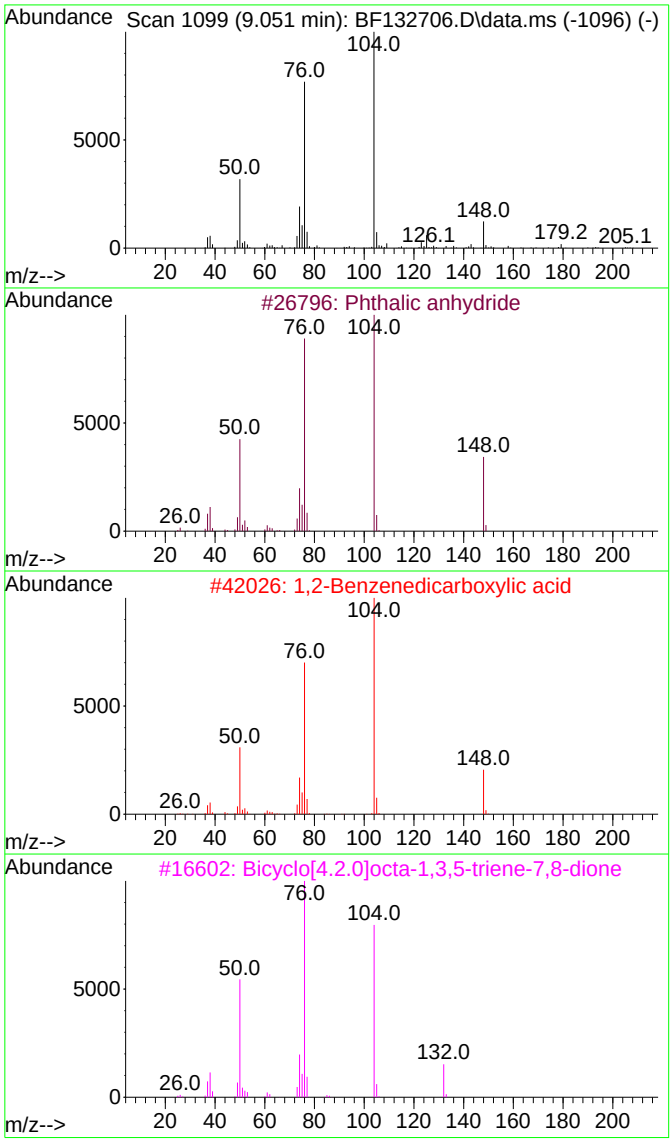
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

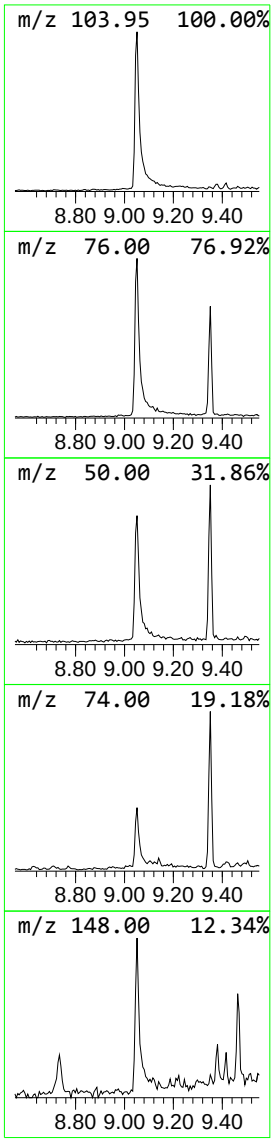
****

Peak Number 5 Phthalic anhydride Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.051	4.56 ng	202943	Naphthalene-d8	8.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic anhydride	148	C8H4O3	000085-44-9	95
2	1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	90
3	Bicyclo[4.2.0]octa-1,3,5-triene-...	132	C8H4O2	006383-11-5	83
4	Indan-1,2,3-trione	160	C9H4O3	000938-24-9	83
5	1H-Isoindole-1,3(2H)-dione, 2-(h...	177	C9H7NO3	000118-29-6	78





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TIC Library : C:\Database\NIST20.L
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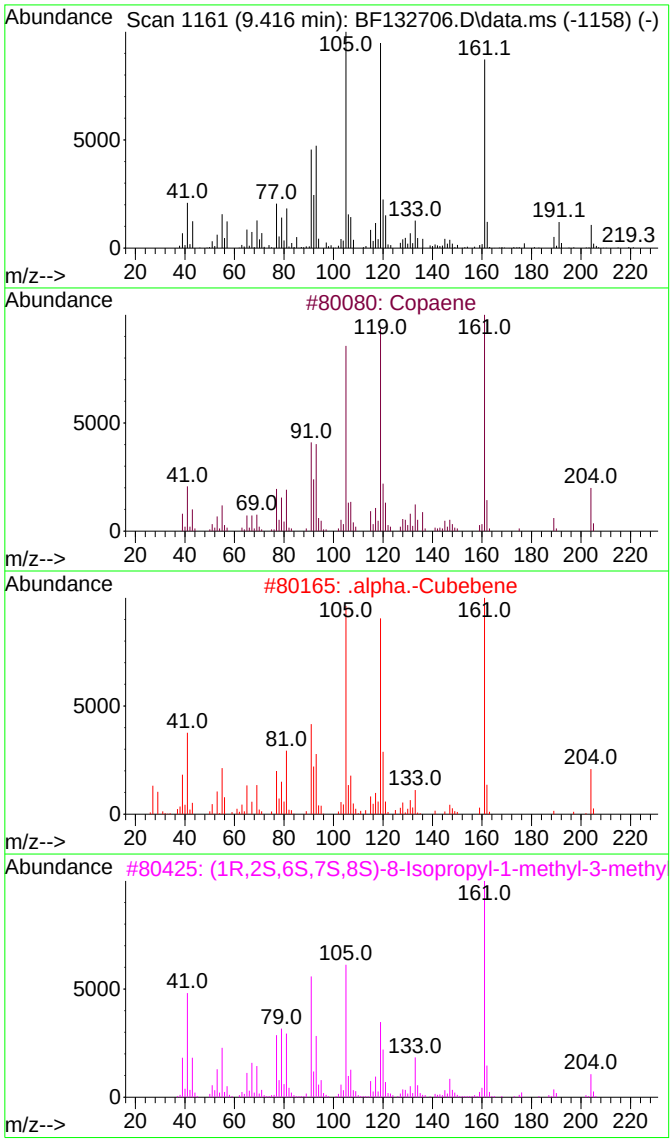
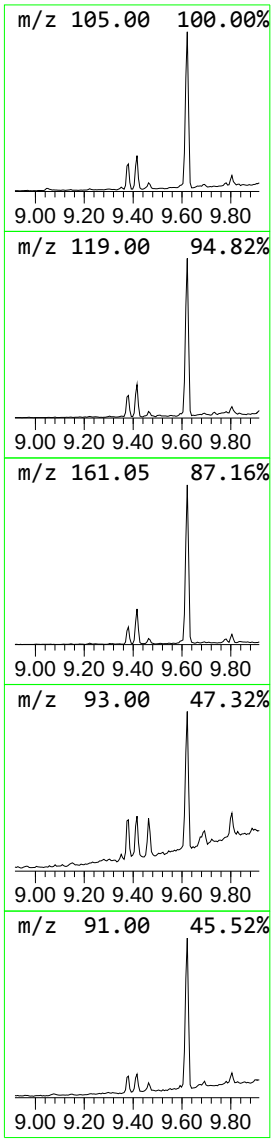
****

Peak Number 6 Copaene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.416	6.51 ng	530821	Acenaphthene-d10	10.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Copaene	204	C15H24	003856-25-5	99
2	.alpha.-Cubebene	204	C15H24	017699-14-8	97
3	(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	78
4	1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	78
5	Tetracyclo[6.1.0.0(2,4).0(5,7)]n...	204	C15H24	051898-92-1	58





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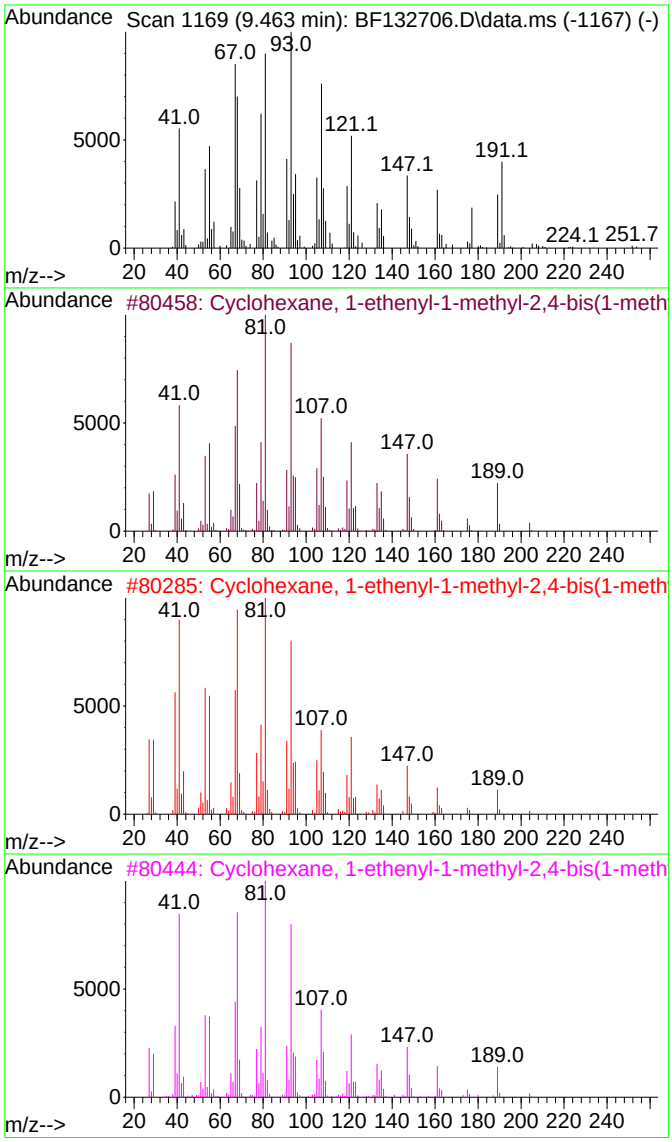
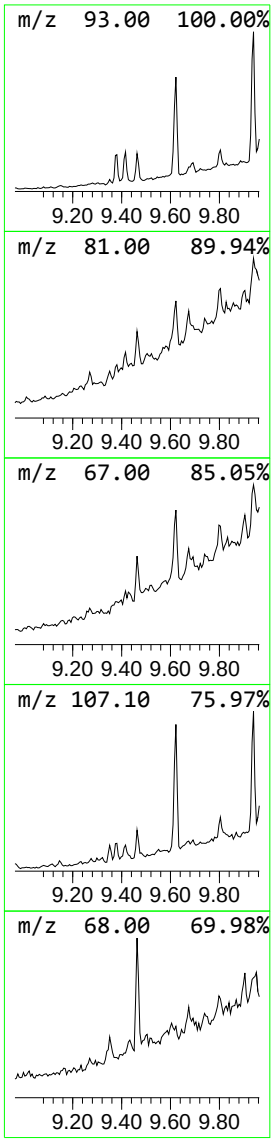
****
Peak Number 7 Cyclohexane, 1-ethenyl-1-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.463	3.93 ng	320301	Acenaphthene-d10	10.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	000515-13-9	70
2	Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	110823-68-2	58
3	Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	033880-83-0	50
4	9,12-Tetradecadien-1-ol, acetate...	252	C16H28O2	031654-77-0	38
5	Bicyclo[10.1.0]tridec-1-ene	178	C13H22	054766-91-5	30





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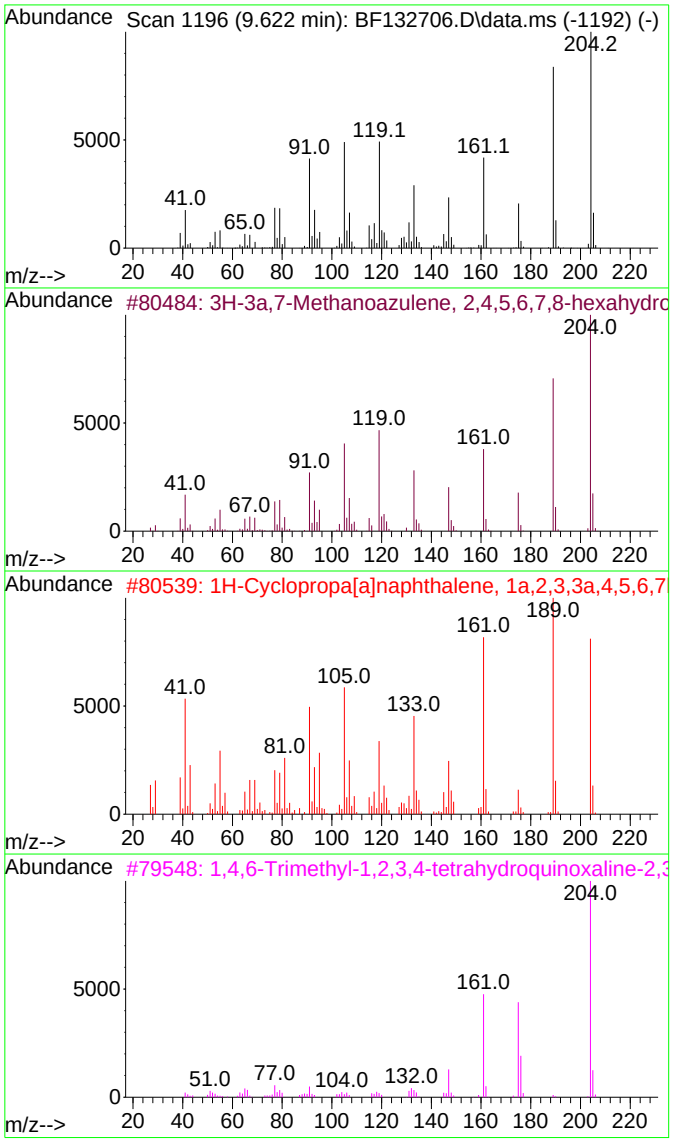
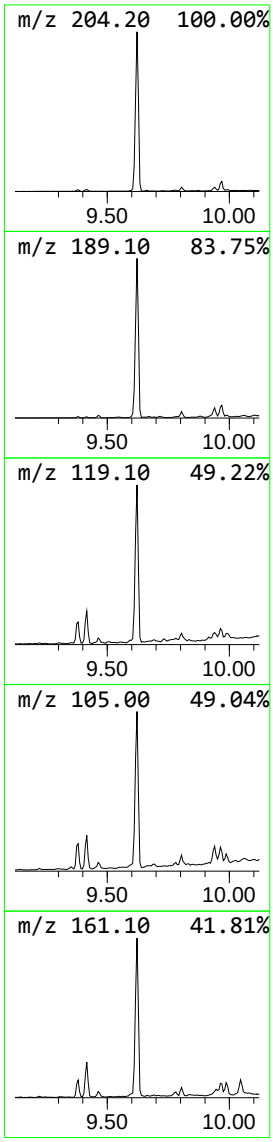
****

Peak Number 8 3H-3a,7-Methanoazulene, 2,4... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.622	55.09 ng	4493220	Acenaphthene-d10	10.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-3a,7-Methanoazulene, 2,4,5,6,...	204	C15H24	002387-78-2	98
2	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	93
3	1,4,6-Trimethyl-1,2,3,4-tetrahyd...	204	C11H12N2O2	004951-03-5	89
4	Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	005951-61-1	89
5	Naphthalene, 2,3,4,4a,5,6-hexahy...	204	C15H24	000473-14-3	76





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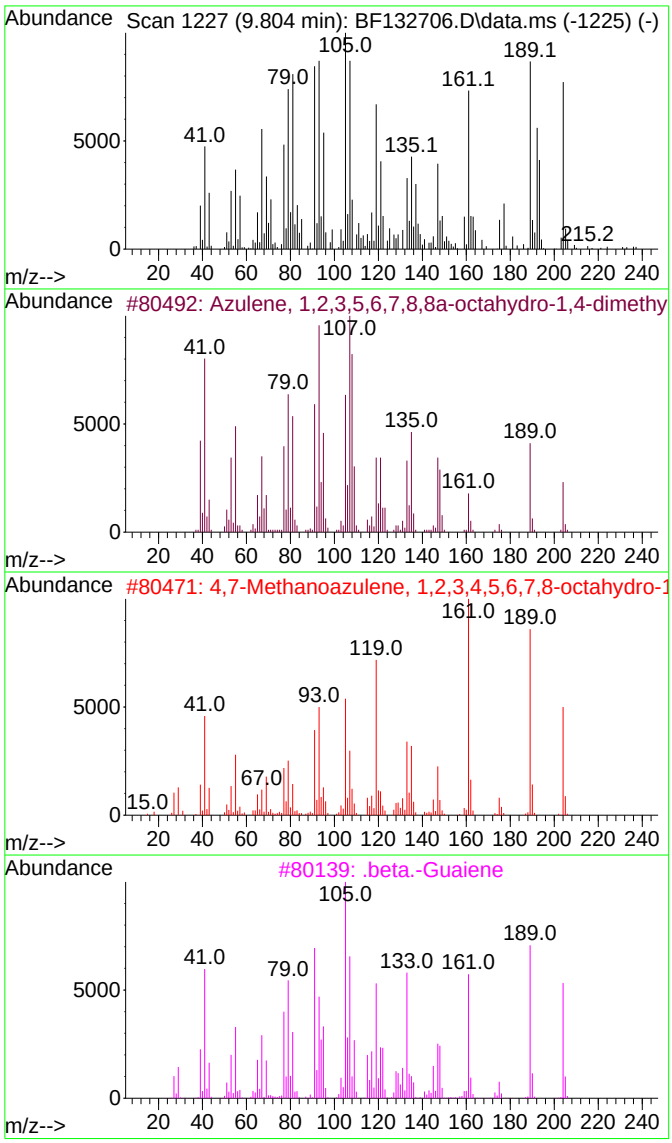
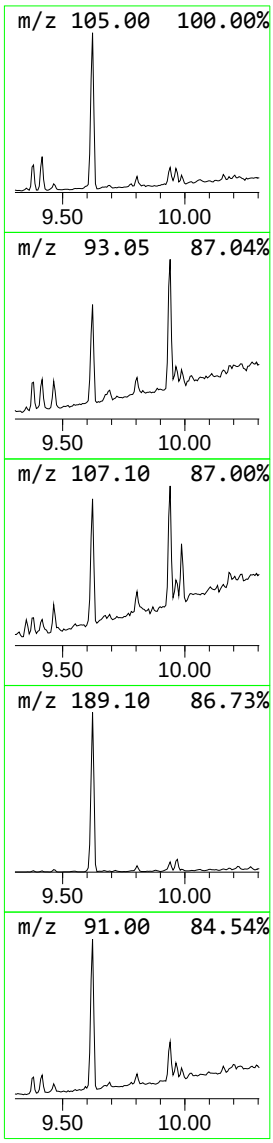
****
Peak Number 9 Azulene, 1,2,3,5,6,7,8,8a-o... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.804	3.80 ng	310322	Acenaphthene-d10	10.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	92
2	4,7-Methanoazulene, 1,2,3,4,5,6,...	204	C15H24	000514-51-2	91
3	.beta.-Guaiene	204	C15H24	000088-84-6	89
4	1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	89
5	(1R,3aS,8aS)-7-Isopropyl-1,4-dim...	204	C15H24	036577-33-0	84





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Data File : BF132706.D
Acq On : 08 Mar 2023 23:42
Operator : CG\JU
Sample : 01829-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-11-20230306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

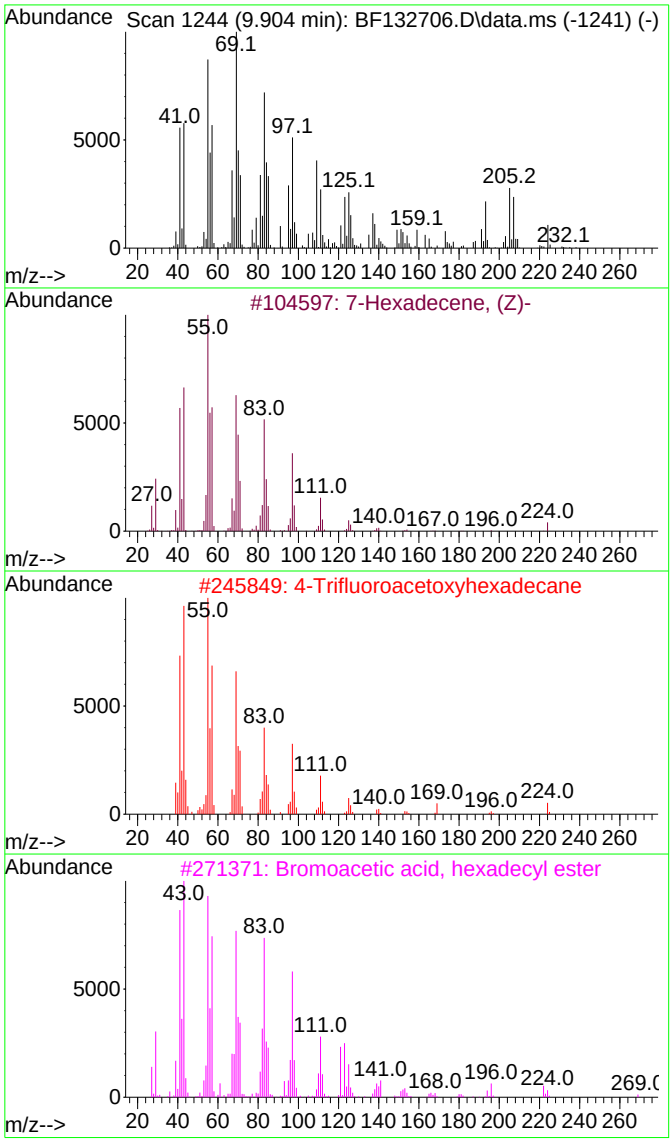
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

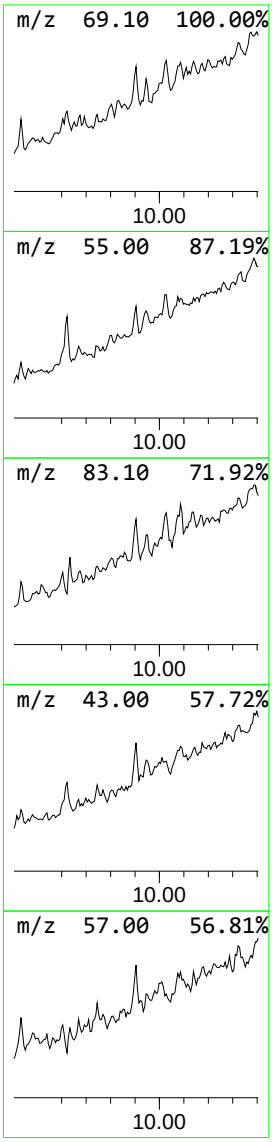
****

Peak Number 10 7-Hexadecene, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.904	8.40 ng	685137	Acenaphthene-d10	10.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	55
2	4-Trifluoroacetoxyhexadecane	338	C18H33F3O2	1000215-97-5	43
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	43
4	2,6-Dodecadien-1-ol, 3,7,11-trim...	224	C15H28O	020576-56-1	41
5	1-Tridecene	182	C13H26	002437-56-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132706.D
Acq On : 08 Mar 2023 23:42
Operator : CG\JU
Sample : 01829-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-11-20230306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

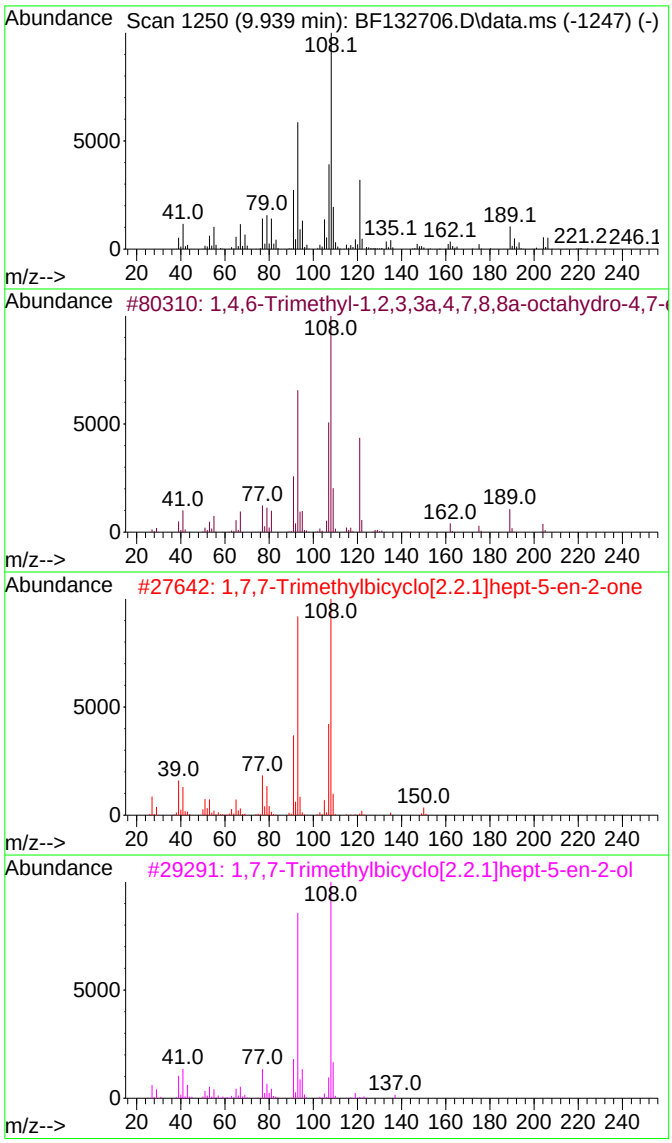
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

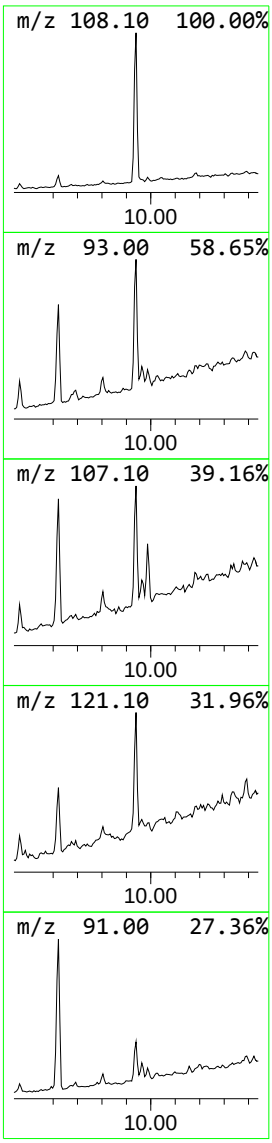
****

Peak Number 11 1,4,6-Trimethyl-1,2,3,3a,4,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.939	20.00 ng	1631320	Acenaphthene-d10	10.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4,6-Trimethyl-1,2,3,3a,4,7,8,8...	204	C15H24	065128-08-7	98
2	1,7,7-Trimethylbicyclo[2.2.1]hep...	150	C10H14O	022516-10-5	64
3	1,7,7-Trimethylbicyclo[2.2.1]hep...	152	C10H16O	1000190-98-1	59
4	Camphenone, 6-	150	C10H14O	055659-42-2	59
5	Tricyclo[3.3.0.0(2,8)]octan-3-on...	150	C10H14O	109915-32-4	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132706.D
Acq On : 08 Mar 2023 23:42
Operator : CG\JU
Sample : 01829-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-11-20230306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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-...	5.216	22.4	ng	898216	1	6.993	803786	20.0
Benzenamine, 2-...	8.157	2.9	ng	128756	2	8.281	890680	20.0
Benzene, 1-isoc...	8.351	12.0	ng	533576	2	8.281	890680	20.0
6-Tridecene, 7-...	8.810	6.3	ng	282011	2	8.281	890680	20.0
Phthalic anhydride	9.051	4.6	ng	202943	2	8.281	890680	20.0
Copaene	9.416	6.5	ng	530821	3	10.045	1631320	20.0
Cyclohexane, 1-...	9.463	3.9	ng	320301	3	10.045	1631320	20.0
3H-3a,7-Methano...	9.622	55.1	ng	4493220	3	10.045	1631320	20.0
Azulene, 1,2,3,...	9.804	3.8	ng	310322	3	10.045	1631320	20.0
7-Hexadecene, (Z)-	9.904	8.4	ng	685137	3	10.045	1631320	20.0
1,4,6-Trimethyl...	9.939	20.0	ng	1631320	3	10.045	1631320	20.0