LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125358.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.510	579	582	587	rVB	299997	285139	7.68%	1.135%
2	6.328	716	721	725	rBV2	250725	273777	7.38%	1.090%
3	6.522	752	754	757	rVB	257663	195974	5.28%	0.780%
4	6.898	815	818	822	rBV	1046109	893826	24.09%	3.558%
5	7.169	858	864	867	rVB5	156008	231648	6.24%	0.922%
6	7.204	867	870	873	rBV2	175975	201094	5.42%	0.801%
7	7.292	881	885	889	rBV5	341579	419692	11.31%	1.671%
8	7.428	903	908	910	rBV4	274374	328000	8.84%	1.306%
9	7.457	910	913	917	rVV	505613	505011	13.61%	2.011%
10	7.545	923	928	931	rVB4	341604	440085	11.86%	1.752%
11	7.592	931	936	939	rBV7	153673	330891	8.92%	1.317%
12	7.680	947	951	953	rBV	342503	405586	10.93%	1.615%
13	7.704	953	955	961	rVB3	591029	529810	14.28%	2.109%
14	7.775	964	967	969	rBV2	441461	406775	10.96%	1.619%
15	7.822	972	975	981	rBV6	669610	870038	23.44%	3.464%
16	7.922	989	992	994	rBV3	291214	296851	8.00%	1.182%
17	7.992	1001	1004	1007	rBV4	206570	253543	6.83%	1.009%
18	8.022	1007	1009	1011	rVB	380921	276224	7.44%	1.100%
19	8.051	1011	1014	1017	rBV2	348365	386204	10.41%	1.538%
20	8.086	1017	1020	1023	rBV4	321095	424810	11.45%	1.691%
21	8.127	1024	1027	1030	rVV2	456673	392352	10.57%	1.562%
22	8.163	1030	1033	1034	rVV2	575400	538001	14.50%	2.142%
23	8.186	1034	1037	1039	rVV2	1326345	1512944	40.77%	6.023%
24	8.233	1042	1045	1048	rVB3	1074434	1090257	29.38%	4.341%
25	8.269	1048	1051	1053	rBV3	642554	730844	19.69%	2.910%
26	8.333	1059	1062	1064	rBV3	198924	268330	7.23%	1.068%
27	8.357	1064	1066	1068	rVB3	361505	248812	6.70%	0.991%
28	8.386	1068	1071	1073	rBV4	311137	283744	7.65%	1.130%
29	8.416	1073	1076	1079	rBV2	624177	747585	20.14%	2.976%
30	8.475	1079	1086	1090	rBV7	1086182	2212507	59.62%	8.808%
31	8.527	1093	1095	1098	rVB3	549016	487004	13.12%	1.939%
32	8.569	1098	1102	1105	rBV3	677700	840248	22.64%	3.345%
33	8.598	1105	1107	1109	rBV2	694773	716161	19.30%	2.851%
34	8.627	1109	1112	1113	rVV2	925144	1055920	28.45%	4.204%
35	8.645	1113	1115	1120	rVB5	1271572	1252773	33.76%	4.988%
36	8.686	1120	1122	1124	rBV3	406767	364207	9.81%	1.450%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.357	1232	1236	1241	rBV4	1740000	3711085	100.00%	14.775%
38	16.745	2489	2492	2502	rVB3	402543	710361	19.14%	2.828%

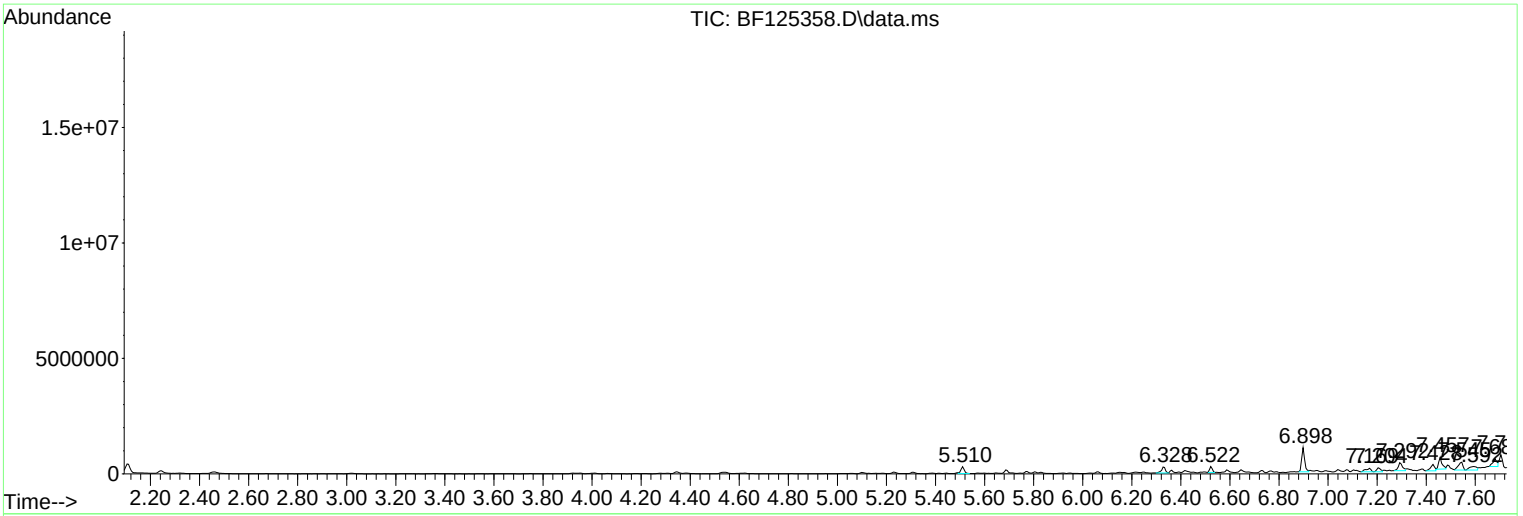
Sum of corrected areas: 25118113

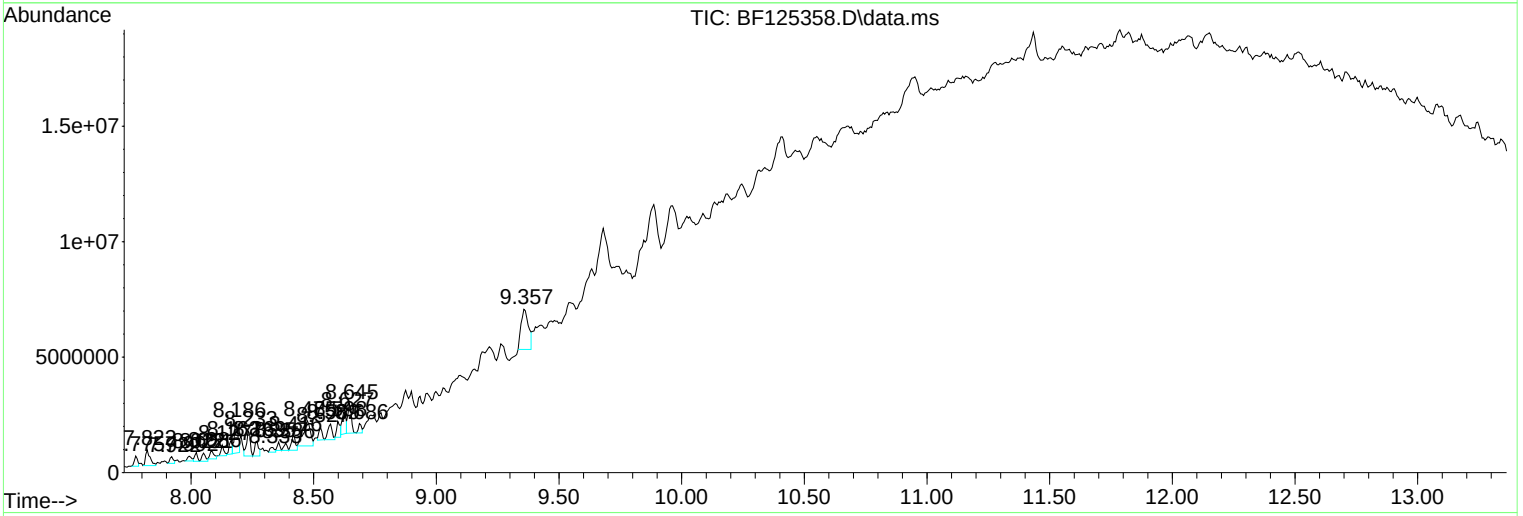
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

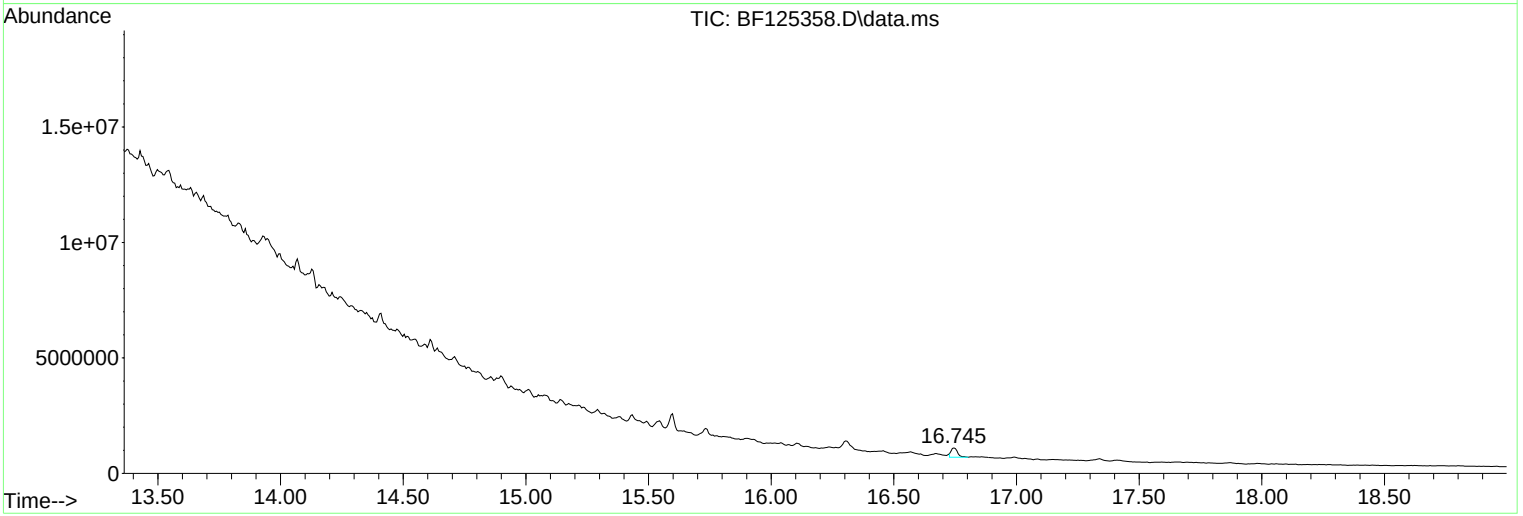
Instrument :
BNA_F
ClientSampleId :
99-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
99-01

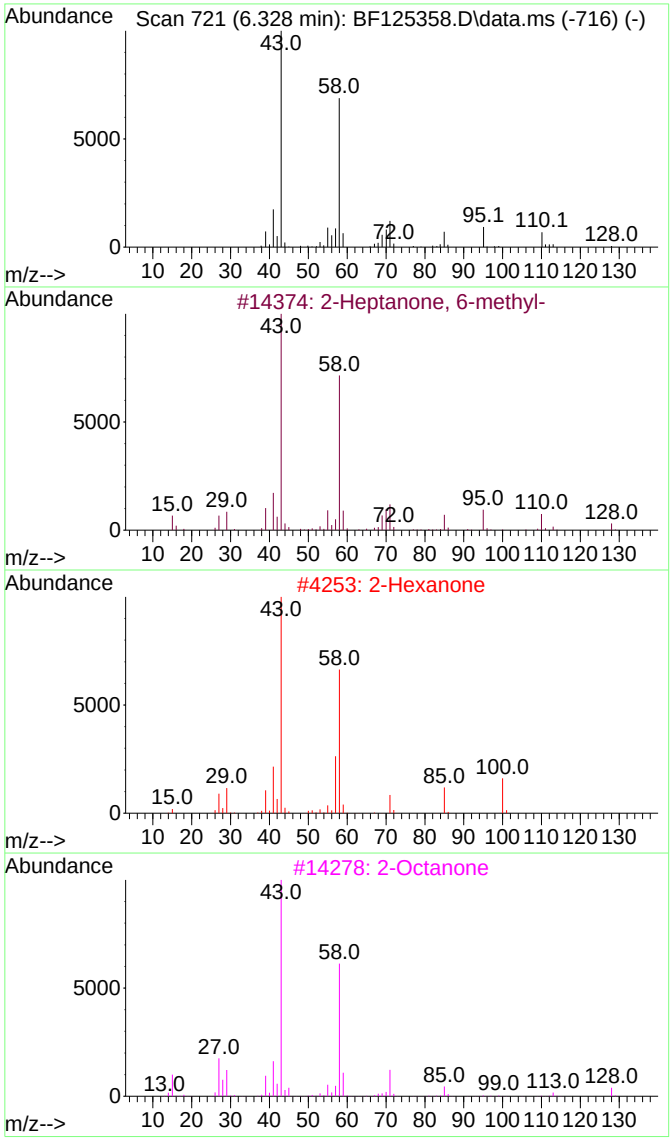
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

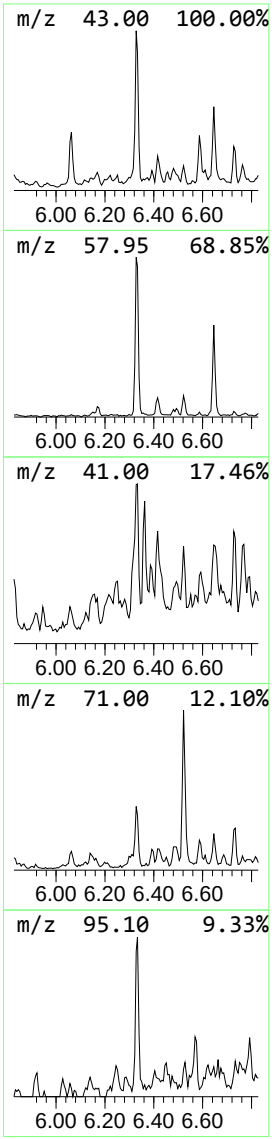
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Heptanone, 6-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.328	6.13 ng	273777	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	90
2	2-Hexanone	100	C6H12O	000591-78-6	59
3	2-Octanone	128	C8H16O	000111-13-7	53
4	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	53
5	2-Hexanone, 4-hydroxy-3-propyl-	158	C9H18O2	062338-17-4	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

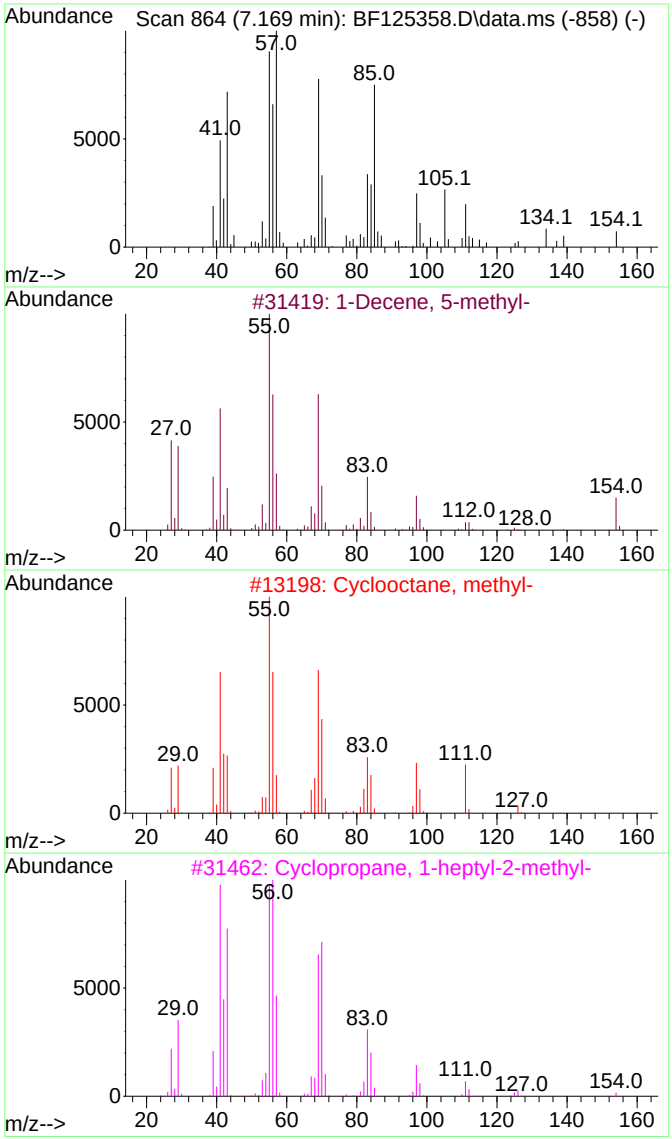
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

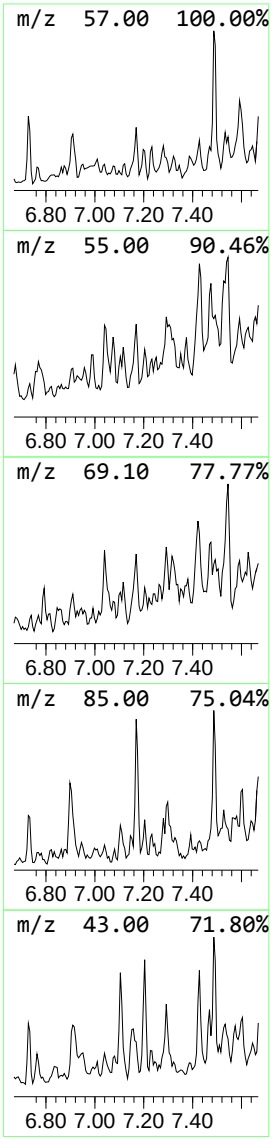
****

Peak Number 2 1-Decene, 5-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.169	5.18 ng	231648	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decene, 5-methyl-	154	C11H22	054244-79-0	60
2	Cyclooctane, methyl-	126	C9H18	001502-38-1	53
3	Cyclopropane, 1-heptyl-2-methyl-	154	C11H22	074663-91-5	53
4	Cyclopropane, 1,2-dibutyl-	154	C11H22	041977-32-6	53
5	4-Decene, 4-methyl-, (E)-	154	C11H22	060366-66-7	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

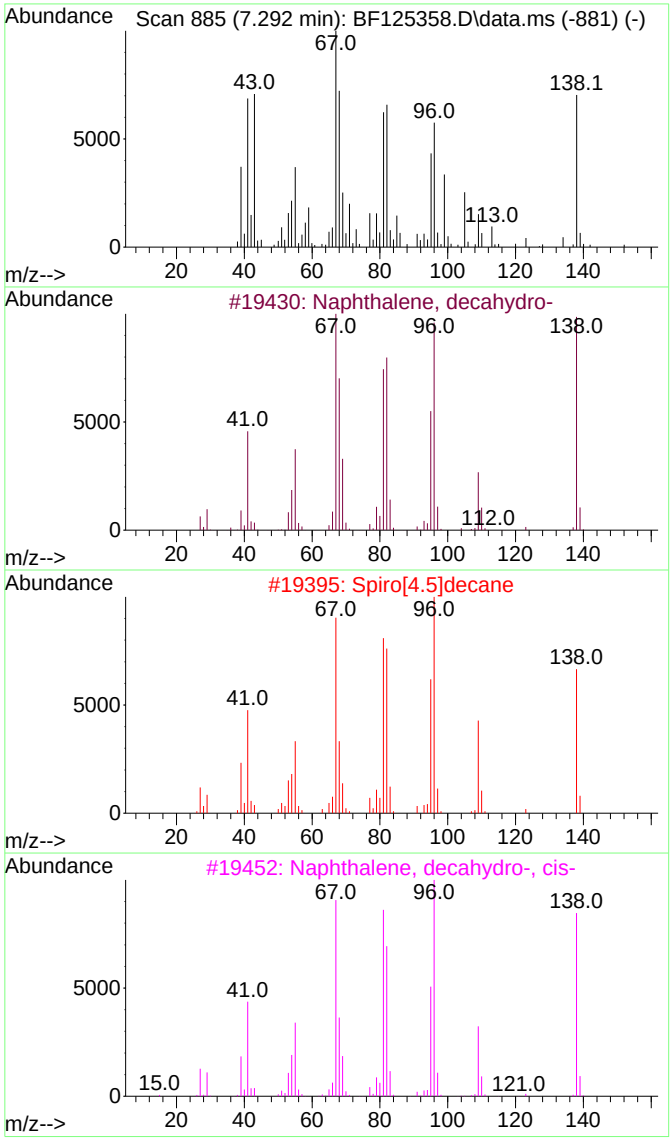
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

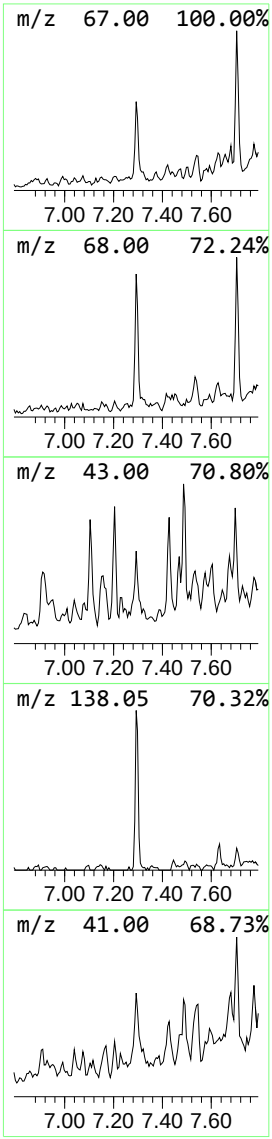
****

Peak Number 3 Naphthalene, decahydro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.292	9.39 ng	419692	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-	138	C10H18	000091-17-8	93
2	Spiro[4.5]decane	138	C10H18	000176-63-6	76
3	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	70
4	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	70
5	5H-Inden-5-one, octahydro-, trans-	138	C9H14O	004668-81-9	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
99-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

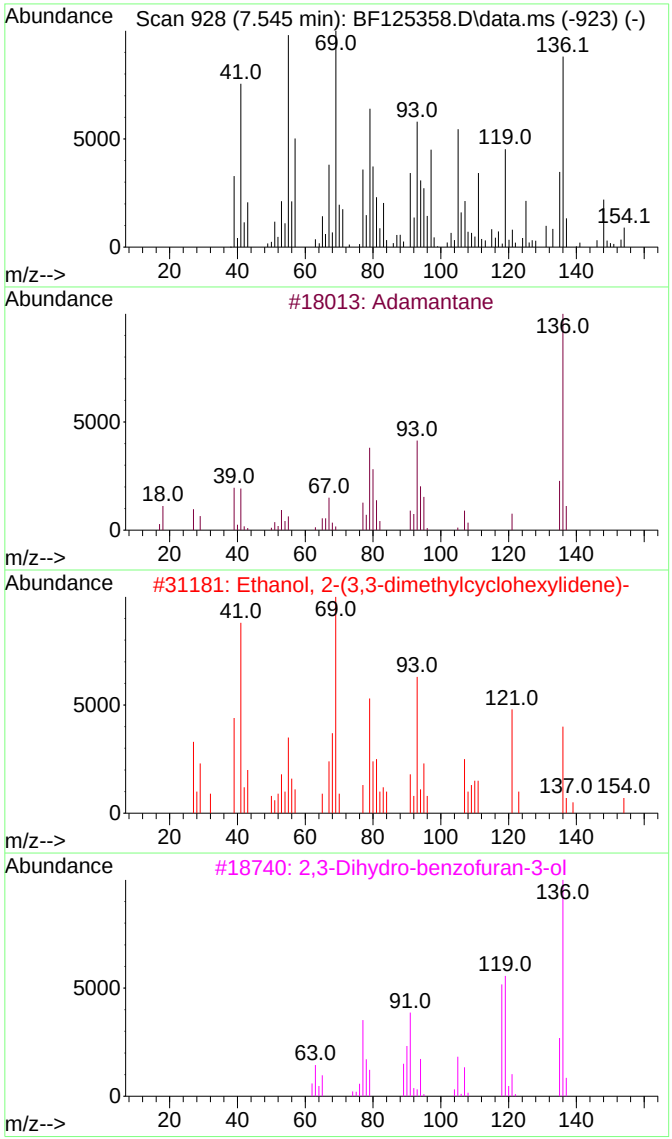
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

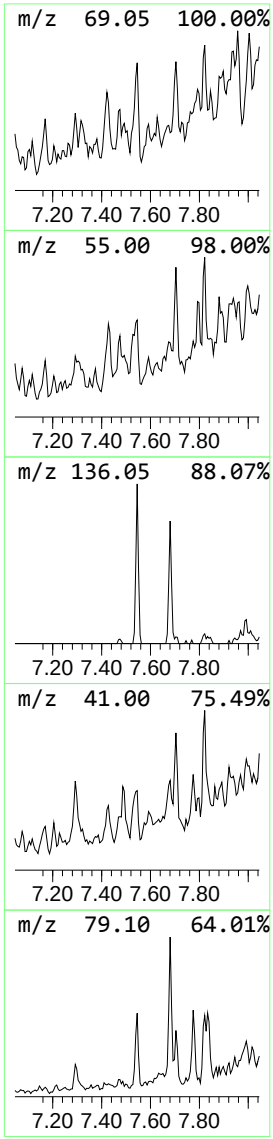
****

Peak Number 4 Adamantane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.545	5.82 ng	440085	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adamantane	136	C10H16	000281-23-2	62
2	Ethanol, 2-(3,3-dimethylcyclohex...	154	C10H18O	041370-29-0	30
3	2,3-Dihydro-benzofuran-3-ol	136	C8H8O2	1000146-26-4	30
4	Bicyclo[4.1.0]heptan-3-ol, 4,7,7...	154	C10H18O	054750-08-2	20
5	2-Carene	136	C10H16	000554-61-0	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

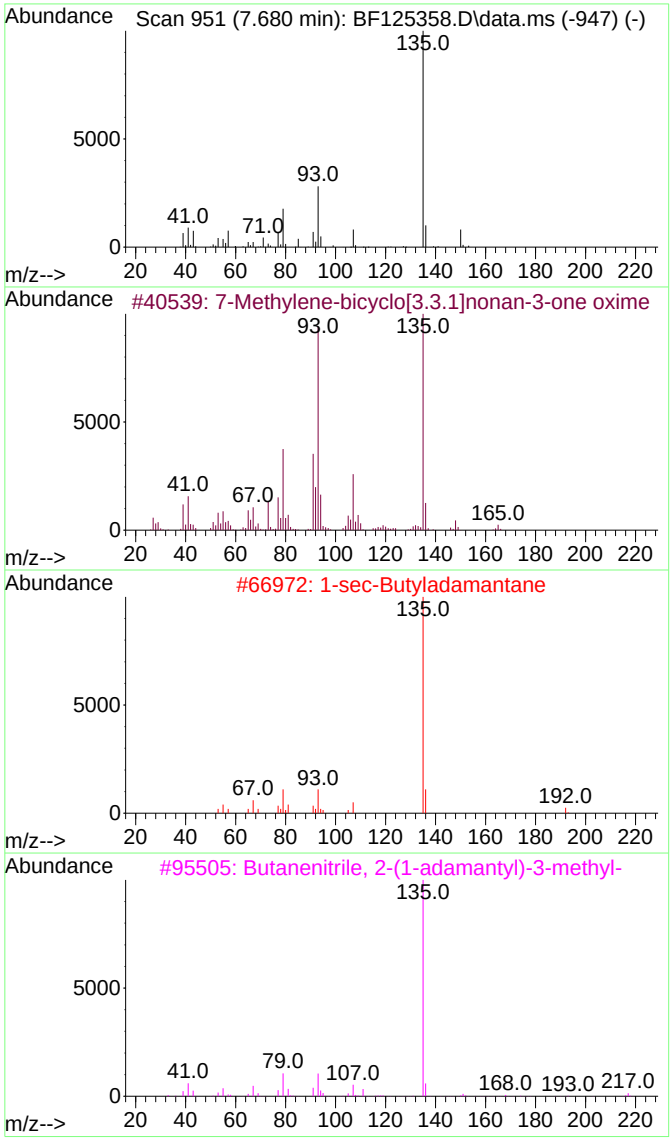
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

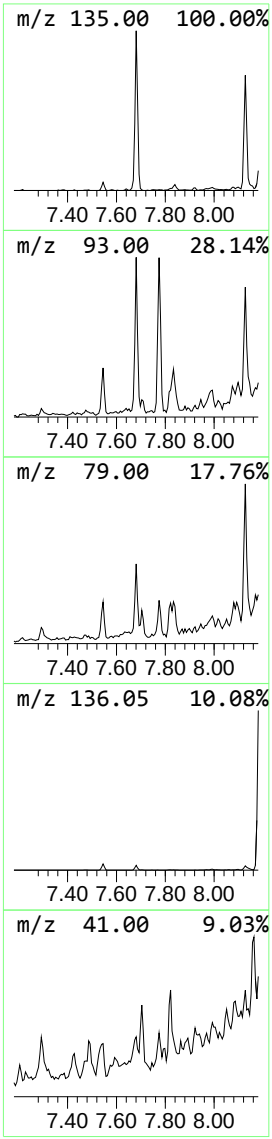
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 7-Methylene-bicyclo[3.3.1]n... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.680	5.36 ng	405586	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Methylene-bicyclo[3.3.1]nonan-...	165	C10H15NO	1000185-68-5	78
2	1-sec-Butyladamantane	192	C14H24	014449-42-4	72
3	Butanenitrile, 2-(1-adamantyl)-3...	217	C15H23N	1000266-44-6	72
4	2-(Adamantan-1-yloxy)-6-chloropy...	263	C15H18ClNO	1000411-33-6	72
5	Tricyclo[3.3.1.1(3,7)]decane, 1-...	181	C10H15NO2	007575-82-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
99-01

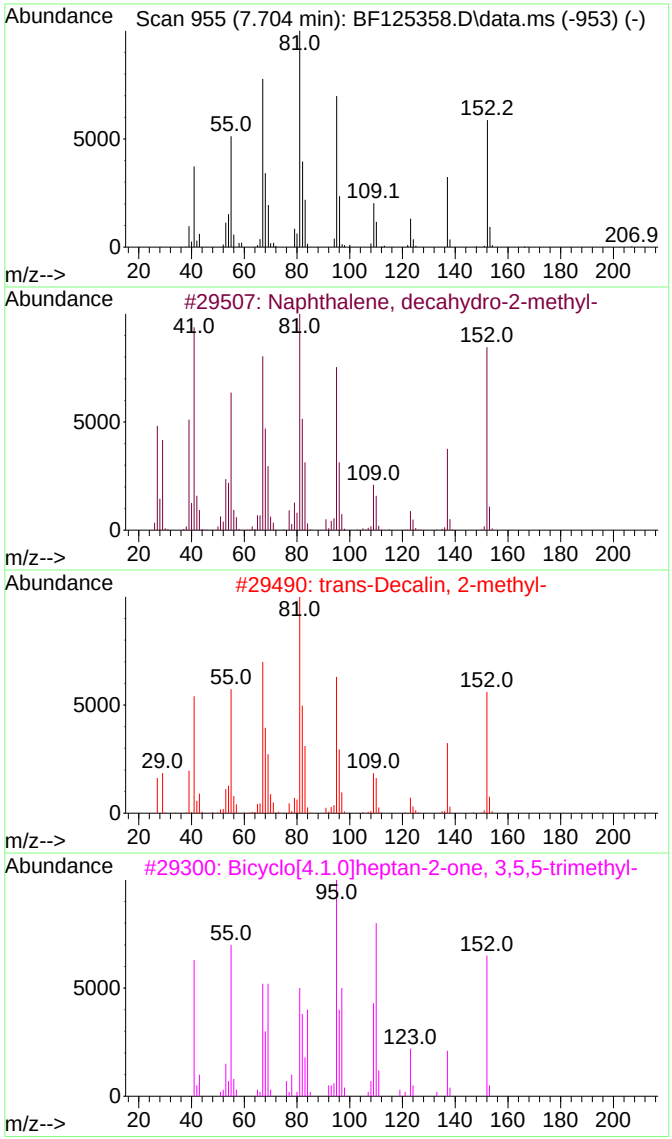
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

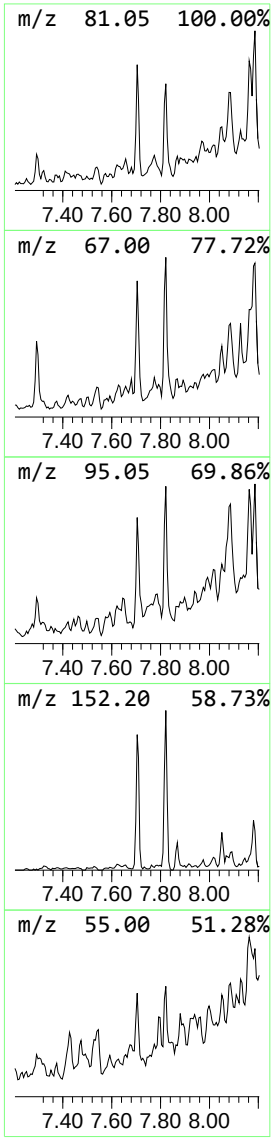
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, decahydro-2-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.704	7.00 ng	529810	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	94
2	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	91
3	Bicyclo[4.1.0]heptan-2-one, 3,5,...	152	C10H16O	029750-24-1	76
4	trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	70
5	Pulegone	152	C10H16O	000089-82-7	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
99-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

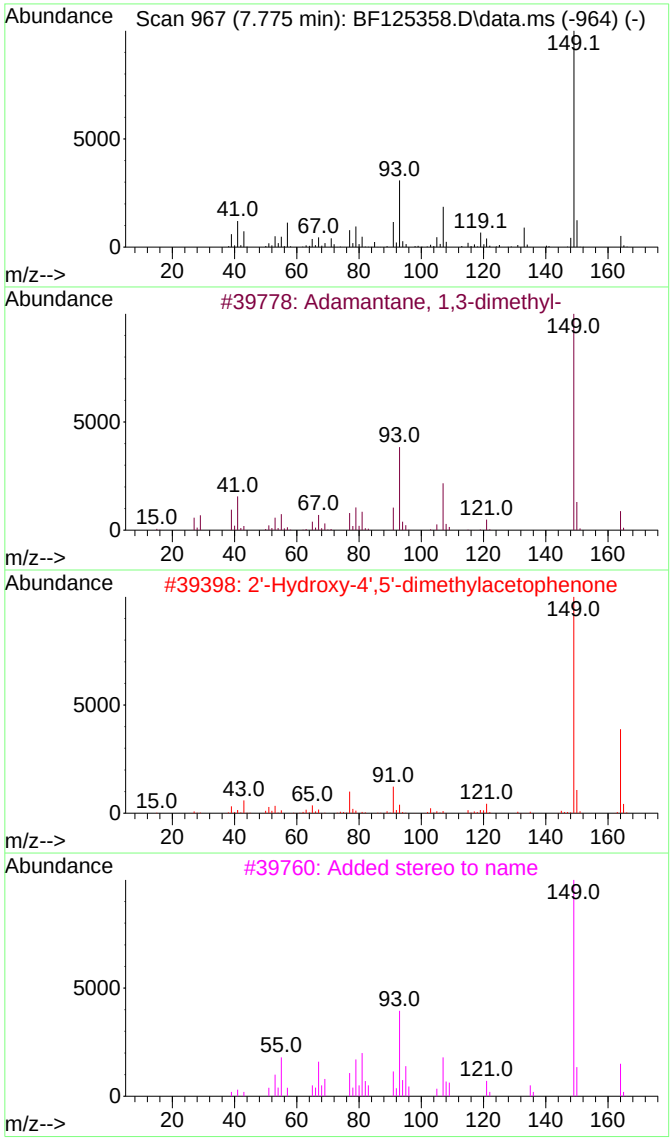
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

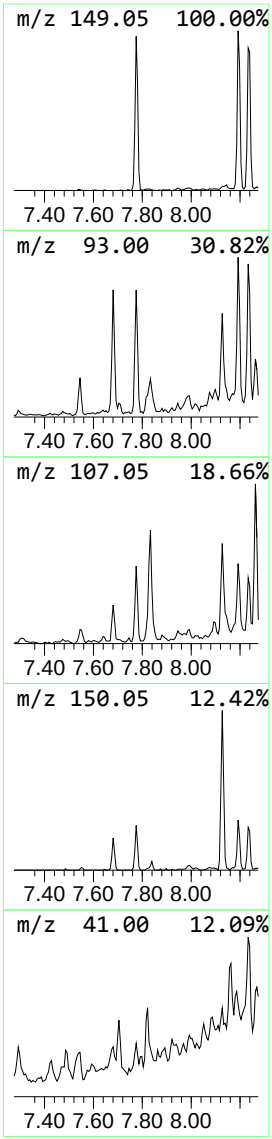
****

Peak Number 7 Adamantane, 1,3-dimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.775	5.38 ng	406775	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	60
2	2'-Hydroxy-4',5'-dimethylacetoph...	164	C10H12O2	036436-65-4	50
3	Added stereo to name	164	C12H20	024145-88-8	50
4	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	50
5	1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

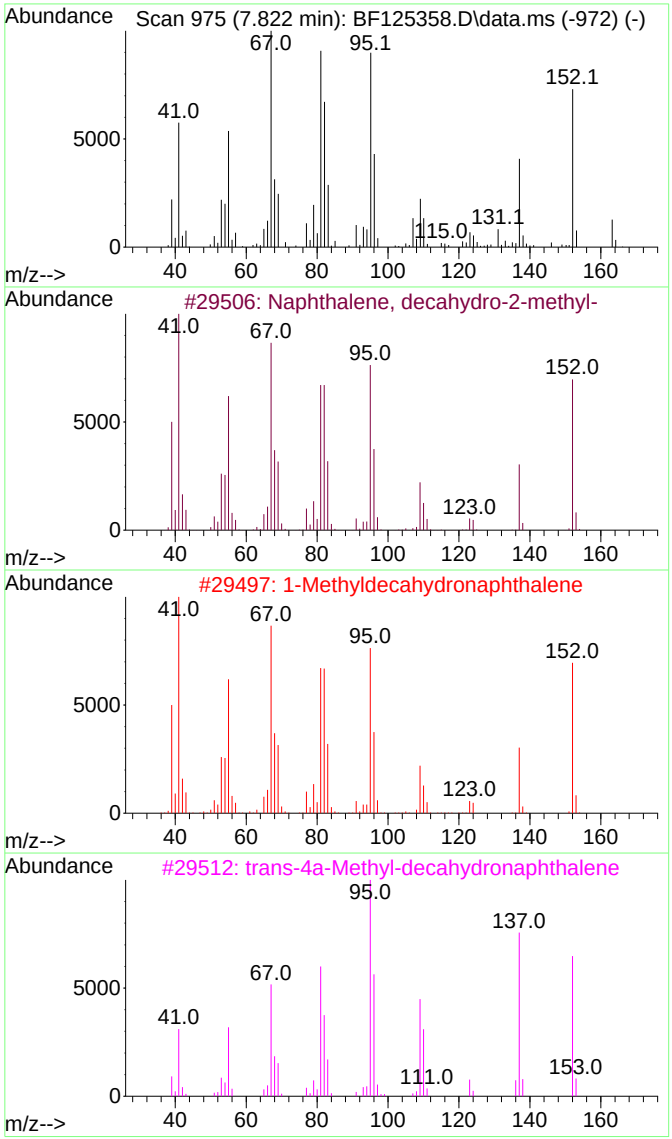
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

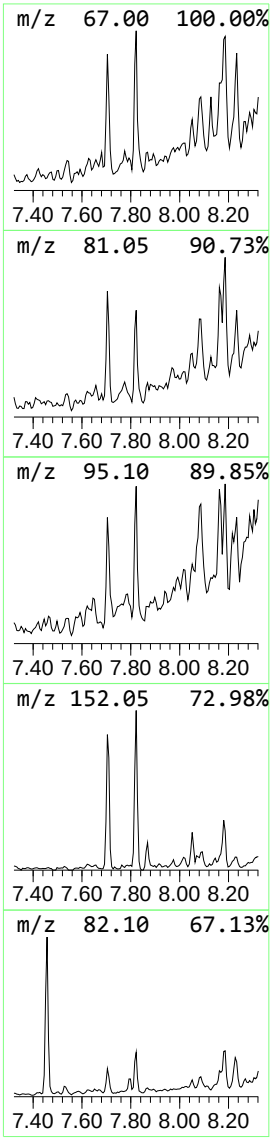
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Methyldecahydronaphthalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.822	11.50 ng	870038	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	98
2	1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	98
3	trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	89
4	cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	83
5	9-Octadecyne	250	C18H34	035365-59-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

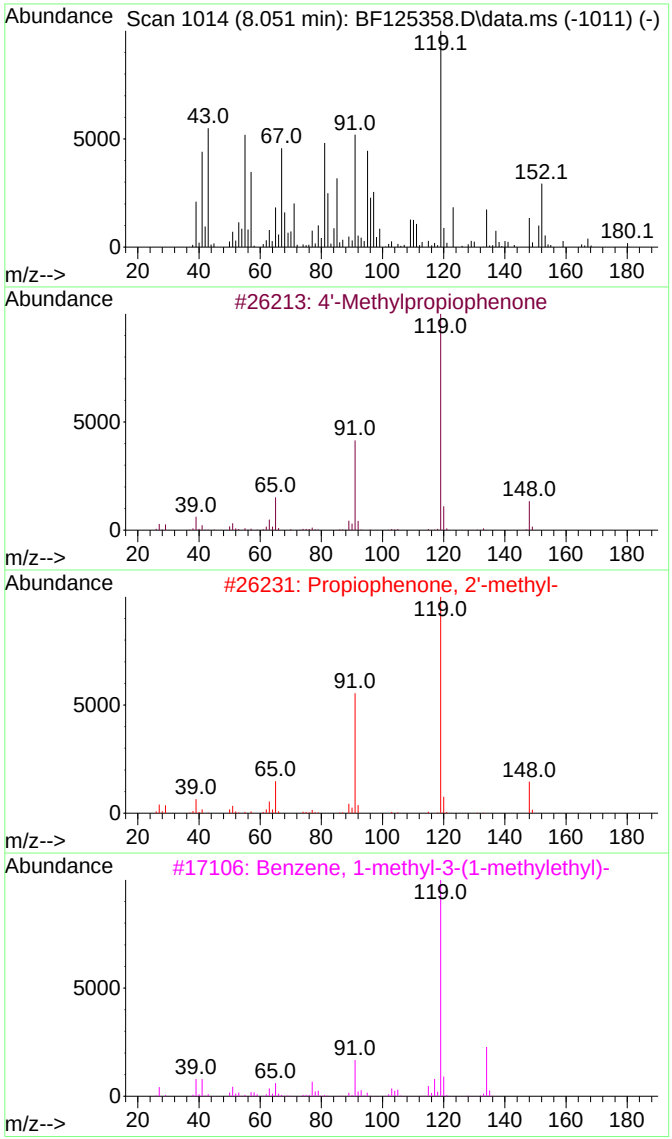
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

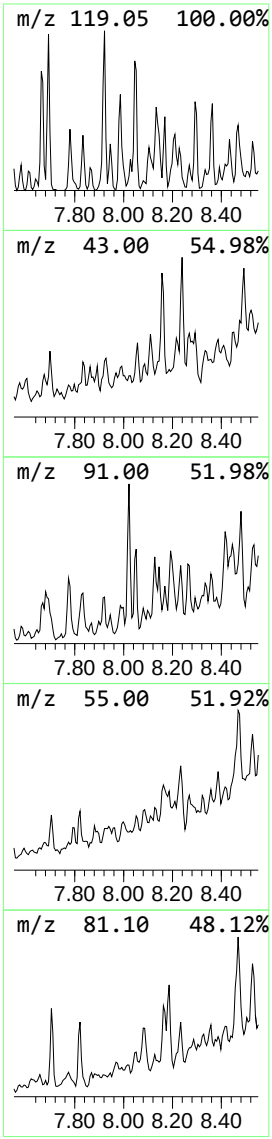
****

Peak Number 9 unknown8.051 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	5.11 ng	386204	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4'-Methylpropiophenone	148	C10H12O	005337-93-9	35
2	Propiophenone, 2'-methyl-	148	C10H12O	002040-14-4	35
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	22
4	N-(m-Toluoyl)glycine	193	C10H11NO3	027115-49-7	22
5	Benzene, isocyanato-	119	C7H5NO	000103-71-9	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

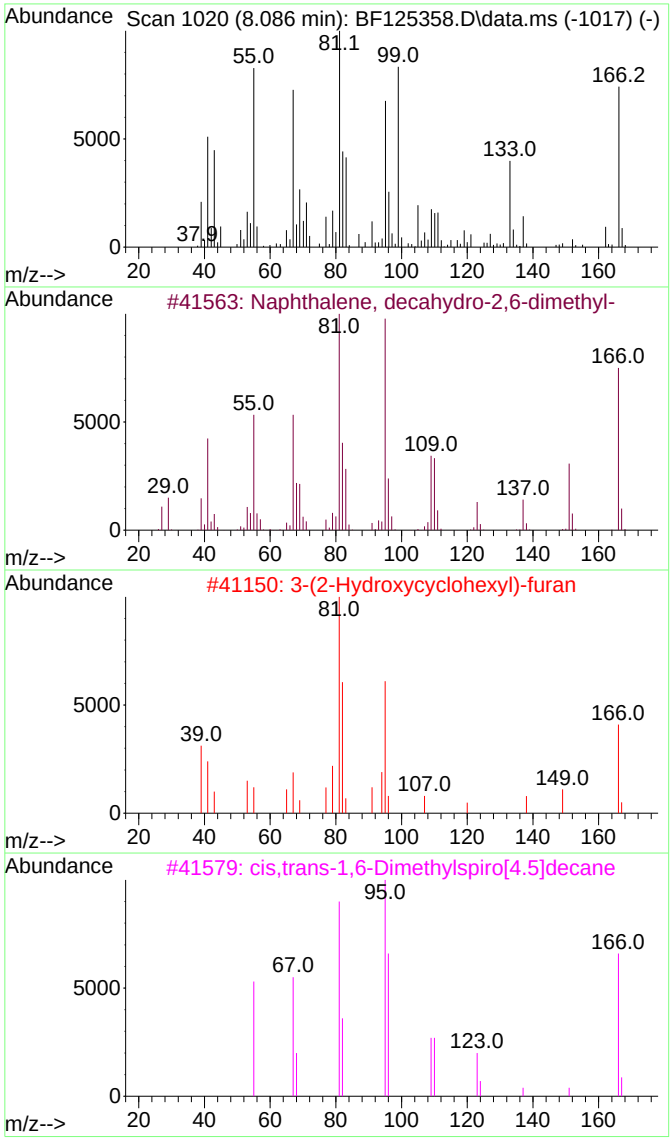
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

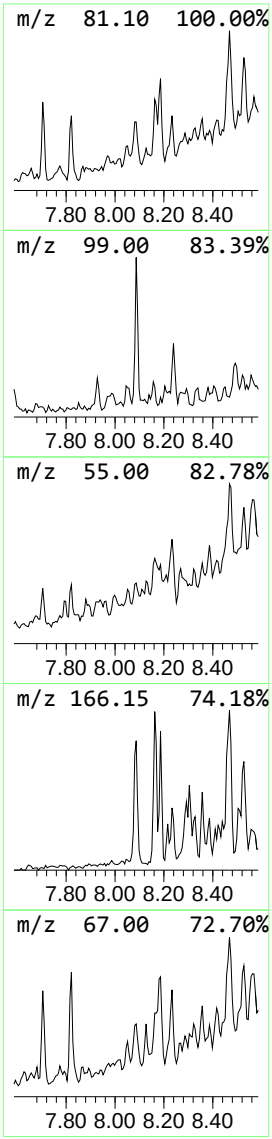
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, decahydro-2,6-... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.086	5.62 ng	424810	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	58
2	3-(2-Hydroxycyclohexyl)-furan	166	C10H14O2	118959-04-9	55
3	cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	53
4	(4aS,7S,7aR)-4,7-Dimethyl-5,6,7,...	166	C10H14O2	021651-62-7	46
5	Naphthalene, decahydro-1,5-dimet...	166	C12H22	066552-62-3	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
99-01

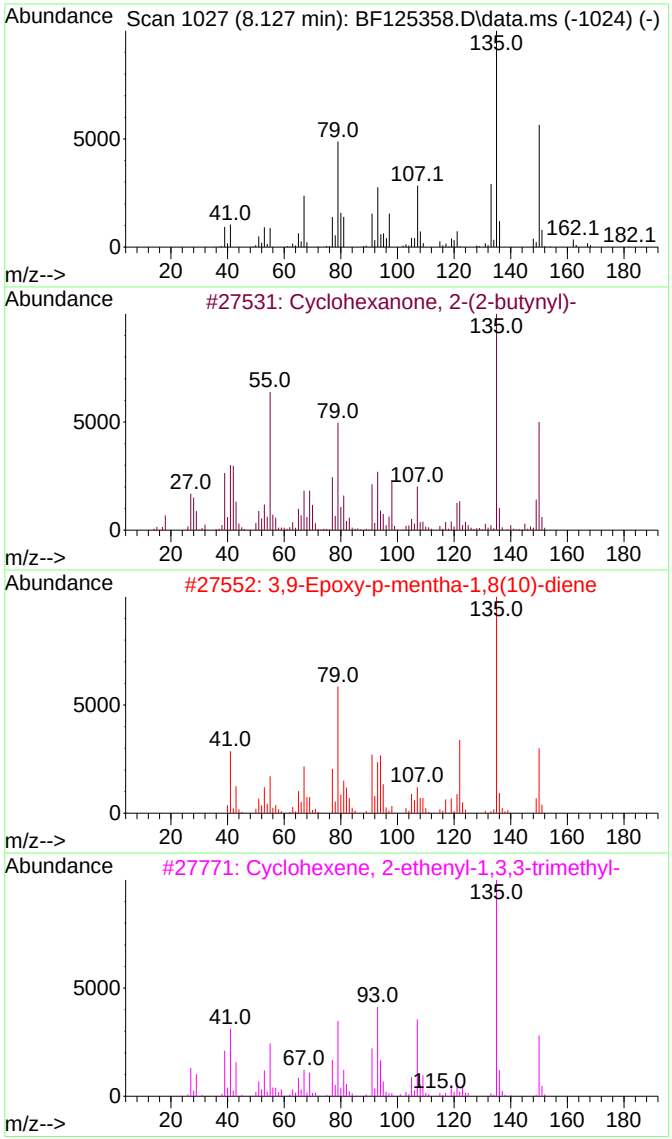
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

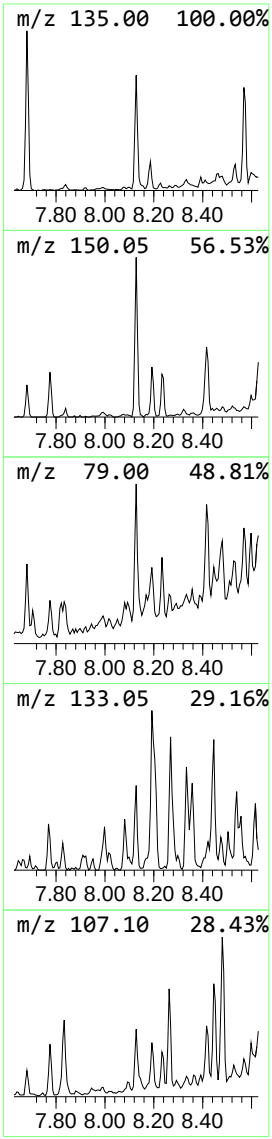
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Cyclohexanone, 2-(2-butynyl)- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.127	5.19 ng	392352	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 2-(2-butynyl)-	150	C10H14O	054166-48-2	74
2	3,9-Epoxy-p-mentha-1,8(10)-diene	150	C10H14O	1000111-14-8	68
3	Cyclohexene, 2-ethenyl-1,3,3-tri...	150	C11H18	005293-90-3	68
4	1-Adamantanethiol	168	C10H16S	034301-54-7	53
5	4-Hydroxy-3-methylacetophenone	150	C9H10O2	000876-02-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
99-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

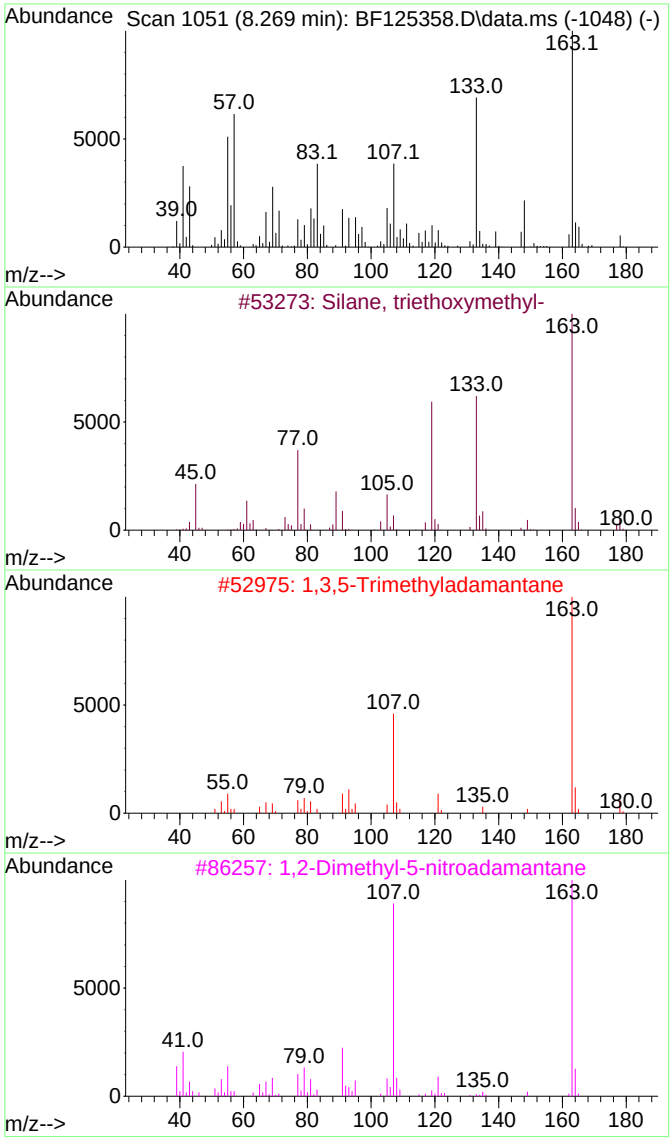
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

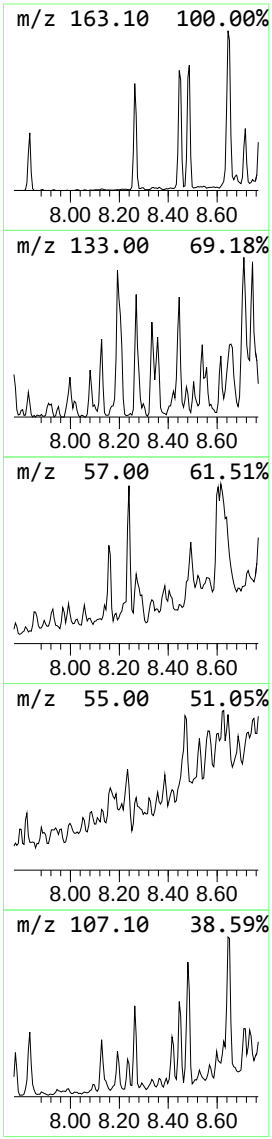
****

Peak Number 12 unknown8.269 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.269	9.66 ng	730844	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, triethoxymethyl-	178	C7H18O3Si	002031-67-6	43
2	1,3,5-Trimethyladamantane	178	C13H22	000707-35-7	38
3	1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	38
4	3,4-Dimethylcumene	148	C11H16	1000370-34-1	25
5	N-(4-Formyl-phenyl)-N-methyl-for...	163	C9H9NO2	079213-80-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

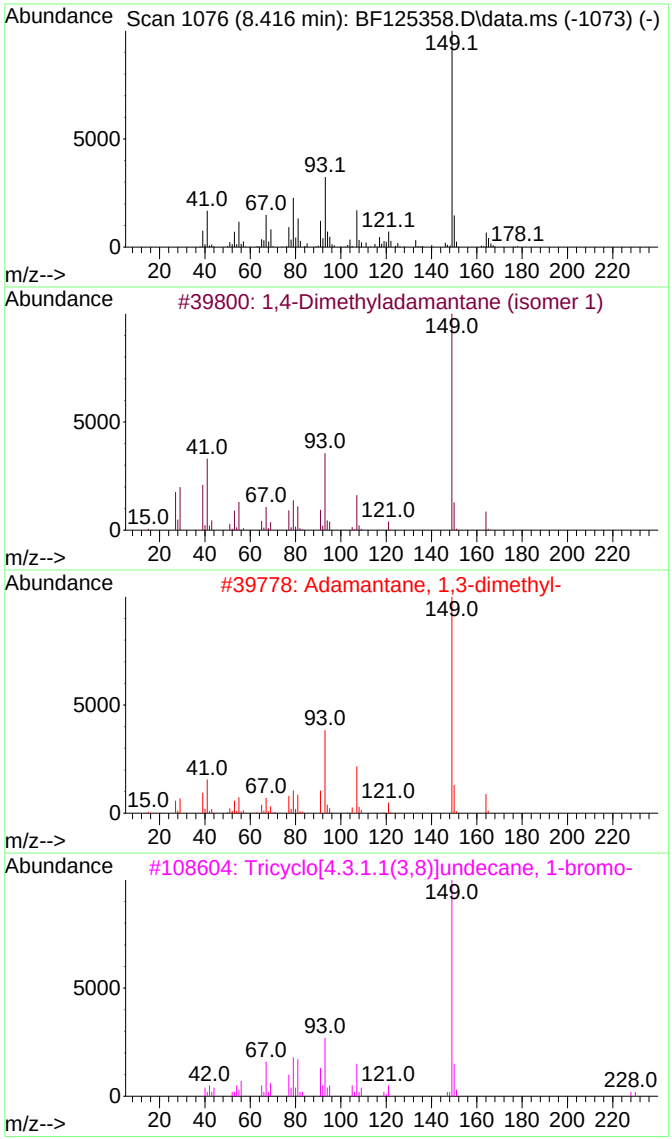
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

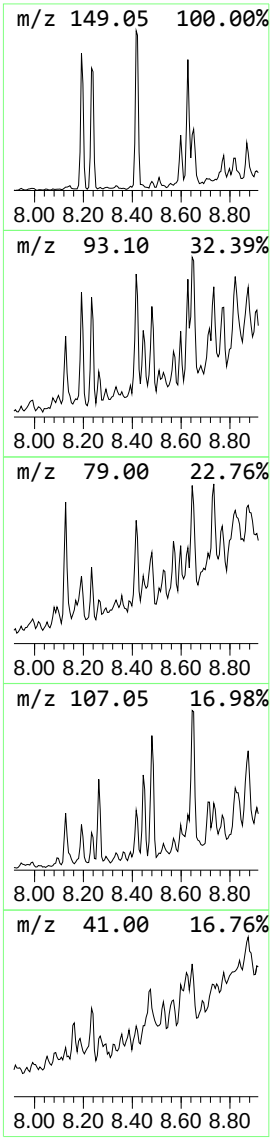
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 1,4-Dimethyladamantane (iso... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.416	9.88 ng	747585	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	93
2	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	81
3	Tricyclo[4.3.1.1(3,8)]undecane, ...	228	C11H17Br	021898-96-4	72
4	Tricyclo[4.3.1.1(3,8)]undecane, ...	184	C11H17Cl	027011-46-7	59
5	1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

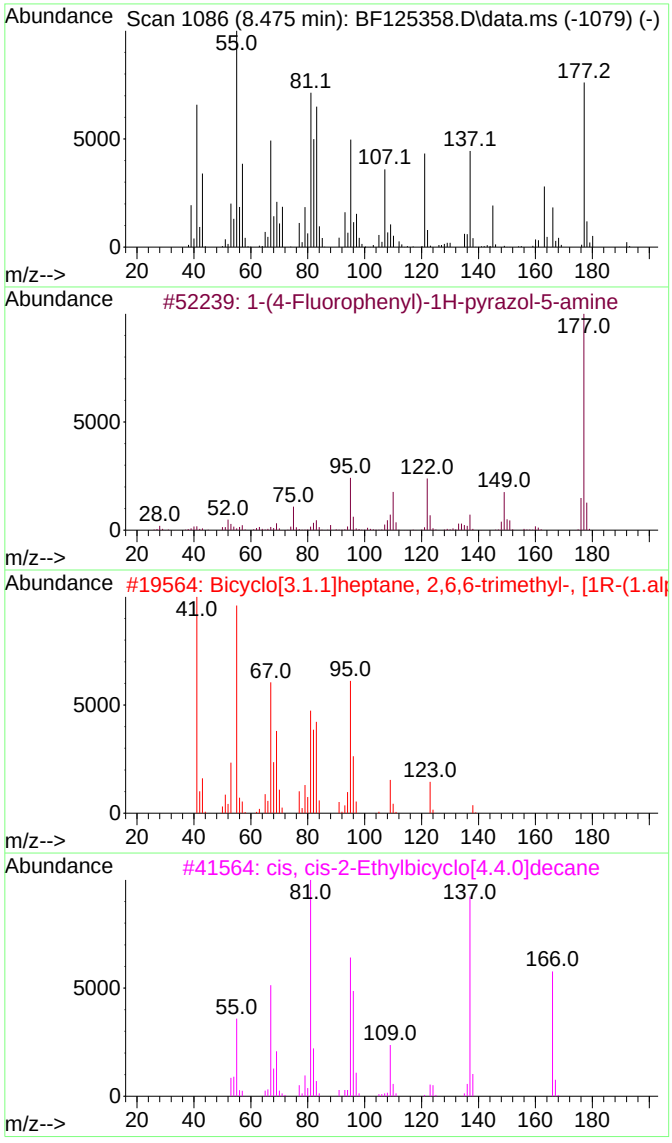
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

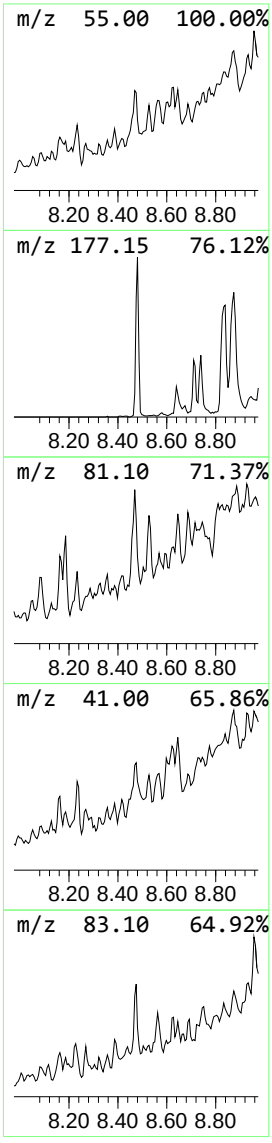
****

Peak Number 14 unknown8.475 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.475	29.25 ng	2212510	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Fluorophenyl)-1H-pyrazol-5-...	177	C9H8FN3	727967-95-5	25
2	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004863-59-6	25
3	cis, cis-2-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-40-0	25
4	Cyclopentane, 1-methyl-2-(2-prop...	124	C9H16	050746-53-7	22
5	trans-.beta.-Ionone	192	C13H20O	000079-77-6	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

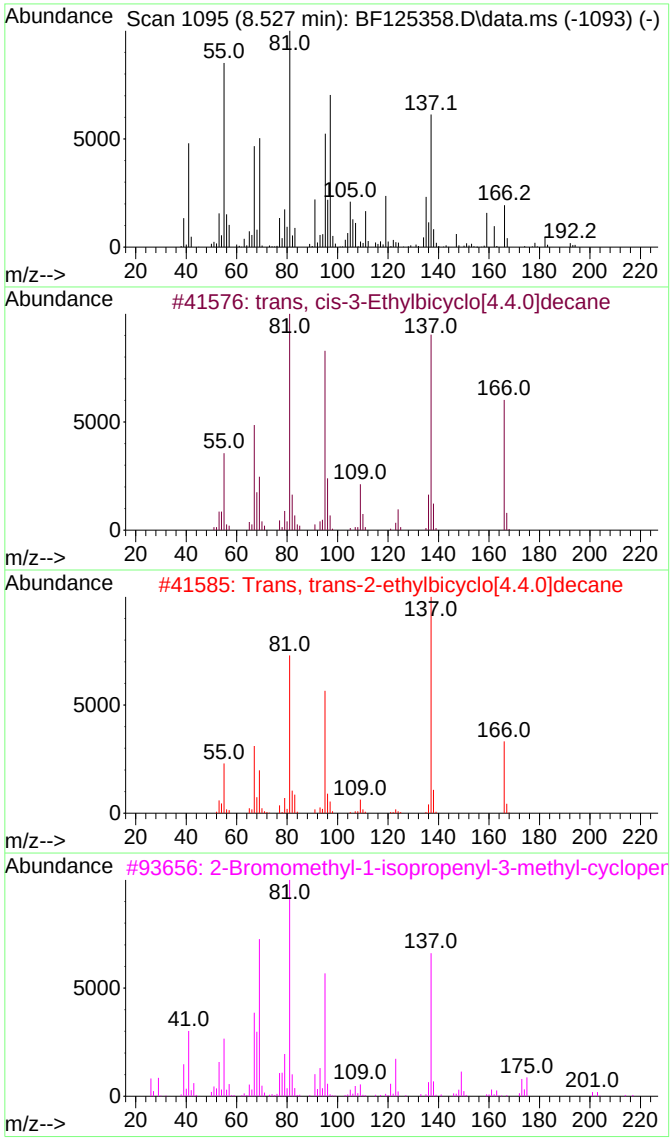
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

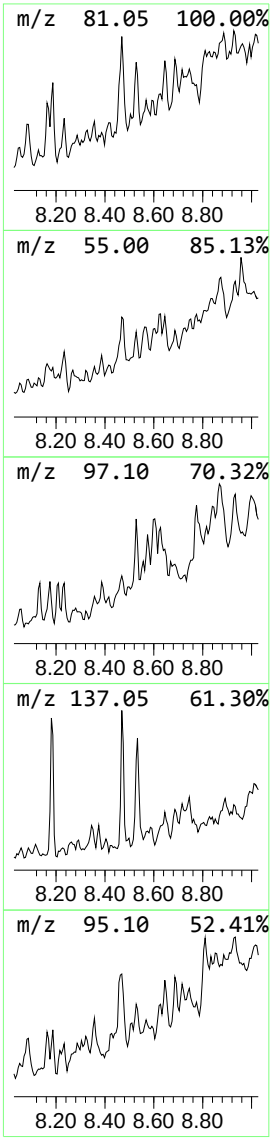
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 trans, cis-3-Ethylbicyclo[4... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.527	6.44 ng	487004	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	68
2	Trans, trans-2-ethylbicyclo[4.4....	166	C12H22	066660-37-5	58
3	2-Bromomethyl-1-isopropenyl-3-me...	216	C10H17Br	1000187-07-8	47
4	Naphthalene, 2-ethyldecahydro-	166	C12H22	001618-23-1	30
5	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

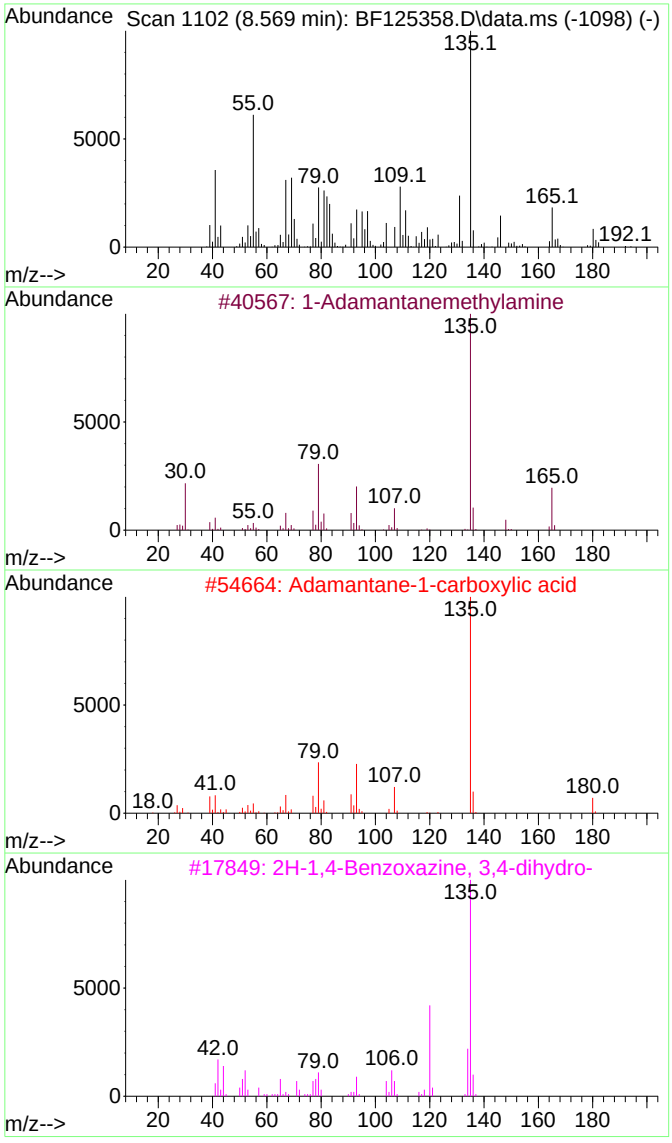
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

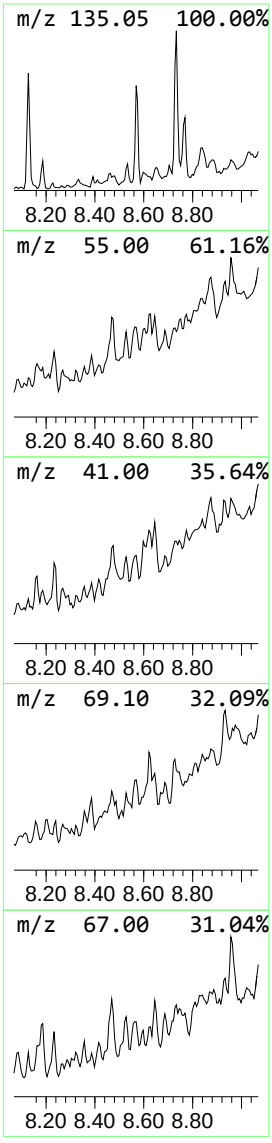
****

Peak Number 16 unknown8.569 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.569	11.11 ng	840248	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Adamantanemethylamine	165	C11H19N	017768-41-1	45
2	Adamantane-1-carboxylic acid	180	C11H16O2	000828-51-3	41
3	2H-1,4-Benzoxazine, 3,4-dihydro-	135	C8H9NO	005735-53-5	38
4	2-Iodoadamantane	262	C10H15I	018971-91-0	38
5	1-Adamantanemethanol	166	C11H18O	000770-71-8	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

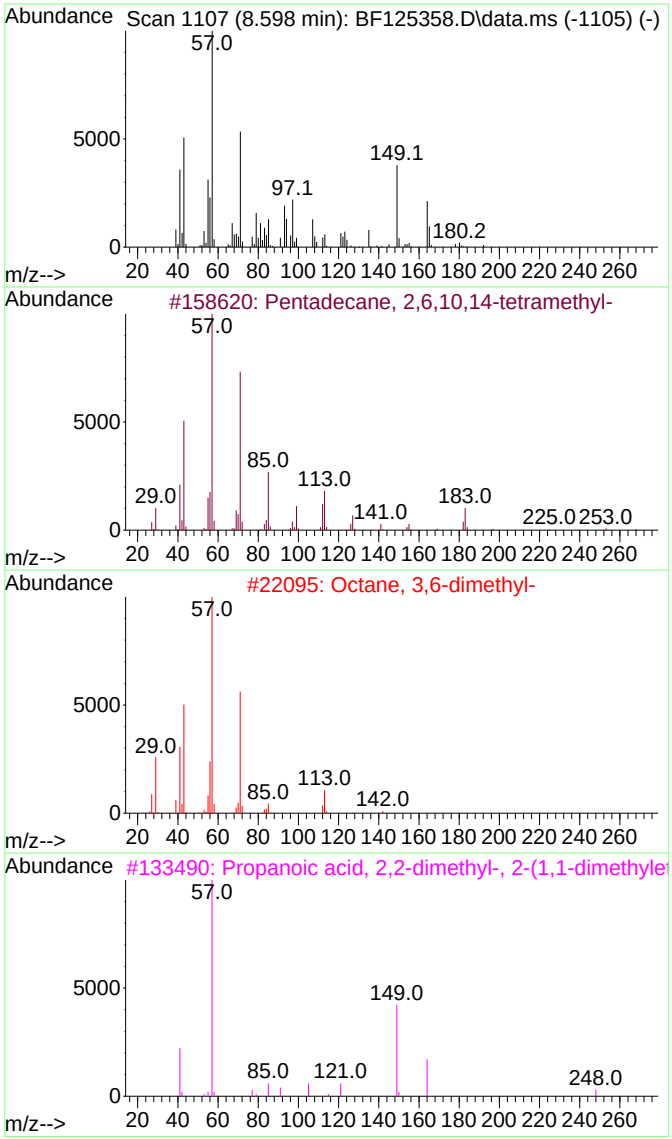
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

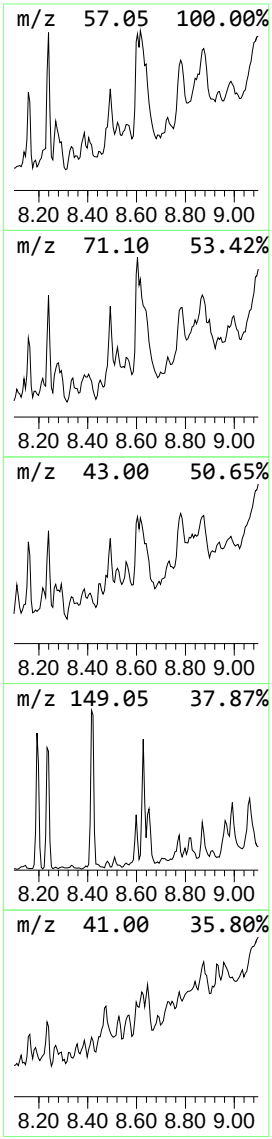
****

Peak Number 17 unknown8.598 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.598	9.47 ng	716161	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	27
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	22
3	Propanoic acid, 2,2-dimethyl-, 2...	248	C16H24O2	054644-42-7	22
4	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	22
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

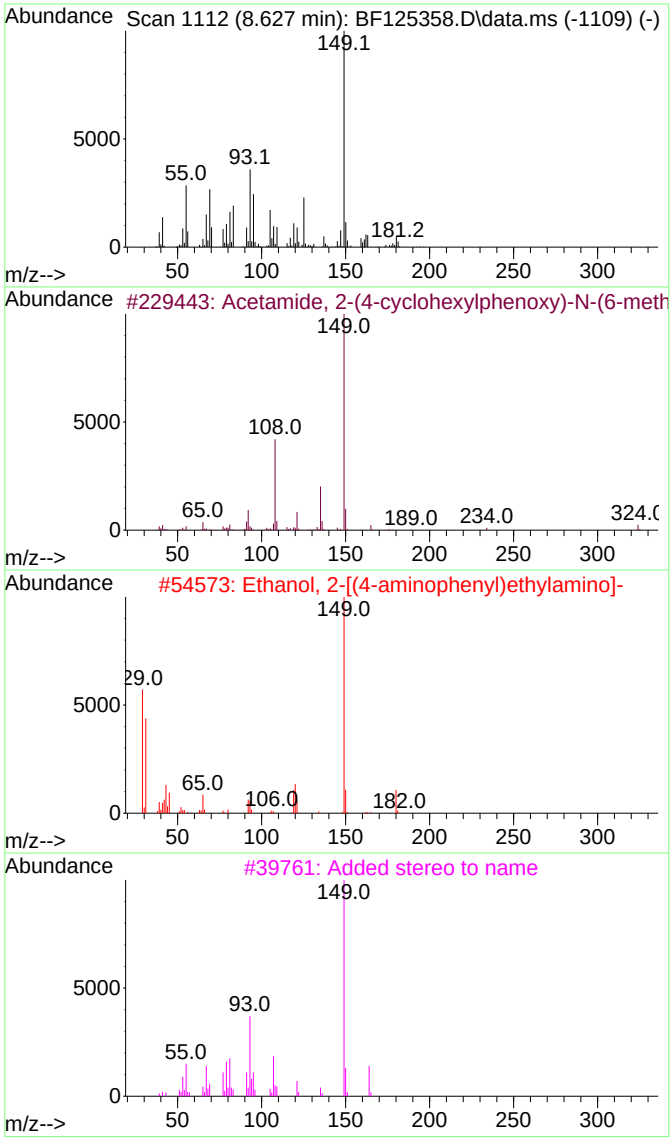
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

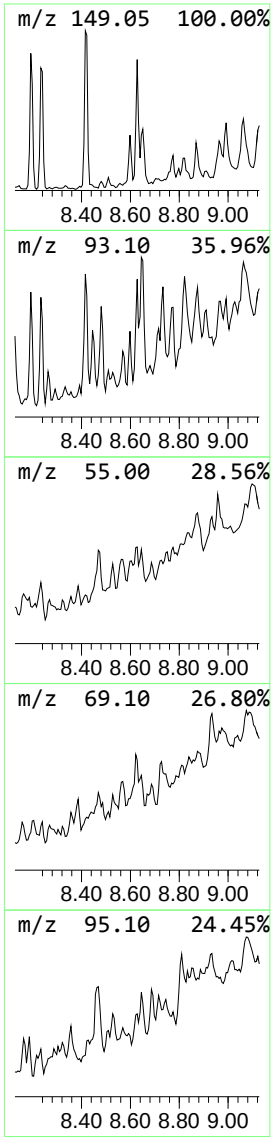
****

Peak Number 18 unknown8.627 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.627	13.96 ng	1055920	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, 2-(4-cyclohexylphenox...	324	C20H24N2O2	1000263-95-6	43
2	Ethanol, 2-[(4-aminophenyl)ethyl...	180	C10H16N2O	000092-65-9	43
3	Added stereo to name	164	C12H20	024145-89-9	40
4	Silane, monochloride, methylviny...	220	C10H21ClOSi	1000420-88-8	40
5	2,4,7,14-Tetramethyl-4-vinyl-tri...	290	C20H34O	1000193-31-2	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

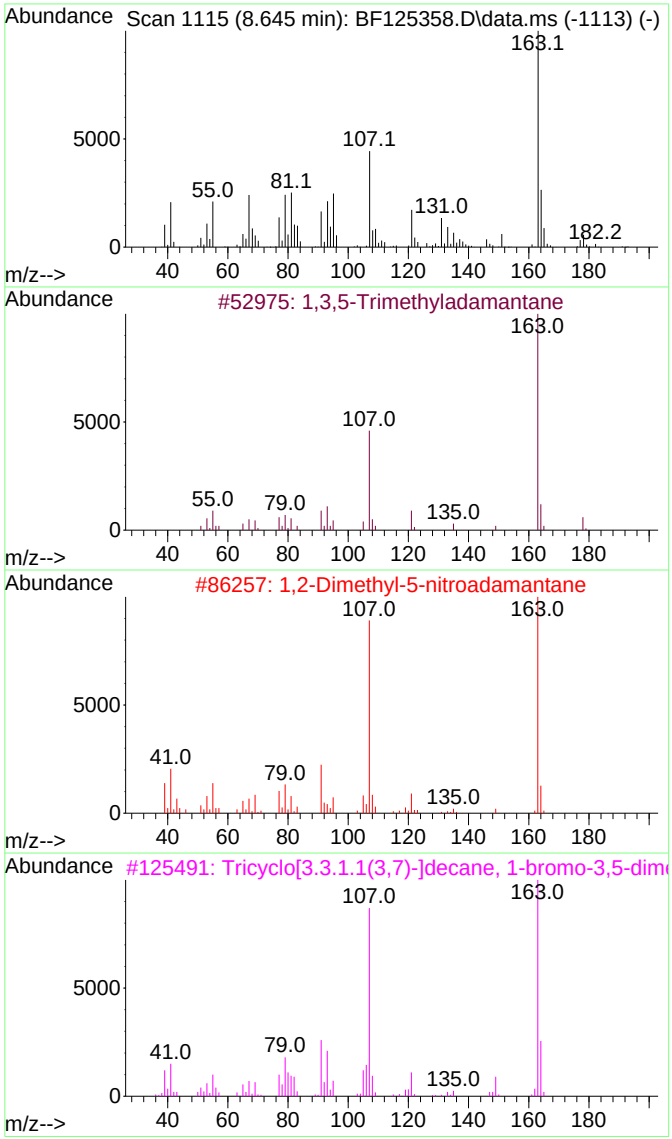
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

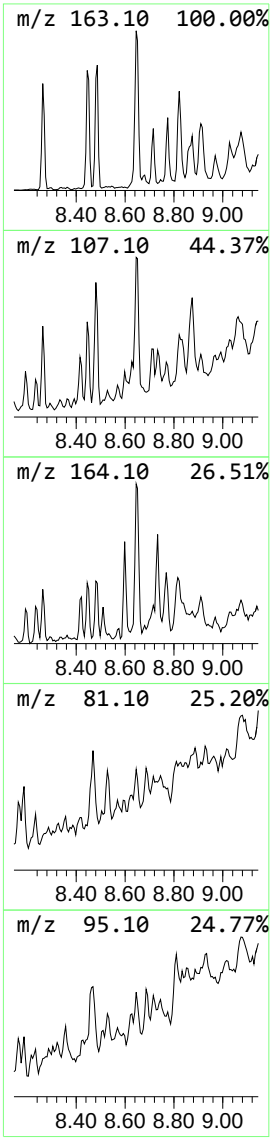
****

Peak Number 19 1,3,5-Trimethyladamantane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.645	16.56 ng	1252770	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Trimethyladamantane	178	C13H22	000707-35-7	52
2	1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	50
3	Tricyclo[3.3.1.1(3,7)-]decane, 1...	242	C12H19Br	000941-37-7	50
4	1,3,6-Trimethyladamantane	178	C13H22	024139-37-5	49
5	benzoxazole, 7-methoxy-2-methyl-	163	C9H9NO2	1000404-43-8	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

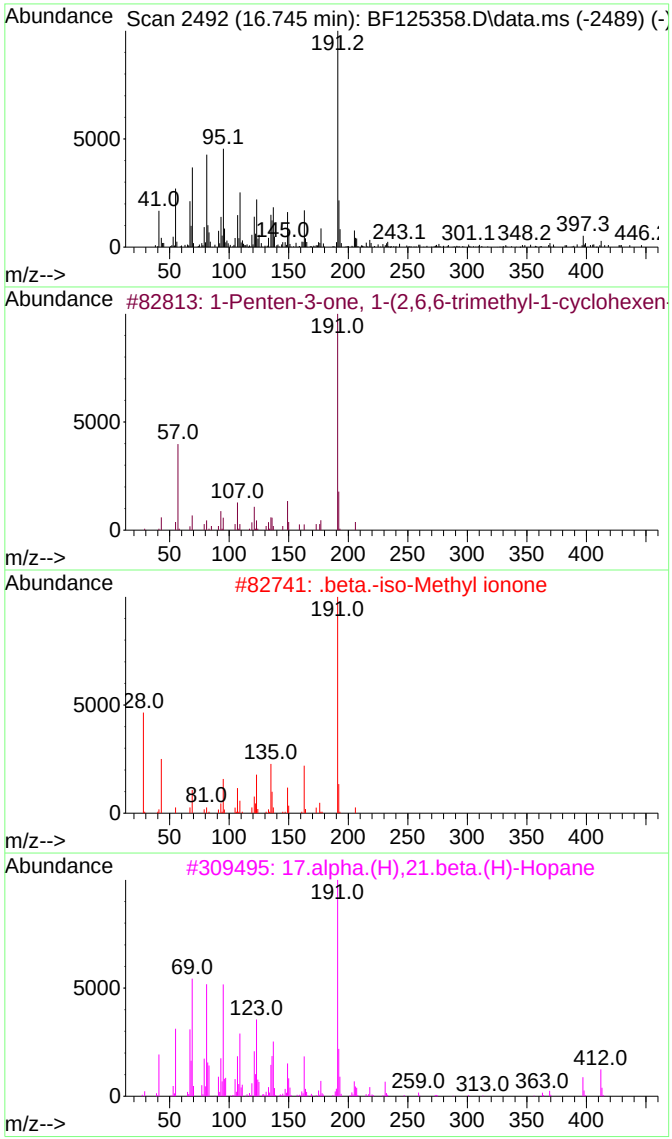
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

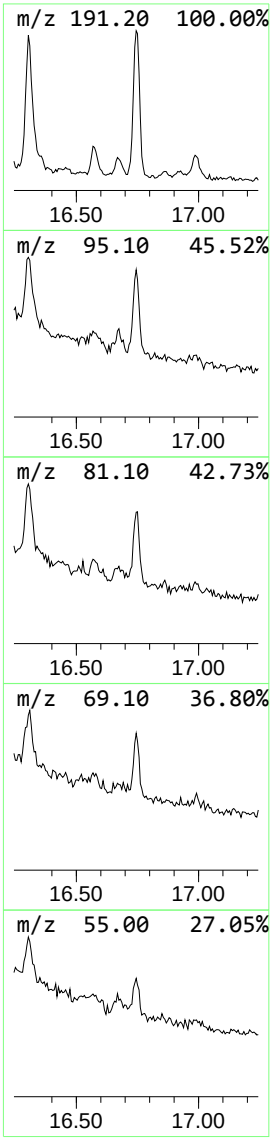
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 1-Penten-3-one, 1-(2,6,6-tr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.745	20.00 ng	710361	Perylene-d12	15.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	87
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	81
3	17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	64
4	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	47
5	Propenamide, 3-(3,4-dimethoxyphe...	313	C18H19NO4	339165-72-9	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090321\
Data File : BF125358.D
Acq On : 3 Sep 2021 21:26
Operator : JU/CG
Sample : M3646-15 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 99-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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-Heptanone, 6-...	6.328	6.1	ng	273777	1	6.898	893826	20.0
1-Decene, 5-met...	7.169	5.2	ng	231648	1	6.898	893826	20.0
Naphthalene, de...	7.292	9.4	ng	419692	1	6.898	893826	20.0
Adamantane	7.545	5.8	ng	440085	2	8.180	1512940	20.0
7-Methylene-bic...	7.680	5.4	ng	405586	2	8.180	1512940	20.0
Naphthalene, de...	7.704	7.0	ng	529810	2	8.180	1512940	20.0
Adamantane, 1,3...	7.775	5.4	ng	406775	2	8.180	1512940	20.0
1-Methyldecahyd...	7.822	11.5	ng	870038	2	8.180	1512940	20.0
unknown8.051	8.051	5.1	ng	386204	2	8.180	1512940	20.0
Naphthalene, de...	8.086	5.6	ng	424810	2	8.180	1512940	20.0
Cyclohexanone, ...	8.127	5.2	ng	392352	2	8.180	1512940	20.0
unknown8.269	8.269	9.7	ng	730844	2	8.180	1512940	20.0
1,4-Dimethylada...	8.416	9.9	ng	747585	2	8.180	1512940	20.0
unknown8.475	8.475	29.3	ng	2212510	2	8.180	1512940	20.0
trans, cis-3-Et...	8.527	6.4	ng	487004	2	8.180	1512940	20.0
unknown8.569	8.569	11.1	ng	840248	2	8.180	1512940	20.0
unknown8.598	8.598	9.5	ng	716161	2	8.180	1512940	20.0
unknown8.627	8.627	14.0	ng	1055920	2	8.180	1512940	20.0
1,3,5-Trimethyl...	8.645	16.6	ng	1252770	2	8.180	1512940	20.0
1-Penten-3-one,...	16.745	20.0	ng	710361	6	15.598	710361	20.0