LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090721\
Data File : BF125391.D
Acq On : 7 Sep 2021 16:58
Operator : JU/CG
Sample : M3658-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-251607

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: BF125391.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	12	18	26	rVB	640318	839252	44.99%	4.429%
2	5.522	580	584	594	rBV	1970355	1865260	100.00%	9.844%
3	6.528	750	755	768	rBV	1723714	1768958	94.84%	9.335%
4	6.898	814	818	821	rBV	871885	693233	37.17%	3.658%
5	7.457	909	913	924	rBV	1251579	1092750	58.58%	5.767%
6	7.922	989	992	996	rBV	167097	147917	7.93%	0.781%
7	8.180	1032	1036	1043	rBV	892379	758236	40.65%	4.002%
8	9.251	1214	1218	1224	rBV	1908989	1812444	97.17%	9.565%
9	9.327	1228	1231	1235	rBV2	194140	266029	14.26%	1.404%
10	9.569	1269	1272	1277	rBV5	265269	481657	25.82%	2.542%
11	9.639	1282	1284	1288	rBV2	382393	433590	23.25%	2.288%
12	9.698	1292	1294	1298	rVV3	298977	342665	18.37%	1.808%
13	9.804	1309	1312	1314	rBV2	699037	786033	42.14%	4.148%
14	9.845	1317	1319	1322	rVB	994472	877209	47.03%	4.629%
15	9.886	1324	1326	1328	rBV2	320631	311542	16.70%	1.644%
16	9.939	1333	1335	1337	rVB	949427	783836	42.02%	4.137%
17	10.351	1402	1405	1407	rVB	925008	824606	44.21%	4.352%
18	13.021	1857	1859	1868	rVB	1782669	1766123	94.69%	9.321%
19	13.933	2012	2014	2021	rVB	589567	731855	39.24%	3.862%
20	14.074	2035	2038	2041	rVB	875962	793101	42.52%	4.186%
21	15.121	2213	2216	2222	rVV2	108436	189608	10.17%	1.001%
22	15.180	2223	2226	2232	rVB	123931	173290	9.29%	0.915%
23	15.562	2286	2291	2306	rVB	810914	1102994	59.13%	5.821%
24	16.015	2365	2368	2373	rVB	80292	106573	5.71%	0.562%

Sum of corrected areas: 18948761

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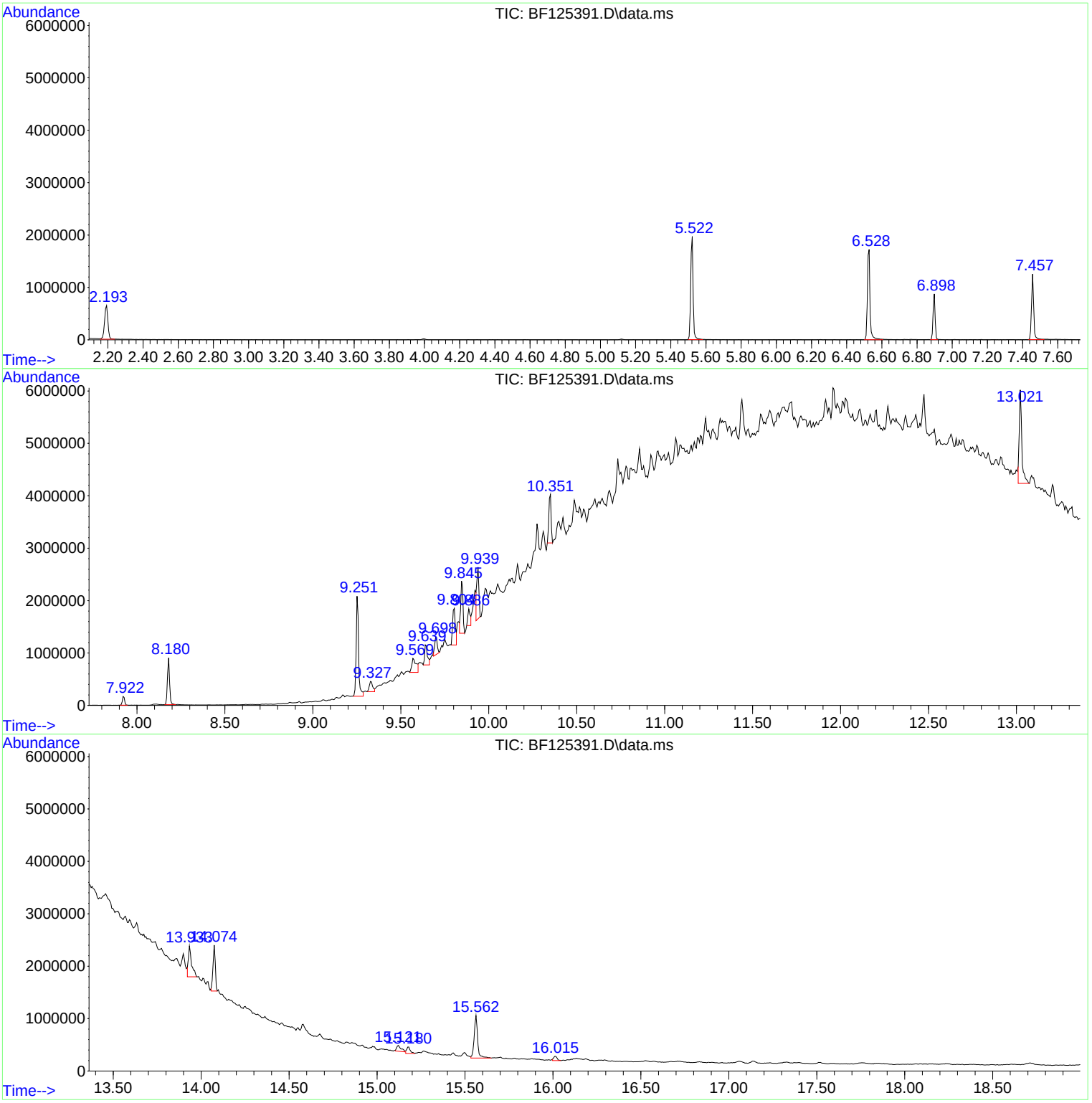
ClientSampleId :
RBR-251607

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



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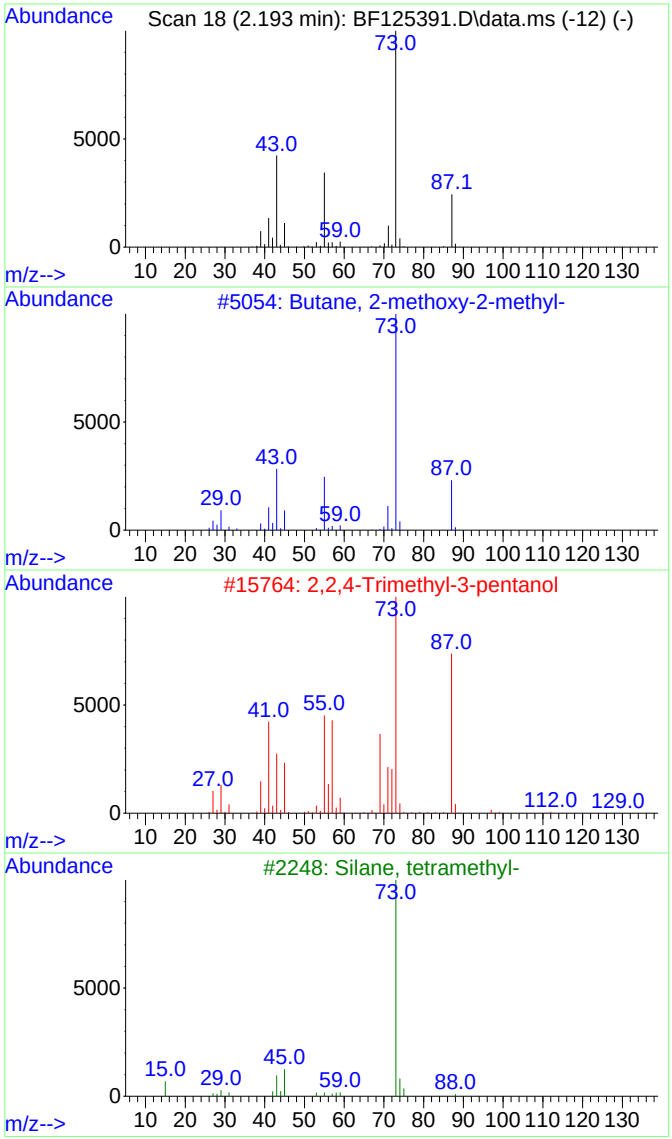
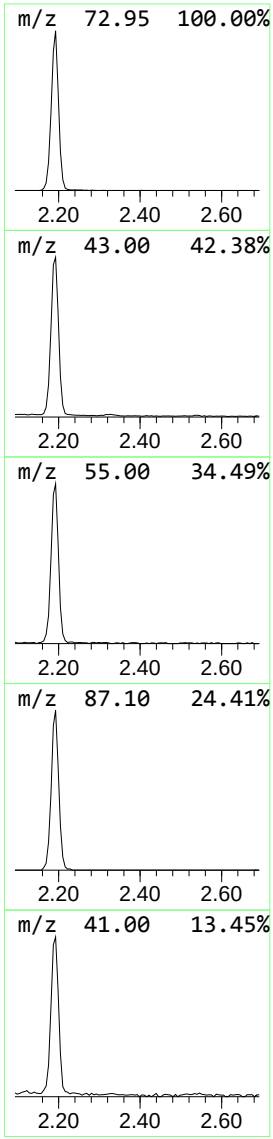
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	24.21 ng	839252	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23





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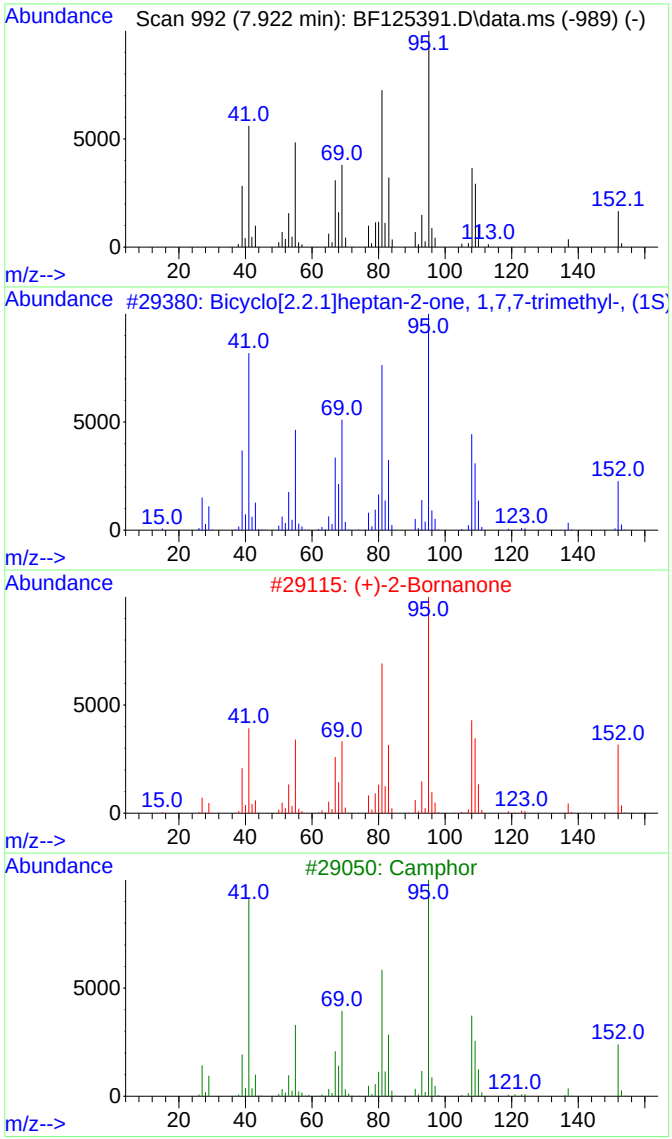
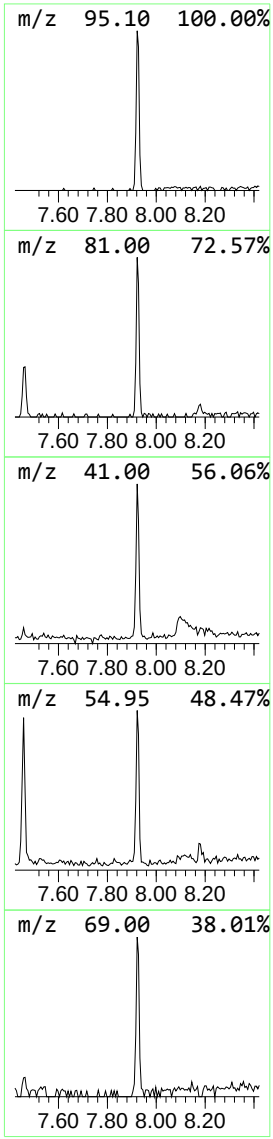
****
Peak Number 2 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.922	3.90 ng	147917	Naphthalene-d8	8.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
2	(+)-2-Bornanone	152	C10H16O	000464-49-3	97
3	Camphor	152	C10H16O	000076-22-2	96
4	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	43
5	Ketone, 1,5-dimethylbicyclo[2.1....	138	C9H14O	024081-57-0	43





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ClientSampleId : RBR-251607

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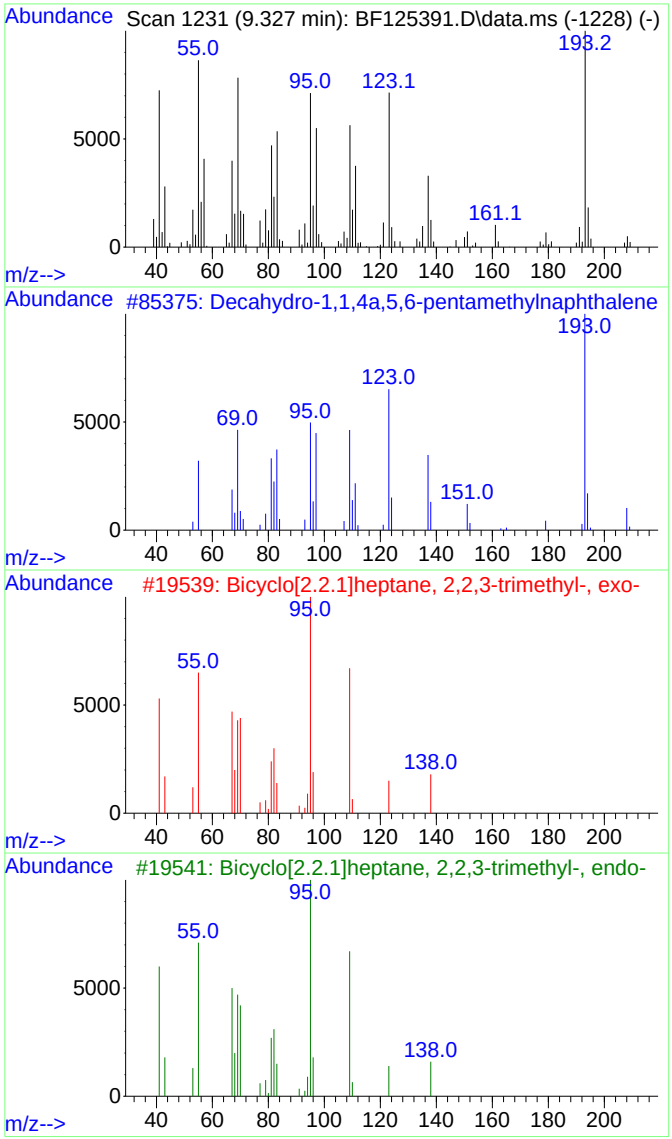
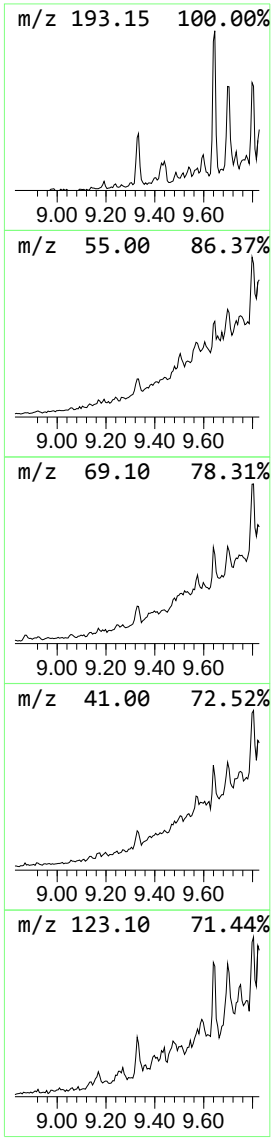
****
Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.327	6.79 ng	266029	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	64
2	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	35
3	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	20
4	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	18
5	Bicyclo[3.1.1]heptan-2-one, 6,6-...	138	C9H14O	038651-65-9	18





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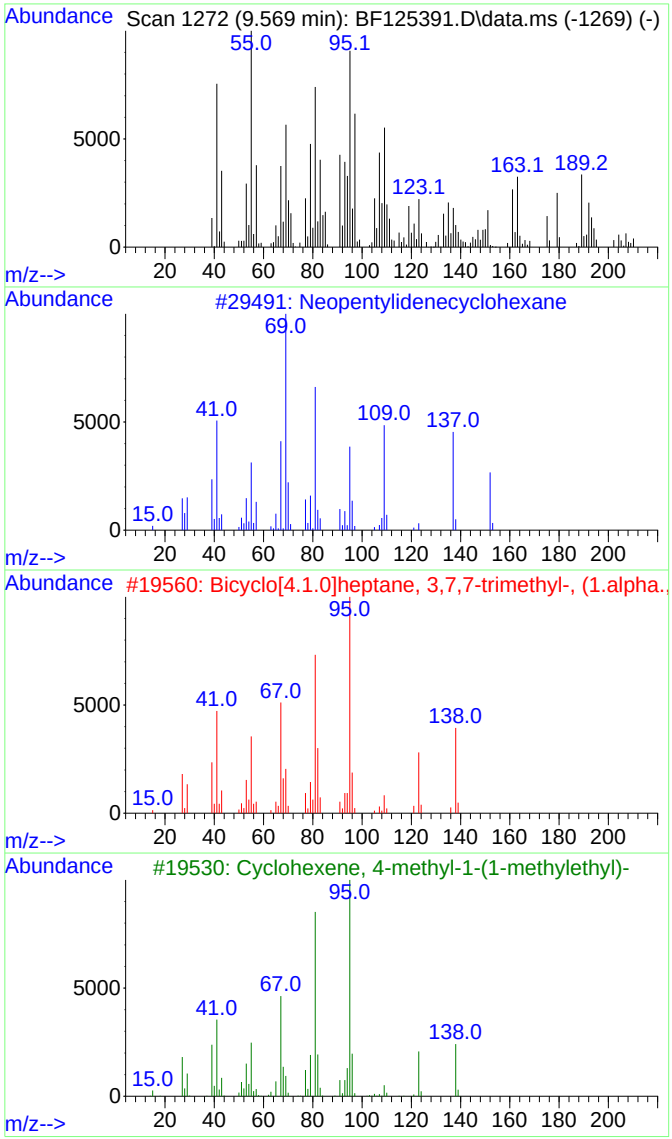
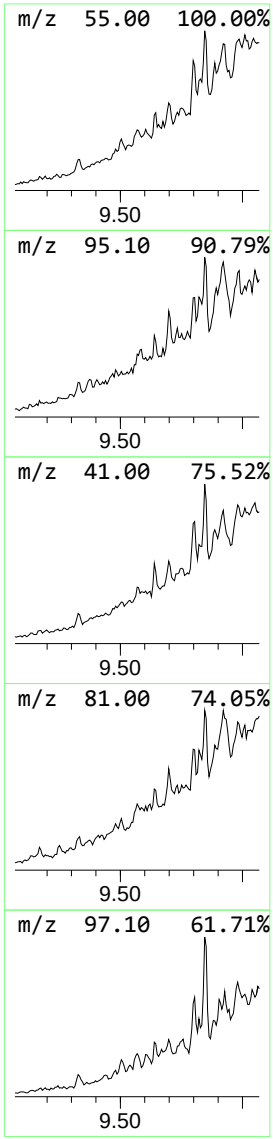
****

Peak Number 4 unknown9.569 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.569	12.29 ng	481657	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neopentylidenecyclohexane	152	C11H20	039546-80-0	27
2	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	27
3	Cyclohexene, 4-methyl-1-(1-methy...	138	C10H18	000500-00-5	27
4	Albene	162	C12H18	038451-64-8	25
5	Cyclohexane, ethylidene-	110	C8H14	001003-64-1	15





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Sample : M3658-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-251607

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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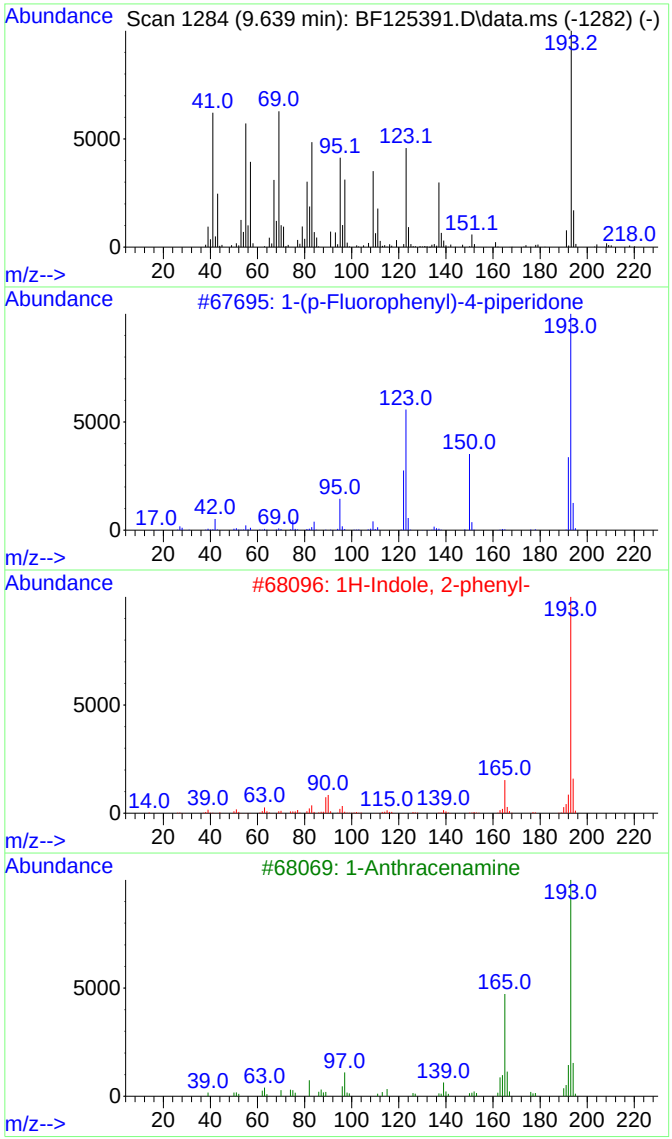
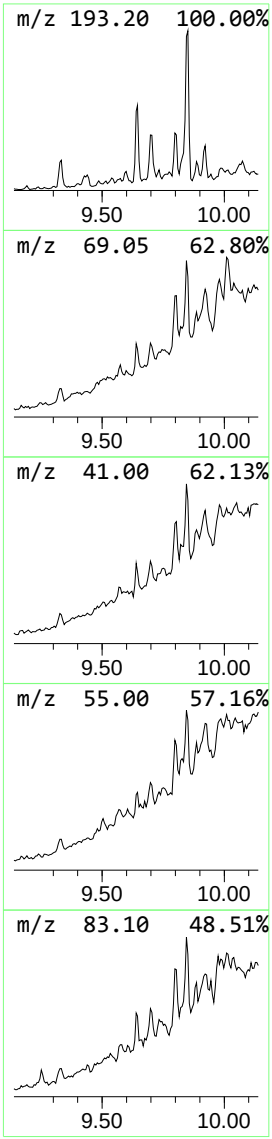
****

Peak Number 5 unknown9.639 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.639	11.06 ng	433590	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	46
2	1H-Indole, 2-phenyl-	193	C14H11N	000948-65-2	25
3	1-Anthracenamine	193	C14H11N	000610-49-1	22
4	Acetylene, 1-(2-aminophenyl)-2-p...	193	C14H11N	1000380-73-4	22
5	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	22





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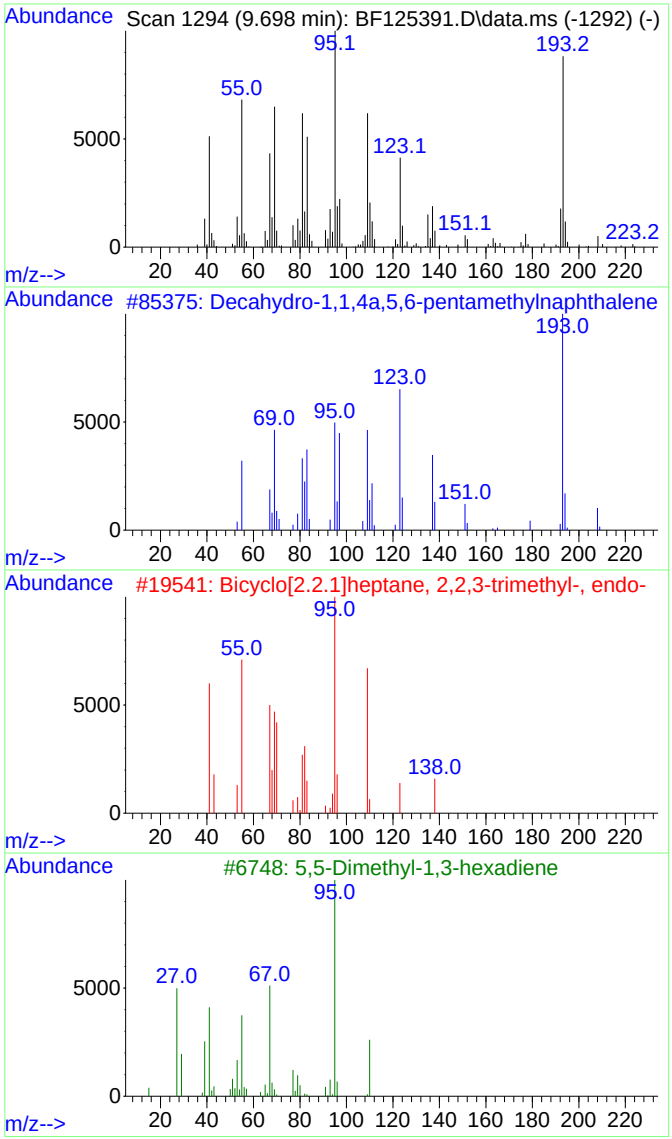
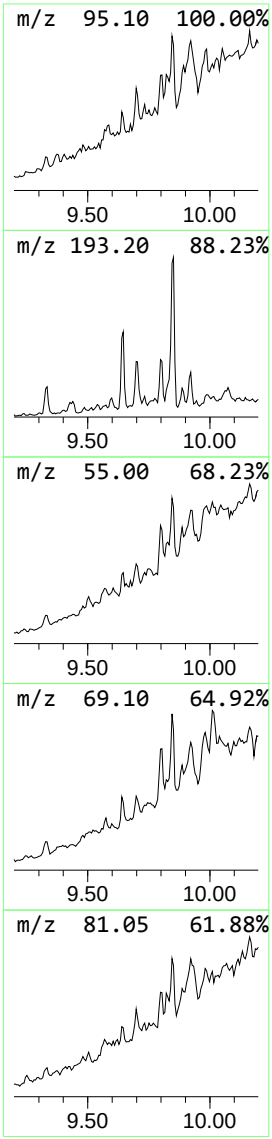
Peak Number 6 unknown9.698 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.698	8.74 ng	342665	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	46
2	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	41
3	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	30
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	25
5	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	25





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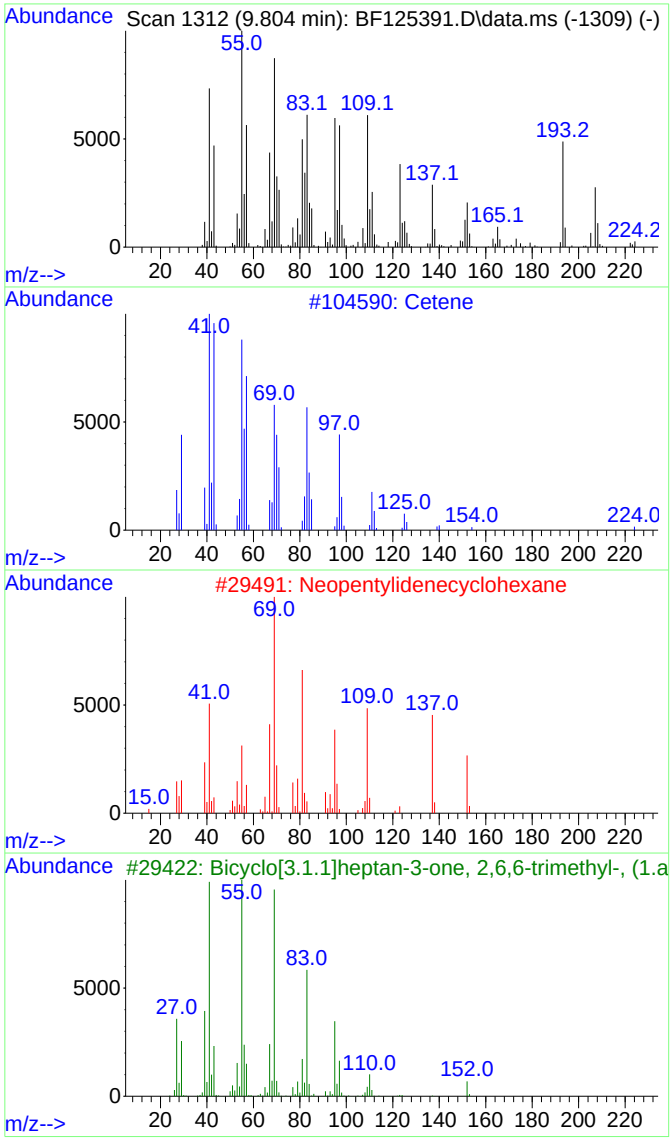
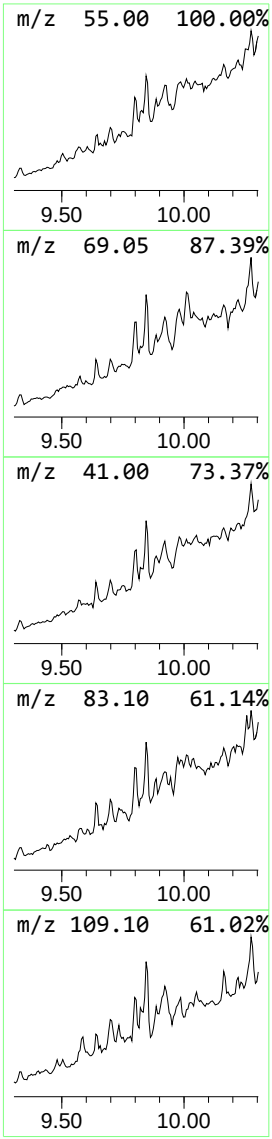
Peak Number 7 unknown9.804 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.804	20.06 ng	786033	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	38
2	Neopentylidenecyclohexane	152	C11H20	039546-80-0	30
3	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	27
4	Naphthalene, decahydro-1,4a-dime...	208	C15H28	030824-81-8	25
5	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	22





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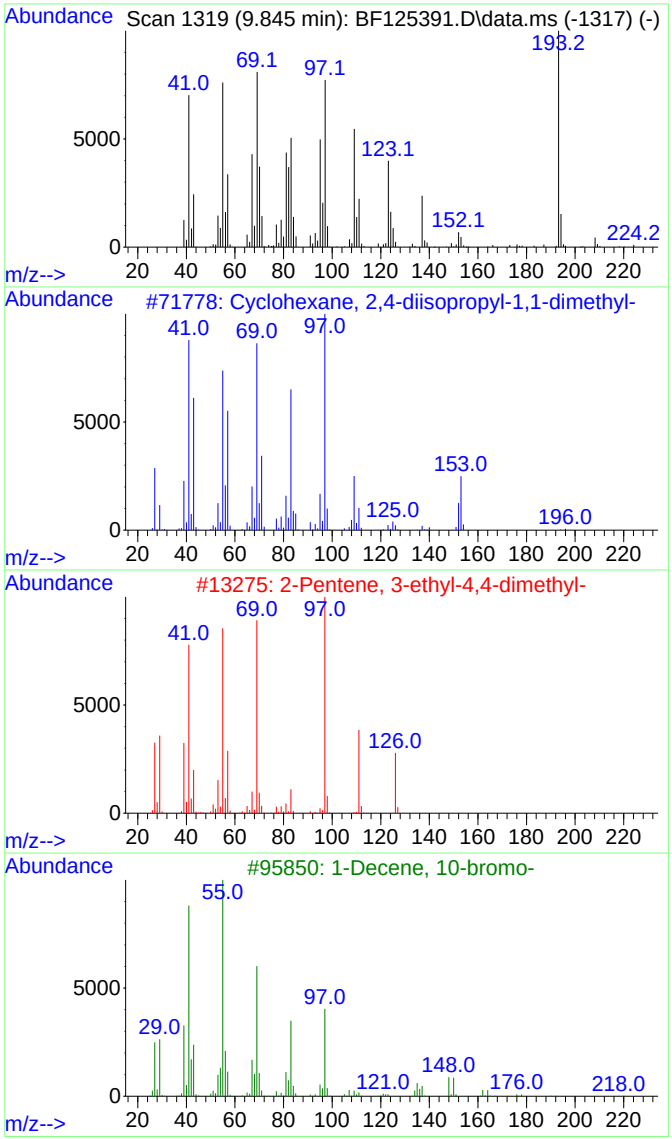
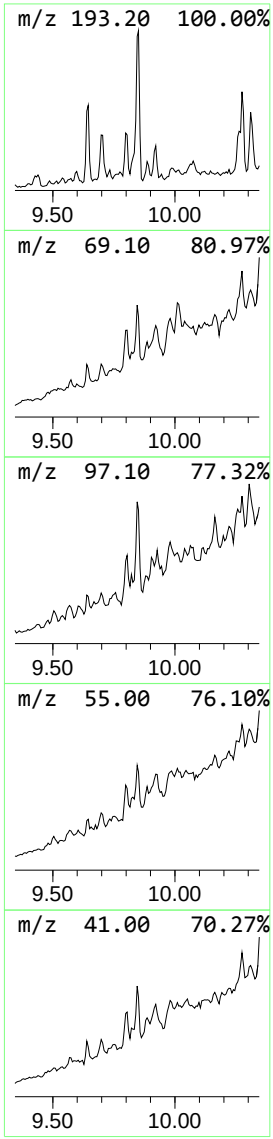
Peak Number 8 unknown9.845 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.845	22.38 ng	877209	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 2,4-diisopropyl-1,1...	196	C14H28	1000149-60-5	35
2	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	30
3	1-Decene, 10-bromo-	218	C10H19Br	062871-09-4	27
4	Cyclohexane, 1,2,4,5-tetraethyl-...	196	C14H28	061142-24-3	25
5	2H-Spiro[1-benzofuran-3,2'-[1,3]...	193	C10H11NO3	1000387-33-4	25





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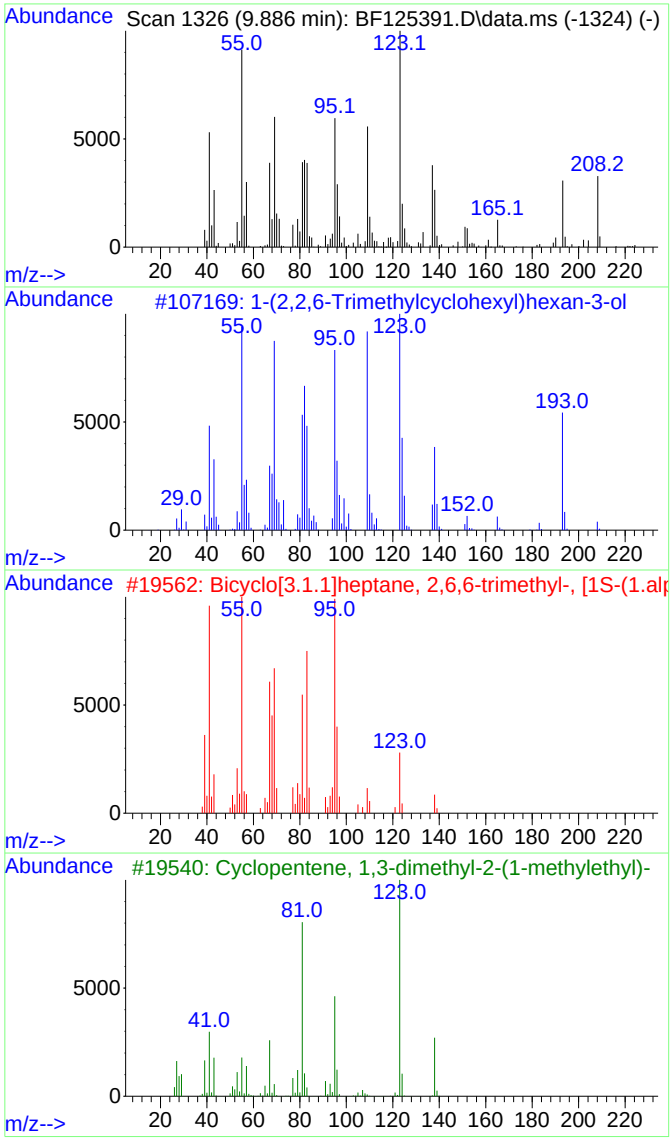
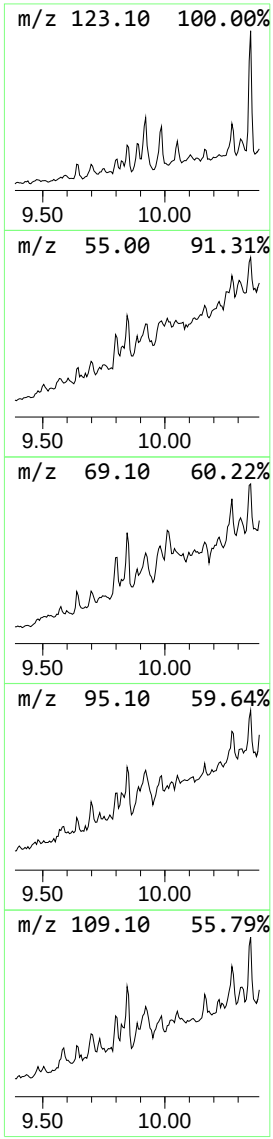
****
Peak Number 9 1-(2,2,6-Trimethylcyclohexy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.886	7.95 ng	311542	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2,2,6-Trimethylcyclohexyl)hex...	226	C15H30O	070788-30-6	50
2	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004755-33-3	46
3	Cyclopentene, 1,3-dimethyl-2-(1-...	138	C10H18	061142-32-3	43
4	Cyclooctene, 1,2-dimethyl-	138	C10H18	054299-96-6	25
5	Cyclopentene, 1-isopropyl-2,3-di...	138	C10H18	007712-73-4	25





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Instrument : BNA_F
ClientSampleId : RBR-251607

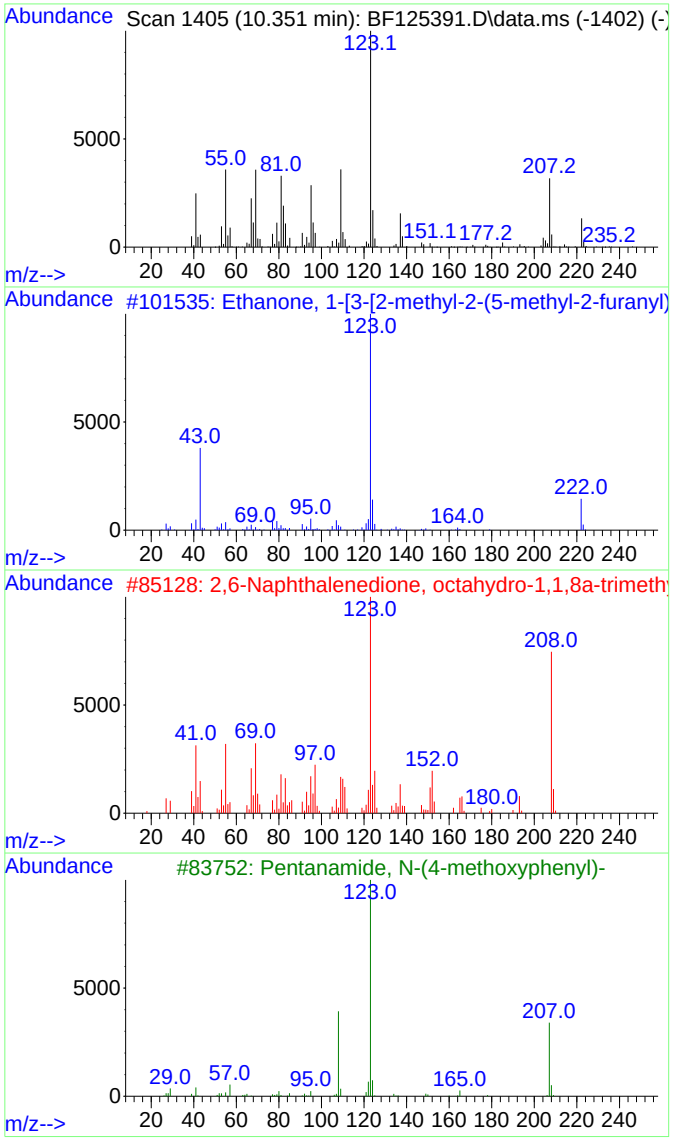
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

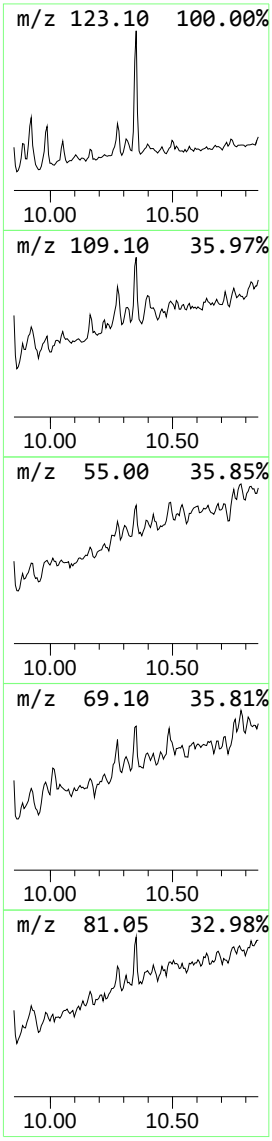
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Ethanone, 1-[3-[2-methyl-2-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.351	21.04 ng	824606	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	50
2	2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-17-5	50
3	Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	43
4	(Phenylthio)acetic acid, cyclobu...	222	C12H14O2S	1010299-95-5	43
5	1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090721\
Data File : BF125391.D
Acq On : 7 Sep 2021 16:58
Operator : JU/CG
Sample : M3658-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-251607

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

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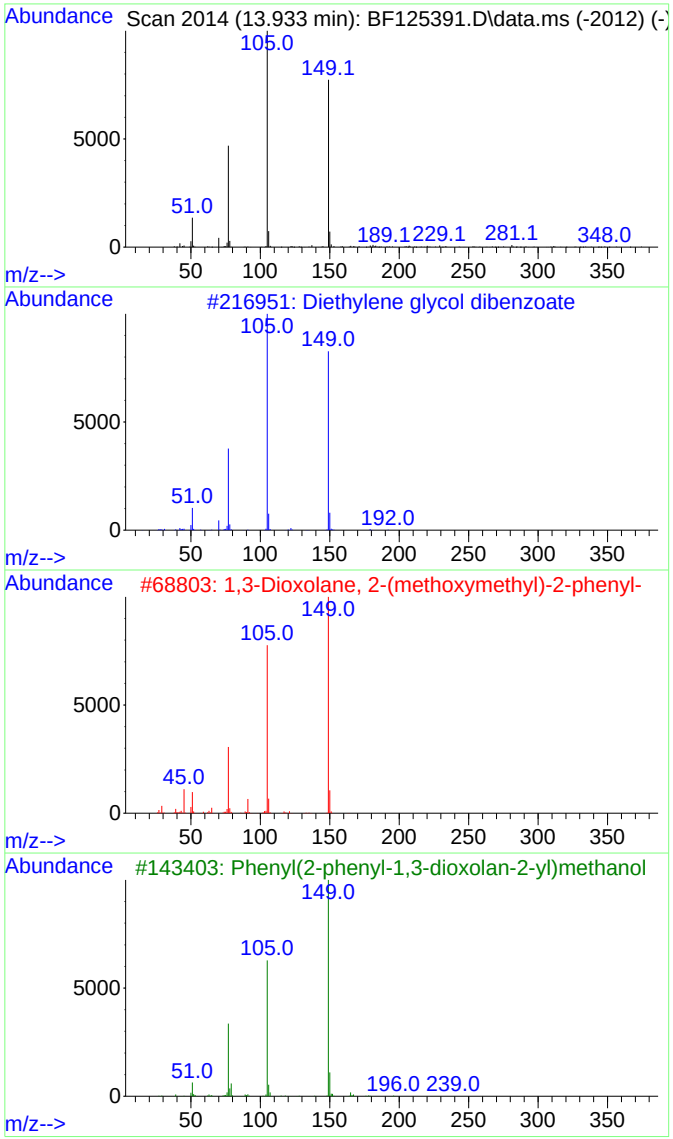
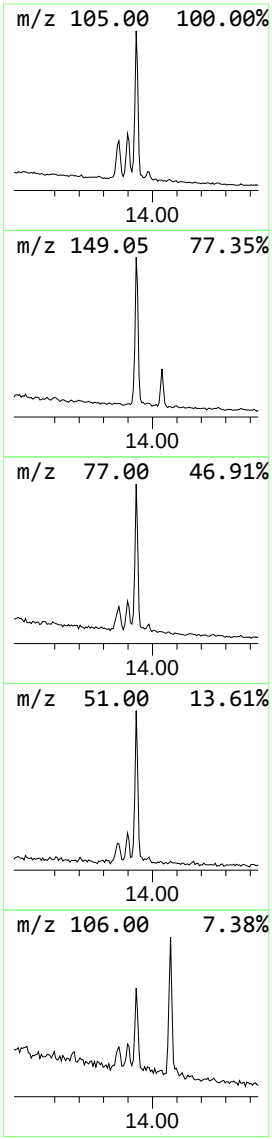
Peak Number 11 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	18.46 ng	731855	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
3	Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	72
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
5	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090721\
Data File : BF125391.D
Acq On : 7 Sep 2021 16:58
Operator : JU/CG
Sample : M3658-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-251607

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

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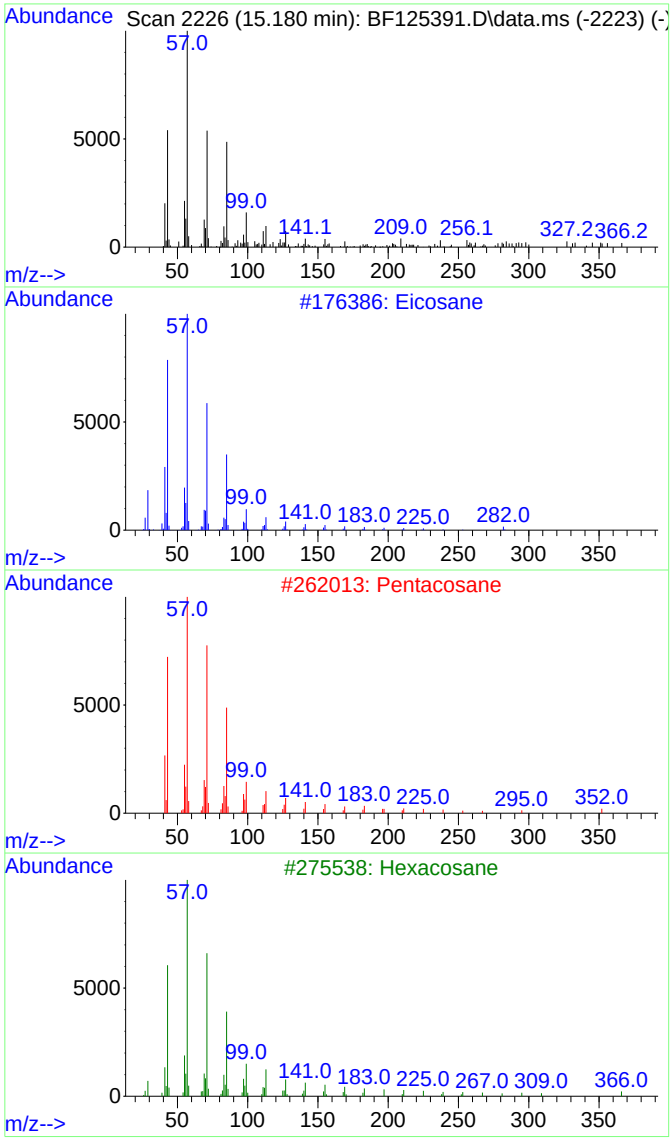
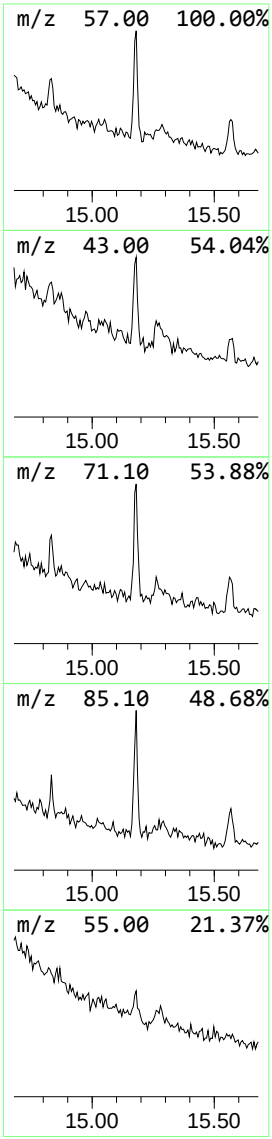
Peak Number 12 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.180	3.14 ng	173290	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Pentacosane	352	C25H52	000629-99-2	92
3	Hexacosane	366	C26H54	000630-01-3	86
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090721\
Data File : BF125391.D
Acq On : 7 Sep 2021 16:58
Operator : JU/CG
Sample : M3658-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-251607

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
Butane, 2-metho...	2.193	24.2	ng	839252	1	6.898	693233	20.0
Bicyclo[2.2.1]h...	7.922	3.9	ng	147917	2	8.180	758236	20.0
Decahydro-1,1,4...	9.327	6.8	ng	266029	3	9.939	783836	20.0
unknown9.569	9.569	12.3	ng	481657	3	9.939	783836	20.0
unknown9.639	9.639	11.1	ng	433590	3	9.939	783836	20.0
unknown9.698	9.698	8.7	ng	342665	3	9.939	783836	20.0
unknown9.804	9.804	20.1	ng	786033	3	9.939	783836	20.0
unknown9.845	9.845	22.4	ng	877209	3	9.939	783836	20.0
1-(2,2,6-Trimet...	9.886	8.0	ng	311542	3	9.939	783836	20.0
Ethanone, 1-[3-...	10.351	21.0	ng	824606	3	9.939	783836	20.0
Diethylene glyc...	13.933	18.5	ng	731855	5	14.074	793101	20.0
Eicosane	15.180	3.1	ng	173290	6	15.562	1102990	20.0