LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090721\
Data File : BF125392.D
Acq On : 7 Sep 2021 17:32
Operator : JU/CG
Sample : M3658-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-400027

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: BF125392.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	11	16	23	rVB	1000746	1317486	56.71%	5.842%
2	5.522	579	584	598	rBV	2446800	2323381	100.00%	10.303%
3	6.528	750	755	769	rBV	2297051	2192323	94.36%	9.721%
4	6.898	814	818	821	rBV	877298	715486	30.80%	3.173%
5	7.457	909	913	924	rBV	1535154	1325233	57.04%	5.876%
6	8.092	1016	1021	1032	rBV	83051	219109	9.43%	0.972%
7	8.181	1032	1036	1043	rVB	921765	805793	34.68%	3.573%
8	9.251	1214	1218	1223	rBV	2195777	2132534	91.79%	9.456%
9	9.328	1228	1231	1235	rBV2	297590	411688	17.72%	1.826%
10	9.575	1270	1273	1276	rBV4	262650	398488	17.15%	1.767%
11	9.645	1282	1285	1289	rBV2	743438	1002879	43.16%	4.447%
12	9.698	1292	1294	1298	rVB3	463962	485337	20.89%	2.152%
13	9.751	1301	1303	1306	rVB2	376034	299142	12.88%	1.326%
14	9.804	1309	1312	1314	rBV2	1203975	1305473	56.19%	5.789%
15	9.851	1317	1320	1322	rVB	1700162	1510413	65.01%	6.698%
16	9.886	1324	1326	1328	rBV3	555532	578954	24.92%	2.567%
17	10.357	1403	1406	1409	rVB	1414006	1301616	56.02%	5.772%
18	13.033	1859	1861	1864	rVB	1749838	1315463	56.62%	5.833%
19	14.080	2036	2039	2042	rVB2	848813	830293	35.74%	3.682%
20	15.121	2213	2216	2220	rBV	250050	371034	15.97%	1.645%
21	15.180	2223	2226	2233	rVB	153065	197369	8.49%	0.875%
22	15.433	2266	2269	2276	rVB	145060	192591	8.29%	0.854%
23	15.498	2277	2280	2286	rVB	181903	233031	10.03%	1.033%
24	15.562	2287	2291	2296	rBV2	735669	918748	39.54%	4.074%
25	16.015	2365	2368	2374	rVB	128689	167665	7.22%	0.743%

Sum of corrected areas: 22551529

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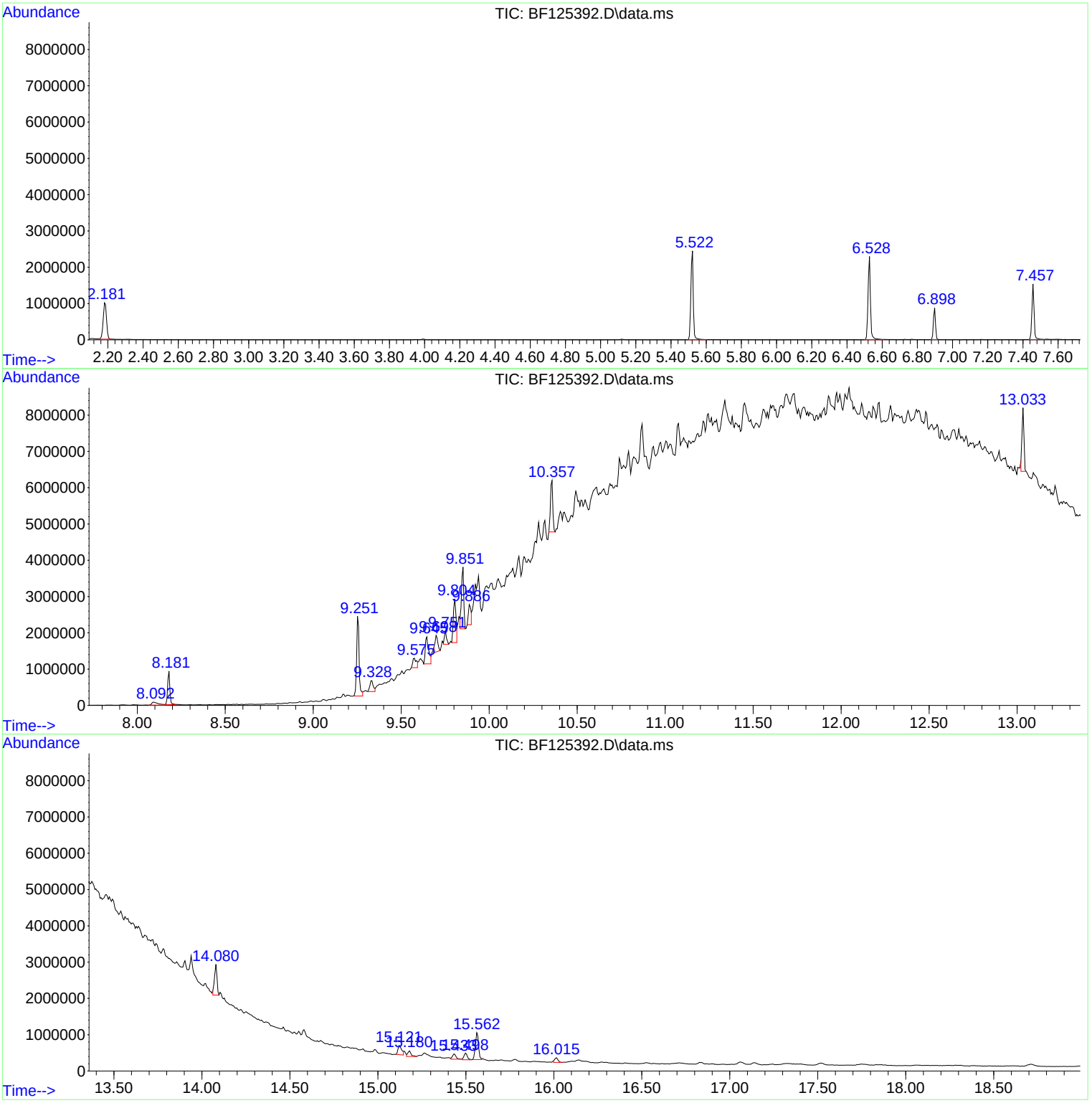
ClientSampleId :
RBR-400027

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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Data File : BF125392.D
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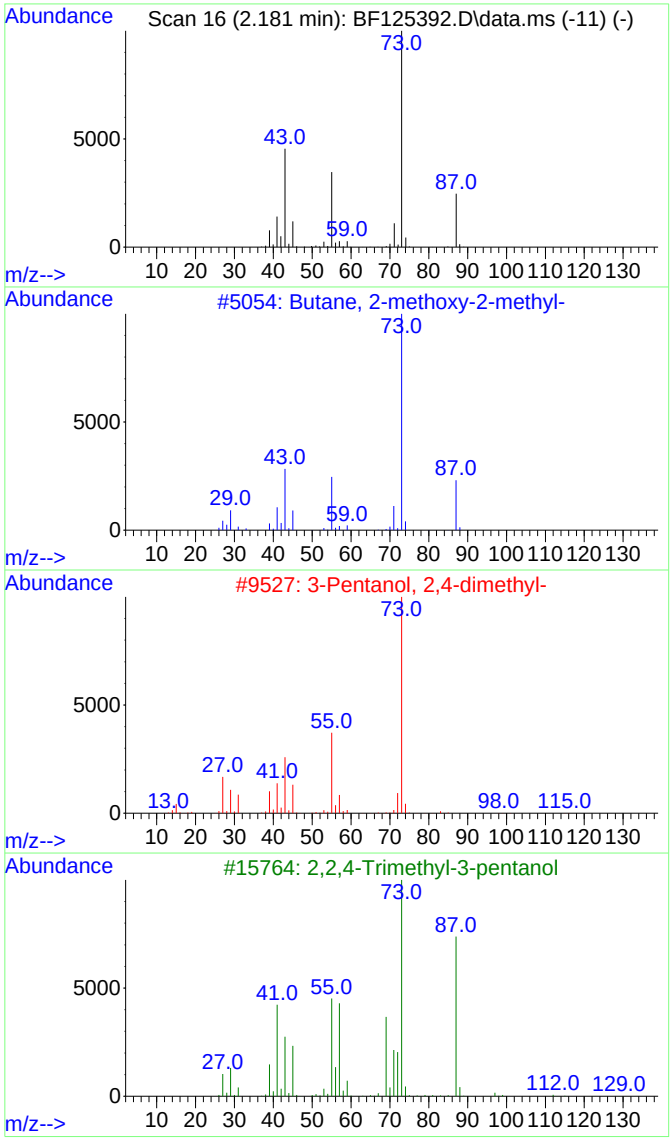
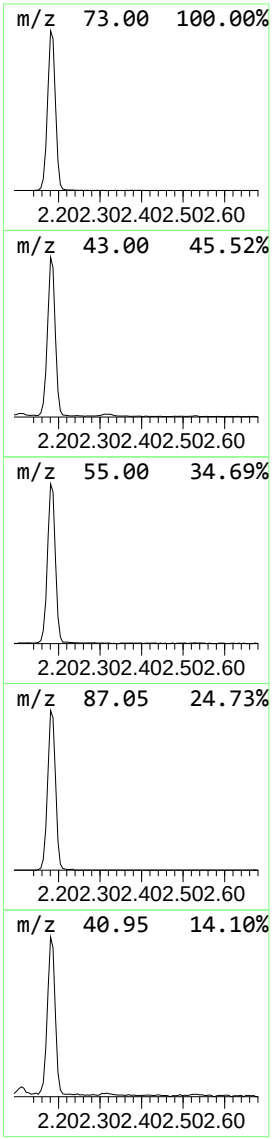
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	36.83 ng	1317490	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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23





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Operator : JU/CG
Sample : M3658-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-400027

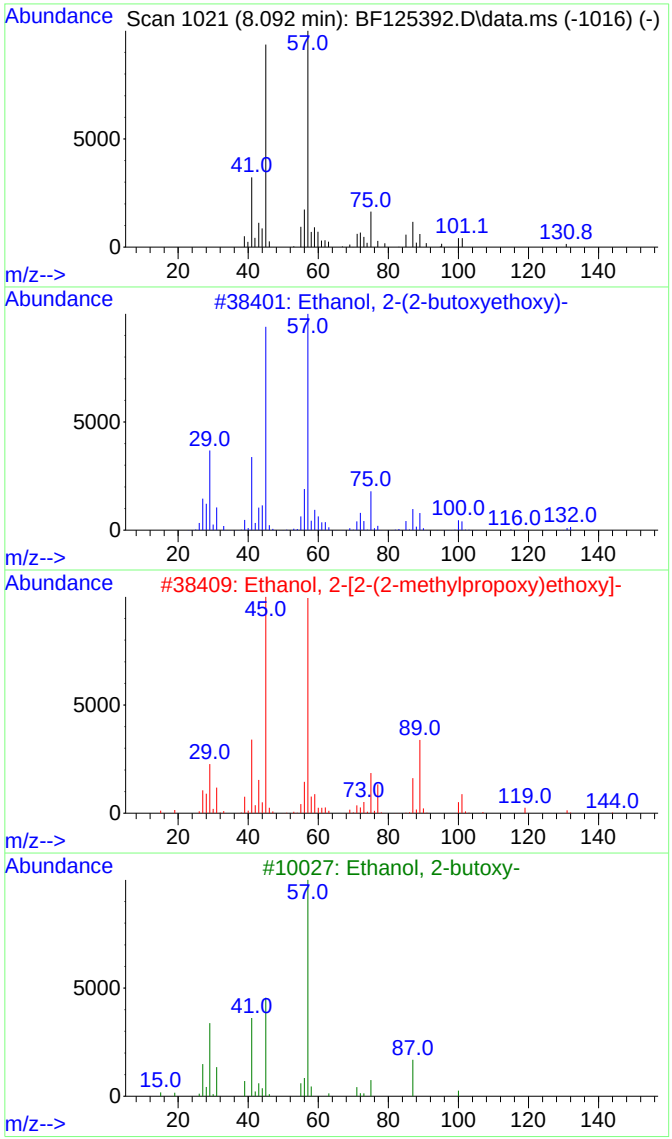
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

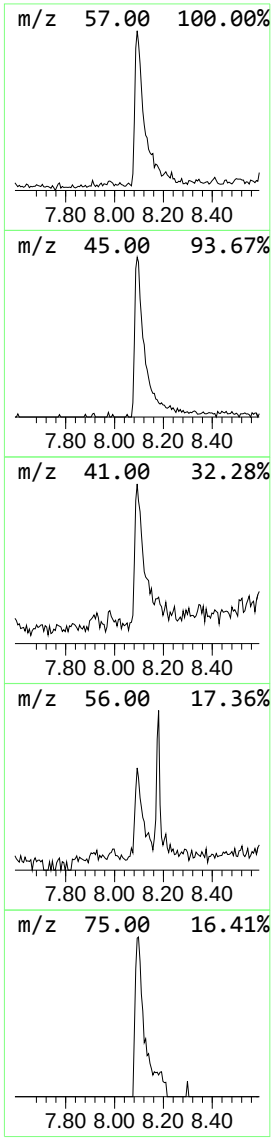
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	5.44 ng	219109	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	47
4	3,6,9,12-Tetraoxatetradeca-1,13-...	202	C10H18O4	000765-12-8	45
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45





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Operator : JU/CG
Sample : M3658-05
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ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-400027

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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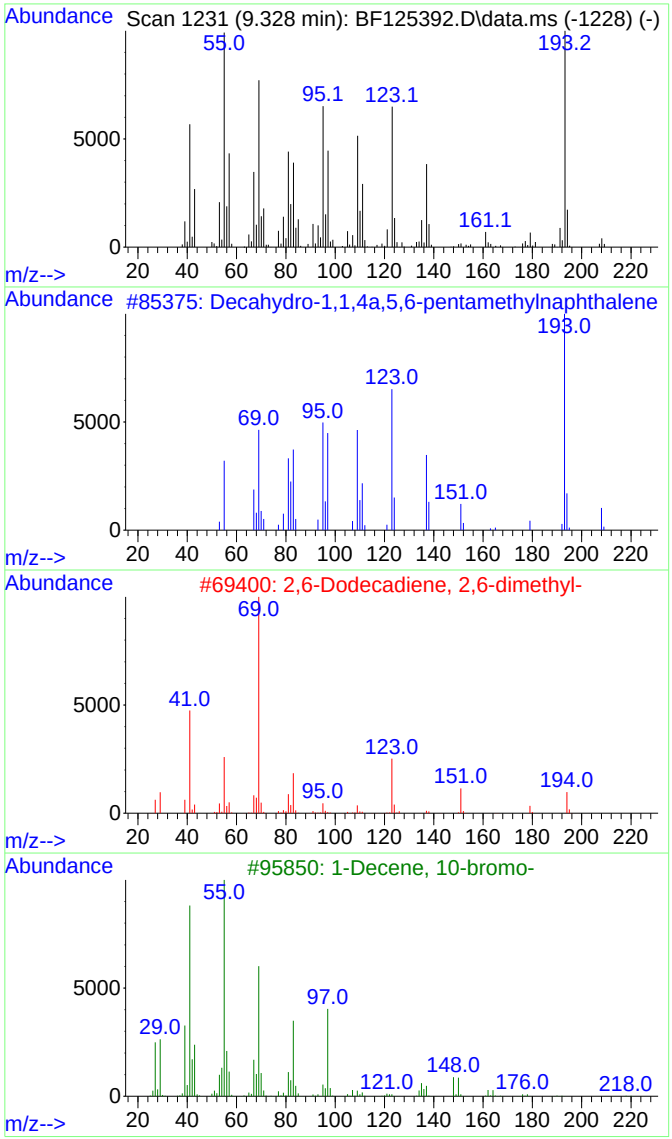
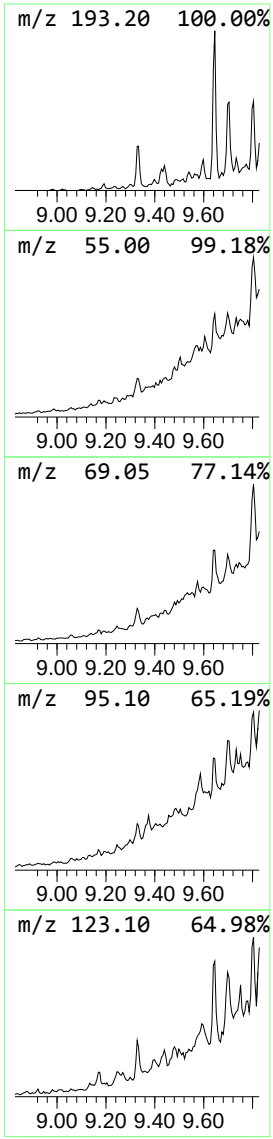
****
Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.328	14.22 ng	411688	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	81
2	2,6-Dodecadiene, 2,6-dimethyl-	194	C14H26	1000164-67-6	27
3	1-Decene, 10-bromo-	218	C10H19Br	062871-09-4	27
4	Cyclohexane, 1-(cyclohexylmethyl...	208	C15H28	054934-94-0	25
5	1-(2-Furyl)-4,4,4-trifluoro-1,3-...	206	C8H5F3O3	000326-90-9	22





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Operator : JU/CG
Sample : M3658-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-400027

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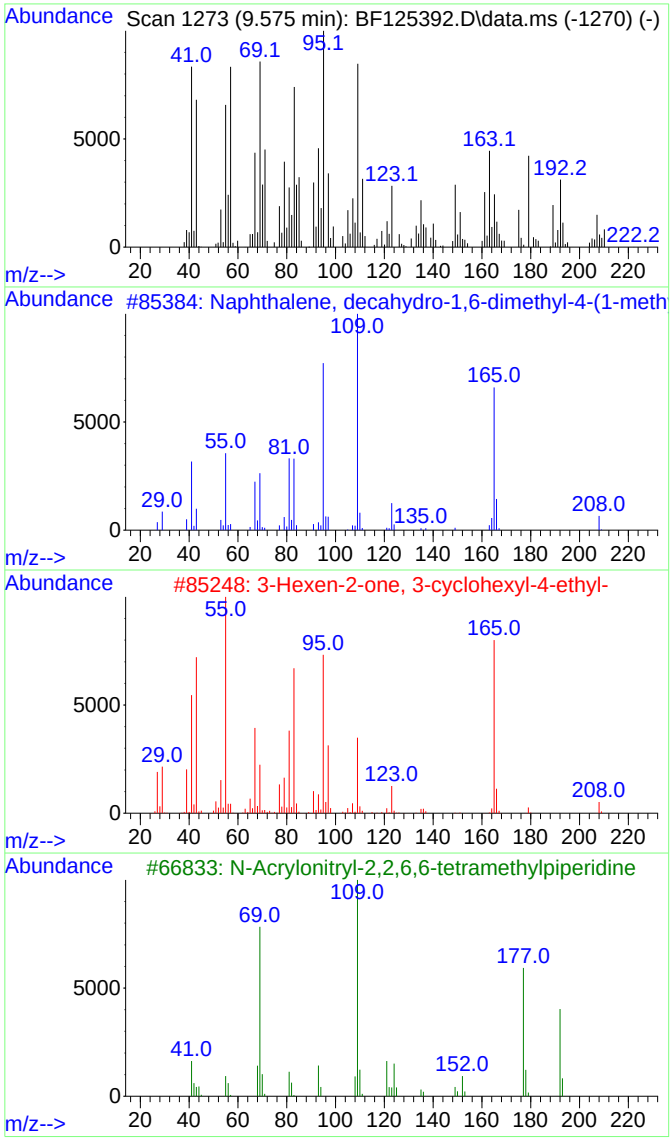
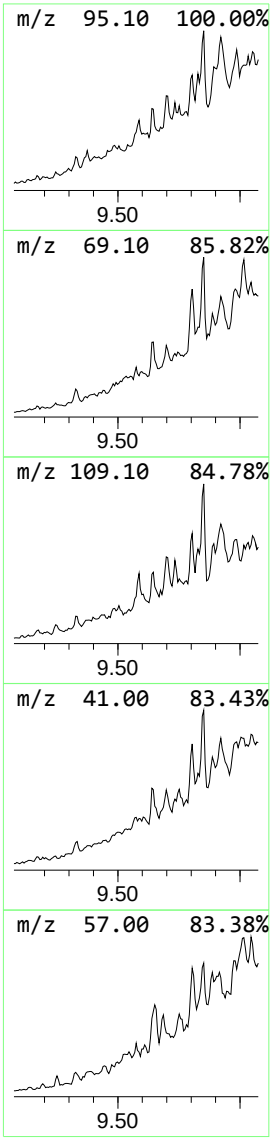
****

Peak Number 4 unknown9.575 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.575	13.77 ng	398488	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-1,6-dimet...	208	C15H28	029788-41-8	35
2	3-Hexen-2-one, 3-cyclohexyl-4-et...	208	C14H24O	1000150-19-1	25
3	N-Acrylonitryl-2,2,6,6-tetrameth...	192	C12H20N2	077376-88-6	25
4	Bicyclo[2.2.1]heptane-2,3-dione,...	166	C10H14O2	010334-26-6	22
5	3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	18





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Operator : JU/CG
Sample : M3658-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-400027

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
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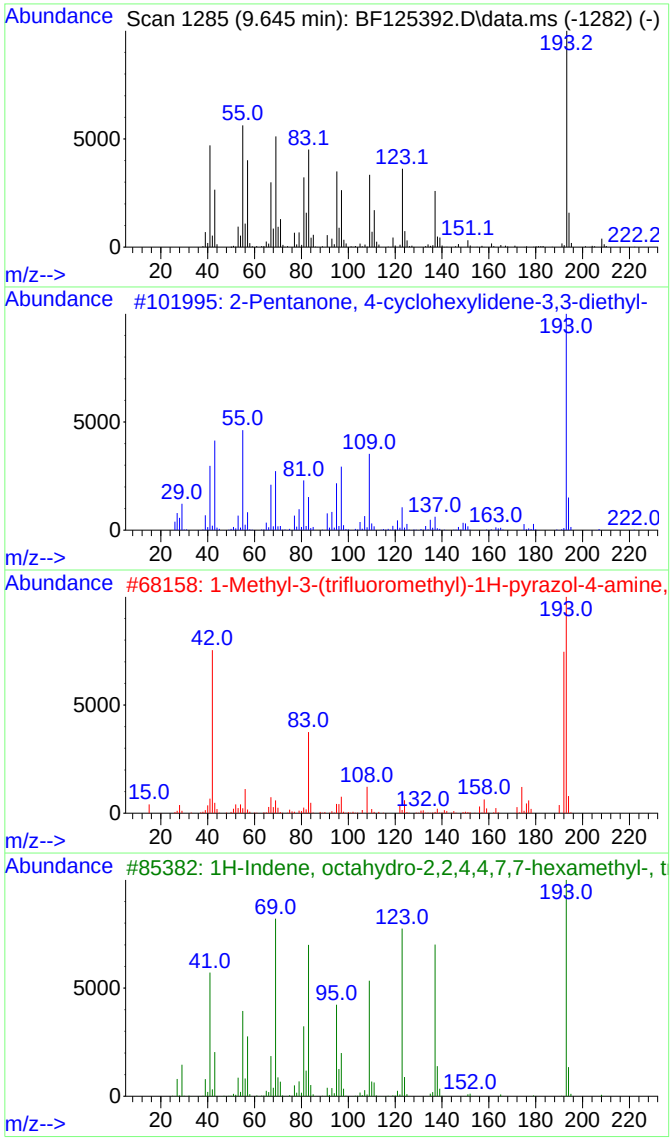
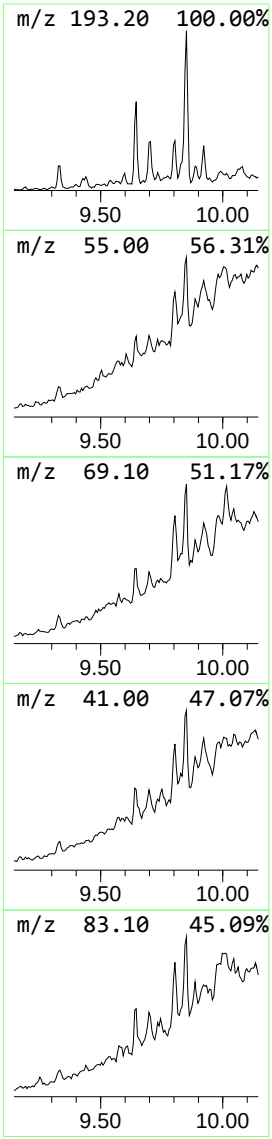
****
Peak Number 5 2-Pentanone, 4-cyclohexylid... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.645	34.64 ng	1002880	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	50
2	1-Methyl-3-(trifluoromethyl)-1H-...	193	C7H10F3N3	1000511-73-1	43
3	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	43
4	Iminostilbene	193	C14H11N	000256-96-2	35
5	9-Phenanthrenamine	193	C14H11N	000947-73-9	35





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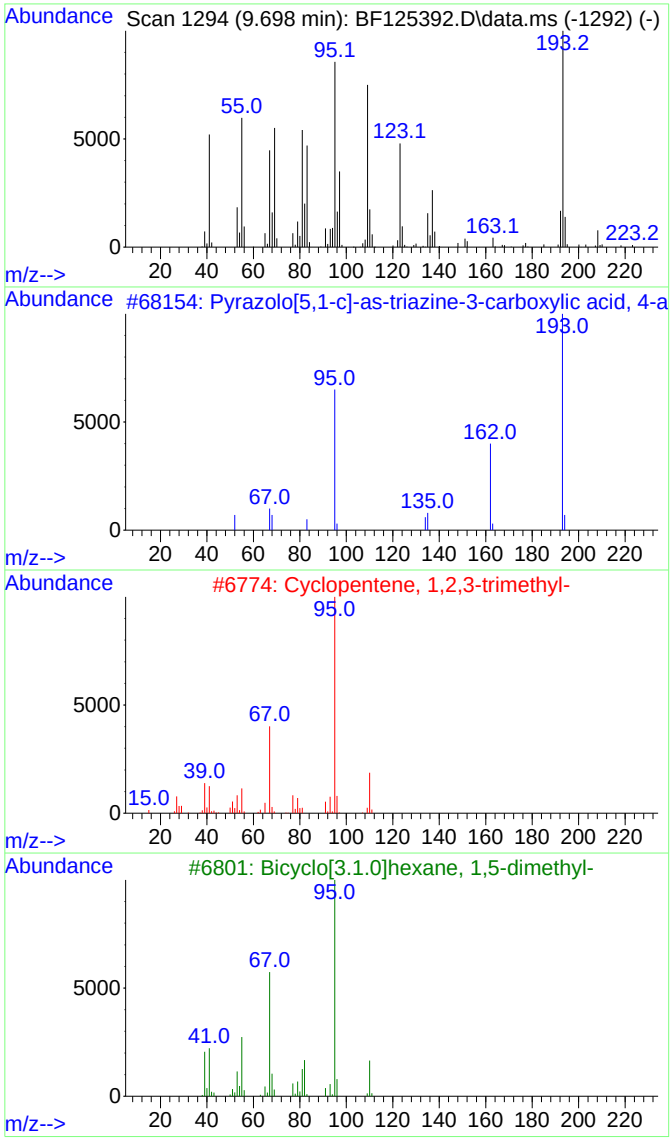
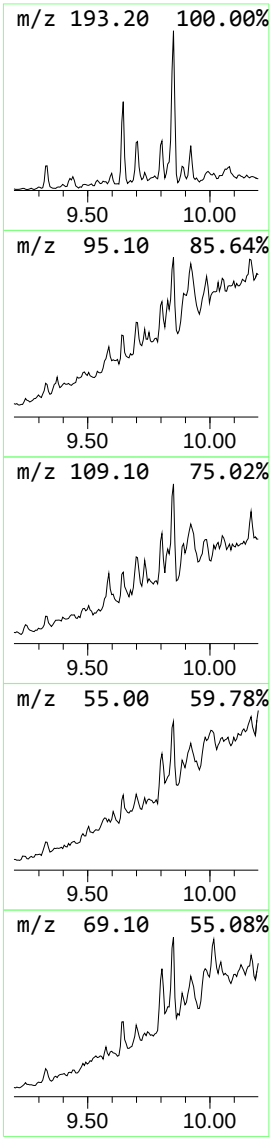
****

Peak Number 6 unknown9.698 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.698	16.77 ng	485337	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrazolo[5,1-c]-as-triazine-3-ca...	193	C6H7N7O	016111-78-7	35
2	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	18
3	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	18
4	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	18
5	Cyclopentane, 2-ethylidene-1,1-d...	124	C9H16	056324-66-4	14





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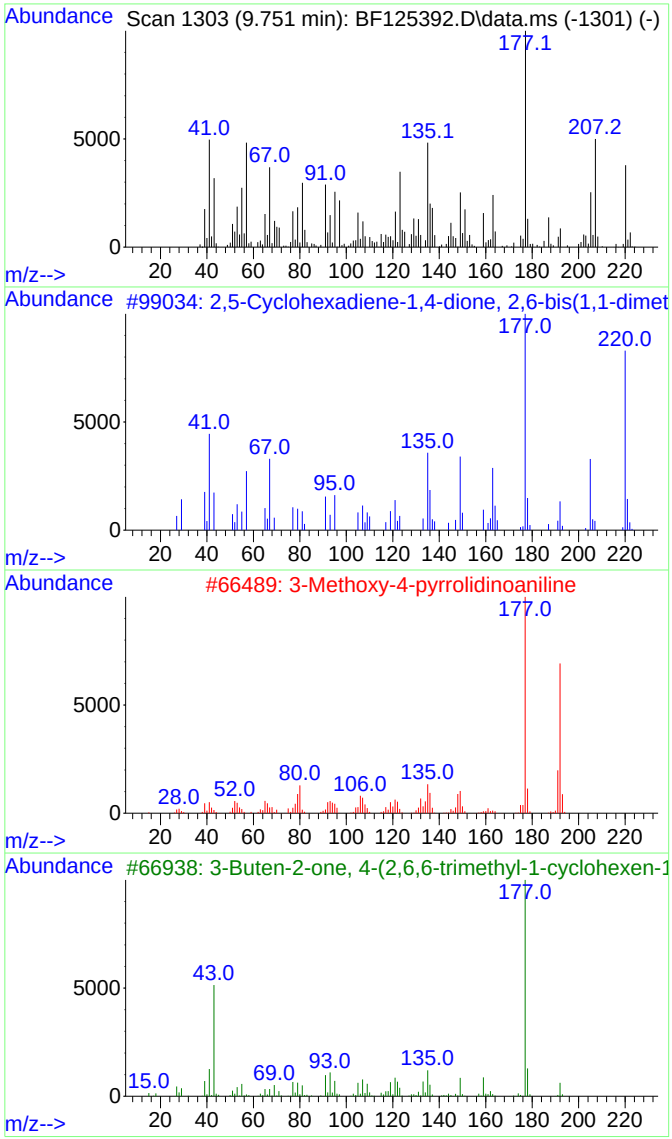
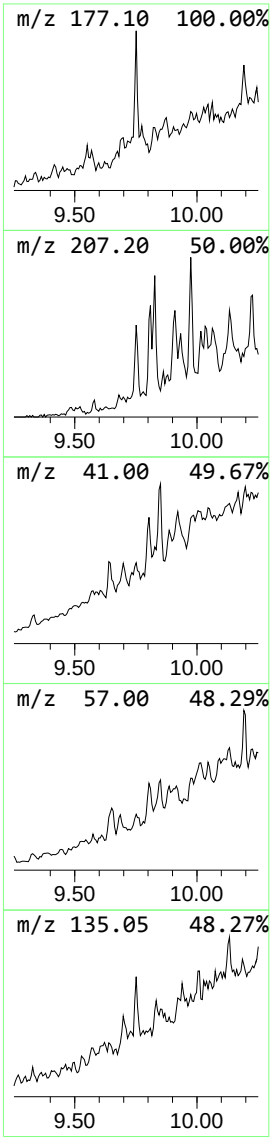
****
Peak Number 7 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.751	10.33 ng	299142	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	83
2	3-Methoxy-4-pyrrolidinoaniline	192	C11H16N2O	016089-42-2	38
3	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	25
4	N-Cyclohexyl-2-nitroaniline	220	C12H16N2O2	006373-71-3	22
5	1,4-Benzenediamine, N,N'-bis(1-m...	192	C12H20N2	004251-01-8	22





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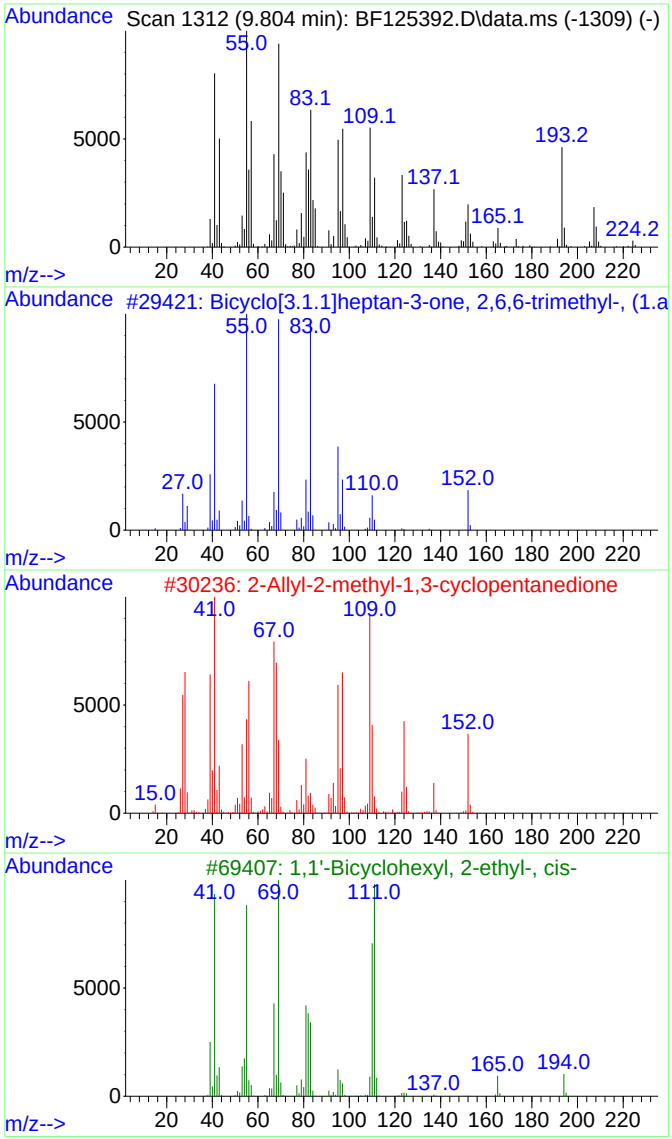
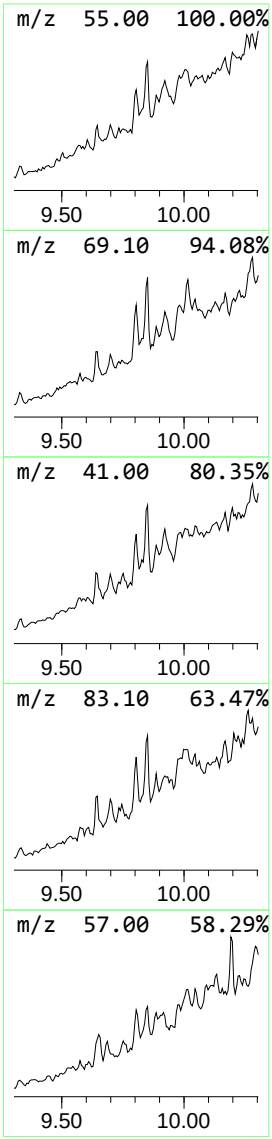
Peak Number 8 unknown9.804 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.804	45.10 ng	1305470	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	43
2	2-Allyl-2-methyl-1,3-cyclopentan...	152	C9H12O2	026828-48-8	41
3	1,1'-Bicyclohexyl, 2-ethyl-, cis-	194	C14H26	050991-12-3	38
4	Cyclohexane, 1-(cyclohexylmethyl...	208	C15H28	054934-92-8	38
5	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-12-7	30





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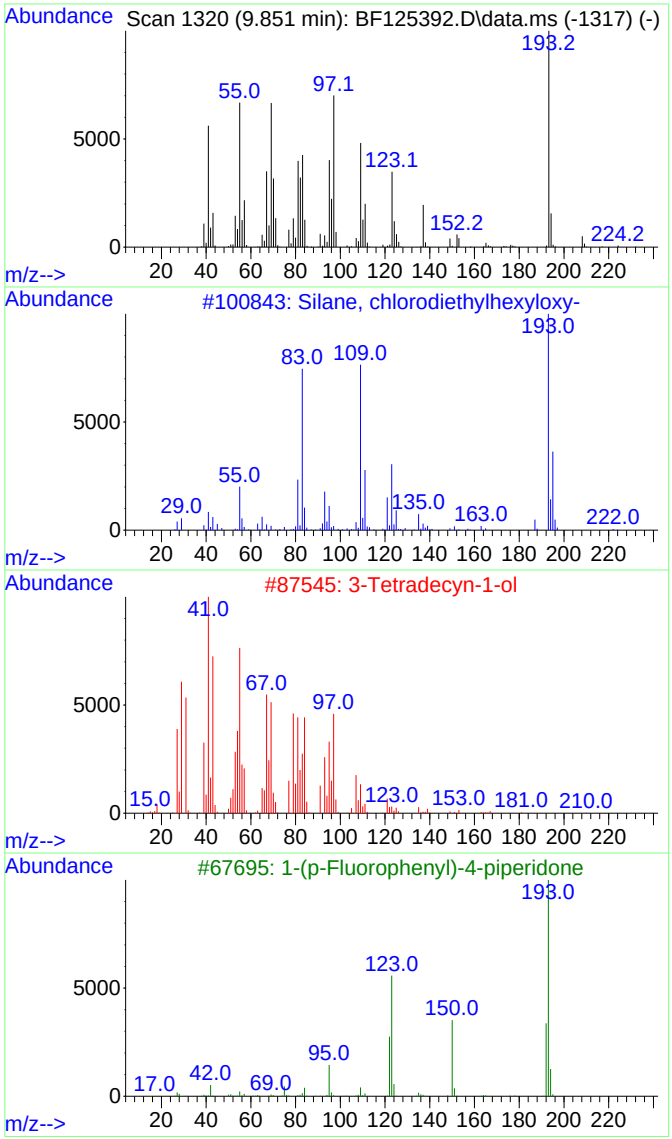
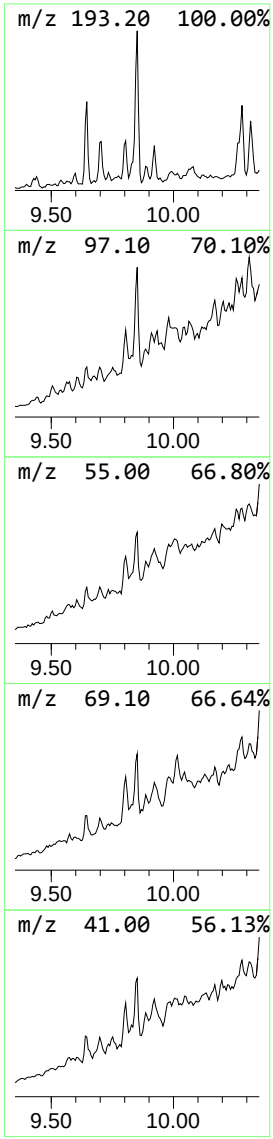
Peak Number 9 unknown9.851 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.851	52.18 ng	1510410	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	38
2	3-Tetradecyn-1-ol	210	C14H26O	055182-74-6	35
3	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27
4	Succinic acid, tridec-2-yn-1-yl ...	420	C26H44O4	1010391-10-5	25
5	Hexadecanedinitrile	248	C16H28N2	006812-44-8	22





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Data File : BF125392.D
Acq On : 7 Sep 2021 17:32
Operator : JU/CG
Sample : M3658-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-400027

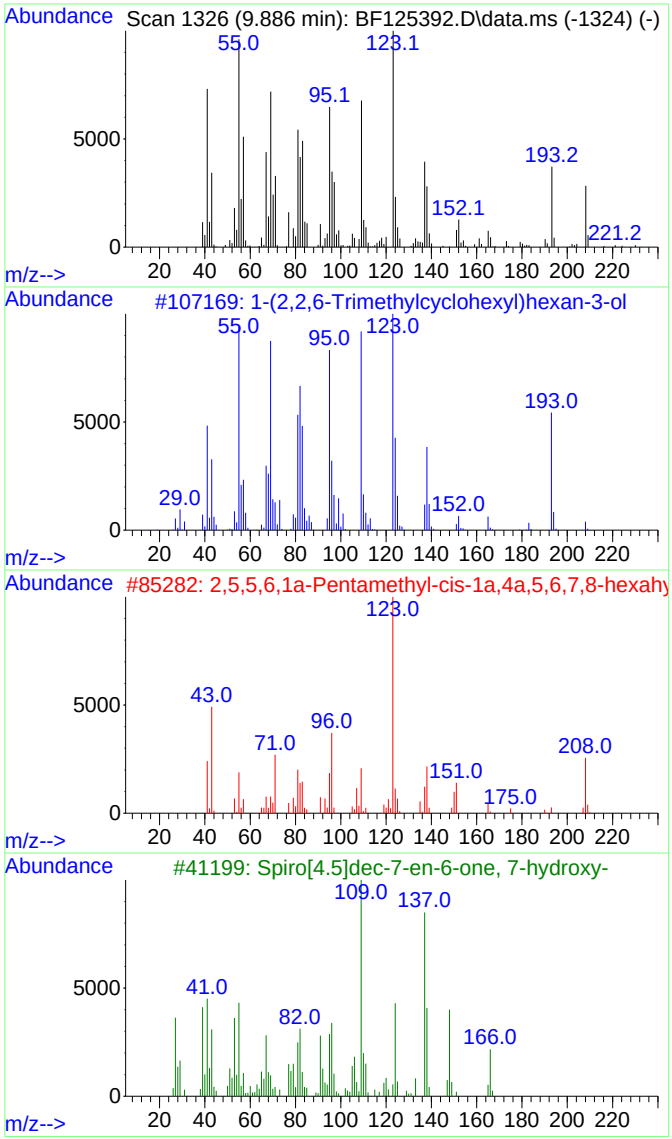
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

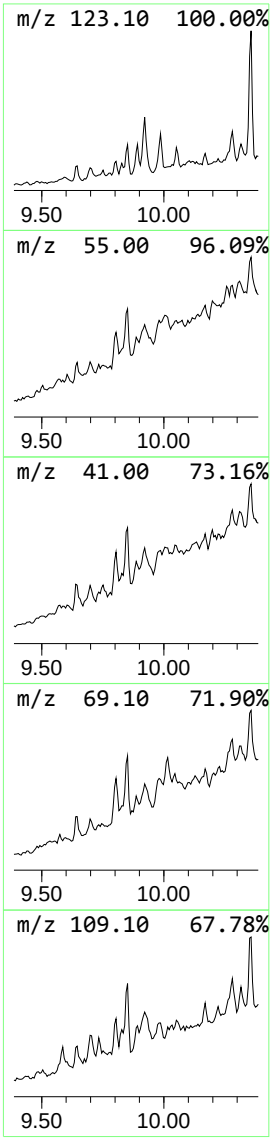
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-(2,2,6-Trimethylcyclohexy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.886	20.00 ng	578954	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	53
2	2,5,5,6,1a-Pentamethyl-cis-1a,4a...	208	C14H24O	1010215-77-9	53
3	Spiro[4.5]dec-7-en-6-one, 7-hydr...	166	C10H14O2	108573-05-3	46
4	2-(3,3-Dimethyl-oxiran-2-yl)-5-e...	209	C11H15NO3	1000194-95-4	38
5	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004755-33-3	38





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

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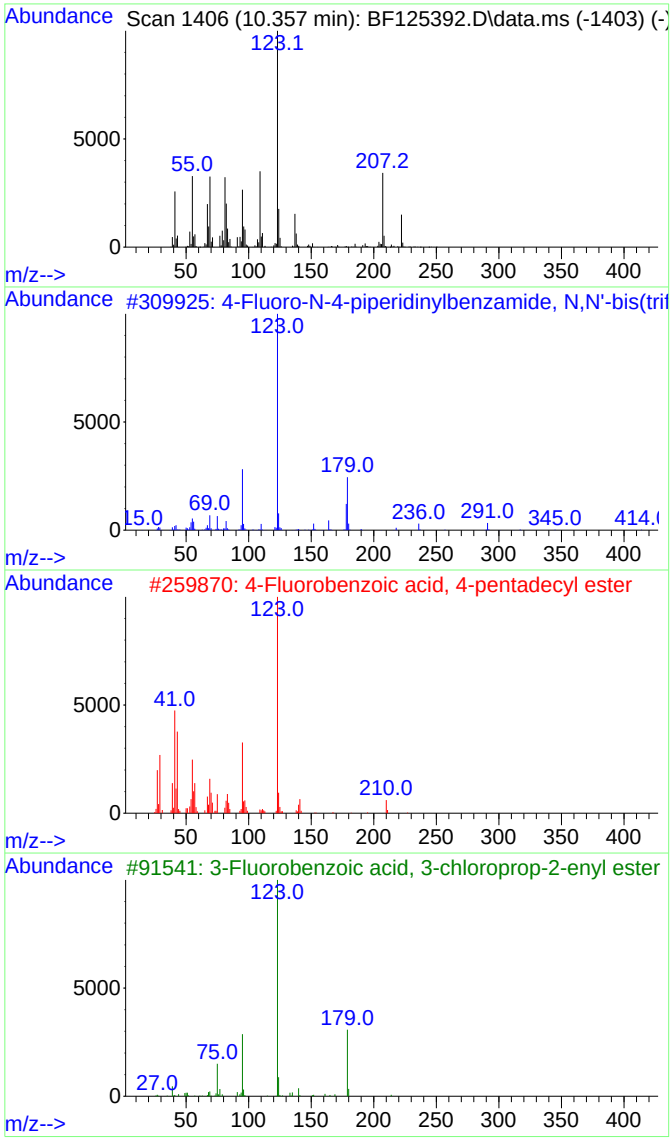
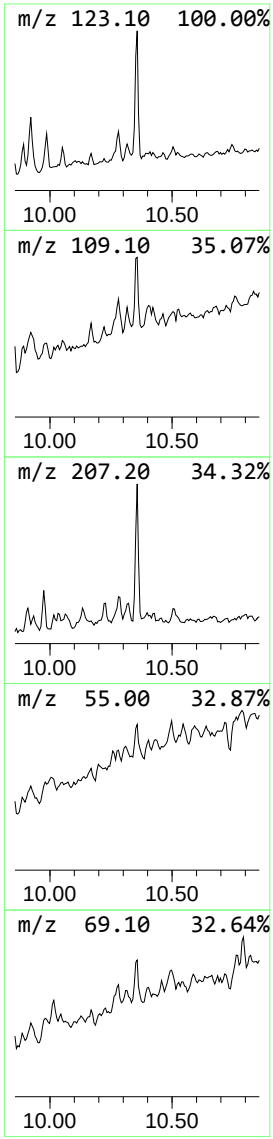
Peak Number 11 unknown10.357 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.357	44.96 ng	1301620	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Fluoro-N-4-piperidinylbenzamid...	414	C16H13F7N2O3	1000470-11-1	43
2	4-Fluorobenzoic acid, 4-pentadec...	350	C22H35FO2	1000280-68-5	43
3	3-Fluorobenzoic acid, 3-chloropr...	214	C10H8ClFO2	1000292-61-0	43
4	Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	43
5	Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	43





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-400027

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
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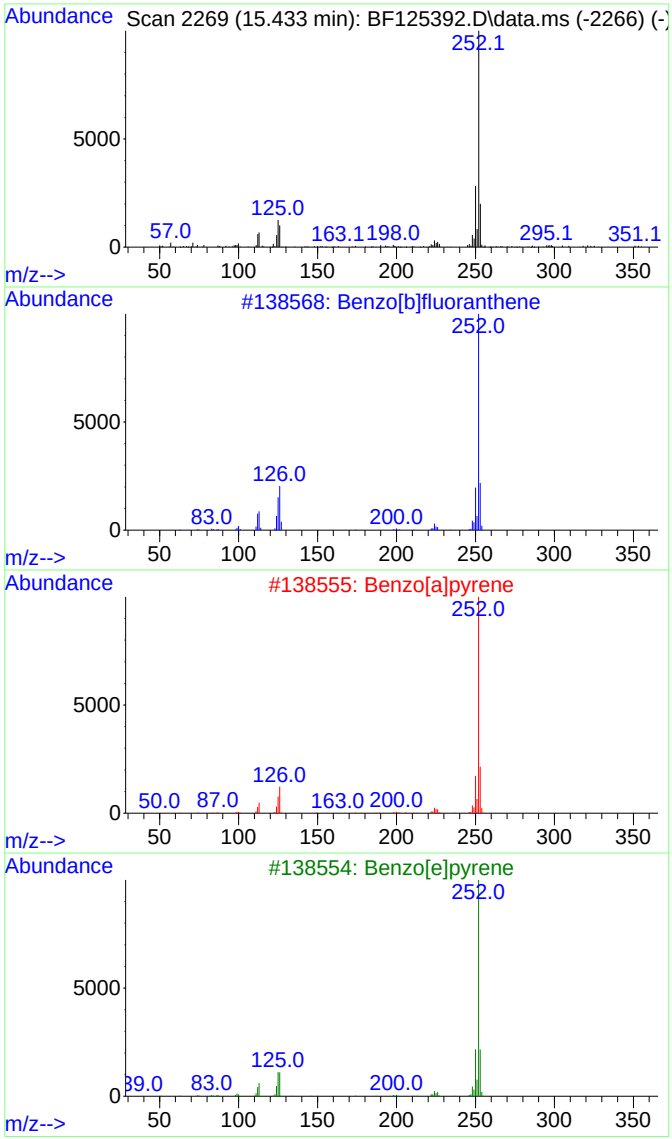
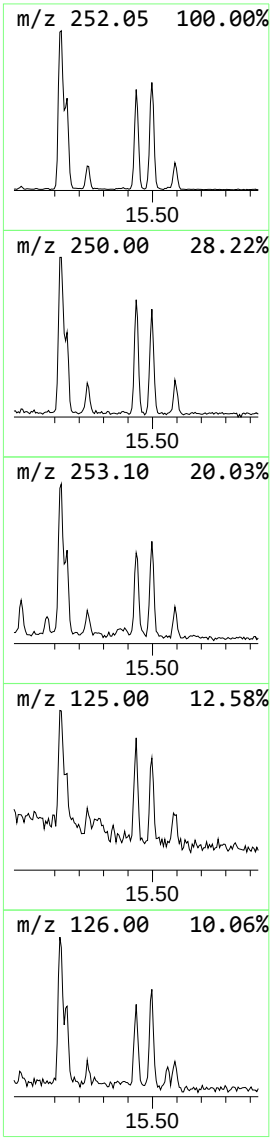
Peak Number 12 Benzo[e]pyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.433	4.19 ng	192591	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
2	Benzo[a]pyrene	252	C20H12	000050-32-8	91
3	Benzo[e]pyrene	252	C20H12	000192-97-2	91
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
5	Perylene	252	C20H12	000198-55-0	81





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Instrument : BNA_F
ClientSampleId : RBR-400027

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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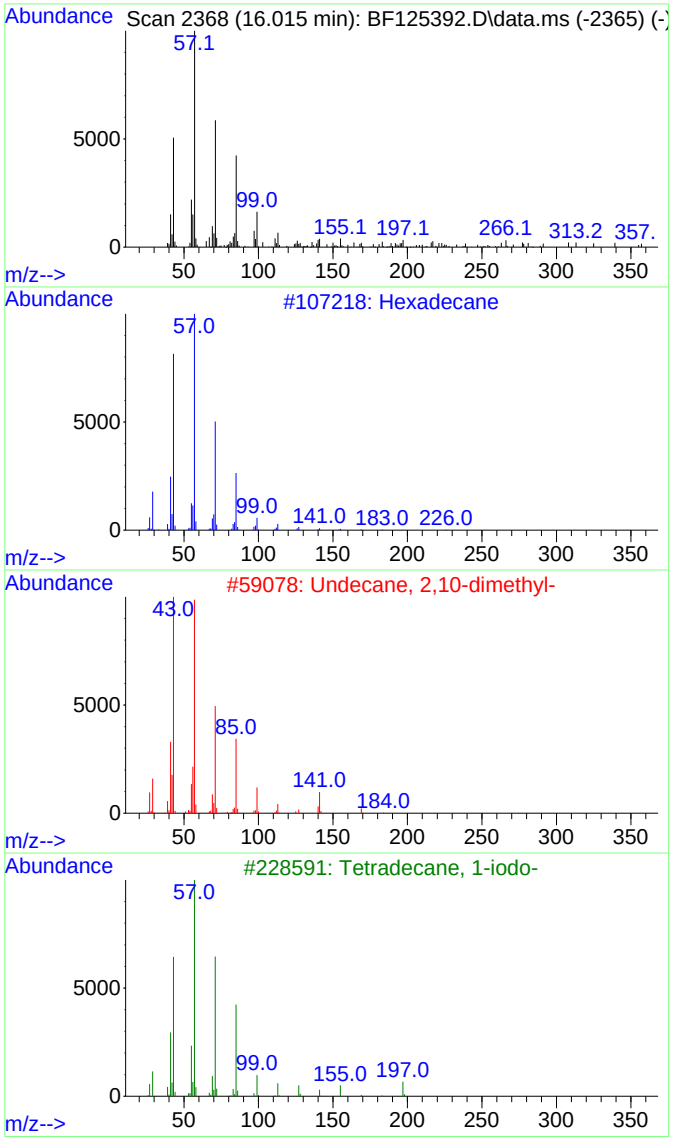
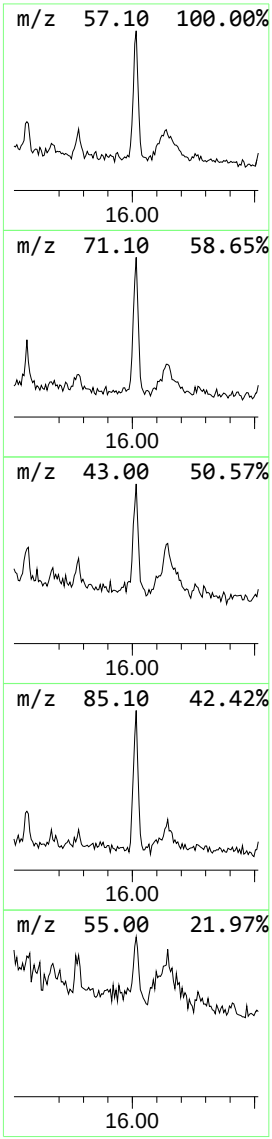
Peak Number 13 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.015	3.65 ng	167665	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	80
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
4	Octadecane	254	C18H38	000593-45-3	80
5	Heptadecane	240	C17H36	000629-78-7	80





Tentatively Identified Compound (LSC) summary

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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...	2.181	36.8	ng	1317490	1	6.898	715486	20.0
Ethanol, 2-(2-b...	8.092	5.4	ng	219109	2	8.181	805793	20.0
Decahydro-1,1,4...	9.328	14.2	ng	411688	3	9.939	578954	20.0
unknown9.575	9.575	13.8	ng	398488	3	9.939	578954	20.0
2-Pentanone, 4-...	9.645	34.6	ng	1002880	3	9.939	578954	20.0
unknown9.698	9.698	16.8	ng	485337	3	9.939	578954	20.0
2,5-Cyclohexadi...	9.751	10.3	ng	299142	3	9.939	578954	20.0
unknown9.804	9.804	45.1	ng	1305470	3	9.939	578954	20.0
unknown9.851	9.851	52.2	ng	1510410	3	9.939	578954	20.0
1-(2,2,6-Trimet...	9.886	20.0	ng	578954	3	9.939	578954	20.0
unknown10.357	10.357	45.0	ng	1301620	3	9.939	578954	20.0
Benzo[e]pyrene	15.433	4.2	ng	192591	6	15.562	918748	20.0
Hexadecane	16.015	3.6	ng	167665	6	15.562	918748	20.0