LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124240.D
Acq On : 10 Jun 2021 19:16
Operator : JU/CG
Sample : M2634-01 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-1

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124240.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.475	572	576	587	rBB	138057	134393	8.73%	1.413%
2	6.487	745	748	758	rVB	172279	154662	10.05%	1.626%
3	6.845	806	809	813	rBV	273186	214202	13.92%	2.252%
4	7.404	901	904	908	rBV	133547	107951	7.01%	1.135%
5	8.128	1024	1027	1030	rBV	310753	277883	18.05%	2.922%
6	9.016	1172	1178	1180	rBV7	36986	66647	4.33%	0.701%
7	9.122	1194	1196	1198	rBV3	52911	48320	3.14%	0.508%
8	9.151	1198	1201	1205	rVB3	61155	49188	3.20%	0.517%
9	9.204	1205	1210	1213	rBV	331147	295516	19.20%	3.107%
10	9.286	1220	1224	1227	rBV3	165928	207412	13.47%	2.181%
11	9.328	1228	1231	1233	rVV2	73176	73224	4.76%	0.770%
12	9.433	1247	1249	1251	rBV3	47774	45981	2.99%	0.483%
13	9.528	1261	1265	1266	rBV3	80381	114408	7.43%	1.203%
14	9.545	1266	1268	1270	rBV3	78961	78818	5.12%	0.829%
15	9.598	1274	1277	1278	rBV	423455	369132	23.98%	3.881%
16	9.757	1301	1304	1307	rBV4	624752	815741	52.99%	8.577%
17	9.804	1309	1312	1315	rVB	1056298	865186	56.21%	9.096%
18	9.845	1315	1319	1321	rBV3	263511	355910	23.12%	3.742%
19	9.875	1321	1324	1325	rBV2	531697	558489	36.28%	5.872%
20	9.933	1332	1334	1337	rBV3	278090	396396	25.75%	4.168%
21	10.157	1370	1372	1375	rBV2	621226	606304	39.39%	6.375%
22	10.216	1380	1382	1384	rBV3	346970	404179	26.26%	4.249%
23	10.269	1388	1391	1394	rBV4	533146	623538	40.51%	6.556%
24	10.316	1395	1399	1404	rBV3	1123143	1539323	100.00%	16.184%
25	14.027	2027	2030	2037	rVB	321594	346593	22.52%	3.644%
26	14.539	2114	2117	2122	rVB4	129189	147833	9.60%	1.554%
27	15.498	2275	2280	2286	rBV	216776	289280	18.79%	3.041%
28	15.945	2352	2356	2362	rVB	80997	118323	7.69%	1.244%
29	17.051	2539	2544	2550	rVB6	52463	115884	7.53%	1.218%
30	17.298	2583	2586	2593	rVB9	23372	43234	2.81%	0.455%
31	17.574	2627	2633	2638	rBV9	23546	47348	3.08%	0.498%

Sum of corrected areas: 9511298

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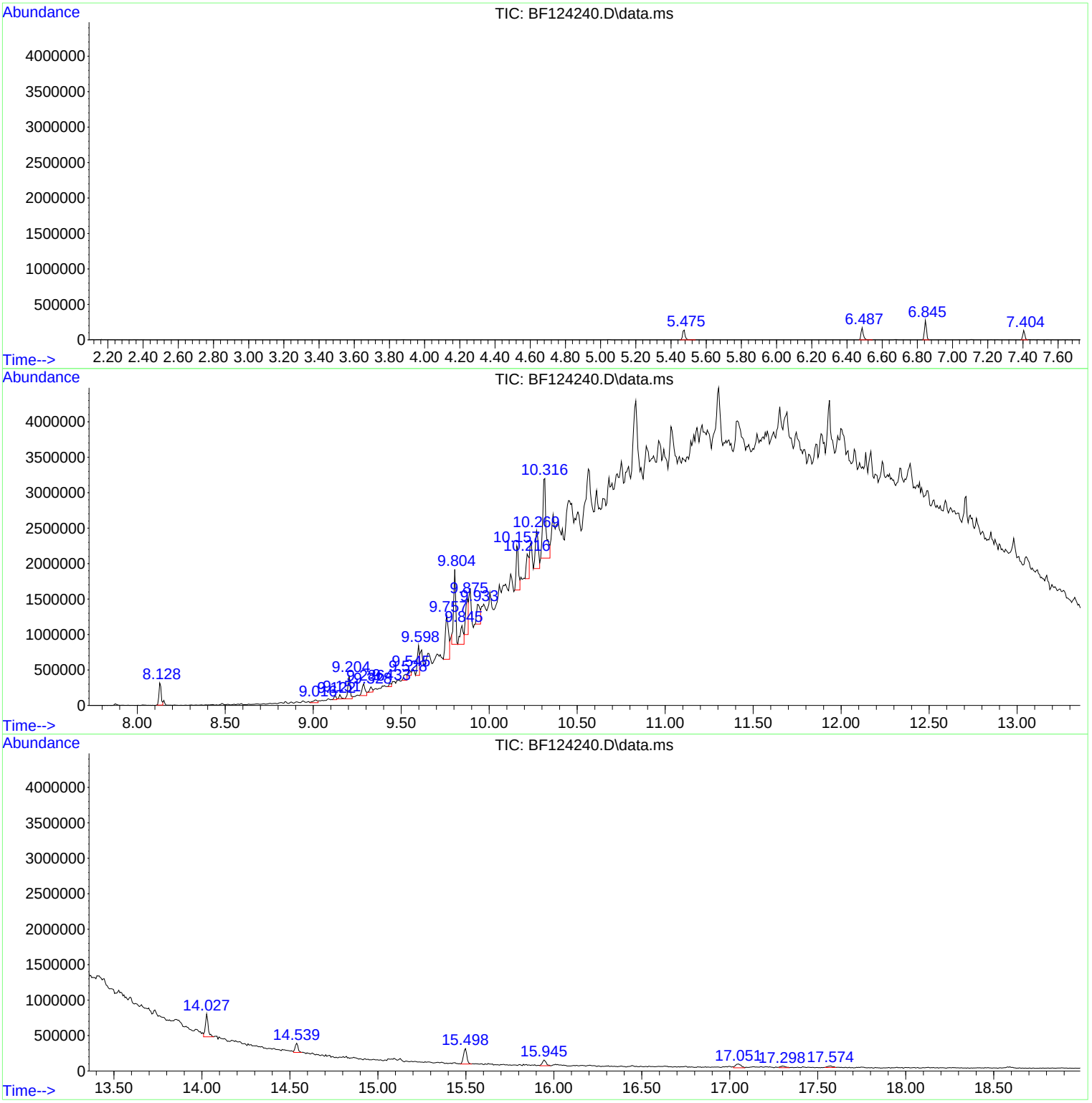
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R44-STONE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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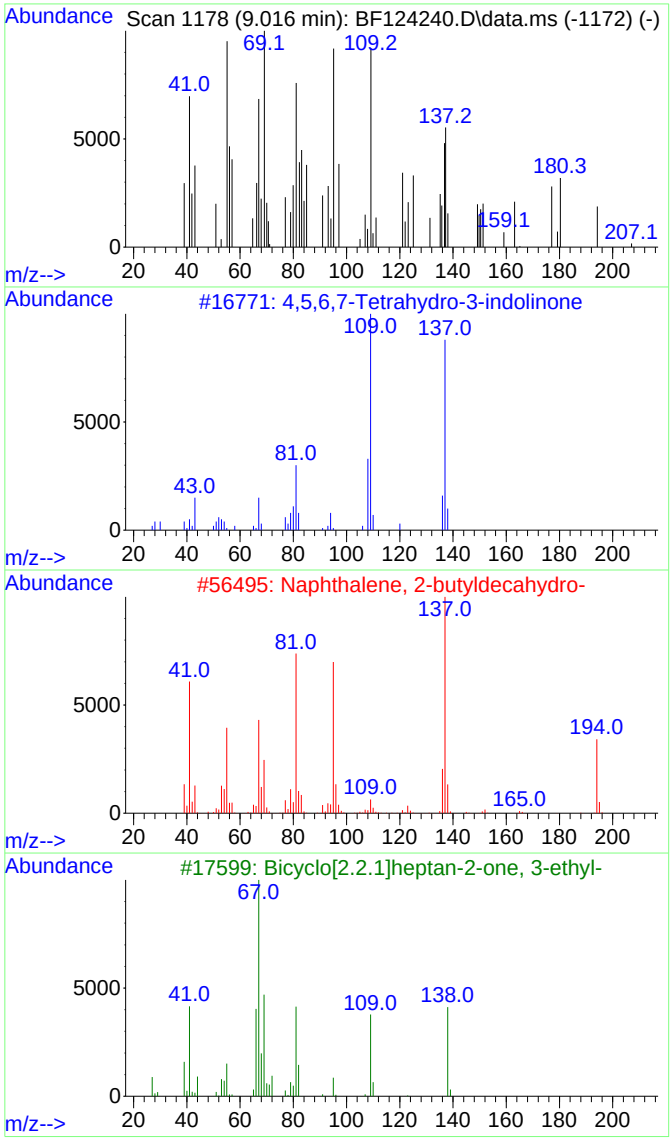
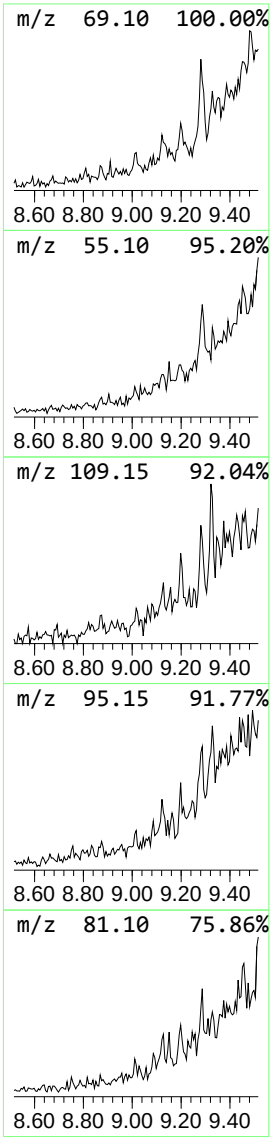
Peak Number 1 unknown9.016 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.016	2.39 ng	66647	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,5,6,7-Tetrahydro-3-indolinone	137	C8H11NO	058074-25-2	42
2	Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	41
3	Bicyclo[2.2.1]heptan-2-one, 3-et...	138	C9H14O	054345-87-8	41
4	2(1H)-Pyridinone, 1-ethyl-6-methyl-	137	C8H11NO	019038-36-9	30
5	4,6-Heptadien-2-one, 3,6-dimethy...	180	C12H20O	077822-50-5	30





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Data File : BF124240.D
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Operator : JU/CG
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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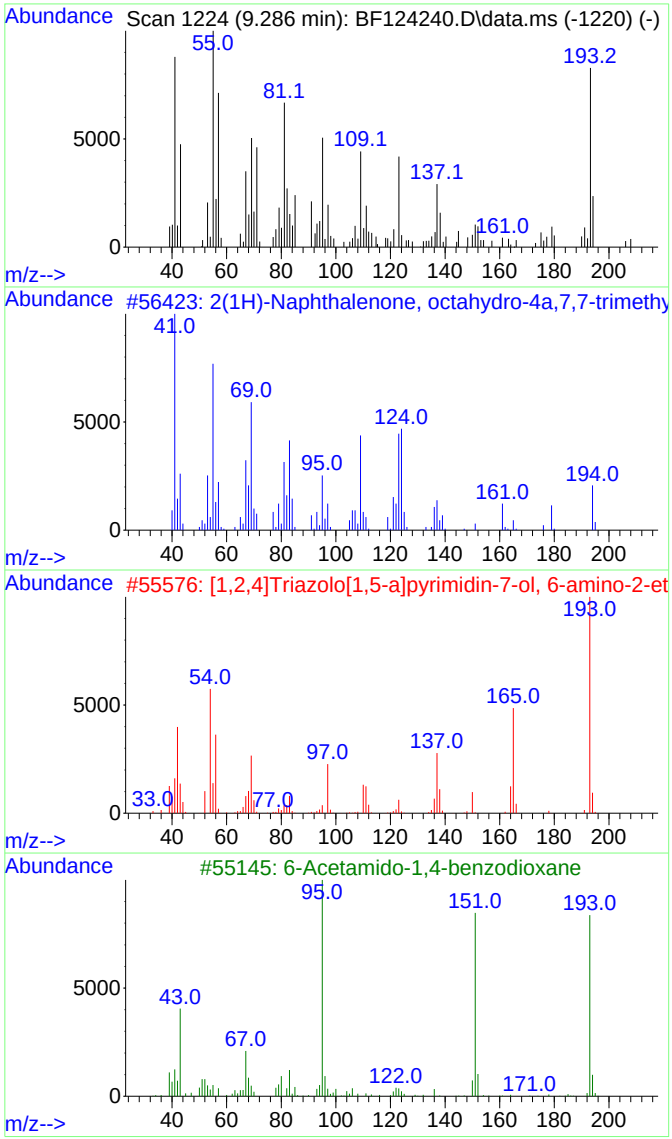
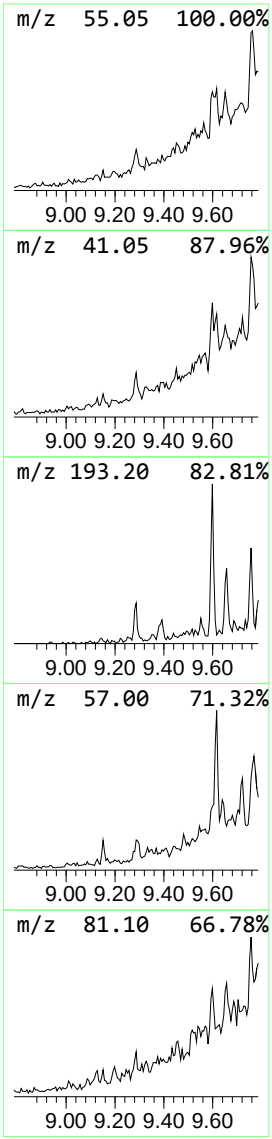
Peak Number 2 unknown9.286 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.286	7.43 ng	207412	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, octahydro-4...	194	C13H22O	007056-56-6	30
2	[1,2,4]Triazolo[1,5-a]pyrimidin-...	193	C8H11N5O	1000351-50-1	25
3	6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	22
4	Trisiloxane, 1,1,3,3,5,5-hexamet...	208	C6H20O2Si3	001189-93-1	18
5	Butanoic acid, 3-methyl-, 3,7-di...	240	C15H28O2	068922-10-1	18





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Sample : M2634-01 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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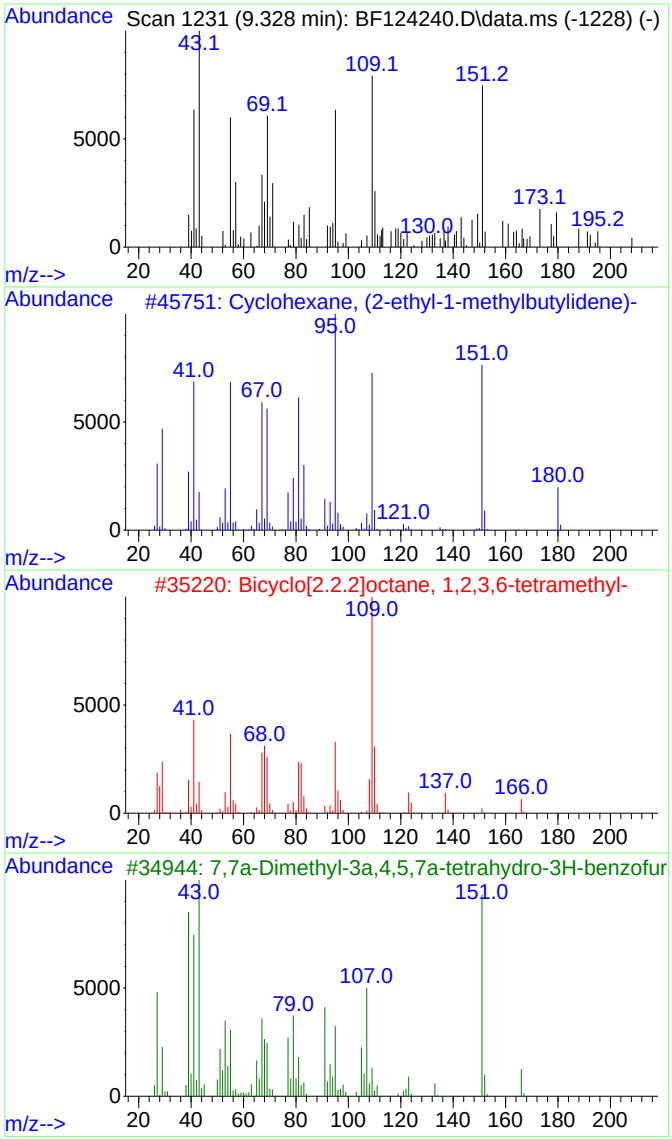
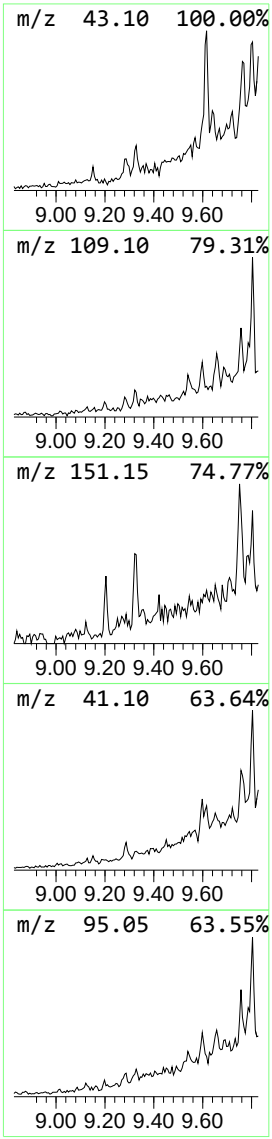
Peak Number 3 unknown9.328 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.328	2.62 ng	73224	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, (2-ethyl-1-methylbu...	180	C13H24	074810-41-6	47
2	Bicyclo[2.2.2]octane, 1,2,3,6-te...	166	C12H22	062338-45-8	35
3	7,7a-Dimethyl-3a,4,5,7a-tetrahyd...	166	C10H14O2	1000186-11-2	27
4	2,4-Diamino-6-cyanamino-1,3,5-tr...	151	C4H5N7	003496-98-8	25
5	(4-Fluorophenyl) methanol, n-pro...	168	C10H13FO	1000374-63-7	25





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Acq On : 10 Jun 2021 19:16
Operator : JU/CG
Sample : M2634-01 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R44-STONE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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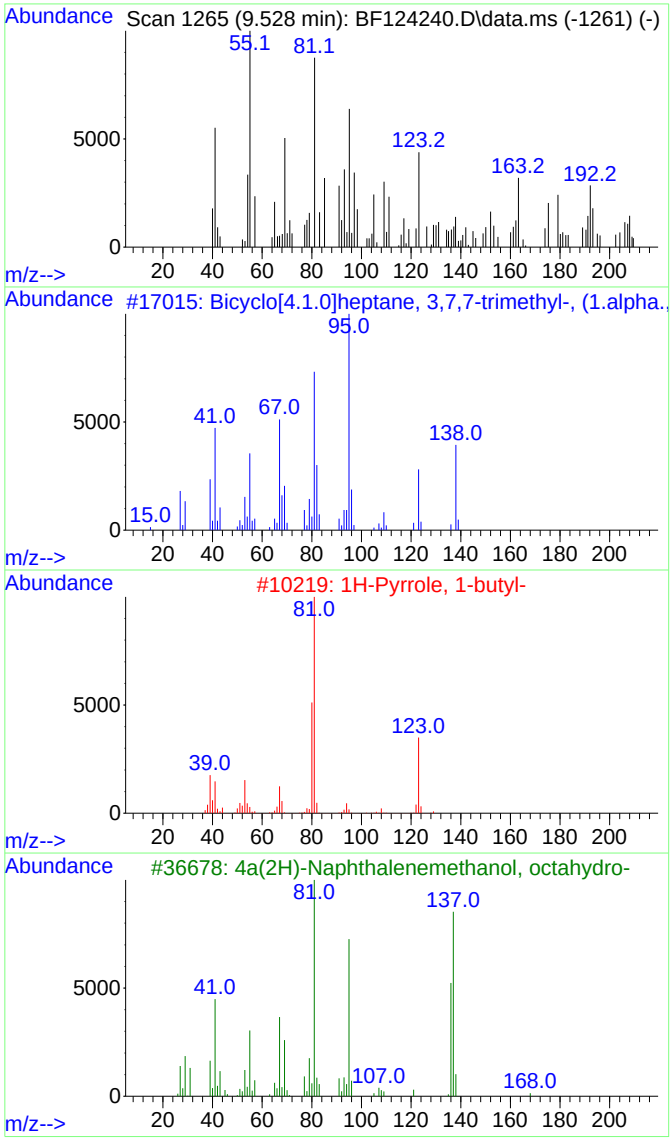
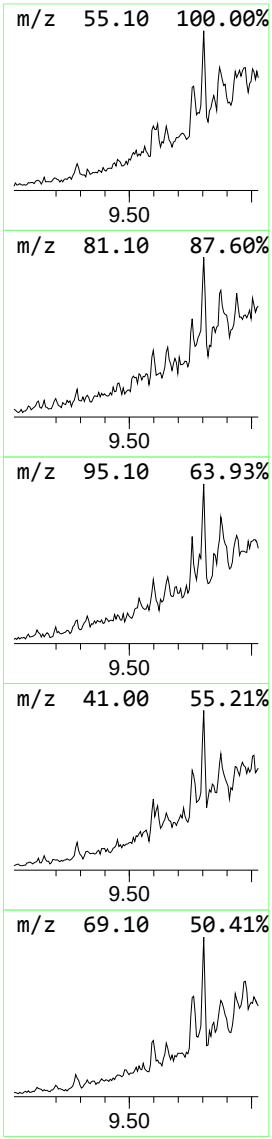
Peak Number 4 unknown9.528 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.528	4.10 ng	114408	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	35
2	1H-Pyrrole, 1-butyl-	123	C8H13N	000589-33-3	27
3	4a(2H)-Naphthalenemethanol, octa...	168	C11H20O	099992-19-5	27
4	Cyclopentane, 1-isobutylidene-3-...	138	C10H18	1000150-62-1	27
5	Bicyclo[2.2.1]heptan-2-one, 4,7,...	152	C10H16O	010292-98-5	22





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Data File : BF124240.D
Acq On : 10 Jun 2021 19:16
Operator : JU/CG
Sample : M2634-01 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R44-STONE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
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TIC Library : C:\DATABASE\NIST11.L
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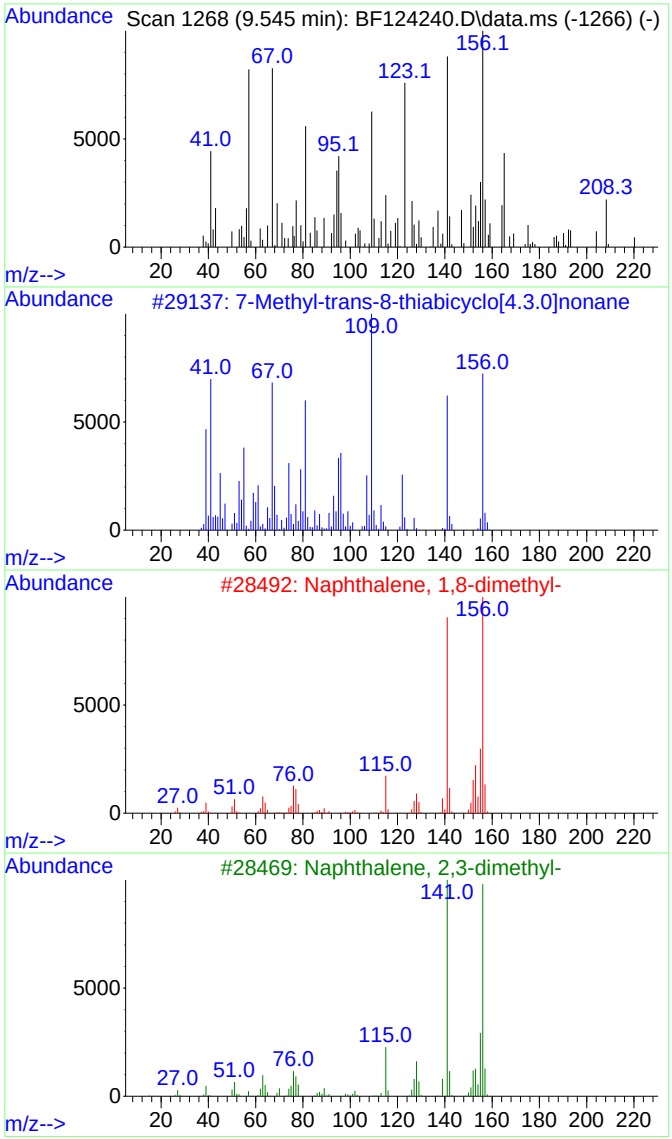
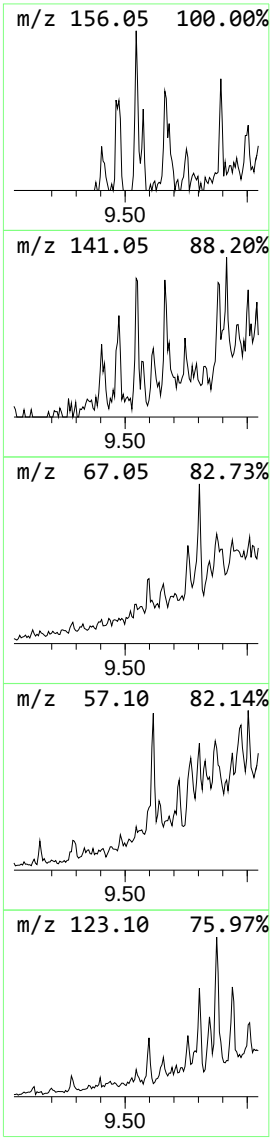
Peak Number 5 unknown9.545 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.545	2.82 ng	78818	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Methyl-trans-8-thiabicyclo[4.3...	156	C9H16S	1000215-96-1	49
2	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	35
3	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	35
4	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	35
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	35





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Instrument : BNA_F
ClientSampleId : R44-STONE-1

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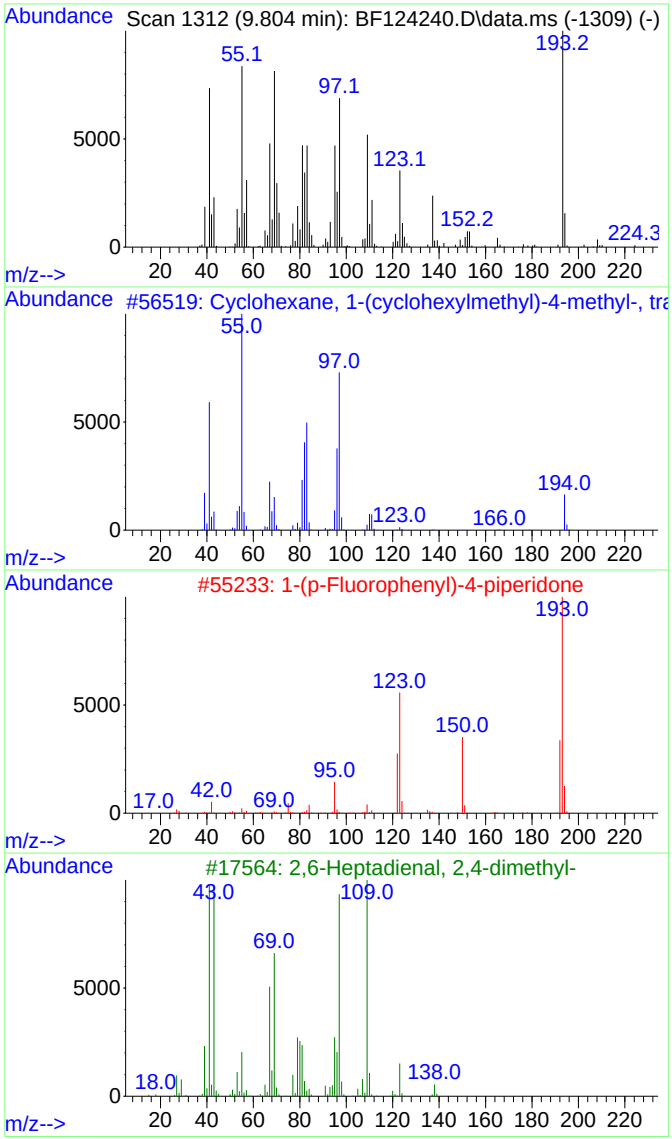
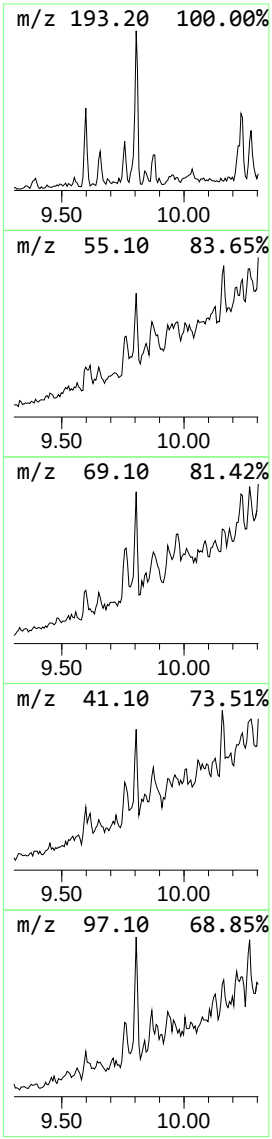
Peak Number 6 unknown9.804 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.804	30.98 ng	865186	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-98-2	25
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	22
3	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	18
4	1,1'-Bicyclohexyl, 2-ethyl-, cis-	194	C14H26	050991-12-3	18
5	Cyclohexylmethanol, trifluoroace...	210	C9H13F3O2	164071-20-9	14





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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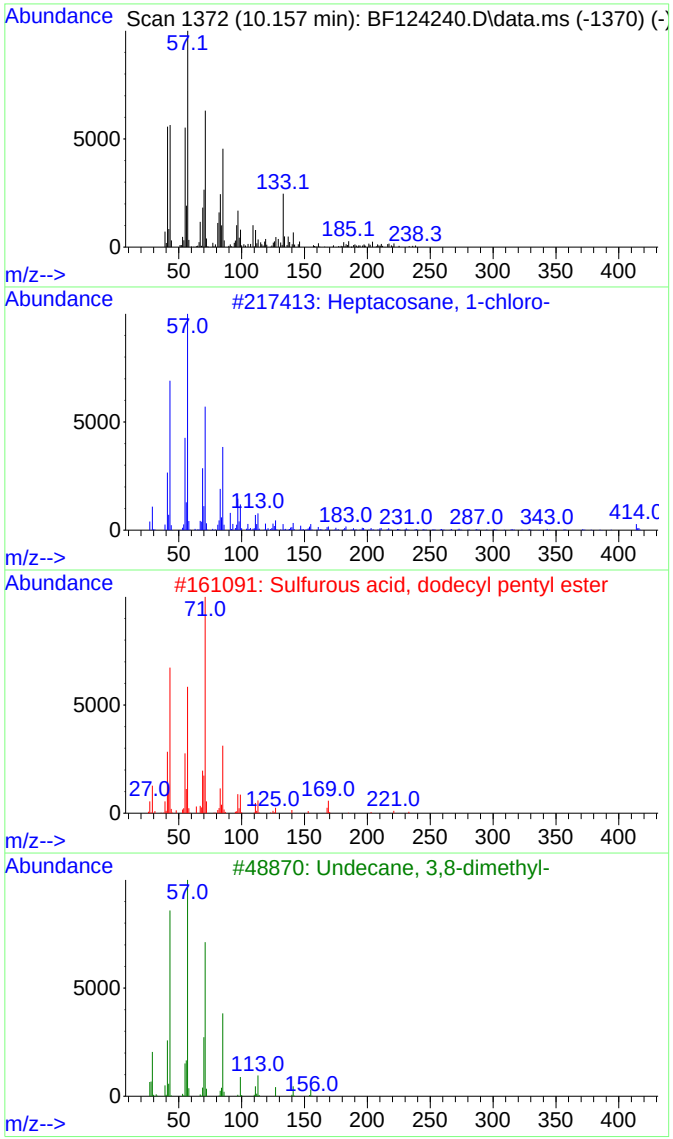
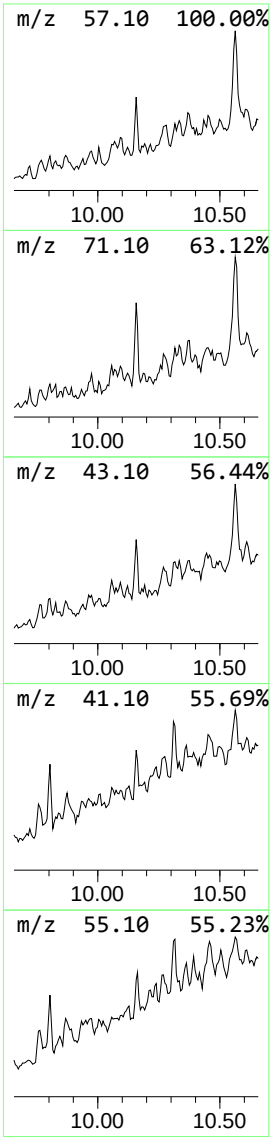
Peak Number 7 Heptacosane, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.157	21.71 ng	606304	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	64
2	Sulfurous acid, dodecyl pentyl e...	320	C17H36O3S	1000309-14-5	49
3	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	49
4	Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	46
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	43





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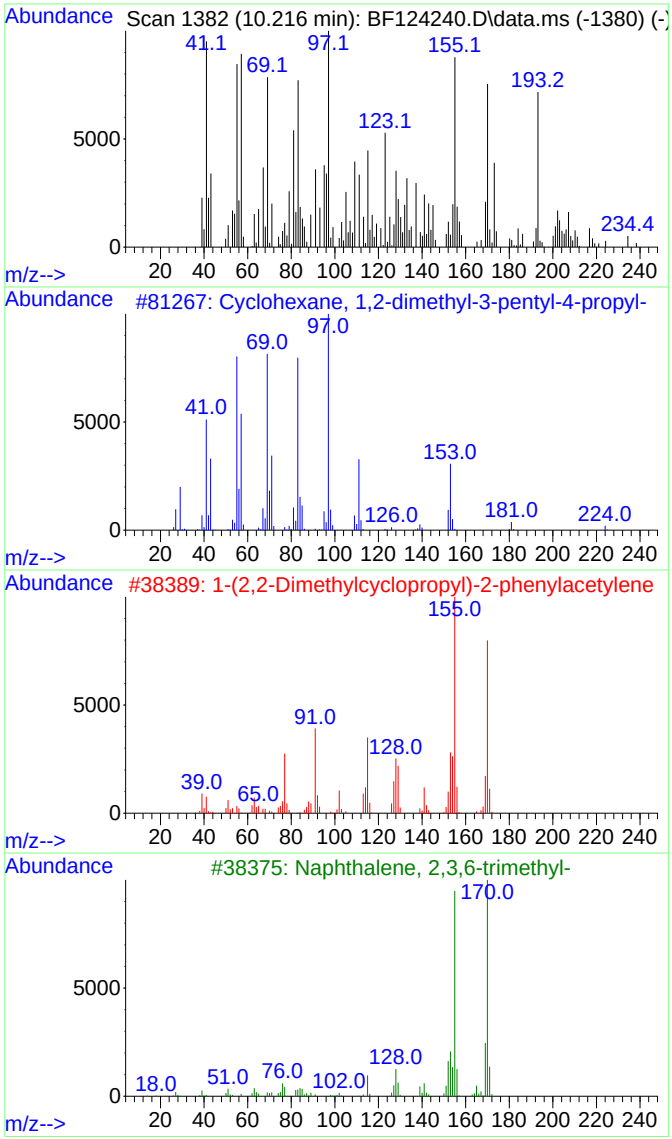
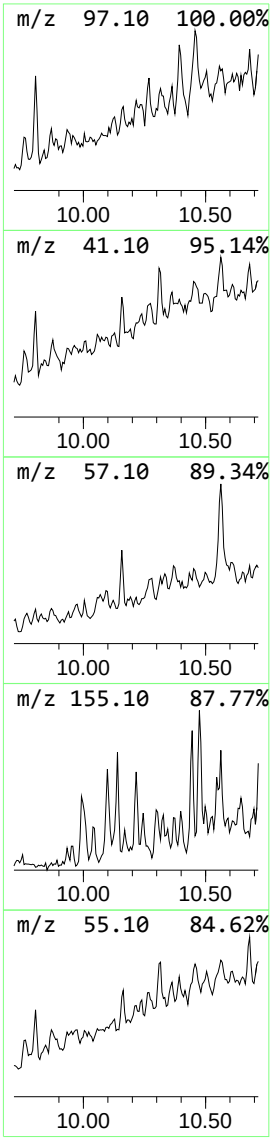
Peak Number 8 Cyclohexane, 1,2-dimethyl-3... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.216	14.47 ng	404179	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	59
2	1-(2,2-Dimethylcyclopropyl)-2-ph...	170	C13H14	1000294-91-1	35
3	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	35
4	3-(2-Methyl-propenyl)-1H-indene	170	C13H14	1000187-78-5	35
5	Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	35





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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST11.L
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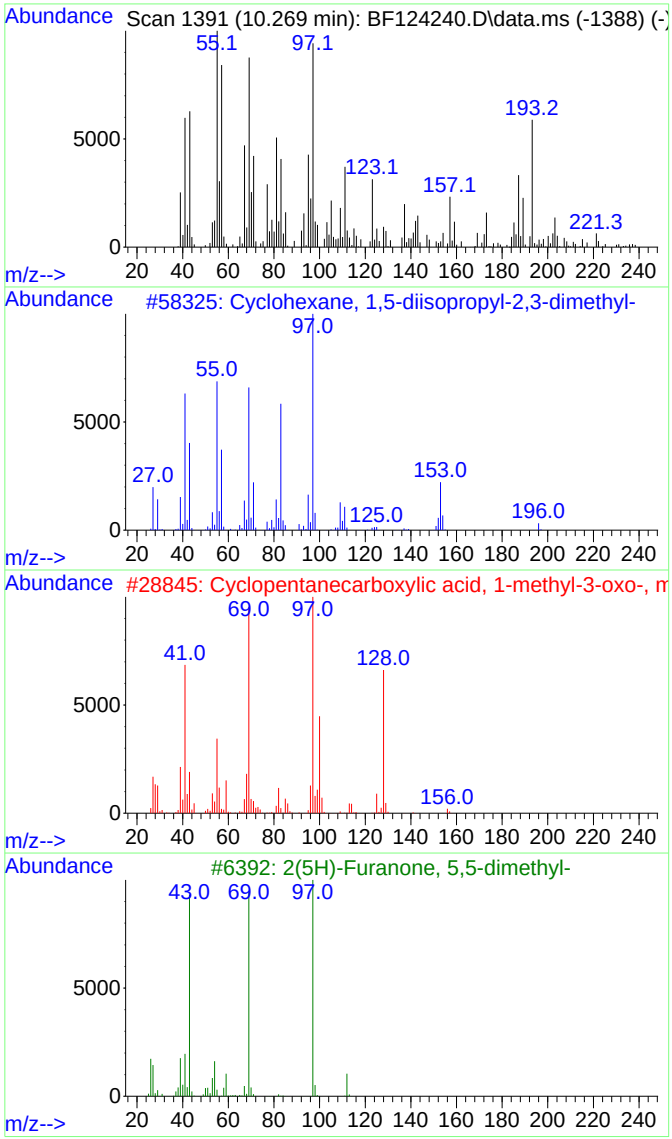
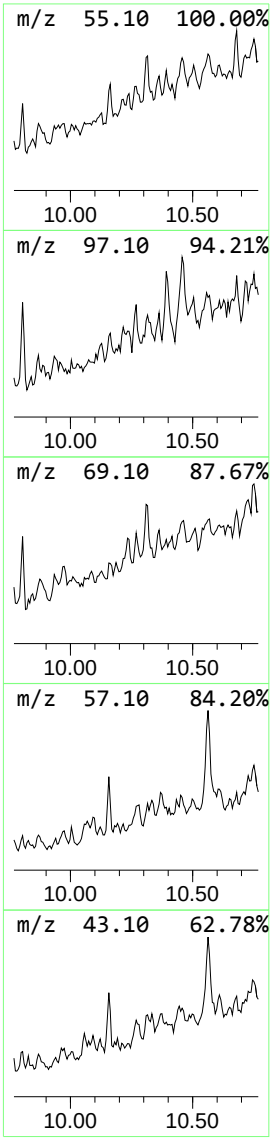
Peak Number 9 unknown10.269 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.269	22.33 ng	623538	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,5-diisopropyl-2,3...	196	C14H28	1000149-58-8	43
2	Cyclopentanecarboxylic acid, 1-m...	156	C8H12O3	032436-10-5	38
3	2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	38
4	Cyclohexane, 1,2,4,5-tetraethyl-...	196	C14H28	061142-24-3	27
5	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	27





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Data File : BF124240.D
Acq On : 10 Jun 2021 19:16
Operator : JU/CG
Sample : M2634-01 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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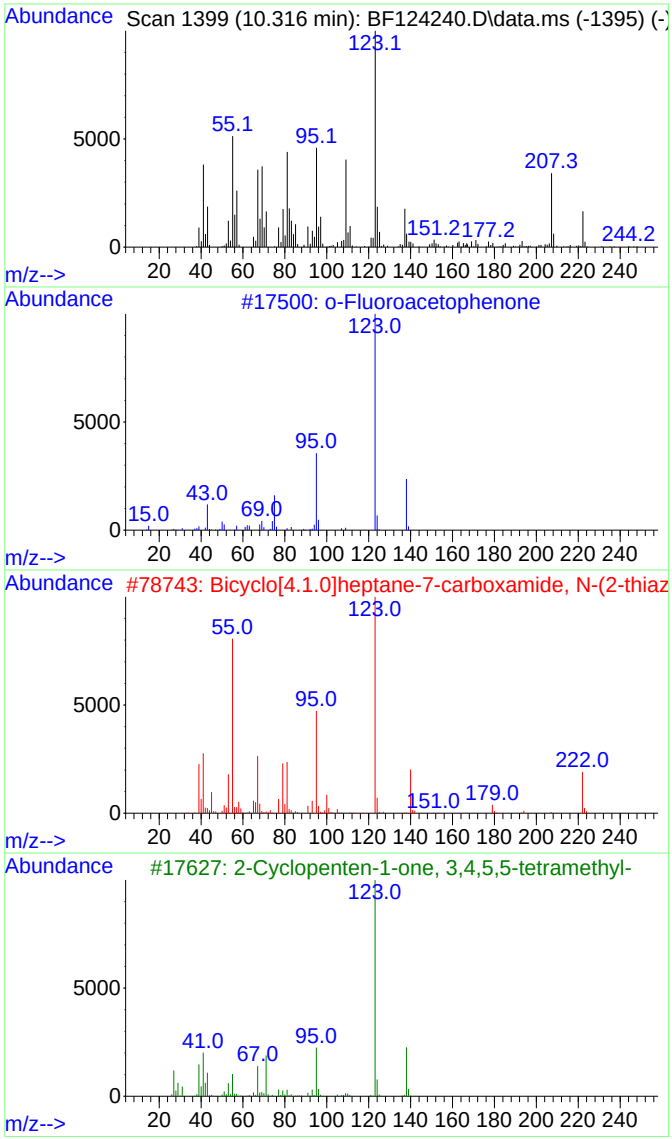
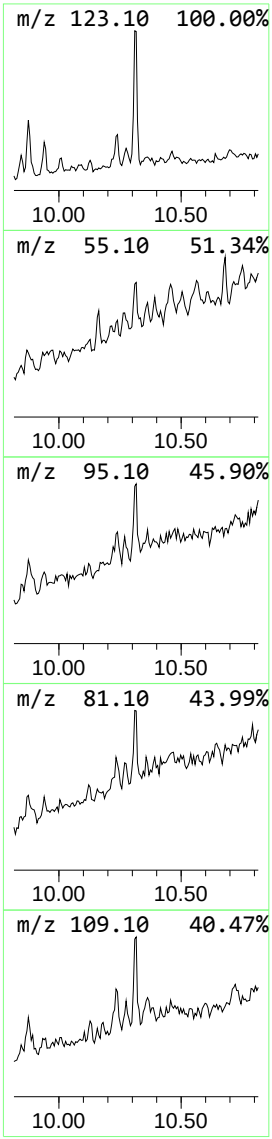
Peak Number 10 unknown10.316 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.316	55.12 ng	1539320	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Fluoroacetophenone	138	C8H7FO	000445-27-2	46
2	Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2OS	329912-72-3	46
3	2-Cyclopenten-1-one, 3,4,5,5-tet...	138	C9H14O	090611-02-2	43
4	3-Fluoro-N-[2-(N-hydroxycarbamim...	239	C11H14FN3O2	1000297-41-5	43
5	.alpha.-Chloro-p-fluoroacetophenone	172	C8H6ClFO	000456-04-2	43





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Operator : JU/CG
Sample : M2634-01 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R44-STONE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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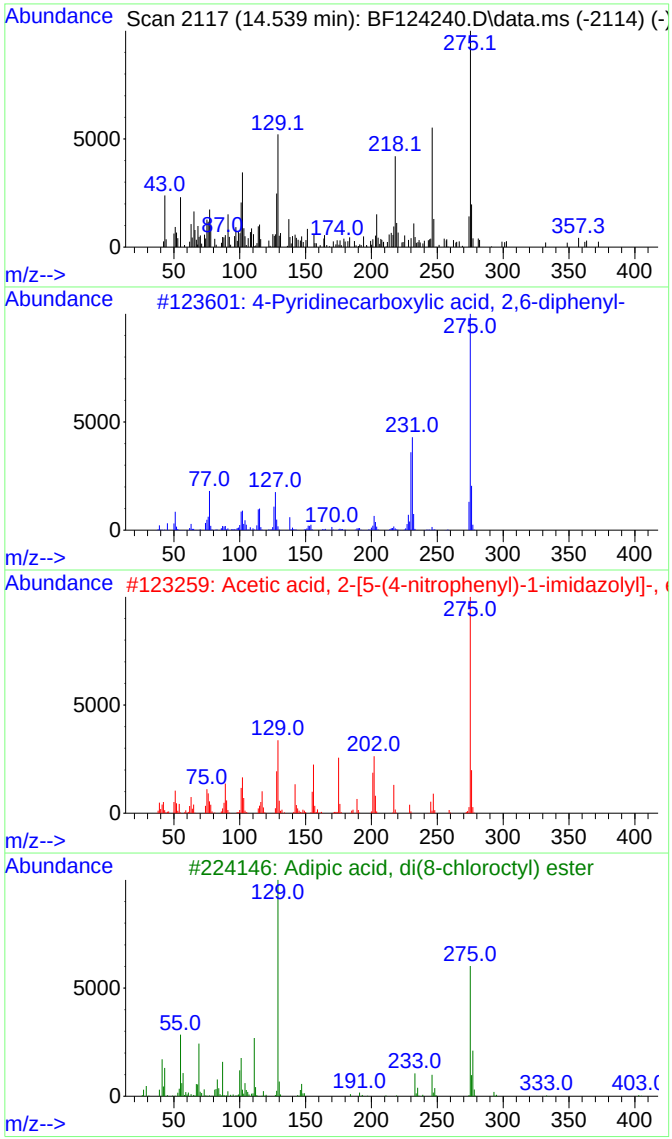
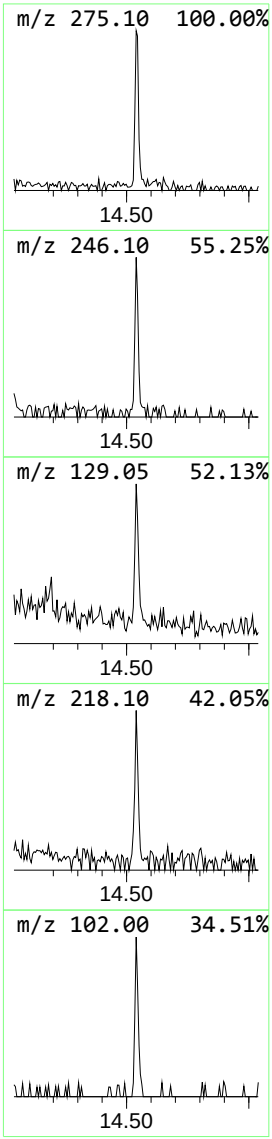
Peak Number 11 unknown14.539 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	8.53 ng	147833	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pyridinecarboxylic acid, 2,6-d...	275	C18H13NO2	1000338-16-2	45
2	Acetic acid, 2-[5-(4-nitrophenyl...	275	C13H13N3O4	351064-45-4	43
3	Adipic acid, di(8-chloroctyl) ester	438	C22H40Cl2O4	1000349-77-4	43
4	1,1':4',1''-Terphenyl, 4-nitro-	275	C18H13NO2	010355-53-0	42
5	1H-Indole, 2-cyclohexyl-3-phenyl-	275	C20H21N	1000163-87-0	38





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Operator : JU/CG
Sample : M2634-01 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R44-STONE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
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TIC Library : C:\DATABASE\NIST11.L
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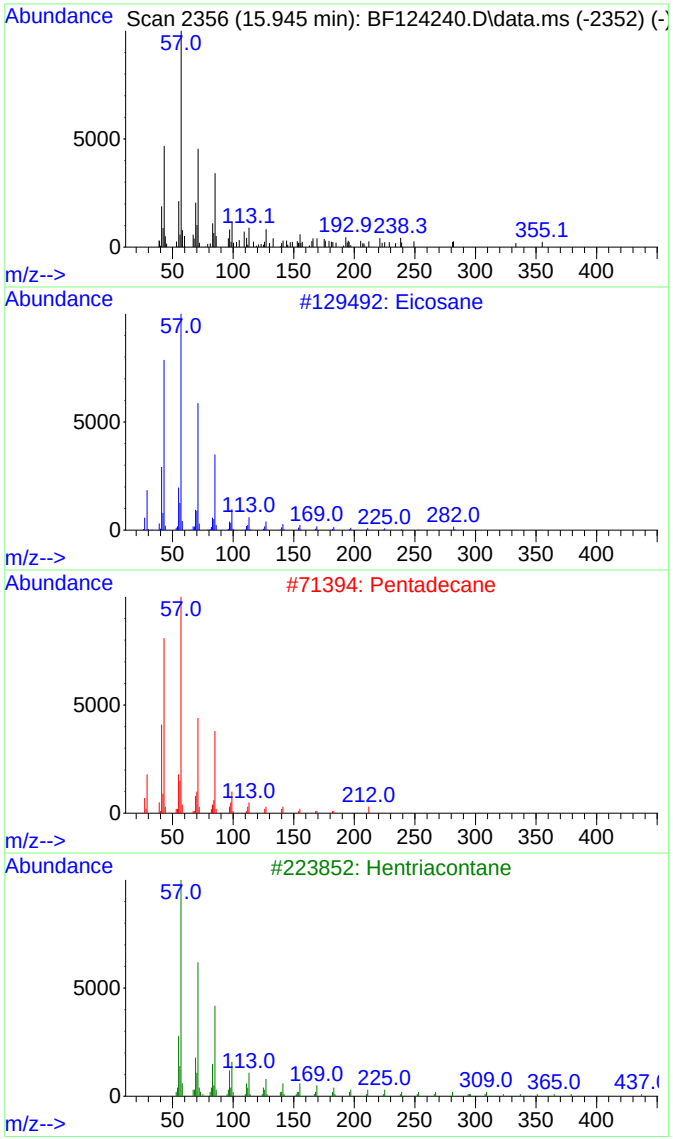
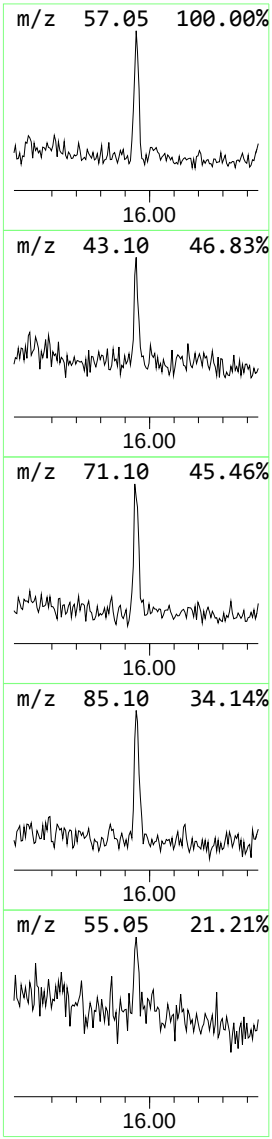
Peak Number 12 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	8.18 ng	118323	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	Pentadecane	212	C15H32	000629-62-9	81
3	Hentriacontane	437	C31H64	000630-04-6	72
4	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	72
5	Tetratetracontane	619	C44H90	007098-22-8	72





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Data File : BF124240.D
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Operator : JU/CG
Sample : M2634-01 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R44-STONE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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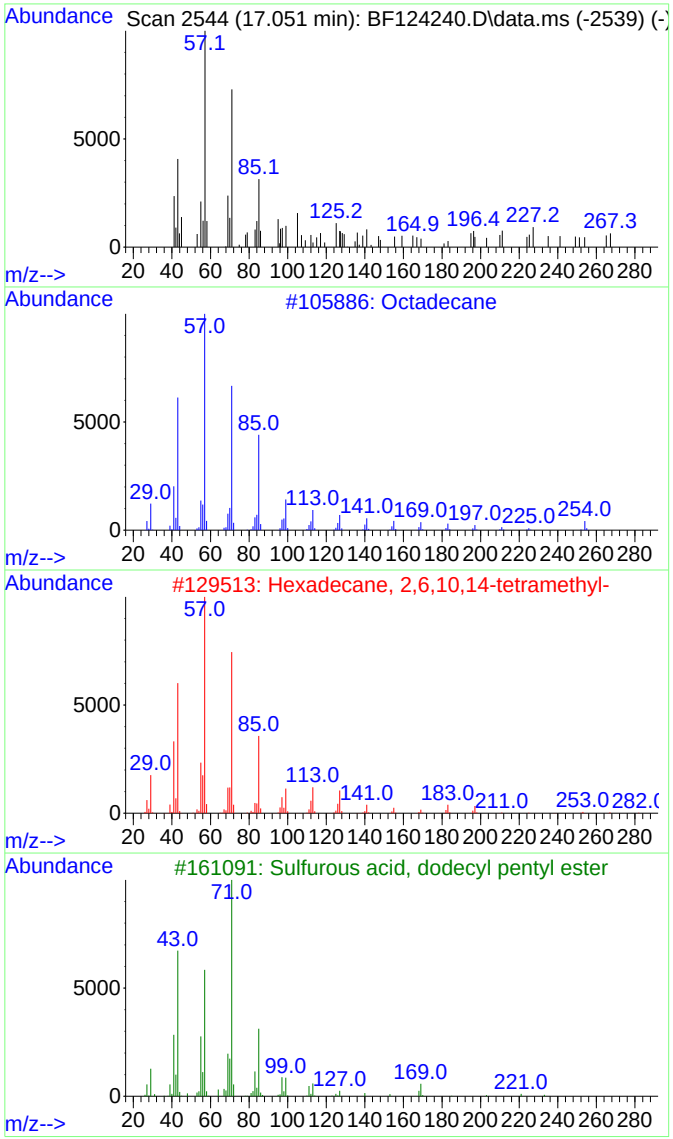
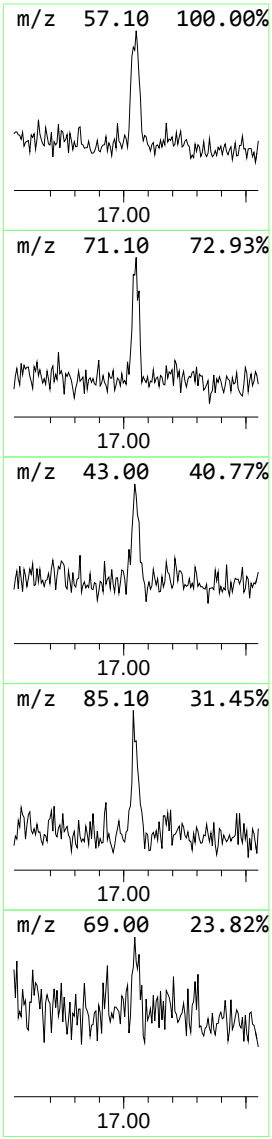
Peak Number 13 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.051	8.01 ng	115884	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	50
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	43
3	Sulfurous acid, dodecyl pentyl e...	320	C17H36O3S	1000309-14-5	43
4	Hexacosane	366	C26H54	000630-01-3	43
5	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	43





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Acq On : 10 Jun 2021 19:16
Operator : JU/CG
Sample : M2634-01 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R44-STONE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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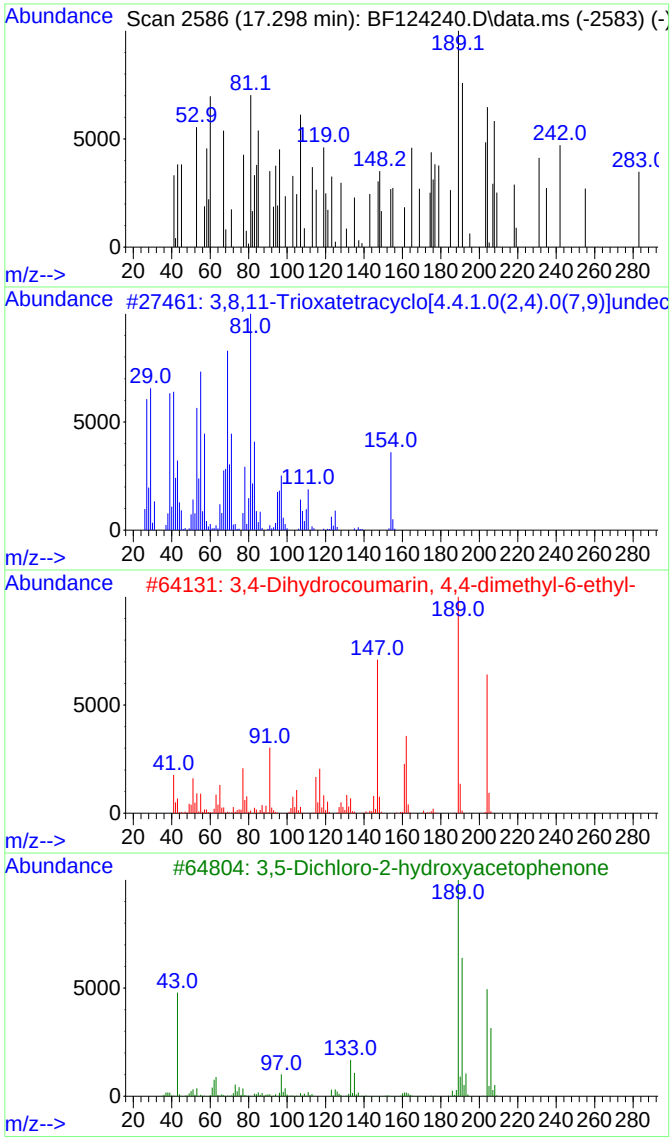
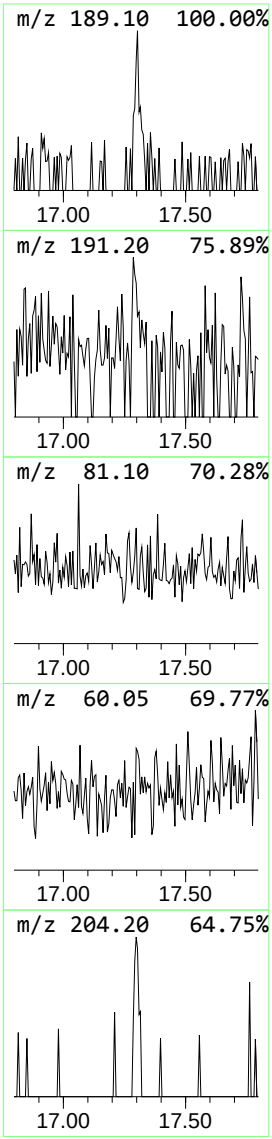
Peak Number 14 unknown17.298 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.298	2.99 ng	43234	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,8,11-Trioxatetracyclo[4.4.1.0(...	154	C8H10O3	050267-11-3	10
2	3,4-Dihydrocoumarin, 4,4-dimethy...	204	C13H16O2	029423-74-3	10
3	3,5-Dichloro-2-hydroxyacetophenone	204	C8H6Cl2O2	003321-92-4	10
4	1,3-Cyclopentanedione, 2-bromo-4...	204	C7H9BrO2	057157-02-5	10
5	4-Bromo-2-fluoroaniline	189	C6H5BrFN	000367-24-8	10





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Data File : BF124240.D
Acq On : 10 Jun 2021 19:16
Operator : JU/CG
Sample : M2634-01 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R44-STONE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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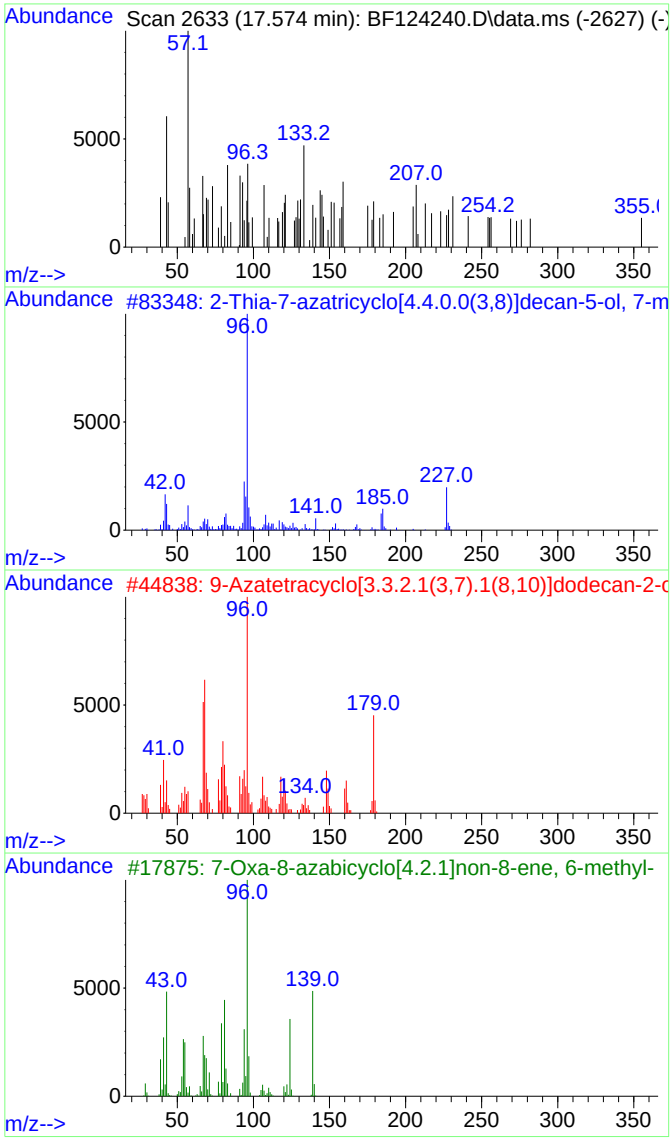
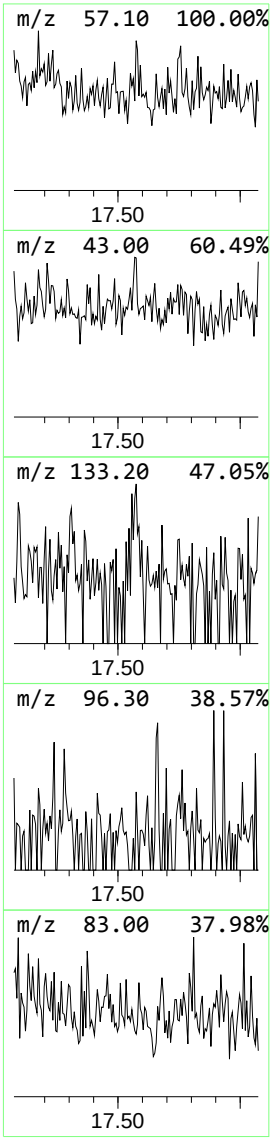
Peak Number 15 unknown17.574 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.574	3.27 ng	47348	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thia-7-azatricyclo[4.4.0.0(3,8...	227	C11H17NO2S	062545-78-2	10
2	9-Azatetracyclo[3.3.2.1(3,7).1(8...	179	C11H17NO	1000191-19-5	10
3	7-Oxa-8-azabicyclo[4.2.1]non-8-e...	139	C8H13NO	1000362-10-7	10
4	Methylselenol	96	CH4Se	006486-05-1	10
5	1H-Indole, octahydro-3-methyl-	139	C9H17N	037865-94-4	9





Tentatively Identified Compound (LSC) summary

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Data File : BF124240.D
Acq On : 10 Jun 2021 19:16
Operator : JU/CG
Sample : M2634-01 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown9.016	9.016	2.4	ng	66647	3	9.892	558489	20.0
unknown9.286	9.286	7.4	ng	207412	3	9.892	558489	20.0
unknown9.328	9.328	2.6	ng	73224	3	9.892	558489	20.0
unknown9.528	9.528	4.1	ng	114408	3	9.892	558489	20.0
unknown9.545	9.545	2.8	ng	78818	3	9.892	558489	20.0
unknown9.804	9.804	31.0	ng	865186	3	9.892	558489	20.0
Heptacosane, 1-...	10.157	21.7	ng	606304	3	9.892	558489	20.0
Cyclohexane, 1,...	10.216	14.5	ng	404179	3	9.892	558489	20.0
unknown10.269	10.269	22.3	ng	623538	3	9.892	558489	20.0
unknown10.316	10.316	55.1	ng	1539320	3	9.892	558489	20.0
unknown14.539	14.539	8.5	ng	147833	5	14.027	346593	20.0
Eicosane	15.945	8.2	ng	118323	6	15.498	289280	20.0
Octadecane	17.051	8.0	ng	115884	6	15.498	289280	20.0
unknown17.298	17.298	3.0	ng	43234	6	15.498	289280	20.0
unknown17.574	17.574	3.3	ng	47348	6	15.498	289280	20.0