LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124220.D
Acq On : 9 Jun 2021 21:32
Operator : JU/CG
Sample : M2634-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-2

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: BF124220.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	573	576	583	rBB	160766	145424	8.68%	1.362%
2	6.487	745	748	755	rBV	182339	153595	9.17%	1.438%
3	6.851	806	810	813	rBV	270313	218163	13.03%	2.043%
4	7.410	901	905	909	rBV	119748	104114	6.22%	0.975%
5	8.134	1025	1028	1030	rBV	359978	273241	16.31%	2.559%
6	8.151	1030	1031	1035	rVB	74529	54176	3.23%	0.507%
7	9.016	1173	1178	1180	rBV5	39299	66467	3.97%	0.622%
8	9.092	1186	1191	1193	rBV6	42717	66794	3.99%	0.626%
9	9.128	1194	1197	1199	rVV3	82118	71701	4.28%	0.671%
10	9.157	1199	1202	1206	rBV4	86293	88816	5.30%	0.832%
11	9.204	1207	1210	1213	rBV	282985	254025	15.17%	2.379%
12	9.292	1221	1225	1228	rBV4	195091	263782	15.75%	2.470%
13	9.334	1229	1232	1234	rBV4	68209	85656	5.11%	0.802%
14	9.439	1248	1250	1251	rBV2	68741	57297	3.42%	0.537%
15	9.486	1256	1258	1260	rBV3	80107	87903	5.25%	0.823%
16	9.604	1275	1278	1279	rBV	519915	475706	28.40%	4.455%
17	9.622	1279	1281	1284	rVV2	419553	419494	25.05%	3.929%
18	9.657	1285	1287	1292	rVB5	257805	359113	21.44%	3.363%
19	9.763	1302	1305	1308	rBV3	770949	1077693	64.35%	10.093%
20	9.810	1310	1313	1316	rVB	1343516	1293728	77.25%	12.116%
21	9.881	1322	1325	1327	rBV3	662457	926410	55.31%	8.676%
22	9.945	1333	1336	1338	rBV2	344196	441386	26.35%	4.134%
23	10.169	1371	1374	1376	rBV2	658562	662314	39.55%	6.203%
24	10.275	1390	1392	1396	rBV4	559885	649973	38.81%	6.087%
25	10.322	1396	1400	1402	rBV2	1526745	1674800	100.00%	15.685%
26	14.033	2029	2031	2034	rVB	290473	275646	16.46%	2.581%
27	15.504	2277	2281	2286	rVB	131834	197432	11.79%	1.849%
28	15.951	2353	2357	2365	rVB2	90398	154336	9.22%	1.445%
29	17.057	2541	2545	2551	rVB4	41989	78565	4.69%	0.736%

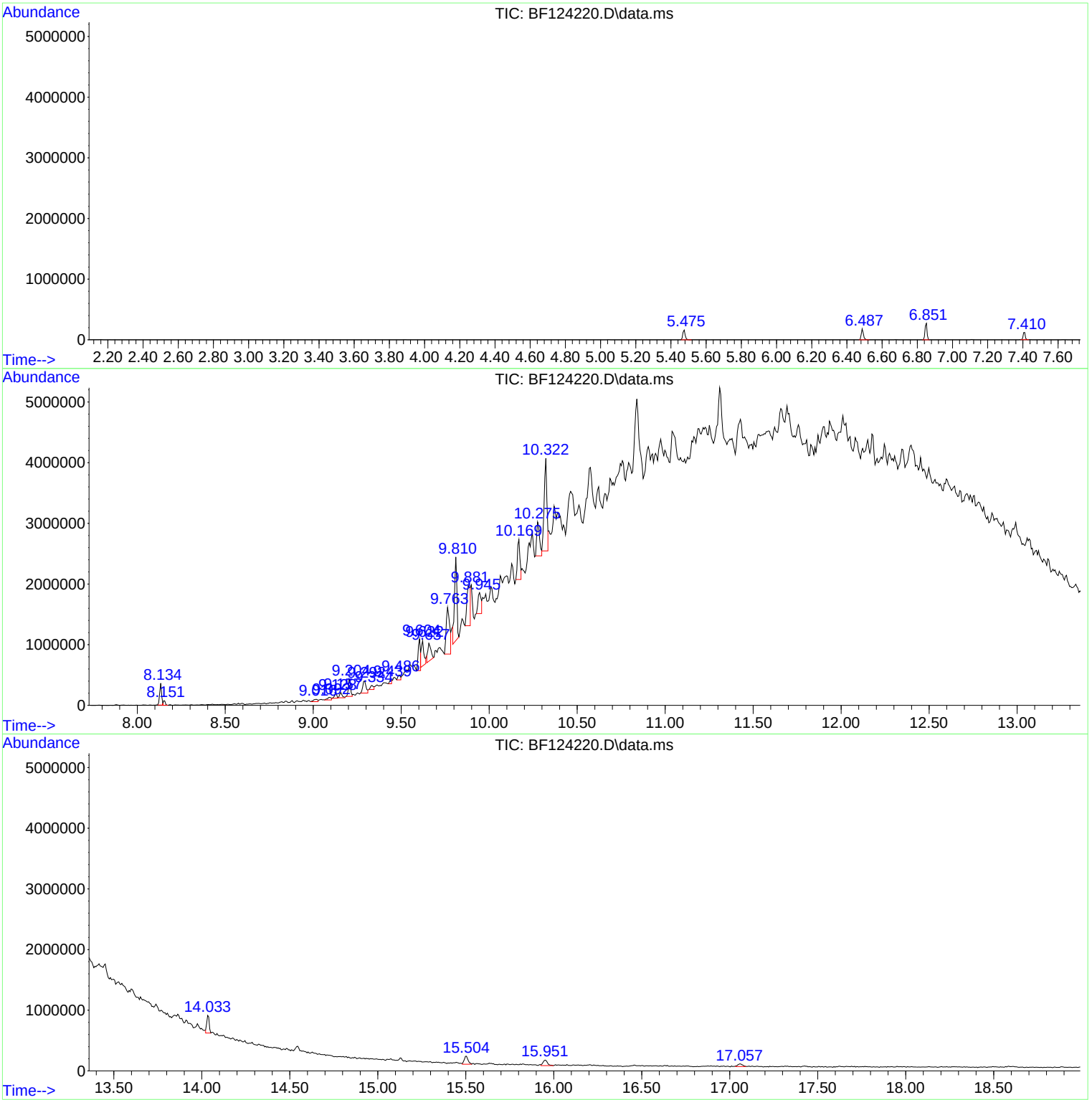
Sum of corrected areas: 10677750

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124220.D
Acq On : 9 Jun 2021 21:32
Operator : JU/CG
Sample : M2634-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R44-STONE-2

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124220.D
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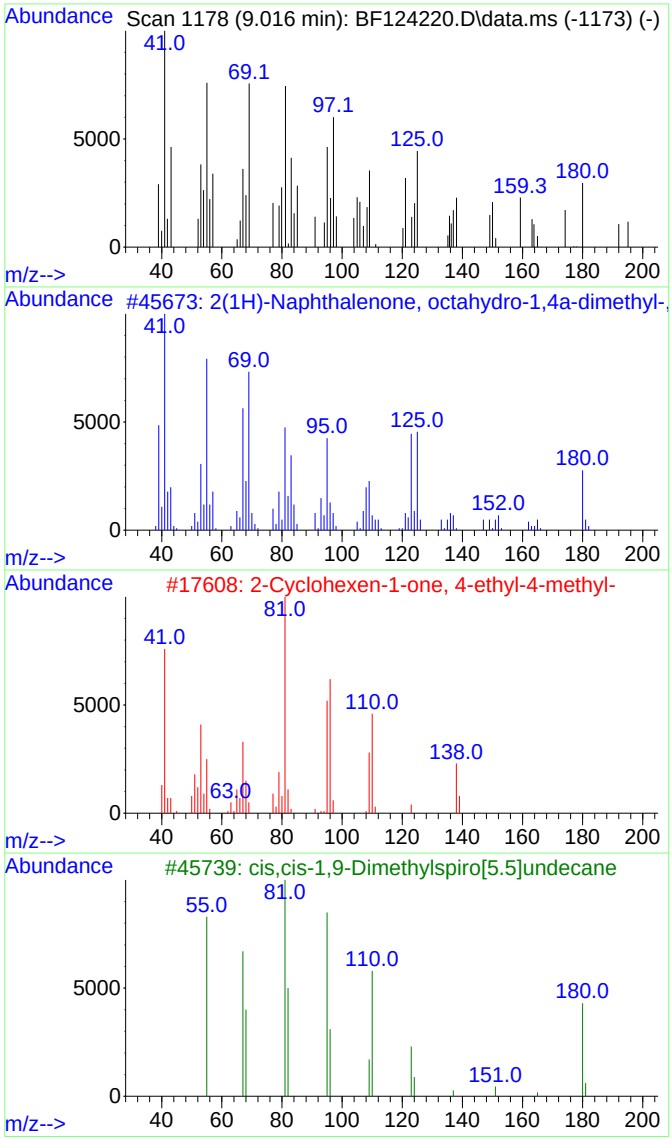
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

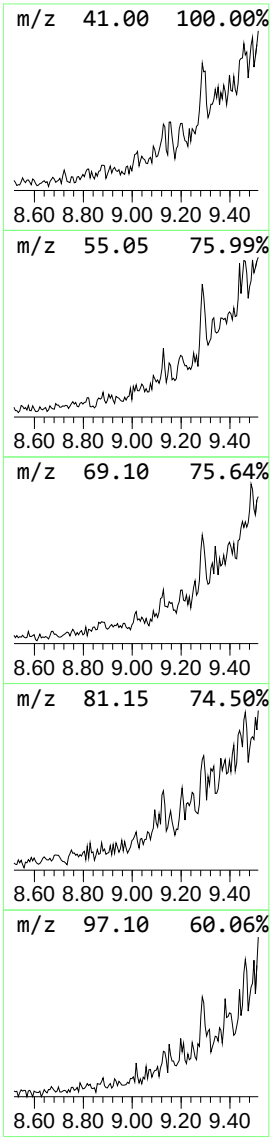
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2(1H)-Naphthalenone, octahy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.016	4.87 ng	66467	Naphthalene-d8	8.134

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, octahydro-1...	180	C12H20O	022738-31-4	83
2	2-Cyclohexen-1-one, 4-ethyl-4-me...	138	C9H14O	017429-32-2	46
3	cis,cis-1,9-Dimethylspiro[5.5]un...	180	C13H24	1000111-73-4	42
4	2-Butene, 1-chloro-2-methyl-	104	C5H9Cl	013417-43-1	35
5	2,4-Octadienal, (E,E)-	124	C8H12O	030361-28-5	35





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Data File : BF124220.D
Acq On : 9 Jun 2021 21:32
Operator : JU/CG
Sample : M2634-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-2

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

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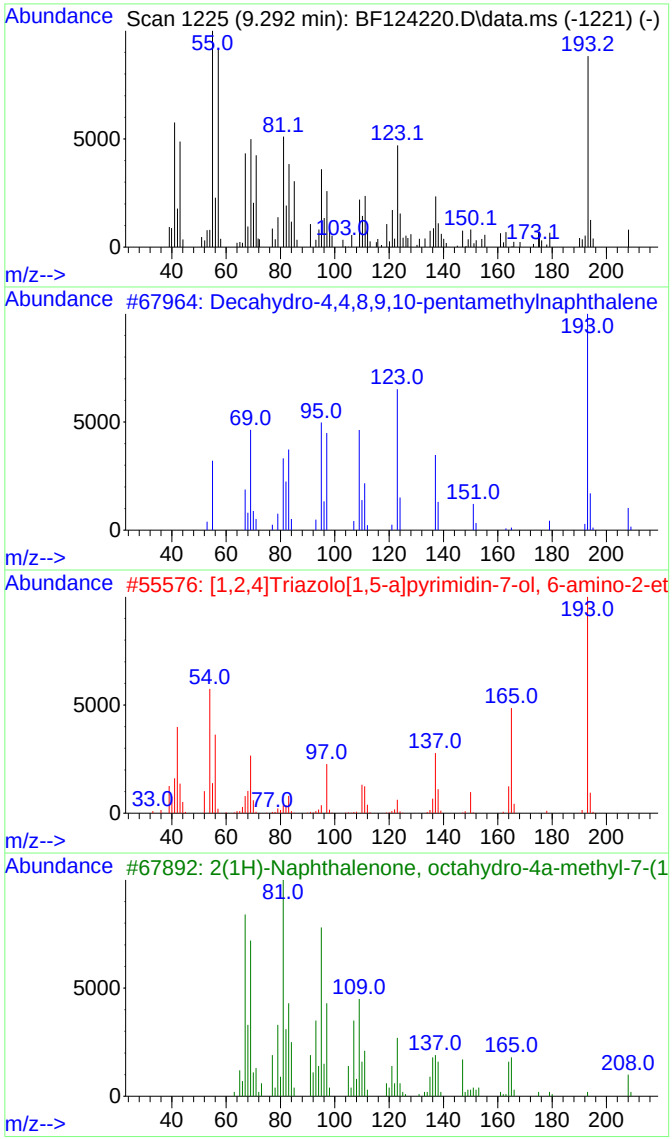
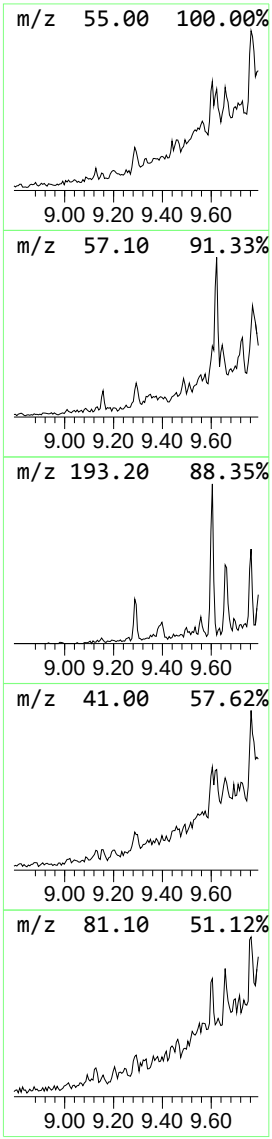
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Decahydro-4,4,8,9,10-pentam... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.292	5.69 ng	263782	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	64
2	[1,2,4]Triazolo[1,5-a]pyrimidin-...	193	C8H11N5O	1000351-50-1	43
3	2(1H)-Naphthalenone, octahydro-4...	208	C14H24O	054594-42-2	38
4	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	30
5	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	30





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Data File : BF124220.D
Acq On : 9 Jun 2021 21:32
Operator : JU/CG
Sample : M2634-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-2

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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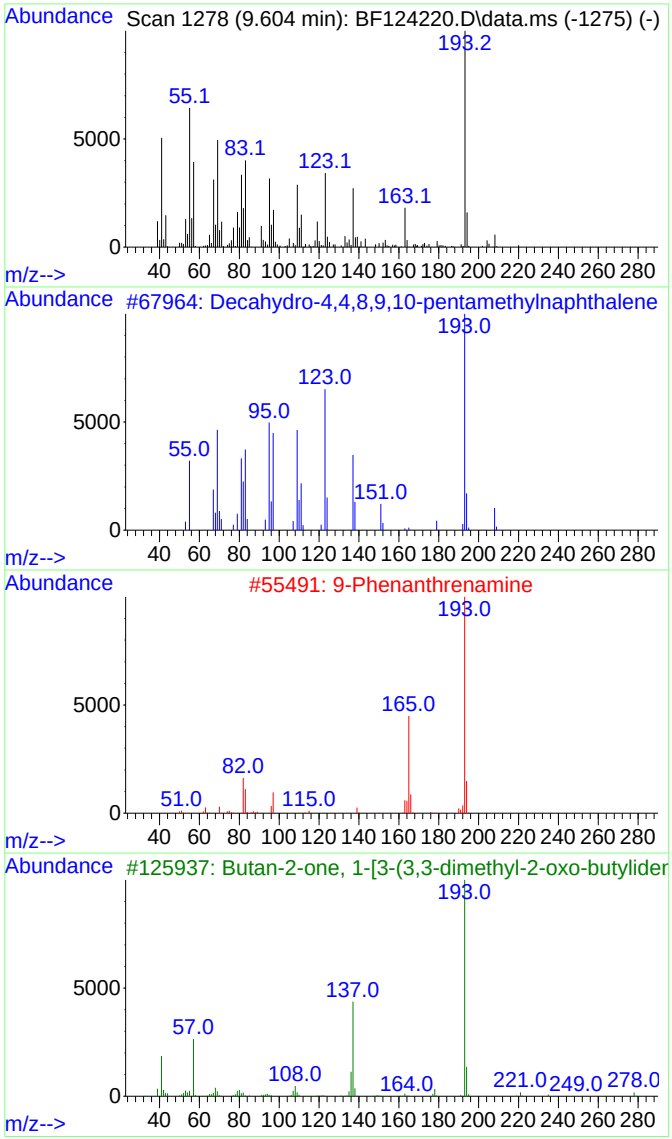
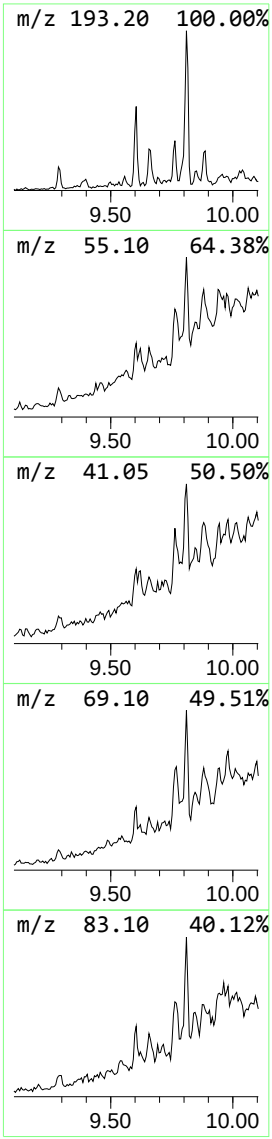
****

Peak Number 3 unknown9.604 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.604	10.27 ng	475706	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	64
2	9-Phenanthrenamine	193	C14H11N	000947-73-9	35
3	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	35
4	Pyrazole, 5-methyl-3-(5-nitro-2-...	193	C8H7N3O3	016239-90-0	35
5	Acridine, 9-methyl-	193	C14H11N	000611-64-3	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124220.D
Acq On : 9 Jun 2021 21:32
Operator : JU/CG
Sample : M2634-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R44-STONE-2

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

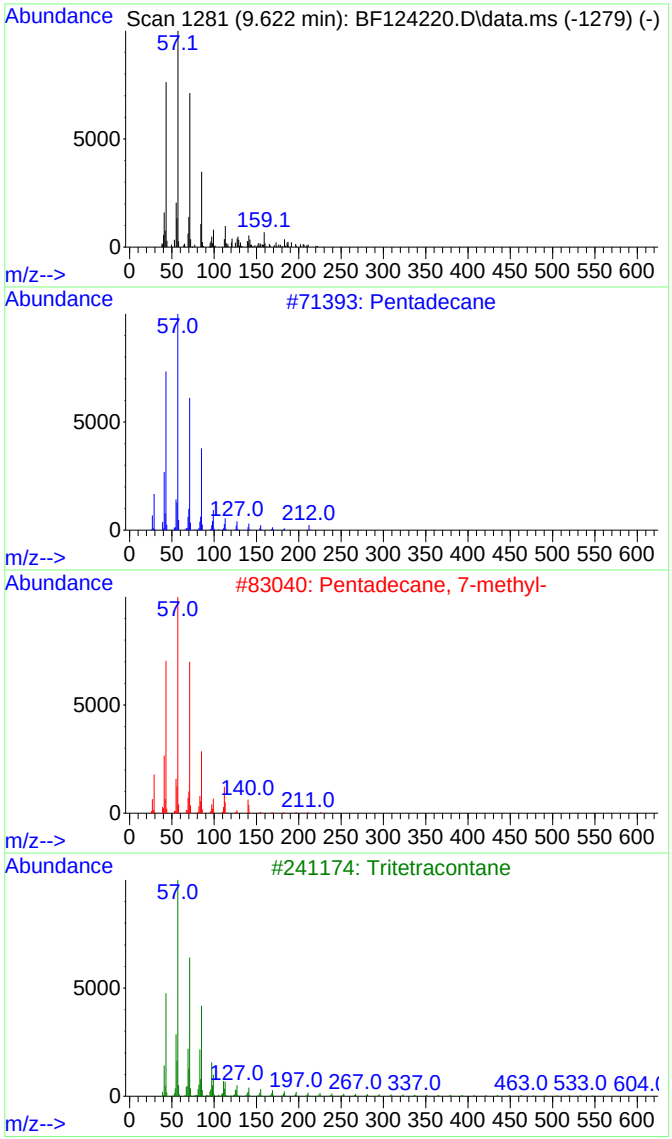
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

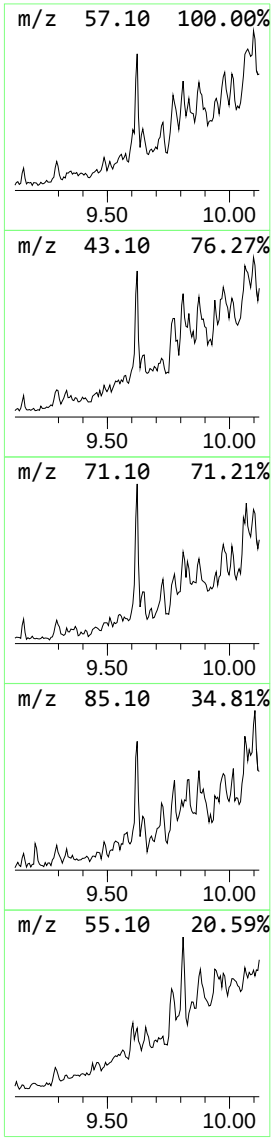
****

Peak Number 4 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.622	9.06 ng	419494	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	80
2	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	80
3	Tritetracontane	605	C43H88	007098-21-7	80
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	74
5	Undecane, 6-ethyl-	184	C13H28	017312-60-6	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124220.D
Acq On : 9 Jun 2021 21:32
Operator : JU/CG
Sample : M2634-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-2

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

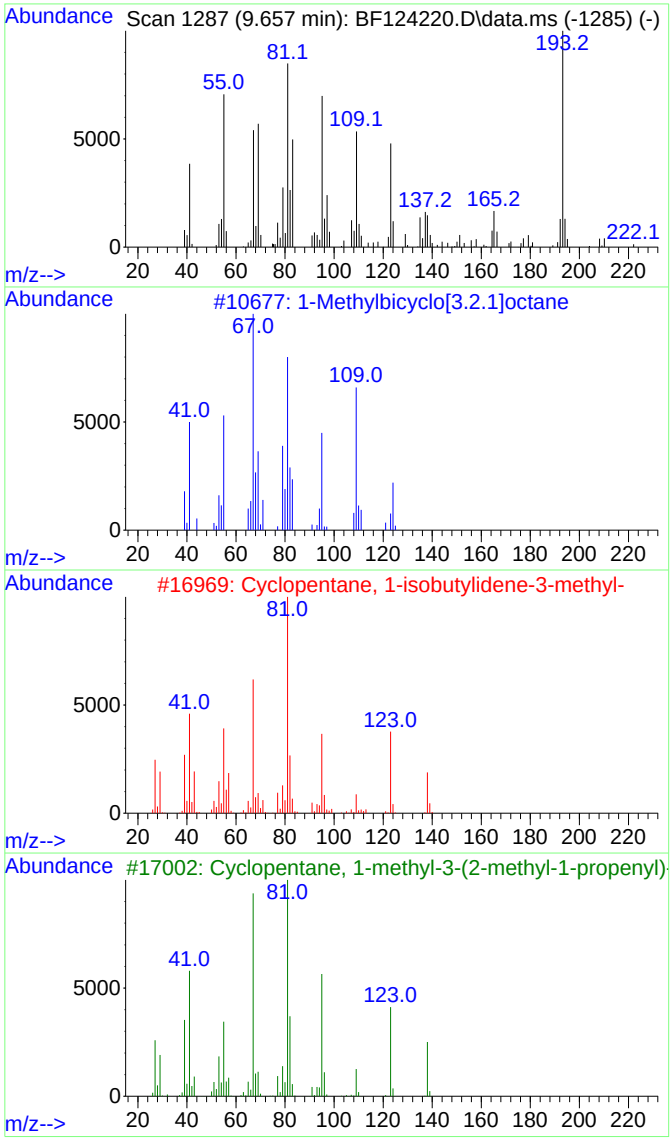
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

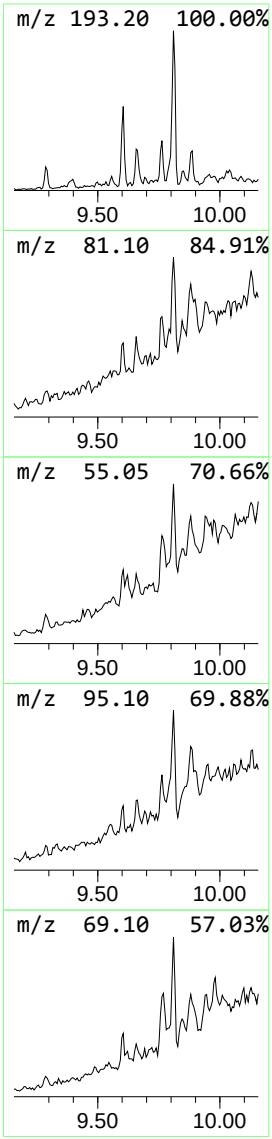
****

Peak Number 5 unknown9.657 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.657	7.75 ng	359113	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methylbicyclo[3.2.1]octane	124	C9H16	119972-41-7	45
2	Cyclopentane, 1-isobutylidene-3-...	138	C10H18	1000150-62-1	38
3	Cyclopentane, 1-methyl-3-(2-meth...	138	C10H18	075873-01-7	38
4	Muurolane-B	208	C15H28	1000121-63-7	30
5	3-Hexen-2-one, 3-cyclohexyl-4-et...	208	C14H24O	1000150-19-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124220.D
Acq On : 9 Jun 2021 21:32
Operator : JU/CG
Sample : M2634-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R44-STONE-2

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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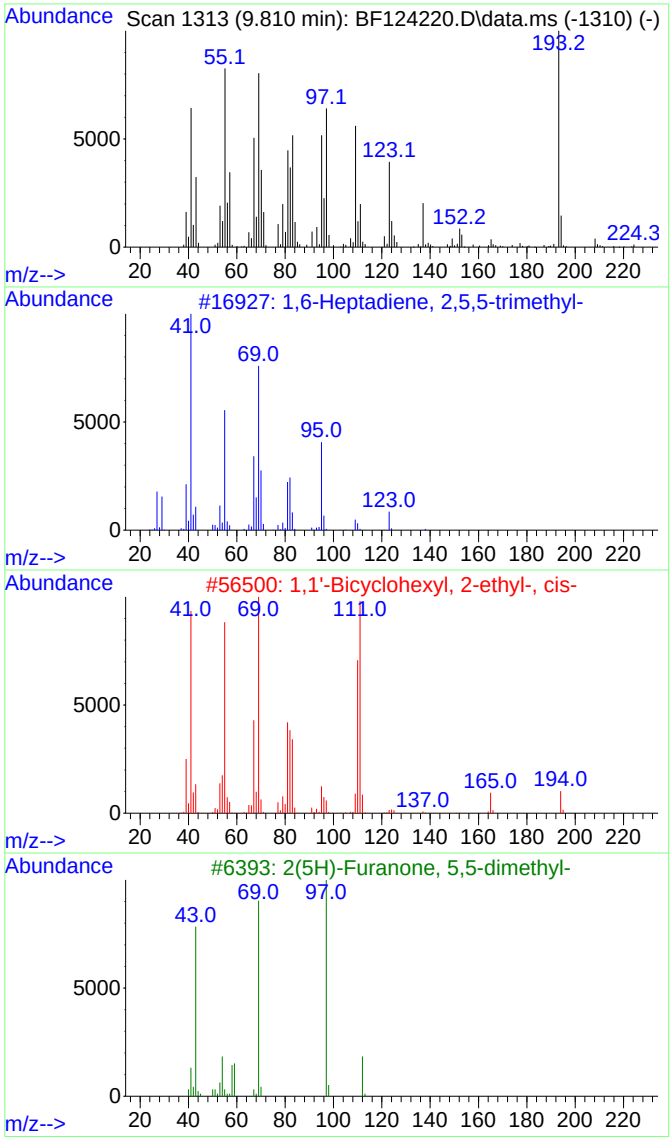
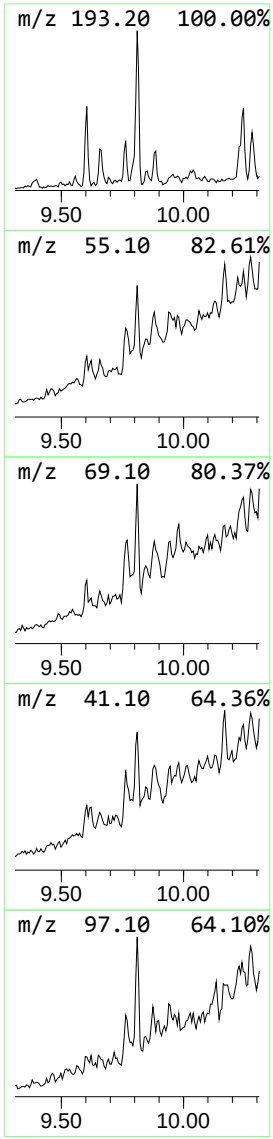
****

Peak Number 6 unknown9.810 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.810	27.93 ng	1293730	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Heptadiene, 2,5,5-trimethyl-	138	C10H18	062238-28-2	25
2	1,1'-Bicyclohexyl, 2-ethyl-, cis-	194	C14H26	050991-12-3	20
3	2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	18
4	Cyclohexane, 1,3-dimethyl-2-meth...	124	C9H16	020348-74-7	15
5	5-Hexen-1-ol, 2-(2-methyl-1-prop...	154	C10H18O	018675-19-9	14





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Acq On : 9 Jun 2021 21:32
Operator : JU/CG
Sample : M2634-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R44-STONE-2

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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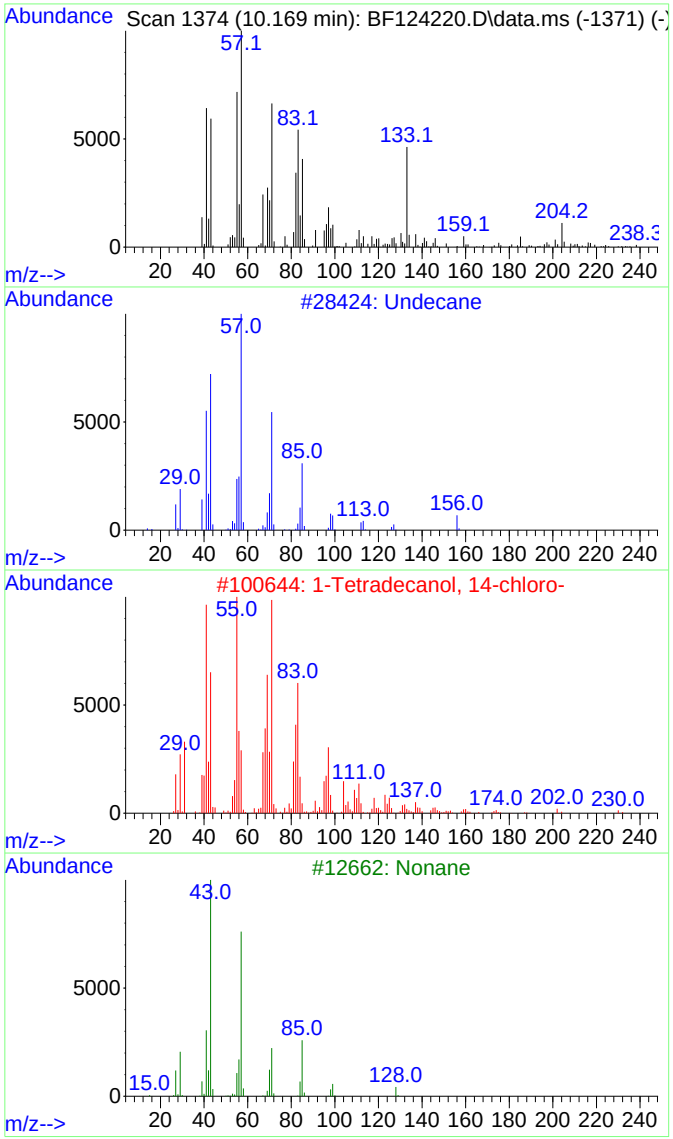
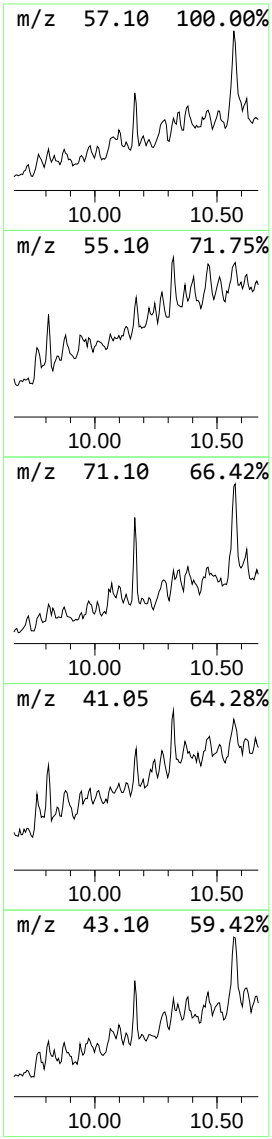
Peak Number 7 unknown10.169 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.169	14.30 ng	662314	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	42
2	1-Tetradecanol, 14-chloro-	248	C14H29ClO	073937-05-0	38
3	Nonane	128	C9H20	000111-84-2	38
4	Sulfurous acid, hexyl pentadecyl...	376	C21H44O3S	1000309-13-7	30
5	Tridecane	184	C13H28	000629-50-5	30





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-2

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

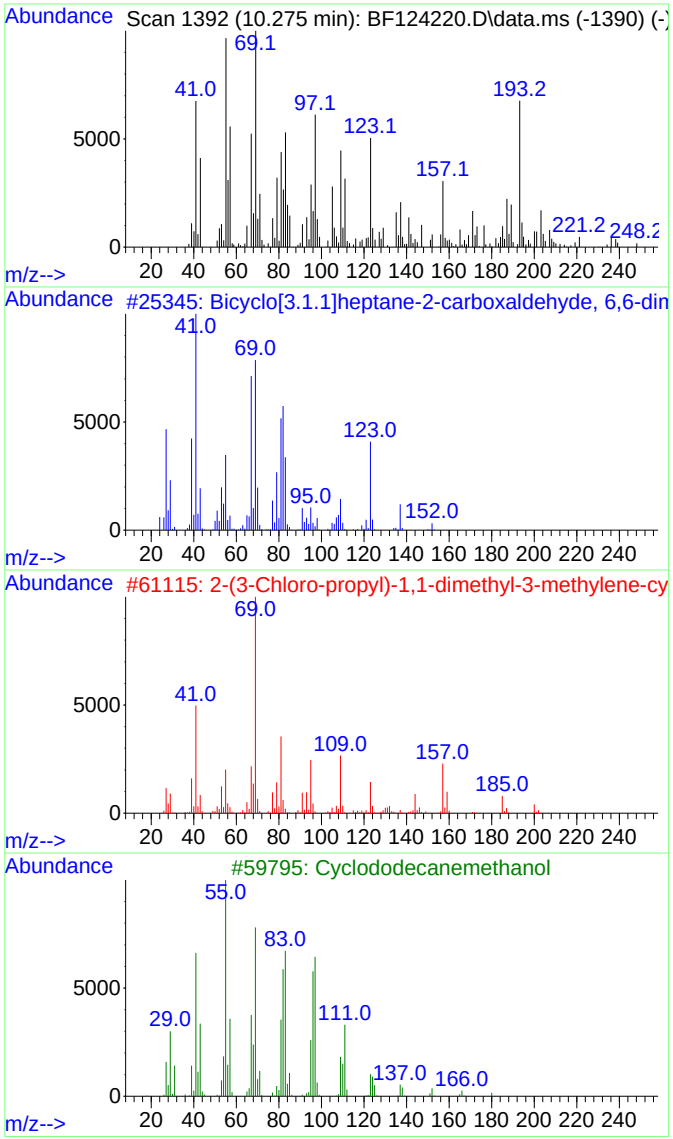
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

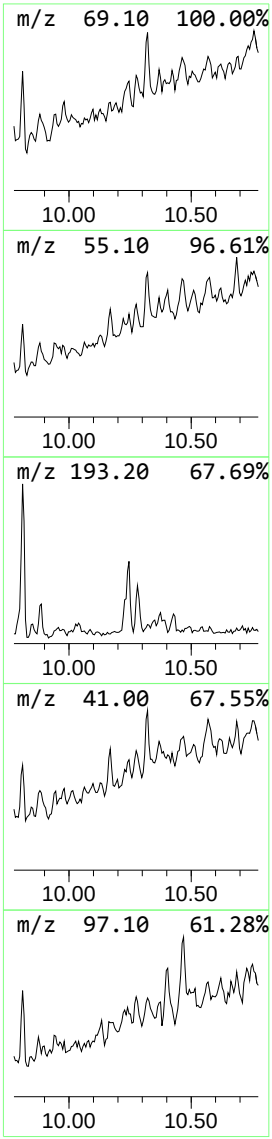
****

Peak Number 8 unknown10.275 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.275	14.03 ng	649973	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptane-2-carboxal...	152	C10H16O	004764-14-1	38
2	2-(3-Chloro-propyl)-1,1-dimethyl...	200	C12H21Cl	1000191-45-6	38
3	Cyclododecanemethanol	198	C13H26O	001892-12-2	30
4	Cyclopropanemethanol, 2-methyl-2...	168	C11H20O	098678-70-7	27
5	1,7-Nonadiene, 4,8-dimethyl-	152	C11H20	062108-28-5	27





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Data File : BF124220.D
Acq On : 9 Jun 2021 21:32
Operator : JU/CG
Sample : M2634-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-2

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

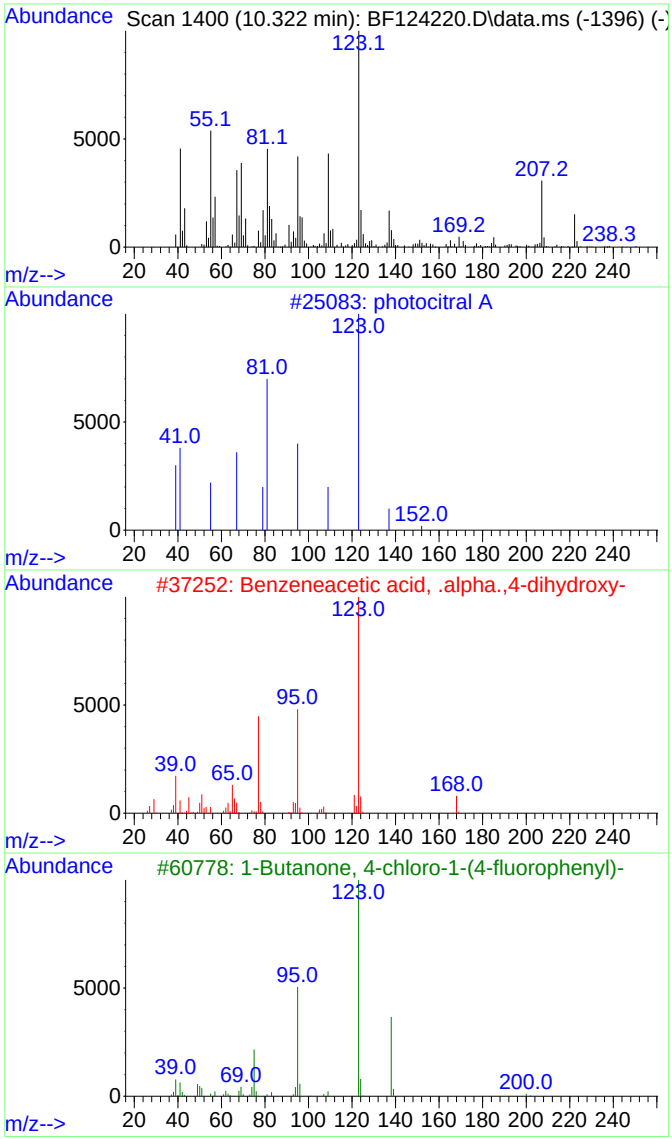
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

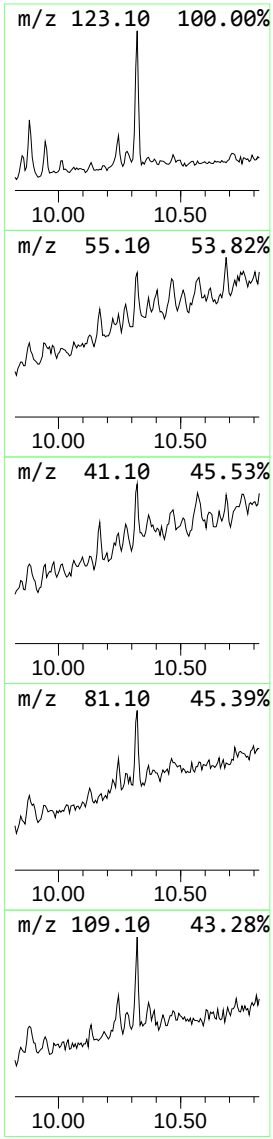
****

Peak Number 9 unknown10.322 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.322	36.16 ng	1674800	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	photocitral A	152	C10H16O	055253-28-6	43
2	Benzeneacetic acid, .alpha.,4-di...	168	C8H8O4	001198-84-1	43
3	1-Butanone, 4-chloro-1-(4-fluoro...	200	C10H10ClFO	003874-54-2	43
4	1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	43
5	1,3-Diazocin-2-one, perhydro-1-(...	250	C13H15FN2O2	1000267-45-2	43





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Data File : BF124220.D
Acq On : 9 Jun 2021 21:32
Operator : JU/CG
Sample : M2634-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-2

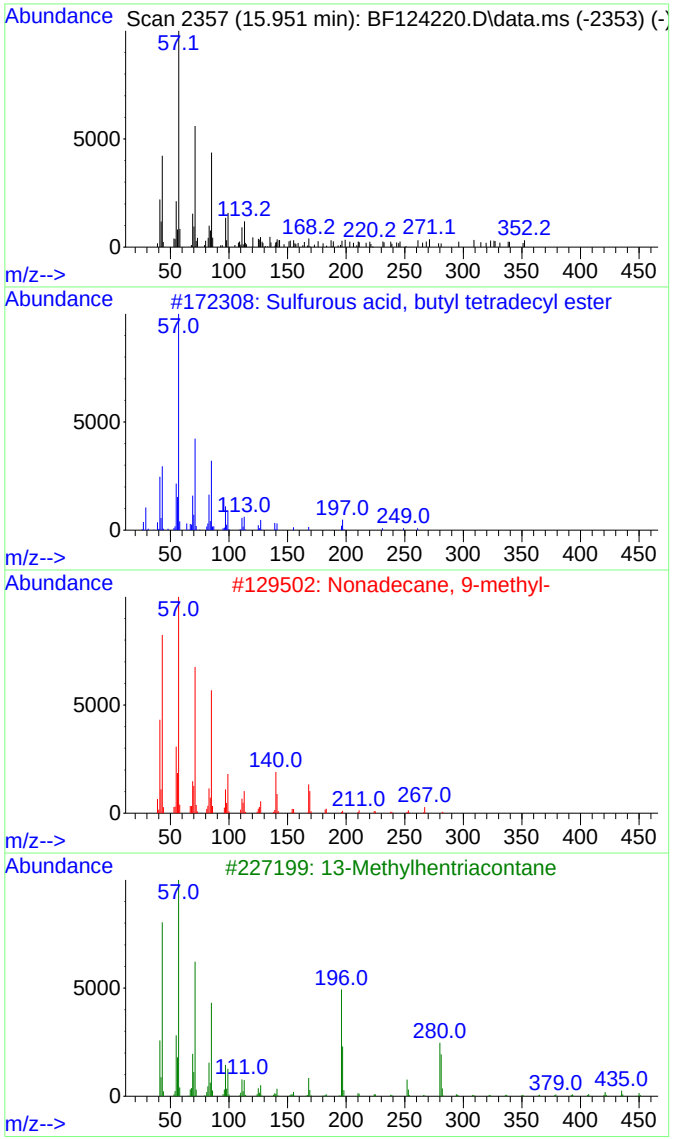
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

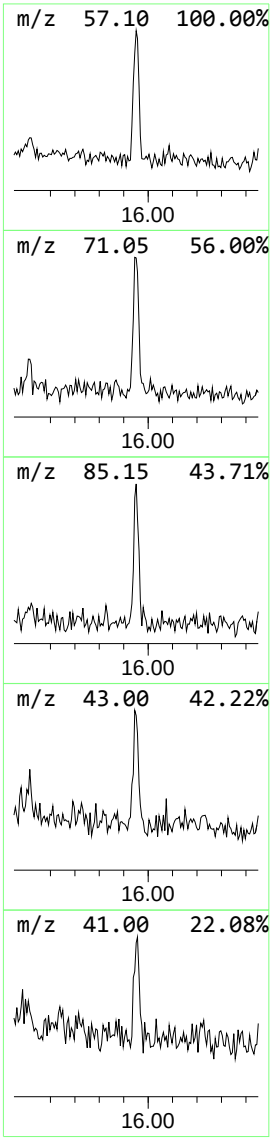
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Sulfurous acid, butyl tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	15.63 ng	154336	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	90
2	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90
3	13-Methylhentriacontane	451	C32H66	1000131-19-4	90
4	Tetracosane	338	C24H50	000646-31-1	83
5	Heneicosane	296	C21H44	000629-94-7	81





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Data File : BF124220.D
Acq On : 9 Jun 2021 21:32
Operator : JU/CG
Sample : M2634-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-2

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

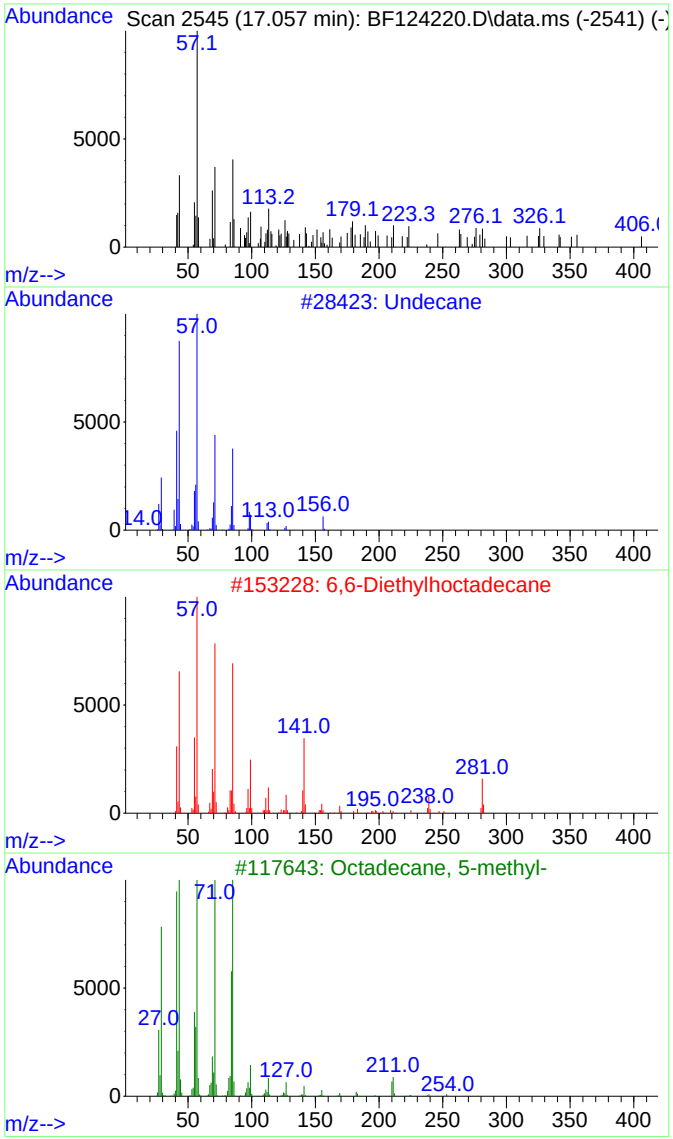
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

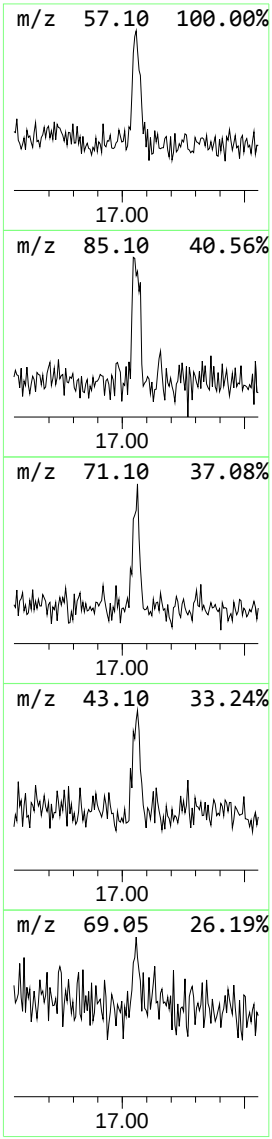
****

Peak Number 11 unknown17.057 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.057	7.96 ng	78565	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	35
2	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	35
3	Octadecane, 5-methyl-	268	C19H40	025117-35-5	35
4	3,5-Dimethyldodecane	198	C14H30	107770-99-0	35
5	3-Hexanone, 2,5-dimethyl-	128	C8H16O	001888-57-9	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124220.D
Acq On : 9 Jun 2021 21:32
Operator : JU/CG
Sample : M2634-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R44-STONE-2

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
2(1H)-Naphthale...	9.016	4.9	ng	66467	2	8.134	273241	20.0
Decahydro-4,4,8...	9.292	5.7	ng	263782	3	9.898	926410	20.0
unknown9.604	9.604	10.3	ng	475706	3	9.898	926410	20.0
Pentadecane	9.622	9.1	ng	419494	3	9.898	926410	20.0
unknown9.657	9.657	7.8	ng	359113	3	9.898	926410	20.0
unknown9.810	9.810	27.9	ng	1293730	3	9.898	926410	20.0
unknown10.169	10.169	14.3	ng	662314	3	9.898	926410	20.0
unknown10.275	10.275	14.0	ng	649973	3	9.898	926410	20.0
unknown10.322	10.322	36.2	ng	1674800	3	9.898	926410	20.0
Sulfurous acid,...	15.951	15.6	ng	154336	6	15.504	197432	20.0
unknown17.057	17.057	8.0	ng	78565	6	15.504	197432	20.0