LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
Operator : JU/CG
Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-3

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_M\Methods\8270-BM121620.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028153.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.728	89	92	101	rBV	28535	44071	1.06%	0.100%
2	5.222	340	346	357	rBV	87965	126433	3.05%	0.288%
3	5.704	421	428	438	rBV	2259091	3355909	80.88%	7.642%
4	7.351	700	708	721	rBV	2206890	3589037	86.50%	8.173%
5	7.792	778	783	796	rBV	146629	234628	5.65%	0.534%
6	8.210	845	854	861	rBV	645741	1007304	24.28%	2.294%
7	9.386	1046	1054	1061	rBV	1372998	2220922	53.52%	5.057%
8	11.039	1328	1335	1342	rBV	772705	1299147	31.31%	2.958%
9	13.463	1739	1747	1754	rBV	2709569	4016517	96.80%	9.146%
10	13.716	1785	1790	1799	rVB	216882	328551	7.92%	0.748%
11	14.280	1878	1886	1893	rBV	303073	418908	10.10%	0.954%
12	14.563	1928	1934	1941	rBV	98623	152537	3.68%	0.347%
13	14.839	1973	1981	1987	rBV	918360	1389238	33.48%	3.164%
14	15.921	2160	2165	2174	rVB	85086	123725	2.98%	0.282%
15	16.310	2224	2231	2237	rBV	1719979	2449143	59.02%	5.577%
16	16.898	2327	2331	2335	rBV2	42725	51773	1.25%	0.118%
17	17.151	2367	2374	2381	rBV	33980	52796	1.27%	0.120%
18	17.556	2437	2443	2447	rBV	986533	1382480	33.32%	3.148%
19	17.598	2447	2450	2457	rVV	300441	396816	9.56%	0.904%
20	17.686	2460	2465	2470	rVV	144576	211221	5.09%	0.481%
21	17.733	2470	2473	2480	rVB3	23312	43067	1.04%	0.098%
22	17.951	2505	2510	2515	rVB	48683	75432	1.82%	0.172%
23	18.409	2583	2588	2594	rBV2	232660	347344	8.37%	0.791%
24	18.468	2594	2598	2605	rVB2	54281	124802	3.01%	0.284%
25	18.545	2608	2611	2616	rVB	34020	46846	1.13%	0.107%
26	18.615	2616	2623	2627	rBV2	72333	142213	3.43%	0.324%
27	18.703	2634	2638	2643	rBV6	23601	41973	1.01%	0.096%
28	19.262	2729	2733	2738	rBV3	49751	68291	1.65%	0.156%
29	19.321	2740	2743	2749	rVB4	30170	44294	1.07%	0.101%
30	19.580	2782	2787	2793	rVB	646523	860883	20.75%	1.960%
31	19.662	2798	2801	2807	rBV3	72411	99842	2.41%	0.227%
32	19.939	2837	2848	2855	rBV	541051	994997	23.98%	2.266%
33	20.127	2875	2880	2885	rBV	3270584	3974354	95.78%	9.050%
34	20.521	2944	2947	2951	rVB	67604	75214	1.81%	0.171%
35	20.715	2978	2980	2984	rBV2	61806	61372	1.48%	0.140%
36	21.356	3085	3089	3093	rBV	1020223	1187146	28.61%	2.703%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
Operator : JU/CG
Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-3

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_M\Methods\8270-BM121620.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.668	3136	3142	3146	rBV2	1285402	2208447	53.22%	5.029%
38	21.703	3146	3148	3157	rVB	343197	432651	10.43%	0.985%
39	21.833	3166	3170	3175	rBV2	545444	643540	15.51%	1.465%
40	21.886	3175	3179	3183	rBV	699991	868579	20.93%	1.978%
41	21.933	3184	3187	3189	rBV2	229186	257201	6.20%	0.586%
42	22.850	3337	3343	3352	rBV	2747334	4149377	100.00%	9.449%
43	23.321	3418	3423	3427	rBV3	596348	1286698	31.01%	2.930%
44	23.833	3506	3510	3521	rVB	381361	705335	17.00%	1.606%
45	23.933	3523	3527	3536	rVB	507421	951254	22.93%	2.166%
46	24.038	3540	3545	3551	rVV	781570	1372047	33.07%	3.124%

Sum of corrected areas: 43914355

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
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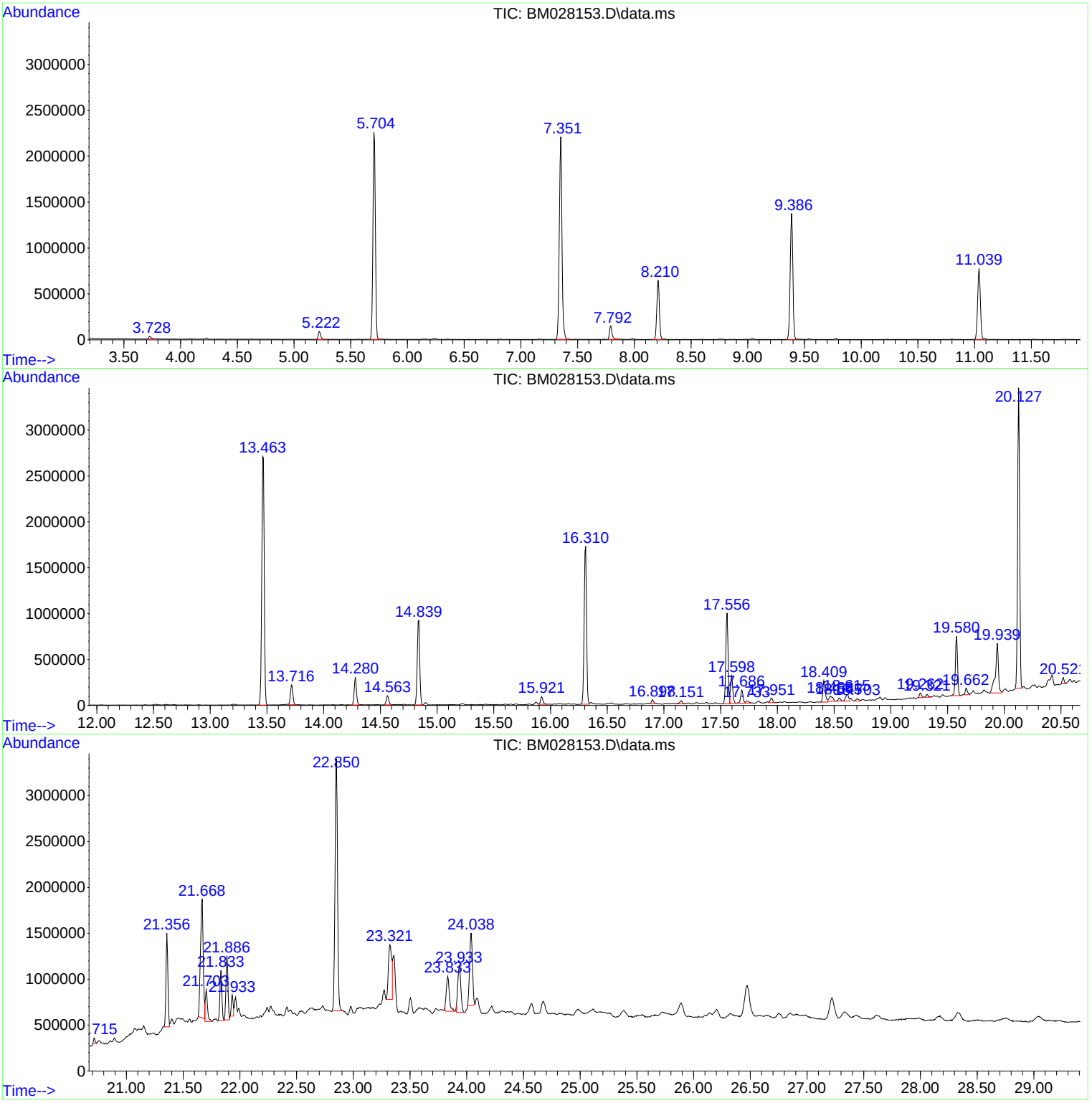
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.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_M\Data\BM121720\
Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
Operator : JU/CG
Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-3

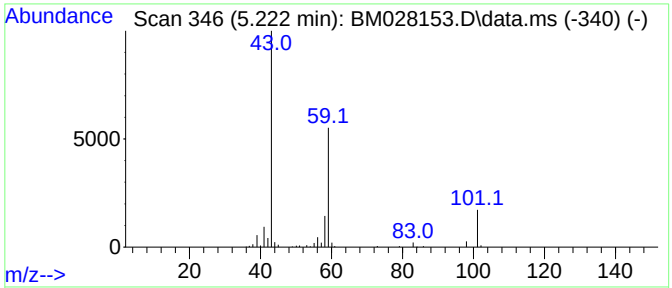
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

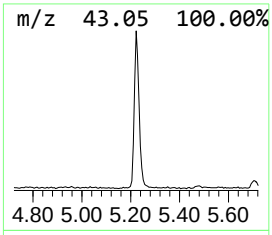
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

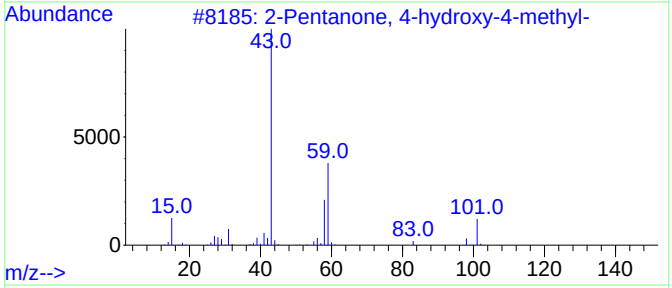
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

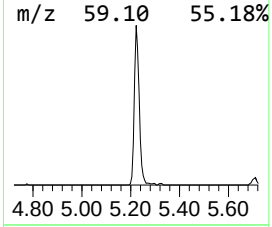
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.222	2.51 ng	126433	1,4-Dichlorobenzene-d4	8.210

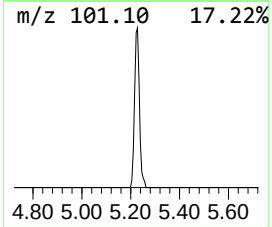
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2-Pentanone	86	C5H10O	000107-87-9	10

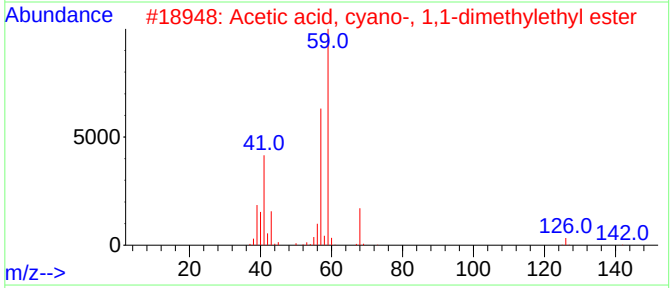


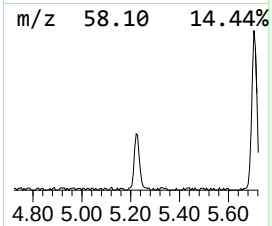


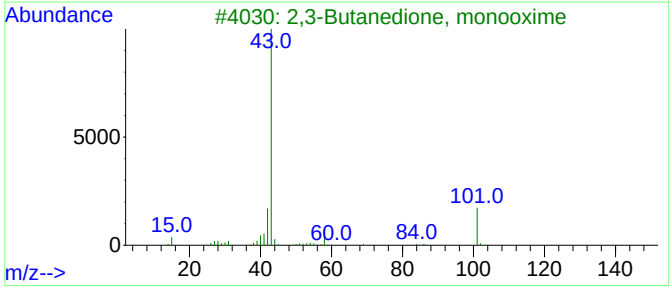


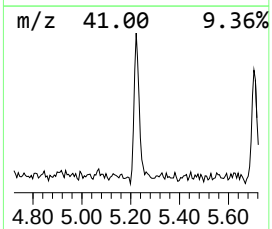












Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
Operator : JU/CG
Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-3

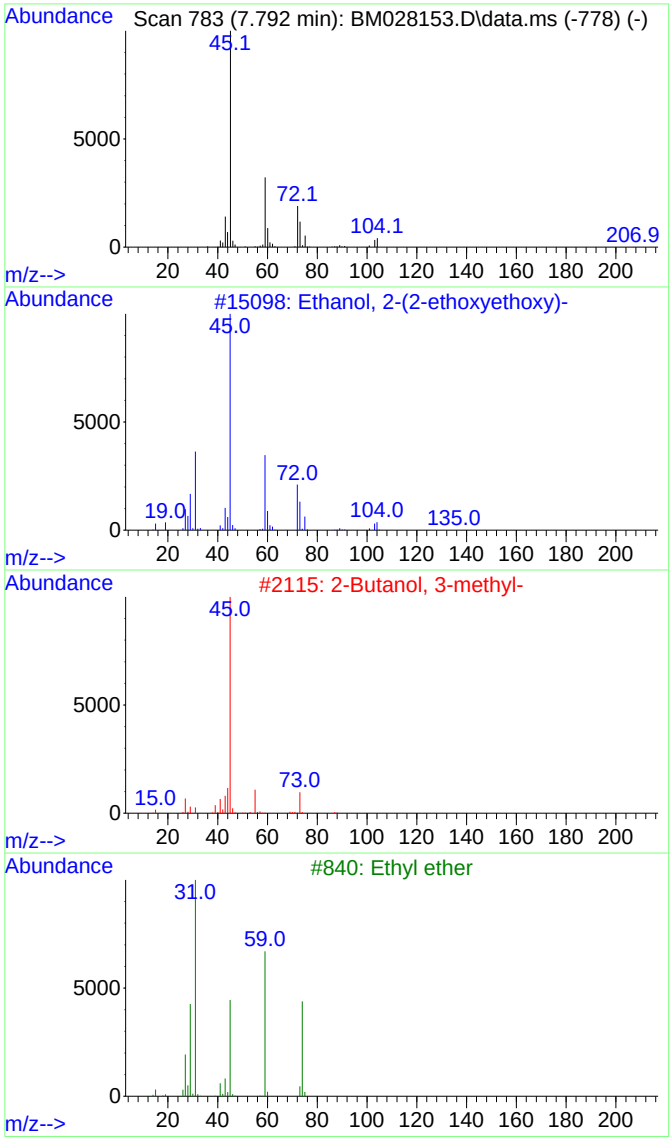
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

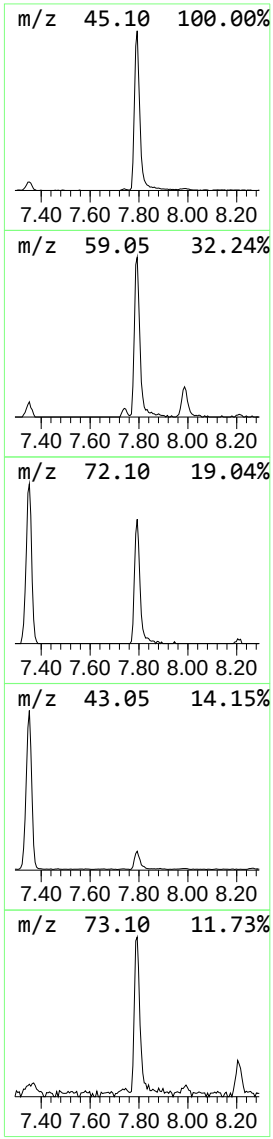
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.792	4.66 ng	234628	1,4-Dichlorobenzene-d4	8.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	47
3	Ethyl ether	74	C4H10O	000060-29-7	33
4	Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	33
5	(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
Operator : JU/CG
Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-3

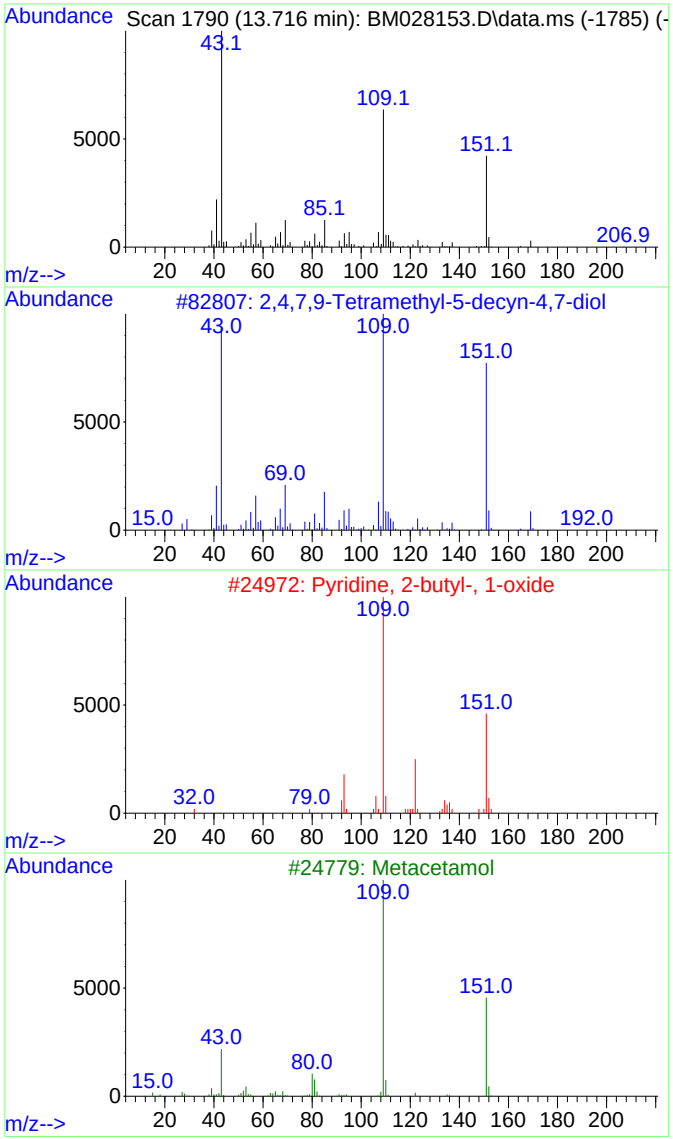
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

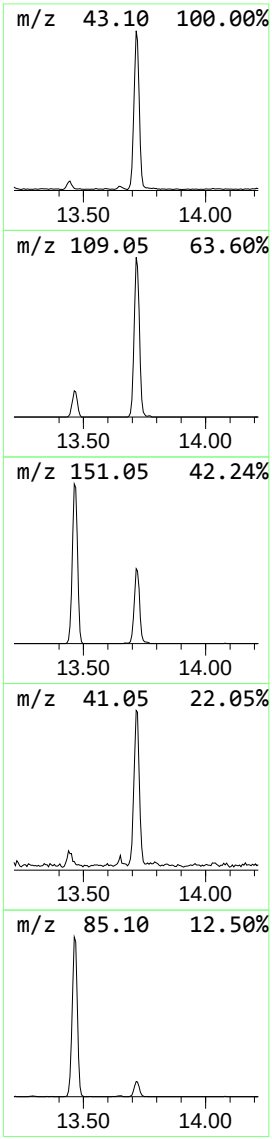
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.716	4.73 ng	328551	Acenaphthene-d10	14.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	83
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	Metacetamol	151	C8H9NO2	000621-42-1	52
4	Acetaminophen	151	C8H9NO2	000103-90-2	50
5	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
Operator : JU/CG
Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

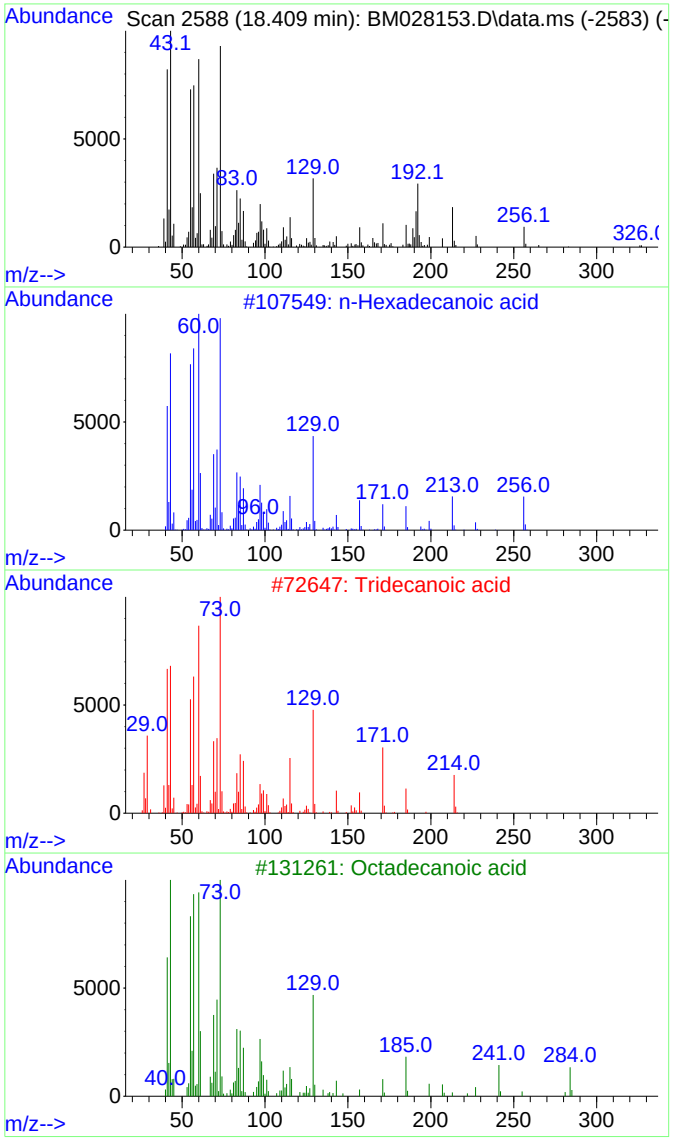
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

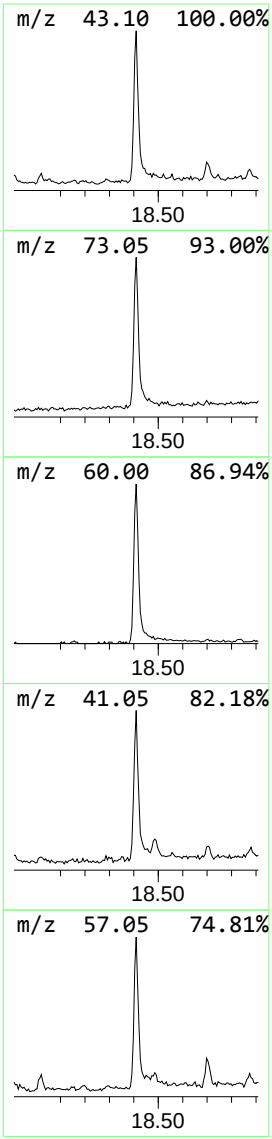
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.409	5.02 ng	347344	Phenanthrene-d10	17.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Octadecanoic acid	284	C18H36O2	000057-11-4	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
Operator : JU/CG
Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-3

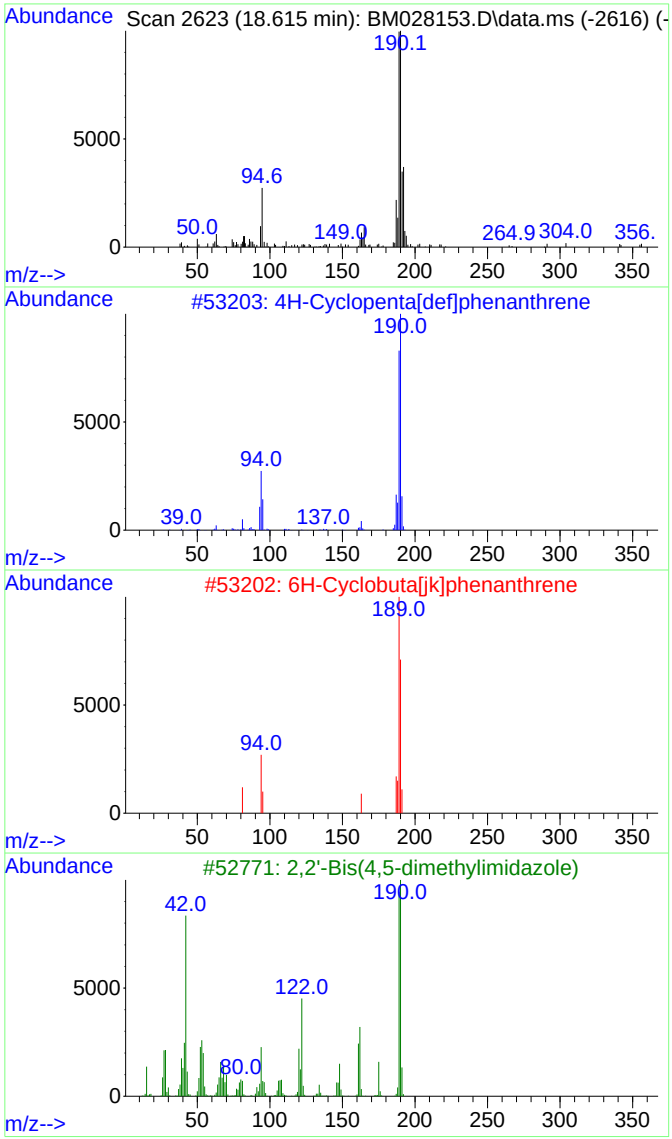
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

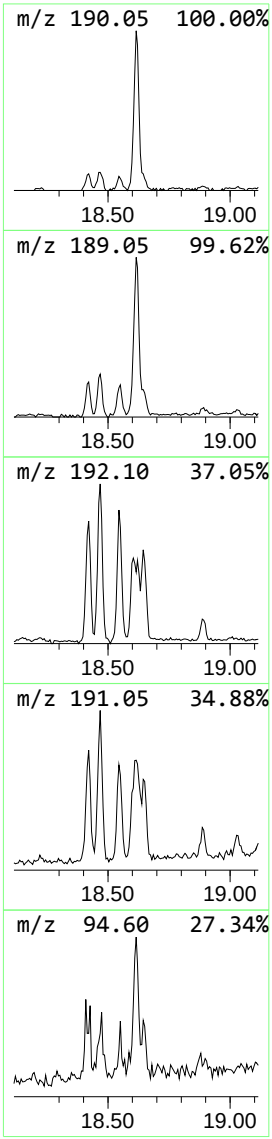
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.615	2.06 ng	142213	Phenanthrene-d10	17.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	72
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	36
4	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25
5	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	25





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Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
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Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

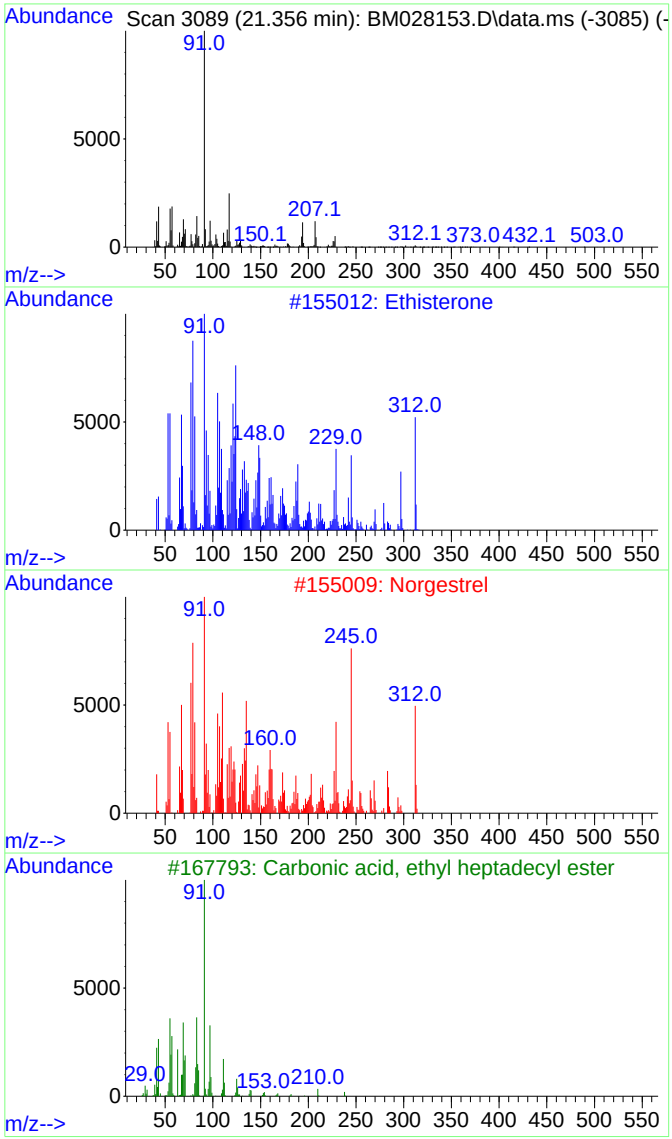
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

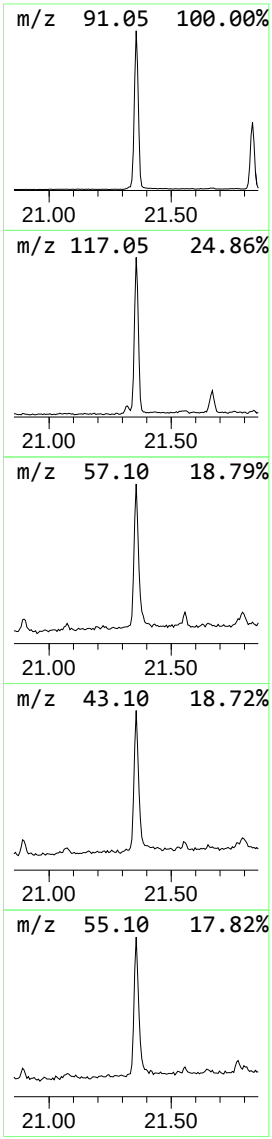
****

Peak Number 6 unknown21.356 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.356	10.75 ng	1187150	Chrysene-d12	21.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethisterone	312	C21H28O2	000434-03-7	25
2	Norgestrel	312	C21H28O2	006533-00-2	15
3	Carbonic acid, ethyl heptadecyl ...	328	C20H40O3	1000314-59-7	11
4	Carbonic acid, ethyl octadecyl e...	342	C21H42O3	1000314-59-8	11
5	Butanamide, 3-hydroxy-3-methyl-N...	223	C12H17NO3	1000185-71-6	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
Operator : JU/CG
Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

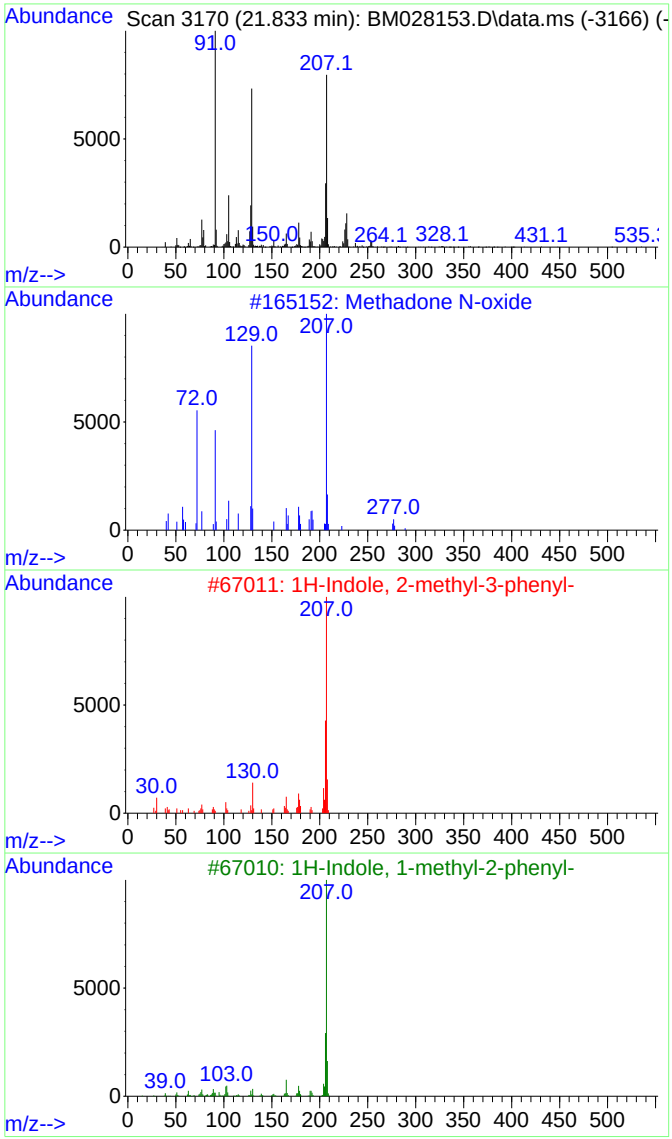
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

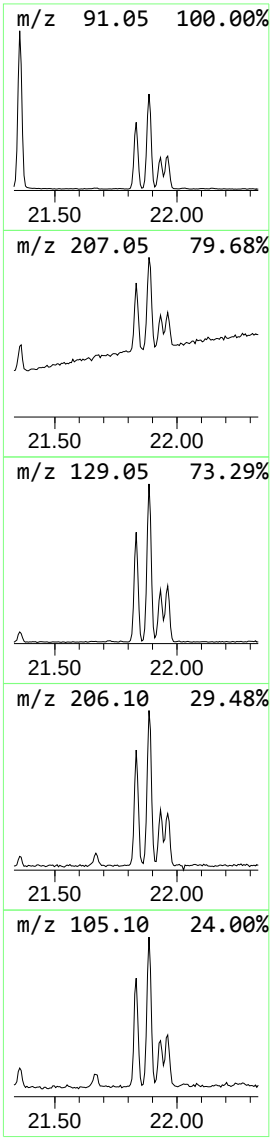
****

Peak Number 7 Methadone N-oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.833	5.83 ng	643540	Chrysene-d12	21.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methadone N-oxide	325	C21H27NO2	1000120-80-7	64
2	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	50
3	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	42
4	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	38
5	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
Operator : JU/CG
Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.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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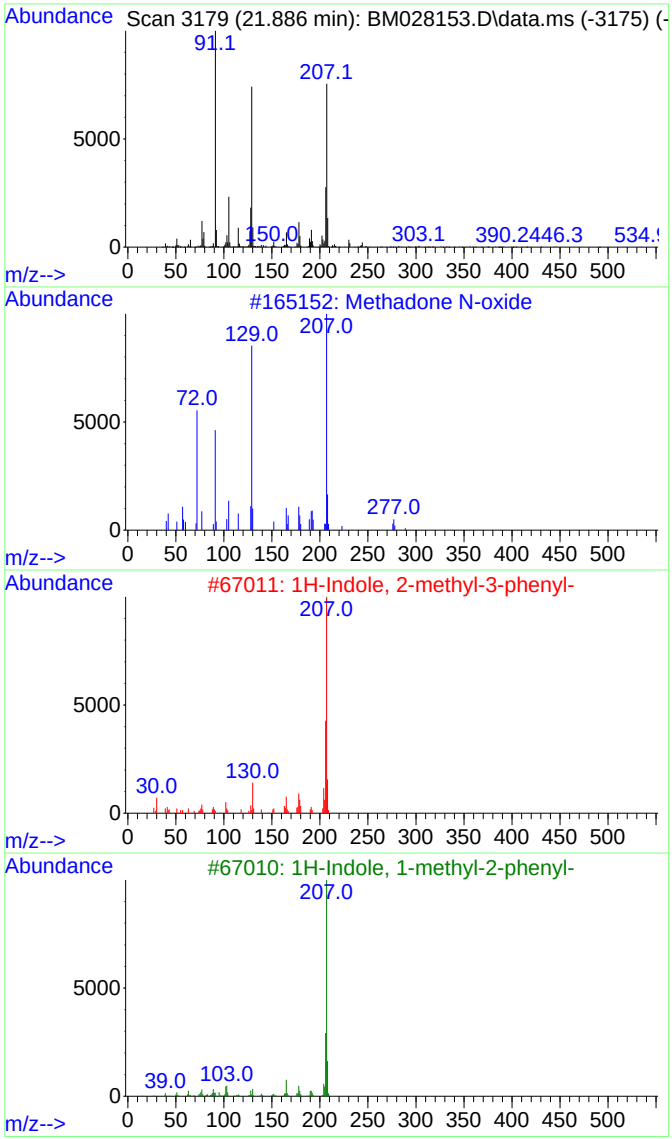
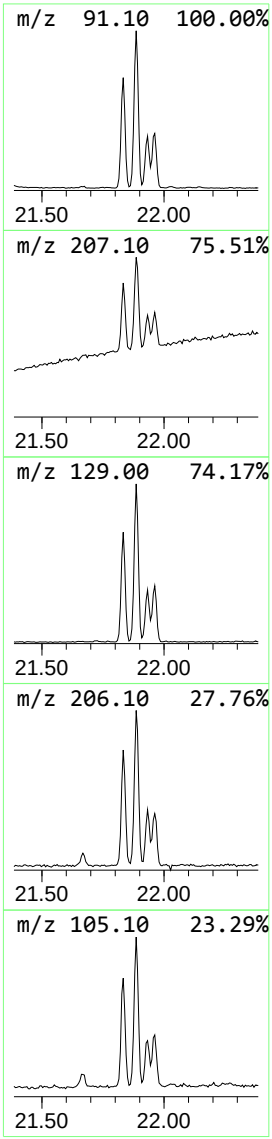
Peak Number 8 unknown21.886 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.886	7.87 ng	868579	Chrysene-d12	21.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methadone N-oxide	325	C21H27NO2	1000120-80-7	64
2	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	45
3	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	38
4	1-benzylindole	207	C15H13N	1000334-31-3	38
5	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
Operator : JU/CG
Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.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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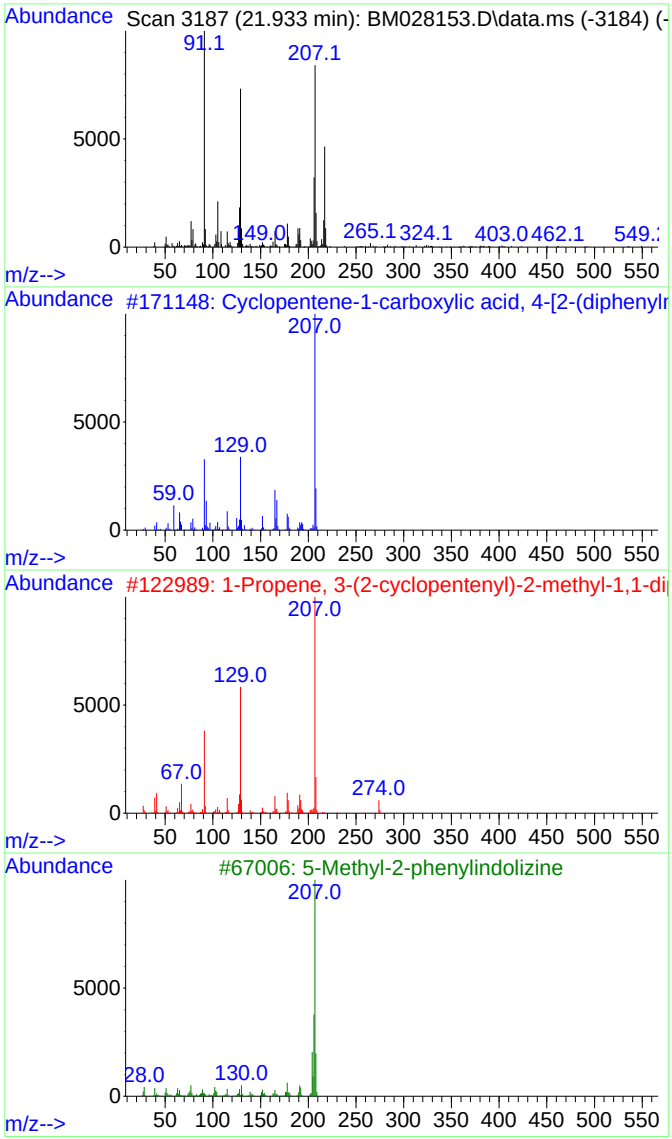
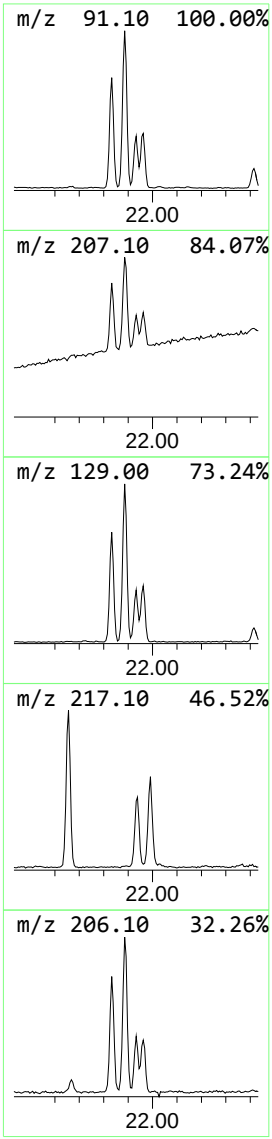
Peak Number 9 unknown21.933 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.933	2.33 ng	257201	Chrysene-d12	21.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene-1-carboxylic acid, ...	332	C23H24O2	1000159-40-6	40
2	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	32
3	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	27
4	6-Methyl-5-[1-piperidinyl]-2,4-p...	207	C10H17N5	164589-37-1	27
5	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
Operator : JU/CG
Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.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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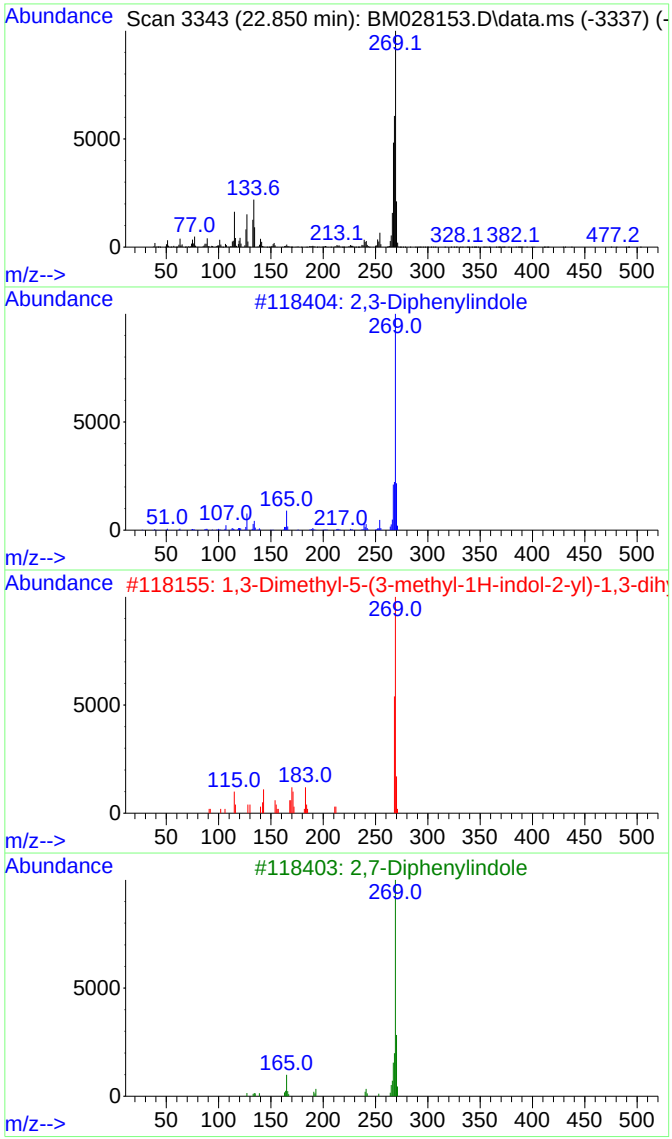
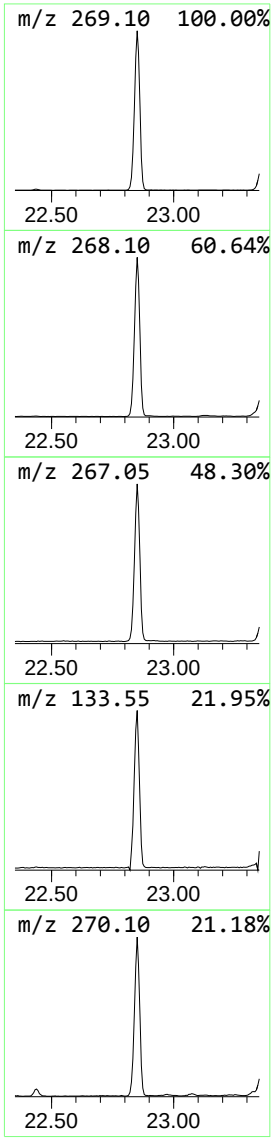
Peak Number 10 2,3-Diphenylindole Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.850	37.58 ng	4149380	Chrysene-d12	21.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Diphenylindole	269	C20H15N	003469-20-3	60
2	1,3-Dimethyl-5-(3-methyl-1H-indo...	269	C15H15N3O2	066723-75-9	47
3	2,7-Diphenylindole	269	C20H15N	001157-17-1	38
4	9H-Xanthene-1-carboxylic acid, 2...	300	C16H12O6	000476-53-9	38
5	2-(Benzylideneamino)fluorene	269	C20H15N	013924-50-0	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
Operator : JU/CG
Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.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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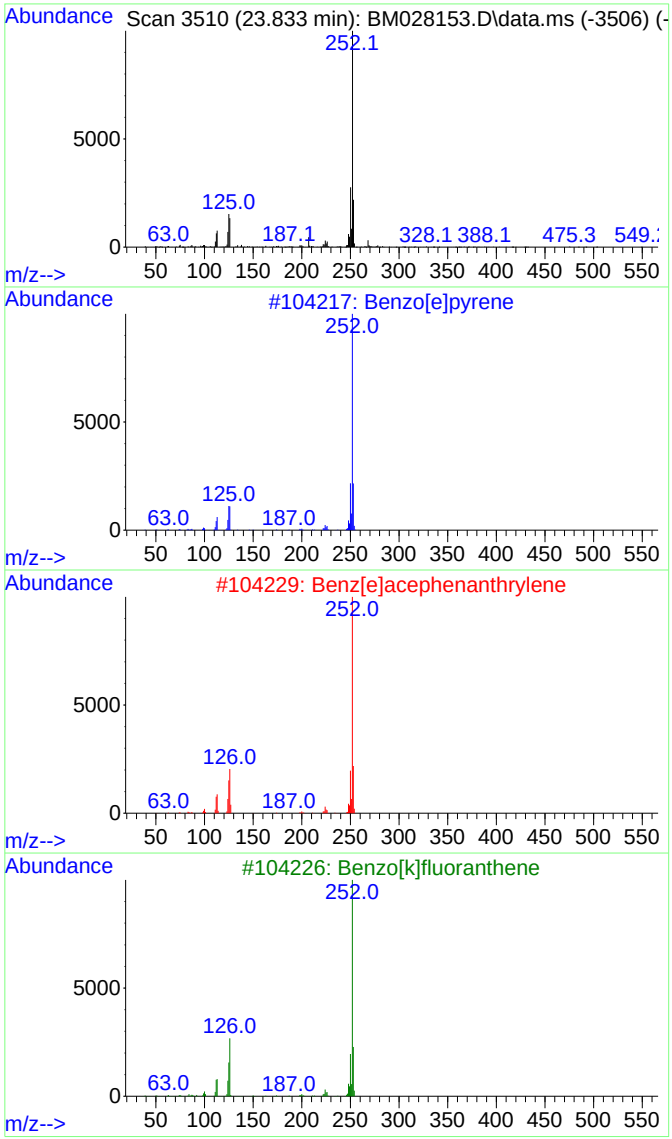
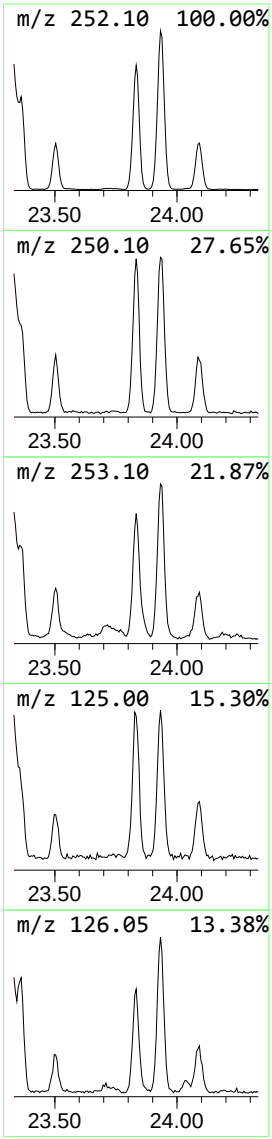
Peak Number 11 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.833	10.28 ng	705335	Perylene-d12	24.038

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	92





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028153.D
Acq On : 17 Dec 2020 22:22
Operator : JU/CG
Sample : L5036-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.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-Pentanone, 4-...	5.222	2.5	ng	126433	1	8.210	1007300	20.0
Ethanol, 2-(2-e...	7.792	4.7	ng	234628	1	8.210	1007300	20.0
2,4,7,9-Tetrame...	13.716	4.7	ng	328551	3	14.839	1389240	20.0
n-Hexadecanoic ...	18.409	5.0	ng	347344	4	17.557	1382480	20.0
4H-Cyclopenta[d...	18.615	2.1	ng	142213	4	17.557	1382480	20.0
unknown21.356	21.356	10.8	ng	1187150	5	21.668	2208450	20.0
Methadone N-oxide	21.833	5.8	ng	643540	5	21.668	2208450	20.0
unknown21.886	21.886	7.9	ng	868579	5	21.668	2208450	20.0
unknown21.933	21.933	2.3	ng	257201	5	21.668	2208450	20.0
2,3-Diphenylindole	22.850	37.6	ng	4149380	5	21.668	2208450	20.0
Benzo[e]pyrene	23.833	10.3	ng	705335	6	24.038	1372050	20.0