LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005270.D
Acq On : 12 Apr 2021 17:25
Operator : CG/JU
Sample : M1967-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB1-B

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_P\Methods\8270E-BP040921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005270.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.822	292	295	304	rVB2	100663	157736	10.77%	1.643%
2	5.281	368	373	379	rVB	653538	926534	63.23%	9.650%
3	6.863	636	642	645	rBV	634876	1081178	73.79%	11.260%
4	7.675	774	780	787	rVV	151392	231186	15.78%	2.408%
5	7.746	788	792	797	rVB2	12388	17525	1.20%	0.183%
6	8.463	908	914	924	rBV4	18740	41587	2.84%	0.433%
7	8.840	970	978	985	rBV	374145	604864	41.28%	6.300%
8	9.240	1040	1046	1053	rVB2	12002	19419	1.33%	0.202%
9	10.469	1247	1255	1260	rBV	168158	279498	19.08%	2.911%
10	11.981	1507	1512	1522	rBV	37916	65844	4.49%	0.686%
11	12.951	1668	1677	1687	rBV	711099	1005986	68.66%	10.477%
12	13.745	1808	1812	1816	rVV6	13206	16279	1.11%	0.170%
13	13.804	1816	1822	1828	rVB3	26782	53178	3.63%	0.554%
14	14.163	1879	1883	1889	rVB8	11092	16545	1.13%	0.172%
15	14.340	1907	1913	1919	rVB2	258530	378517	25.83%	3.942%
16	15.610	2125	2129	2132	rVB5	12137	15442	1.05%	0.161%
17	15.839	2162	2168	2174	rBV	214237	307474	20.98%	3.202%
18	16.086	2207	2210	2215	rVB2	29312	41430	2.83%	0.431%
19	16.186	2223	2227	2231	rBV6	10875	22084	1.51%	0.230%
20	16.916	2348	2351	2360	rVB5	25132	36200	2.47%	0.377%
21	17.104	2377	2383	2387	rBV	336793	485326	33.12%	5.055%
22	17.145	2387	2390	2395	rVB2	19446	27430	1.87%	0.286%
23	17.198	2395	2399	2402	rBV2	44212	55160	3.76%	0.574%
24	18.151	2558	2561	2568	rVB5	31655	50252	3.43%	0.523%
25	18.992	2701	2704	2712	rVB6	33355	60199	4.11%	0.627%
26	19.128	2723	2727	2733	rVB	71750	93967	6.41%	0.979%
27	19.480	2783	2787	2788	rBV	63280	70546	4.81%	0.735%
28	19.504	2788	2791	2797	rVB	97301	130799	8.93%	1.362%
29	19.680	2816	2821	2826	rBV	1233067	1465226	100.00%	15.260%
30	20.927	3028	3033	3039	rVB2	130174	267572	18.26%	2.787%
31	20.986	3039	3043	3050	rVB	241222	294133	20.07%	3.063%
32	21.116	3061	3065	3071	rVB	217240	230881	15.76%	2.405%
33	21.204	3075	3080	3084	rBV	437251	574926	39.24%	5.988%
34	23.474	3461	3466	3472	rVB2	265259	476851	32.54%	4.966%

Sum of corrected areas: 9601774

Instrument :
BNA_P
ClientSampleId :
SB1-B

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005270.D
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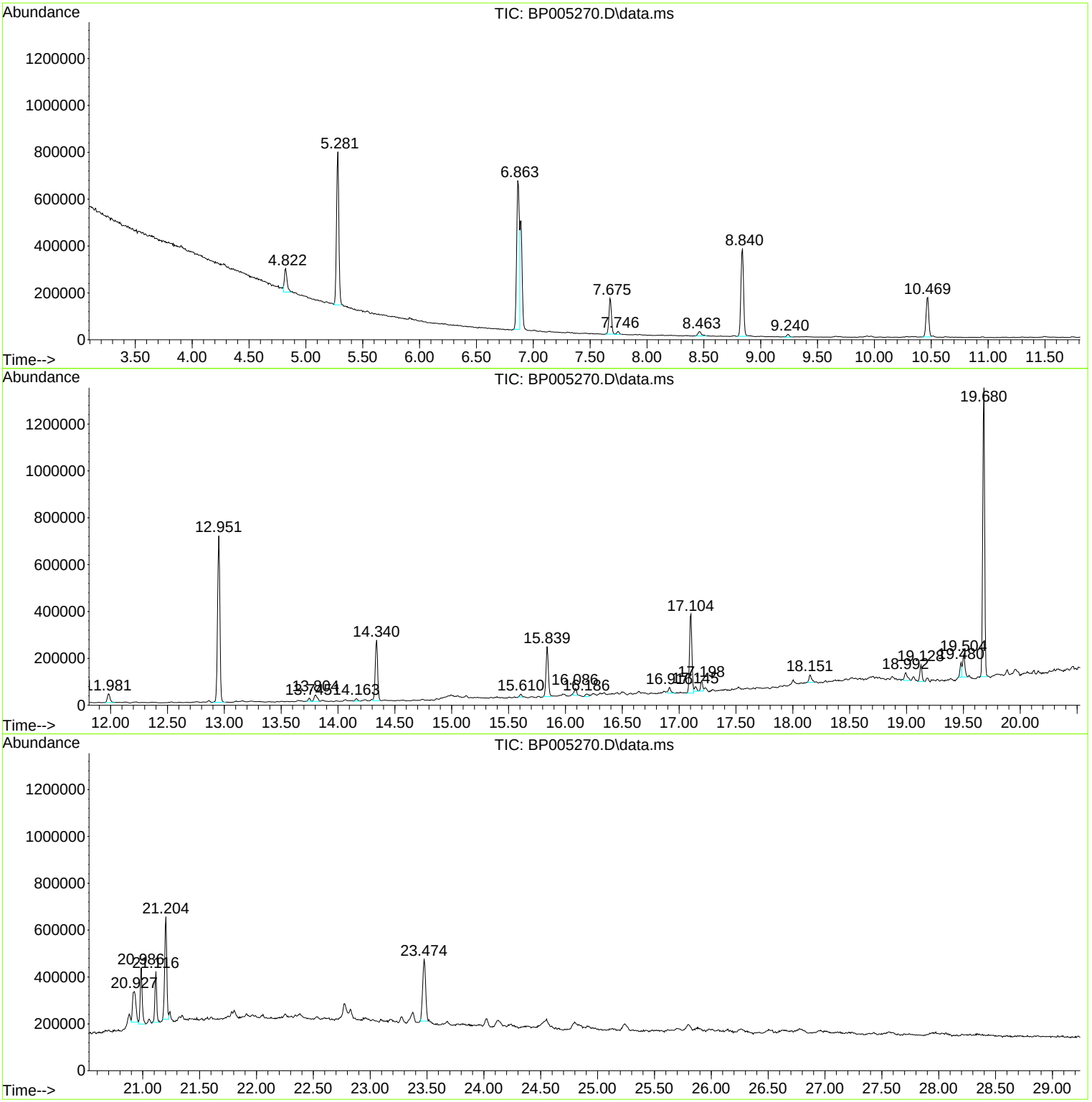
Sample : M1967-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB1-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.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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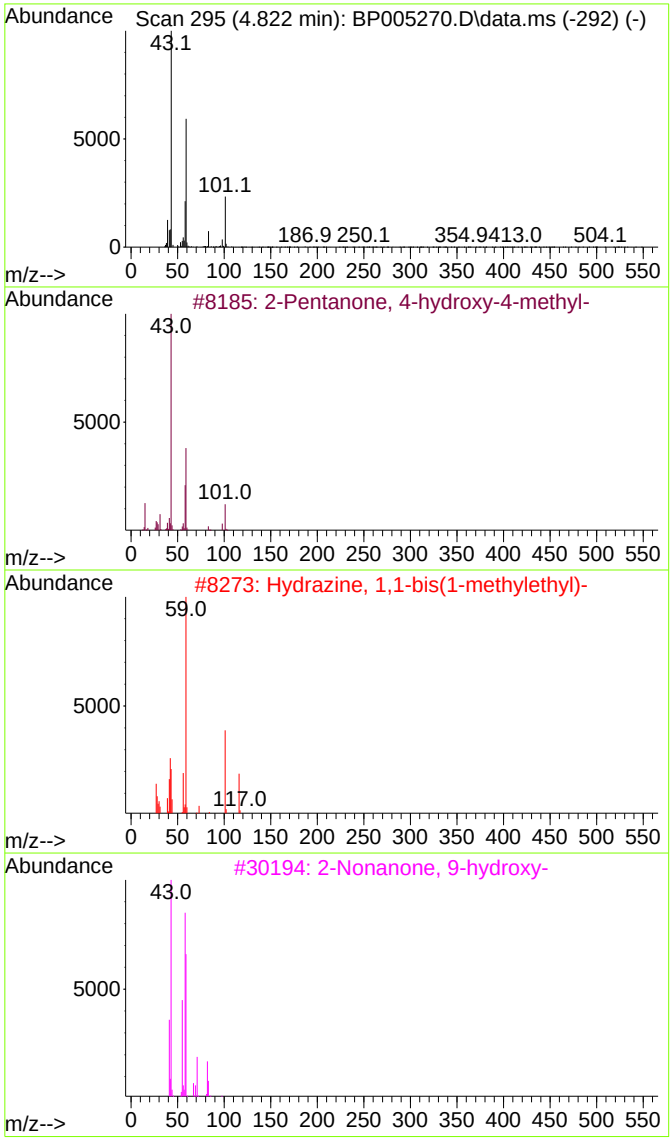
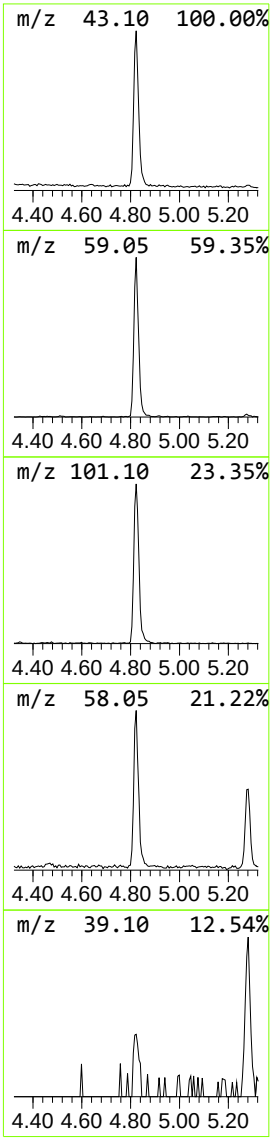
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.822	13.65 ng	157736	1,4-Dichlorobenzene-d4	7.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	37
3	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	25
4	Butyric acid, 3-bromo-, methyl e...	180	C5H9BrO2	021249-59-2	23
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	10





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Data File : BP005270.D
Acq On : 12 Apr 2021 17:25
Operator : CG/JU
Sample : M1967-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB1-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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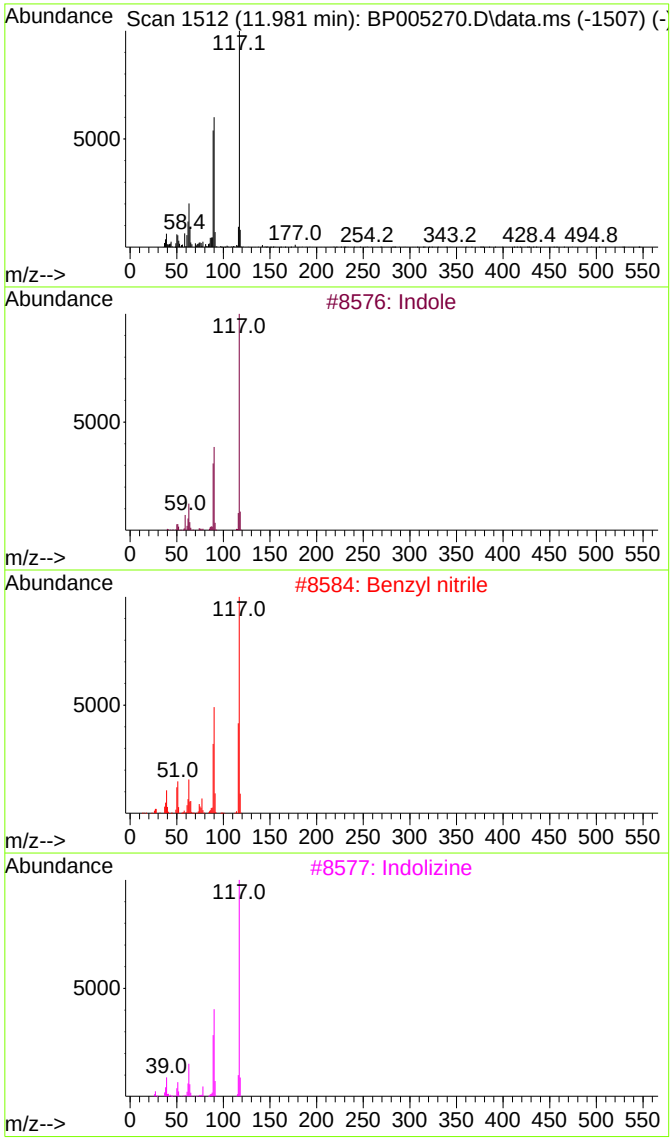
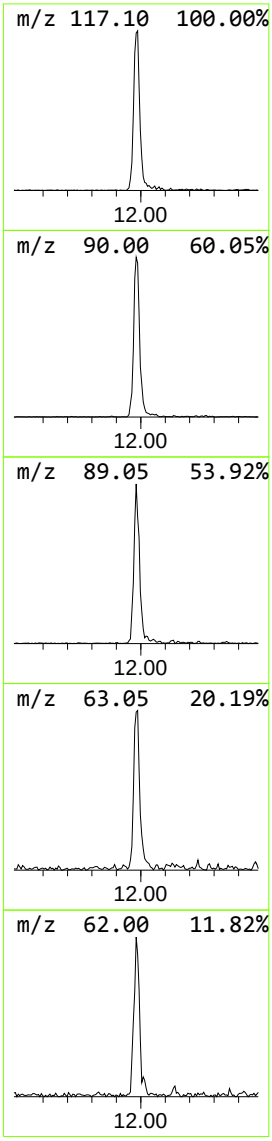
Peak Number 2 Indole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.981	4.71 ng	65844	Naphthalene-d8	10.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole	117	C8H7N	000120-72-9	95
2	Benzyl nitrile	117	C8H7N	000140-29-4	91
3	Indolizine	117	C8H7N	000274-40-8	91
4	m-Aminophenylacetylene	117	C8H7N	054060-30-9	87
5	Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	87





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Acq On : 12 Apr 2021 17:25
Operator : CG/JU
Sample : M1967-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB1-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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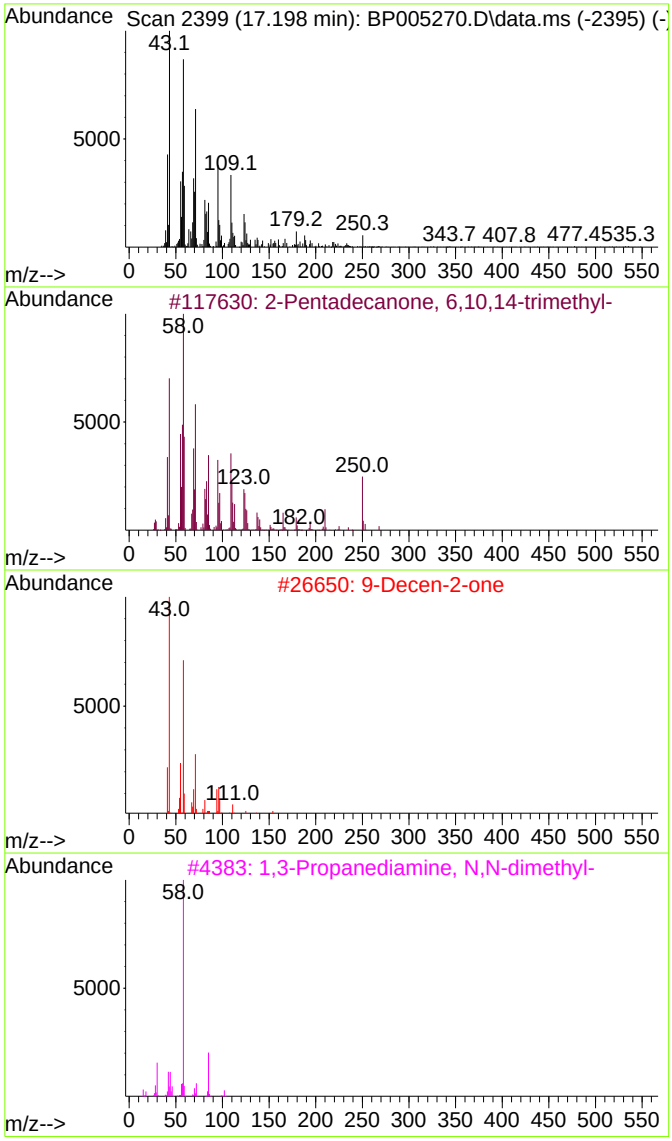
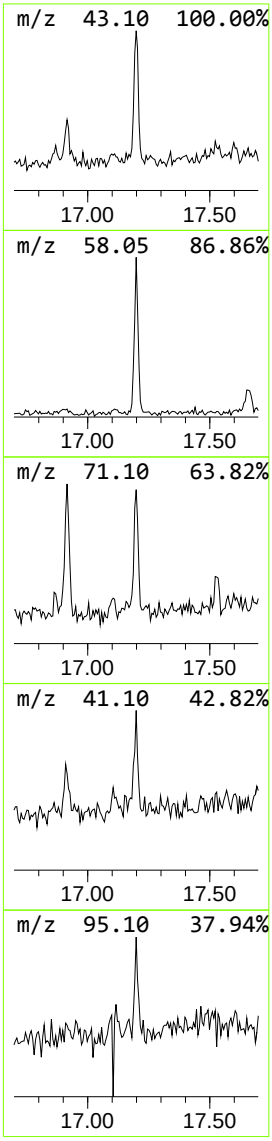
****
Peak Number 3 2-Pentadecanone, 6,10,14-tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.198	2.27 ng	55160	Phenanthrene-d10	17.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentadecanone, 6,10,14-trimethyl-	268	C18H36O	000502-69-2	89
2	9-Decen-2-one	154	C10H18O	035194-30-0	43
3	1,3-Propanediamine, N,N-dimethyl-	102	C5H14N2	000109-55-7	35
4	Pentanal, 2,3-dimethyl-	114	C7H14O	032749-94-3	27
5	Azocino[3,2-c]benzothiophen-2(1H...	320	C18H28N2OS	1000265-50-9	27





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Data File : BP005270.D
Acq On : 12 Apr 2021 17:25
Operator : CG/JU
Sample : M1967-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB1-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

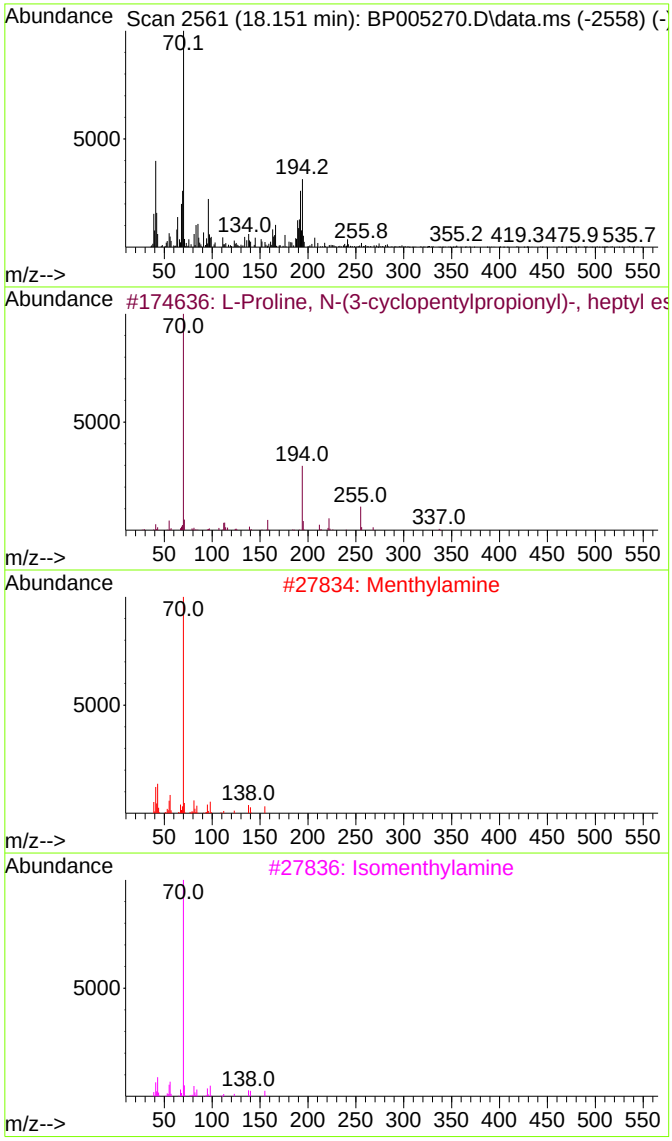
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

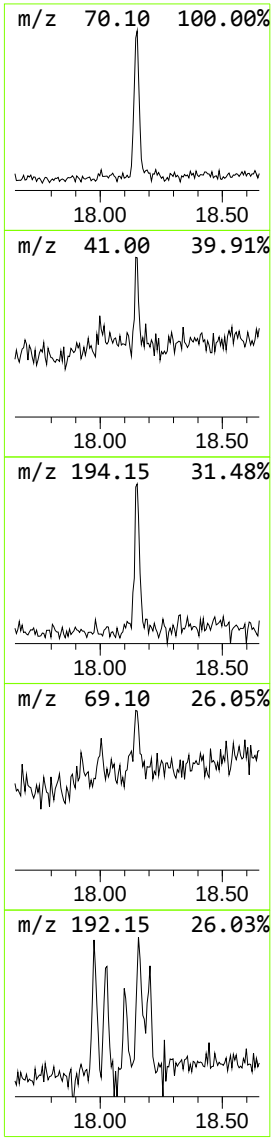
****

Peak Number 4 unknown18.51 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	2.07 ng	50252	Phenanthrene-d10	17.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Proline, N-(3-cyclopentylpropi...	337	C20H35NO3	1000346-41-3	47
2	Menthylamine	155	C10H21N	020706-69-8	43
3	Isomenthylamine	155	C10H21N	004894-99-9	43
4	3a-(4-Chloro-phenyl)-3,3,6,6-tet...	308	C16H17ClO4	1000300-10-3	38
5	2-Acetylpyrrolidine	113	C6H11NO	060026-20-2	38





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Sample : M1967-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB1-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

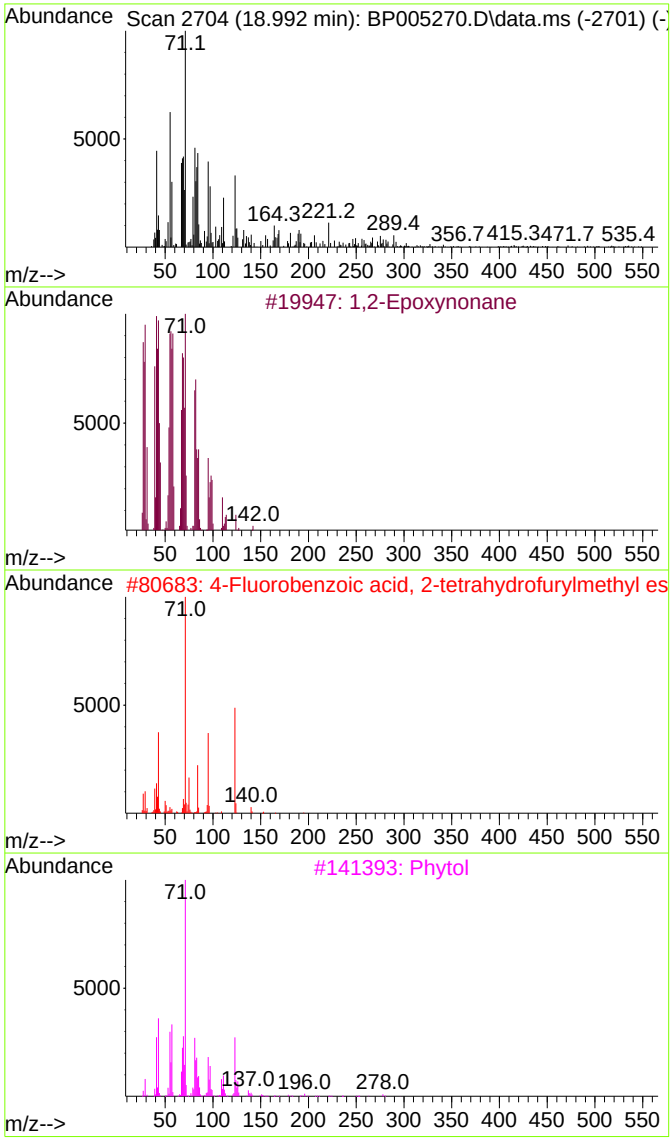
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

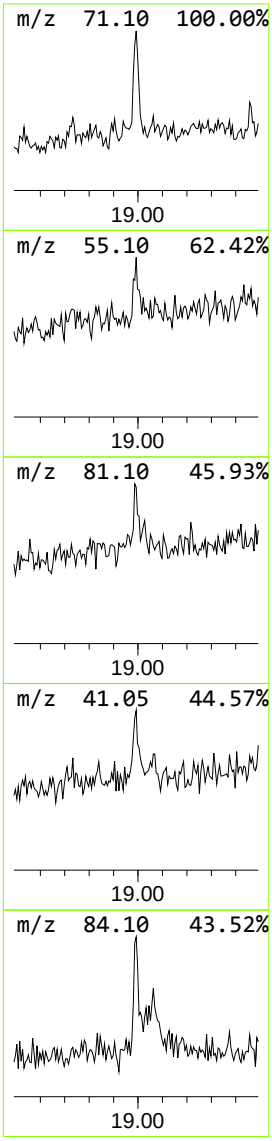
****

Peak Number 5 unknown18.99 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.992	2.48 ng	60199	Phenanthrene-d10	17.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Epoxynonane	142	C9H18O	028114-20-7	47
2	4-Fluorobenzoic acid, 2-tetrahyd...	224	C12H13FO3	1000279-07-0	38
3	Phytol	296	C20H40O	000150-86-7	38
4	Cyclohexanecarboxylic acid, 2-te...	212	C12H20O3	1000279-85-7	35
5	8-Methyloctahydrocoumarin	168	C10H16O2	021197-56-8	30





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Sample : M1967-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB1-B

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TIC Library : C:\DATABASE\NIST11.L
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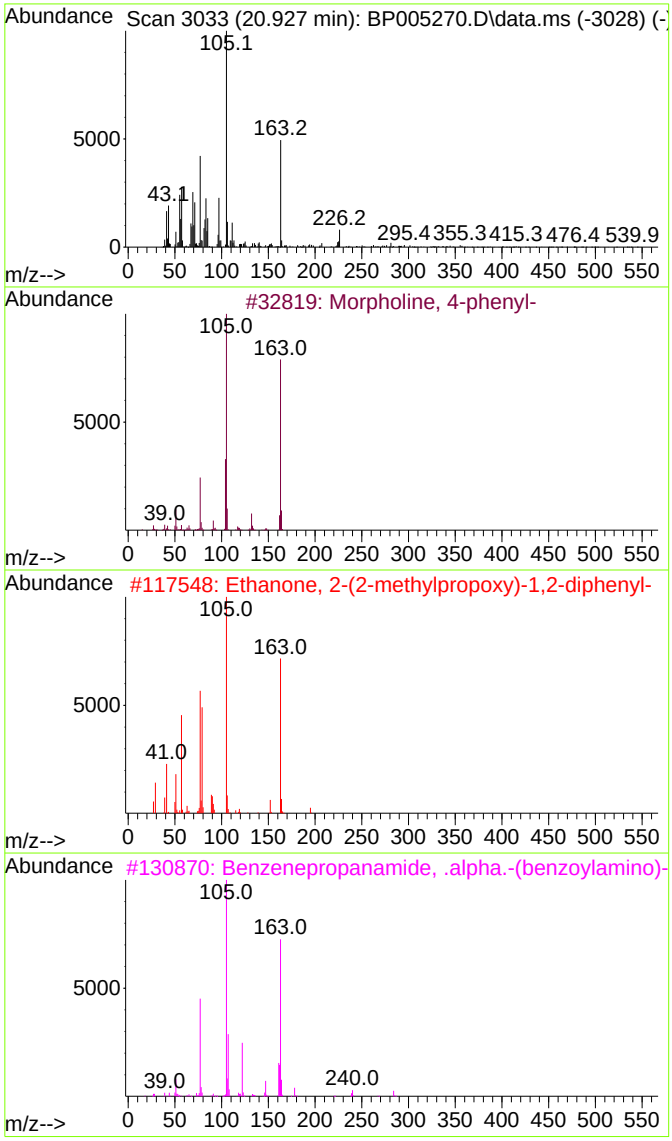
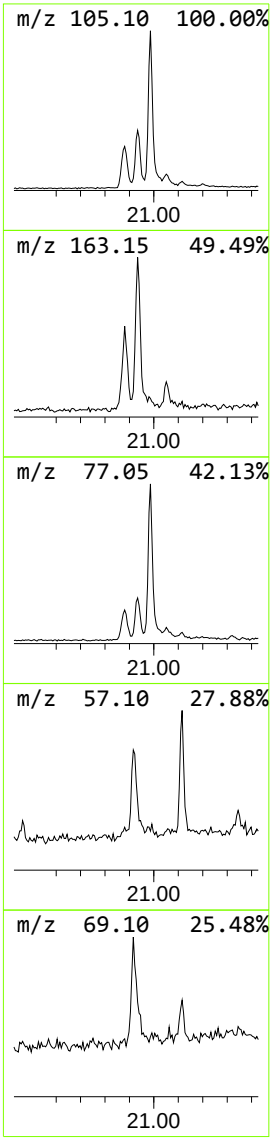
****

Peak Number 6 unknown20.92 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.927	9.31 ng	267572	Chrysene-d12	21.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	43
2	Ethanone, 2-(2-methylpropoxy)-1,...	268	C18H20O2	022499-12-3	37
3	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	37
4	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	25
5	1,3,5-Tribenzoylbenzene	390	C27H18O3	025871-69-6	22





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Sample : M1967-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB1-B

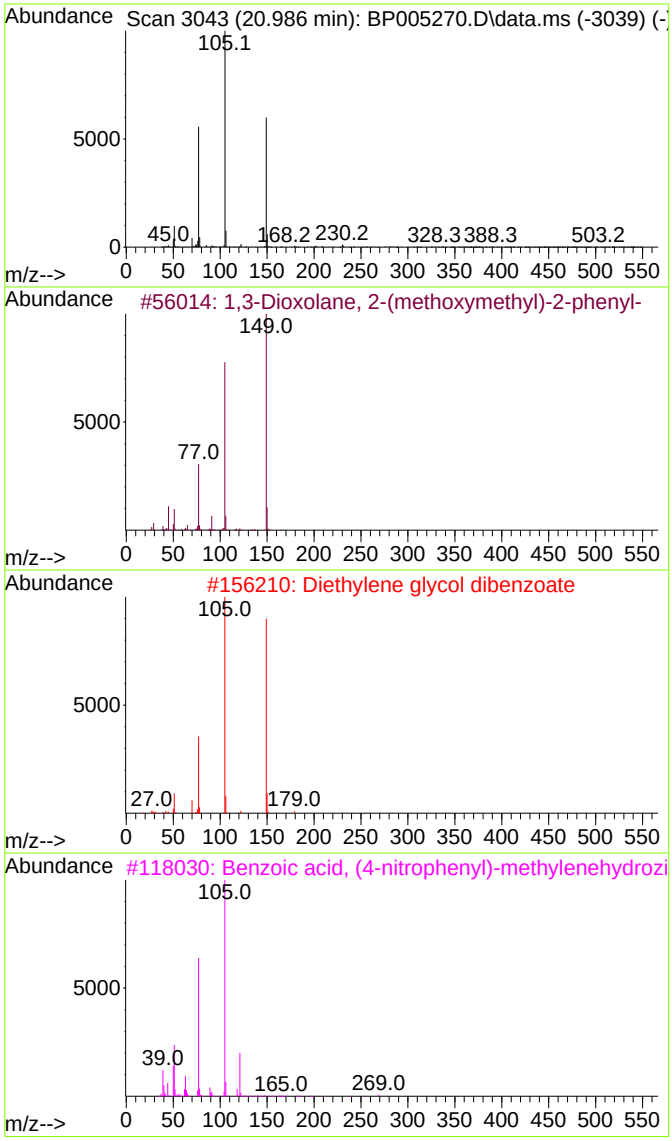
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

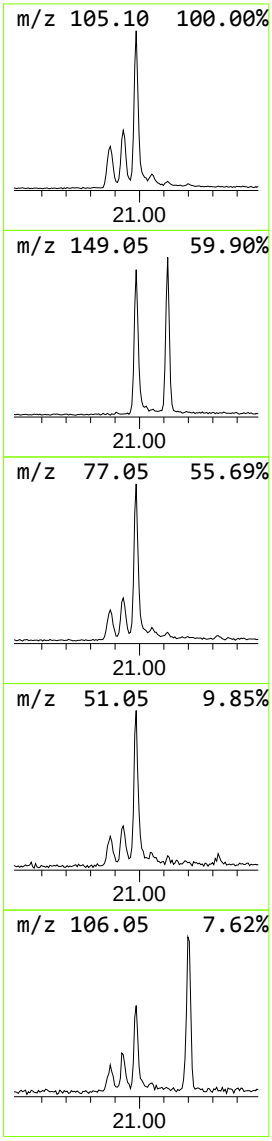
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.986	10.23 ng	294133	Chrysene-d12	21.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	53
3	Benzoic acid, (4-nitrophenyl)-me...	269	C14H11N3O3	028123-77-5	47
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	45
5	.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	43





Tentatively Identified Compound (LSC) summary

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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-...	4.822	13.7	ng	157736	1	7.675	231186	20.0
Indole	11.981	4.7	ng	65844	2	10.469	279498	20.0
2-Pentadecanone...	17.198	2.3	ng	55160	4	17.104	485326	20.0
unknown18.51	18.151	2.1	ng	50252	4	17.104	485326	20.0
unknown18.99	18.992	2.5	ng	60199	4	17.104	485326	20.0
unknown20.92	20.927	9.3	ng	267572	5	21.204	574926	20.0
1,3-Dioxolane, ...	20.986	10.2	ng	294133	5	21.204	574926	20.0