LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041621\
Data File : BP005326.D
Acq On : 16 Apr 2021 19:22
Operator : CG/JU
Sample : M1966-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-110RR

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-BP041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005326.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.264	365	370	380	rVB	350569	520914	19.92%	4.342%
2	6.846	635	639	650	rVB	246985	411887	15.75%	3.433%
3	7.658	772	777	786	rVB	134462	211200	8.08%	1.761%
4	8.822	969	975	981	rVB	361762	541506	20.71%	4.514%
5	9.087	1015	1020	1030	rVB2	39782	66519	2.54%	0.554%
6	9.646	1108	1115	1123	rBV	49476	86239	3.30%	0.719%
7	9.952	1161	1167	1172	rBV2	25638	45533	1.74%	0.380%
8	10.452	1245	1252	1256	rBV	129383	206595	7.90%	1.722%
9	10.499	1256	1260	1266	rVB	40764	65308	2.50%	0.544%
10	10.605	1274	1278	1286	rVB3	17049	29060	1.11%	0.242%
11	12.199	1543	1549	1555	rBV	76156	119431	4.57%	0.996%
12	12.934	1665	1674	1684	rBV	871208	1240074	47.43%	10.337%
13	13.787	1814	1819	1823	rBV	46178	64146	2.45%	0.535%
14	14.163	1873	1883	1888	rBV2	26128	55872	2.14%	0.466%
15	14.322	1904	1910	1916	rBV	233802	343763	13.15%	2.866%
16	15.828	2160	2166	2178	rBV	820507	1169321	44.73%	9.747%
17	15.957	2184	2188	2192	rBV5	29550	44579	1.71%	0.372%
18	16.104	2206	2213	2224	rBV	330252	614070	23.49%	5.119%
19	16.498	2276	2280	2285	rBV4	20642	30790	1.18%	0.257%
20	17.087	2375	2380	2386	rBV	320681	473261	18.10%	3.945%
21	17.222	2400	2403	2410	rVB	41742	59760	2.29%	0.498%
22	18.004	2531	2536	2541	rBV2	185262	278220	10.64%	2.319%
23	18.881	2681	2685	2693	rVB	147187	195937	7.49%	1.633%
24	19.239	2742	2746	2753	rBV2	77522	118253	4.52%	0.986%
25	19.498	2787	2790	2796	rVB	64453	82255	3.15%	0.686%
26	19.669	2814	2819	2824	rBV	2209311	2614431	100.00%	21.794%
27	19.869	2851	2853	2861	rVB2	26941	32799	1.25%	0.273%
28	20.875	3020	3024	3026	rBV	42188	62114	2.38%	0.518%
29	20.904	3026	3029	3037	rVV2	280953	461735	17.66%	3.849%
30	20.975	3038	3041	3050	rVB	219736	296062	11.32%	2.468%
31	21.192	3074	3078	3083	rBV	451421	567099	21.69%	4.727%
32	22.398	3278	3283	3292	rVB	214637	334643	12.80%	2.790%
33	23.463	3458	3464	3474	rVB2	284009	552991	21.15%	4.610%

Sum of corrected areas: 11996367

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041621\
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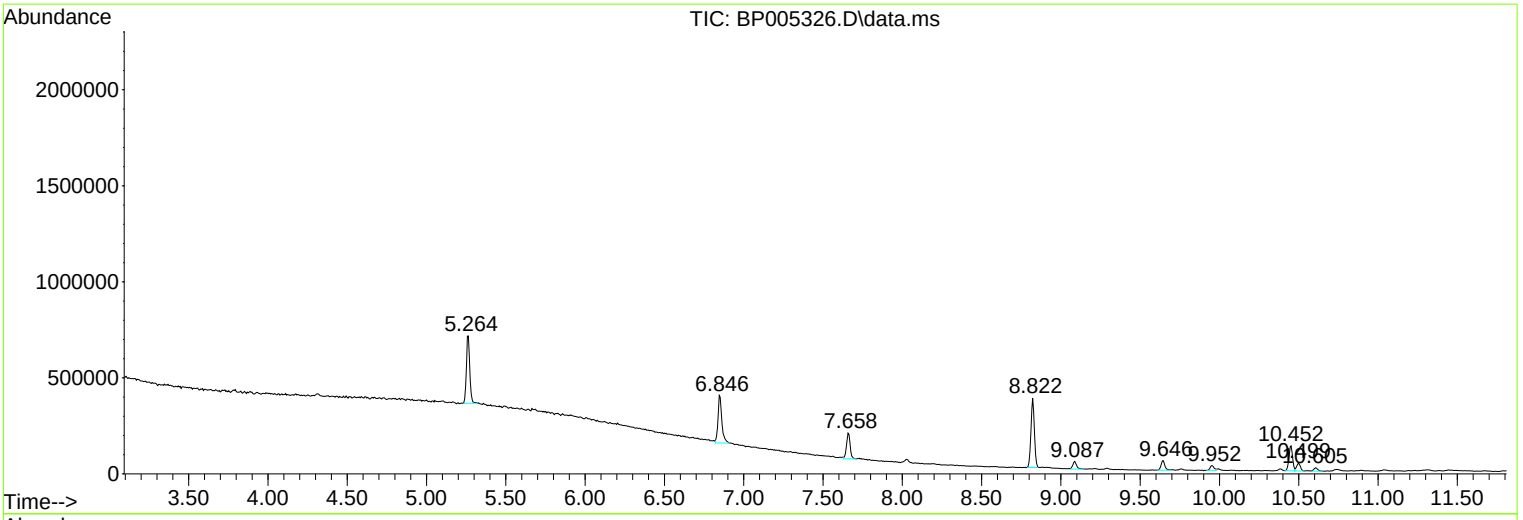
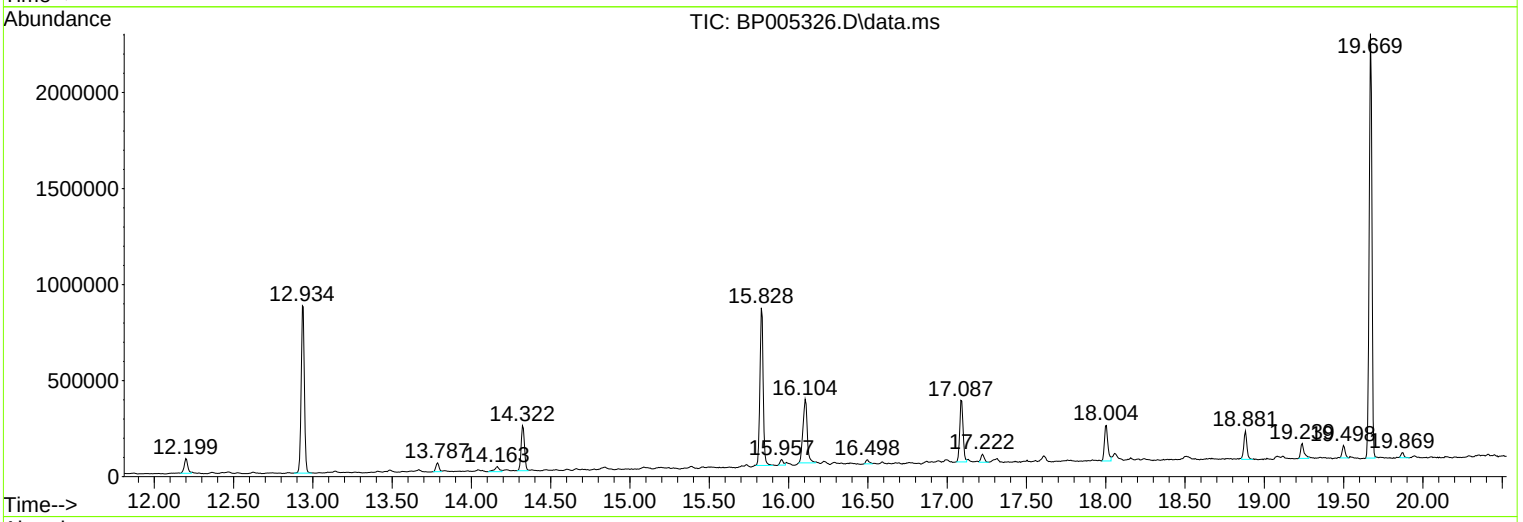
Misc :
ALS Vial : 18 Sample Multiplier: 1

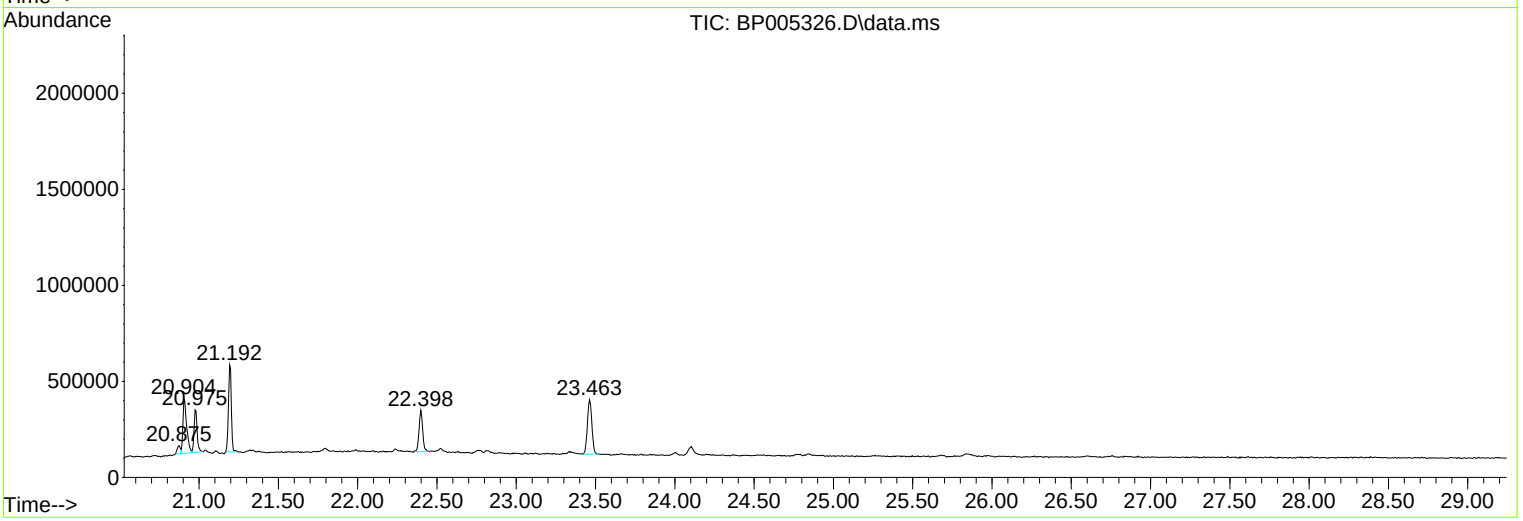
Instrument :
BNA_P
ClientSampleId :
MW-110RR

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.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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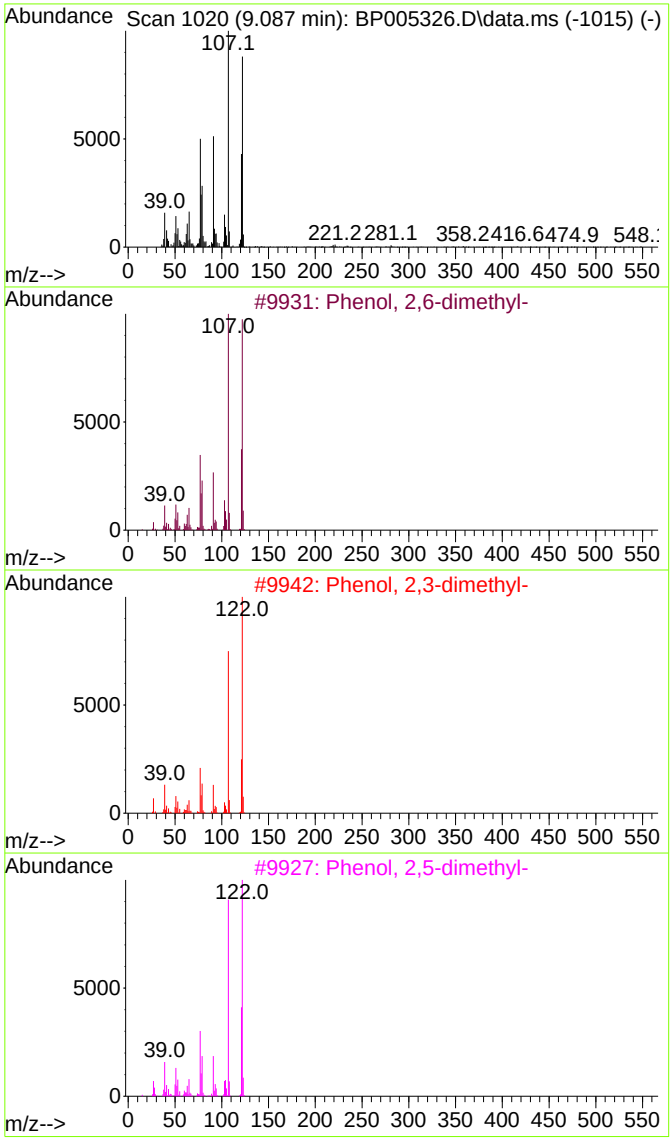
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

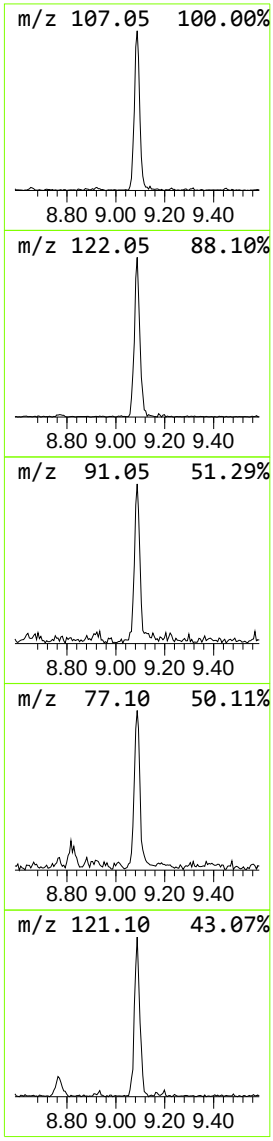
****

Peak Number 1 Phenol, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.087	6.44 ng	66519	Naphthalene-d8	10.452

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dimethyl-	122	C8H10O	000576-26-1	94
2	Phenol, 2,3-dimethyl-	122	C8H10O	000526-75-0	91
3	Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	91
4	Phenol, 2,4-dimethyl-	122	C8H10O	000105-67-9	87
5	Benzenemethanol, 4-methyl-	122	C8H10O	000589-18-4	81





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Data File : BP005326.D
Acq On : 16 Apr 2021 19:22
Operator : CG/JU
Sample : M1966-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-110RR

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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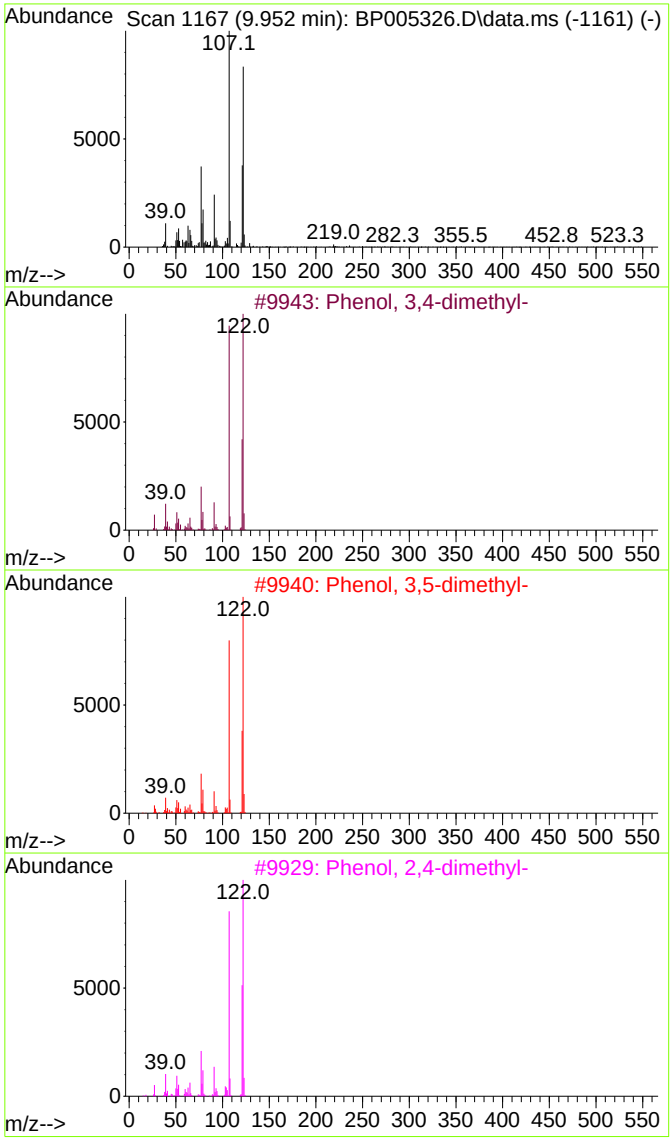
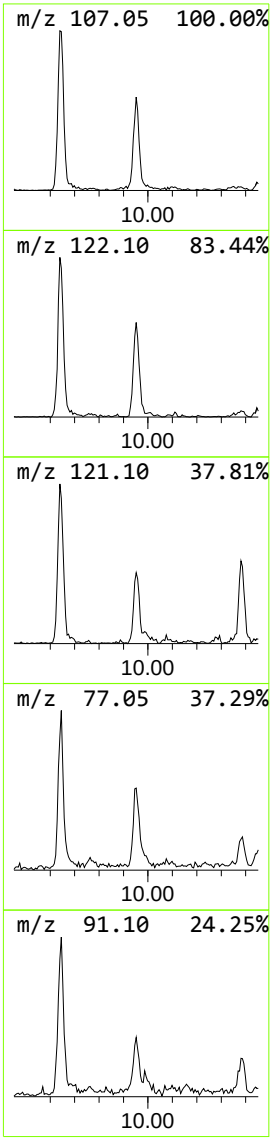
****
Peak Number 2 Phenol, 3,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.952	4.41 ng	45533	Naphthalene-d8	10.452

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3,4-dimethyl-	122	C8H10O	000095-65-8	95
2	Phenol, 3,5-dimethyl-	122	C8H10O	000108-68-9	91
3	Phenol, 2,4-dimethyl-	122	C8H10O	000105-67-9	91
4	Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	91
5	Phenol, 2-ethyl-	122	C8H10O	000090-00-6	90





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Sample : M1966-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-110RR

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.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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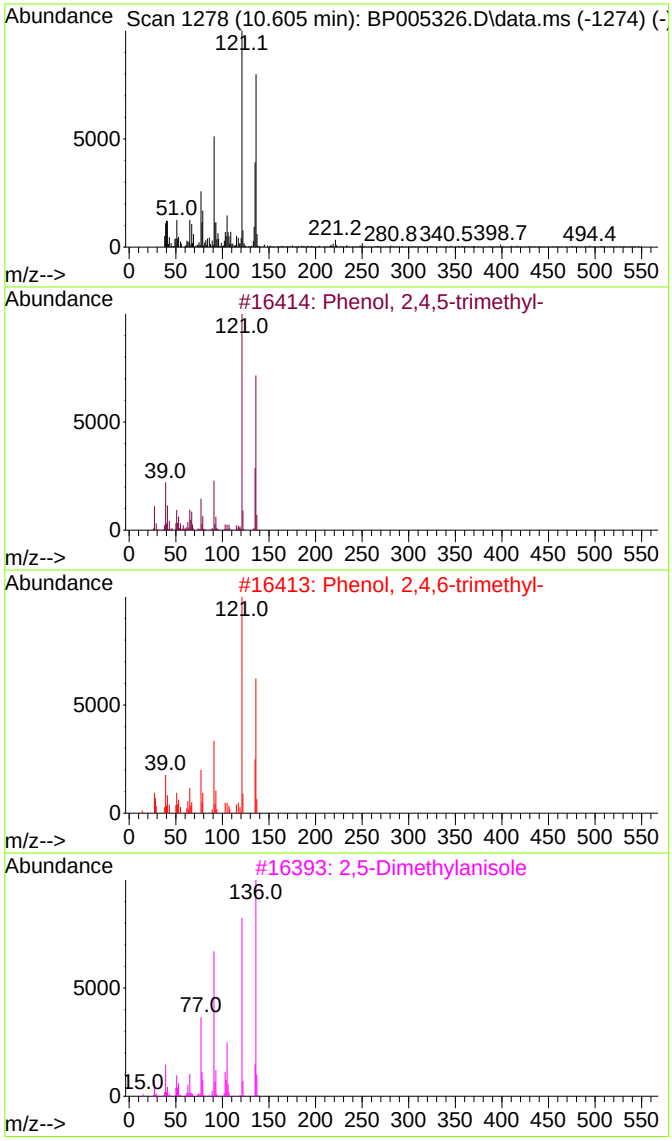
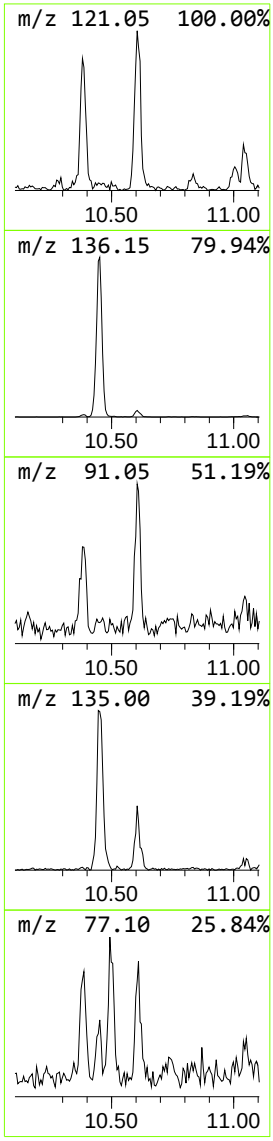
Peak Number 3 Phenol, 2,4,5-trimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.605	2.81 ng	29060	Naphthalene-d8	10.452

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4,5-trimethyl-	136	C9H12O	000496-78-6	87
2	Phenol, 2,4,6-trimethyl-	136	C9H12O	000527-60-6	81
3	2,5-Dimethylanisole	136	C9H12O	001706-11-2	80
4	2,4-Dimethylanisole	136	C9H12O	006738-23-4	76
5	3,4-Dimethylanisole	136	C9H12O	004685-47-6	74





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Operator : CG/JU
Sample : M1966-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-110RR

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
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TIC Library : C:\DATABASE\NIST11.L
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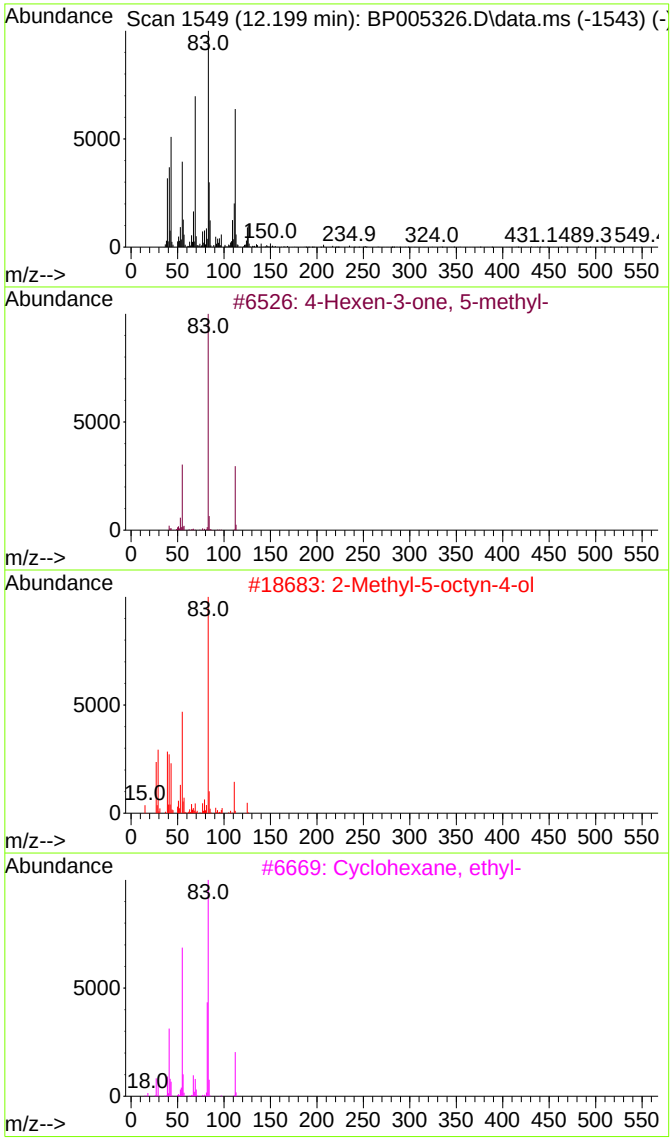
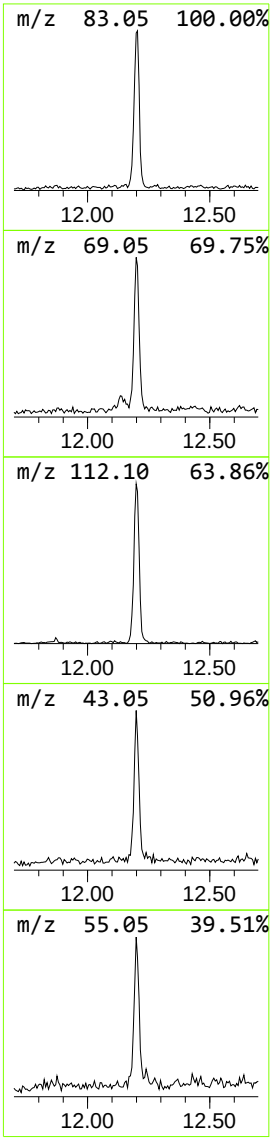
Peak Number 4 unknown12.199 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.199	11.56 ng	119431	Naphthalene-d8	10.452

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Hexen-3-one, 5-methyl-	112	C7H12O	013905-10-7	49
2	2-Methyl-5-octyn-4-ol	140	C9H16O	060657-70-7	47
3	Cyclohexane, ethyl-	112	C8H16	001678-91-7	47
4	2H-Pyran-2-carboxaldehyde, 5,6-d...	112	C6H8O2	053897-26-0	47
5	Cyclohexane, propyl-	126	C9H18	001678-92-8	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041621\
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Sample : M1966-03
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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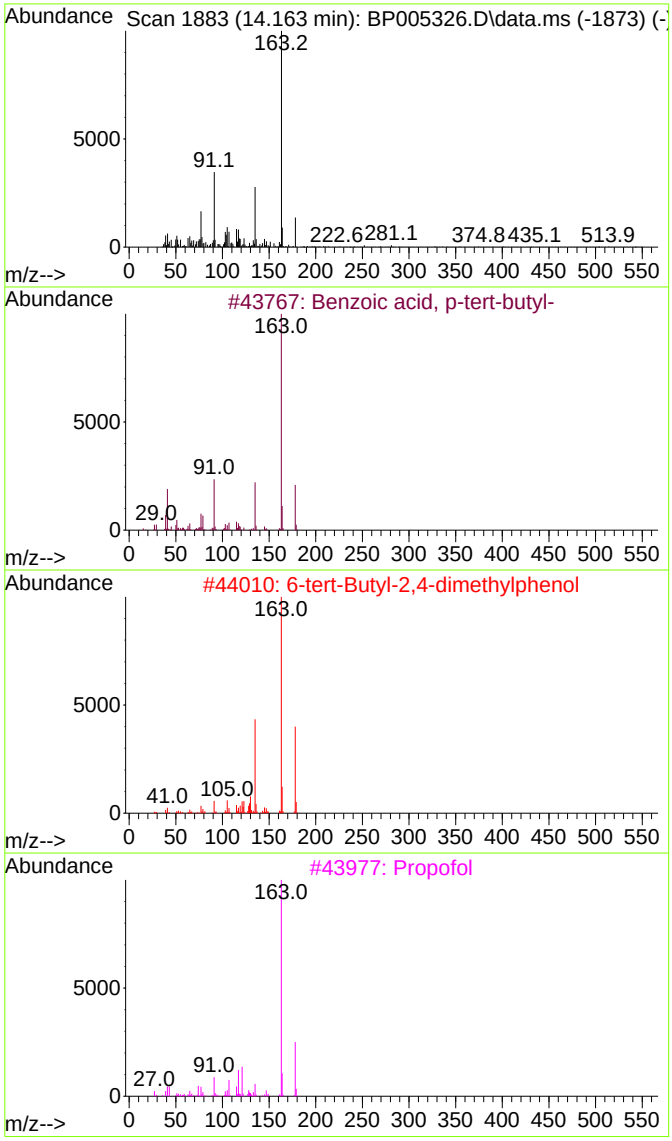
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

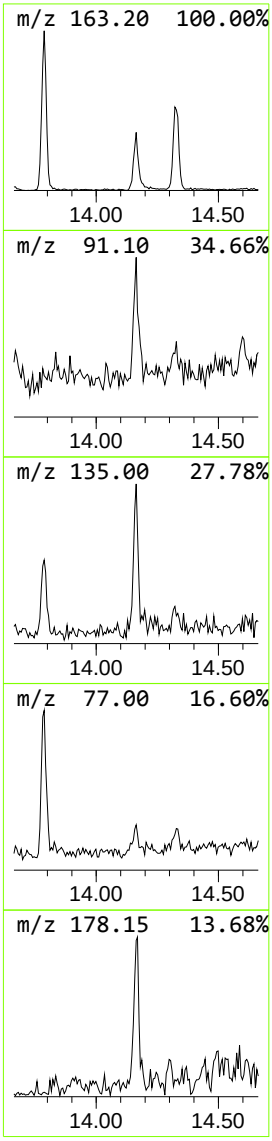
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzoic acid, p-tert-butyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.163	3.25 ng	55872	Acenaphthene-d10	14.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	91
2	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	72
3	Propofol	178	C12H18O	002078-54-8	58
4	Pyrido[2,3-d]pyridazine-5(6H)-th...	163	C7H5N3S	015370-85-1	50
5	Phosphine oxide, cyclohexyl meth...	300	C17H33O2P	1000195-73-8	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041621\
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Sample : M1966-03
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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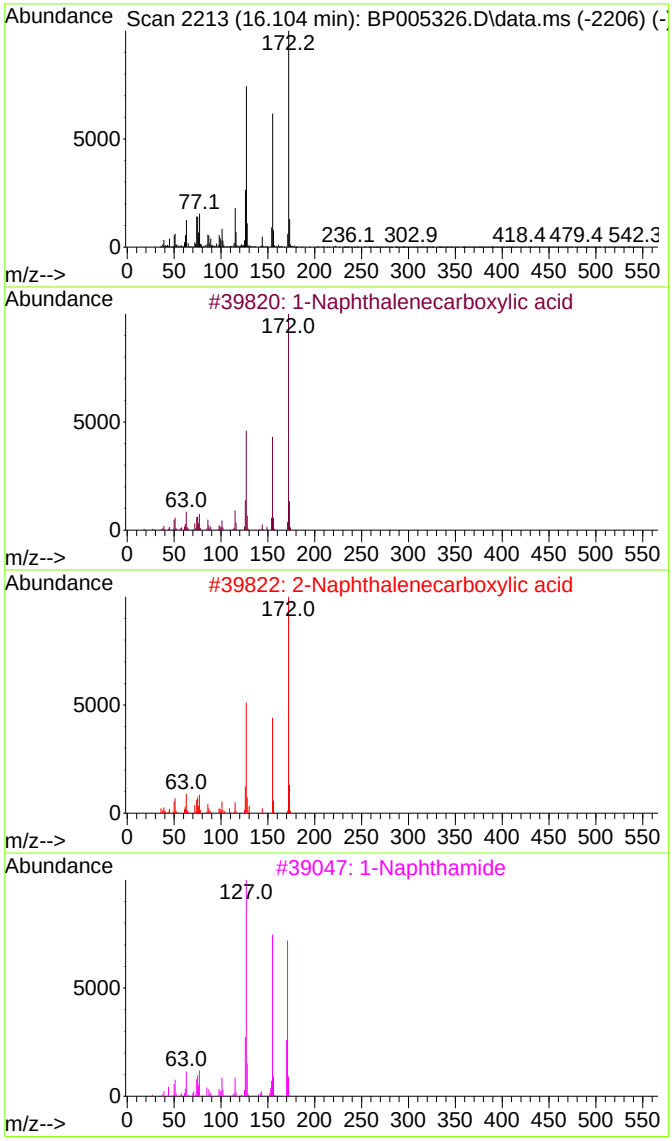
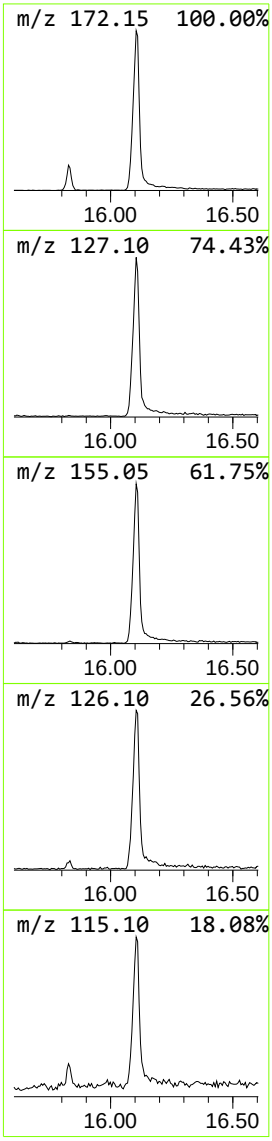
****
Peak Number 6 1-Naphthalenecarboxylic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	25.95 ng	614070	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenecarboxylic acid	172	C11H8O2	000086-55-5	96
2	2-Naphthalenecarboxylic acid	172	C11H8O2	000093-09-4	95
3	1-Naphthamide	171	C11H9NO	002243-81-4	50
4	1-Naphthalenecarbonyl chloride	190	C11H7ClO	000879-18-5	46
5	Naphthalene-1-carbohydrazide, N2...	294	C17H14N2OS	1000263-63-0	46





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Sample : M1966-03
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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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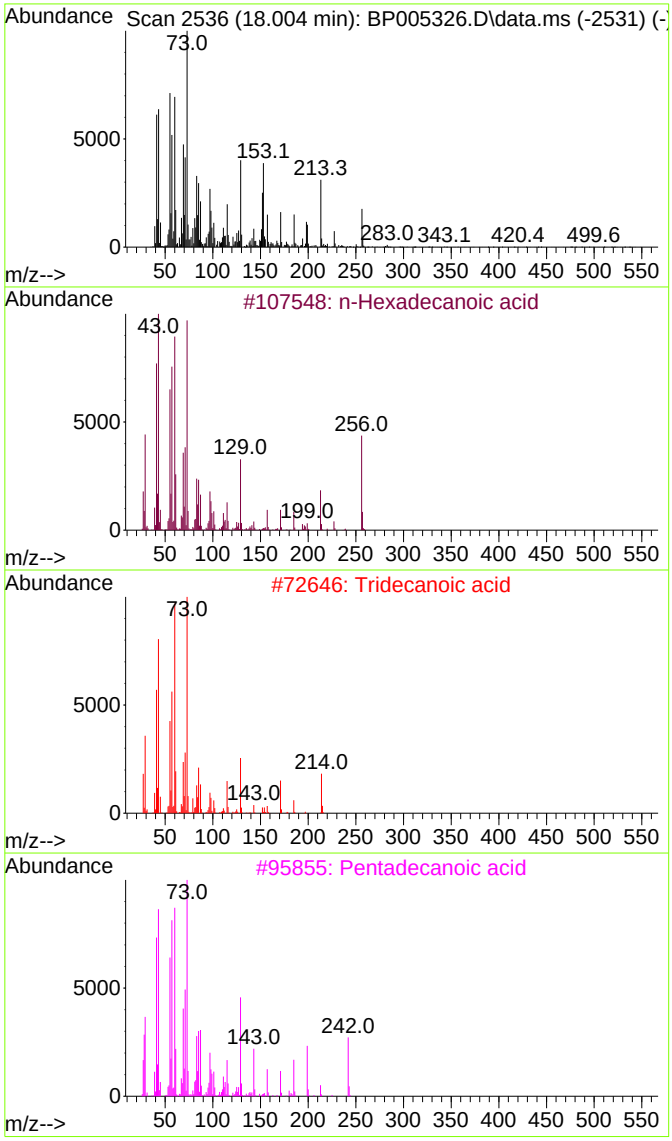
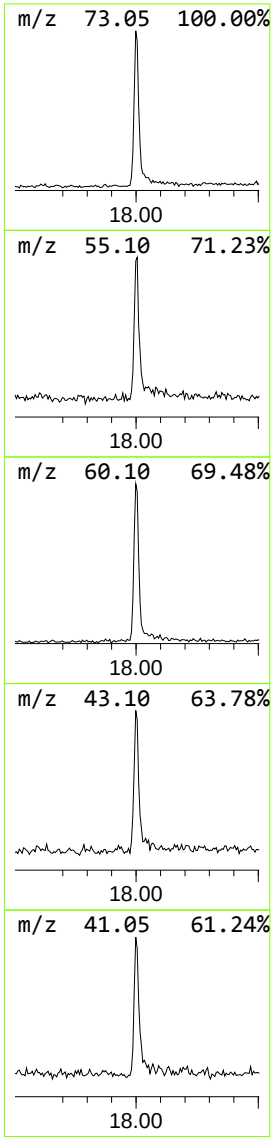
Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.004	11.76 ng	278220	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Undecanoic acid	186	C11H22O2	000112-37-8	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Sample : M1966-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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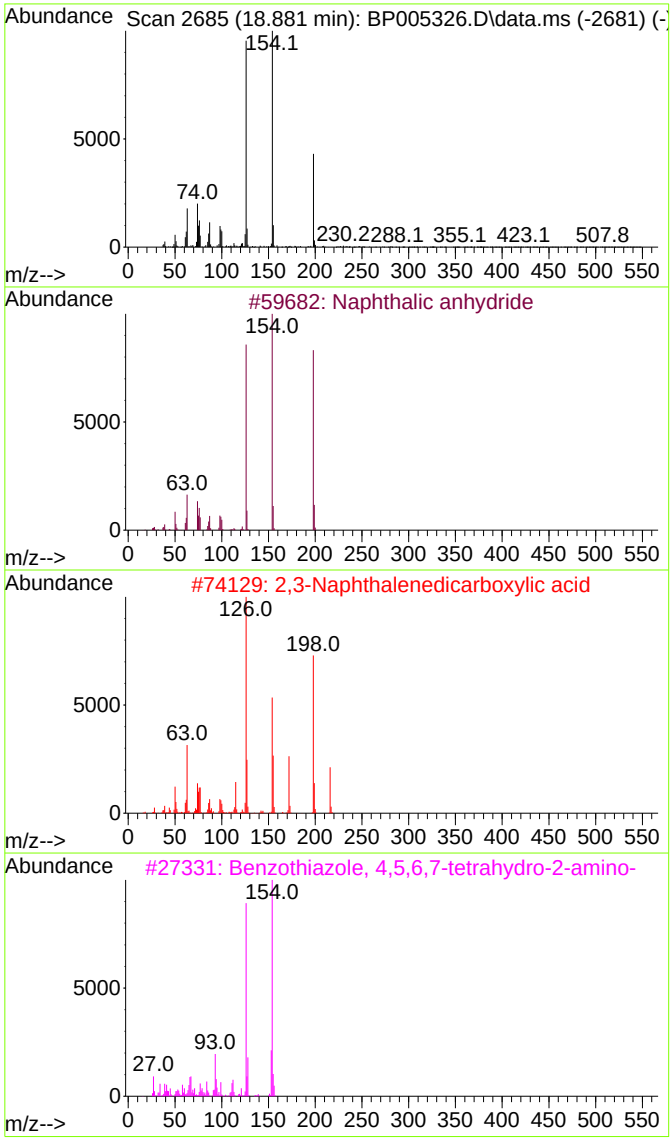
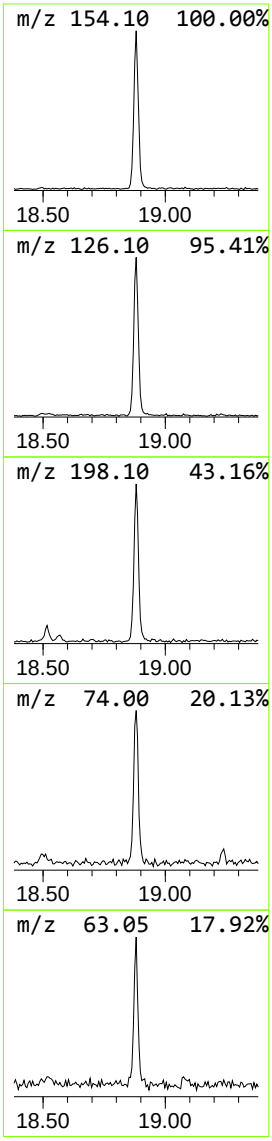
Peak Number 8 Naphthalic anhydride Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.881	8.28 ng	195937	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalic anhydride	198	C12H6O3	000081-84-5	94
2	2,3-Naphthalenedicarboxylic acid	216	C12H8O4	002169-87-1	42
3	Benzothiazole, 4,5,6,7-tetrahydr...	154	C7H10N2S	002933-29-1	40
4	1,4-Diethynylbenzene	126	C10H6	000935-14-8	35
5	1H-Benz[f]indene-1,2,3-trione	210	C13H6O3	020927-01-9	32





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Data File : BP005326.D
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Operator : CG/JU
Sample : M1966-03
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Instrument :
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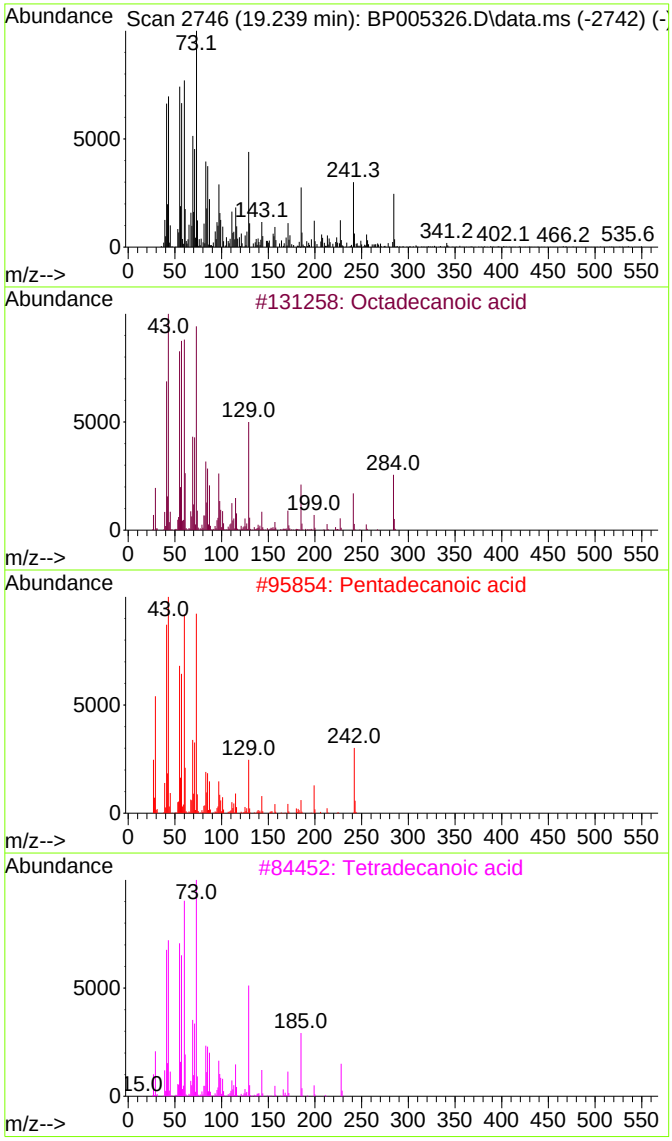
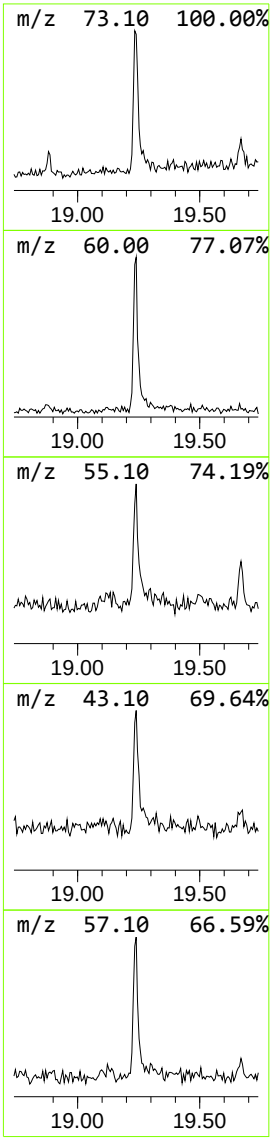
Peak Number 9 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.239	4.17 ng	118253	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





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Data File : BP005326.D
Acq On : 16 Apr 2021 19:22
Operator : CG/JU
Sample : M1966-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-110RR

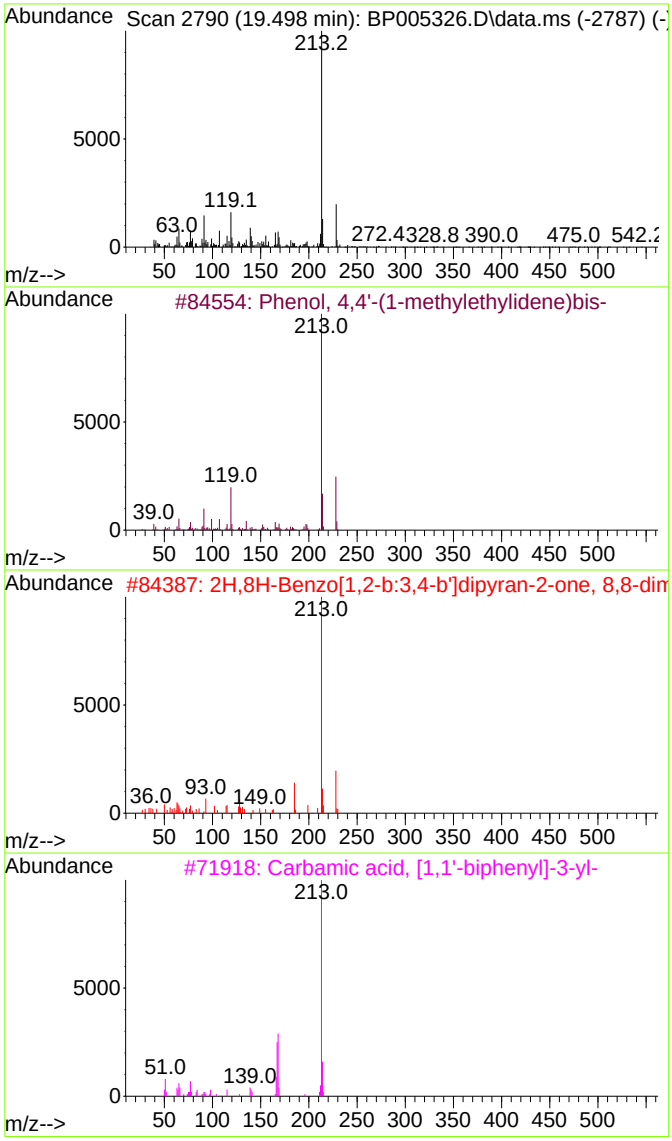
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

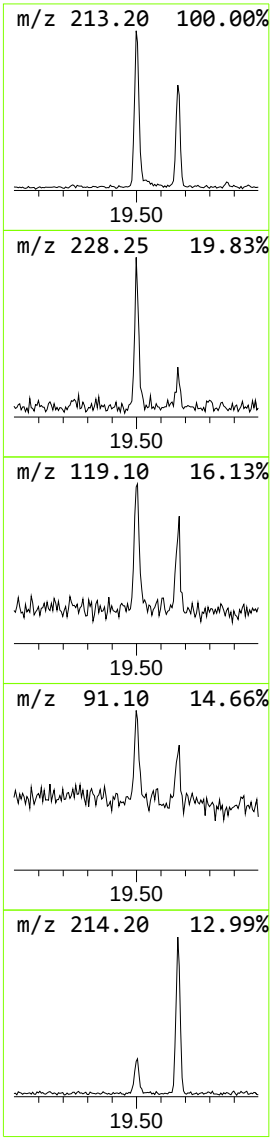
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 4,4'-(1-methylethyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.498	2.90 ng	82255	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	64
3	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	62
4	2,2-Bis-(4-hyxroxyphenyl)-butane	242	C16H18O2	000077-40-7	59
5	4H-Pyrazolo[5,1-c]-1,4-benzodiaz...	213	C11H7N3O2	1000277-20-1	59





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Acq On : 16 Apr 2021 19:22
Operator : CG/JU
Sample : M1966-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-110RR

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

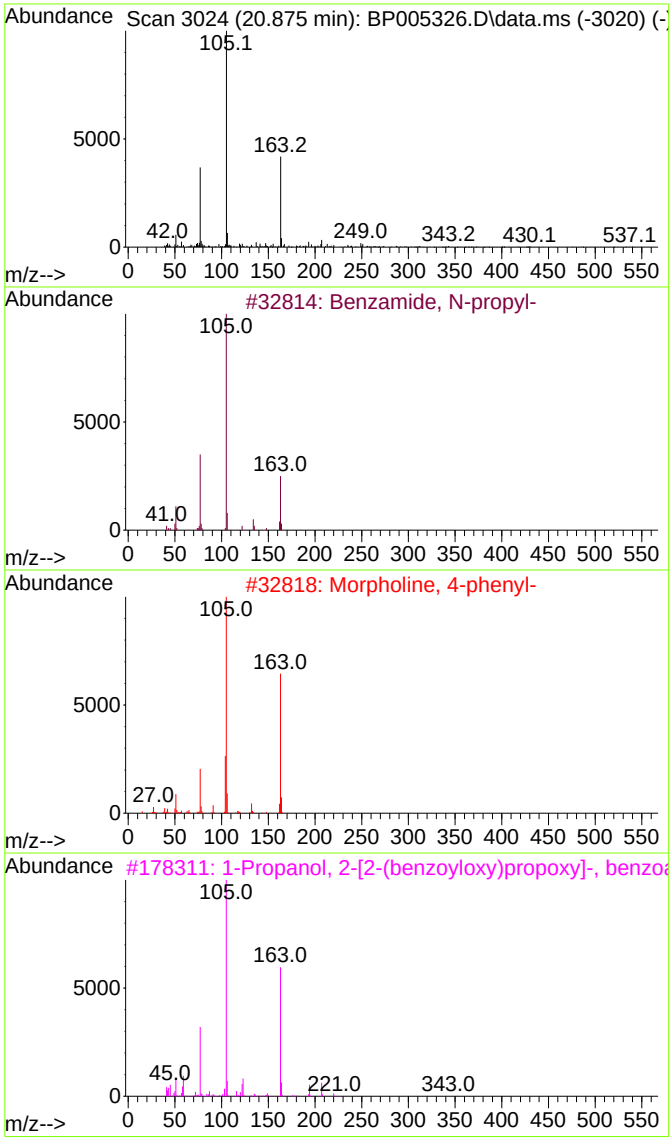
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

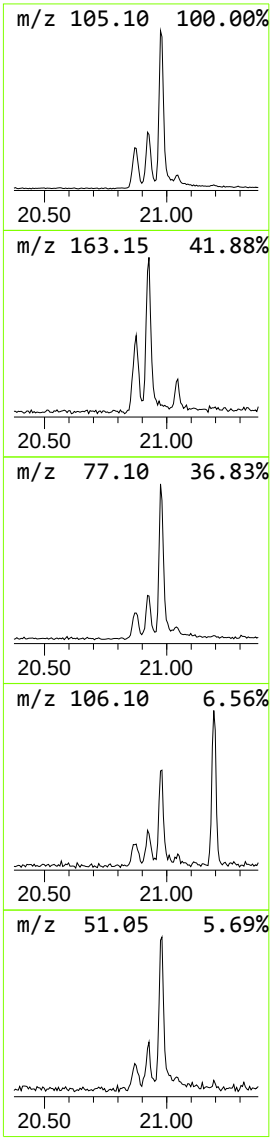
****

Peak Number 11 Benzamide, N-propyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.875	2.19 ng	62114	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	50
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	42
3	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	28
4	Biphenyl, 4,4'-dibenzoyloxy-	394	C26H18O4	1000294-15-4	27
5	Benzamide, N-(2,3-dihydro-6-benz...	395	C24H17N3O3	186965-74-2	16





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Acq On : 16 Apr 2021 19:22
Operator : CG/JU
Sample : M1966-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-110RR

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

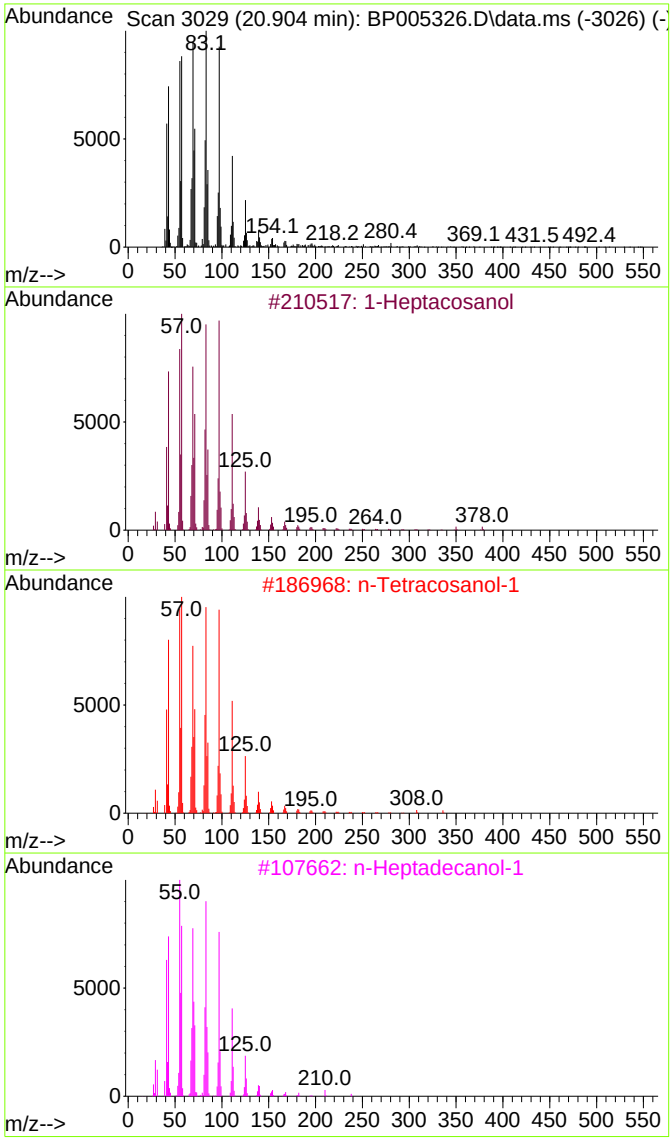
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

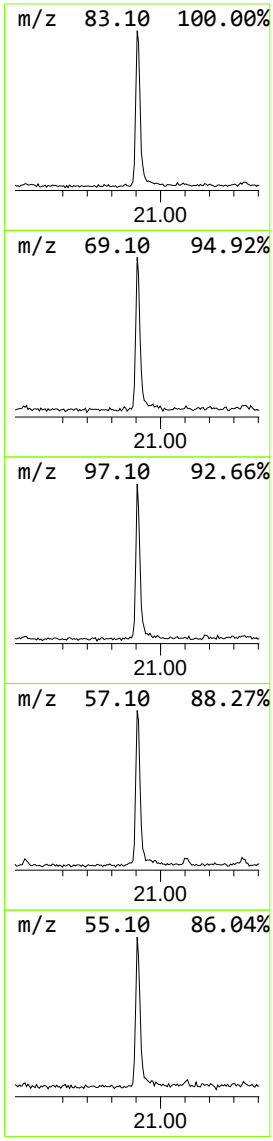
****

Peak Number 12 1-Heptacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.904	16.28 ng	461735	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	83





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Acq On : 16 Apr 2021 19:22
Operator : CG/JU
Sample : M1966-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-110RR

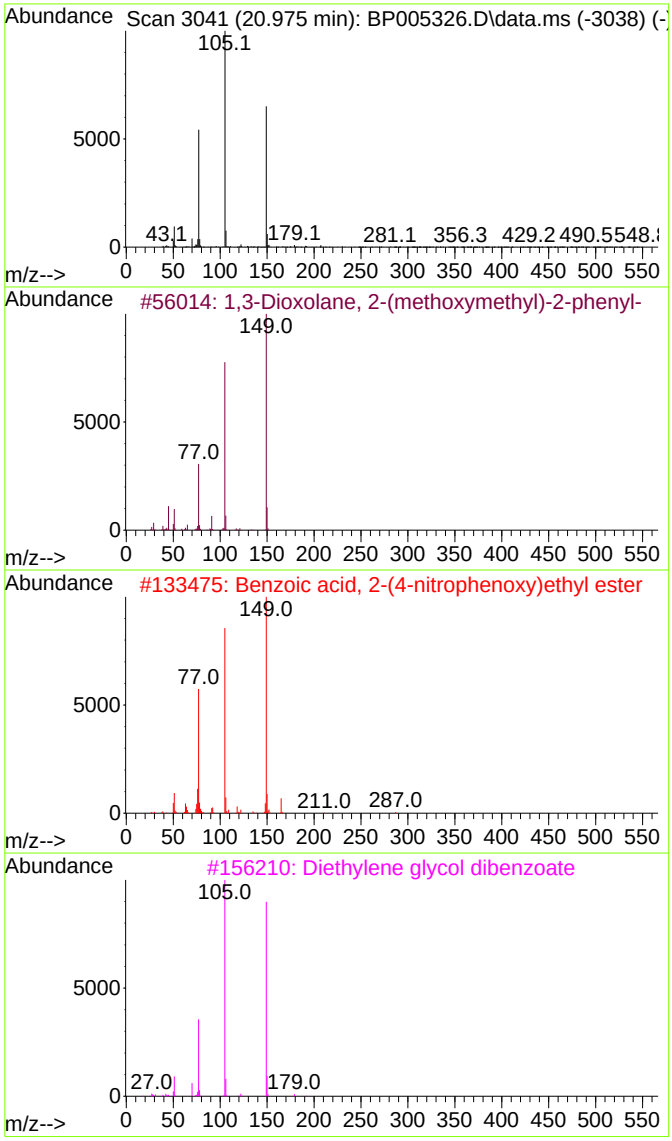
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

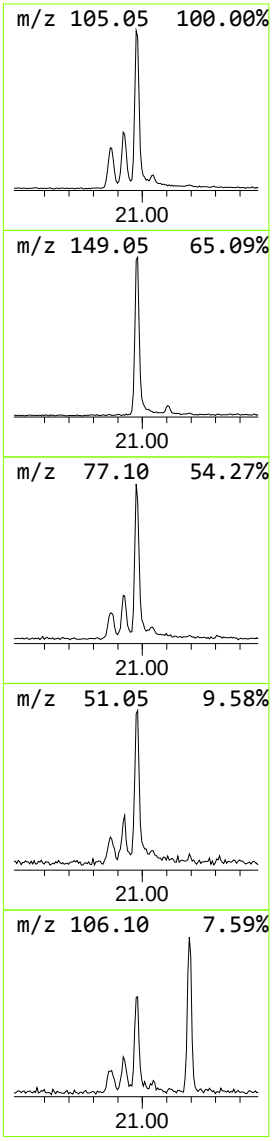
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.975	10.44 ng	296062	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
2	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	56
3	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	53
4	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	50
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47





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Data File : BP005326.D
Acq On : 16 Apr 2021 19:22
Operator : CG/JU
Sample : M1966-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-110RR

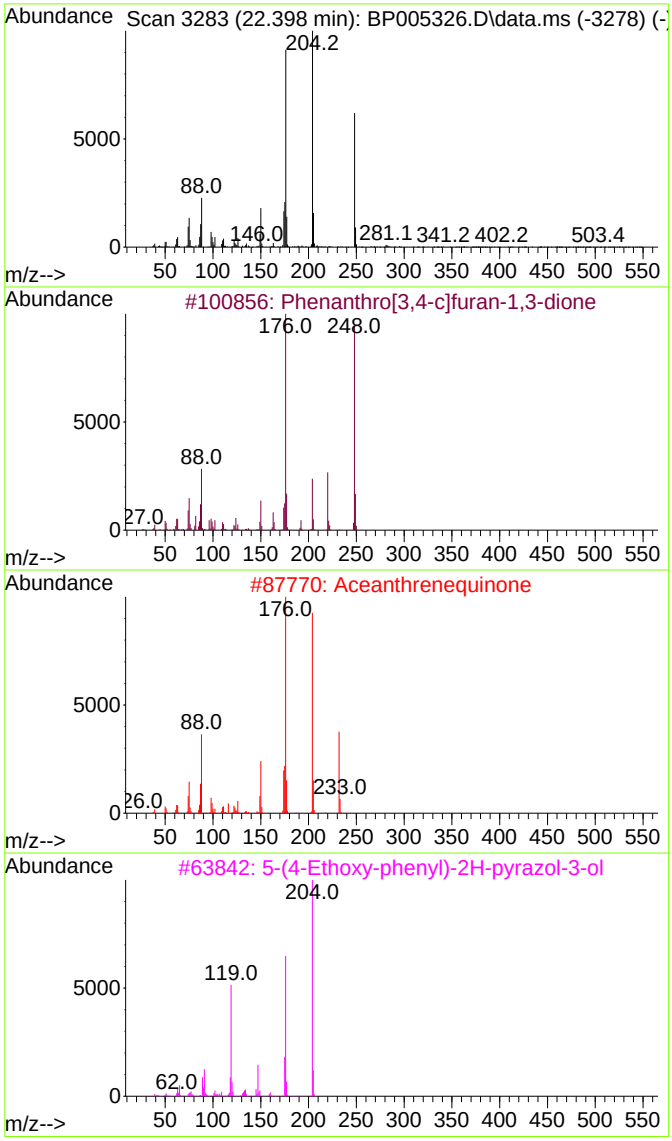
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

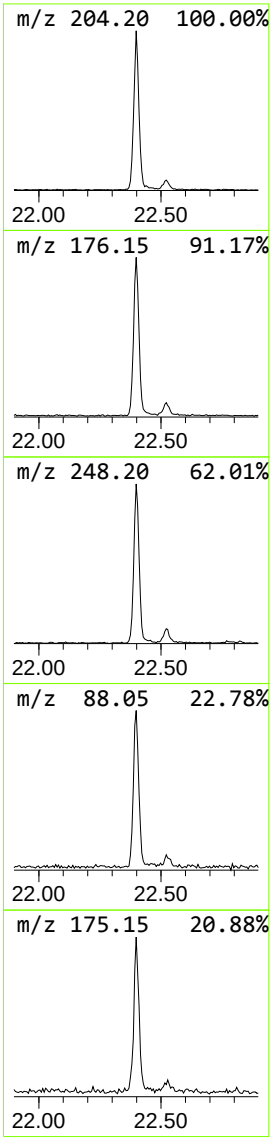
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Phenanthro[3,4-c]furan-1,3-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.398	12.10 ng	334643	Perylene-d12	23.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthro[3,4-c]furan-1,3-dione	248	C16H8O3	005723-54-6	62
2	Aceanthrenequinone	232	C16H8O2	006373-11-1	52
3	5-(4-Ethoxy-phenyl)-2H-pyrazol-3-ol	204	C11H12N2O2	1000278-26-8	50
4	4-Methyl-6,7-methylenedioxycoumarin	204	C11H8O4	015071-04-2	47
5	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041621\
Data File : BP005326.D
Acq On : 16 Apr 2021 19:22
Operator : CG/JU
Sample : M1966-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-110RR

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.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
Phenol, 2,6-dim...	9.087	6.4	ng	66519	2	10.452	206595	20.0
Phenol, 3,4-dim...	9.952	4.4	ng	45533	2	10.452	206595	20.0
Phenol, 2,4,5-t...	10.605	2.8	ng	29060	2	10.452	206595	20.0
unknown12.199	12.199	11.6	ng	119431	2	10.452	206595	20.0
Benzoic acid, p...	14.163	3.3	ng	55872	3	14.322	343763	20.0
1-Naphthaleneca...	16.104	25.9	ng	614070	4	17.087	473261	20.0
n-Hexadecanoic ...	18.004	11.8	ng	278220	4	17.087	473261	20.0
Naphthalic anhy...	18.881	8.3	ng	195937	4	17.087	473261	20.0
Octadecanoic acid	19.239	4.2	ng	118253	5	21.192	567099	20.0
Phenol, 4,4'-(1...	19.498	2.9	ng	82255	5	21.192	567099	20.0
Benzamide, N-pr...	20.875	2.2	ng	62114	5	21.192	567099	20.0
1-Heptacosanol	20.904	16.3	ng	461735	5	21.192	567099	20.0
1,3-Dioxolane, ...	20.975	10.4	ng	296062	5	21.192	567099	20.0
Phenanthro[3,4-...	22.398	12.1	ng	334643	6	23.463	552991	20.0