LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

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-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008251.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.381	400	407	421	rBV	207899	363468	18.85%	3.800%
2	6.981	667	679	693	rBV	105487	217491	11.28%	2.274%
3	7.381	741	747	756	rVB	36316	62380	3.23%	0.652%
4	7.787	809	816	823	rBV	96099	163026	8.45%	1.704%
5	8.945	1006	1013	1023	rBV	361328	631907	32.76%	6.607%
6	9.040	1024	1029	1036	rVB	23809	41645	2.16%	0.435%
7	9.951	1178	1184	1191	rBV	11392	21628	1.12%	0.226%
8	10.581	1285	1291	1304	rBV	124909	224664	11.65%	2.349%
9	11.122	1376	1383	1390	rVB2	16293	27447	1.42%	0.287%
10	12.651	1631	1643	1650	rBV	22539	40568	2.10%	0.424%
11	13.051	1704	1711	1720	rBV	889778	1401990	72.69%	14.658%
12	13.798	1835	1838	1850	rVB6	12294	31769	1.65%	0.332%
13	13.939	1857	1862	1873	rBV3	45764	125658	6.52%	1.314%
14	14.433	1941	1946	1953	rBV	187426	294843	15.29%	3.083%
15	14.539	1960	1964	1971	rBV	28297	46113	2.39%	0.482%
16	14.763	1998	2002	2006	rBV2	91387	123740	6.42%	1.294%
17	15.075	2051	2055	2061	rBV3	29016	48892	2.54%	0.511%
18	15.422	2110	2114	2119	rBV2	28419	41902	2.17%	0.438%
19	15.586	2139	2142	2148	rVB2	22556	32720	1.70%	0.342%
20	15.933	2196	2201	2212	rVB	753522	1179469	61.16%	12.331%
21	16.351	2267	2272	2279	rBV2	126868	179974	9.33%	1.882%
22	16.569	2305	2309	2314	rBV4	53148	75927	3.94%	0.794%
23	16.745	2335	2339	2343	rBV6	24942	42648	2.21%	0.446%
24	16.845	2352	2356	2367	rBV	109169	179990	9.33%	1.882%
25	17.051	2387	2391	2396	rBV	187366	277865	14.41%	2.905%
26	17.198	2411	2416	2424	rBV	249278	375436	19.47%	3.925%
27	17.351	2439	2442	2451	rVB	44065	67280	3.49%	0.703%
28	17.745	2507	2509	2510	rBV	27412	22792	1.18%	0.238%
29	17.845	2523	2526	2530	rBV2	28788	43481	2.25%	0.455%
30	18.098	2566	2569	2575	rBV5	36566	60449	3.13%	0.632%
31	19.768	2848	2853	2860	rBV	1624000	1928623	100.00%	20.164%
32	21.304	3110	3114	3119	rBV	426157	545818	28.30%	5.707%
33	23.698	3516	3521	3529	rVB	313892	643099	33.34%	6.724%

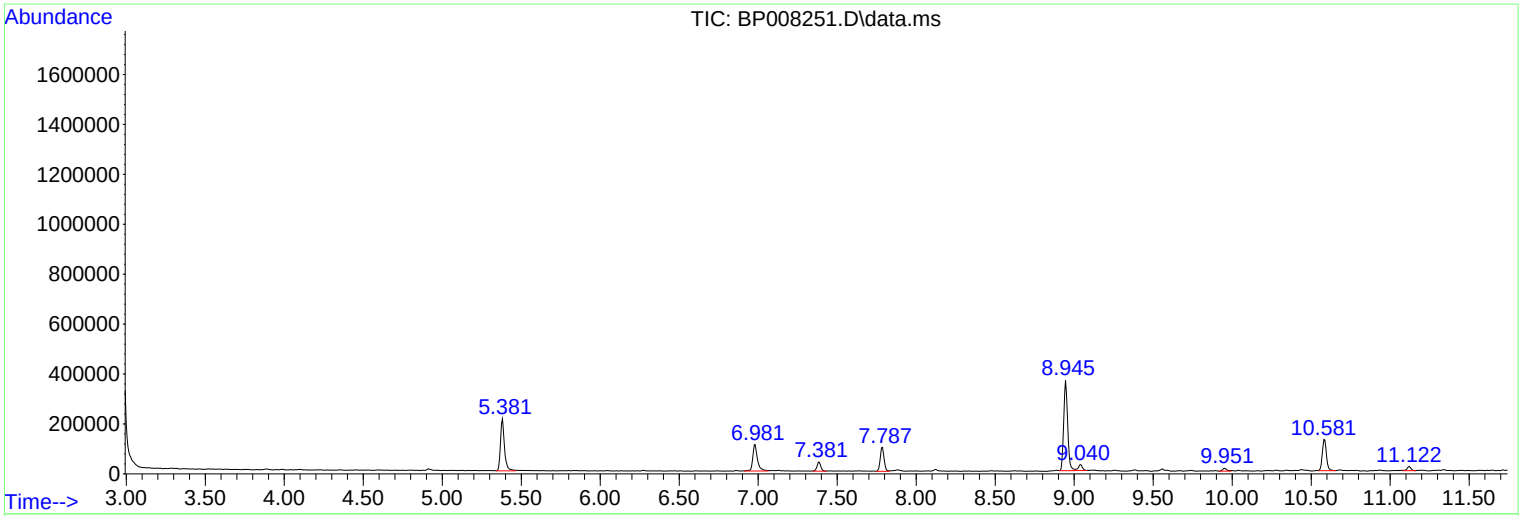
Sum of corrected areas: 9564702

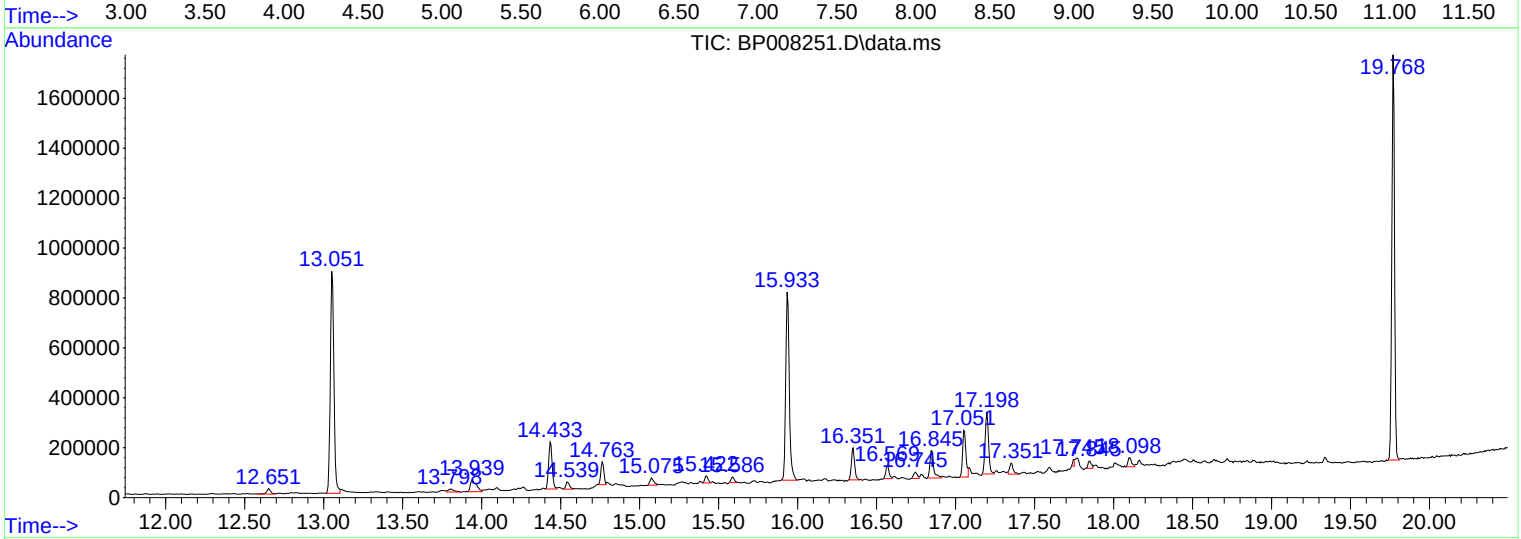
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

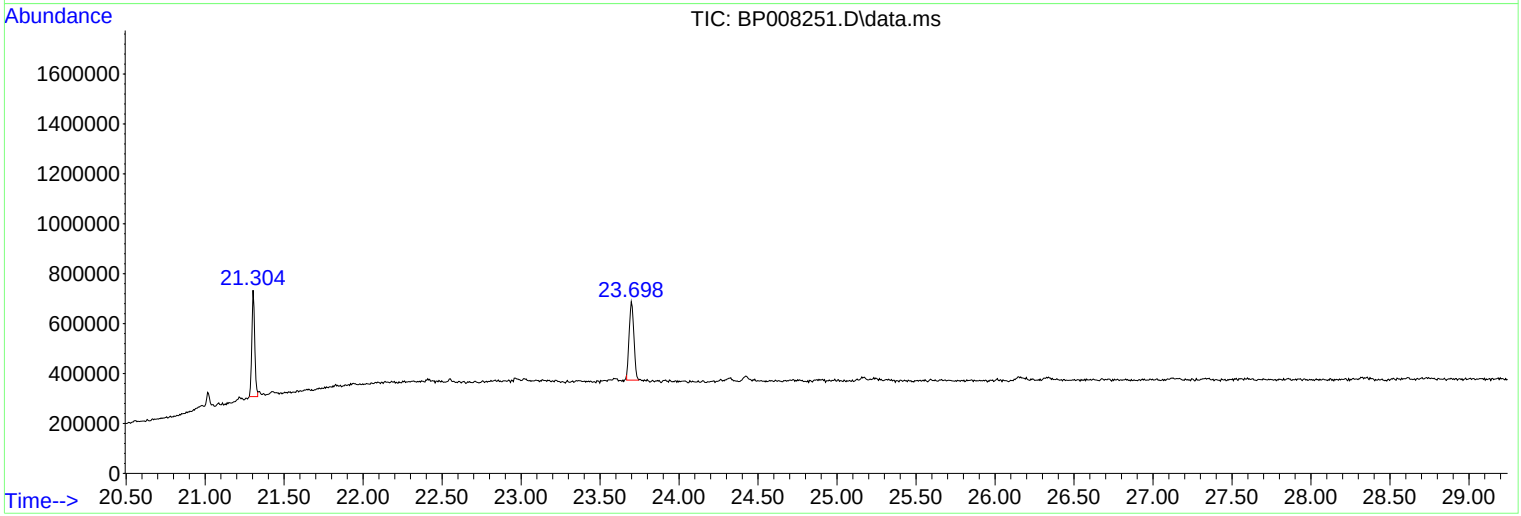
Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

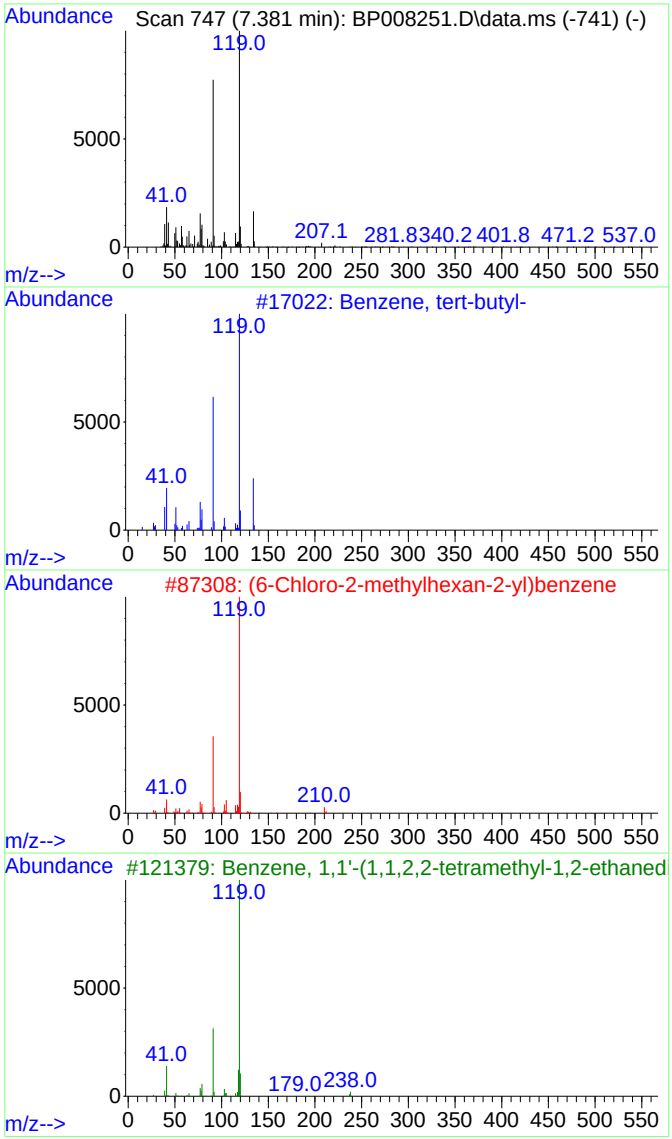
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

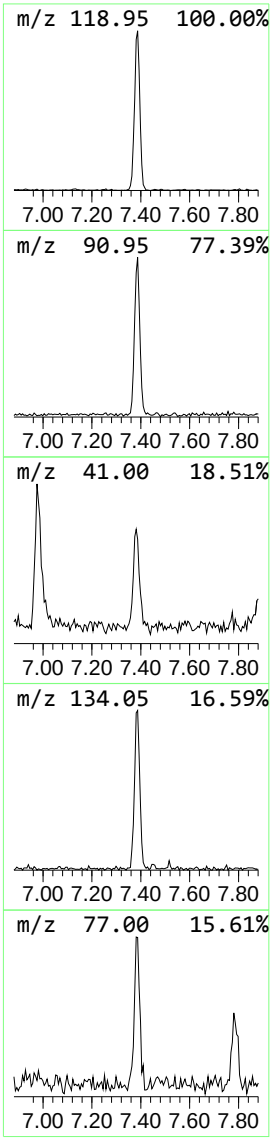
****

Peak Number 1 Benzene, tert-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.381	7.65 ng	62380	1,4-Dichlorobenzene-d4	7.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, tert-butyl-	134	C10H14	000098-06-6	91
2	(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	87
3	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	74
4	1,3,5-Cycloheptatriene, 3,7,7-tr...	134	C10H14	003479-89-8	74
5	trans-Carveol, O-(pentafluoropro...	298	C13H15F5O2	1000454-02-5	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

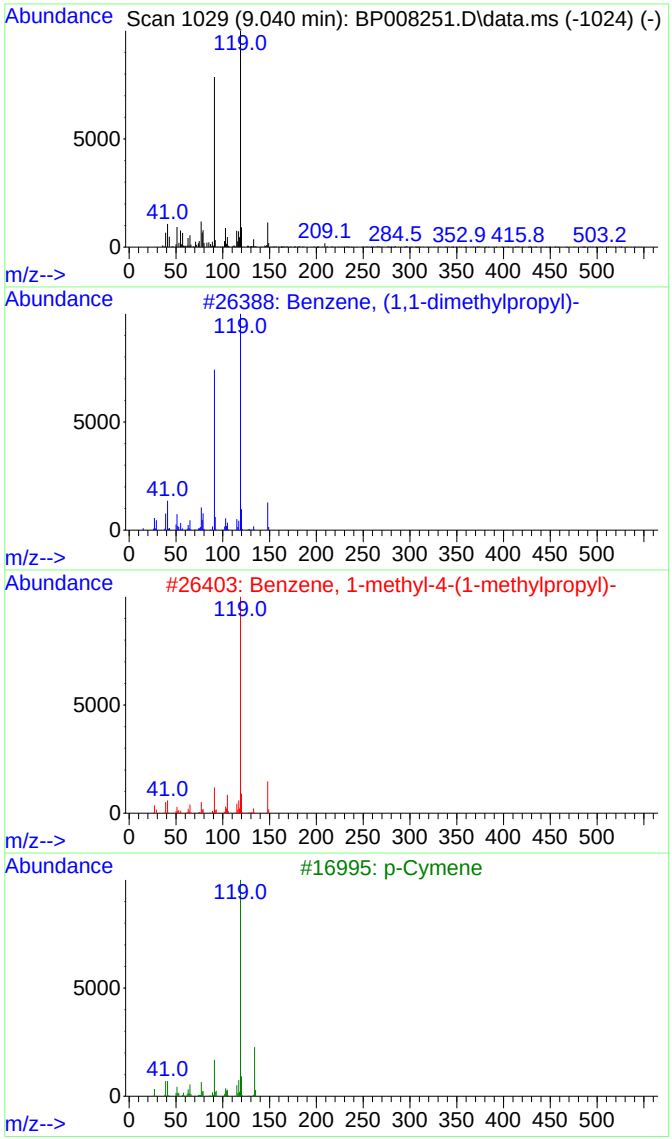
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

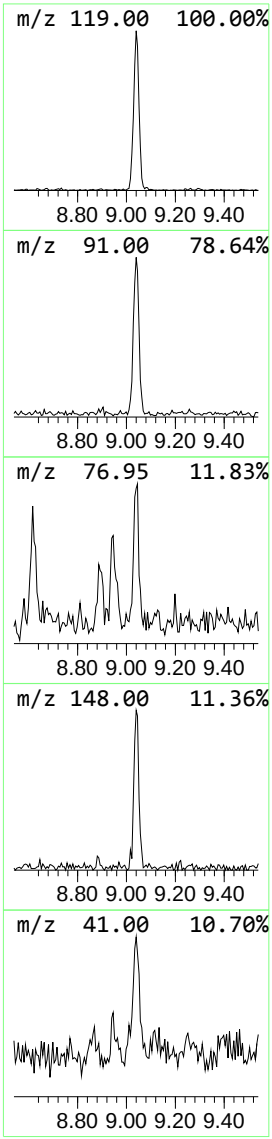
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1-methyl-4-(1-meth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.040	5.11 ng	41645	1,4-Dichlorobenzene-d4	7.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	90
2	Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	78
3	p-Cymene	134	C10H14	000099-87-6	59
4	Benzamide, 3-methyl-N-propyl-N-b...	233	C15H23NO	1000438-12-6	59
5	m-Toluic acid, 2,6-dimethylnon-1...	284	C19H24O2	1010292-49-8	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

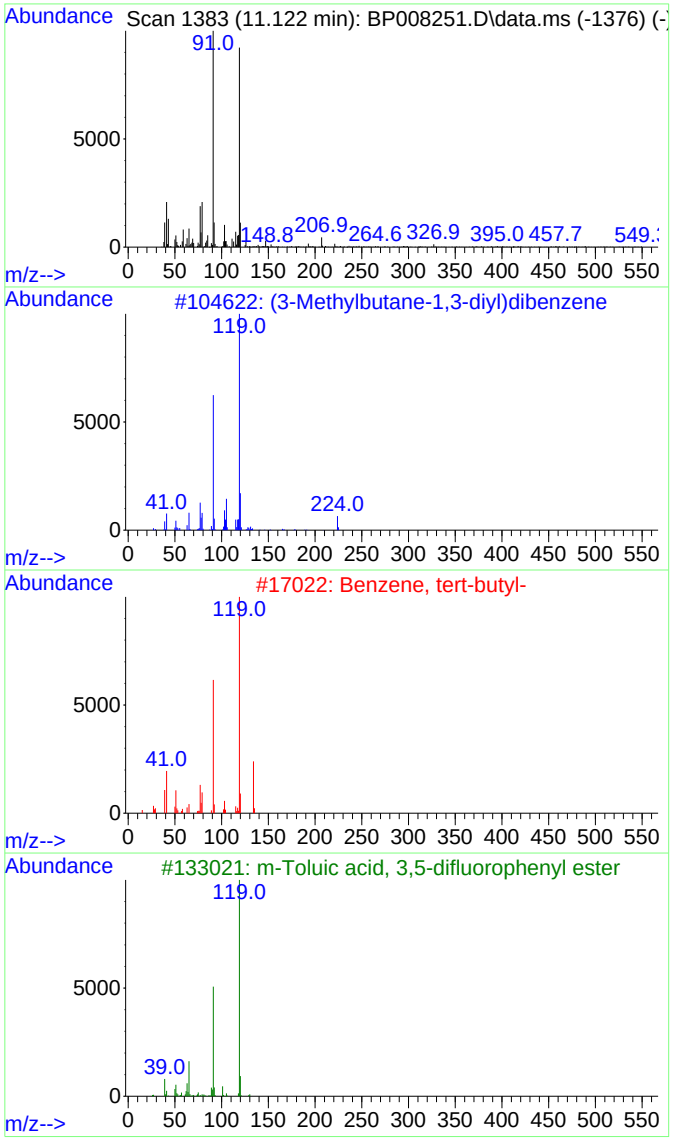
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

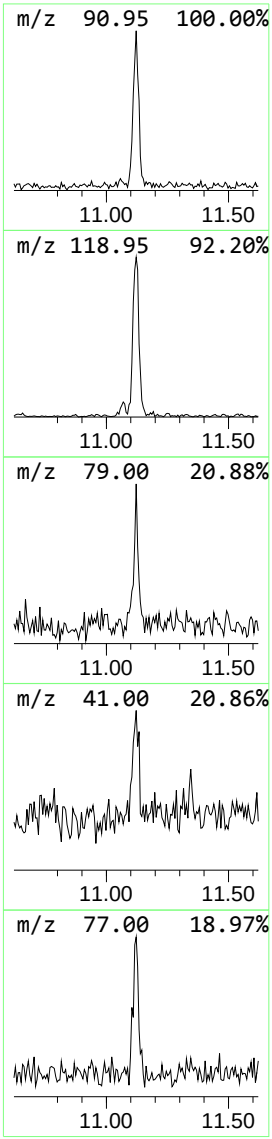
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (3-Methylbutane-1,3-diyl)di... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.122	2.44 ng	27447	Naphthalene-d8	10.581

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3-Methylbutane-1,3-diyl)dibenzene	224	C17H20	001520-43-0	87
2	Benzene, tert-butyl-	134	C10H14	000098-06-6	78
3	m-Toluic acid, 3,5-difluoropheny...	248	C14H10F2O2	1000293-76-6	72
4	Benzene, isocyanato-	119	C7H5NO	000103-71-9	72
5	Benzonitrile, 3-hydroxy-	119	C7H5NO	000873-62-1	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

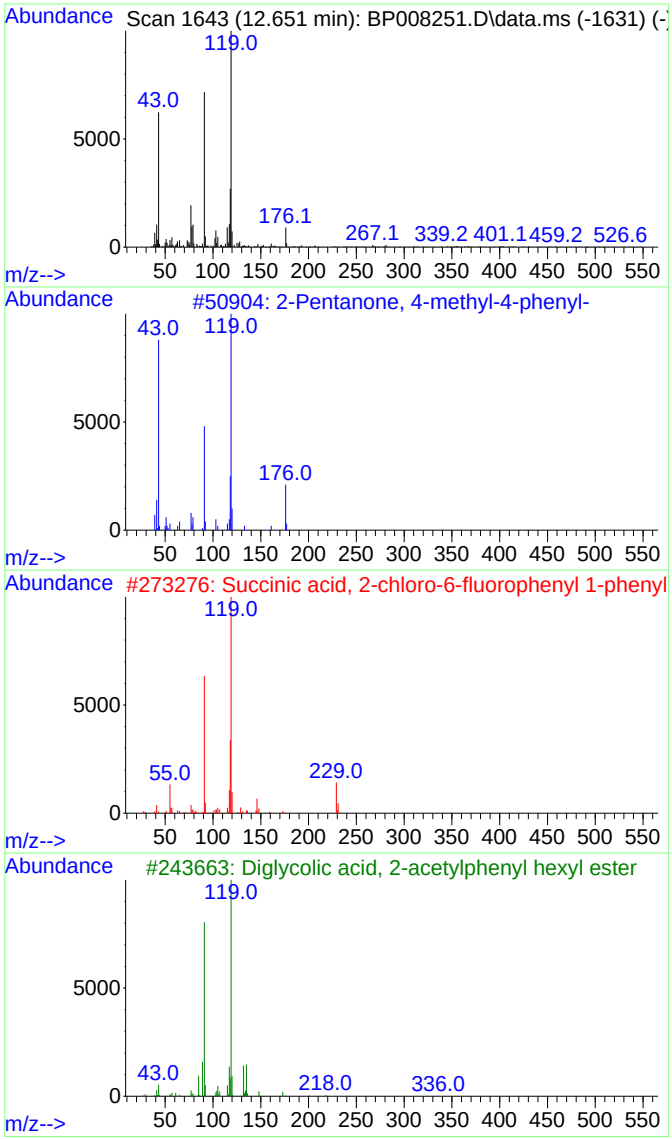
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

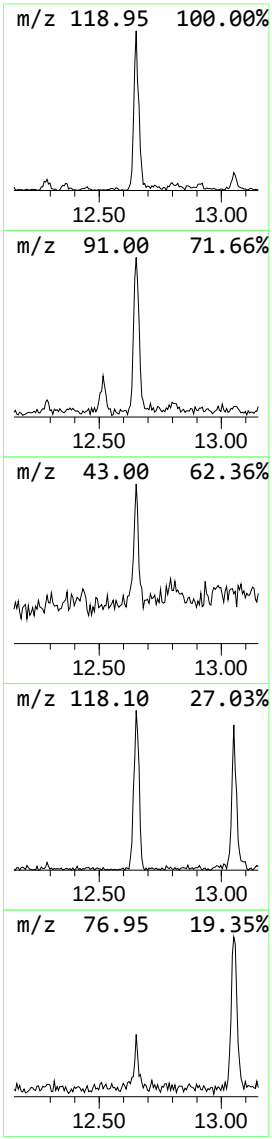
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-methyl-4-phe... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	2.75 ng	40568	Acenaphthene-d10	14.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methyl-4-phenyl-	176	C12H16O	007403-42-1	59
2	Succinic acid, 2-chloro-6-fluoro...	364	C19H18ClFO4	1000389-93-2	59
3	Diglycolic acid, 2-acetylphenyl ...	336	C18H24O6	1000382-72-2	53
4	Pyridine, 5-ethenyl-2-methyl-	119	C8H9N	000140-76-1	50
5	1-Chloro-2-methyl-2-phenylpropane	168	C10H13Cl	000515-40-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

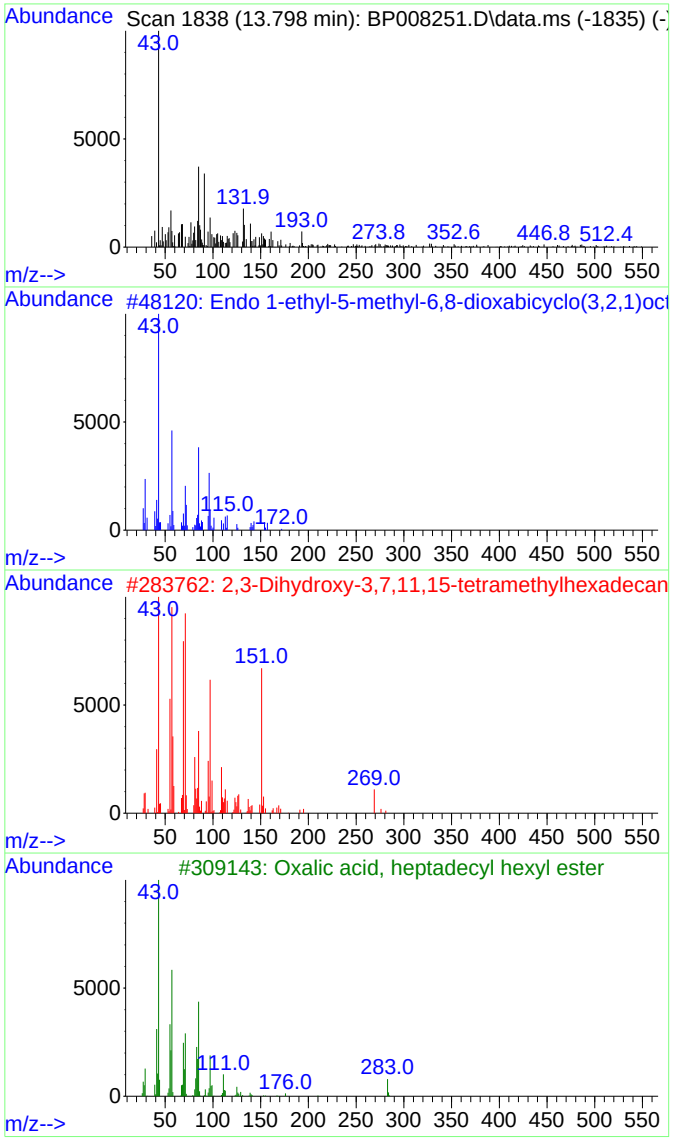
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

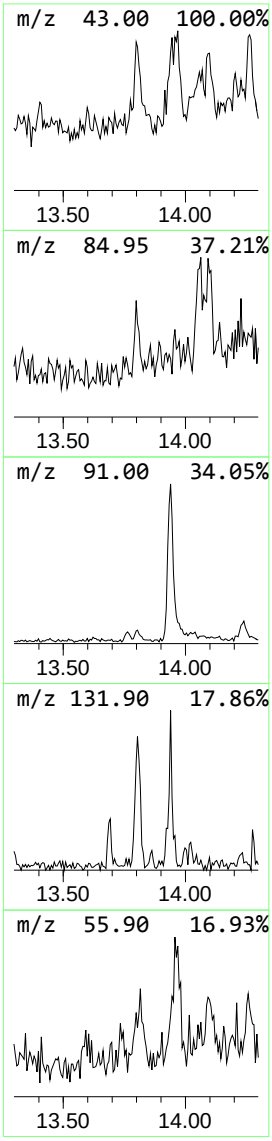
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 unknown13.798 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	2.15 ng	31769	Acenaphthene-d10	14.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Endo 1-ethyl-5-methyl-6,8-dioxab...	172	C9H16O3	1000426-71-4	38
2	2,3-Dihydroxy-3,7,11,15-tetramet...	375	C20H41NO5	1000432-41-1	30
3	Oxalic acid, heptadecyl hexyl ester	412	C25H48O4	1000309-25-1	27
4	Butanoic acid, 3-oxo-, 2-hydroxy...	146	C6H10O4	033736-01-5	27
5	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

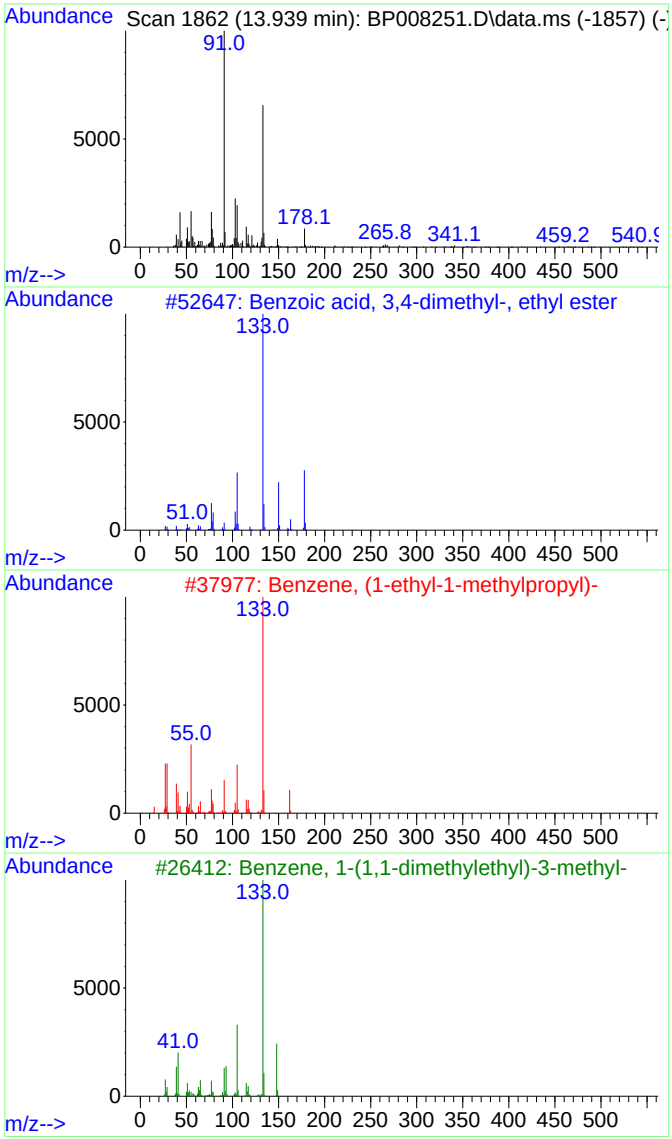
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

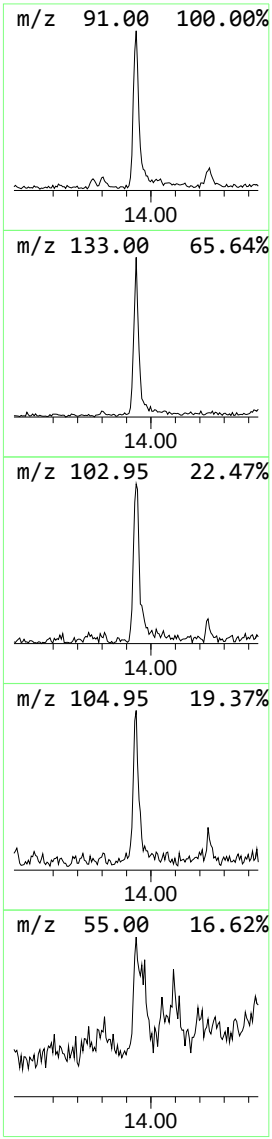
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown13.939 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	8.52 ng	125658	Acenaphthene-d10	14.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 3,4-dimethyl-, eth...	178	C11H14O2	033499-44-4	47
2	Benzene, (1-ethyl-1-methylpropyl)-	162	C12H18	001985-97-3	47
3	Benzene, 1-(1,1-dimethylethyl)-3...	148	C11H16	001075-38-3	47
4	2,5-Pyrrolidinedione, 1-[(3,4-di...	247	C13H13NO4	1000306-84-7	46
5	1H-Indol-4-ol	133	C8H7NO	002380-94-1	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

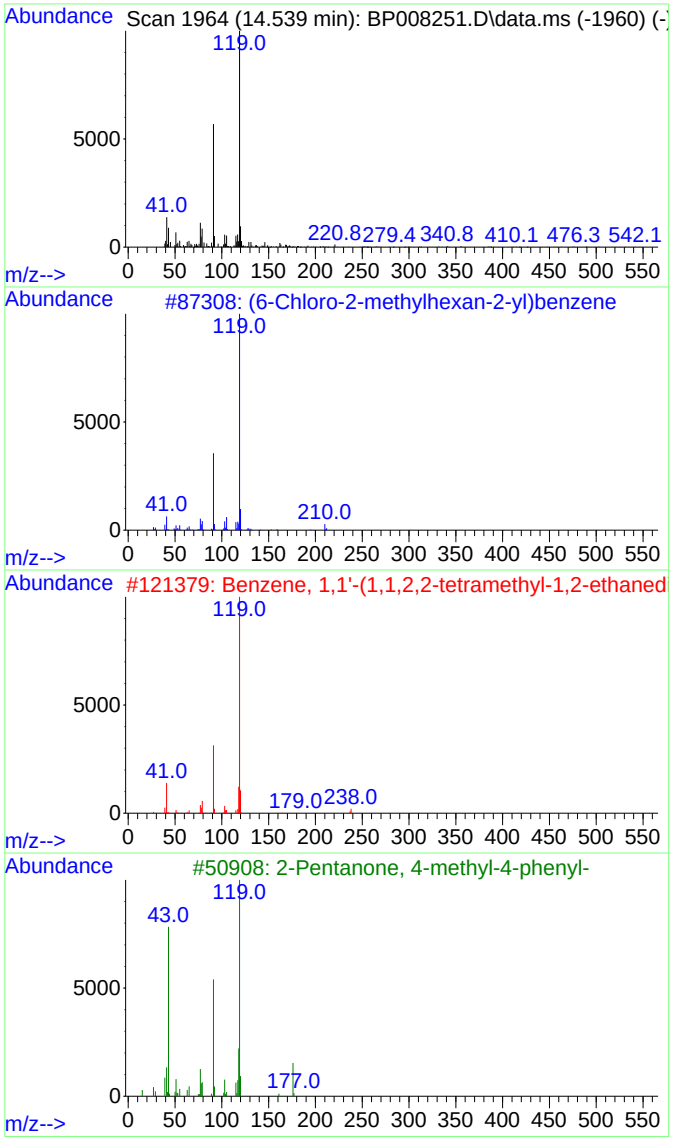
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

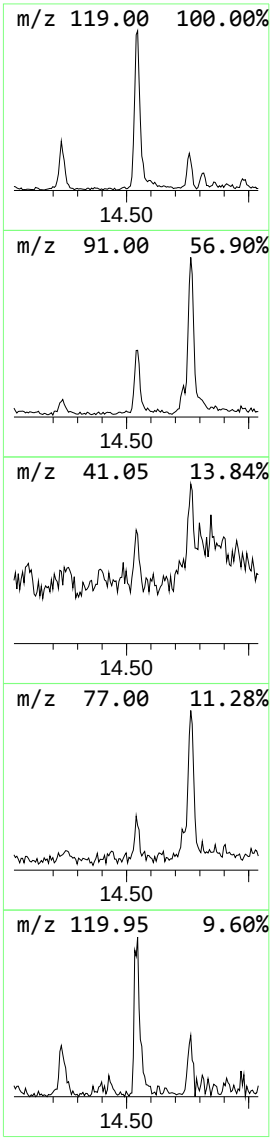
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (6-Chloro-2-methylhexan-2-y... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	3.13 ng	46113	Acenaphthene-d10	14.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	94
2	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	87
3	2-Pentanone, 4-methyl-4-phenyl-	176	C12H16O	007403-42-1	83
4	o-Cymene	134	C10H14	000527-84-4	78
5	Benzene, tert-butyl-	134	C10H14	000098-06-6	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

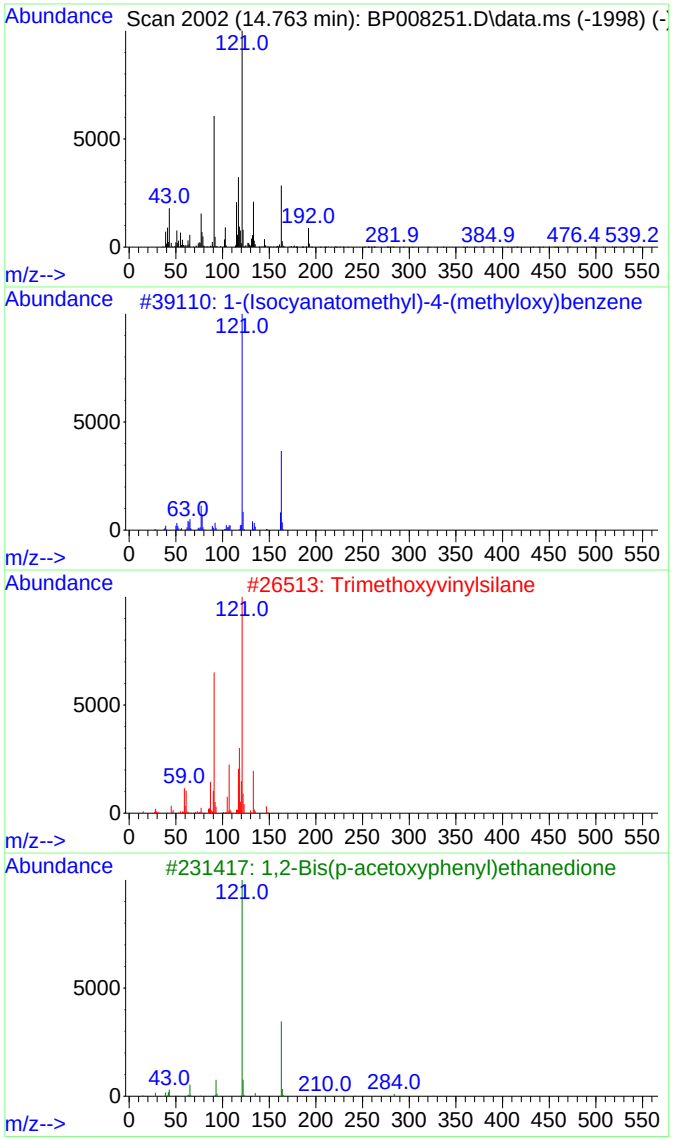
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

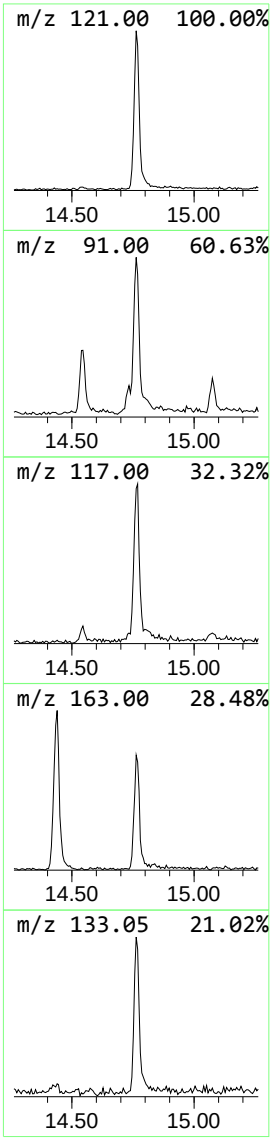
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 unknown14.763 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	8.39 ng	123740	Acenaphthene-d10	14.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(Isocyanatomethyl)-4-(methylox...	163	C9H9NO2	056651-60-6	43
2	Trimethoxyvinylsilane	148	C5H12O3Si	002768-02-7	43
3	1,2-Bis(p-acetoxyphenyl)ethanedione	326	C18H14O6	093655-79-9	38
4	2-Acetamidotropone	163	C9H9NO2	006422-12-4	38
5	1-(4-Pyridinyl)piperazine	163	C9H13N3	001008-91-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

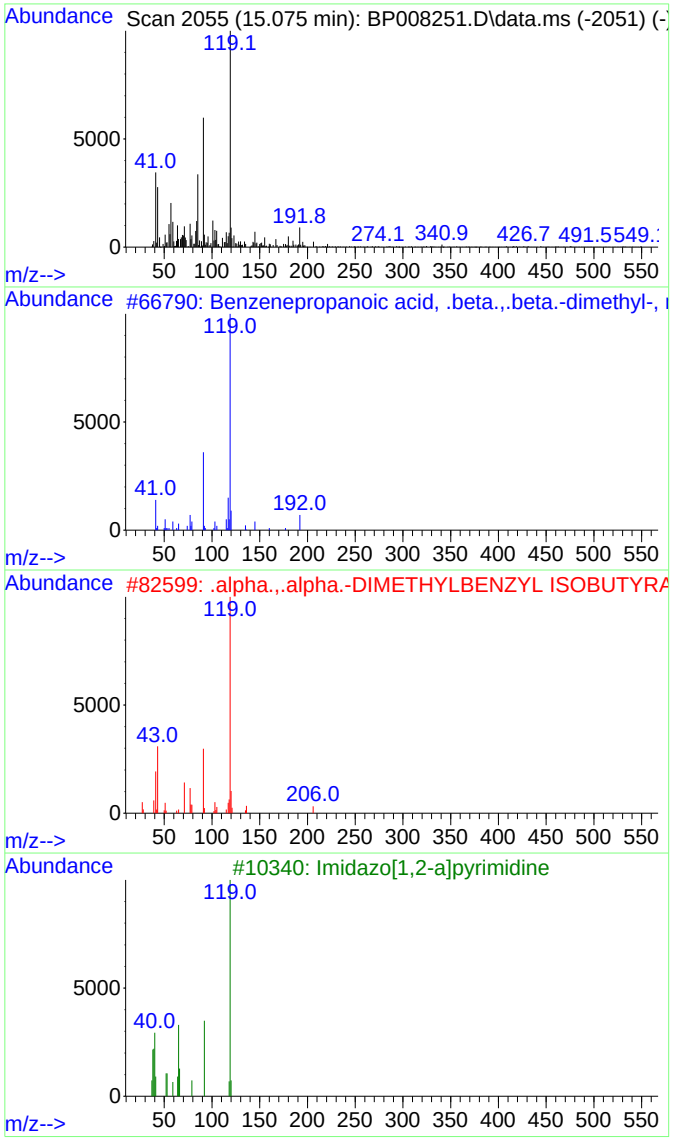
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

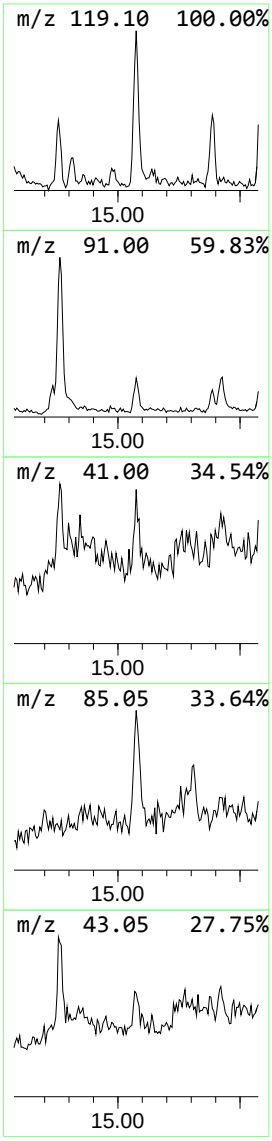
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzenepropanoic acid, .bet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.075	3.32 ng	48892	Acenaphthene-d10	14.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanoic acid, .beta.,.b...	192	C12H16O2	025080-84-6	60
2	.alpha.,.alpha.-DIMETHYLBENZYL I...	206	C13H18O2	1000429-51-9	50
3	Imidazo[1,2-a]pyrimidine	119	C6H5N3	000274-95-3	47
4	Cumene hydroperoxide, TMS deriva...	224	C12H20O2Si	018057-16-4	45
5	2-Isothiocyanato-2,4-dimethyl-4-...	233	C14H19NS	1000293-27-6	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

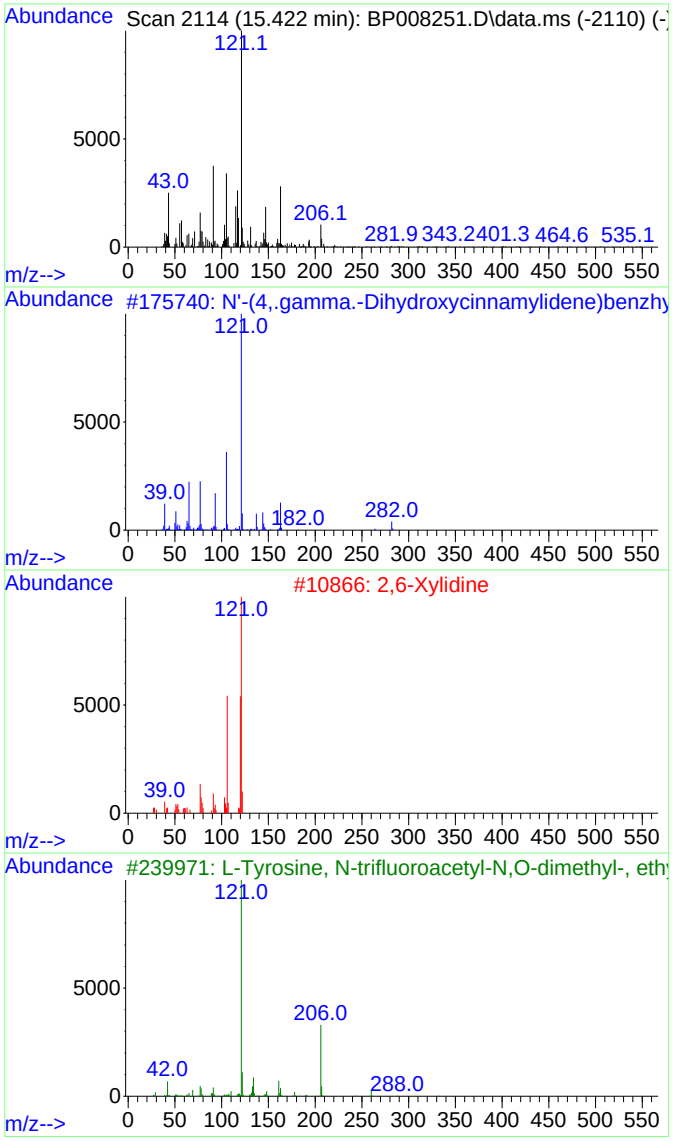
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

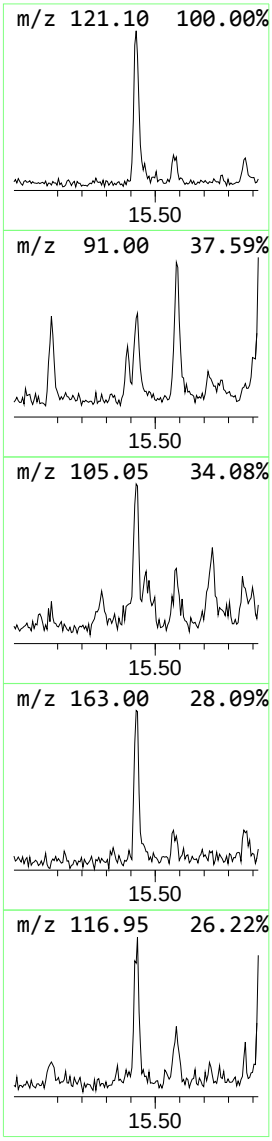
****

Peak Number 10 unknown15.422 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.422	2.84 ng	41902	Acenaphthene-d10	14.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N'-(4,.gamma.-Dihydroxycinnamyli...	282	C16H14N2O3	1000225-23-0	43
2	2,6-Xylidine	121	C8H11N	000087-62-7	43
3	L-Tyrosine, N-trifluoroacetyl-N,...	333	C15H18F3NO4	1000452-69-8	43
4	4-Methoxybenzylamine, N,N-dibutyl-	249	C16H27NO	1000310-38-3	43
5	Aminorex, N,N-dimethyl	190	C11H14N2O	1000447-11-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

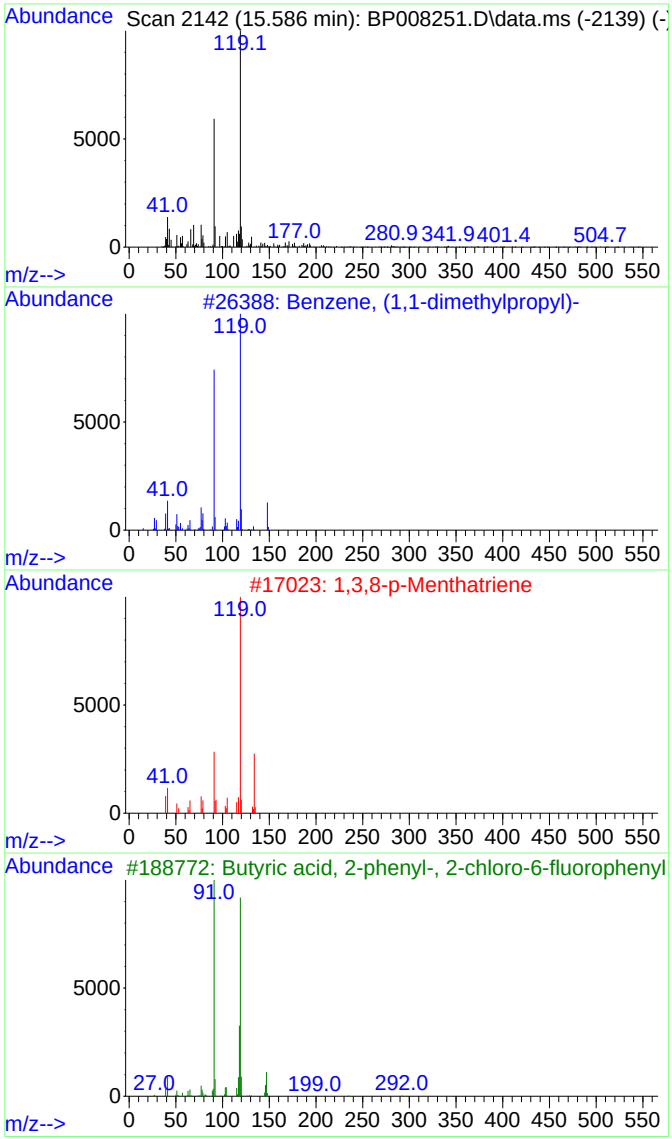
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

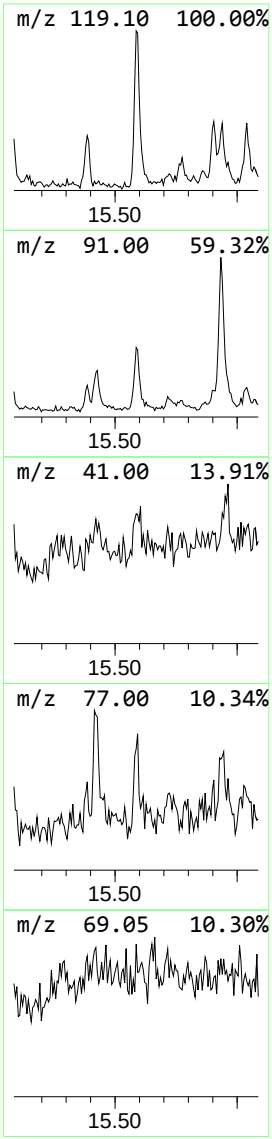
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Benzene, (1,1-dimethylpropyl)- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.586	2.22 ng	32720	Acenaphthene-d10	14.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	64
2	1,3,8-p-Menthatriene	134	C10H14	018368-95-1	64
3	Butyric acid, 2-phenyl-, 2-chlor...	292	C16H14ClFO2	1000406-86-2	64
4	Butyric acid, 2-phenyl-, 2,3-dic...	308	C16H14Cl2O2	1000406-86-5	64
5	Pyridine, 5-ethenyl-2-methyl-	119	C8H9N	000140-76-1	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

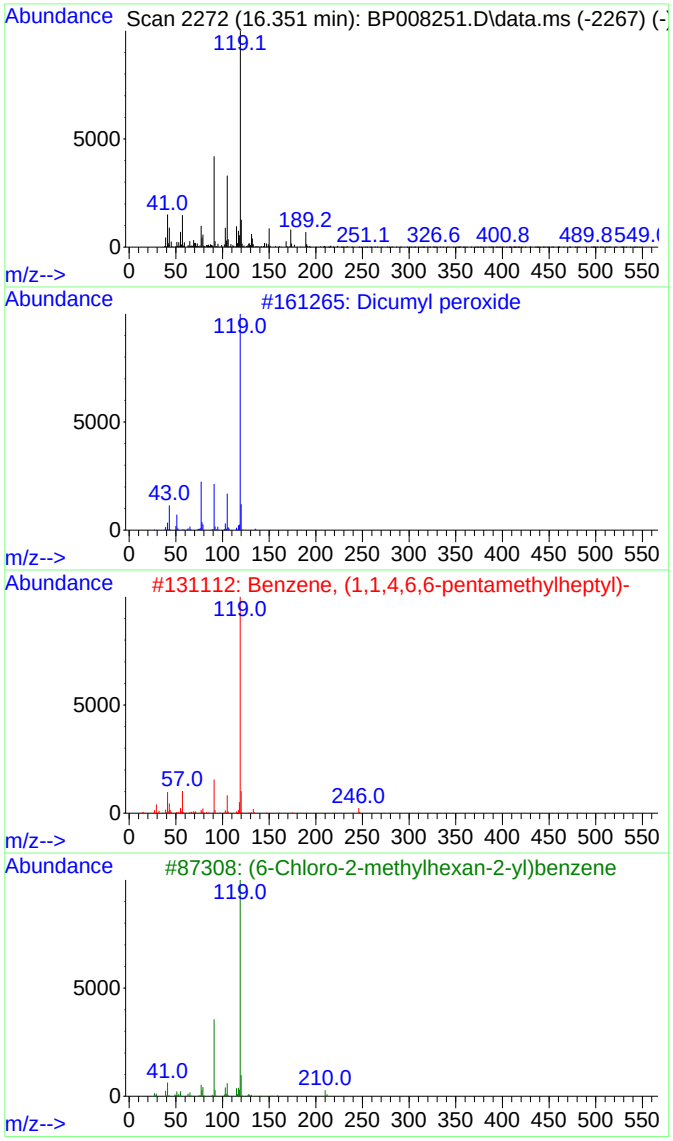
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

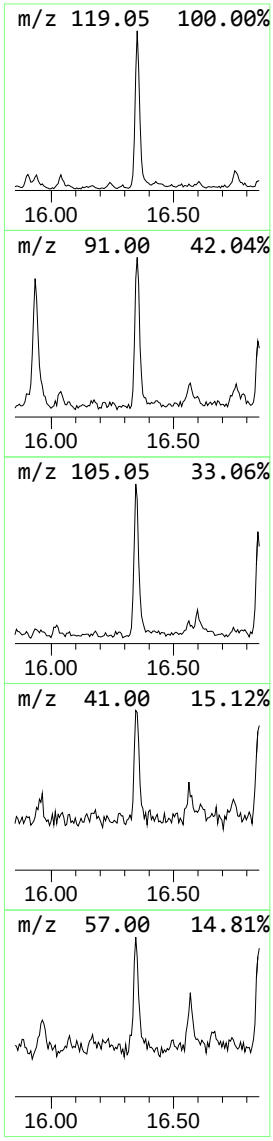
****

Peak Number 12 Dicumyl peroxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.351	9.59 ng	179974	Phenanthrene-d10	17.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dicumyl peroxide	270	C18H22O2	000080-43-3	64
2	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	64
3	(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	62
4	(3-Methylbutane-1,3-diyl)dibenzene	224	C17H20	001520-43-0	59
5	Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

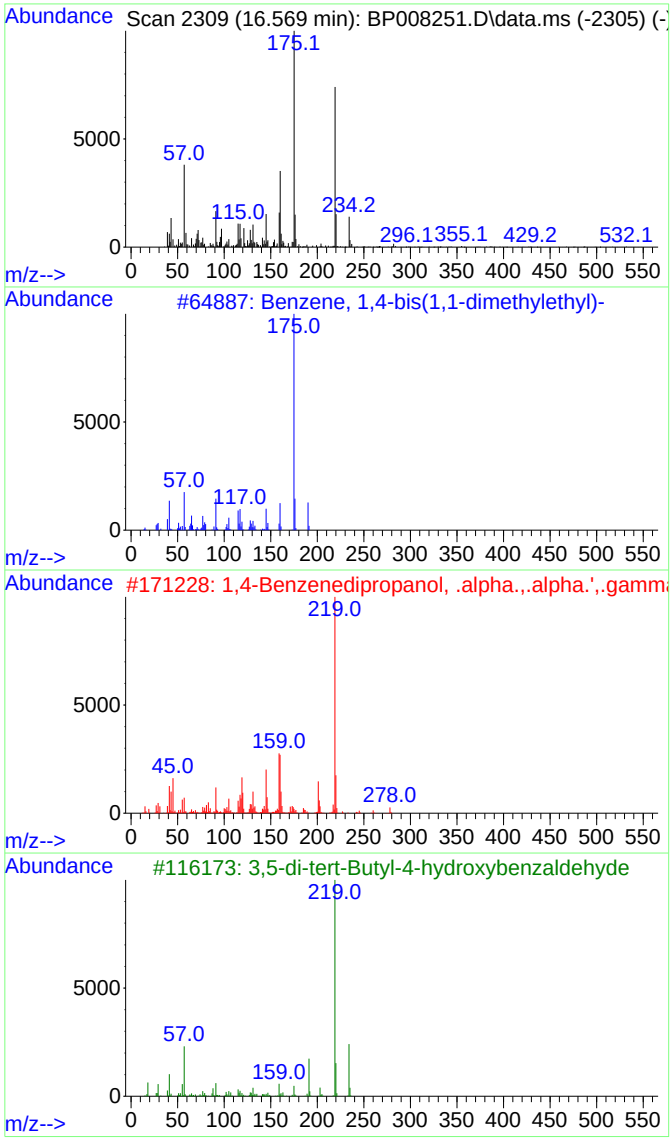
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

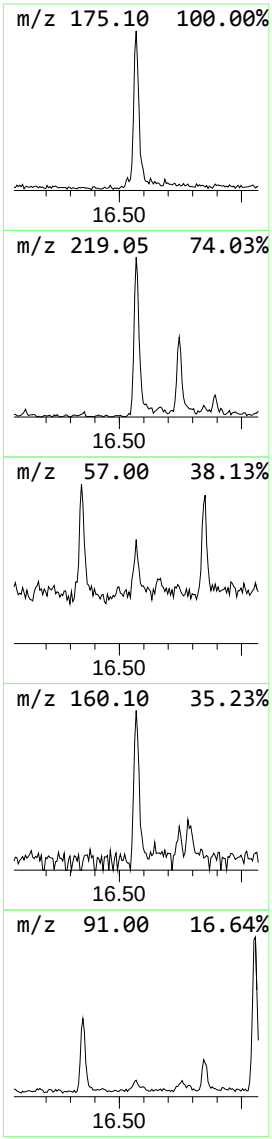
****

Peak Number 13 unknown16.569 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.569	4.04 ng	75927	Phenanthrene-d10	17.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,4-bis(1,1-dimethyleth...	190	C14H22	001012-72-2	38
2	1,4-Benzenedipropanol, .alpha.,....	278	C18H30O2	054964-98-6	38
3	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	35
4	Iron(0), (2-methylbutadiene)-1,2...	386	C19H40FeP2	1000160-76-3	30
5	3,5-Di-tert-butyl-2-hydroxybenza...	234	C15H22O2	037942-07-7	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

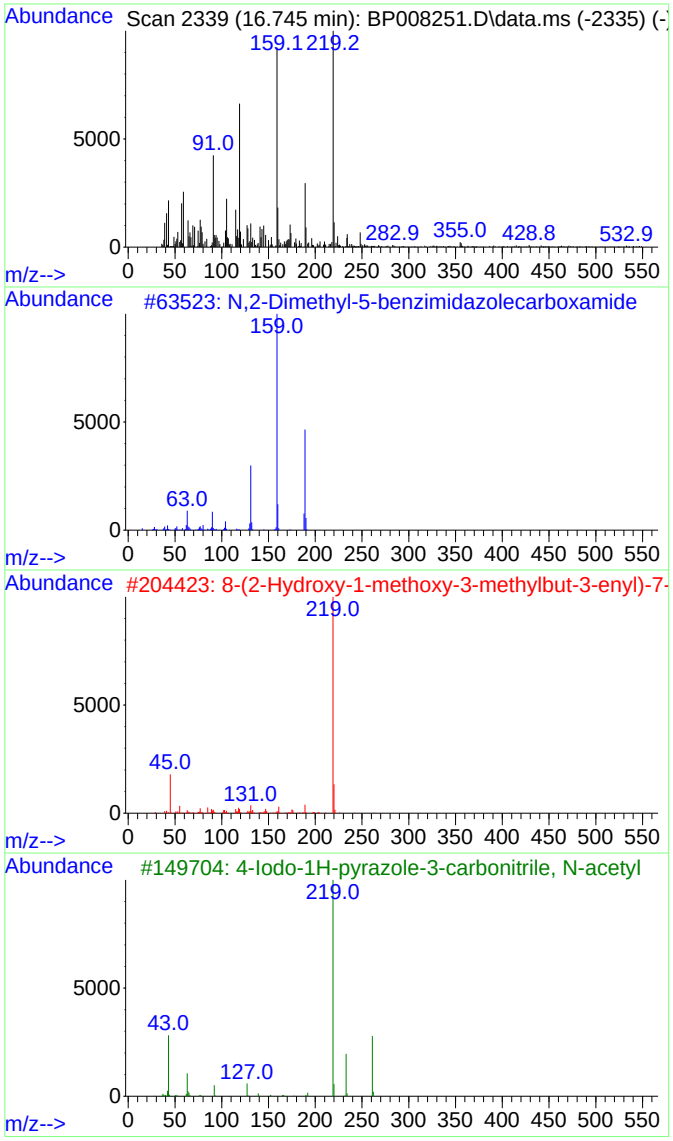
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

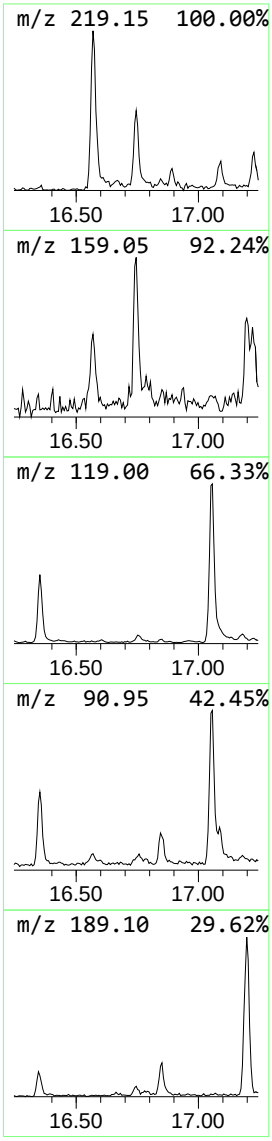
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 unknown16.745 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.745	2.27 ng	42648	Phenanthrene-d10	17.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N,2-Dimethyl-5-benzimidazolecarb...	189	C10H11N3O	093690-15-4	22
2	8-(2-Hydroxy-1-methoxy-3-methylb...	304	C17H20O5	1000493-42-6	22
3	4-Iodo-1H-pyrazole-3-carbonitril...	261	C6H4IN3O	1000512-23-0	22
4	acetamide, 2,2,2-trifluoro-N-(4-...	219	C9H8F3NO2	1010400-75-8	20
5	4-Phenyl-1H-pyrazol-3-ylamine	159	C9H9N3	005591-70-8	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

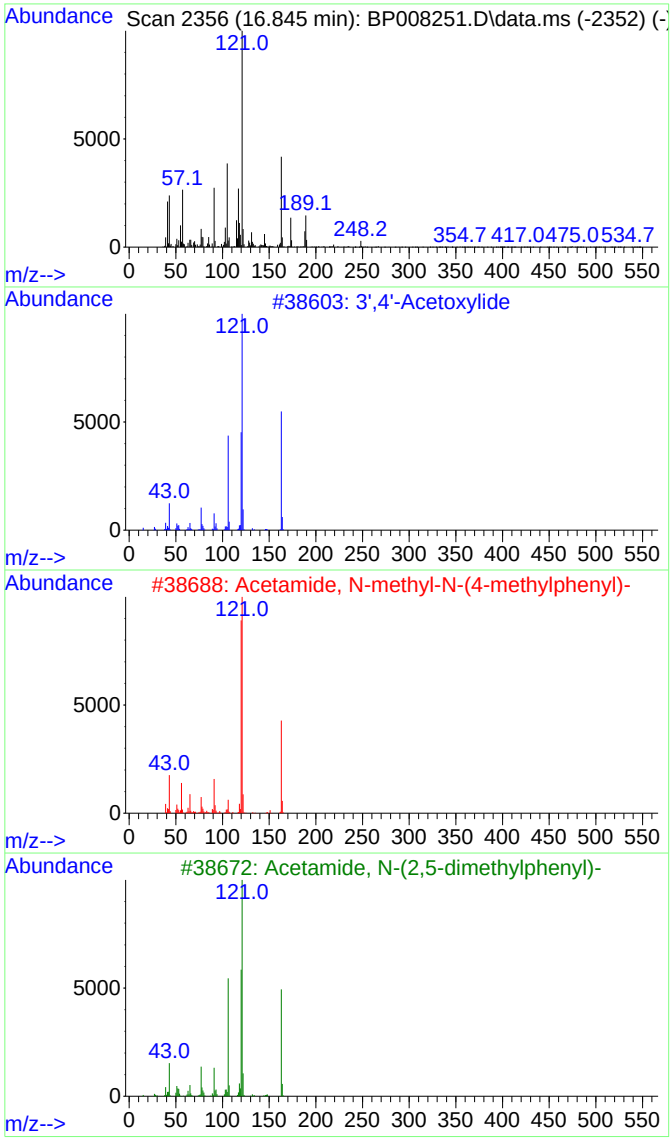
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

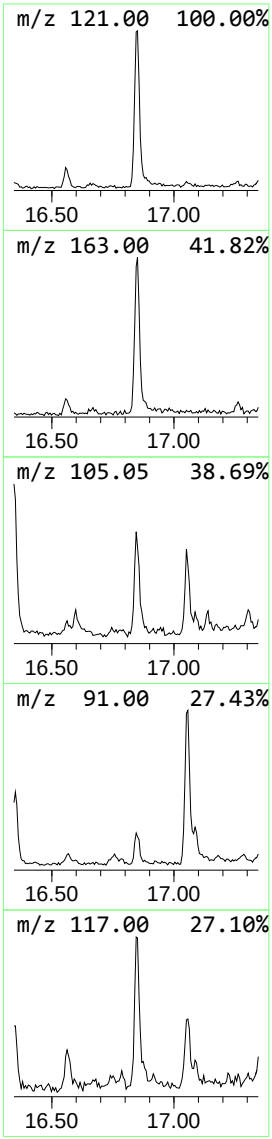
****

Peak Number 15 3',4'-Acetoxylide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.845	9.59 ng	179990	Phenanthrene-d10	17.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3',4'-Acetoxylide	163	C10H13NO	002198-54-1	52
2	Acetamide, N-methyl-N-(4-methylp...	163	C10H13NO	000612-03-3	52
3	Acetamide, N-(2,5-dimethylphenyl)-	163	C10H13NO	002050-44-4	52
4	2-Acetamidotropone	163	C9H9NO2	006422-12-4	47
5	2-sec-Butylphenol, acetate	192	C12H16O2	003056-61-9	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

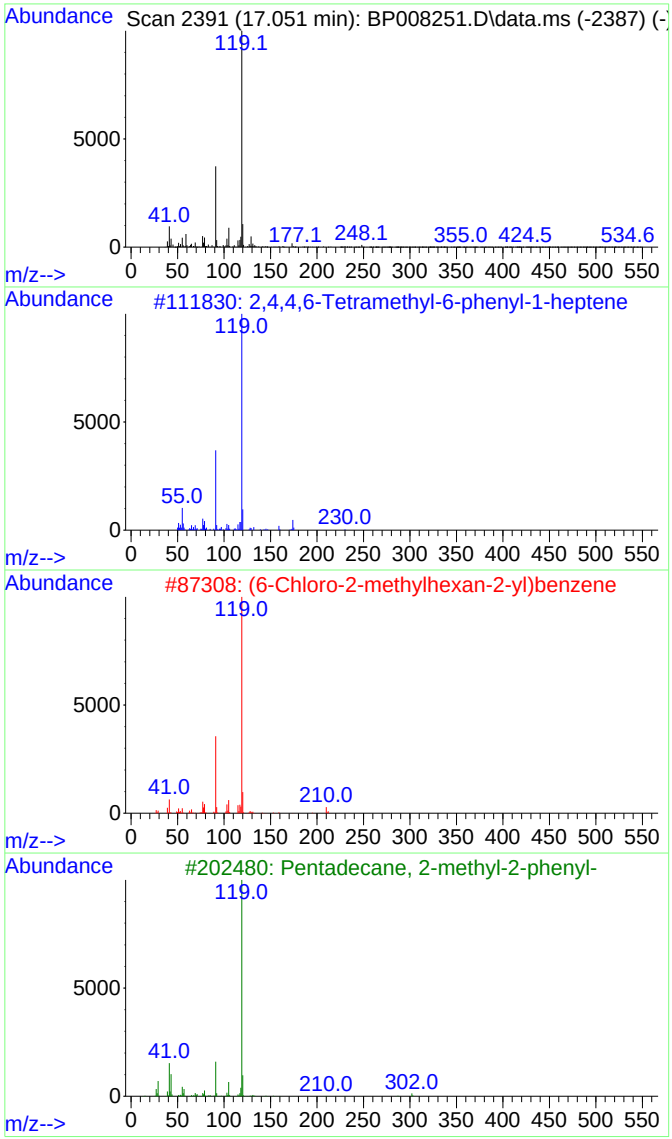
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

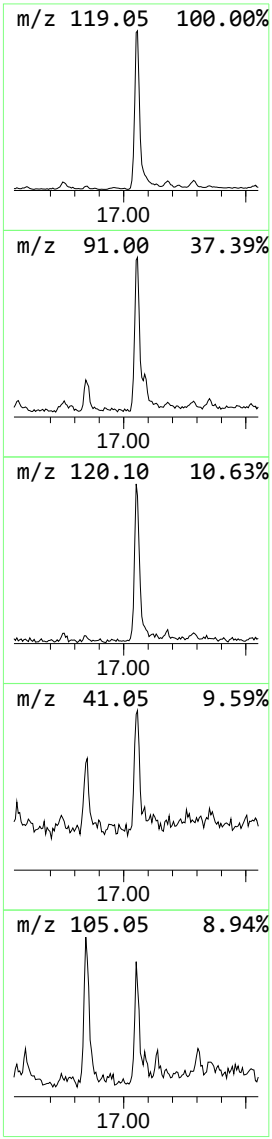
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 2,4,4,6-Tetramethyl-6-pheny... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.051	14.80 ng	277865	Phenanthrene-d10	17.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6-Tetramethyl-6-phenyl-1-h...	230	C17H26	1000293-27-9	83
2	(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	72
3	Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	64
4	2-Hexanone, 5-methyl-5-phenyl-	190	C13H18O	014128-61-1	64
5	Benzene, (1,1-dimethylbutyl)-	162	C12H18	001985-57-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

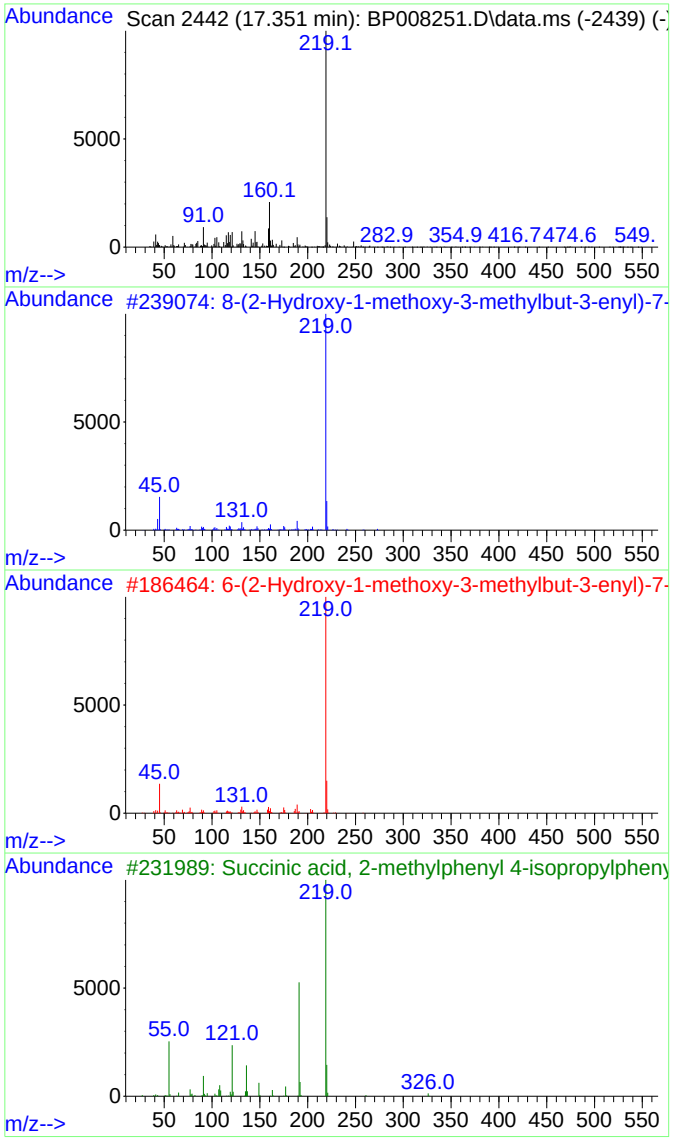
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

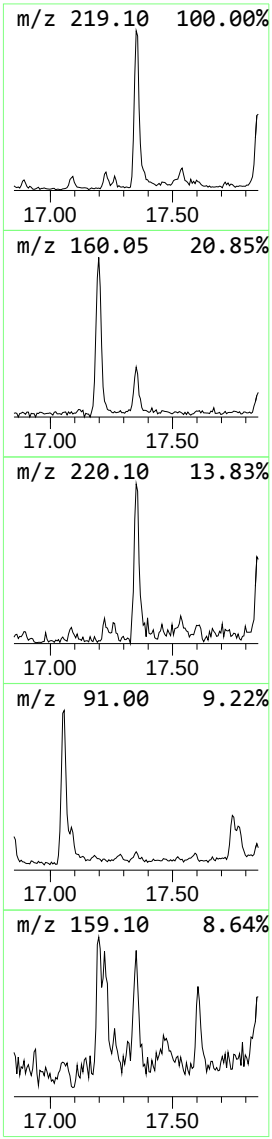
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 8-(2-Hydroxy-1-methoxy-3-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.351	3.58 ng	67280	Phenanthrene-d10	17.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-(2-Hydroxy-1-methoxy-3-methylb...	332	C18H20O6	006432-70-8	53
2	6-(2-Hydroxy-1-methoxy-3-methylb...	290	C16H18O5	1234985-51-3	53
3	Succinic acid, 2-methylphenyl 4-...	326	C20H22O4	1000357-54-1	50
4	Terephthalic acid, pentyl phenyl...	312	C19H20O4	1000324-06-2	50
5	Terephthalic acid, 2-bromo-4-flu...	408	C19H18BrFO4	1000323-70-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

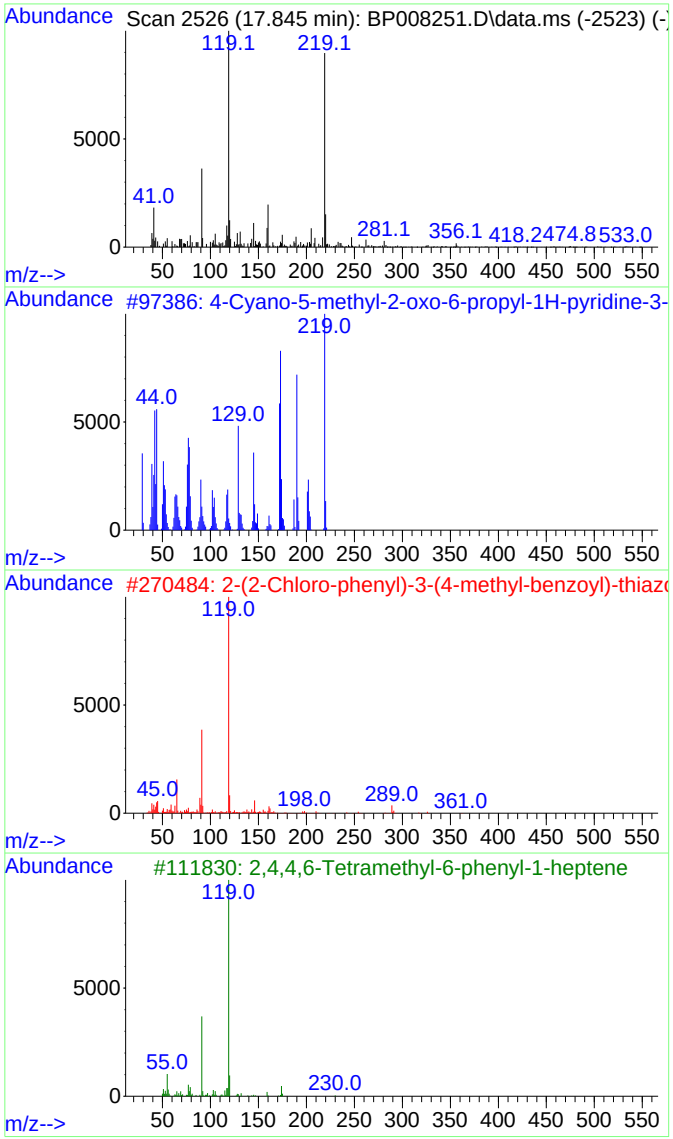
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

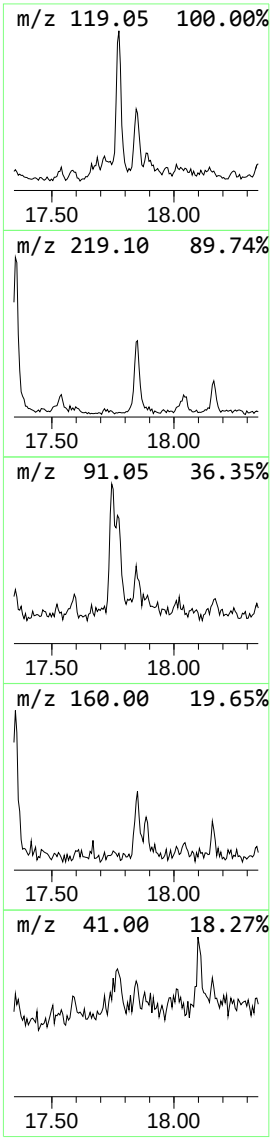
****

Peak Number 18 unknown17.845 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.845	2.32 ng	43481	Phenanthrene-d10	17.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Cyano-5-methyl-2-oxo-6-propyl-...	219	C11H13N3O2	1000459-78-4	30
2	2-(2-Chloro-phenyl)-3-(4-methyl-...	361	C18H16ClNO3S	1000300-65-2	30
3	2,4,4,6-Tetramethyl-6-phenyl-1-h...	230	C17H26	1000293-27-9	30
4	[5-(4-Ethylphenyl)-5-hydroxy-3-t...	376	C20H19F3N2O2	1000311-59-5	30
5	Benzamide, 3-methyl-N-(2-ethylhe...	247	C16H25NO	1000407-41-6	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

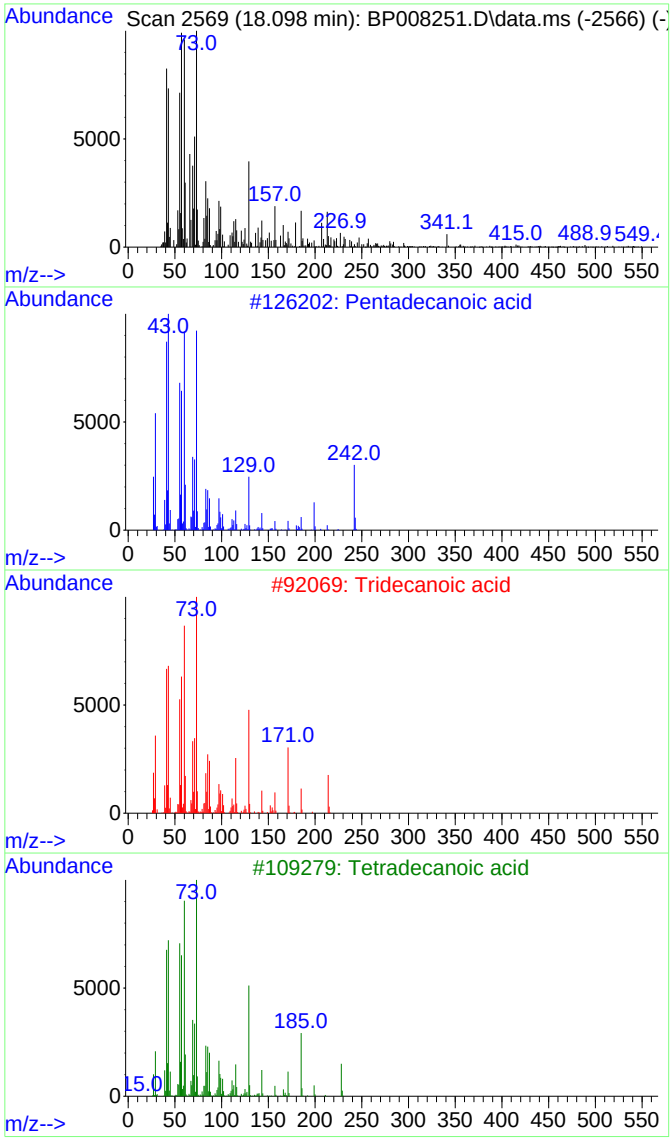
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

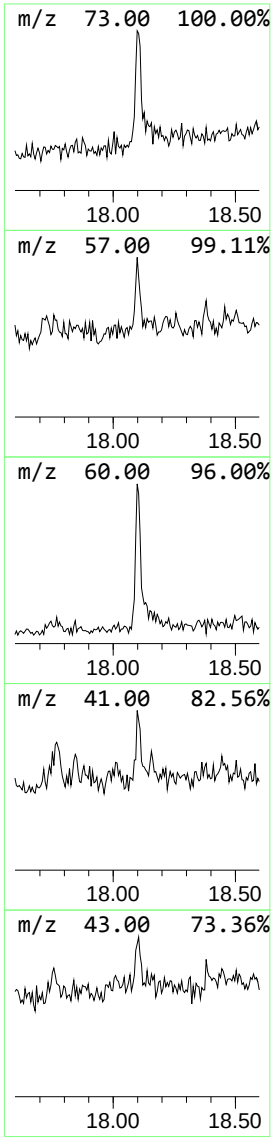
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 unknown18.098 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.098	3.22 ng	60449	Phenanthrene-d10	17.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	46
2	Tridecanoic acid	214	C13H26O2	000638-53-9	45
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43
5	n-Decanoic acid	172	C10H20O2	000334-48-5	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008251.D
Acq On : 07 Dec 2021 14:50
Operator : CG/JU
Sample : M4919-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-MW-3-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Benzene, tert-b...	7.381	7.7	ng	62380	1	7.787	163026	20.0
Benzene, 1-meth...	9.040	5.1	ng	41645	1	7.787	163026	20.0
(3-Methylbutane...	11.122	2.4	ng	27447	2	10.581	224664	20.0
2-Pentanone, 4-...	12.651	2.8	ng	40568	3	14.433	294843	20.0
unknown13.798	13.798	2.1	ng	31769	3	14.433	294843	20.0
unknown13.939	13.939	8.5	ng	125658	3	14.433	294843	20.0
(6-Chloro-2-met...	14.539	3.1	ng	46113	3	14.433	294843	20.0
unknown14.763	14.763	8.4	ng	123740	3	14.433	294843	20.0
Benzenepropanoi...	15.075	3.3	ng	48892	3	14.433	294843	20.0
unknown15.422	15.422	2.8	ng	41902	3	14.433	294843	20.0
Benzene, (1,1-d...	15.586	2.2	ng	32720	3	14.433	294843	20.0
Dicumyl peroxide	16.351	9.6	ng	179974	4	17.198	375436	20.0
unknown16.569	16.569	4.0	ng	75927	4	17.198	375436	20.0
unknown16.745	16.745	2.3	ng	42648	4	17.198	375436	20.0
3',4'-Acetoxylide	16.845	9.6	ng	179990	4	17.198	375436	20.0
2,4,4,6-Tetrame...	17.051	14.8	ng	277865	4	17.198	375436	20.0
8-(2-Hydroxy-1-...	17.351	3.6	ng	67280	4	17.198	375436	20.0
unknown17.845	17.845	2.3	ng	43481	4	17.198	375436	20.0
unknown18.098	18.098	3.2	ng	60449	4	17.198	375436	20.0