LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051221\
Data File : BP005512.D
Acq On : 12 May 2021 19:41
Operator : CG/JU
Sample : M2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-1-20210505

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-BP050521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005512.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.287	369	374	385	rVB3	8837	16904	5.77%	0.876%
2	6.905	645	649	653	rBV4	2180	4080	1.39%	0.212%
3	7.687	774	782	792	rBV	56008	92429	31.53%	4.792%
4	8.799	964	971	976	rBV3	8565	14681	5.01%	0.761%
5	8.863	976	982	991	rVB4	6816	13260	4.52%	0.687%
6	10.481	1249	1257	1267	rBV	58049	95368	32.53%	4.944%
7	11.022	1342	1349	1356	rBV6	2179	4461	1.52%	0.231%
8	12.698	1627	1634	1640	rBV6	6297	12022	4.10%	0.623%
9	12.869	1654	1663	1671	rVB7	3780	8340	2.85%	0.432%
10	12.963	1671	1679	1685	rBV	24088	40233	13.72%	2.086%
11	13.198	1713	1719	1723	rBV6	2240	3405	1.16%	0.177%
12	13.510	1769	1772	1779	rVB4	2845	3976	1.36%	0.206%
13	13.681	1794	1801	1811	rBV2	57249	100021	34.12%	5.186%
14	13.751	1811	1813	1819	rVB7	2282	3187	1.09%	0.165%
15	13.845	1825	1829	1834	rVB6	3540	6598	2.25%	0.342%
16	13.928	1837	1843	1851	rVB5	5864	11718	4.00%	0.608%
17	14.169	1882	1884	1890	rVB4	3085	4005	1.37%	0.208%
18	14.340	1908	1913	1919	rBV	94945	130643	44.57%	6.773%
19	14.522	1937	1944	1953	rBV4	9390	19172	6.54%	0.994%
20	14.616	1953	1960	1963	rVV5	5355	8143	2.78%	0.422%
21	14.675	1963	1970	1974	rVV3	16839	30311	10.34%	1.572%
22	14.722	1974	1978	1986	rVB4	10472	17716	6.04%	0.919%
23	14.863	1998	2002	2007	rVB7	1979	3142	1.07%	0.163%
24	15.228	2060	2064	2067	rBV4	4330	5236	1.79%	0.271%
25	15.275	2067	2072	2076	rVV5	3541	6019	2.05%	0.312%
26	15.328	2076	2081	2083	rVV4	5824	8298	2.83%	0.430%
27	15.363	2083	2087	2099	rVB2	11838	19934	6.80%	1.034%
28	15.492	2104	2109	2113	rBV7	1871	3972	1.35%	0.206%
29	15.557	2117	2120	2123	rVV4	4151	5195	1.77%	0.269%
30	15.598	2123	2127	2128	rVV4	3813	5328	1.82%	0.276%
31	15.622	2128	2131	2137	rVB7	4551	7536	2.57%	0.391%
32	15.798	2155	2161	2164	rBV8	2651	5035	1.72%	0.261%
33	15.839	2164	2168	2176	rBV4	32314	59819	20.41%	3.101%
34	15.957	2184	2188	2194	rVB4	5952	7899	2.69%	0.410%
35	16.075	2205	2208	2213	rVB6	3006	4050	1.38%	0.210%
36	16.145	2213	2220	2223	rBV8	3776	6342	2.16%	0.329%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051221\
Data File : BP005512.D
Acq On : 12 May 2021 19:41
Operator : CG/JU
Sample : M2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-1-20210505

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-BP050521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.251	2232	2238	2246	rVB10	4747	9523	3.25%	0.494%
38	16.469	2270	2275	2287	rVB2	26789	41546	14.17%	2.154%
39	16.551	2287	2289	2294	rBV6	2197	2933	1.00%	0.152%
40	16.645	2300	2305	2309	rBV6	6133	9975	3.40%	0.517%
41	16.710	2310	2316	2319	rVV3	8382	13707	4.68%	0.711%
42	16.745	2319	2322	2327	rVB5	7367	9375	3.20%	0.486%
43	16.951	2352	2357	2363	rBV2	9147	15351	5.24%	0.796%
44	17.098	2376	2382	2390	rBV	144126	214148	73.05%	11.103%
45	17.163	2390	2393	2399	rVV7	8137	15415	5.26%	0.799%
46	17.251	2402	2408	2413	rVV	20135	29444	10.04%	1.527%
47	17.375	2427	2429	2433	rVB4	3182	3584	1.22%	0.186%
48	17.469	2441	2445	2447	rBV3	4166	4990	1.70%	0.259%
49	17.745	2489	2492	2501	rVB3	9659	13849	4.72%	0.718%
50	17.910	2516	2520	2528	rBV8	5793	12578	4.29%	0.652%
51	17.998	2531	2535	2543	rVV8	17000	23934	8.16%	1.241%
52	18.163	2560	2563	2564	rBV3	4395	4204	1.43%	0.218%
53	18.292	2582	2585	2591	rBV8	3539	6898	2.35%	0.358%
54	18.398	2601	2603	2608	rVB6	4664	5632	1.92%	0.292%
55	19.098	2718	2722	2723	rBV4	3023	3552	1.21%	0.184%
56	19.239	2742	2746	2751	rBV5	10924	13925	4.75%	0.722%
57	19.669	2814	2819	2827	rVB	79961	102838	35.08%	5.332%
58	20.039	2876	2882	2885	rBV8	6404	12998	4.43%	0.674%
59	21.198	3074	3079	3085	rBV	229851	293140	100.00%	15.198%
60	23.504	3465	3471	3483	rVB	137312	276756	94.41%	14.349%

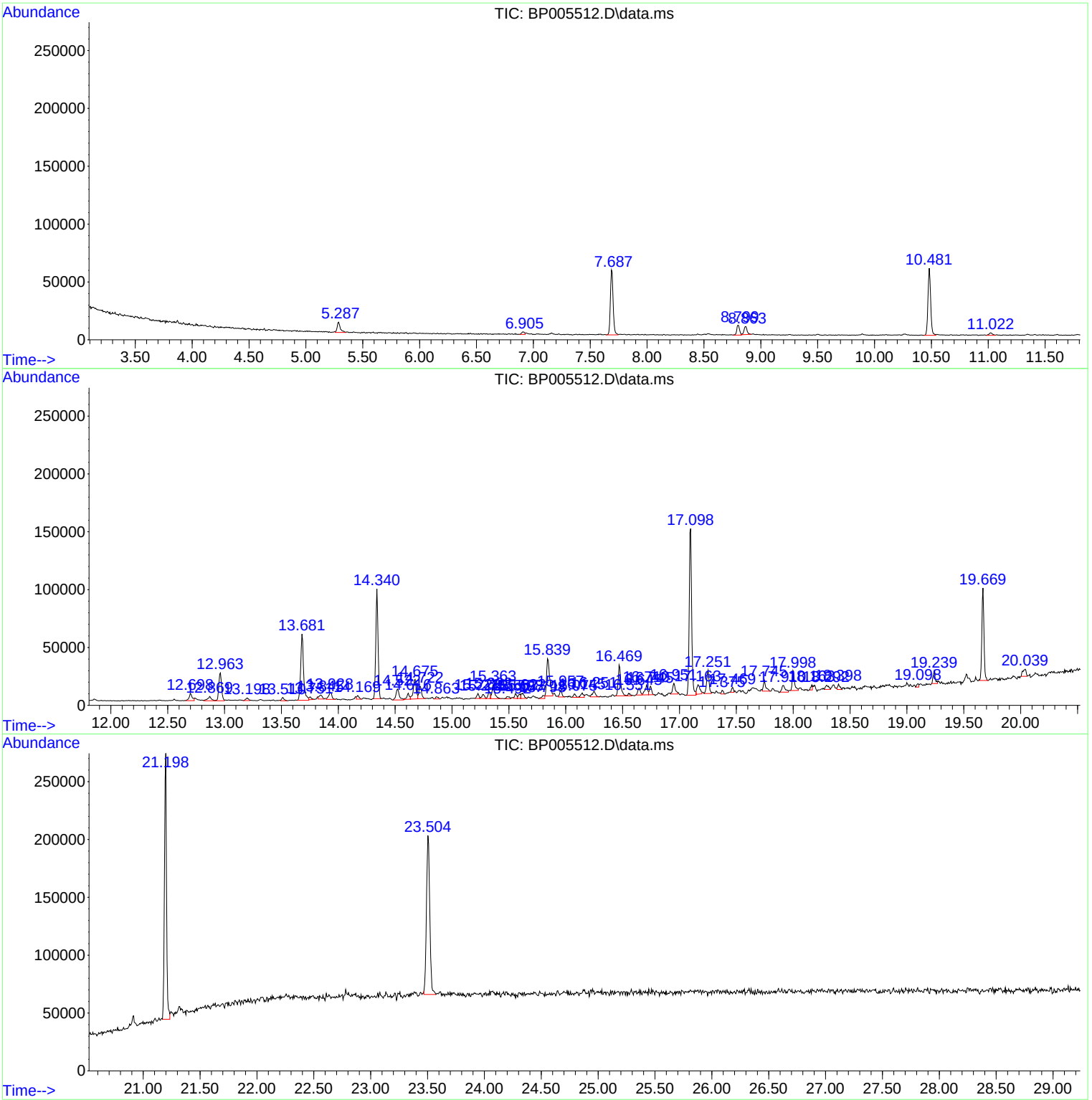
Sum of corrected areas: 1928773

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051221\
Data File : BP005512.D
Acq On : 12 May 2021 19:41
Operator : CG/JU
Sample : M2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1-20210505

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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_P\Data\BP051221\
Data File : BP005512.D
Acq On : 12 May 2021 19:41
Operator : CG/JU
Sample : M2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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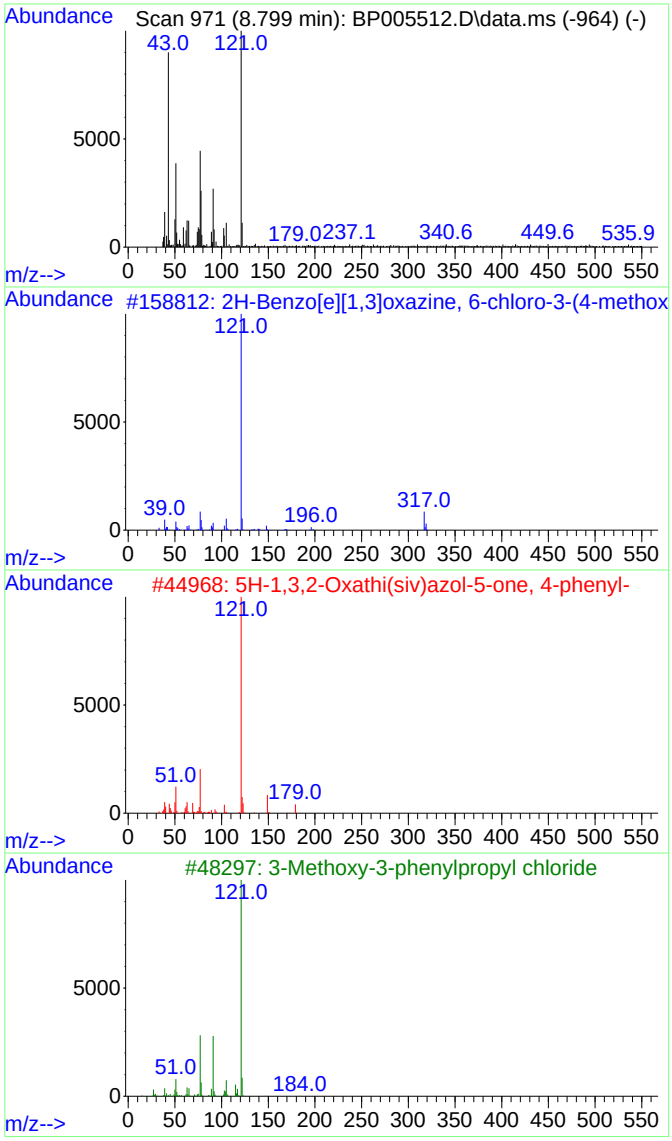
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

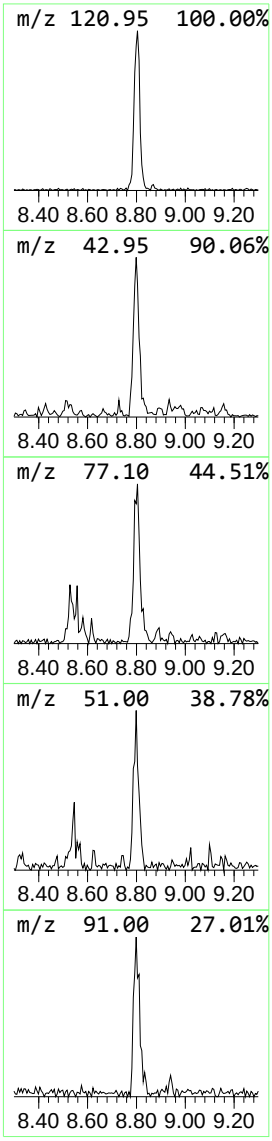
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2H-Benzo[e][1,3]oxazine, 6-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.799	3.18 ng	14681	1,4-Dichlorobenzene-d4	7.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Benzo[e][1,3]oxazine, 6-chlor...	317	C18H20ClNO2	1000310-79-4	90
2	5H-1,3,2-Oxathi(siv)azol-5-one, ...	179	C8H5NO2S	032545-34-9	78
3	3-Methoxy-3-phenylpropyl chloride	184	C10H13ClO	1000370-35-5	78
4	Benzeneacetic acid, .alpha.-meth...	166	C9H10O3	026164-26-1	78
5	Benzenemethanamine, 4-methoxy-N-...	213	C14H15NO	003526-43-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051221\
Data File : BP005512.D
Acq On : 12 May 2021 19:41
Operator : CG/JU
Sample : M2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1-20210505

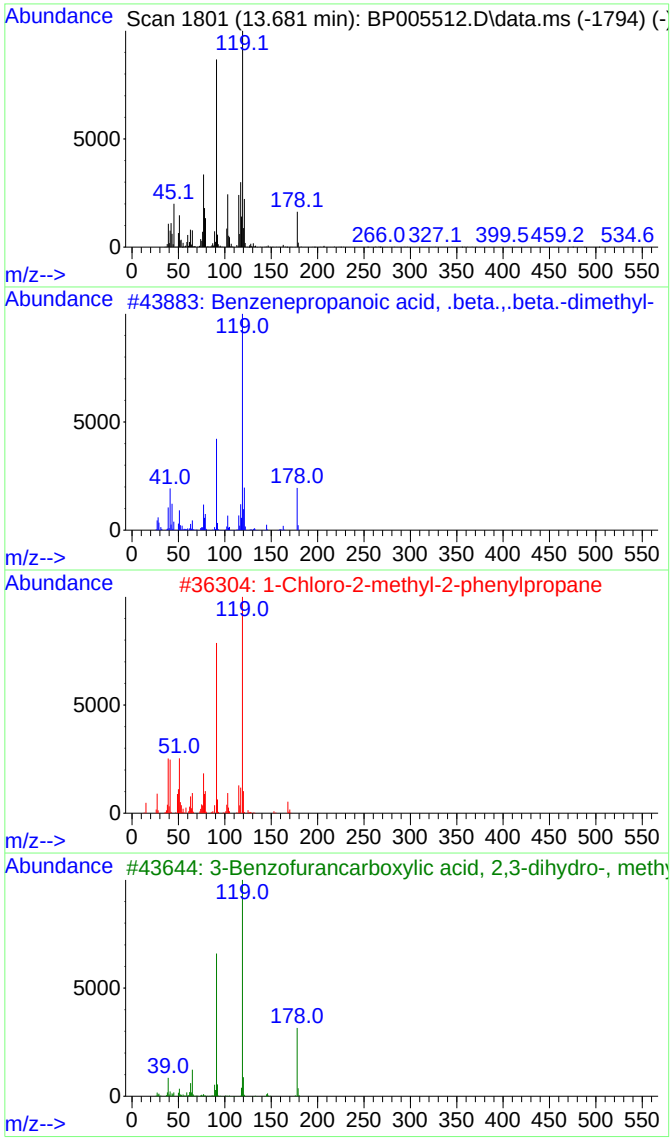
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

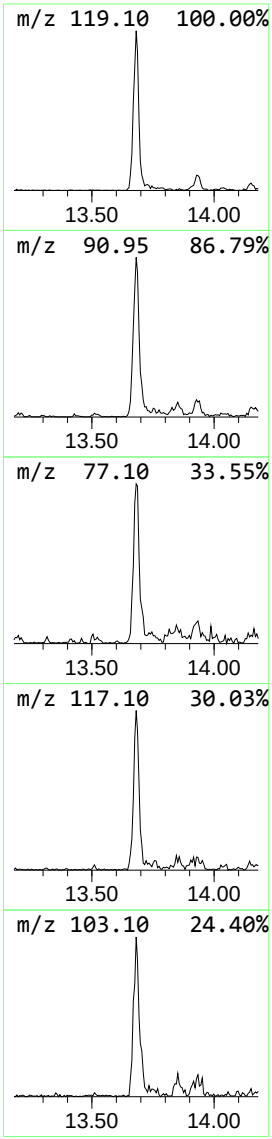
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown13.681 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.681	15.31 ng	100021	Acenaphthene-d10	14.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanoic acid, .beta.,.b...	178	C11H14O2	001010-48-6	49
2	1-Chloro-2-methyl-2-phenylpropane	168	C10H13Cl	000515-40-2	43
3	3-Benzofurancarboxylic acid, 2,3...	178	C10H10O3	039891-56-0	43
4	o-Toluic acid, 2-methylphenyl ester	226	C15H14O2	023597-23-1	38
5	Benzeneacetic acid, .alpha.-ethy...	178	C11H14O2	002294-71-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051221\
Data File : BP005512.D
Acq On : 12 May 2021 19:41
Operator : CG/JU
Sample : M2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1-20210505

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

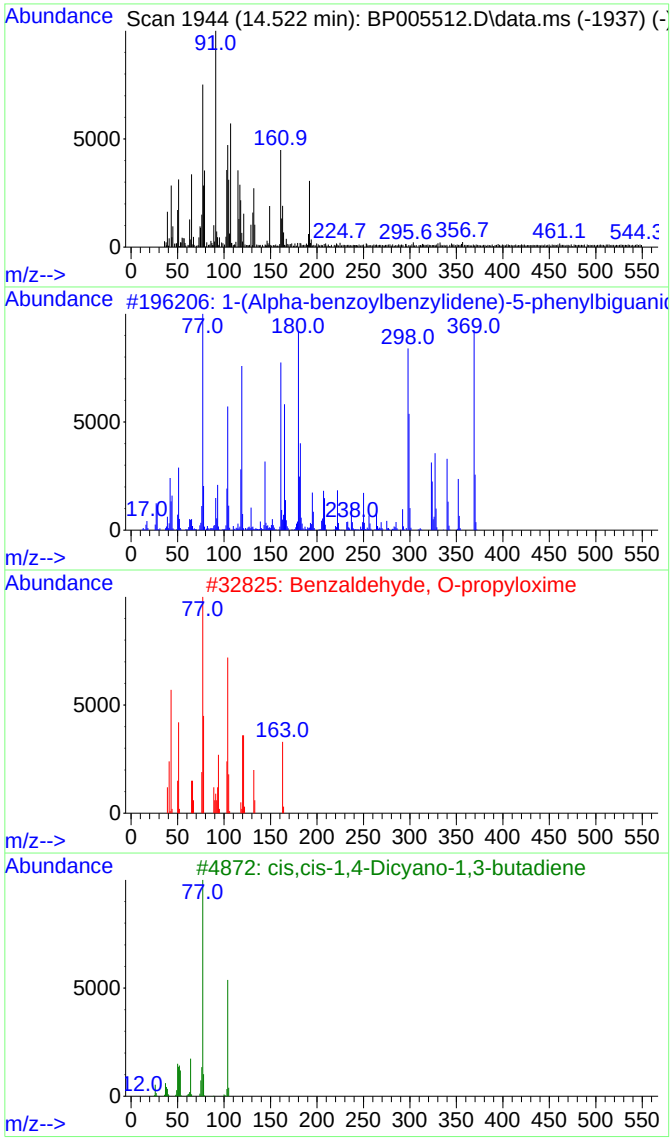
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

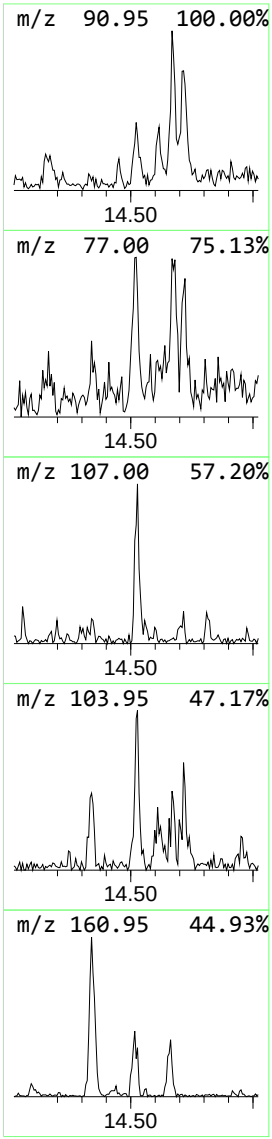
****

Peak Number 3 unknown14.522 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.522	2.94 ng	19172	Acenaphthene-d10	14.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(Alpha-benzoylbenzylidene)-5-p...	369	C22H19N5O	1000241-15-7	47
2	Benzaldehyde, O-propyloxime	163	C10H13NO	033581-40-7	43
3	cis,cis-1,4-Dicyano-1,3-butadiene	104	C6H4N2	001557-59-1	38
4	N-Methyl-4-oxo-4,N-diphenyl-buty...	267	C17H17NO2	181872-71-9	38
5	2-Butanone, 4-(4-hydroxyphenyl)-	164	C10H12O2	005471-51-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051221\
Data File : BP005512.D
Acq On : 12 May 2021 19:41
Operator : CG/JU
Sample : M2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1-20210505

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

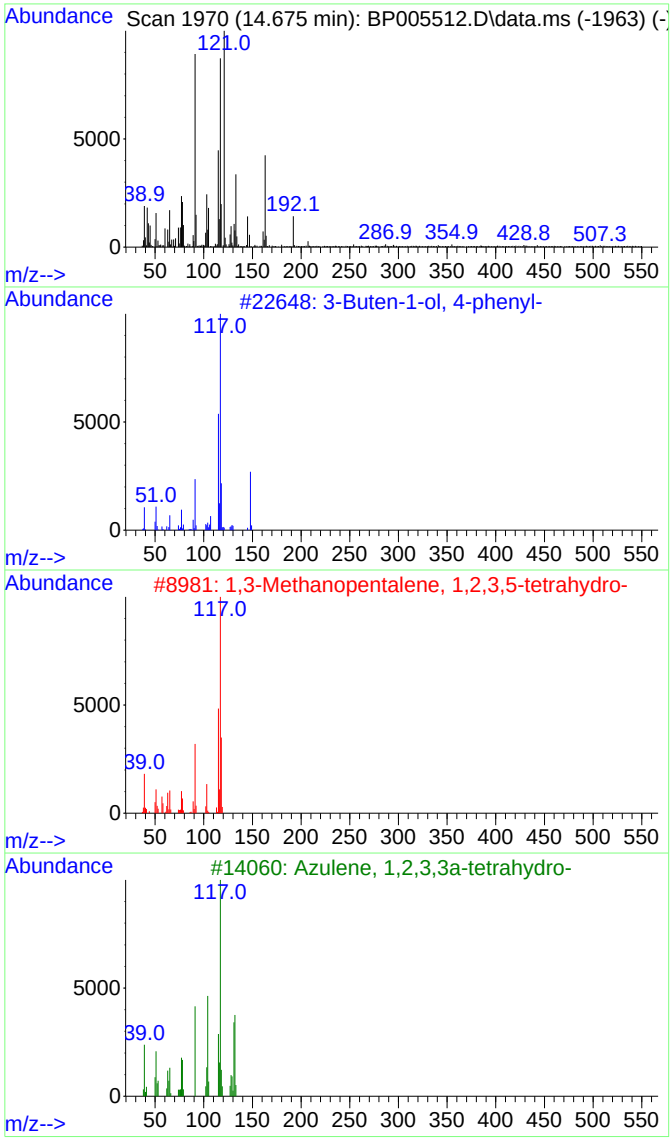
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

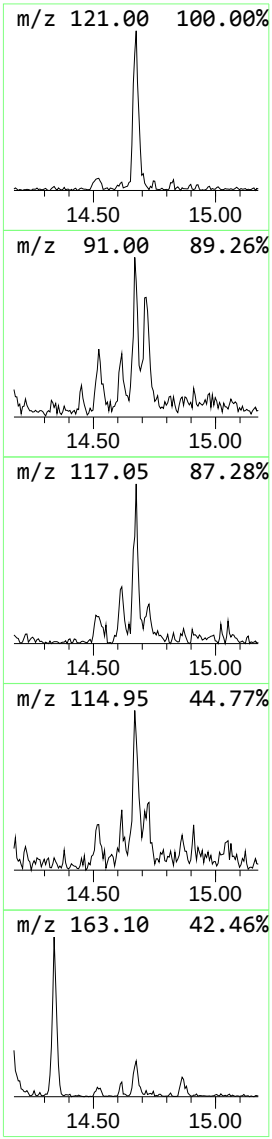
****

Peak Number 4 unknown14.675 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.675	4.64 ng	30311	Acenaphthene-d10	14.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-1-ol, 4-phenyl-	148	C10H12O	000937-58-6	35
2	1,3-Methanopentalene, 1,2,3,5-te...	118	C9H10	128600-88-4	30
3	Azulene, 1,2,3,3a-tetrahydro-	132	C10H12	033877-87-1	30
4	Deltacyclene	118	C9H10	007785-10-6	30
5	5-Methyl-6-phenyltetrahydro-1,3-...	207	C11H13NOS	086071-95-6	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051221\
Data File : BP005512.D
Acq On : 12 May 2021 19:41
Operator : CG/JU
Sample : M2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1-20210505

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

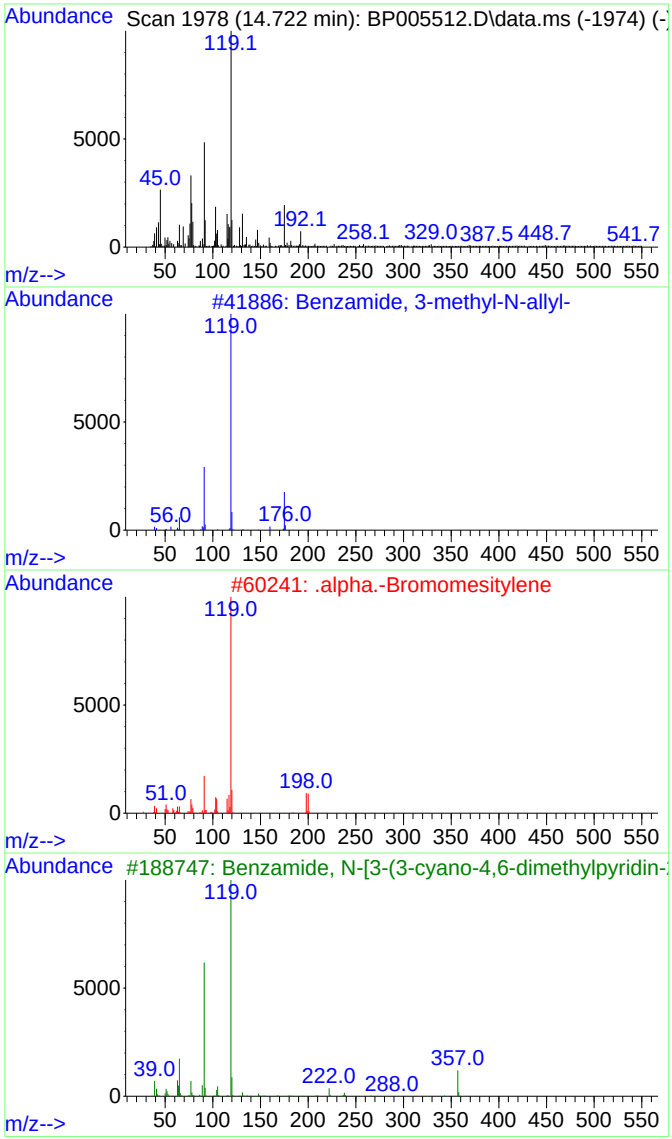
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

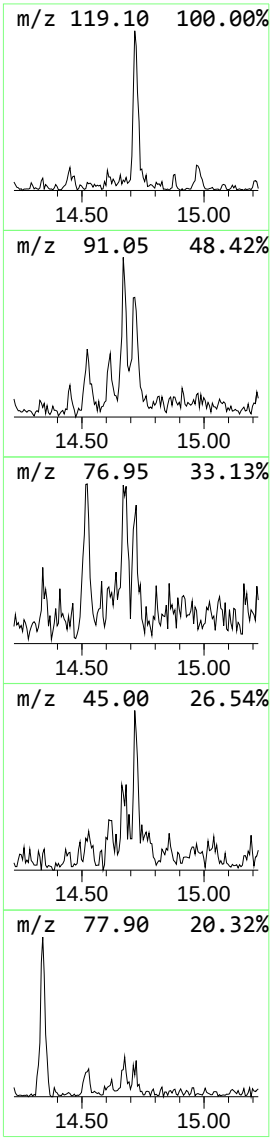
****

Peak Number 5 Benzamide, 3-methyl-N-allyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.722	2.71 ng	17716	Acenaphthene-d10	14.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, 3-methyl-N-allyl-	175	C11H13NO	1000339-09-8	64
2	.alpha.-Bromomesitylene	198	C9H11Br	027129-86-8	58
3	Benzamide, N-[3-(3-cyano-4,6-dim...	357	C22H19N3O2	1000303-00-9	58
4	Benzoic acid, 3-methyl-, 4-metho...	236	C14H20O3	1000355-71-0	52
5	Benzamide, N-[2-acetyl-1,1-di(tr...	383	C16H15F6NO3	1000276-52-7	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051221\
Data File : BP005512.D
Acq On : 12 May 2021 19:41
Operator : CG/JU
Sample : M2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1-20210505

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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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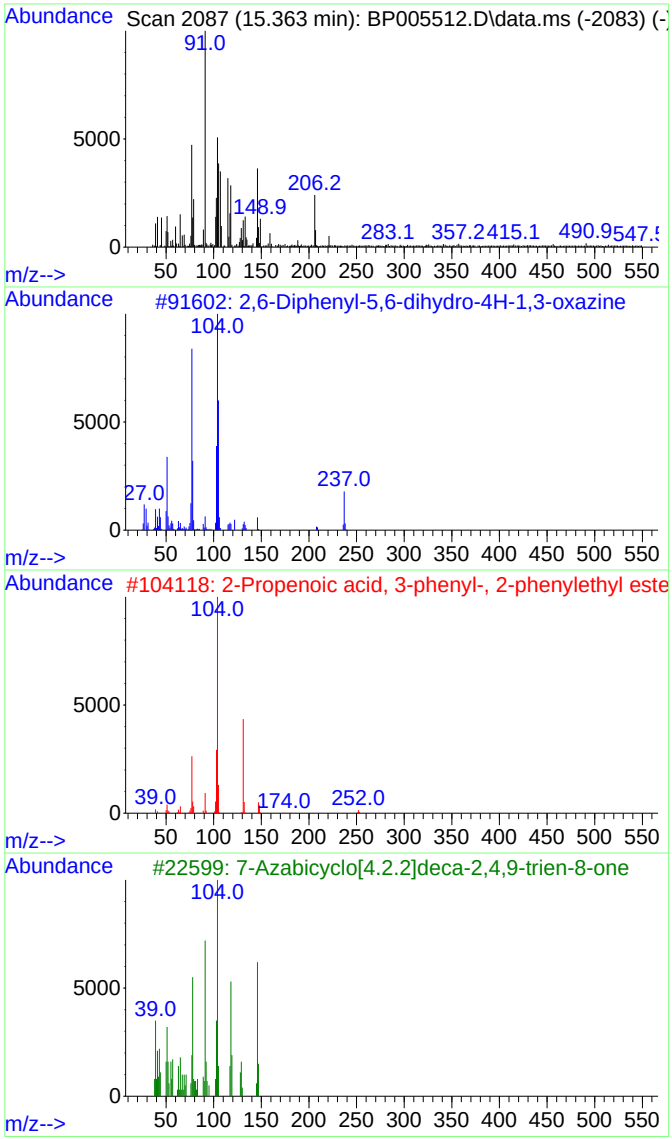
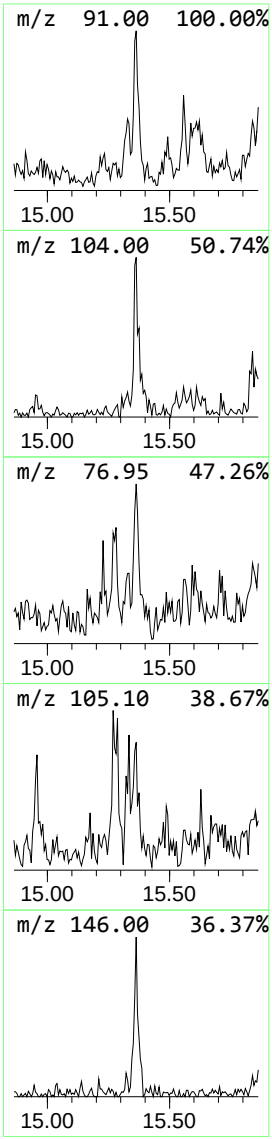
Peak Number 6 unknown15.363 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.363	3.05 ng	19934	Acenaphthene-d10	14.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Diphenyl-5,6-dihydro-4H-1,3-...	237	C16H15NO	013157-48-7	43
2	2-Propenoic acid, 3-phenyl-, 2-p...	252	C17H16O2	000103-53-7	38
3	7-Azabicyclo[4.2.2]deca-2,4,9-tr...	147	C9H9NO	017198-06-0	38
4	1-Cyclopropyl-2-phenylethane	146	C11H14	037904-33-9	38
5	Benzenepropanoic acid, 2-methylp...	206	C13H18O2	028048-94-4	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051221\
Data File : BP005512.D
Acq On : 12 May 2021 19:41
Operator : CG/JU
Sample : M2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1-20210505

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

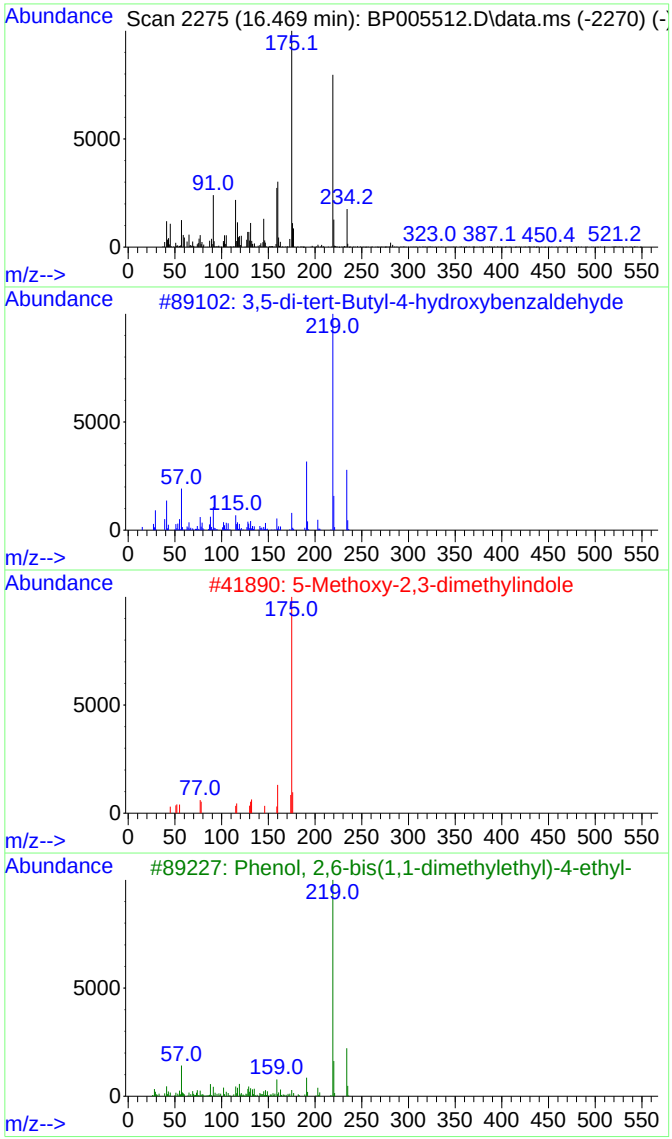
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

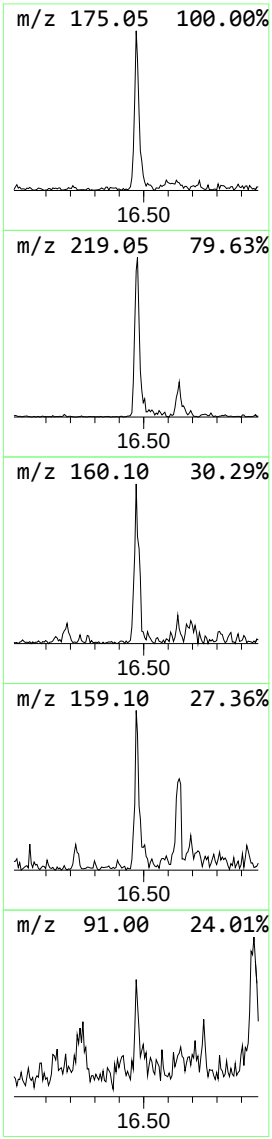
****

Peak Number 7 unknown16.469 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.469	3.88 ng	41546	Phenanthrene-d10	17.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	43
2	5-Methoxy-2,3-dimethylindole	175	C11H13NO	000828-94-4	38
3	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	38
4	12-Azabicyclo[9.2.2]pentadeca-1(...	219	C14H21NO	1000185-25-1	30
5	Isoquinolin-3(2H)-one, 6,7-dimet...	219	C12H13NO3	016535-98-1	27





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Acq On : 12 May 2021 19:41
Operator : CG/JU
Sample : M2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1-20210505

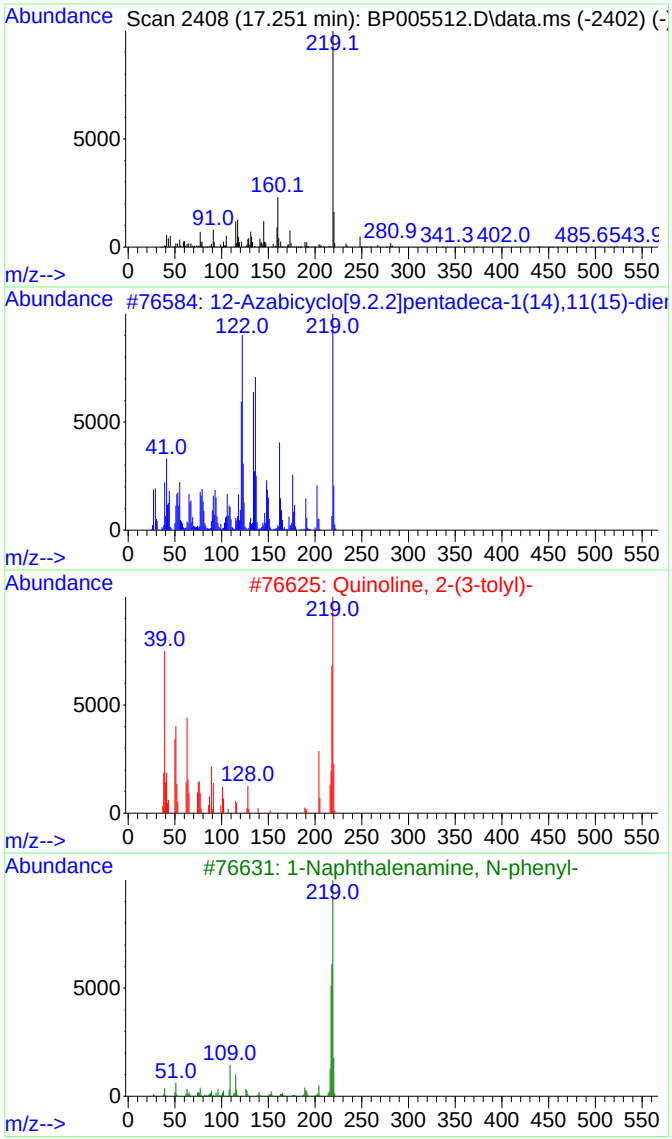
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

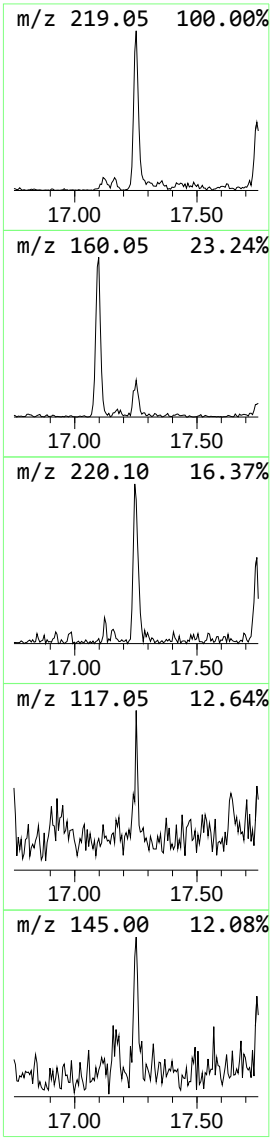
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 12-Azabicyclo[9.2.2]pentade... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.251	2.75 ng	29444	Phenanthrene-d10	17.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Azabicyclo[9.2.2]pentadeca-1(...	219	C14H21NO	1000185-25-1	53
2	Quinoline, 2-(3-tolyl)-	219	C16H13N	024641-30-3	49
3	1-Naphthalenamine, N-phenyl-	219	C16H13N	000090-30-2	47
4	5-(4-Ethoxy-phenyl)-5-methyl-imi...	234	C12H14N2O3	1000297-64-8	47
5	p-Hexylbenzaldehyde diethyl acetal	264	C17H28O2	089511-01-3	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051221\
Data File : BP005512.D
Acq On : 12 May 2021 19:41
Operator : CG/JU
Sample : M2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1-20210505

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

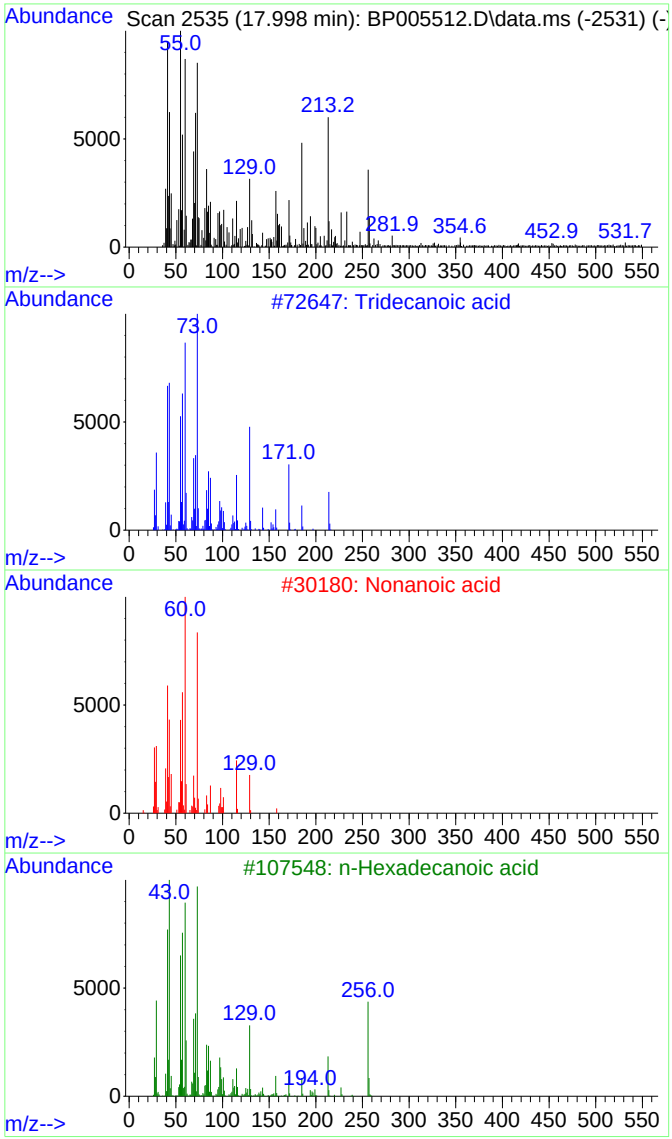
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

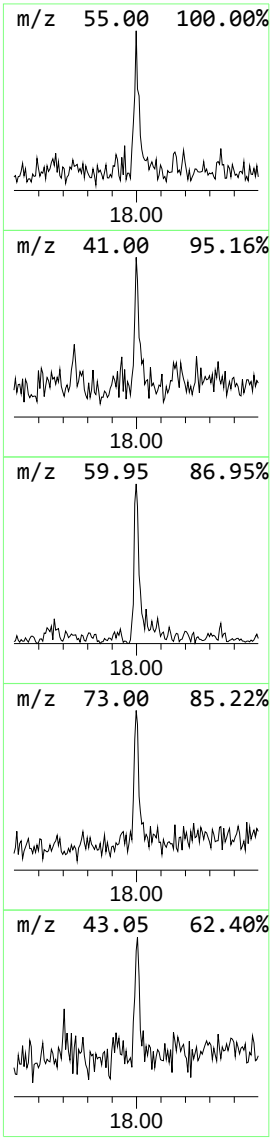
****

Peak Number 9 Tridecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.998	2.24 ng	23934	Phenanthrene-d10	17.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	90
2	Nonanoic acid	158	C9H18O2	000112-05-0	38
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	38
4	Dodecanoic acid	200	C12H24O2	000143-07-7	30
5	n-Decanoic acid	172	C10H20O2	000334-48-5	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051221\
Data File : BP005512.D
Acq On : 12 May 2021 19:41
Operator : CG/JU
Sample : M2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-1-20210505

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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
2H-Benzo[e][1,3...	8.799	3.2	ng	14681	1	7.693	92429	20.0
unknown13.681	13.681	15.3	ng	100021	3	14.339	130643	20.0
unknown14.522	14.522	2.9	ng	19172	3	14.339	130643	20.0
unknown14.675	14.675	4.6	ng	30311	3	14.339	130643	20.0
Benzamide, 3-me...	14.722	2.7	ng	17716	3	14.339	130643	20.0
unknown15.363	15.363	3.0	ng	19934	3	14.339	130643	20.0
unknown16.469	16.469	3.9	ng	41546	4	17.098	214148	20.0
12-Azabicyclo[9...	17.251	2.8	ng	29444	4	17.098	214148	20.0
Tridecanoic acid	17.998	2.2	ng	23934	4	17.098	214148	20.0