LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 17-B6(20-24)

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-BP060821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005941.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.117	3	5	15	rVB	64819	75419	1.98%	0.309%
2	5.034	327	331	341	rVB	28169	41318	1.09%	0.169%
3	5.499	403	410	417	rBV	1071719	1615022	42.49%	6.614%
4	5.558	417	420	430	rVB	36698	77318	2.03%	0.317%
5	7.105	672	683	696	rBV	1019593	1677391	44.13%	6.869%
6	7.934	815	824	830	rBV	258802	412487	10.85%	1.689%
7	8.722	950	958	963	rBV	30639	62443	1.64%	0.256%
8	9.034	1004	1011	1015	rBV2	25744	50469	1.33%	0.207%
9	9.099	1015	1022	1031	rVB	599119	1012965	26.65%	4.148%
10	9.916	1155	1161	1164	rBV2	30009	51772	1.36%	0.212%
11	10.222	1210	1213	1221	rVB2	22900	41096	1.08%	0.168%
12	10.522	1258	1264	1267	rBV2	24533	46264	1.22%	0.189%
13	10.646	1281	1285	1292	rVB	43318	76866	2.02%	0.315%
14	10.734	1293	1300	1307	rBV	334286	540617	14.22%	2.214%
15	11.281	1386	1393	1398	rBV2	22736	44634	1.17%	0.183%
16	11.569	1434	1442	1447	rBV3	35524	80024	2.11%	0.328%
17	11.675	1453	1460	1468	rVB5	19609	38869	1.02%	0.159%
18	11.904	1493	1499	1504	rBV	75761	124569	3.28%	0.510%
19	12.781	1641	1648	1651	rBV6	17645	39924	1.05%	0.163%
20	12.834	1651	1657	1666	rVB	260976	401239	10.56%	1.643%
21	13.057	1691	1695	1705	rVB	55265	87033	2.29%	0.356%
22	13.187	1705	1717	1725	rBV	1759922	2566130	67.52%	10.509%
23	13.369	1743	1748	1756	rVB5	28901	53998	1.42%	0.221%
24	13.704	1801	1805	1809	rBV4	22540	45457	1.20%	0.186%
25	13.916	1832	1841	1849	rBV	403460	616072	16.21%	2.523%
26	13.987	1849	1853	1856	rBV2	30913	42326	1.11%	0.173%
27	14.416	1915	1926	1936	rBV6	59921	200465	5.27%	0.821%
28	14.557	1943	1950	1957	rBV	522063	782388	20.59%	3.204%
29	14.716	1971	1977	1989	rVB	505464	730197	19.21%	2.990%
30	14.816	1989	1994	1998	rBV	58132	91823	2.42%	0.376%
31	14.945	2013	2016	2027	rVB9	24692	66721	1.76%	0.273%
32	15.434	2096	2099	2105	rVB2	83640	108917	2.87%	0.446%
33	15.504	2105	2111	2116	rBV	408550	547386	14.40%	2.242%
34	15.592	2123	2126	2134	rVB7	19021	39345	1.04%	0.161%
35	15.969	2186	2190	2192	rBV	38932	46840	1.23%	0.192%
36	16.045	2197	2203	2211	rVB	1639046	2263421	59.55%	9.269%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 17-B6(20-24)

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-BP060821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.339	2248	2253	2259	rVB2	75670	110707	2.91%	0.453%
38	16.598	2292	2297	2303	rBV	139329	197634	5.20%	0.809%
39	16.851	2335	2340	2347	rVB	131422	210051	5.53%	0.860%
40	17.304	2411	2417	2422	rBV	688087	972588	25.59%	3.983%
41	17.798	2497	2501	2506	rBV4	46171	68926	1.81%	0.282%
42	18.186	2562	2567	2579	rBV2	216161	353769	9.31%	1.449%
43	18.463	2612	2614	2618	rVB2	33723	39092	1.03%	0.160%
44	19.298	2753	2756	2764	rVB4	91920	139354	3.67%	0.571%
45	19.410	2771	2775	2785	rBV	126790	174424	4.59%	0.714%
46	19.604	2804	2808	2810	rBV	94236	109701	2.89%	0.449%
47	19.628	2810	2812	2816	rVB	48346	50142	1.32%	0.205%
48	19.851	2844	2850	2855	rBV	3182967	3800624	100.00%	15.564%
49	20.145	2898	2900	2904	rVB2	49564	49189	1.29%	0.201%
50	20.586	2972	2975	2976	rBV	53094	52677	1.39%	0.216%
51	20.610	2976	2979	2990	rVB5	126143	225223	5.93%	0.922%
52	21.075	3054	3058	3065	rBV	400904	516253	13.58%	2.114%
53	21.275	3090	3092	3097	rVB	74395	80422	2.12%	0.329%
54	21.375	3104	3109	3115	rBV	938353	1192783	31.38%	4.885%
55	23.786	3512	3519	3528	rVB2	621581	1276013	33.57%	5.226%

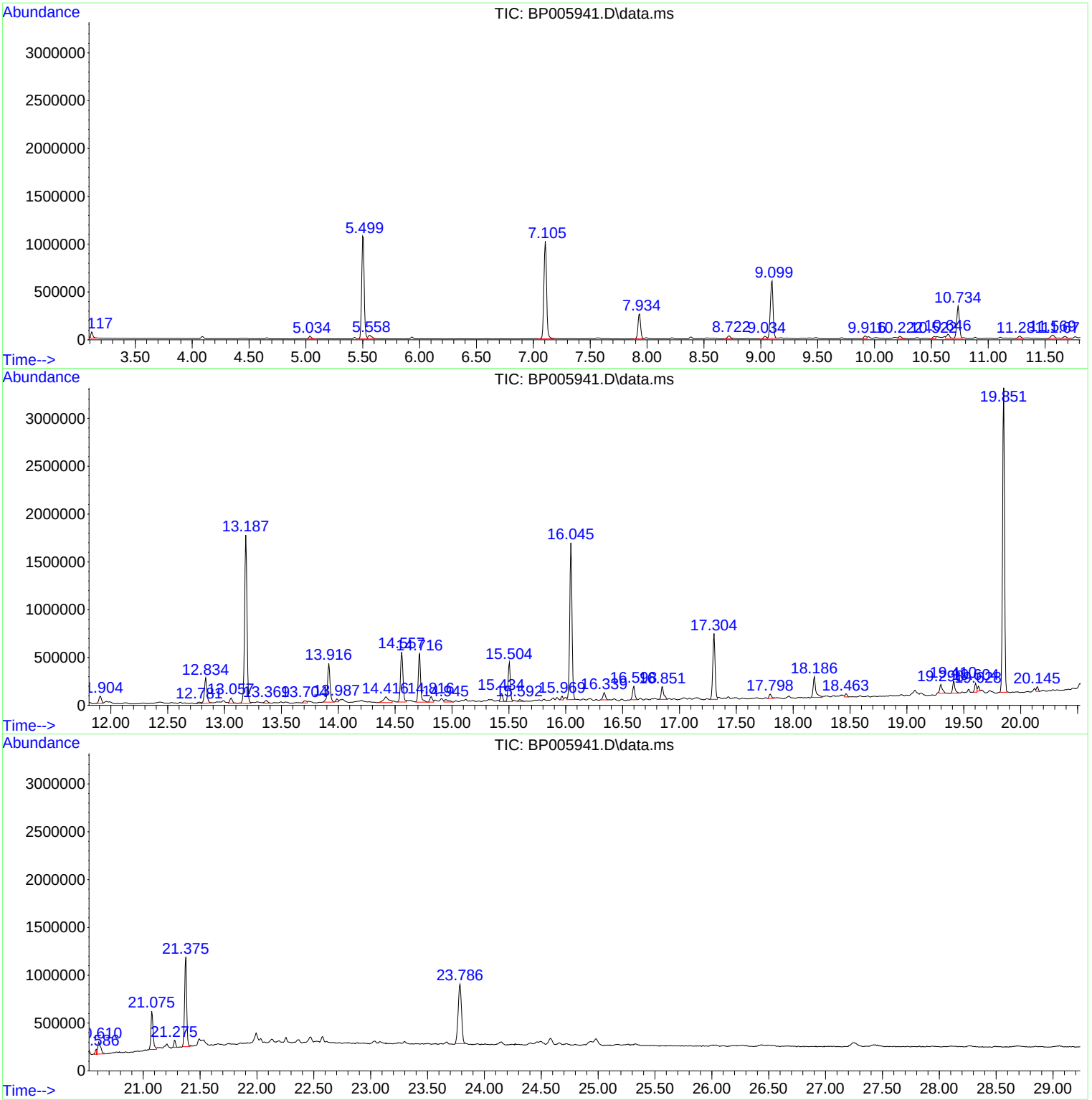
Sum of corrected areas: 24418797

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

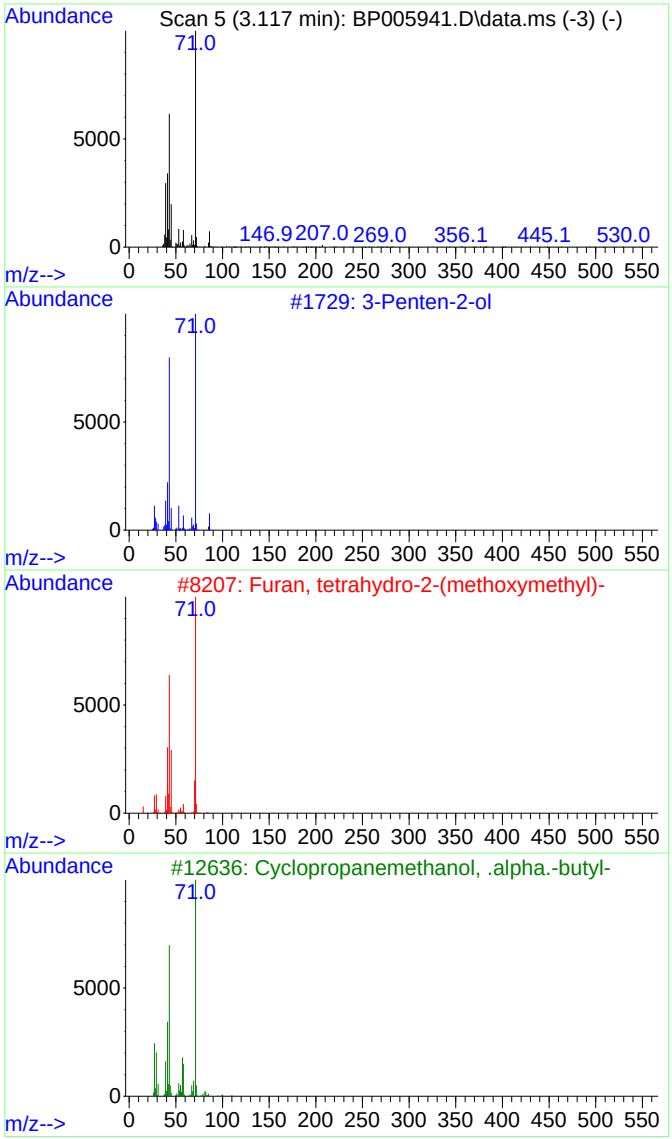
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

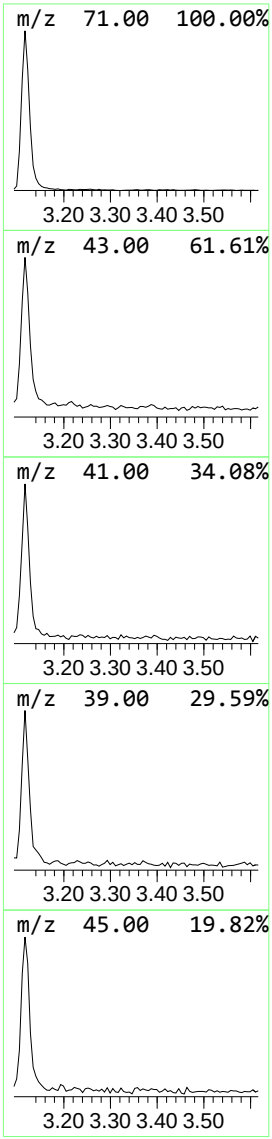
****

Peak Number 1 3-Penten-2-ol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.117	3.66 ng	75419	1,4-Dichlorobenzene-d4	7.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	64
2	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	56
3	Cyclopropanemethanol, .alpha.-bu...	128	C8H16O	004379-16-2	45
4	3-Heptanone, 2,4-dimethyl-	142	C9H18O	018641-71-9	42
5	2-Furanmethanol, tetrahydro-	102	C5H10O2	000097-99-4	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

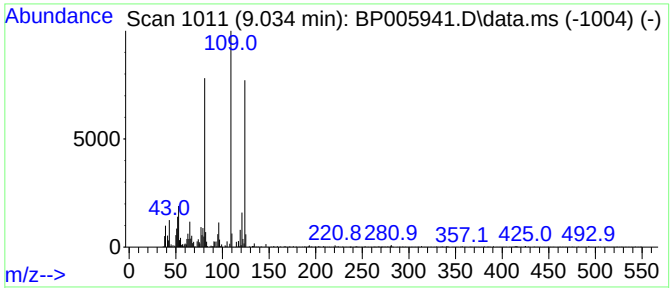
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

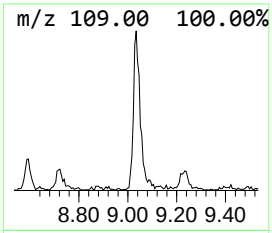
****

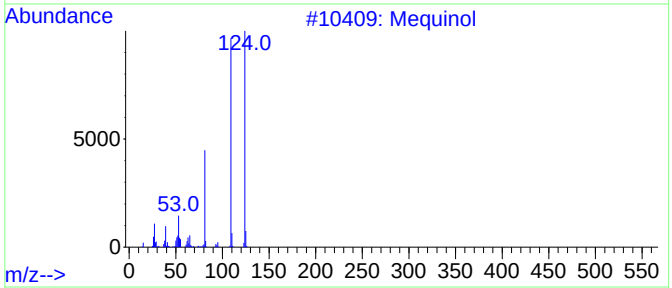
Peak Number 3 Mequinol Concentration Rank 19

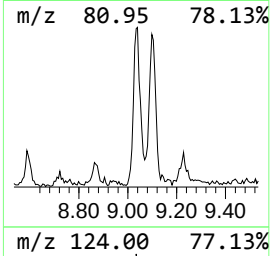
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.034	2.45 ng	50469	1,4-Dichlorobenzene-d4	7.934

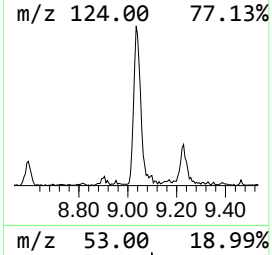
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mequinol	124	C7H8O2	000150-76-5	87
2	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	87
3	2-Cyclopenten-1-one, 3,4,4-trime...	124	C8H12O	030434-65-2	86
4	3-Fluoro-o-xylene	124	C8H9F	000443-82-3	49
5	Ethanone, 1-(2-methyl-1-cyclopen...	124	C8H12O	003168-90-9	49

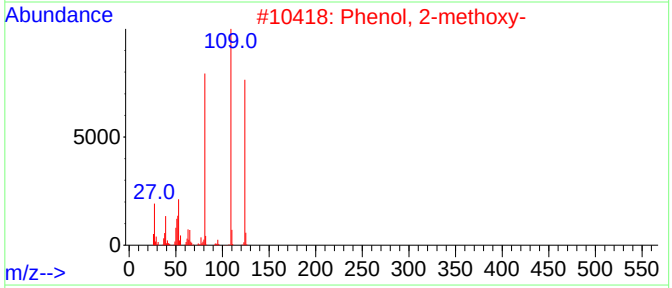


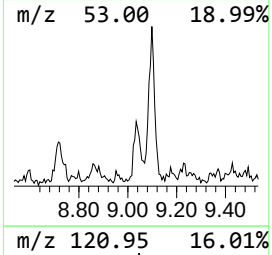


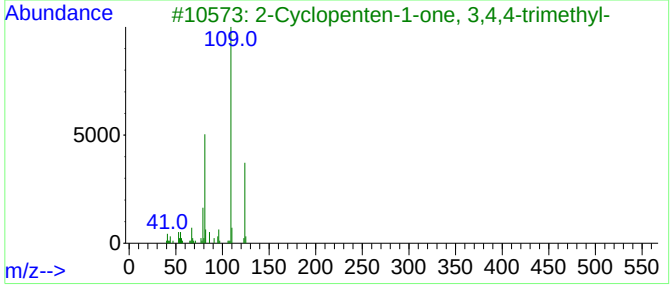


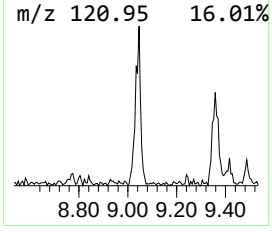












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

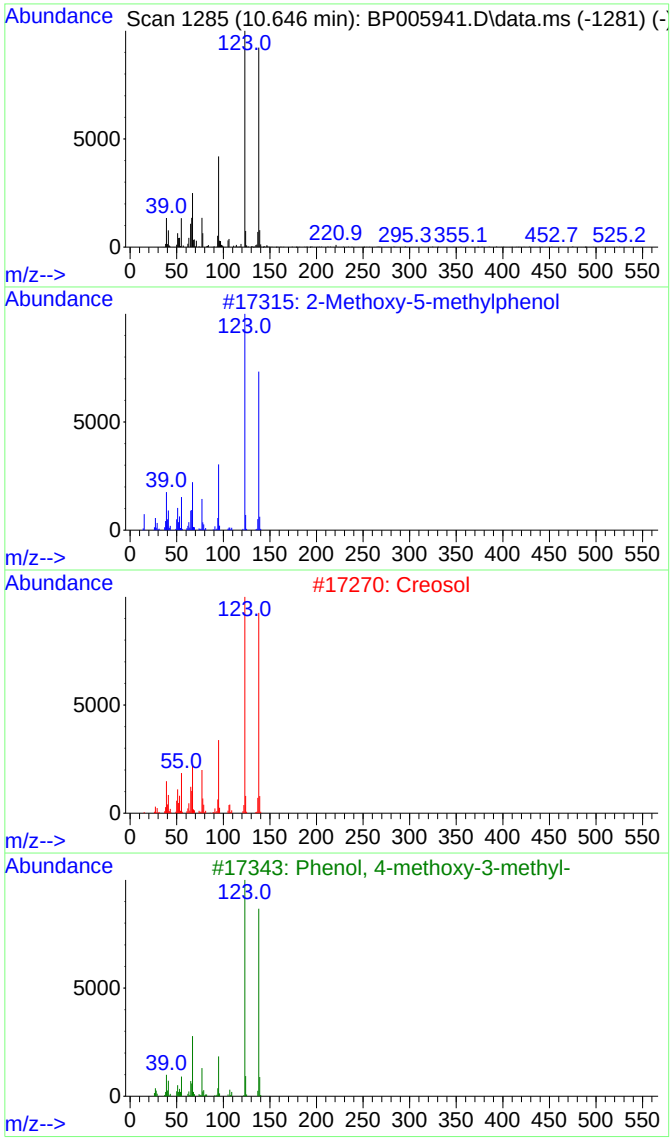
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

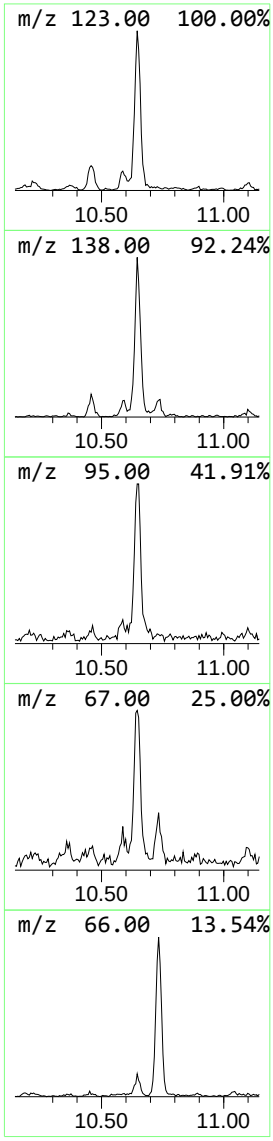
****

Peak Number 4 2-Methoxy-5-methylphenol Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.646	2.84 ng	76866	Naphthalene-d8	10.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methoxy-5-methylphenol	138	C8H10O2	001195-09-1	91
2	Creosol	138	C8H10O2	000093-51-6	91
3	Phenol, 4-methoxy-3-methyl-	138	C8H10O2	014786-82-4	81
4	Benzene, 1,4-dimethoxy-	138	C8H10O2	000150-78-7	80
5	1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

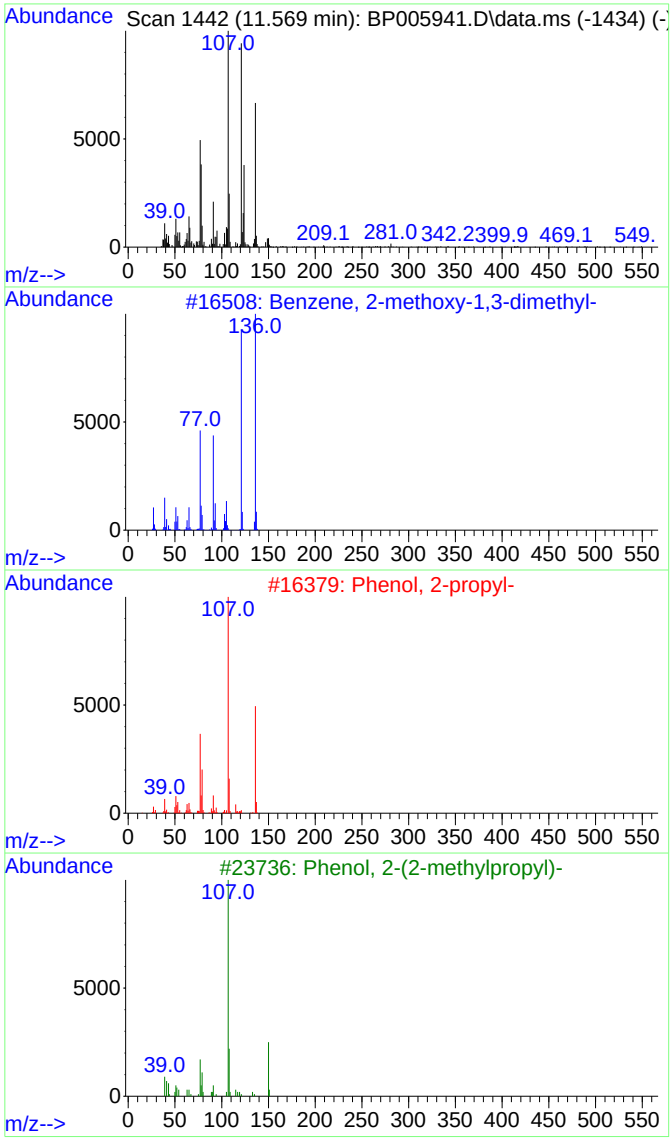
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

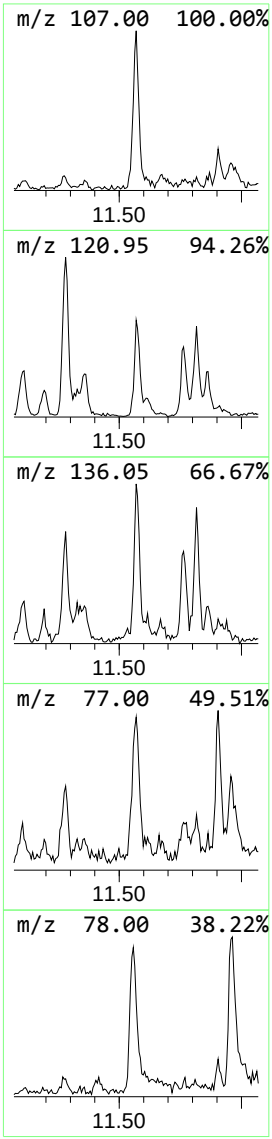
****

Peak Number 5 unknown11.569 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.569	2.96 ng	80024	Naphthalene-d8	10.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-methoxy-1,3-dimethyl-	136	C9H12O	001004-66-6	43
2	Phenol, 2-propyl-	136	C9H12O	000644-35-9	43
3	Phenol, 2-(2-methylpropyl)-	150	C10H14O	004167-75-3	35
4	Phenol, 2,3,6-trimethyl-	136	C9H12O	002416-94-6	30
5	Phenol, 2,4,5-trimethyl-	136	C9H12O	000496-78-6	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

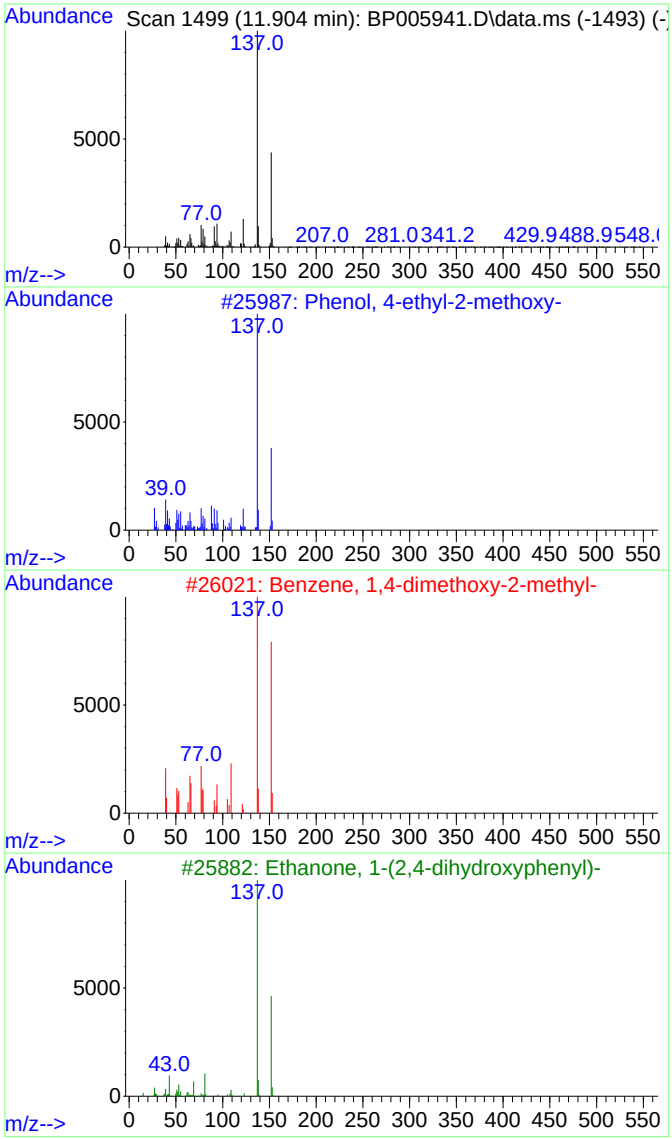
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

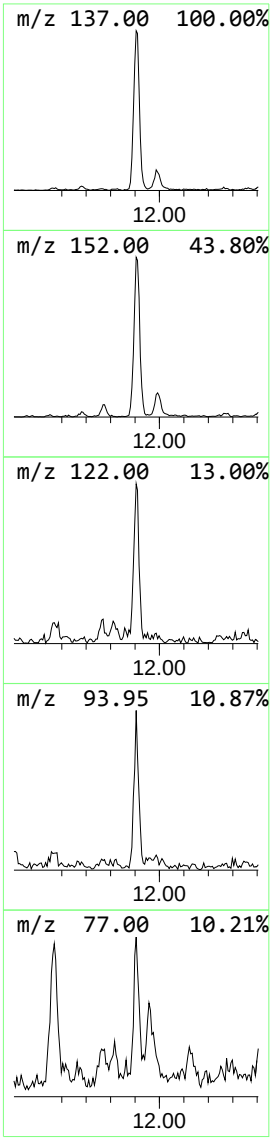
****

Peak Number 6 Phenol, 4-ethyl-2-methoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	4.61 ng	124569	Naphthalene-d8	10.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-ethyl-2-methoxy-	152	C9H12O2	002785-89-9	91
2	Benzene, 1,4-dimethoxy-2-methyl-	152	C9H12O2	024599-58-4	83
3	Ethanone, 1-(2,4-dihydroxyphenyl)-	152	C8H8O3	000089-84-9	68
4	O-Methoxy-.alpha.-methylbenzyl a...	152	C9H12O2	013513-82-1	64
5	Resorcinol, 2-acetyl-	152	C8H8O3	000699-83-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

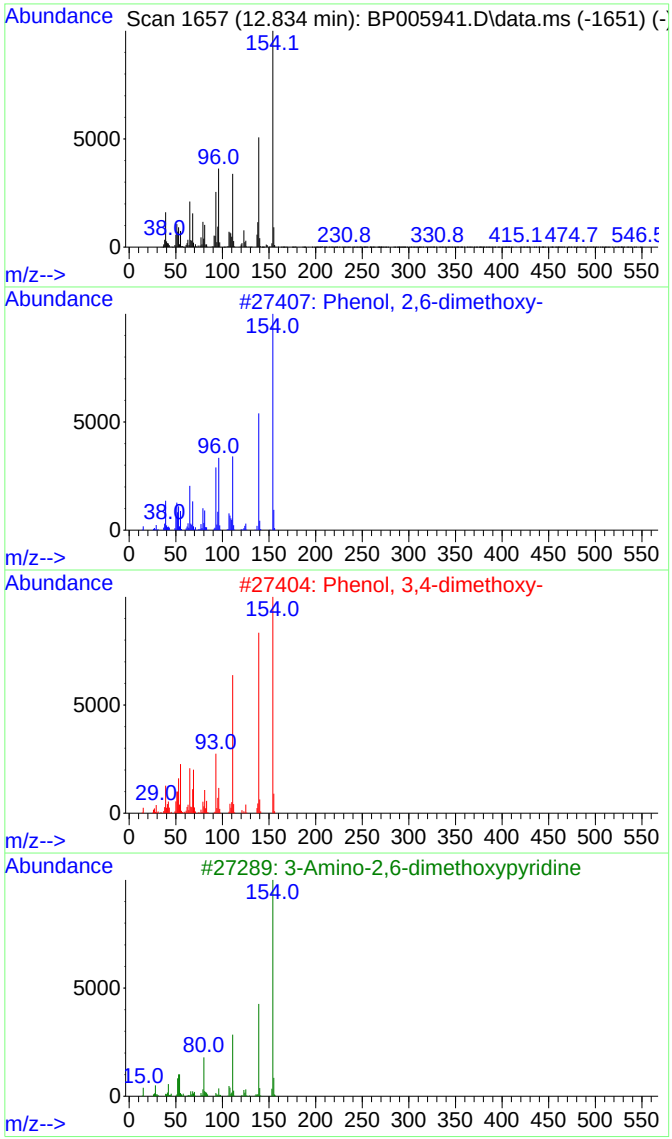
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

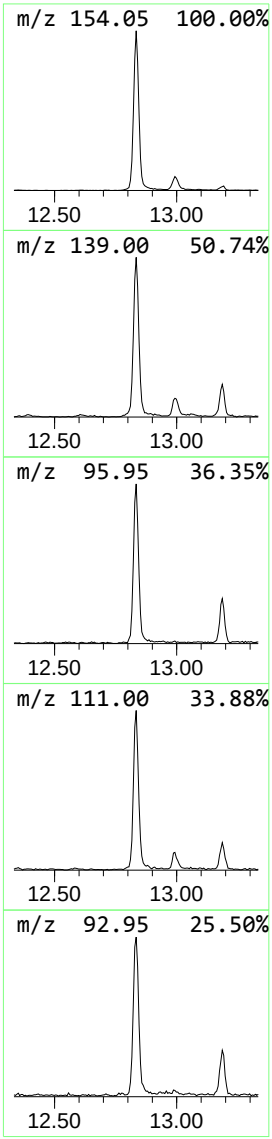
****

Peak Number 7 Phenol, 2,6-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.834	10.26 ng	401239	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dimethoxy-	154	C8H10O3	000091-10-1	97
2	Phenol, 3,4-dimethoxy-	154	C8H10O3	002033-89-8	74
3	3-Amino-2,6-dimethoxypyridine	154	C7H10N2O2	028020-37-3	64
4	Formic acid, 2,6-dimethoxyphenyl...	182	C9H10O4	1000368-91-0	50
5	Phenol, 3,4-dimethoxy-, acetate	196	C10H12O4	007203-46-5	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

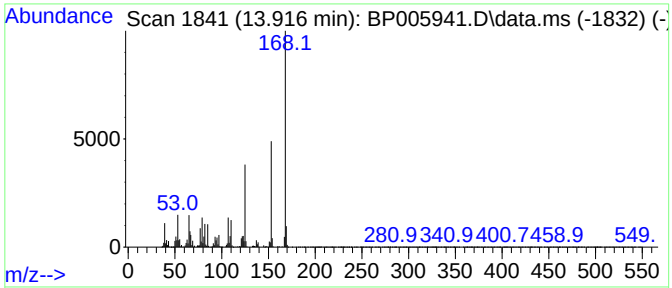
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

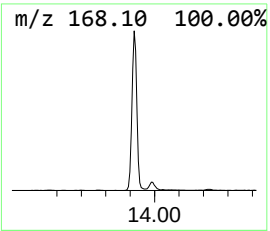
****

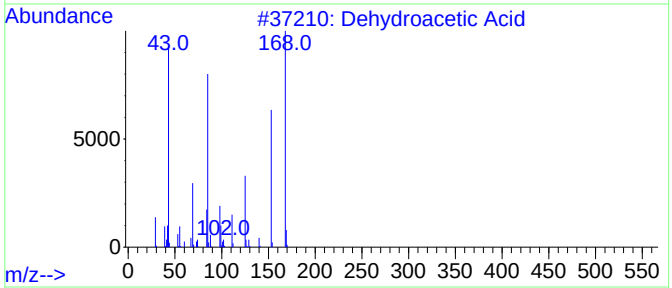
Peak Number 8 Dehydroacetic Acid Concentration Rank 2

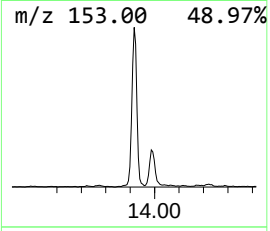
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	15.75 ng	616072	Acenaphthene-d10	14.557

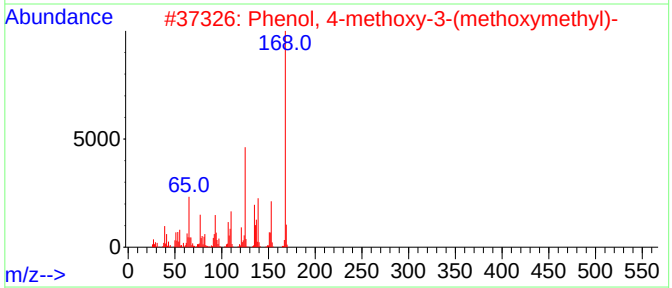
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dehydroacetic Acid	168	C8H8O4	000520-45-6	59
2	Phenol, 4-methoxy-3-(methoxymeth...	168	C9H12O3	059907-65-2	59
3	3-Hydroxy-4-methoxybenzoic acid	168	C8H8O4	000645-08-9	58
4	Benzoic acid, 4-hydroxy-3-methoxy-	168	C8H8O4	000121-34-6	53
5	4-Methoxy-2-methyl-1-(methylthio...	168	C9H12OS	022583-04-6	53

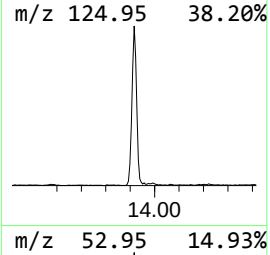


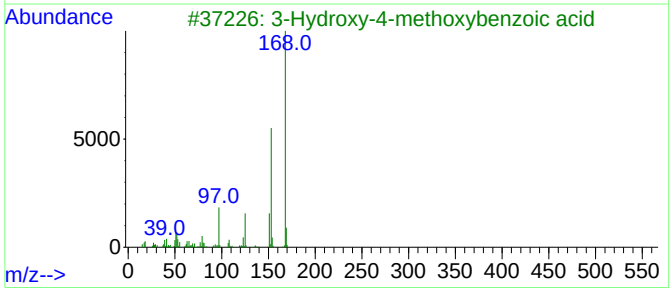


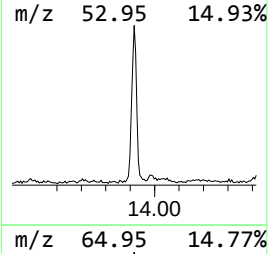


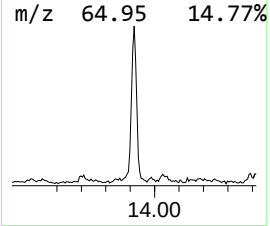












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

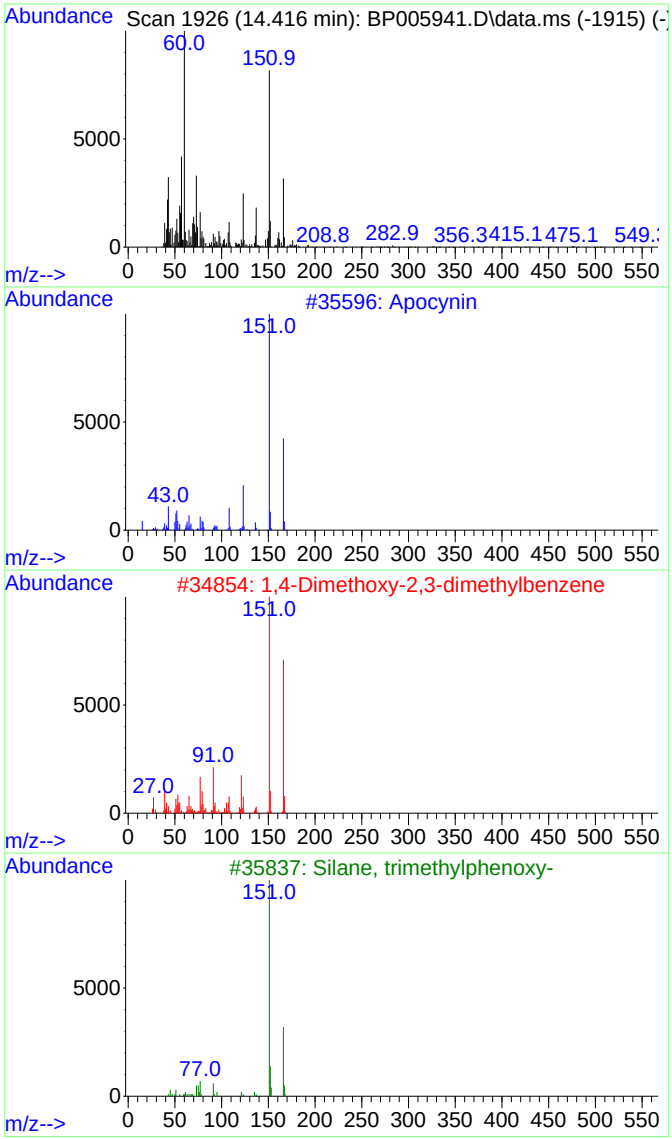
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

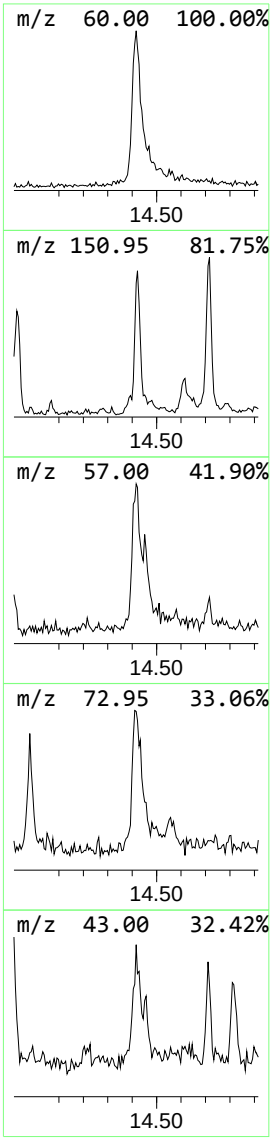
****

Peak Number 9 Apocynin Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.416	5.12 ng	200465	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Apocynin	166	C9H10O3	000498-02-2	89
2	1,4-Dimethoxy-2,3-dimethylbenzene	166	C10H14O2	039021-83-5	41
3	Silane, trimethylphenoxy-	166	C9H14OSi	001529-17-5	38
4	Ethanone, 1-[4-(methylthio)phenyl]-	166	C9H10OS	001778-09-2	38
5	Ethanone, 1-(2-hydroxy-6-methoxy...	166	C9H10O3	000703-23-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

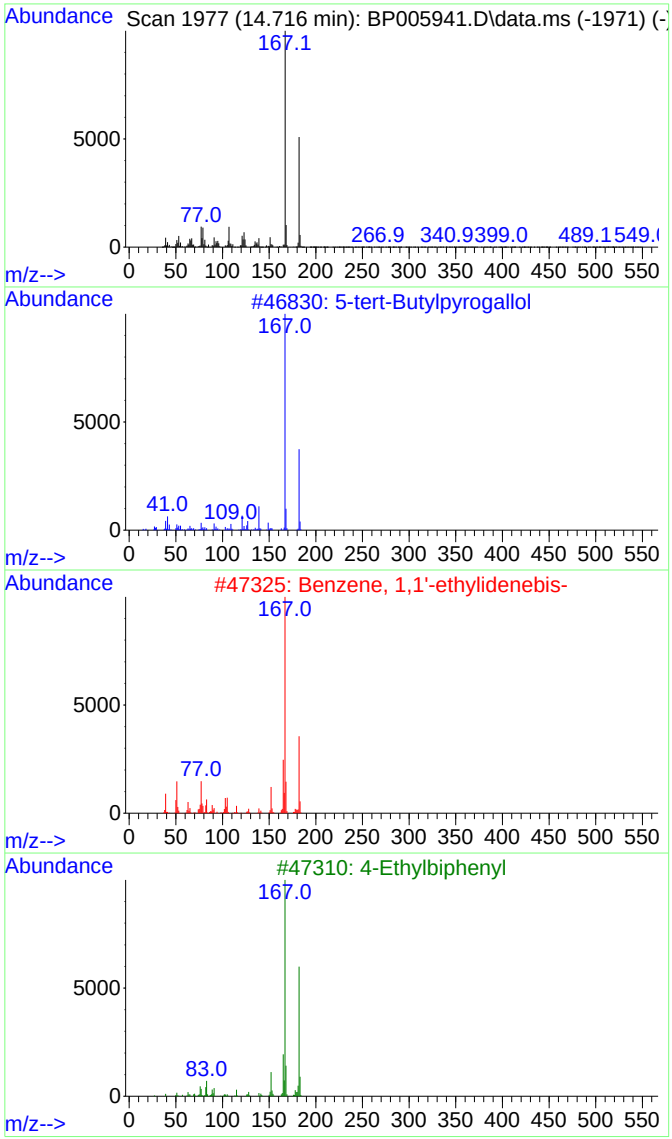
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

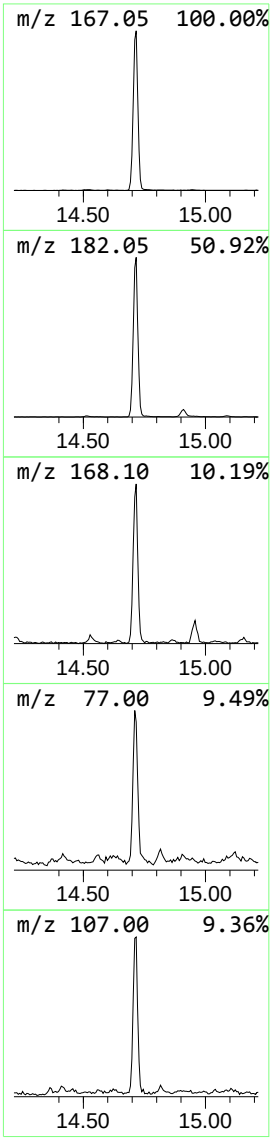
****

Peak Number 10 5-tert-Butylpyrogallol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.716	18.67 ng	730197	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-tert-Butylpyrogallol	182	C10H14O3	020481-17-8	72
2	Benzene, 1,1'-ethylidenebis-	182	C14H14	000612-00-0	64
3	4-Ethylbiphenyl	182	C14H14	005707-44-8	64
4	Hydroquinone mono-trimethylsilyl...	182	C9H14O2Si	017881-87-7	64
5	Benzene, 1,2,3-trimethoxy-5-methyl-	182	C10H14O3	006443-69-2	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

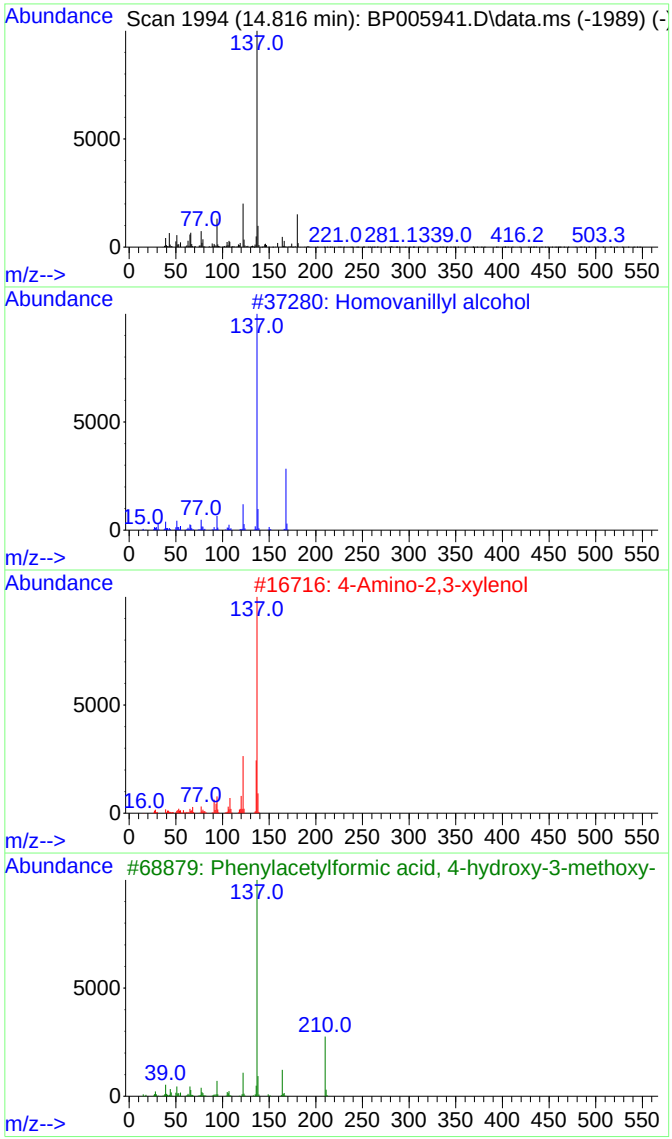
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

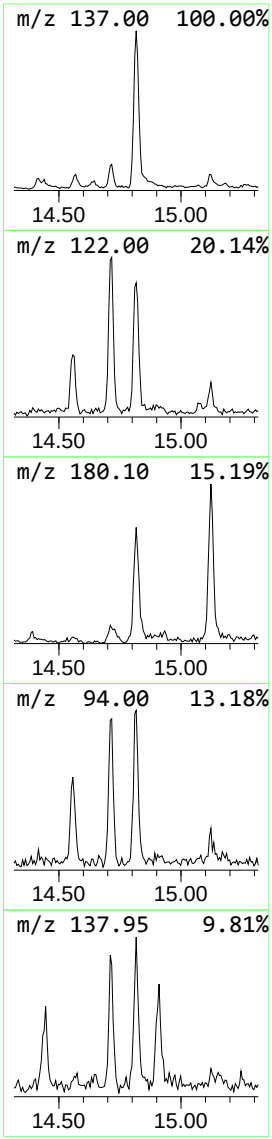
****

Peak Number 11 Homovanillyl alcohol Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	2.35 ng	91823	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Homovanillyl alcohol	168	C9H12O3	002380-78-1	72
2	4-Amino-2,3-xylenol	137	C8H11NO	003096-69-3	64
3	Phenylacetylformic acid, 4-hydro...	210	C10H10O5	001081-71-6	59
4	Homovanillic acid	182	C9H10O4	000306-08-1	56
5	Benzeneacetic acid, .alpha.-hydr...	196	C10H12O4	013305-14-1	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

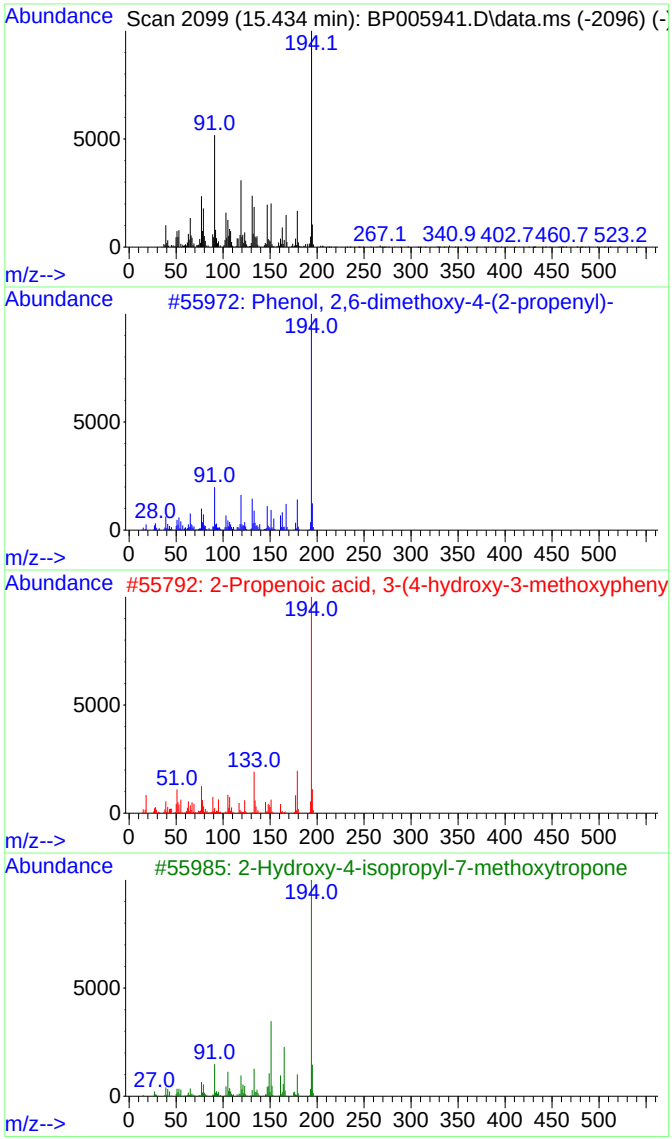
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

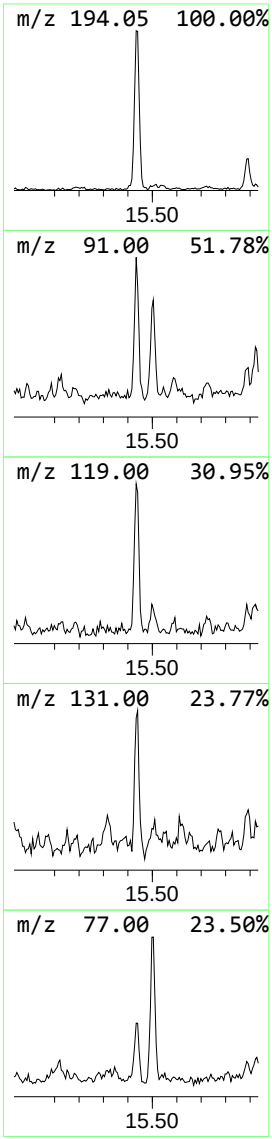
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Phenol, 2,6-dimethoxy-4-(2-... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.434	2.78 ng	108917	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dimethoxy-4-(2-prope...	194	C11H14O3	006627-88-9	94
2	2-Propenoic acid, 3-(4-hydroxy-3...	194	C10H10O4	001135-24-6	70
3	2-Hydroxy-4-isopropyl-7-methoxyt...	194	C11H14O3	089647-85-8	52
4	2-Propenoic acid, 3-(4-hydroxy-3...	194	C10H10O4	000537-98-4	46
5	4-Oxoadamantane-1-carboxylic acid	194	C11H14O3	1000302-82-2	41





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

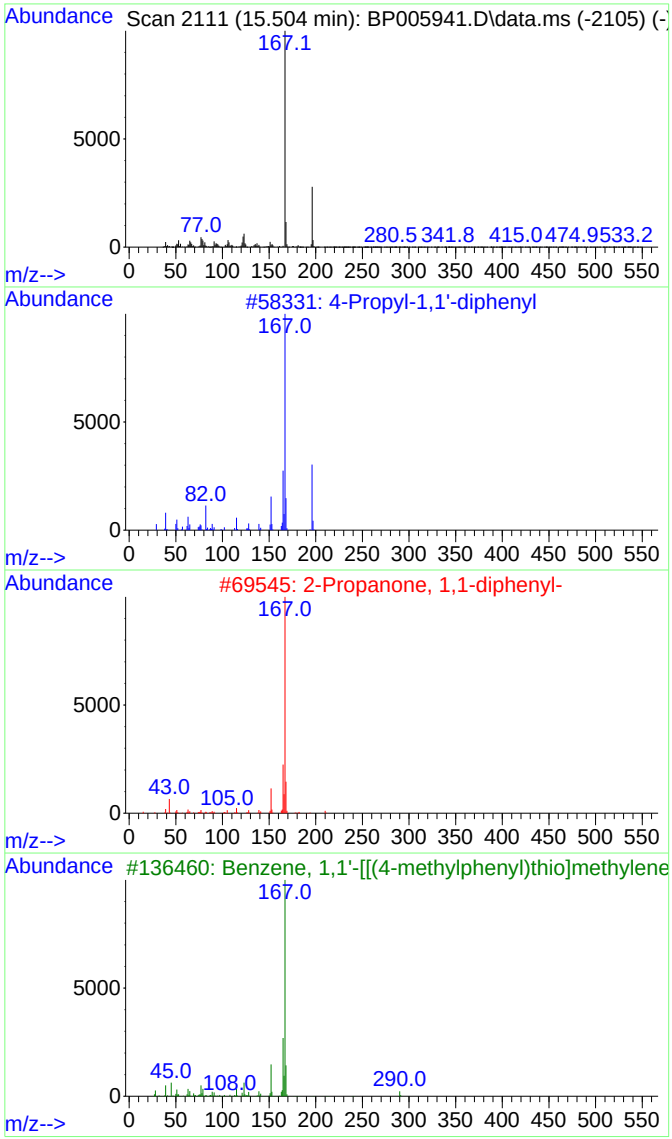
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

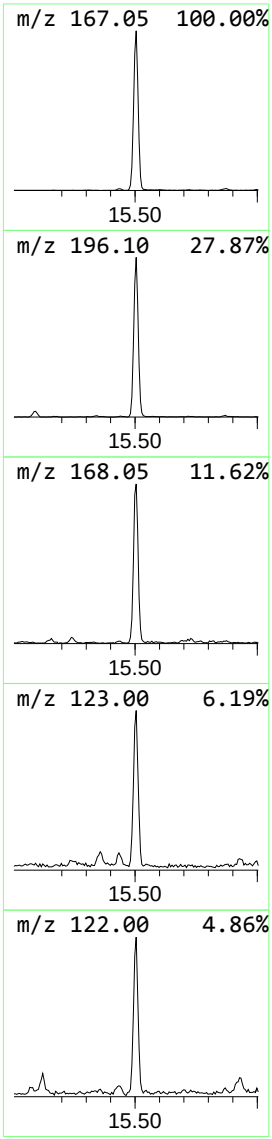
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 4-Propyl-1,1'-diphenyl Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.504	13.99 ng	547386	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Propyl-1,1'-diphenyl	196	C15H16	010289-45-9	72
2	2-Propanone, 1,1-diphenyl-	210	C15H14O	000781-35-1	42
3	Benzene, 1,1'-[[(4-methylphenyl)...	290	C20H18S	032110-49-9	36
4	2,4-Hexadienedioic acid, 3-methy...	226	C12H18O4	069796-13-0	36
5	Benzene, 1,1',1'',1'''-(1,2-etha...	334	C26H22	000632-50-8	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

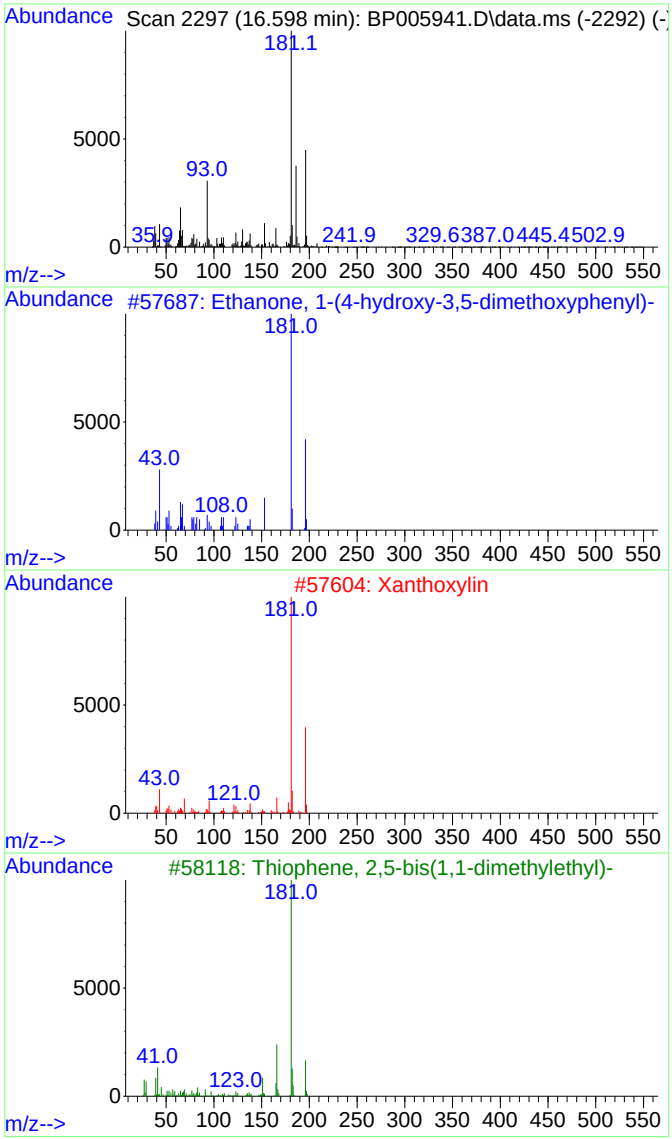
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

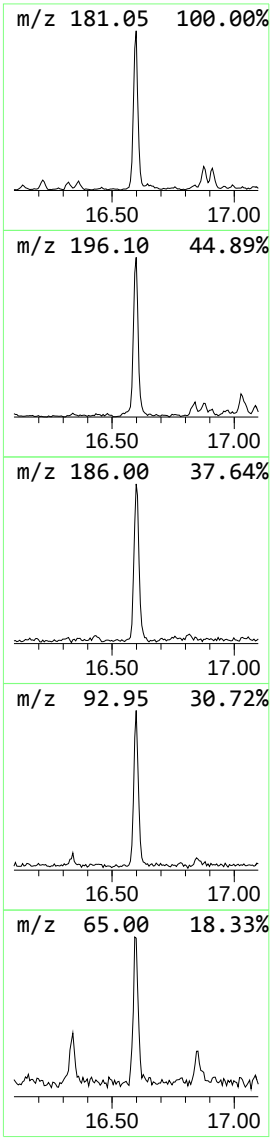
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Ethanone, 1-(4-hydroxy-3,5-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.598	4.06 ng	197634	Phenanthrene-d10	17.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(4-hydroxy-3,5-dimet...	196	C10H12O4	002478-38-8	95
2	Xanthoxylin	196	C10H12O4	000090-24-4	62
3	Thiophene, 2,5-bis(1,1-dimethyle...	196	C12H20S	001689-77-6	53
4	Silane, (3-methoxyphenoxy)trimet...	196	C10H16O2Si	033285-71-1	42
5	5H-Indeno[1,2-b]pyridin-5-one	181	C12H7NO	003882-46-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

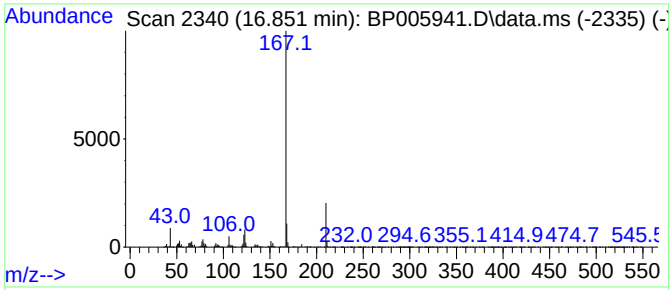
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

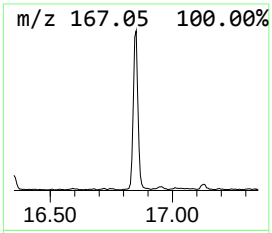
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

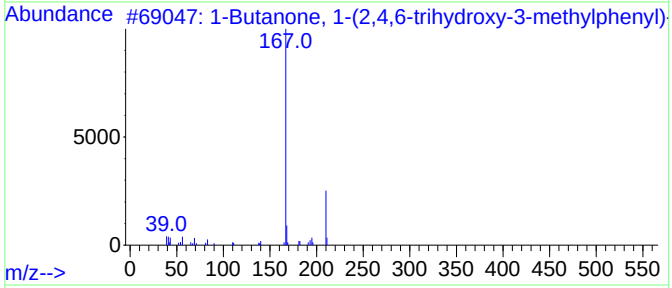
****
Peak Number 15 1-Butanone, 1-(2,4,6-trihyd... Concentration Rank 9

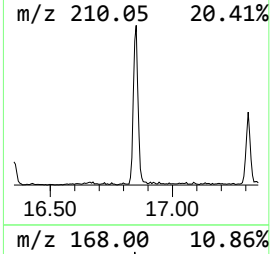
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.851	4.32 ng	210051	Phenanthrene-d10	17.304

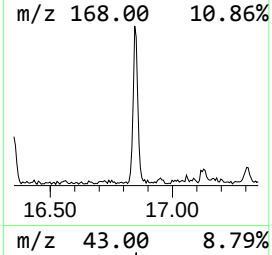
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanone, 1-(2,4,6-trihydroxy-...	210	C11H14O4	001509-06-4	64
2	2-Pentanone, 1-(2,4,6-trihydroxy...	210	C11H14O4	1000116-22-3	50
3	Diphenylmethoxy acetic acid	242	C15H14O3	021409-25-6	40
4	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	38
5	Heptane, 1,1-diphenyl-	252	C19H24	001530-05-8	33

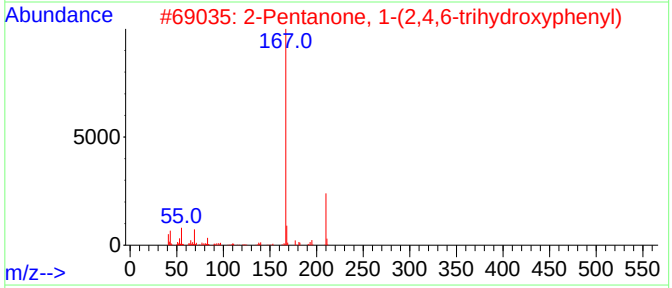


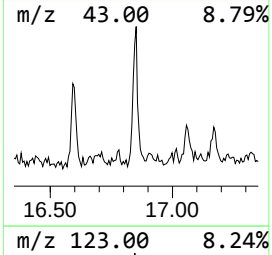


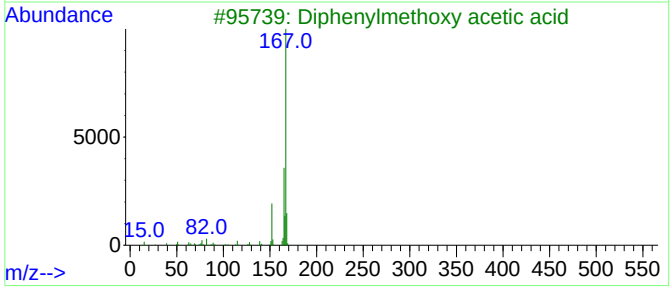


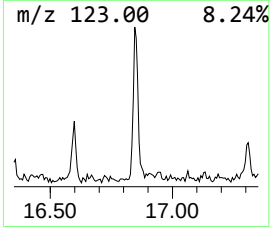












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

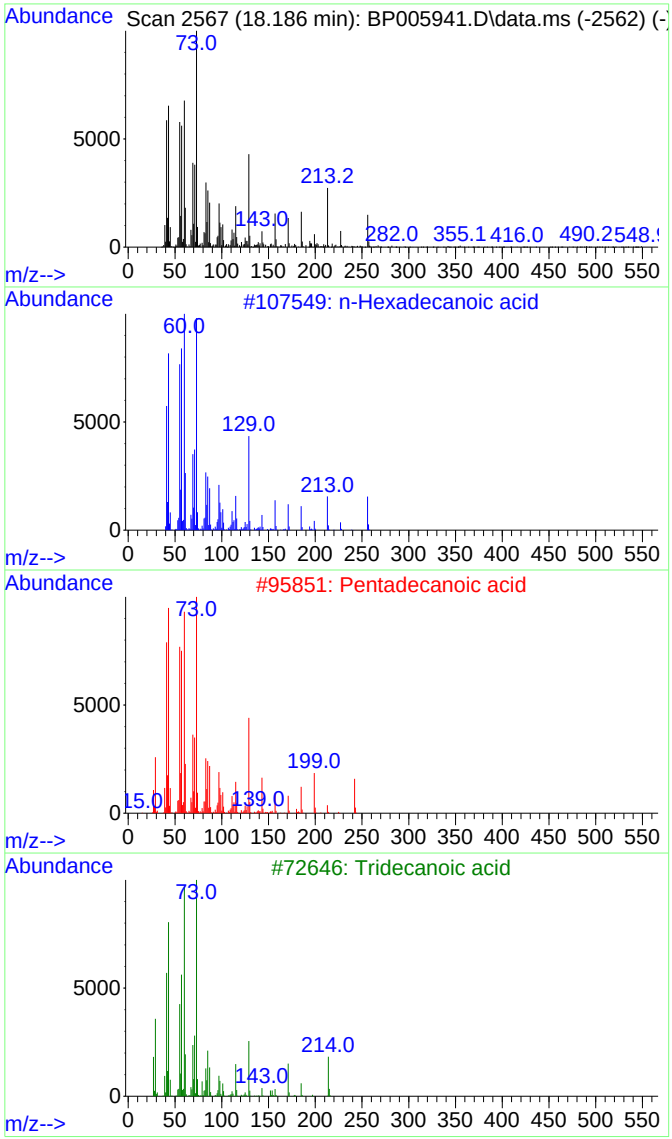
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

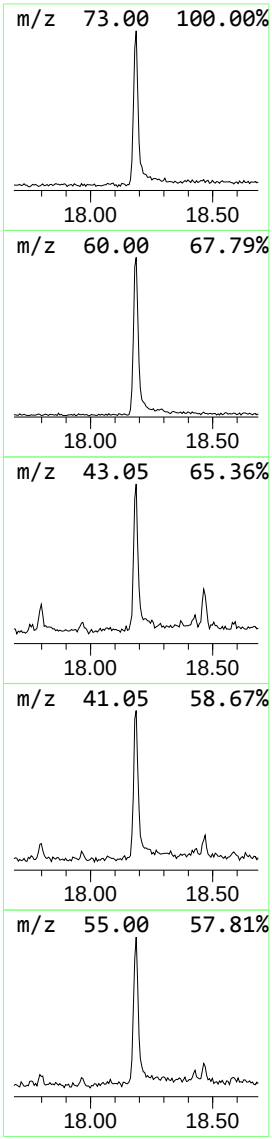
****

Peak Number 16 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	7.27 ng	353769	Phenanthrene-d10	17.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Octadecanoic acid	284	C18H36O2	000057-11-4	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

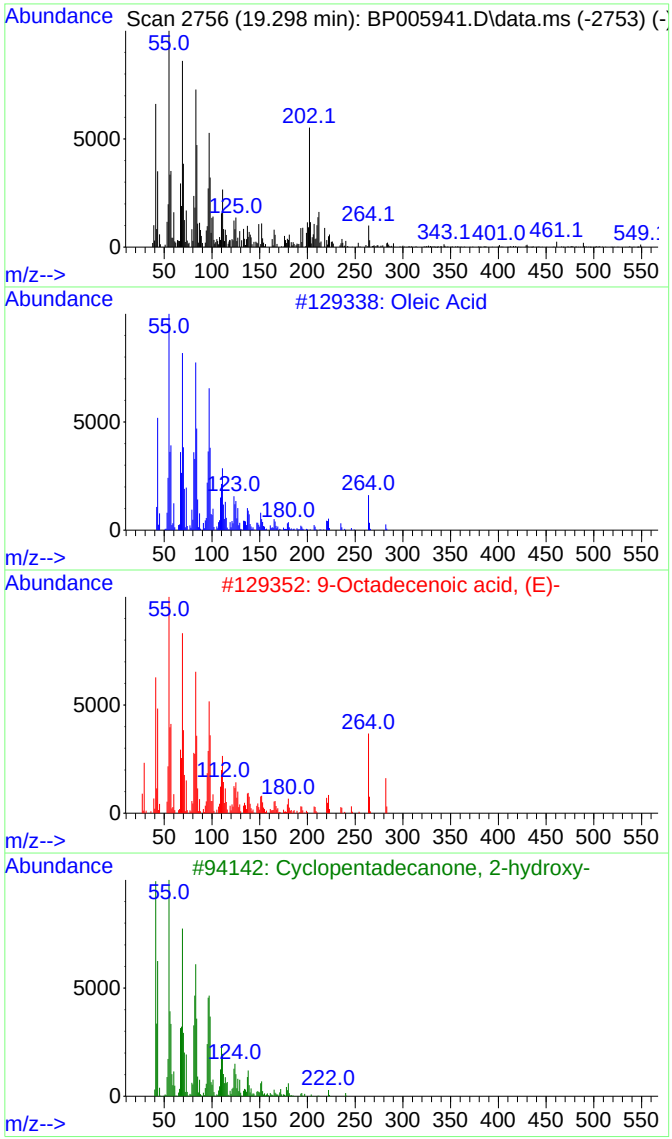
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

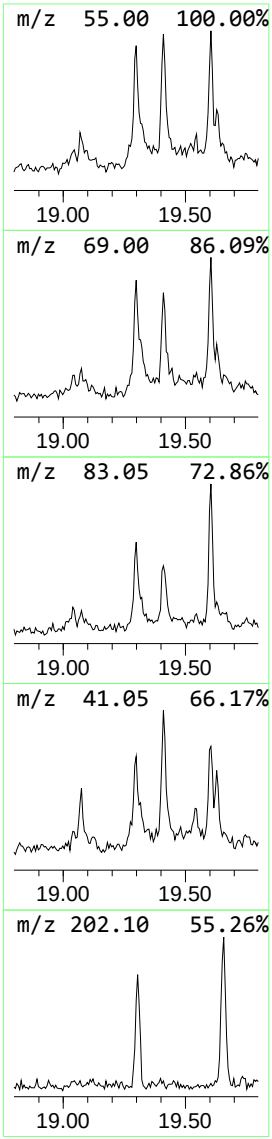
****

Peak Number 17 Oleic Acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.298	2.87 ng	139354	Phenanthrene-d10	17.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	76
2	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	62
3	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	52
4	4-Undecene, 4-methyl-, (Z)-	168	C12H24	074630-57-2	47
5	Cyclopentane, 1,1'-[3-(2-cyclope...	304	C22H40	055255-85-1	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

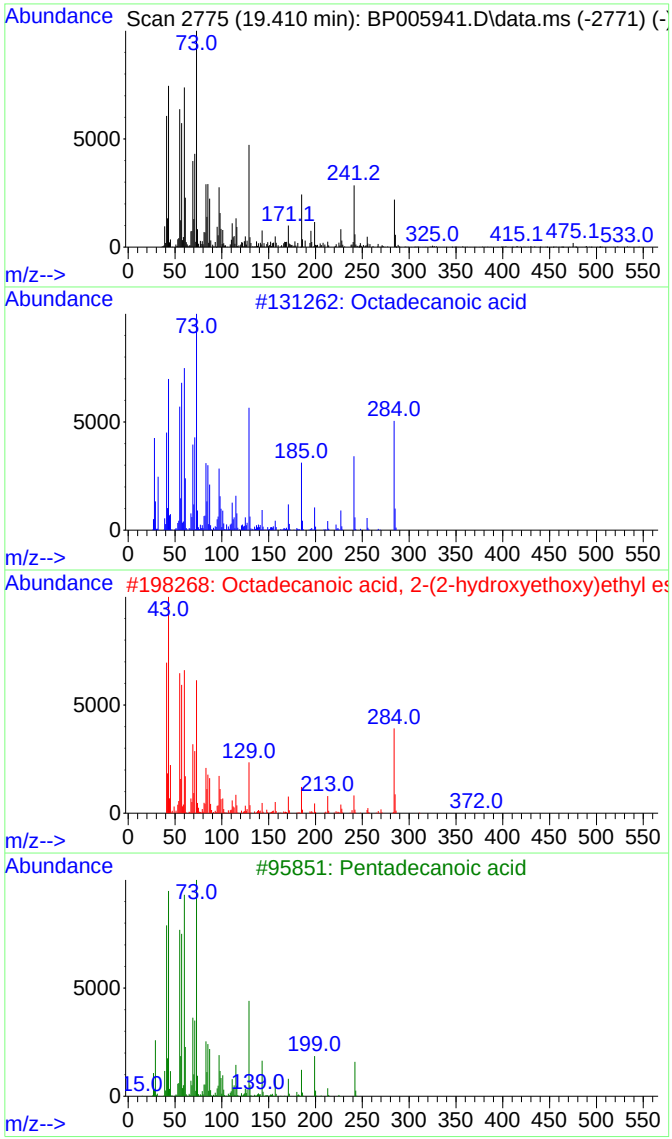
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

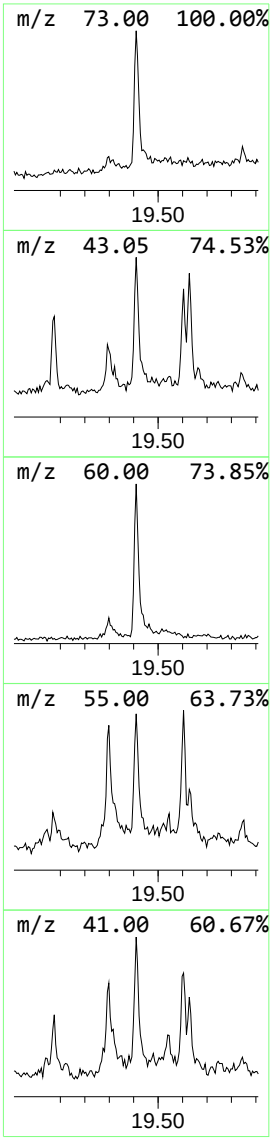
****

Peak Number 18 Octadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.410	2.92 ng	174424	Chrysene-d12	21.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Octadecanoic acid, 2-hydroxy-1,3...	625	C39H76O5	000504-40-5	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 17-B6(20-24)

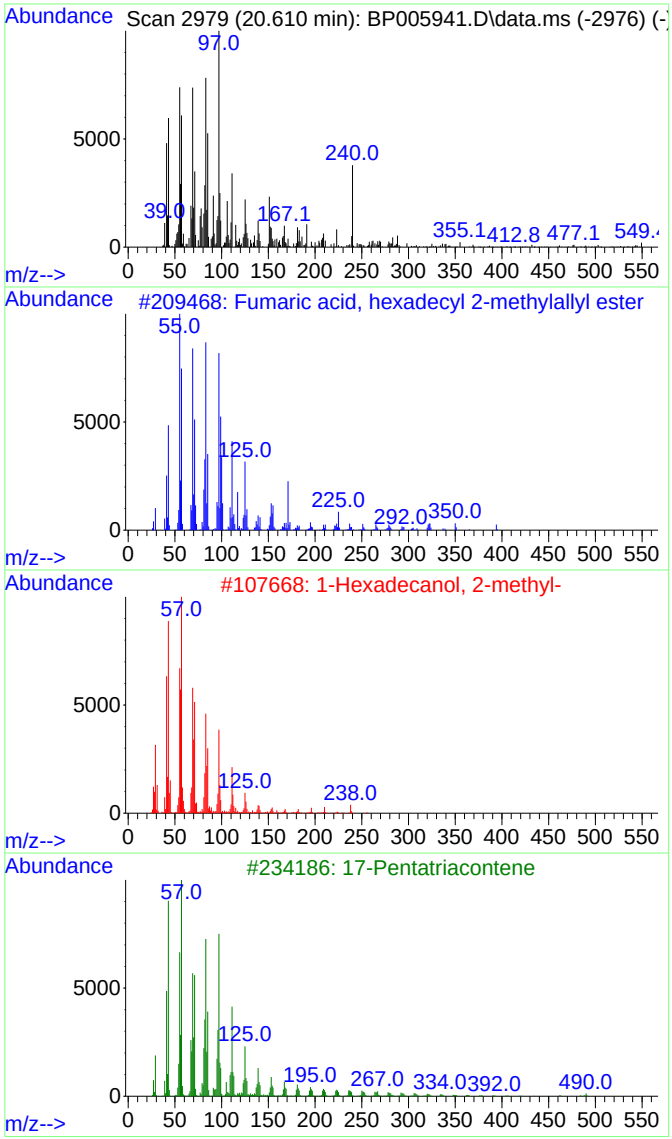
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

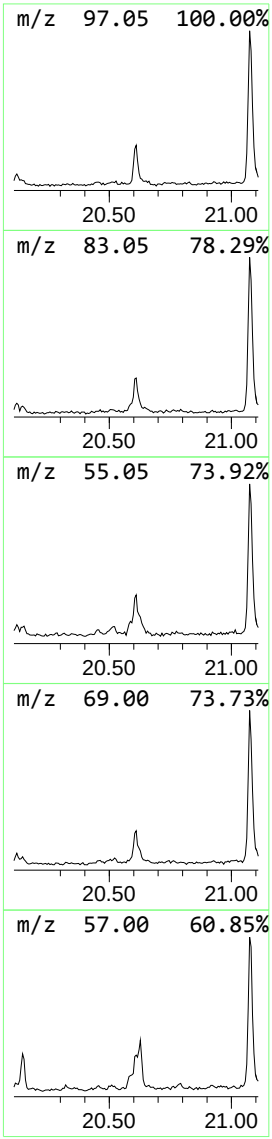
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Fumaric acid, hexadecyl 2-m... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.610	3.78 ng	225223	Chrysene-d12	21.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, hexadecyl 2-methyl...	394	C24H42O4	1000330-55-5	58
2	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	55
3	17-Pentatriacontene	491	C35H70	006971-40-0	51
4	1-Docosene	308	C22H44	001599-67-3	49
5	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

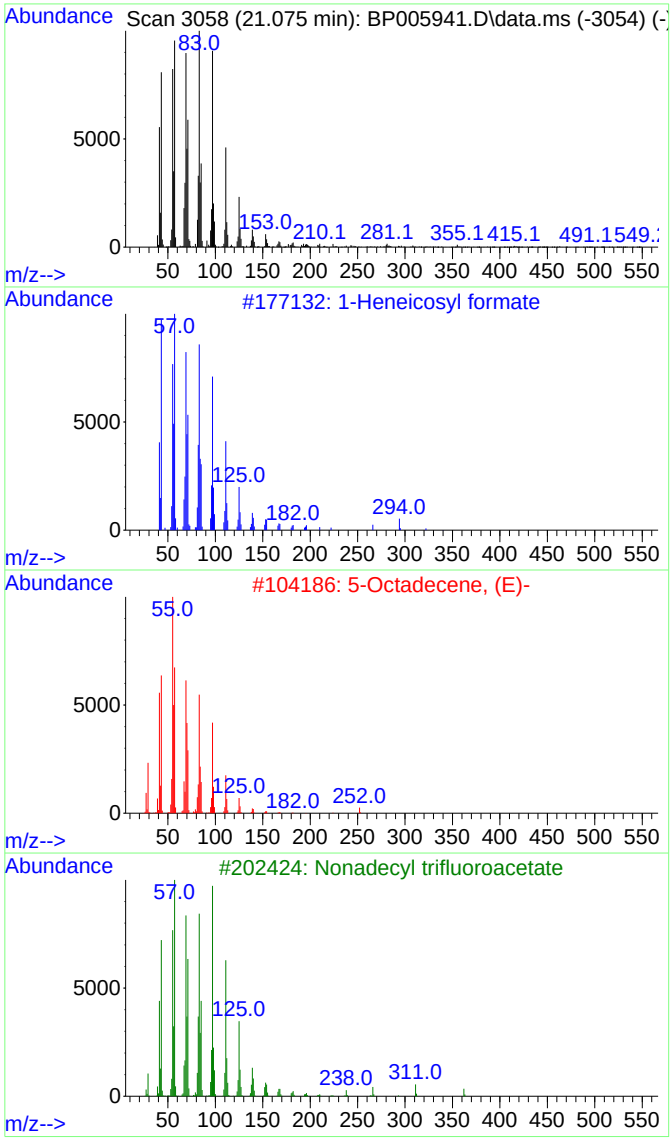
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

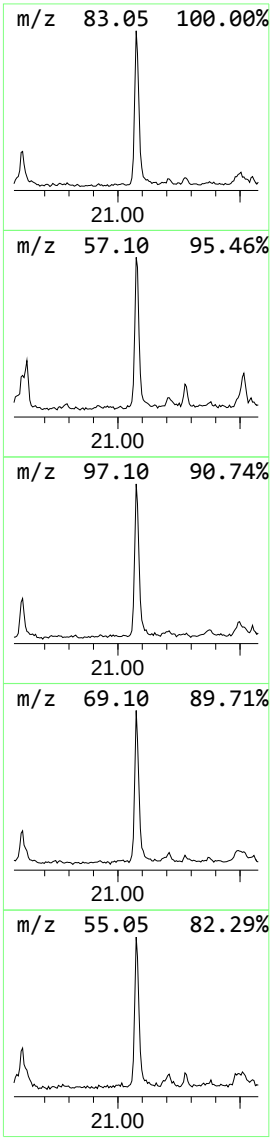
****

Peak Number 20 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.075	8.66 ng	516253	Chrysene-d12	21.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
3	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	Cyclopentadecane	210	C15H30	000295-48-7	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005941.D
Acq On : 15 Jun 2021 21:10
Operator : CG/JU
Sample : M2672-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 17-B6(20-24)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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
3-Penten-2-ol	3.117	3.7	ng	75419	1	7.934	412487	20.0
Mequinol	9.034	2.5	ng	50469	1	7.934	412487	20.0
2-Methoxy-5-met...	10.646	2.8	ng	76866	2	10.734	540617	20.0
unknown11.569	11.569	3.0	ng	80024	2	10.734	540617	20.0
Phenol, 4-ethyl...	11.904	4.6	ng	124569	2	10.734	540617	20.0
Phenol, 2,6-dim...	12.834	10.3	ng	401239	3	14.557	782388	20.0
Dehydroacetic Acid	13.916	15.8	ng	616072	3	14.557	782388	20.0
Apocynin	14.416	5.1	ng	200465	3	14.557	782388	20.0
5-tert-Butylpyr...	14.716	18.7	ng	730197	3	14.557	782388	20.0
Homovanillyl al...	14.816	2.4	ng	91823	3	14.557	782388	20.0
Phenol, 2,6-dim...	15.434	2.8	ng	108917	3	14.557	782388	20.0
4-Propyl-1,1'-d...	15.504	14.0	ng	547386	3	14.557	782388	20.0
Ethanone, 1-(4-...	16.598	4.1	ng	197634	4	17.304	972588	20.0
1-Butanone, 1-(...	16.851	4.3	ng	210051	4	17.304	972588	20.0
n-Hexadecanoic ...	18.186	7.3	ng	353769	4	17.304	972588	20.0
Oleic Acid	19.298	2.9	ng	139354	4	17.304	972588	20.0
Octadecanoic acid	19.410	2.9	ng	174424	5	21.375	1192780	20.0
Fumaric acid, h...	20.610	3.8	ng	225223	5	21.375	1192780	20.0
1-Heneicosyl fo...	21.075	8.7	ng	516253	5	21.375	1192780	20.0