LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007041.D
Acq On : 17 Sep 2021 23:36
Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-CB-04-(1.5)

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-BP091621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007041.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.317	204	209	219	rBV	217553	325955	1.69%	0.242%
2	4.728	274	279	282	rBV	164485	254979	1.33%	0.189%
3	4.811	283	293	303	rVV	395890	1139599	5.92%	0.845%
4	5.023	325	329	339	rVB	253887	371911	1.93%	0.276%
5	5.481	400	407	416	rBV	2882367	4119357	21.41%	3.054%
6	7.069	670	677	687	rBV	1644088	2686226	13.96%	1.991%
7	7.905	812	819	828	rBV	1232741	2021250	10.51%	1.498%
8	8.669	939	949	956	rBV	939343	1515874	7.88%	1.124%
9	9.069	1001	1017	1026	rBV	3634619	6015563	31.27%	4.459%
10	9.428	1051	1078	1094	rBV	1111984	4887482	25.41%	3.623%
11	9.628	1106	1112	1119	rBV4	115356	212045	1.10%	0.157%
12	9.963	1156	1169	1175	rBV	212455	455679	2.37%	0.338%
13	10.152	1191	1201	1211	rBV	3410711	5837016	30.34%	4.327%
14	10.487	1250	1258	1267	rBV2	242495	444706	2.31%	0.330%
15	10.705	1287	1295	1300	rBV	1661155	2792537	14.52%	2.070%
16	10.757	1300	1304	1311	rVB	492937	818511	4.26%	0.607%
17	11.263	1376	1390	1402	rBV	665297	1523213	7.92%	1.129%
18	12.416	1575	1586	1595	rBV	2250905	4103898	21.33%	3.042%
19	12.587	1595	1615	1633	rVB	3832105	14038627	72.98%	10.407%
20	13.163	1706	1713	1724	rVB	9790506	14152041	73.57%	10.491%
21	13.334	1736	1742	1753	rBV	239034	413493	2.15%	0.307%
22	13.499	1765	1770	1780	rBV	316183	492176	2.56%	0.365%
23	14.346	1908	1914	1925	rVB2	123874	241537	1.26%	0.179%
24	14.534	1936	1946	1956	rBV	2516012	3789600	19.70%	2.809%
25	15.081	2034	2039	2049	rVB2	100193	201223	1.05%	0.149%
26	15.410	2088	2095	2102	rBV2	207502	310810	1.62%	0.230%
27	15.734	2144	2150	2157	rBV	126907	218297	1.13%	0.162%
28	15.910	2170	2180	2184	rBV2	324151	568725	2.96%	0.422%
29	16.022	2189	2199	2209	rBV	6936318	10428784	54.21%	7.731%
30	16.204	2220	2230	2234	rBV	365958	674841	3.51%	0.500%
31	16.287	2239	2244	2253	rVB	953850	1310454	6.81%	0.971%
32	16.369	2253	2258	2263	rBV	1049369	1350649	7.02%	1.001%
33	16.787	2321	2329	2348	rBV	2885864	4935844	25.66%	3.659%
34	17.281	2406	2413	2417	rBV	2996526	4288894	22.30%	3.179%
35	17.328	2417	2421	2425	rVB2	561670	765006	3.98%	0.567%
36	17.498	2446	2450	2460	rVB3	227986	428877	2.23%	0.318%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007041.D
Acq On : 17 Sep 2021 23:36
Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-CB-04-(1.5)

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-BP091621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.651	2472	2476	2489	rVB2	199247	290136	1.51%	0.215%
38	18.169	2559	2564	2572	rBV	844498	1223279	6.36%	0.907%
39	19.398	2769	2773	2780	rBV	417568	552014	2.87%	0.409%
40	19.833	2842	2847	2853	rBV	15421031	19236387	100.00%	14.260%
41	20.533	2963	2966	2972	rVB3	227343	299959	1.56%	0.222%
42	21.045	3049	3053	3055	rBV2	321728	440392	2.29%	0.326%
43	21.069	3055	3057	3065	rVB	646063	743456	3.86%	0.551%
44	21.357	3101	3106	3116	rBV	3619323	4638929	24.12%	3.439%
45	21.510	3129	3132	3137	rVB	267619	290162	1.51%	0.215%
46	21.975	3208	3211	3218	rVB	226250	292898	1.52%	0.217%
47	22.322	3267	3270	3276	rVB3	223160	309137	1.61%	0.229%
48	22.475	3293	3296	3301	rVB	253849	322645	1.68%	0.239%
49	23.469	3460	3465	3473	rVB2	732889	1339936	6.97%	0.993%
50	23.769	3509	3516	3527	rVB2	2381248	4708281	24.48%	3.490%
51	24.986	3717	3723	3736	rVB	873684	2077184	10.80%	1.540%

Sum of corrected areas: 134900474

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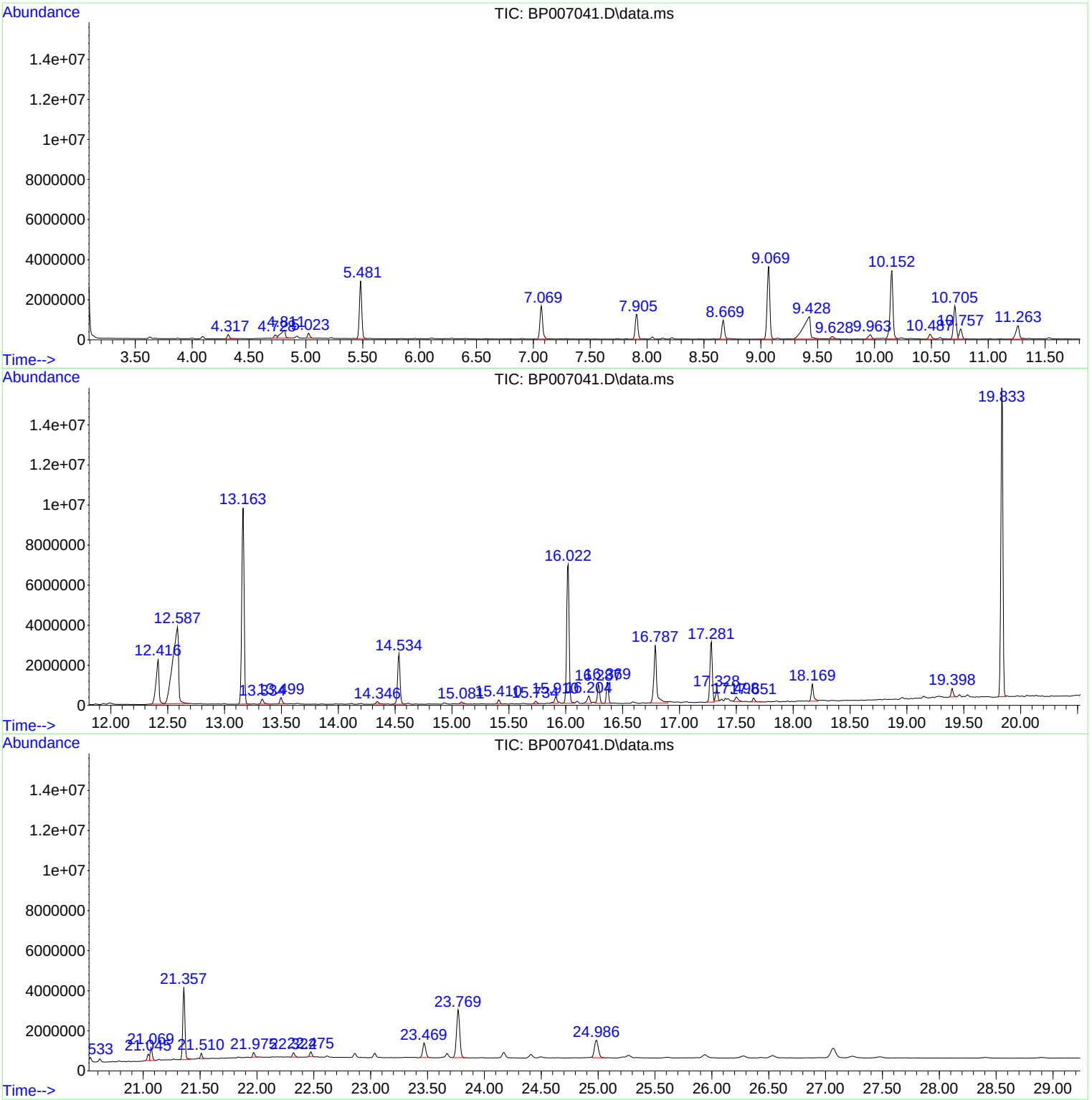
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.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\BP091721\
Data File : BP007041.D
Acq On : 17 Sep 2021 23:36
Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

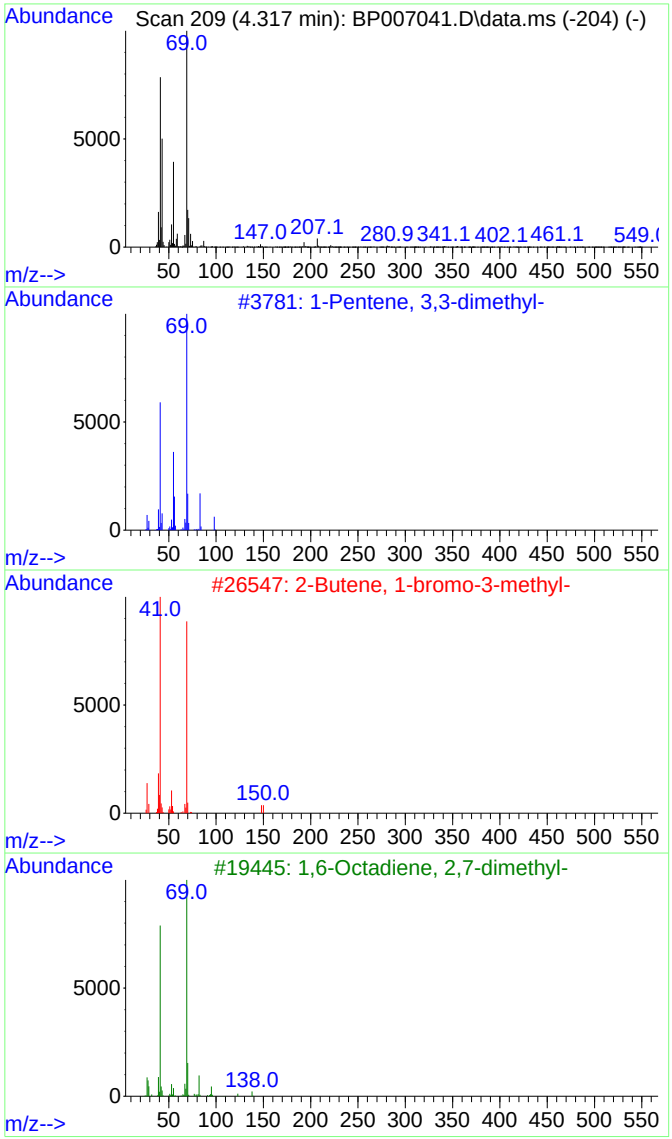
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

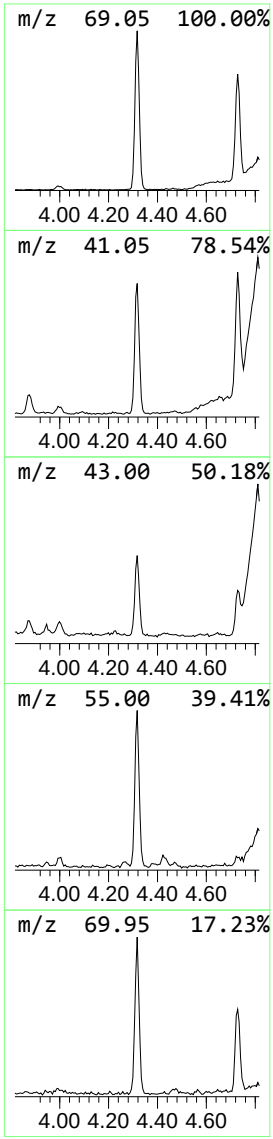
****

Peak Number 1 unknown4.317 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.317	3.23 ng	325955	1,4-Dichlorobenzene-d4	7.911

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	45
2	2-Butene, 1-bromo-3-methyl-	148	C5H9Br	000870-63-3	40
3	1,6-Octadiene, 2,7-dimethyl-	138	C10H18	040195-09-3	36
4	1-Octene, 3,3-dimethyl-	140	C10H20	074511-51-6	33
5	1-Butene, 3,3-dimethyl-	84	C6H12	000558-37-2	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007041.D
Acq On : 17 Sep 2021 23:36
Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

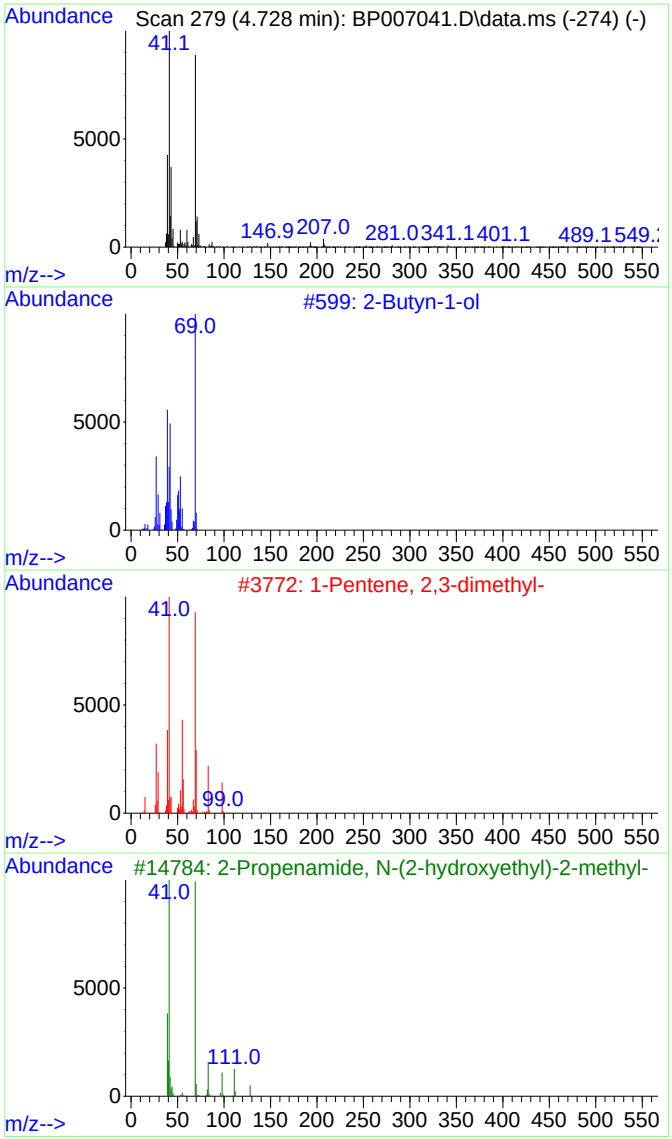
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

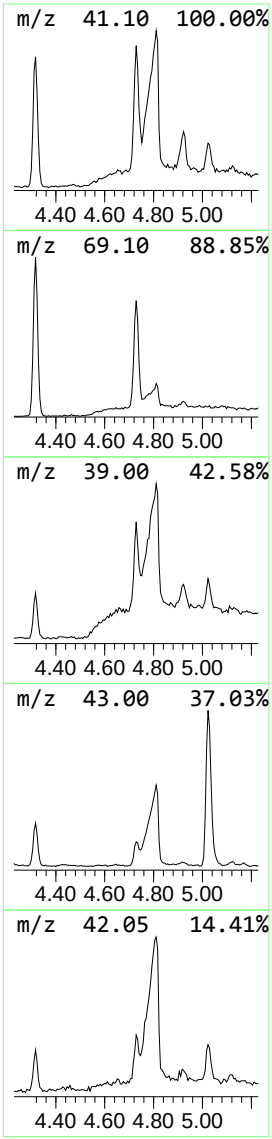
****

Peak Number 2 2-Butyn-1-ol Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.728	2.52 ng	254979	1,4-Dichlorobenzene-d4	7.911

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butyn-1-ol	70	C4H6O	000764-01-2	59
2	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	38
3	2-Propenamide, N-(2-hydroxyethyl...	129	C6H11NO2	005238-56-2	38
4	Ethane, 1,1,1-trifluoro-	84	C2H3F3	000420-46-2	32
5	2-Propenoic acid, 2-methyl-, 1-m...	128	C7H12O2	004655-34-9	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007041.D
Acq On : 17 Sep 2021 23:36
Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

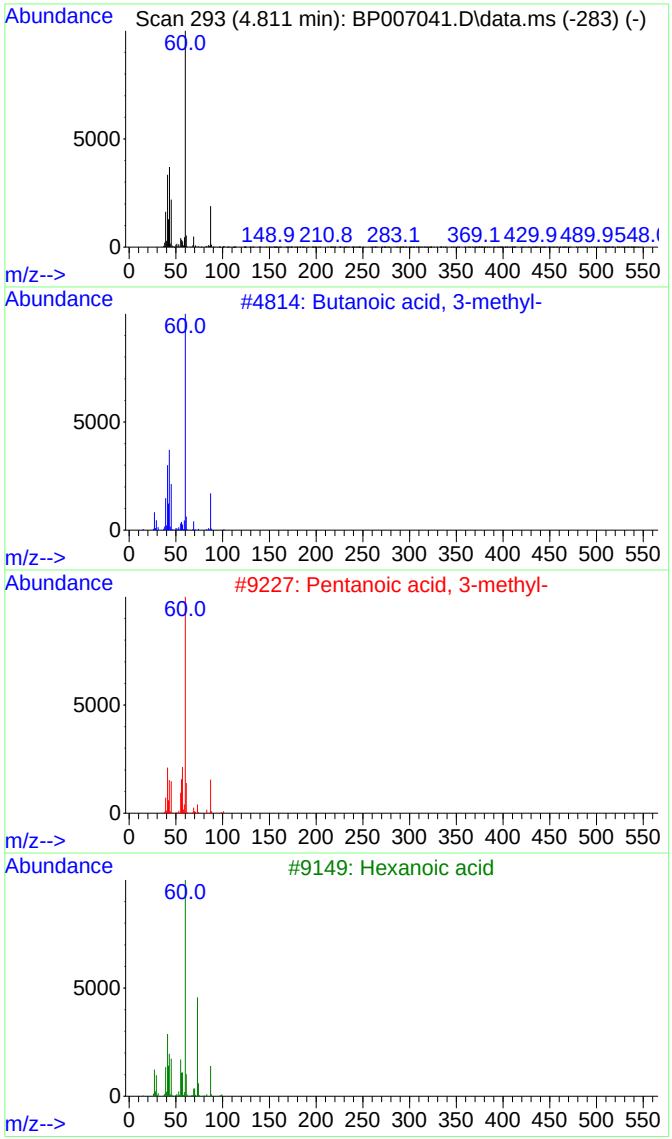
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

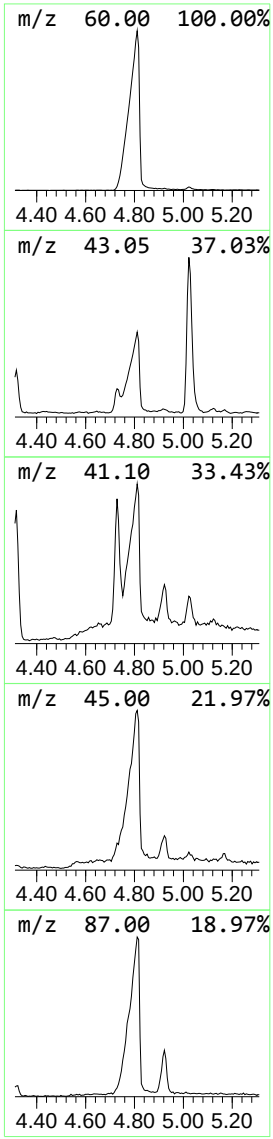
****

Peak Number 3 Butanoic acid, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.811	11.28 ng	1139600	1,4-Dichlorobenzene-d4	7.911

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	90
2	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	56
3	Hexanoic acid	116	C6H12O2	000142-62-1	40
4	Heptanoic acid	130	C7H14O2	000111-14-8	39
5	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
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Acq On : 17 Sep 2021 23:36
Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-CB-04-(1.5)

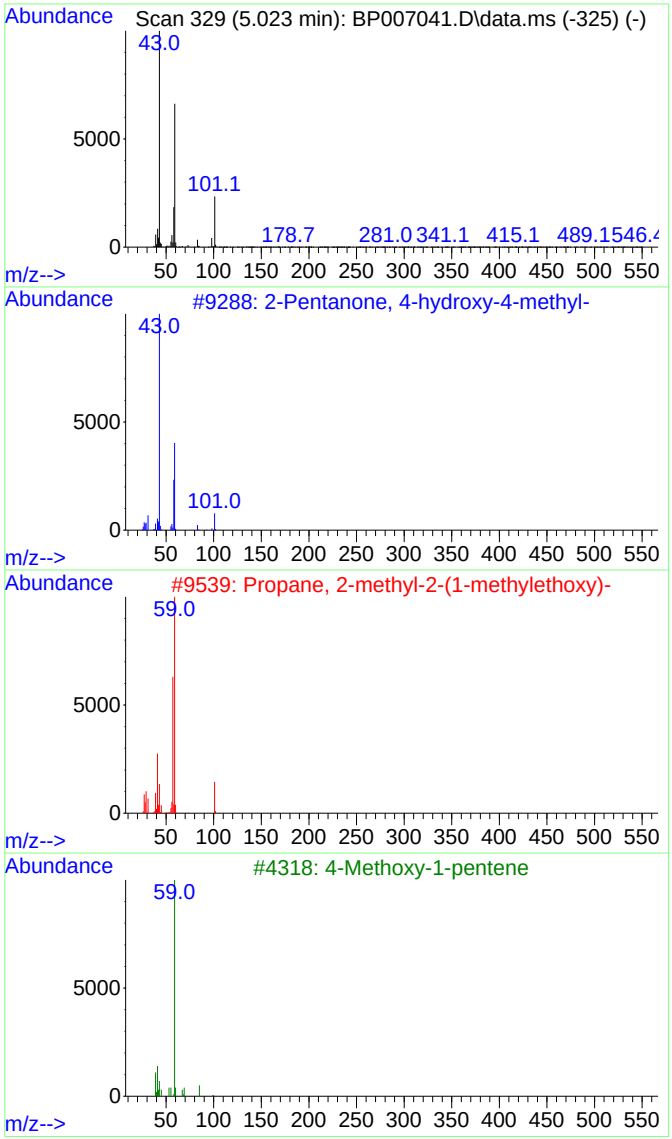
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

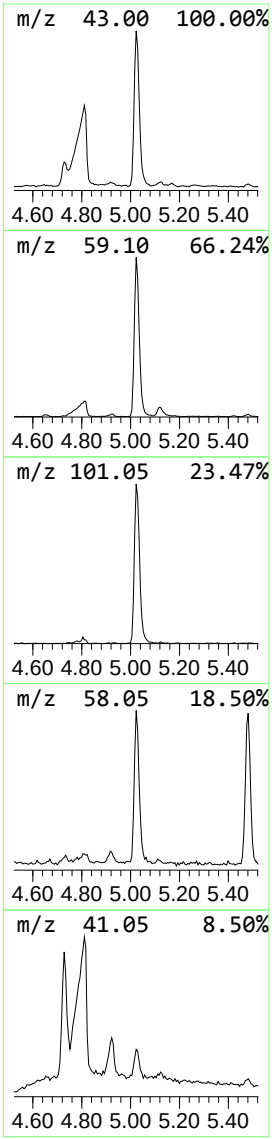
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.023	3.68 ng	371911	1,4-Dichlorobenzene-d4	7.911

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	40
3	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	35
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Tetraglyme	222	C10H22O5	000143-24-8	23





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Data File : BP007041.D
Acq On : 17 Sep 2021 23:36
Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

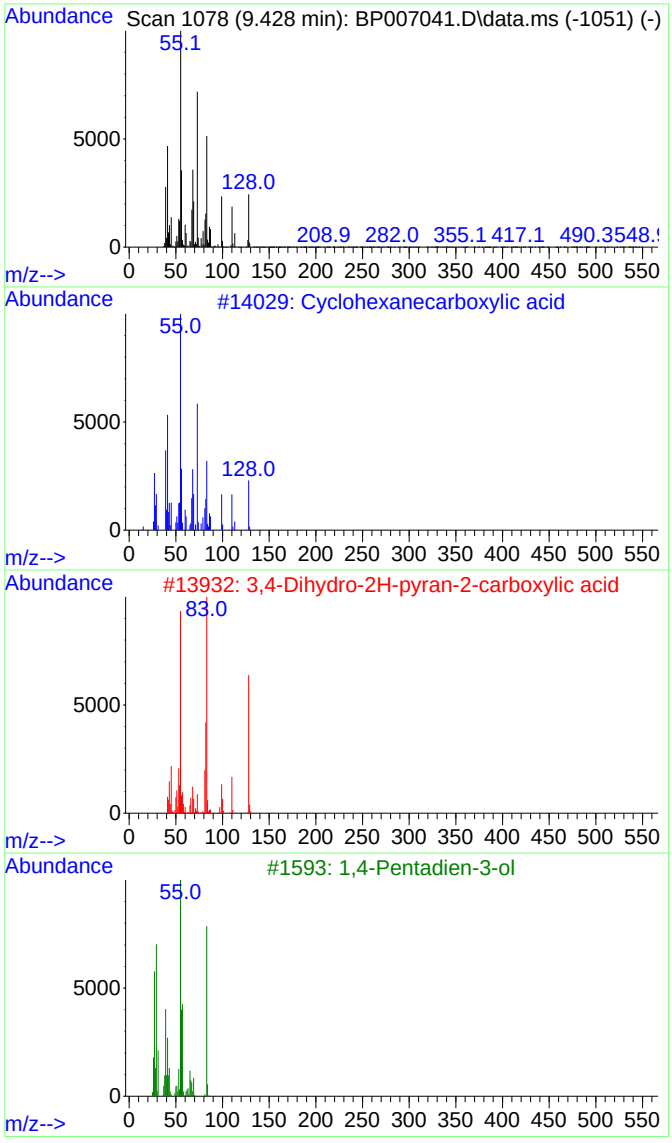
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

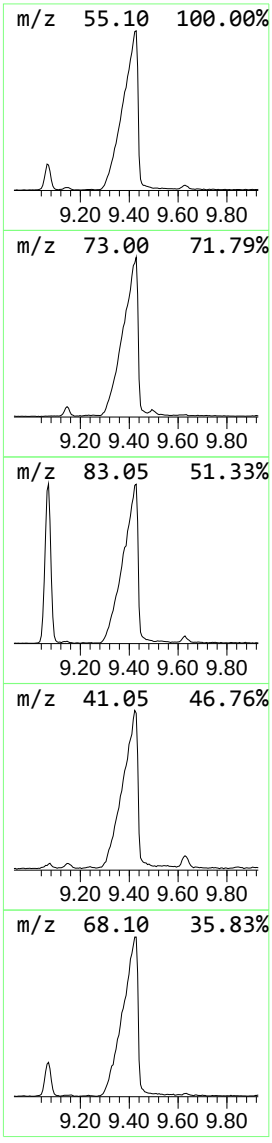
****

Peak Number 5 Cyclohexanecarboxylic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.428	35.00 ng	4887480	Naphthalene-d8	10.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	96
2	3,4-Dihydro-2H-pyran-2-carboxyli...	128	C6H8O3	1010132-10-4	41
3	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	35
4	1-Cyclohexylethanol, pentafluoro...	274	C11H15F5O2	1000365-50-1	25
5	5-Methyl-1-heptanol	130	C8H18O	007212-53-5	25





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BNA_P
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SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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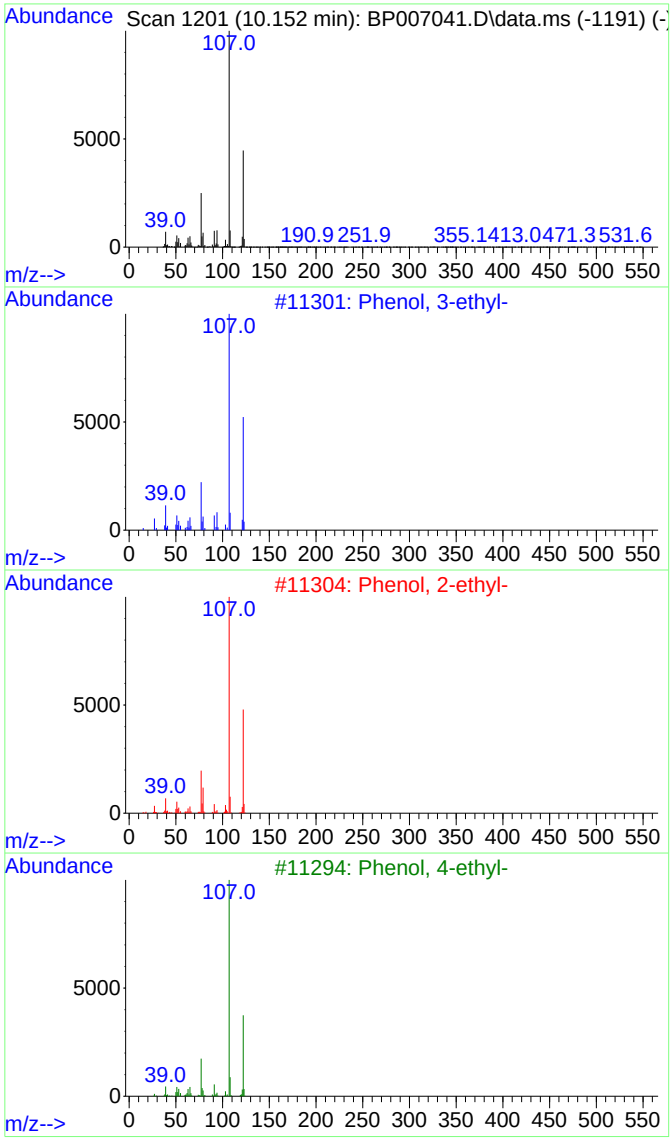
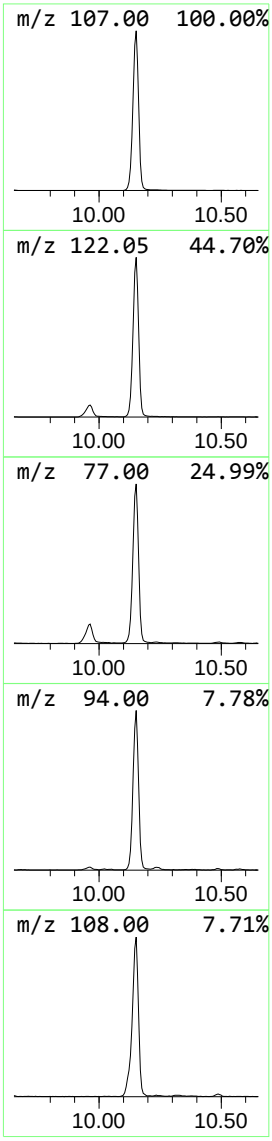
Peak Number 6 Phenol, 3-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.152	41.80 ng	5837020	Naphthalene-d8	10.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-ethyl-	122	C8H10O	000620-17-7	97
2	Phenol, 2-ethyl-	122	C8H10O	000090-00-6	91
3	Phenol, 4-ethyl-	122	C8H10O	000123-07-9	90
4	Phenol, 3,4-dimethyl-	122	C8H10O	000095-65-8	78
5	Silane, 1,3-butadiynyltrimethyl-	122	C7H10Si	004526-06-1	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007041.D
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Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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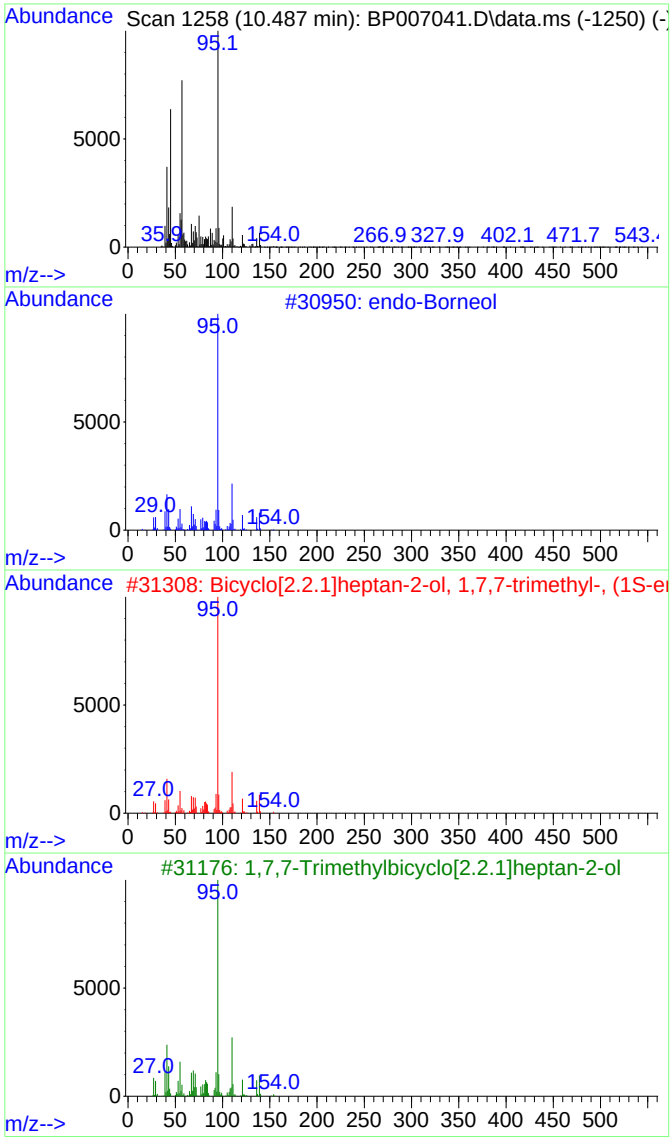
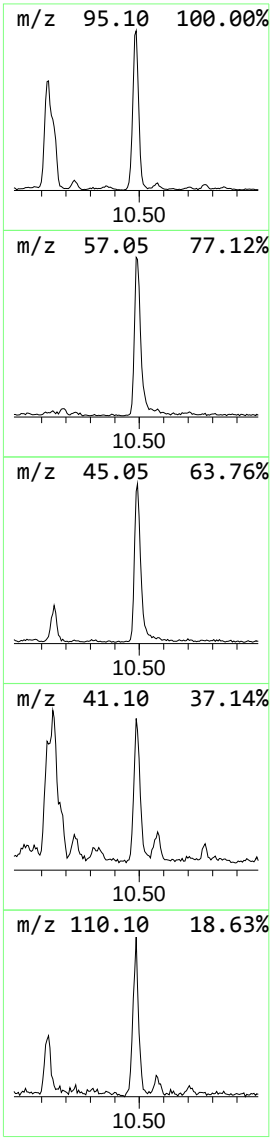
Peak Number 7 endo-Borneol Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.487	3.18 ng	444706	Naphthalene-d8	10.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	endo-Borneol	154	C10H18O	000507-70-0	92
2	Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	154	C10H18O	000464-45-9	91
3	1,7,7-Trimethylbicyclo[2.2.1]hep...	154	C10H18O	010385-78-1	80
4	Isoborneol	154	C10H18O	000124-76-5	46
5	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007041.D
Acq On : 17 Sep 2021 23:36
Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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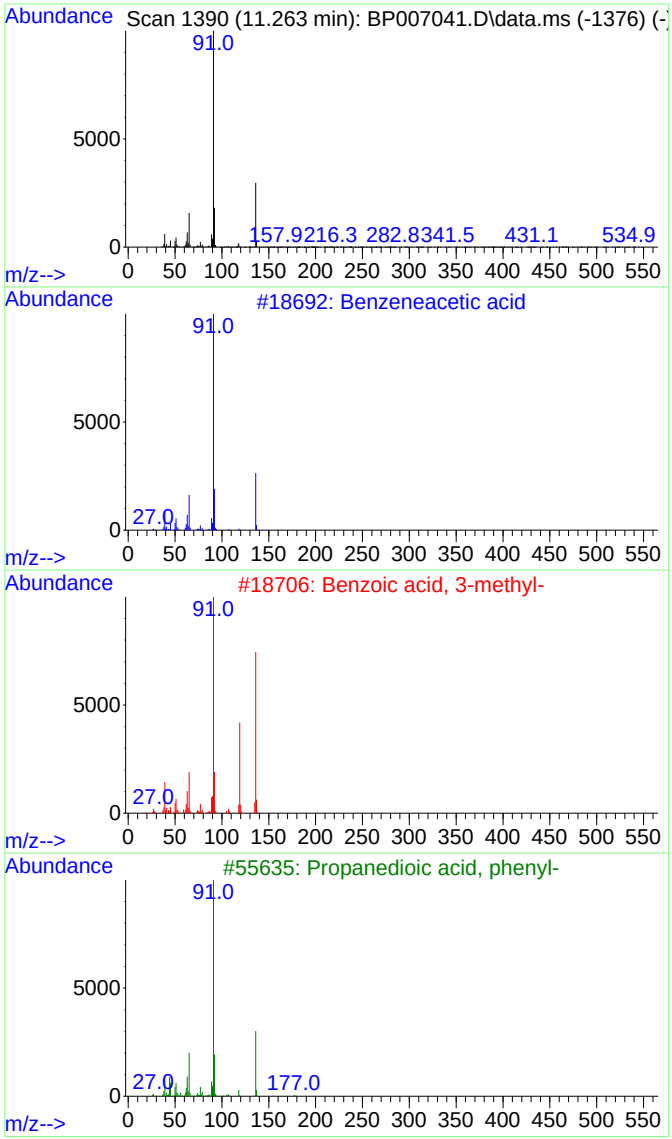
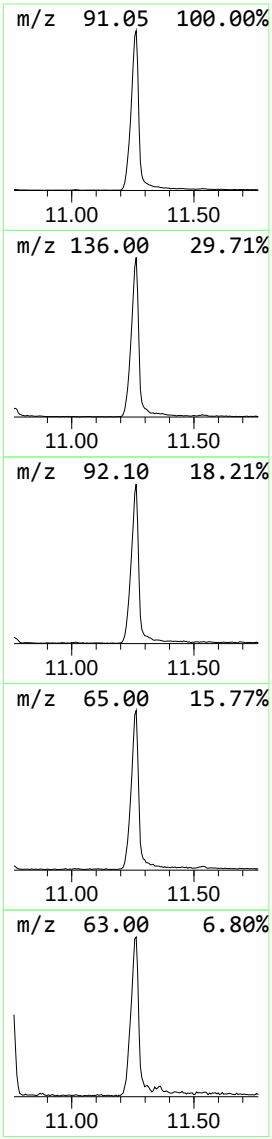
Peak Number 8 Benzeneacetic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.263	10.91 ng	1523210	Naphthalene-d8	10.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	95
2	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	64
3	Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	59
4	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	53
5	Benzene, (2-methoxyethyl)-	136	C9H12O	003558-60-9	50





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Data File : BP007041.D
Acq On : 17 Sep 2021 23:36
Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

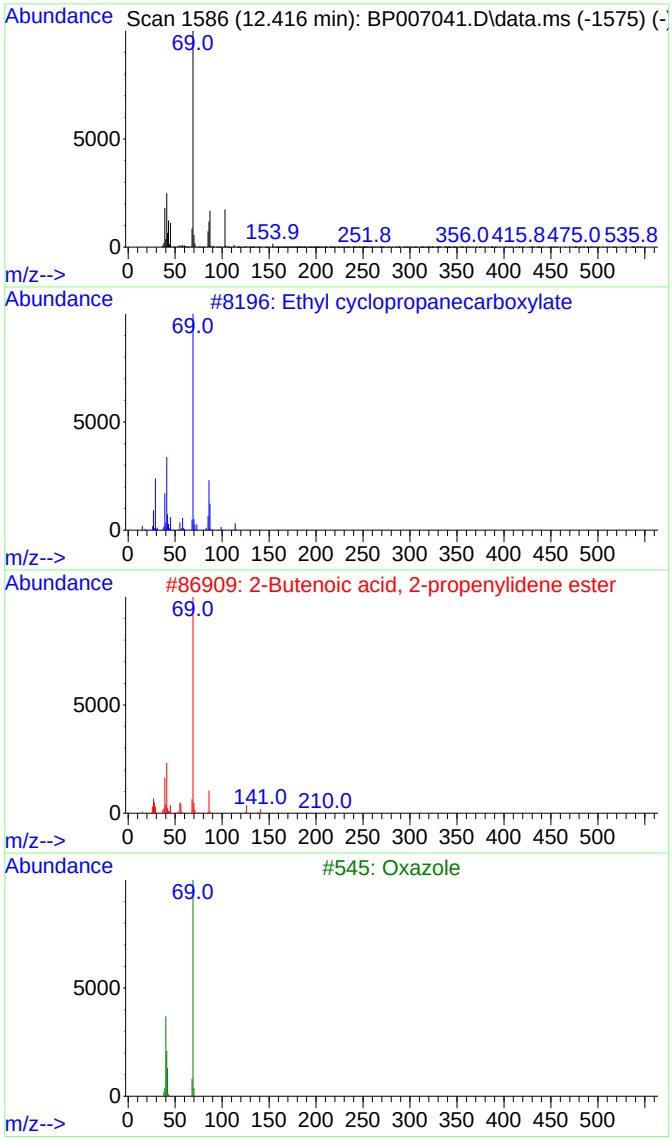
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

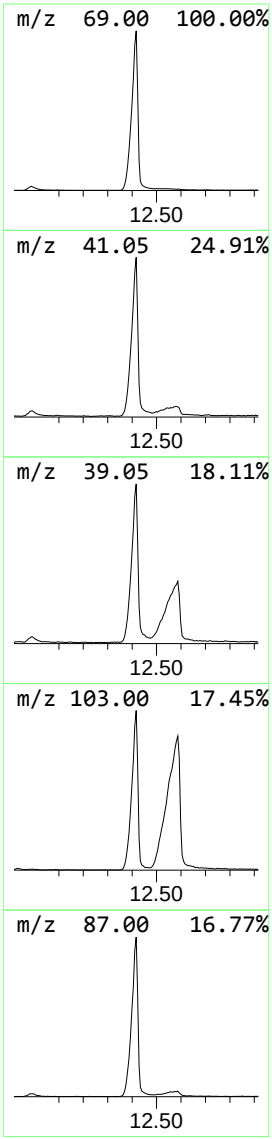
****

Peak Number 9 unknown12.416 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.416	29.39 ng	4103900	Naphthalene-d8	10.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	40
2	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	36
3	Oxazole	69	C3H3NO	000288-42-6	9
4	Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	9
5	Cyclopropanecarboxylic acid,buty...	142	C8H14O2	054947-39-6	9





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Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-CB-04-(1.5)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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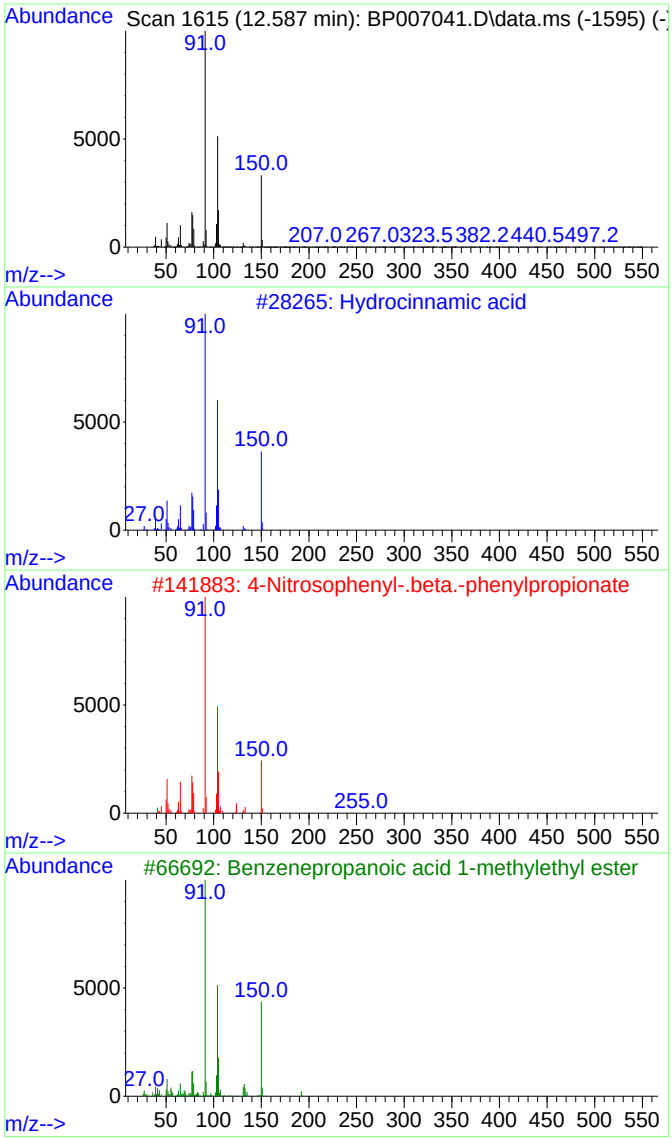
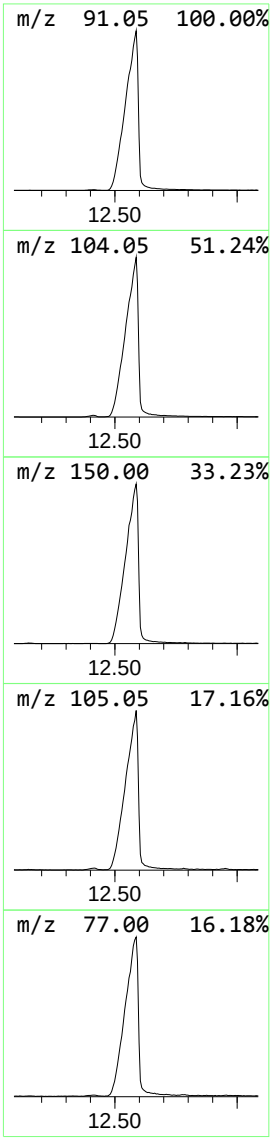
Peak Number 10 Hydrocinnamic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.587	100.54 ng	14038600	Naphthalene-d8	10.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrocinnamic acid	150	C9H10O2	000501-52-0	96
2	4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	86
3	Benzenepropanoic acid 1-methylet...	192	C12H16O2	022767-95-9	72
4	Acetic acid, trifluoro-, 2-pheny...	218	C10H9F3O2	055419-66-4	53
5	Benzenepropanoic acid, silver(1+...	256	C9H9AgO2	075112-79-7	53





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-CB-04-(1.5)

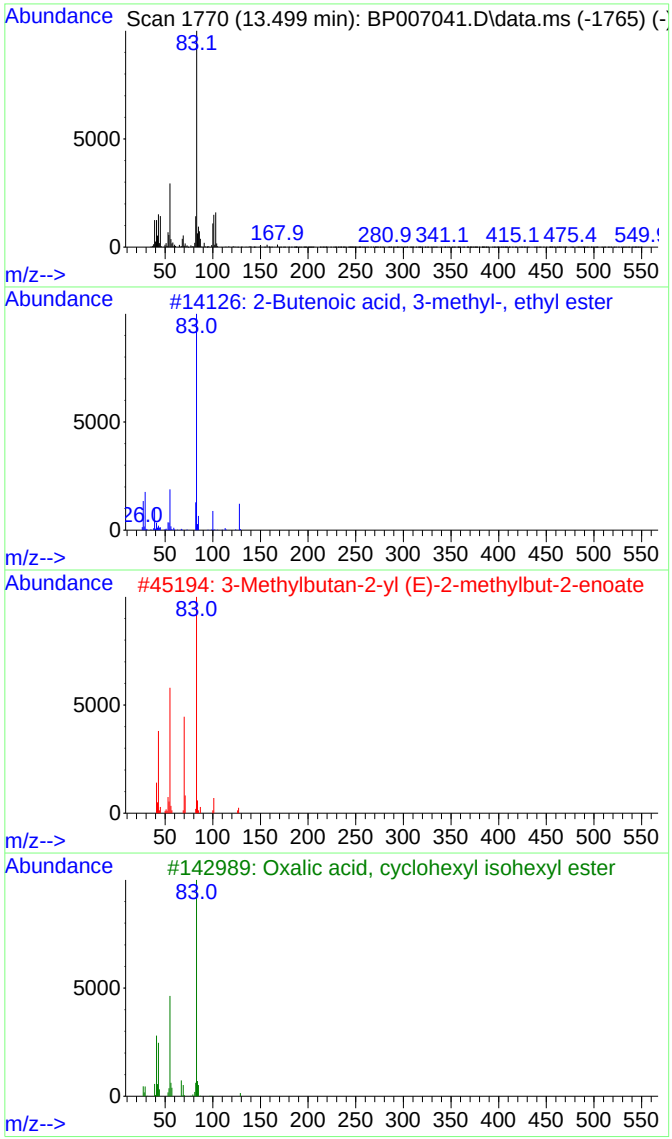
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

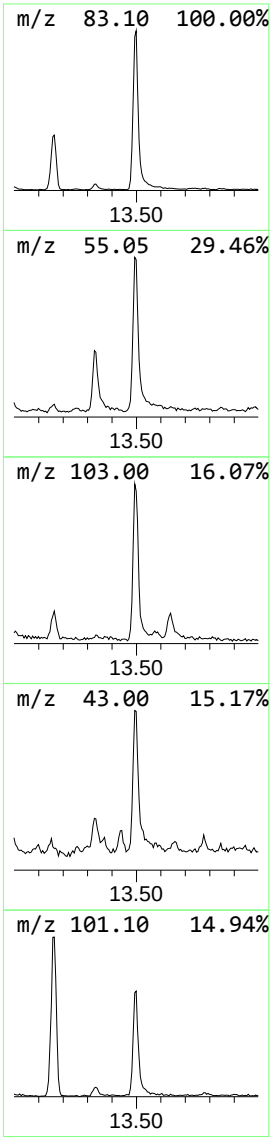
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 2-Butenoic acid, 3-methyl-,... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.499	2.60 ng	492176	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 3-methyl-, ethy...	128	C7H12O2	000638-10-8	59
2	3-Methylbutan-2-yl (E)-2-methylb...	170	C10H18O2	1000373-73-4	53
3	Oxalic acid, cyclohexyl isohexyl...	256	C14H24O4	1010309-30-7	50
4	2,6-Dimethyl-6-nitro-2-hepten-4-one	185	C9H15NO3	073583-56-9	47
5	3-Methyl-2-butenoic acid, cyclop...	168	C10H16O2	1000279-23-3	45





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Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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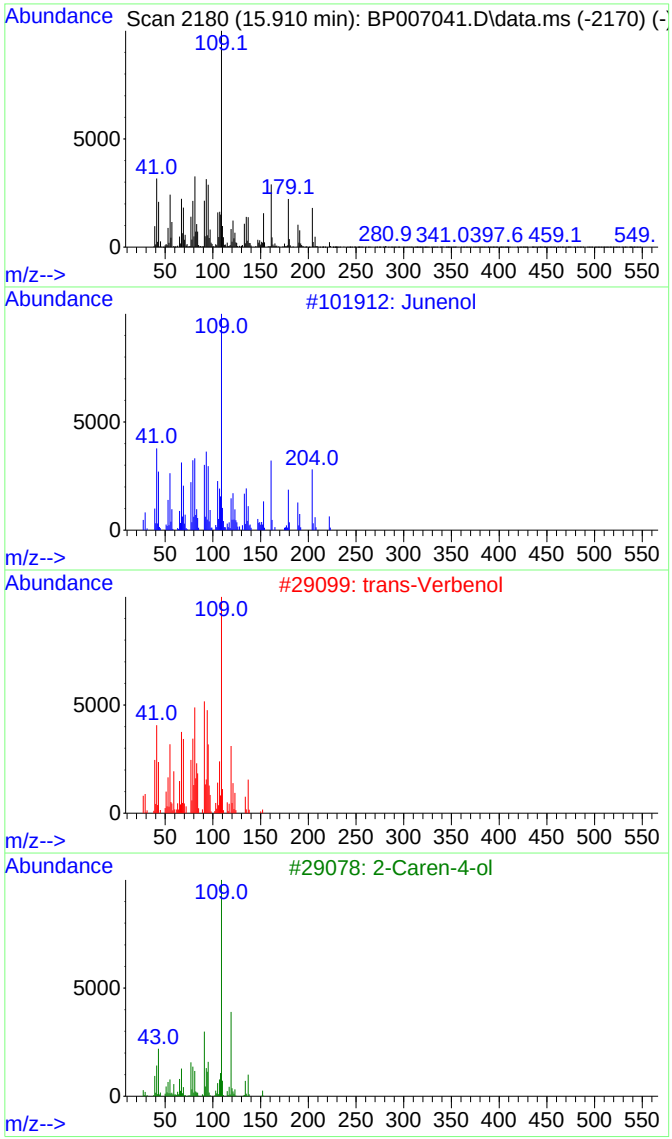
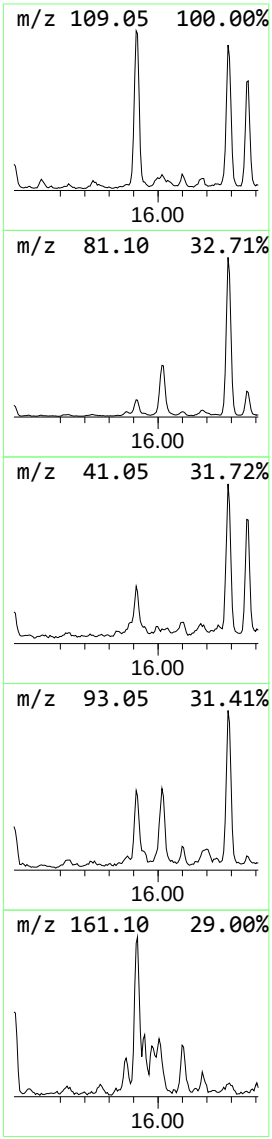
Peak Number 12 Junenol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.910	2.65 ng	568725	Phenanthrene-d10	17.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Junenol	222	C15H26O	000472-07-1	93
2	trans-Verbenol	152	C10H16O	001820-09-3	43
3	2-Caren-4-ol	152	C10H16O	006617-35-2	43
4	Butanamide, N-(4-hydroxyphenyl)-	179	C10H13NO2	000101-91-7	38
5	4-Pentyloxyaniline	179	C11H17NO	039905-50-5	38





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Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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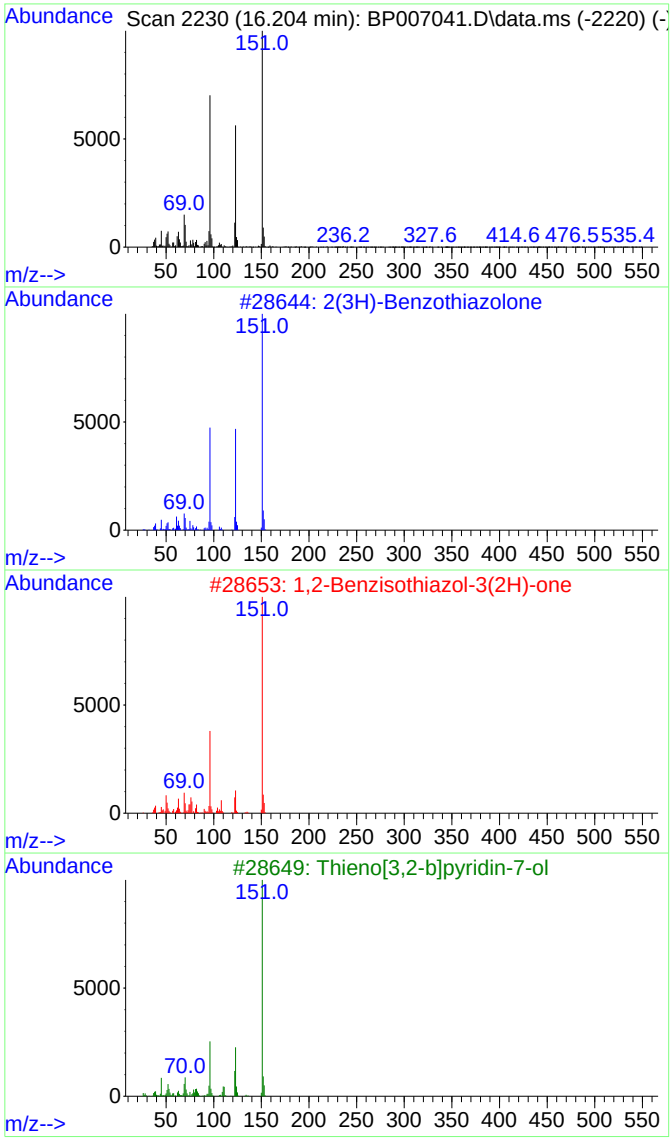
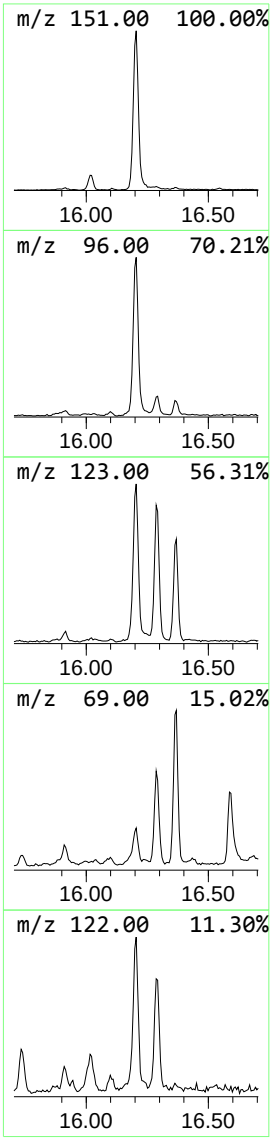
Peak Number 13 2(3H)-Benzothiazolone Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.204	3.15 ng	674841	Phenanthrene-d10	17.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	94
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	64
3	Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	64
4	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	52
5	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	50





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Sample : M3791-05
Misc :
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Instrument : BNA_P
ClientSampleId : SW-CB-04-(1.5)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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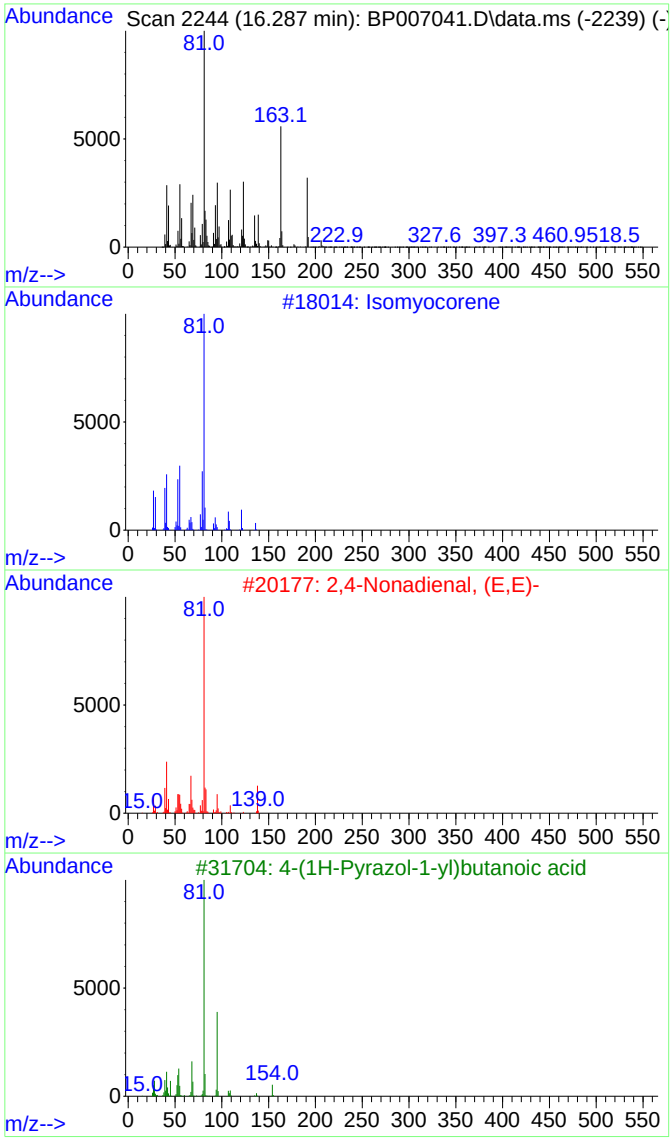
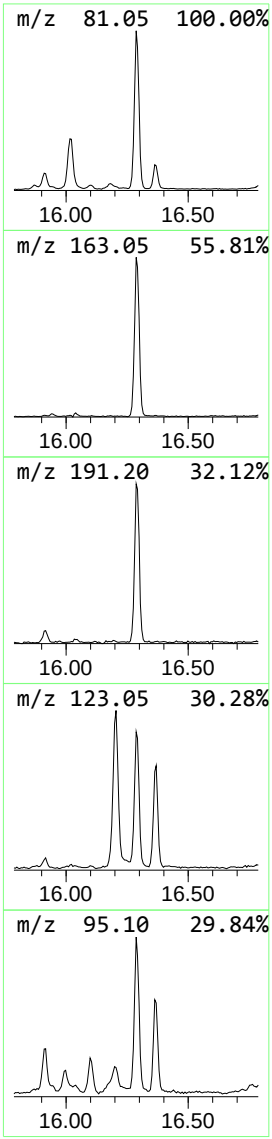
Peak Number 14 unknown16.287 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.287	6.11 ng	1310450	Phenanthrene-d10	17.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isomyocorene	136	C10H16	006876-07-9	27
2	2,4-Nonadienal, (E,E)-	138	C9H14O	005910-87-2	27
3	4-(1H-Pyrazol-1-yl)butanoic acid	154	C7H10N2O2	1010468-88-1	25
4	Zinc, bis(2,2-dimethyl-3(cis)-(1...	310	C18H30Zn	081069-88-7	25
5	2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	16





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Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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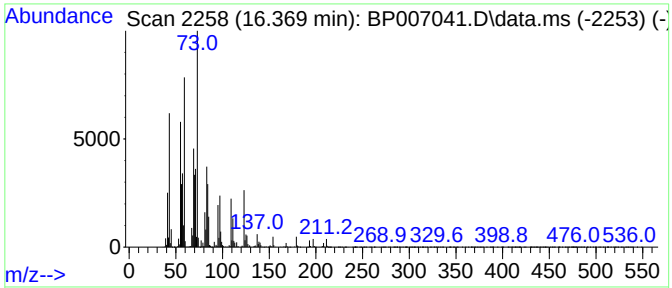
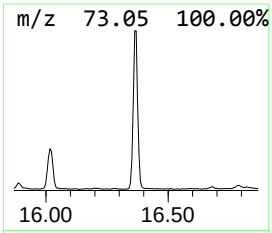
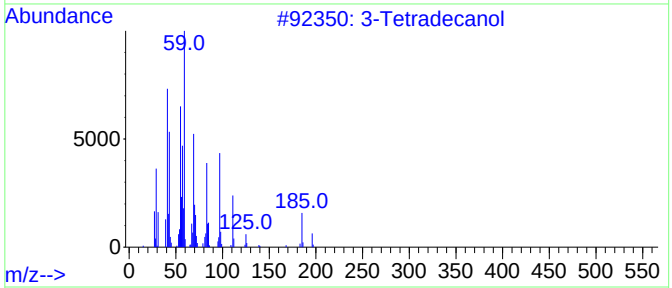
Peak Number 15 unknown16.369 Concentration Rank 9

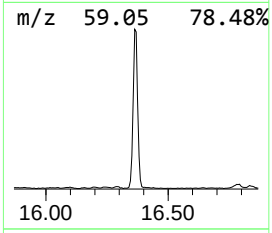
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.369	6.30 ng	1350650	Phenanthrene-d10	17.281

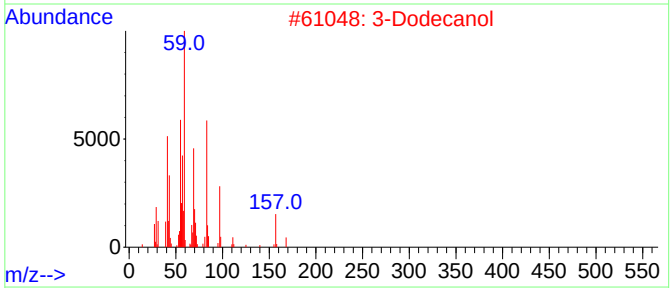
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Tetradecanol	214	C14H30O	001653-32-3	43
2	3-Dodecanol	186	C12H26O	010203-30-2	43
3	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	27
4	Bromoacetic acid, tridecyl ester	320	C15H29BrO2	1000281-85-0	27
5	Hexylene glycol	118	C6H14O2	000107-41-5	22

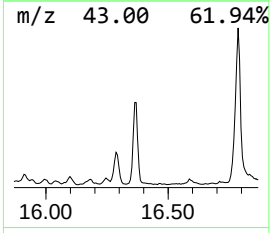


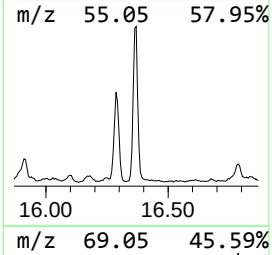


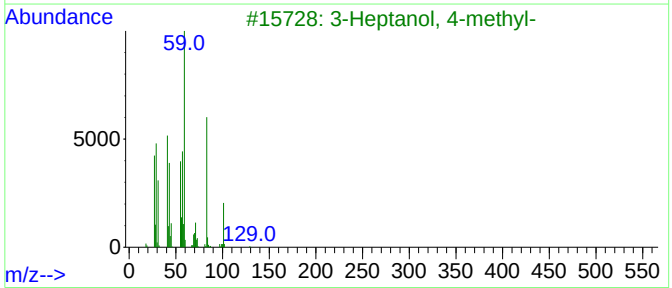


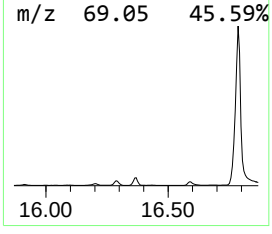












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Acq On : 17 Sep 2021 23:36
Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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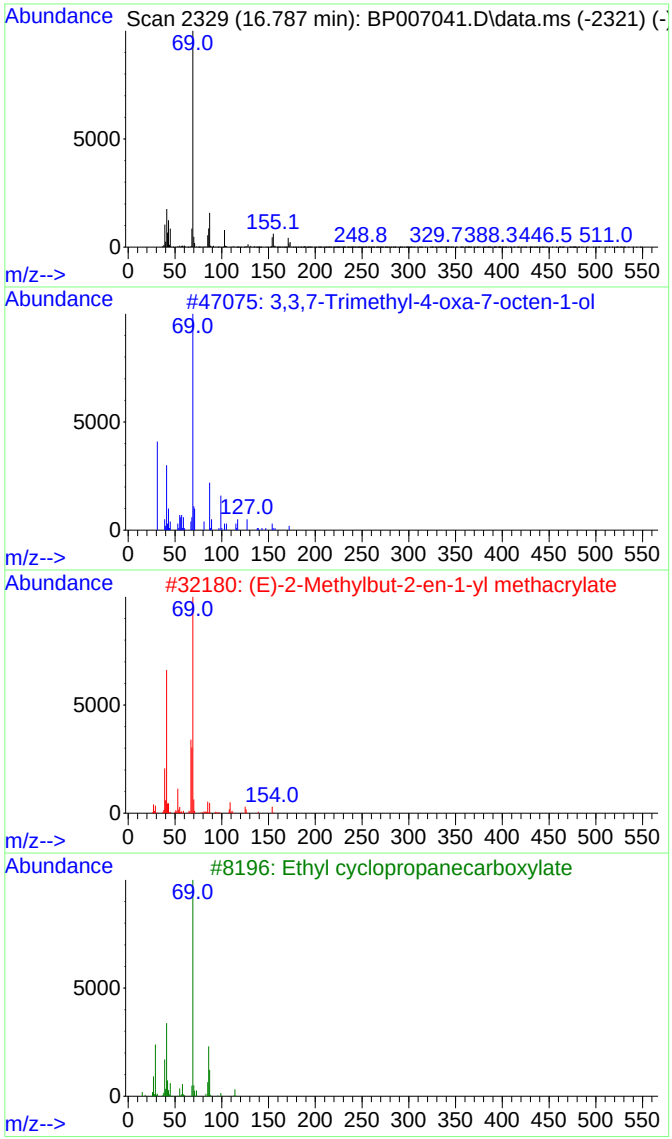
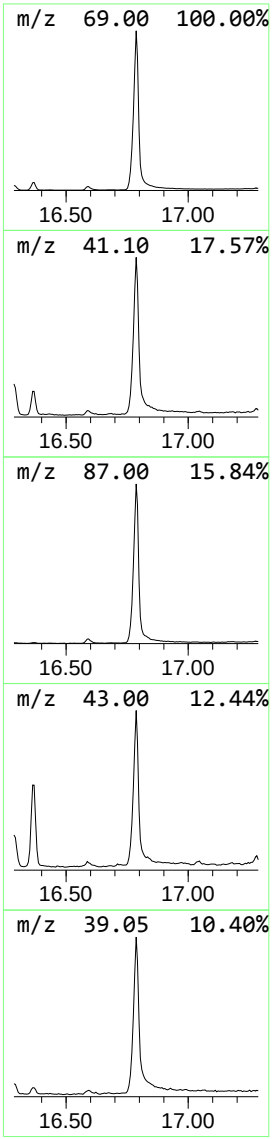
Peak Number 16 unknown16.787 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.787	23.02 ng	4935840	Phenanthrene-d10	17.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3,7-Trimethyl-4-oxa-7-octen-1-ol	172	C10H20O2	069161-47-3	39
2	(E)-2-Methylbut-2-en-1-yl methac...	154	C9H14O2	088142-95-4	38
3	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	36
4	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	33
5	Cyclopropanecarboxylic acid,buty...	142	C8H14O2	054947-39-6	9





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SW-CB-04-(1.5)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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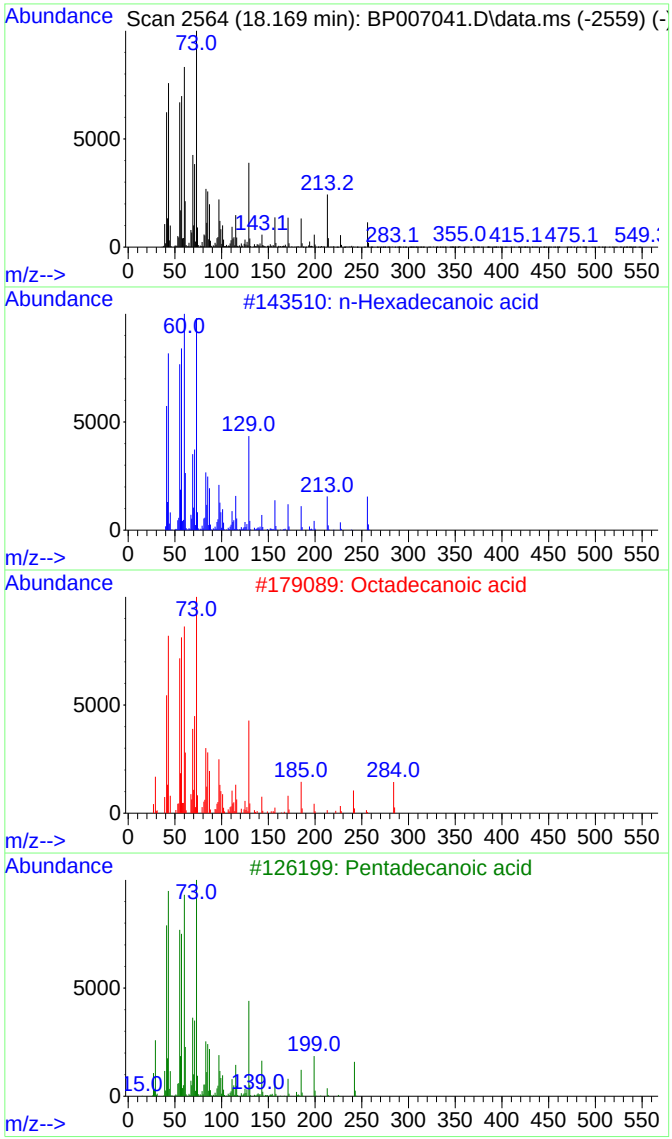
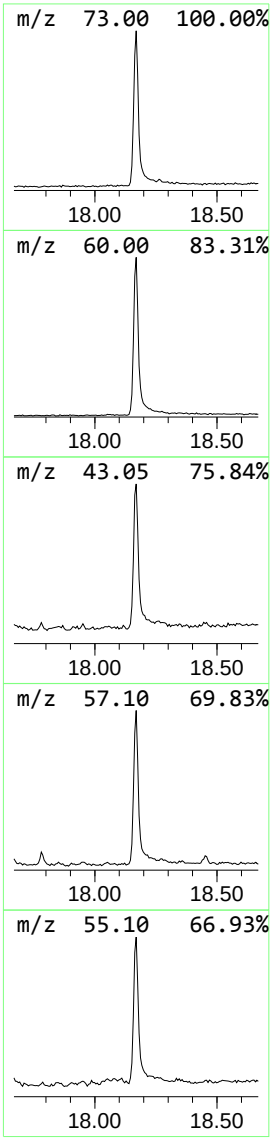
Peak Number 17 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	5.70 ng	1223280	Phenanthrene-d10	17.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	92
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80





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ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-CB-04-(1.5)

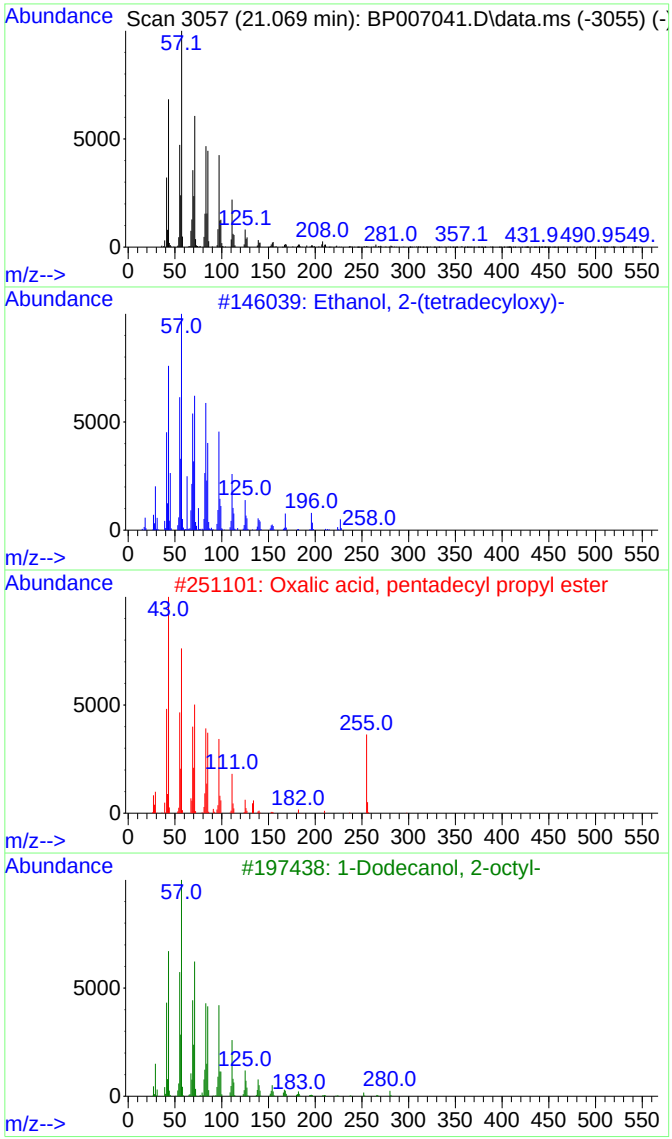
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

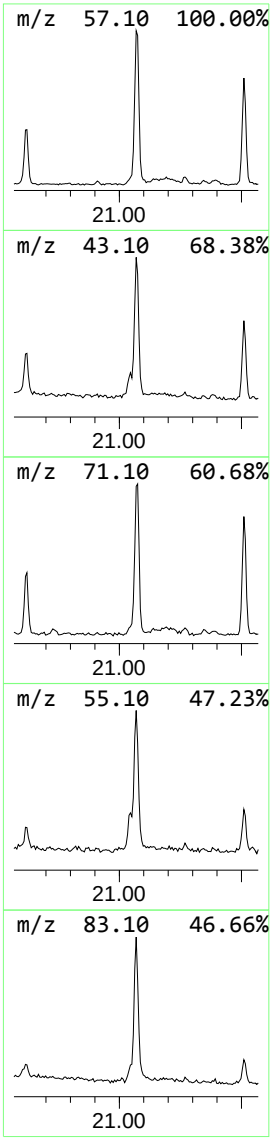
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Ethanol, 2-(tetradecyloxy)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.069	3.21 ng	743456	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	92
2	Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	91
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
4	Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	91
5	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007041.D
Acq On : 17 Sep 2021 23:36
Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

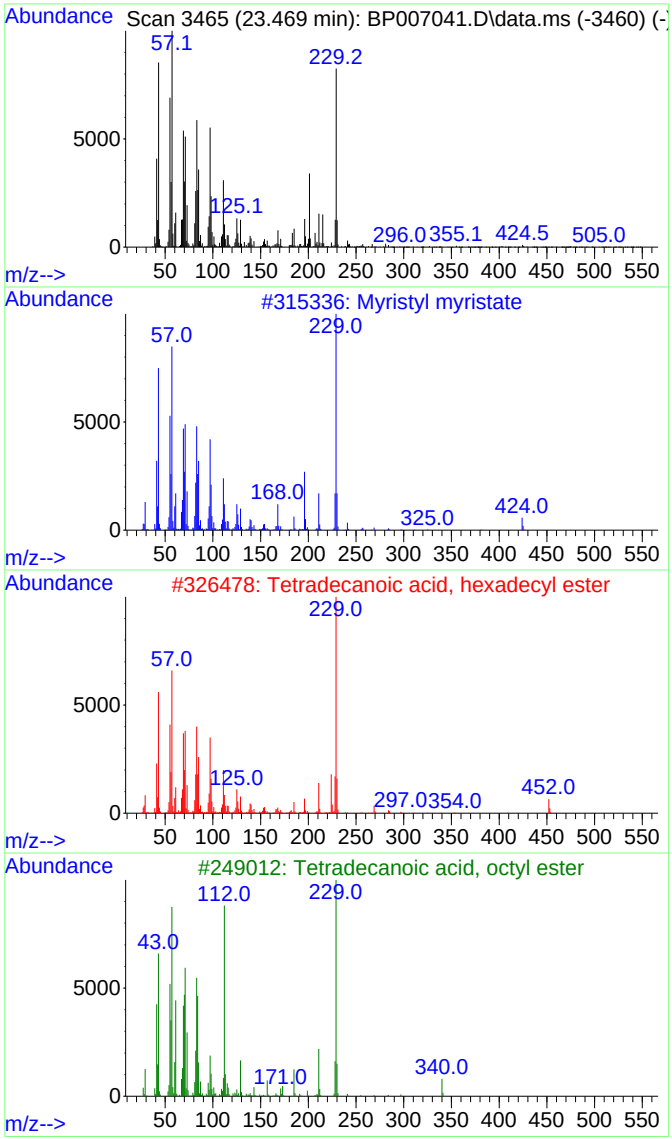
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

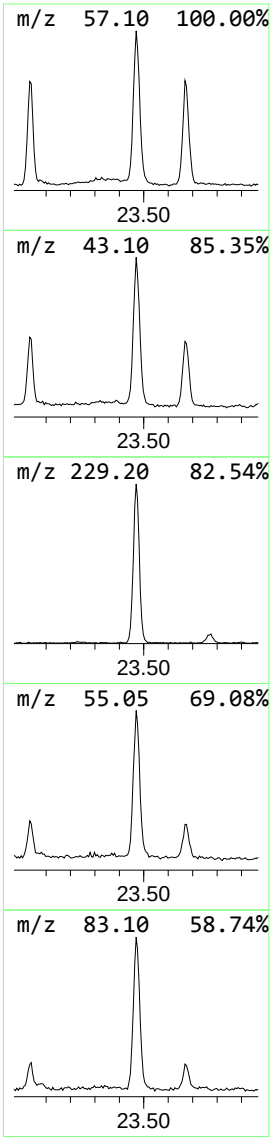
****

Peak Number 19 Myristyl myristate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.469	5.69 ng	1339940	Perylene-d12	23.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristyl myristate	424	C28H56O2	003234-85-3	93
2	Tetradecanoic acid, hexadecyl ester	452	C30H60O2	002599-01-1	90
3	Tetradecanoic acid, octyl ester	340	C22H44O2	016260-26-7	38
4	Hexadecanoic acid, dodecyl ester	424	C28H56O2	042232-29-1	38
5	4-Acetyl-2,3-O-acetone-d-mannosan	244	C11H16O6	014440-55-2	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007041.D
Acq On : 17 Sep 2021 23:36
Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-CB-04-(1.5)

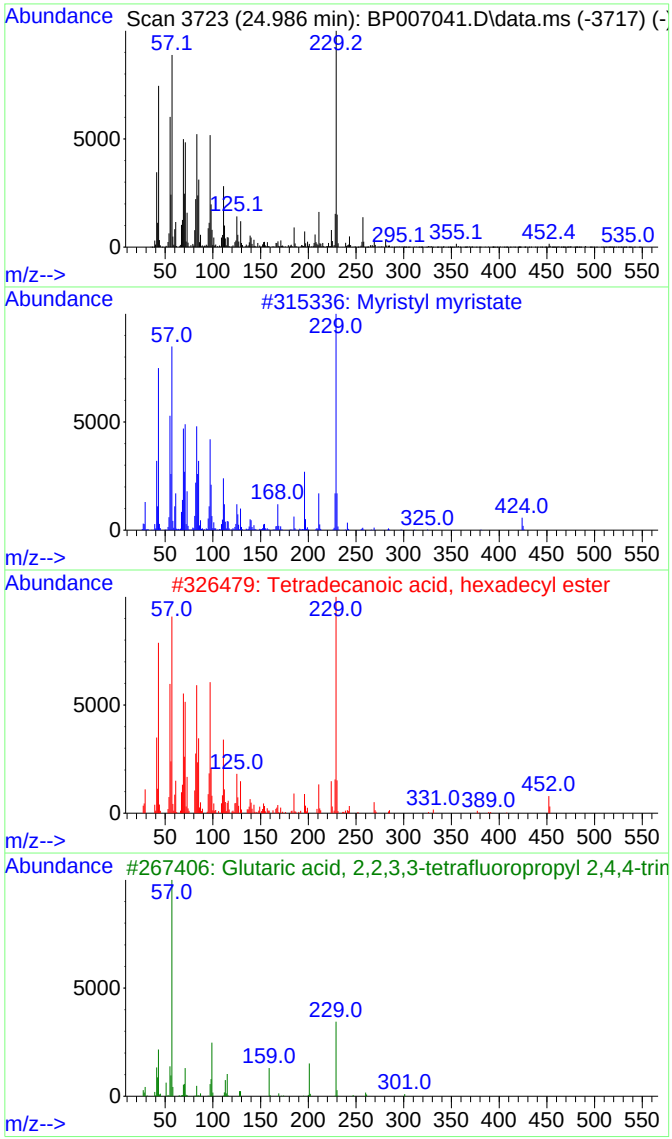
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

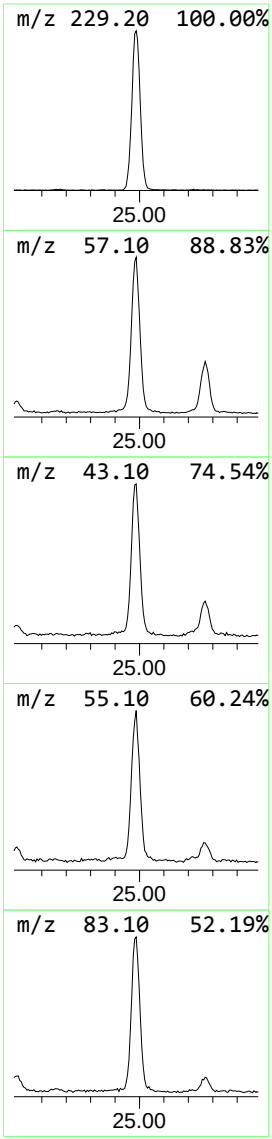
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 Tetradecanoic acid, hexadec... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.986	8.82 ng	2077180	Perylene-d12	23.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristyl myristate	424	C28H56O2	003234-85-3	94
2	Tetradecanoic acid, hexadecyl ester	452	C30H60O2	002599-01-1	91
3	Glutaric acid, 2,2,3,3-tetrafluo...	358	C16H26F4O4	1000391-52-3	37
4	2-(5-Nitro-2-furyl)benzimidazole...	229	C11H7N3O3	003945-78-6	18
5	Benzo(a)acridine	229	C17H11N	000225-11-6	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007041.D
Acq On : 17 Sep 2021 23:36
Operator : CG/JU
Sample : M3791-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SW-CB-04-(1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown4.317	4.317	3.2	ng	325955	1	7.911	2021250	20.0
2-Butyn-1-ol	4.728	2.5	ng	254979	1	7.911	2021250	20.0
Butanoic acid, ...	4.811	11.3	ng	1139600	1	7.911	2021250	20.0
2-Pentanone, 4-...	5.023	3.7	ng	371911	1	7.911	2021250	20.0
Cyclohexanecarb...	9.428	35.0	ng	4887480	2	10.704	2792540	20.0
Phenol, 3-ethyl-	10.152	41.8	ng	5837020	2	10.704	2792540	20.0
endo-Borneol	10.487	3.2	ng	444706	2	10.704	2792540	20.0
Benzeneacetic acid	11.263	10.9	ng	1523210	2	10.704	2792540	20.0
unknown12.416	12.416	29.4	ng	4103900	2	10.704	2792540	20.0
Hydrocinnamic acid	12.587	100.5	ng	14038600	2	10.704	2792540	20.0
2-Butenoic acid...	13.499	2.6	ng	492176	3	14.534	3789600	20.0
Junenol	15.910	2.6	ng	568725	4	17.281	4288890	20.0
2(3H)-Benzothia...	16.204	3.1	ng	674841	4	17.281	4288890	20.0
unknown16.287	16.287	6.1	ng	1310450	4	17.281	4288890	20.0
unknown16.369	16.369	6.3	ng	1350650	4	17.281	4288890	20.0
unknown16.787	16.787	23.0	ng	4935840	4	17.281	4288890	20.0
n-Hexadecanoic ...	18.169	5.7	ng	1223280	4	17.281	4288890	20.0
Ethanol, 2-(tet...	21.069	3.2	ng	743456	5	21.357	4638930	20.0
Myristyl myristate	23.469	5.7	ng	1339940	6	23.769	4708280	20.0
Tetradecanoic a...	24.986	8.8	ng	2077180	6	23.769	4708280	20.0