LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

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-BP110221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007845.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.487	369	374	383	rVB	371139	579516	2.80%	0.248%
2	7.093	639	647	654	rBV	179807	389282	1.88%	0.166%
3	7.516	713	719	725	rVB	282572	443024	2.14%	0.189%
4	7.910	780	786	792	rBV	769088	1160190	5.61%	0.496%
5	8.181	823	832	841	rBV	1193733	2145134	10.37%	0.917%
6	8.263	841	846	855	rVB	147521	244278	1.18%	0.104%
7	9.005	966	972	977	rBV	454215	807667	3.90%	0.345%
8	9.069	978	983	986	rBV	380431	584164	2.82%	0.250%
9	9.175	994	1001	1007	rVB2	696388	1266763	6.12%	0.542%
10	9.252	1007	1014	1018	rBV3	106741	240052	1.16%	0.103%
11	9.940	1126	1131	1139	rBV6	135294	375303	1.81%	0.160%
12	10.016	1139	1144	1150	rVV3	186194	309541	1.50%	0.132%
13	10.281	1183	1189	1198	rVB	222790	426644	2.06%	0.182%
14	10.416	1208	1212	1217	rVB	394650	631476	3.05%	0.270%
15	10.716	1257	1263	1269	rBV	1014733	1724622	8.33%	0.737%
16	11.046	1312	1319	1324	rBV6	152207	434365	2.10%	0.186%
17	11.110	1325	1330	1339	rVB3	287362	726227	3.51%	0.311%
18	11.210	1342	1347	1352	rVV	276207	463655	2.24%	0.198%
19	11.299	1359	1362	1369	rVB4	250729	432739	2.09%	0.185%
20	11.369	1370	1374	1380	rBV3	161159	317804	1.54%	0.136%
21	11.646	1415	1421	1428	rBV4	411239	1053693	5.09%	0.451%
22	11.728	1430	1435	1439	rBV2	277134	526447	2.54%	0.225%
23	11.787	1442	1445	1449	rVV	291381	412230	1.99%	0.176%
24	11.881	1458	1461	1464	rBV2	219720	303604	1.47%	0.130%
25	11.969	1471	1476	1481	rBV	1923161	3034627	14.67%	1.298%
26	12.010	1481	1483	1488	rVB3	235463	385824	1.86%	0.165%
27	12.110	1494	1500	1503	rBV4	640457	1385396	6.70%	0.592%
28	12.263	1523	1526	1530	rVB3	586967	814571	3.94%	0.348%
29	12.328	1532	1537	1540	rBV3	818527	1584429	7.66%	0.678%
30	12.516	1562	1569	1577	rBV4	650261	1893575	9.15%	0.810%
31	12.881	1628	1631	1636	rVB3	1219362	1975041	9.55%	0.845%
32	12.998	1646	1651	1655	rBV2	1998858	3590611	17.35%	1.535%
33	13.175	1679	1681	1685	rVB	1331988	1646692	7.96%	0.704%
34	13.522	1737	1740	1744	rBV2	860532	1341442	6.48%	0.574%
35	13.610	1750	1755	1756	rBV2	2000133	3028588	14.64%	1.295%
36	13.722	1770	1774	1778	rBV3	1295556	1952244	9.43%	0.835%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

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-BP110221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.034	1823	1827	1833	rBV3	1458459	2793321	13.50%	1.194%
38	14.334	1875	1878	1882	rBV	1229894	1507169	7.28%	0.645%
39	14.557	1912	1916	1921	rVB2	1480738	2194123	10.60%	0.938%
40	14.616	1922	1926	1931	rVB2	857750	1458928	7.05%	0.624%
41	14.740	1944	1947	1951	rVB	1397199	1661098	8.03%	0.710%
42	14.981	1984	1988	1992	rBV5	1096759	1836920	8.88%	0.786%
43	15.034	1994	1997	1999	rBV	743910	879514	4.25%	0.376%
44	15.528	2075	2081	2085	rVB2	3311439	6635123	32.07%	2.837%
45	15.610	2092	2095	2107	rVB3	3389483	6849170	33.10%	2.929%
46	15.845	2130	2135	2143	rBV2	4240353	11011529	53.22%	4.709%
47	15.916	2143	2147	2151	rBV3	3789886	5580905	26.97%	2.387%
48	15.992	2156	2160	2164	rBV	4793953	7257535	35.07%	3.104%
49	16.034	2164	2167	2171	rVB	3064795	4117730	19.90%	1.761%
50	16.110	2177	2180	2183	rVB	3345205	4009337	19.38%	1.714%
51	16.210	2192	2197	2201	rBV	7839209	10414728	50.33%	4.454%
52	16.375	2221	2225	2228	rVB	5397739	6568571	31.74%	2.809%
53	16.486	2239	2244	2252	rVB	7964756	13767796	66.54%	5.887%
54	16.563	2252	2257	2260	rBV2	3662416	6202232	29.97%	2.652%
55	16.981	2324	2328	2334	rBV2	3341583	5263930	25.44%	2.251%
56	17.086	2341	2346	2352	rBV	5047745	11499711	55.58%	4.918%
57	17.251	2366	2374	2380	rBV2	6385254	19893267	96.14%	8.507%
58	17.416	2398	2402	2407	rBV2	4263983	7062548	34.13%	3.020%
59	17.481	2409	2413	2414	rBV3	3008845	4193084	20.26%	1.793%
60	17.645	2438	2441	2448	rVB3	2664229	5429470	26.24%	2.322%
61	17.722	2450	2454	2459	rBV2	6307806	10911596	52.73%	4.666%
62	17.869	2473	2479	2486	rBV2	8345107	20691692	100.00%	8.848%
63	17.992	2497	2500	2502	rBV	3844284	5306025	25.64%	2.269%
64	18.022	2502	2505	2508	rVB	4852006	6607938	31.94%	2.826%
65	18.104	2516	2519	2522	rBV	3346116	3613537	17.46%	1.545%

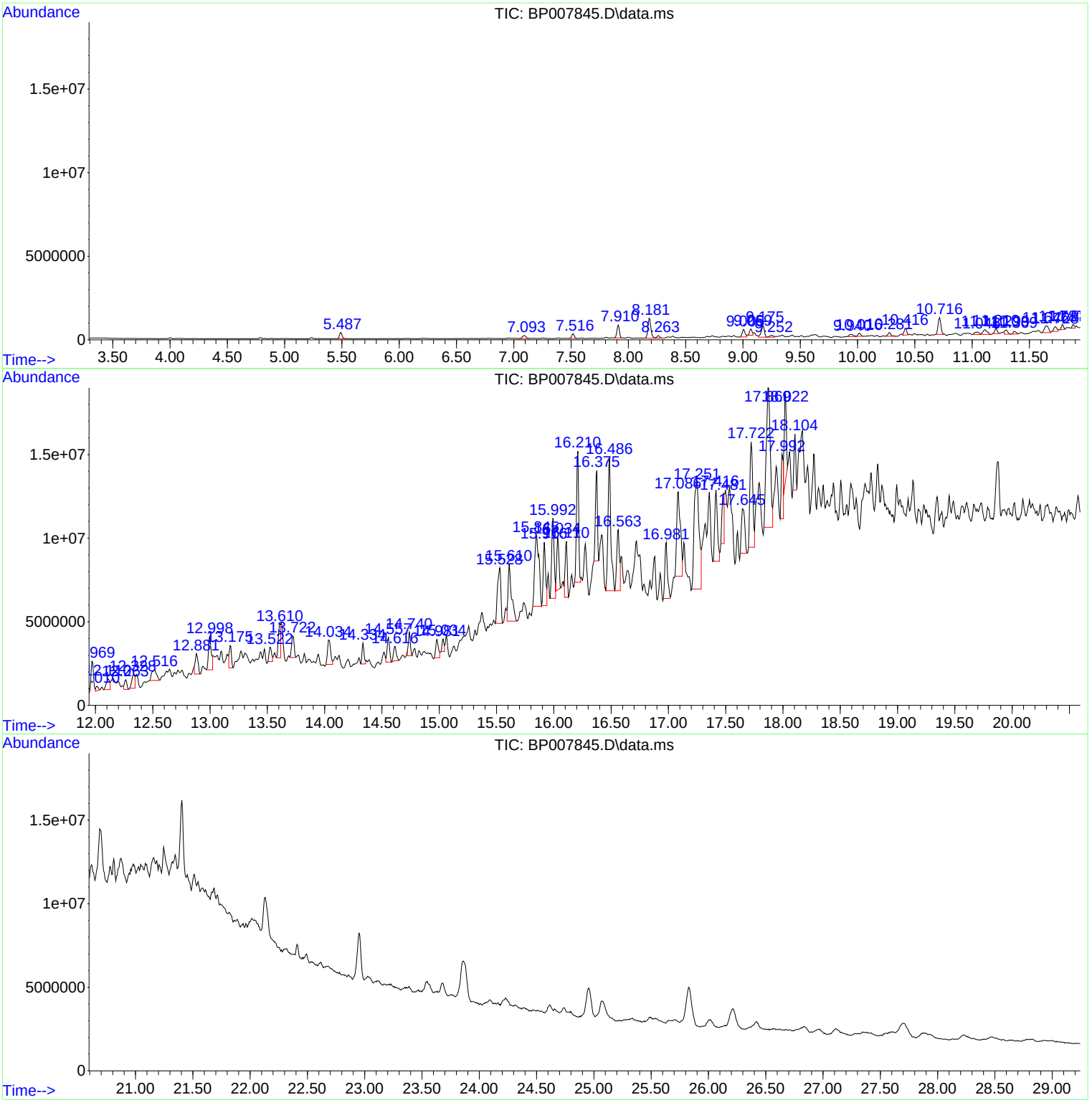
Sum of corrected areas: 233849987

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.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\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

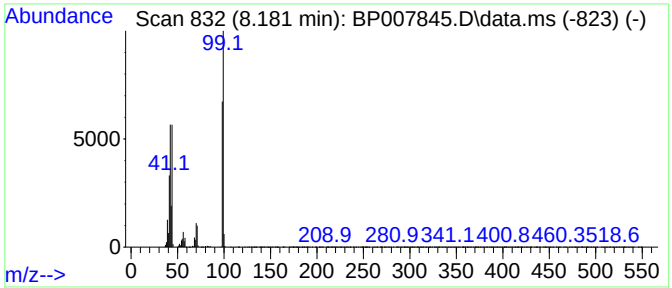
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

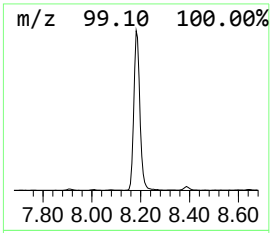
****

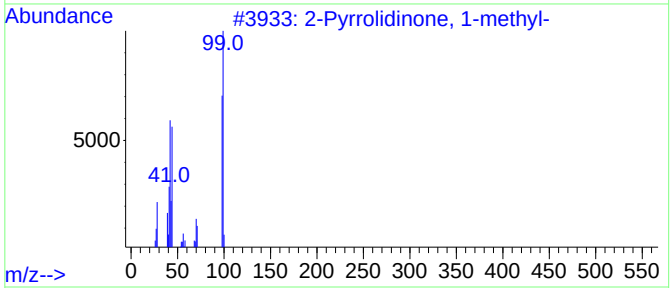
Peak Number 1 2-Pyrrolidinone, 1-methyl- Concentration Rank 5

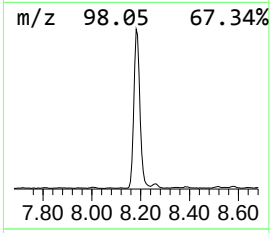
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.181	36.98 ng	2145130	1,4-Dichlorobenzene-d4	7.910

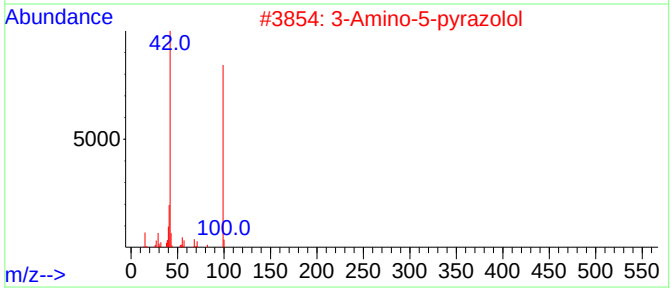
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	95
2	3-Amino-5-pyrazolol	99	C3H5N3O	006126-22-3	43
3	5-Amino-3-methyl-1,2,4-oxadiazole	99	C3H5N3O	003663-39-6	38
4	4-Piperidone	99	C5H9NO	041661-47-6	37
5	2-Piperidinone	99	C5H9NO	000675-20-7	37

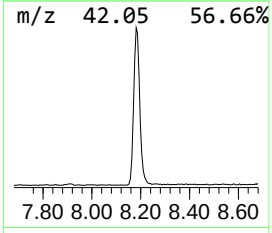


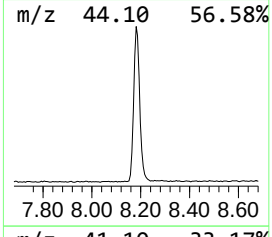


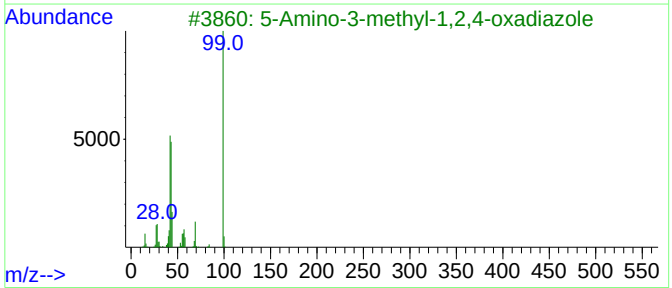


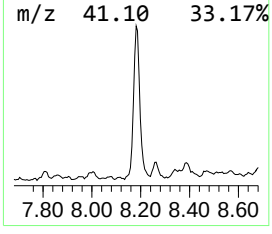












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

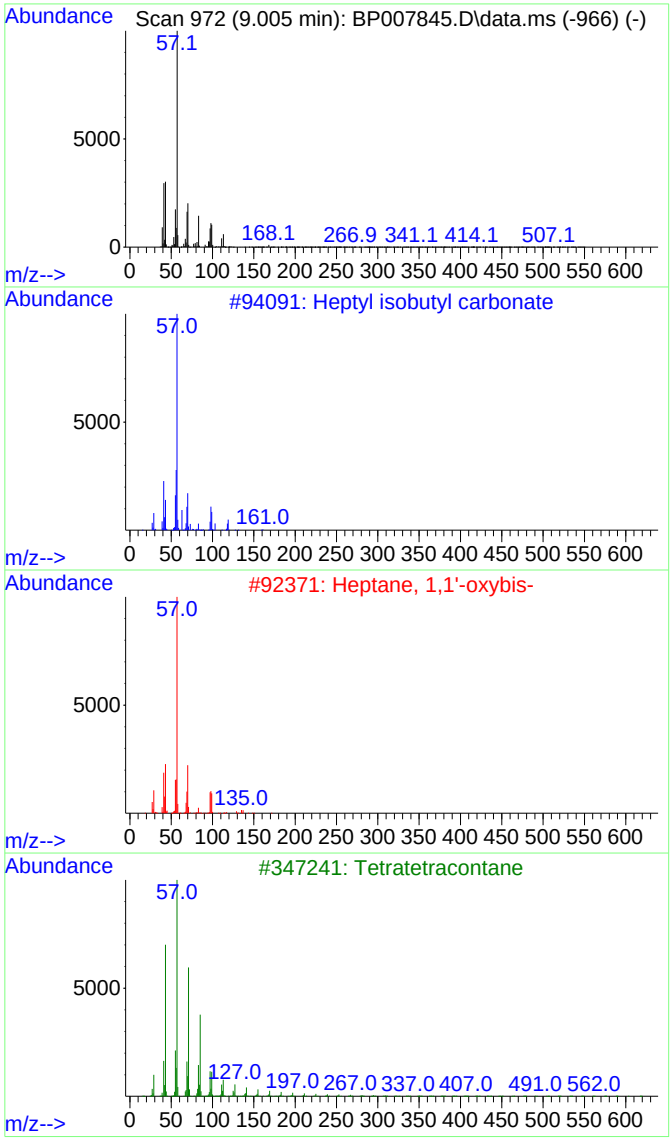
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

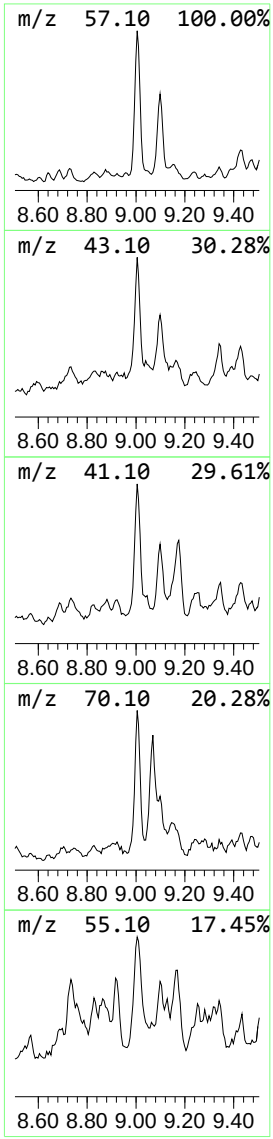
****

Peak Number 2 Heptyl isobutyl carbonate Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.005	13.92 ng	807667	1,4-Dichlorobenzene-d4	7.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	64
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
3	Tetratetracontane	619	C44H90	007098-22-8	45
4	Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	40
5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

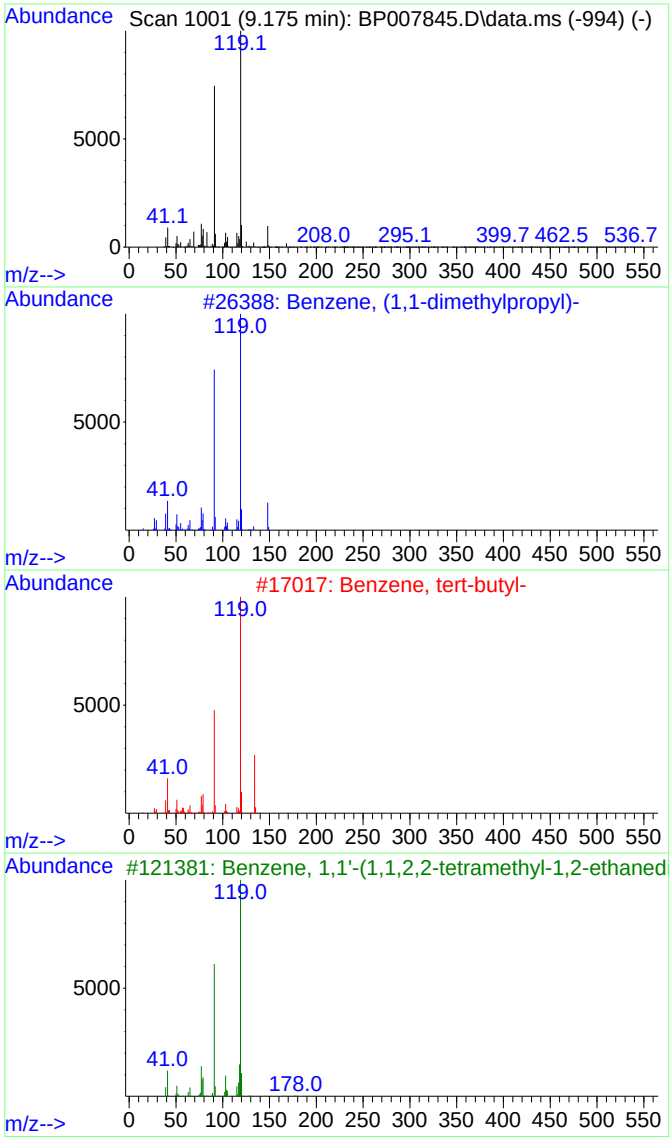
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

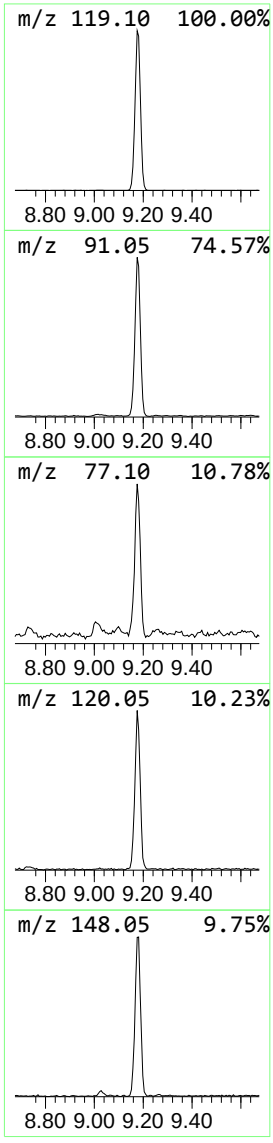
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, (1,1-dimethylpropyl)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.175	21.84 ng	1266760	1,4-Dichlorobenzene-d4	7.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	94
2	Benzene, tert-butyl-	134	C10H14	000098-06-6	83
3	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	72
4	Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	64
5	4'-Methylpropiophenone	148	C10H12O	005337-93-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

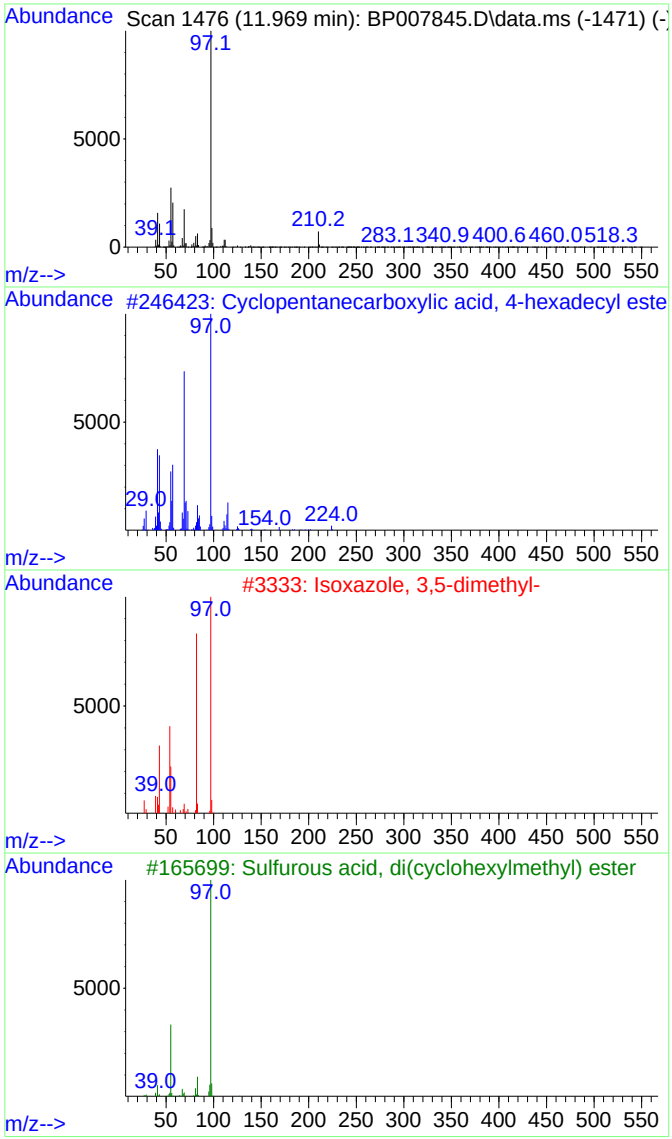
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

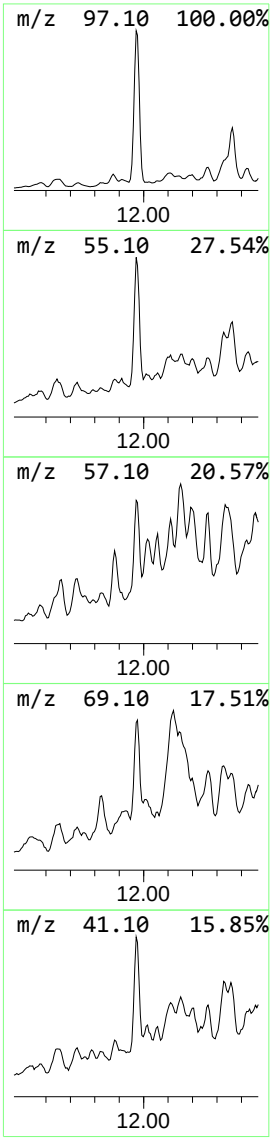
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentanecarboxylic acid... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	35.19 ng	3034630	Naphthalene-d8	10.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	64
2	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	64
3	Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1010309-22-7	59
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	56
5	Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

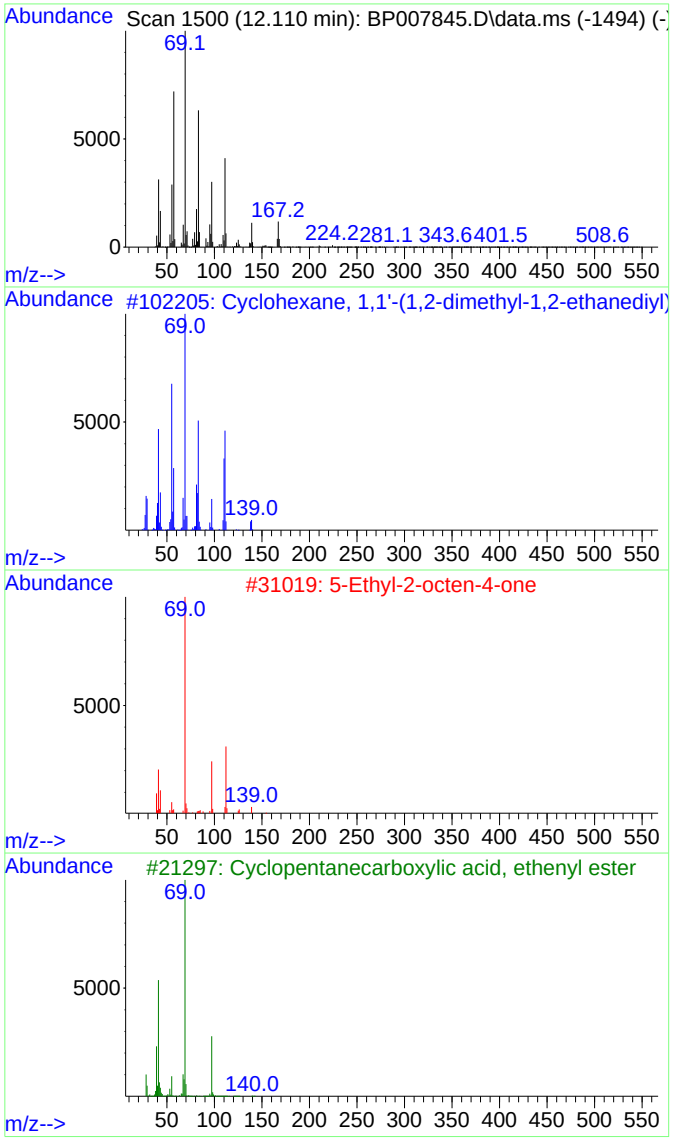
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

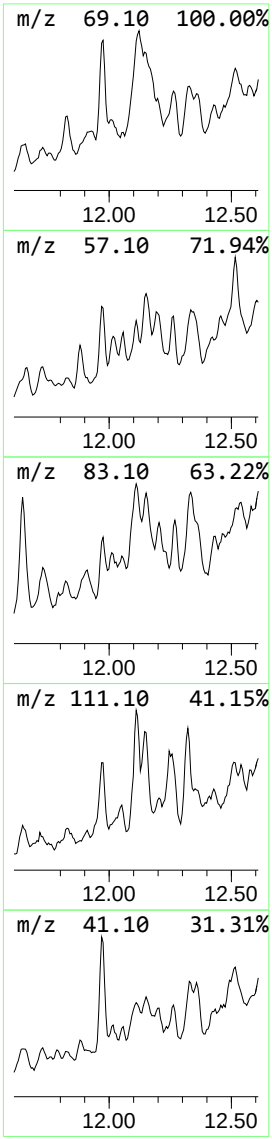
****

Peak Number 5 Cyclohexane, 1,1'-(1,2-dime... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.110	16.07 ng	1385400	Naphthalene-d8	10.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1'-(1,2-dimethyl-...	222	C16H30	074663-71-1	50
2	5-Ethyl-2-octen-4-one	154	C10H18O	1000374-14-3	38
3	Cyclopentanecarboxylic acid, eth...	140	C8H12O2	016523-06-1	35
4	4-Nonene, 2,3,3-trimethyl-, (Z)-	168	C12H24	063830-68-2	35
5	2-Propenoic acid, 2-methyl-, 3-m...	166	C10H14O2	076003-37-7	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

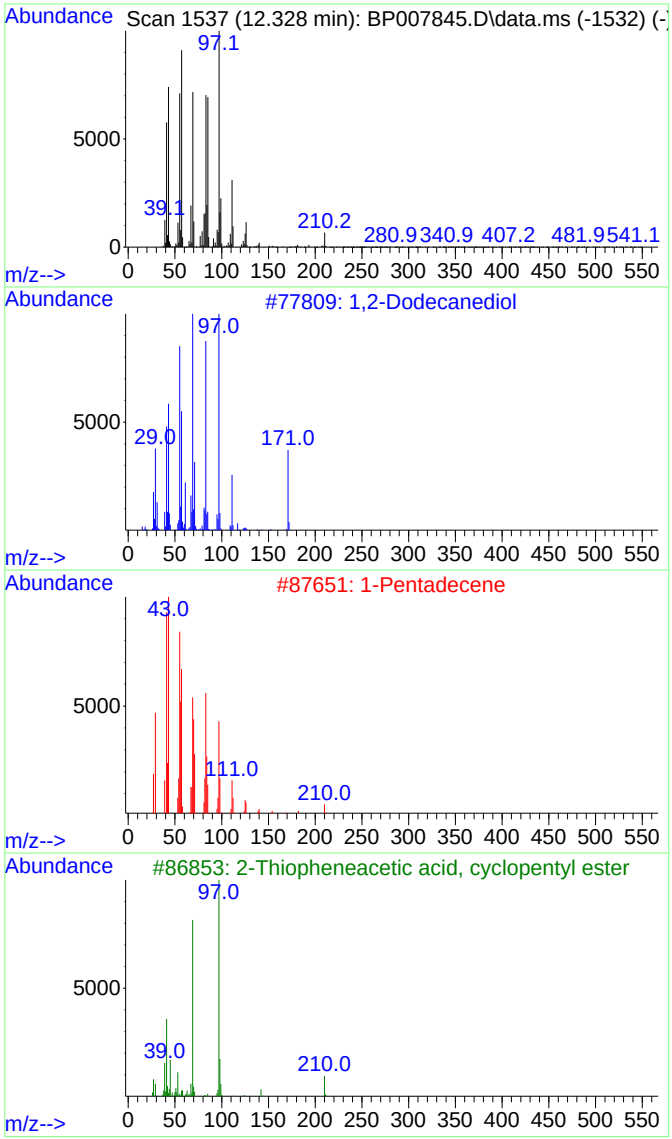
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

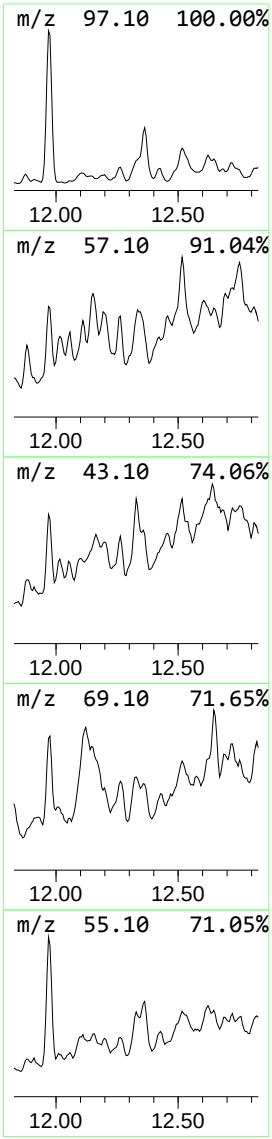
****

Peak Number 6 unknown12.328 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.328	18.37 ng	1584430	Naphthalene-d8	10.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Dodecanediol	202	C12H26O2	001119-87-5	43
2	1-Pentadecene	210	C15H30	013360-61-7	38
3	2-Thiopheneacetic acid, cyclopen...	210	C11H14O2S	1000278-95-8	30
4	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054824-04-3	27
5	2-Thiopheneacetic acid, 2-ethylc...	252	C14H20O2S	1000278-96-1	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

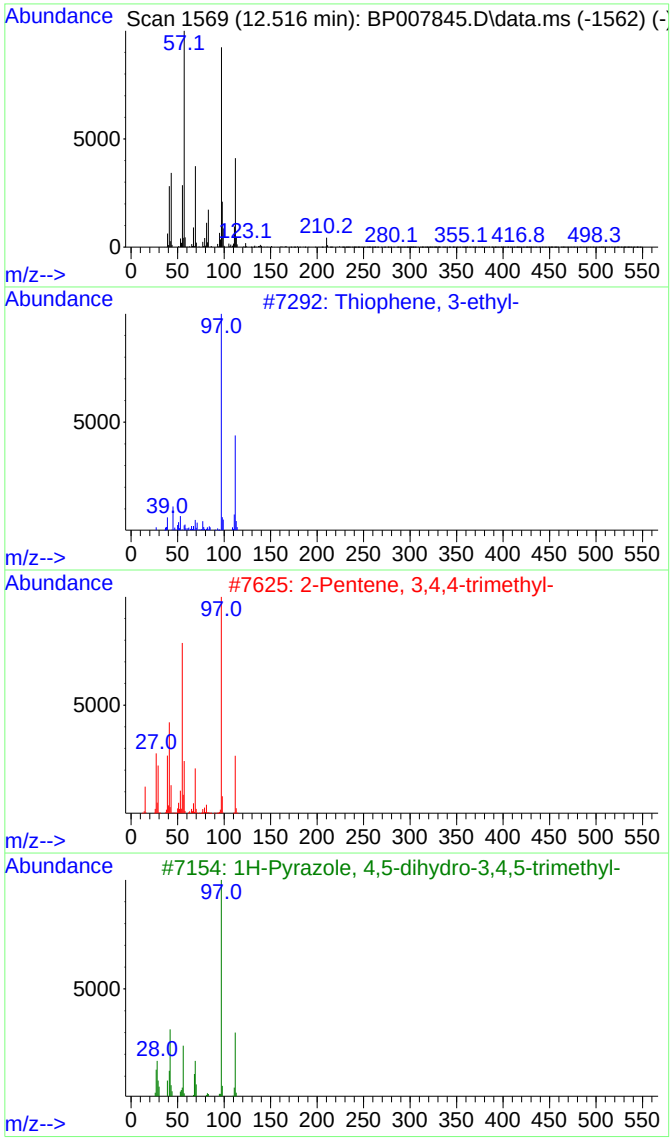
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

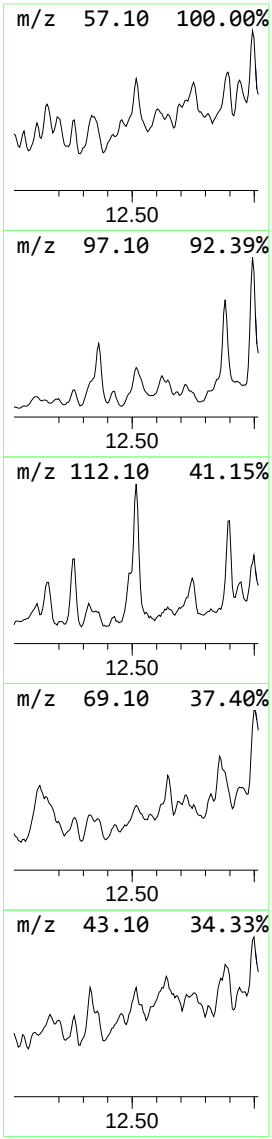
****

Peak Number 7 Thiophene, 3-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.516	21.96 ng	1893580	Naphthalene-d8	10.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 3-ethyl-	112	C6H8S	001795-01-3	59
2	2-Pentene, 3,4,4-trimethyl-	112	C8H16	000598-96-9	59
3	1H-Pyrazole, 4,5-dihydro-3,4,5-t...	112	C6H12N2	022591-95-3	59
4	Thiophene, 2-ethyl-	112	C6H8S	000872-55-9	53
5	1,1-Dimethyl-1-silacyclo-3-pentene	112	C6H12Si	016054-12-9	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

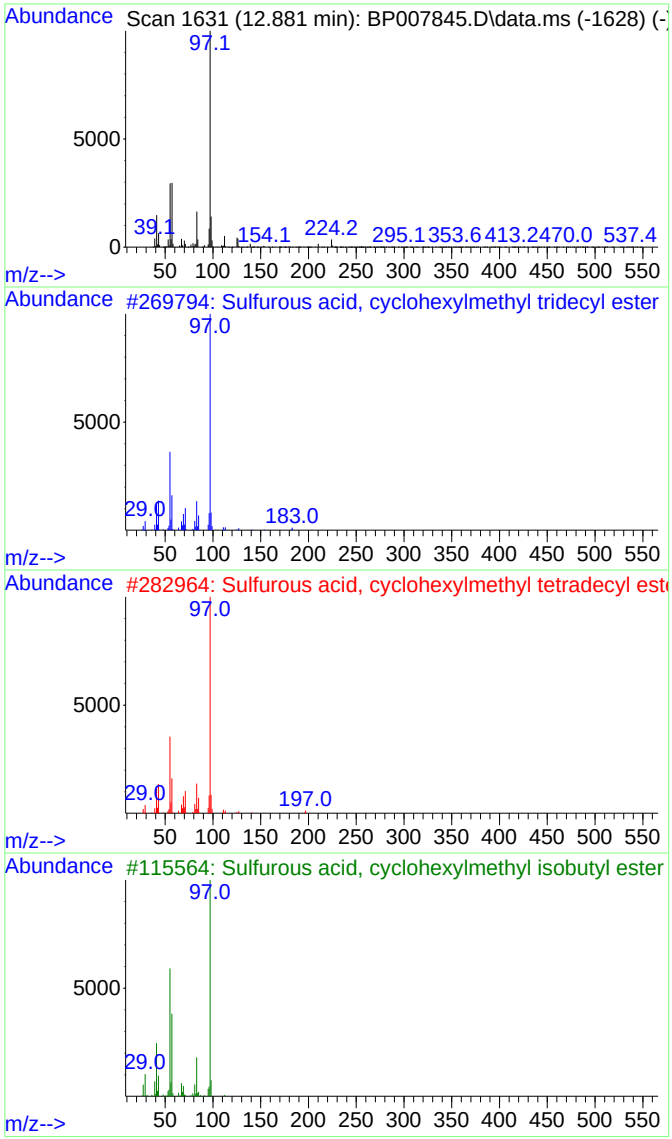
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

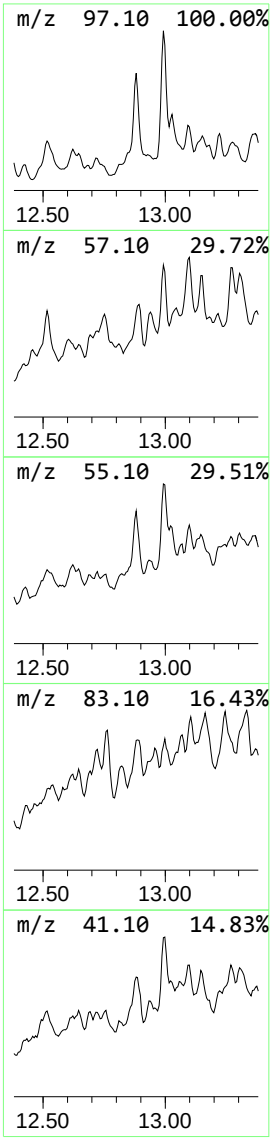
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Sulfurous acid, cyclohexylm... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.881	18.00 ng	1975040	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	360	C20H40O3S	1000309-22-1	64
2	Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	64
3	Sulfurous acid, cyclohexylmethyl...	234	C11H22O3S	1000309-21-3	59
4	Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	53
5	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1010309-21-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

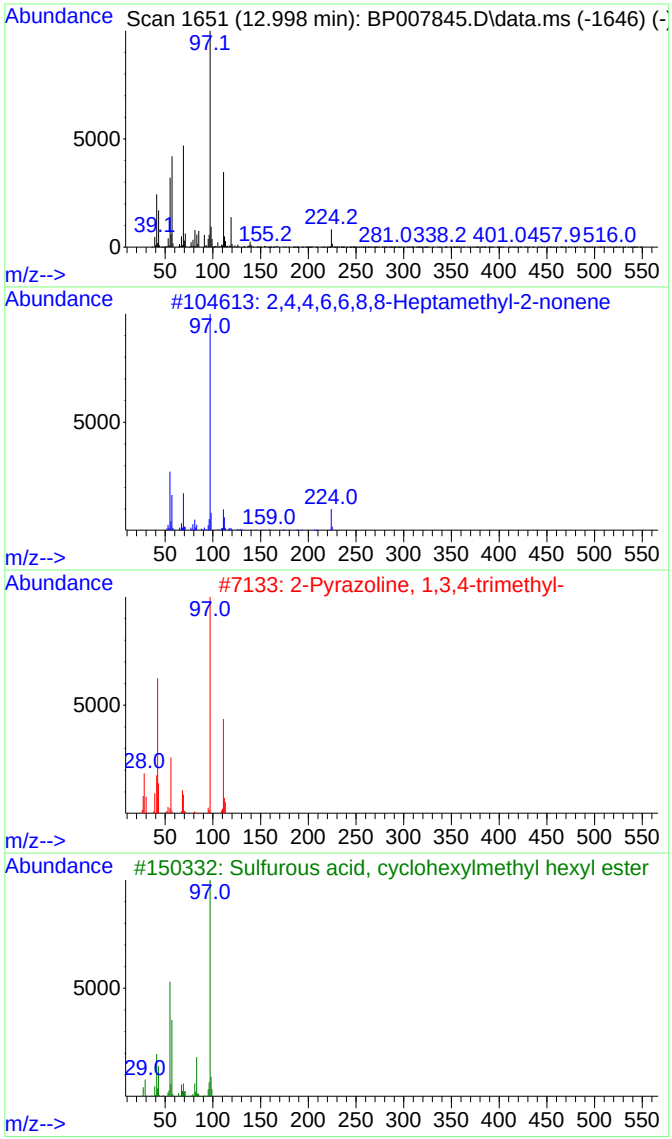
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

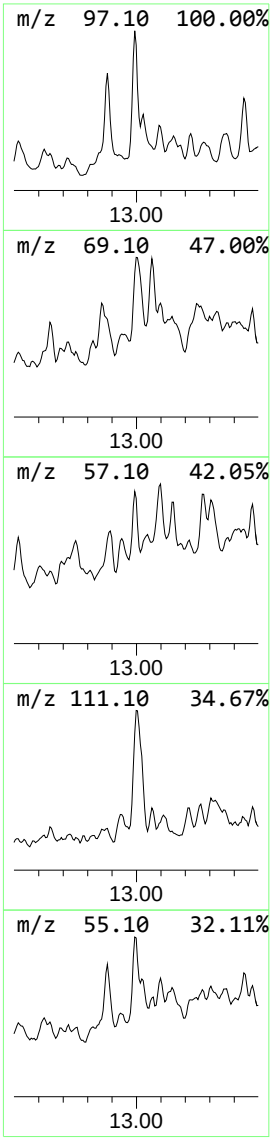
****

Peak Number 9 2,4,4,6,6,8,8-Heptamethyl-2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.998	32.73 ng	3590610	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-2-nonene	224	C16H32	039761-73-4	76
2	2-Pyrazoline, 1,3,4-trimethyl-	112	C6H12N2	014044-41-8	59
3	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1010309-21-6	53
4	2H-Pyran-2-one, 5,6-dihydro-6-pe...	168	C10H16O2	054814-64-1	53
5	Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

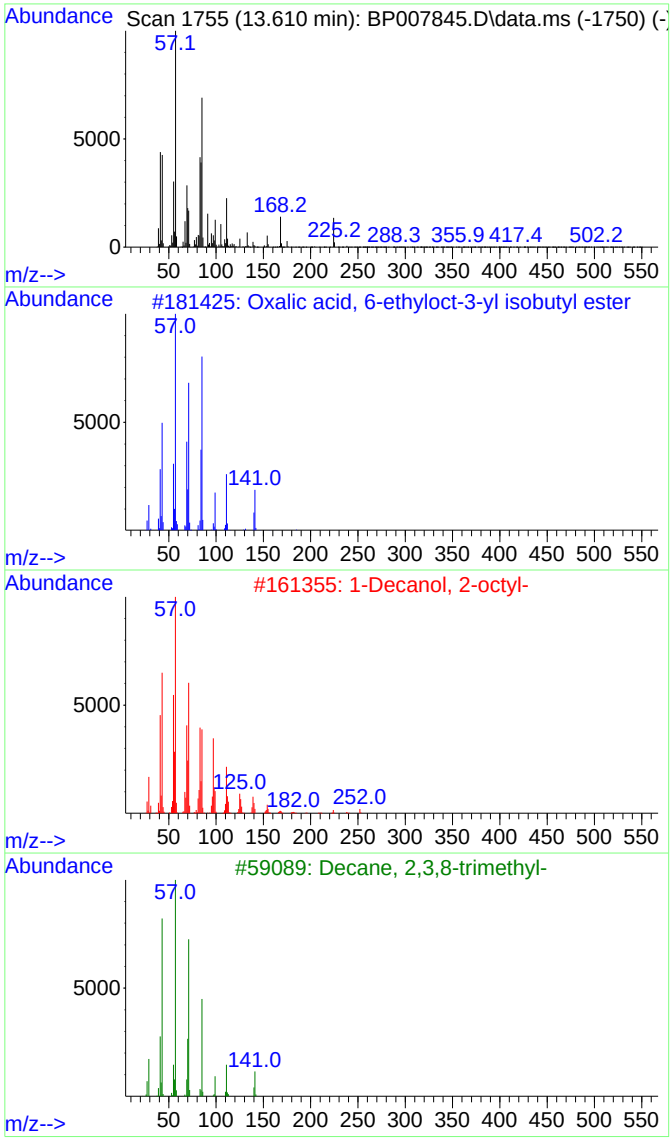
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

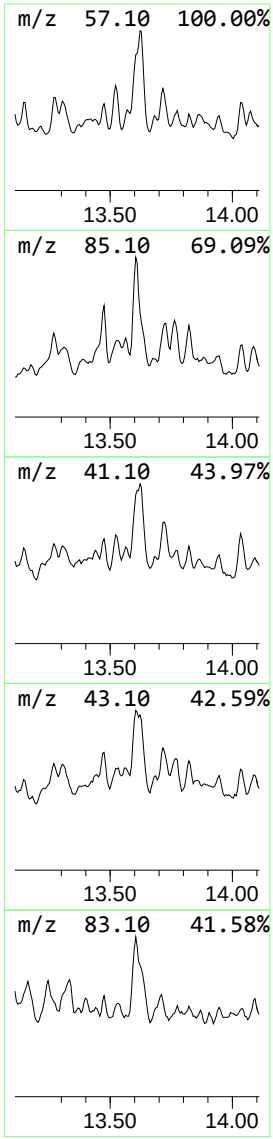
****

Peak Number 10 unknown13.610 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.610	27.61 ng	3028590	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, 6-ethyloct-3-yl iso...	286	C16H30O4	1010309-34-1	43
2	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	38
3	Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	35
4	Oxalic acid, butyl 6-ethyloct-3-...	286	C16H30O4	1000309-34-2	32
5	Oxalic acid, heptyl isohexyl ester	272	C15H28O4	1000309-33-1	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

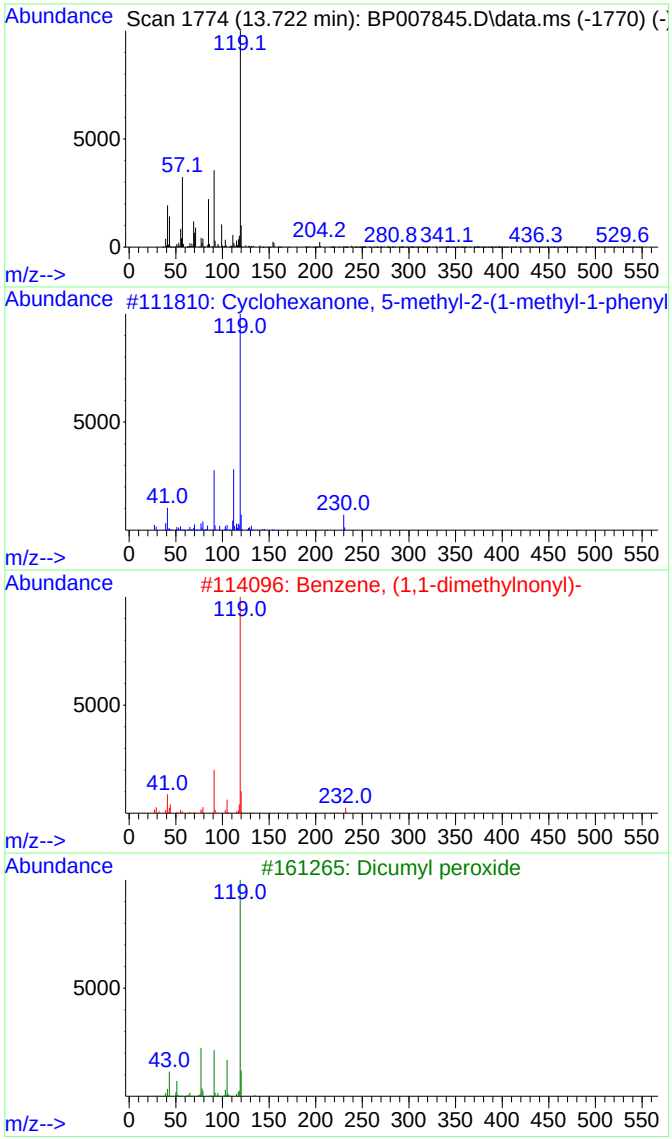
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

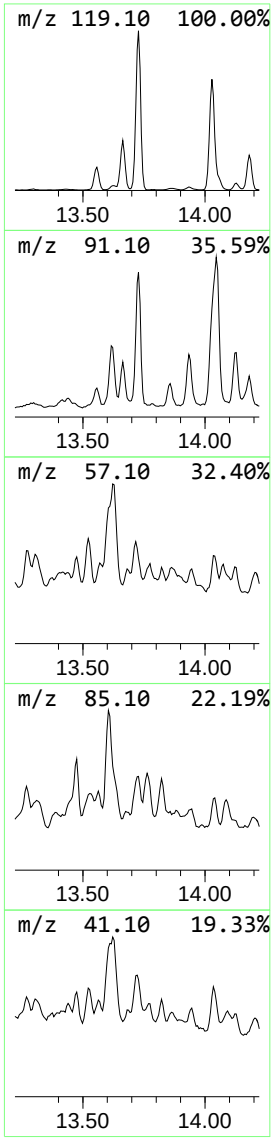
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Cyclohexanone, 5-methyl-2-(... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.722	17.80 ng	1952240	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 5-methyl-2-(1-met...	230	C16H22O	097275-48-4	50
2	Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	50
3	Dicumyl peroxide	270	C18H22O2	000080-43-3	50
4	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	50
5	Cumene hydroperoxide, TMS deriva...	224	C12H20O2Si	018057-16-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

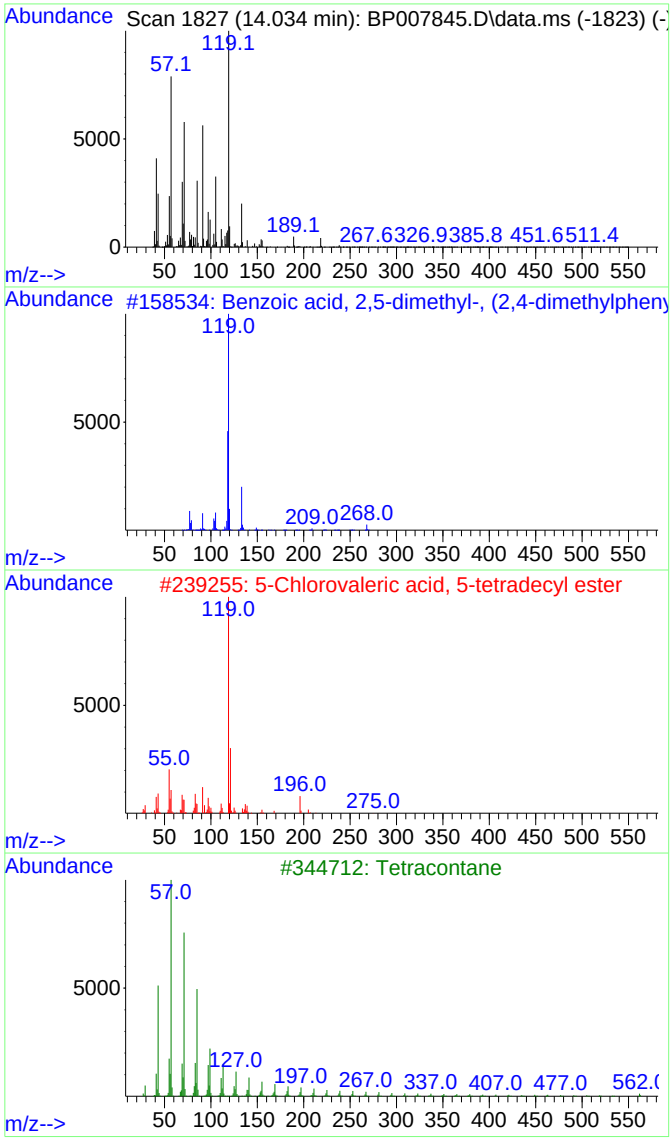
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

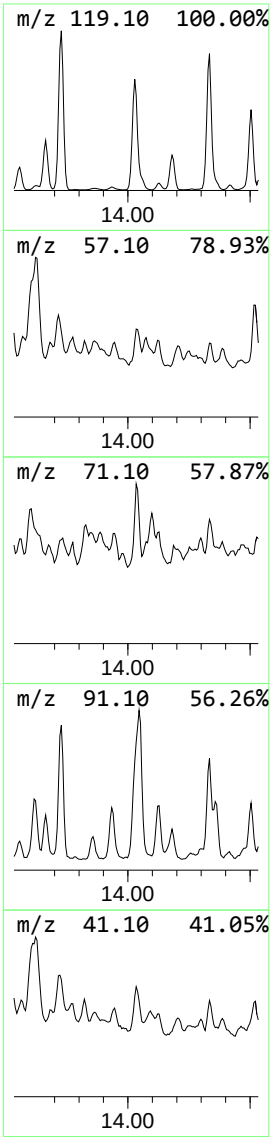
****

Peak Number 12 Benzoic acid, 2,5-dimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.034	25.46 ng	2793320	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,5-dimethyl-, (2,...	268	C18H20O2	055000-48-1	50
2	5-Chlorovaleric acid, 5-tetradec...	332	C19H37ClO2	1000299-91-9	43
3	Tetracontane	563	C40H82	004181-95-7	27
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	27
5	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

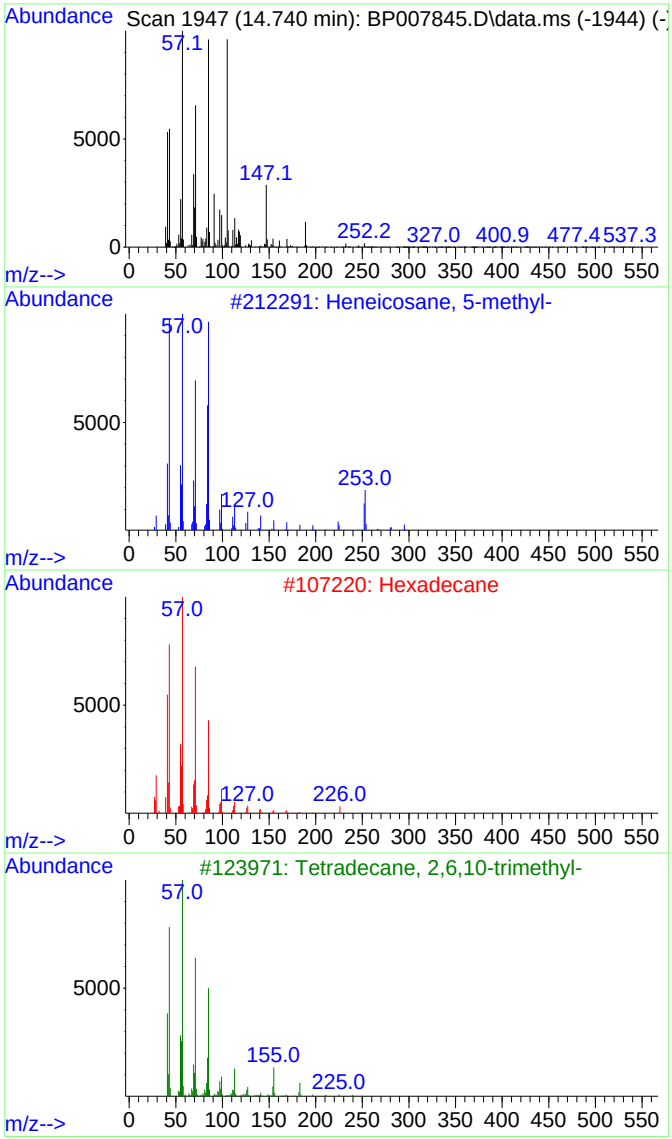
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

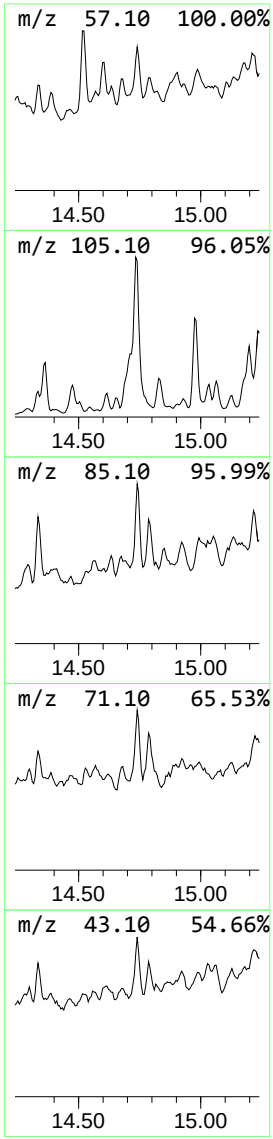
****

Peak Number 13 Heneicosane, 5-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.740	15.14 ng	1661100	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 5-methyl-	310	C22H46	025117-37-7	59
2	Hexadecane	226	C16H34	000544-76-3	43
3	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	43
4	Heptane, 2,4,6-trimethyl-	142	C10H22	002613-61-8	43
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

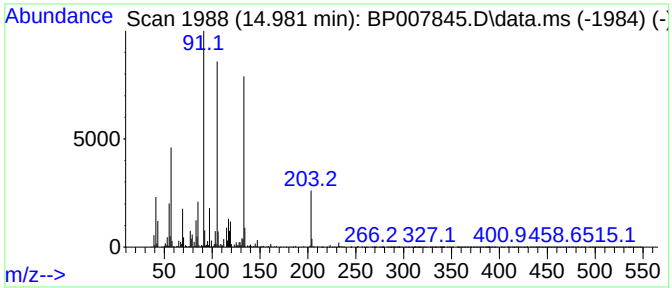
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

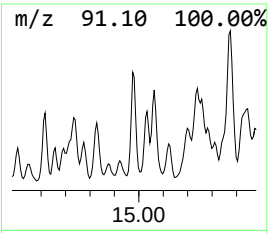
****

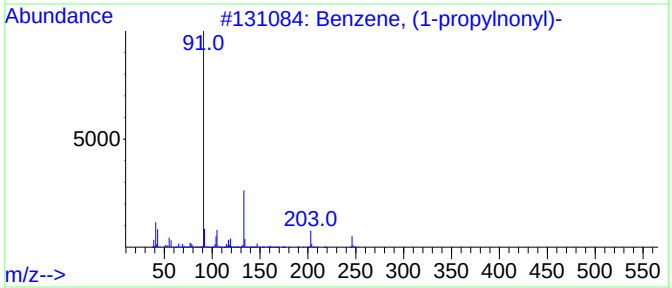
Peak Number 14 unknown14.981 Concentration Rank 17

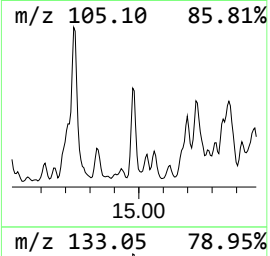
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.981	16.74 ng	1836920	Acenaphthene-d10	14.557

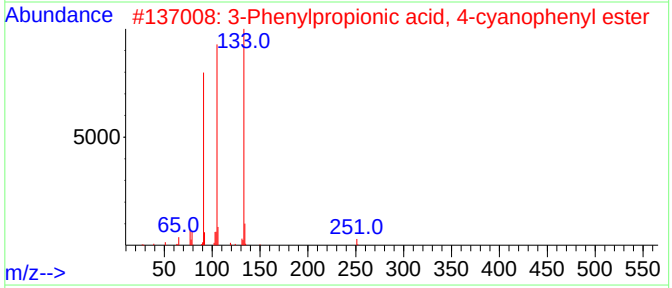
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-propylnonyl)-	246	C18H30	002719-64-4	47
2	3-Phenylpropionic acid, 4-cyanop...	251	C16H13NO2	1000307-78-4	46
3	Oxalamide, N-(2-hydroxyethyl)-N'...	278	C14H18N2O4	1000304-26-2	46
4	3-Phenylpropionic acid, 2,3-dich...	294	C15H12Cl2O2	1000331-06-3	43
5	3-Benzofuranmethanol, 2,3-dihydr...	164	C10H12O2	039891-58-2	43

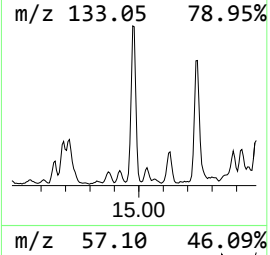


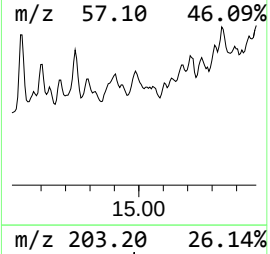


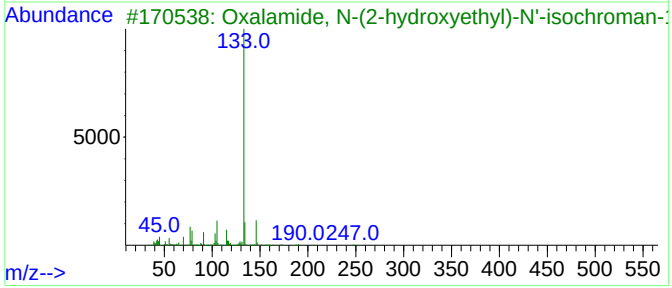


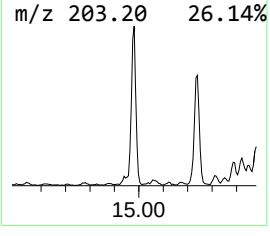












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

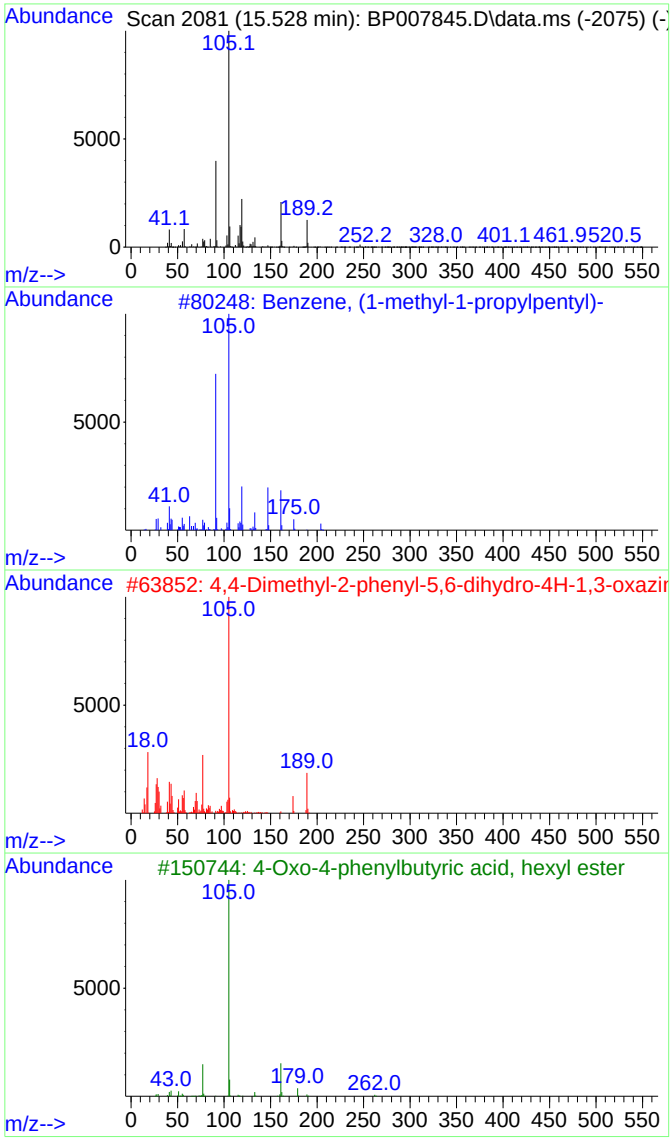
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

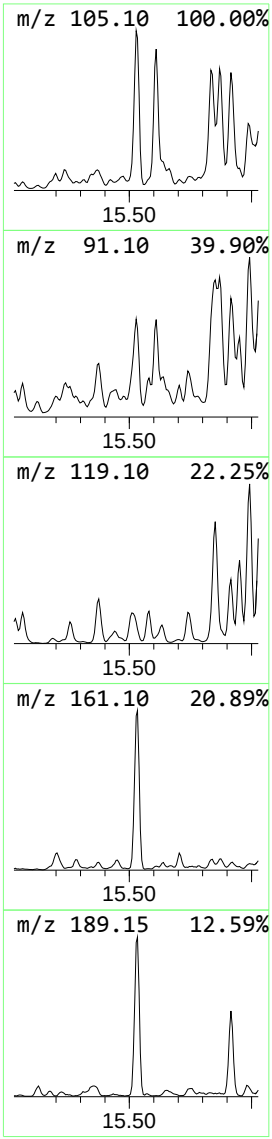
****

Peak Number 15 unknown15.528 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.528	60.48 ng	6635120	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-propylpentyl)-	204	C15H24	054932-91-1	40
2	4,4-Dimethyl-2-phenyl-5,6-dihydr...	189	C12H15NO	037139-43-8	27
3	4-Oxo-4-phenylbutyric acid, hexy...	262	C16H22O3	1000405-97-7	25
4	4-Oxo-4-phenylbutyric acid, isob...	234	C14H18O3	1000405-97-4	25
5	4-Oxo-4-phenylbutyric acid, octy...	290	C18H26O3	1010405-97-9	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

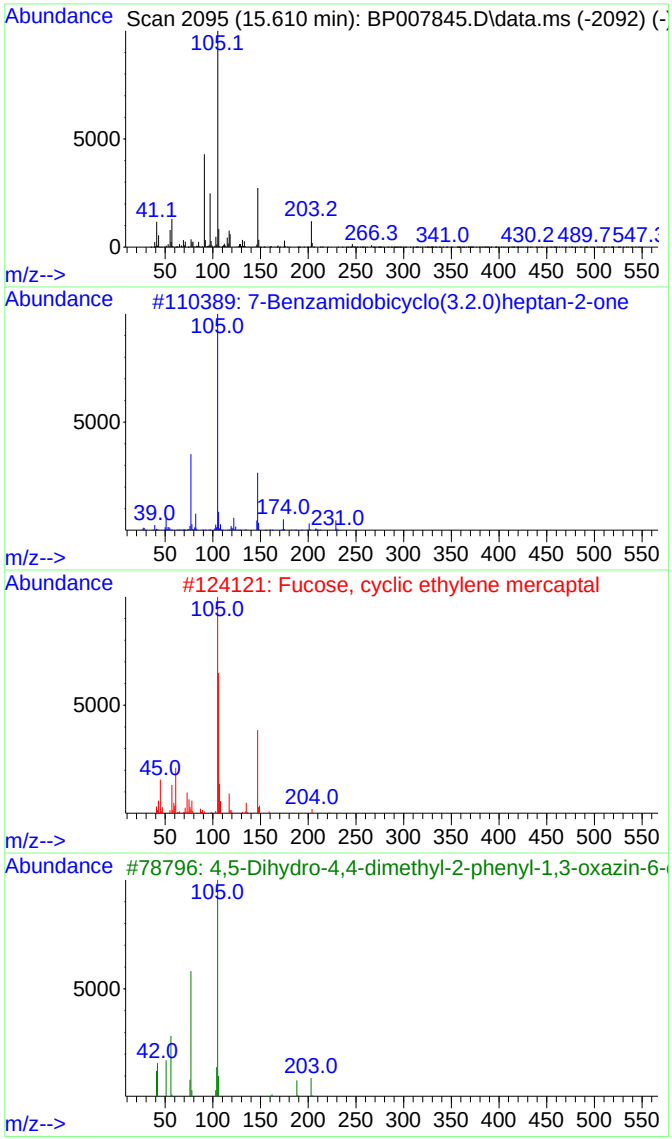
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

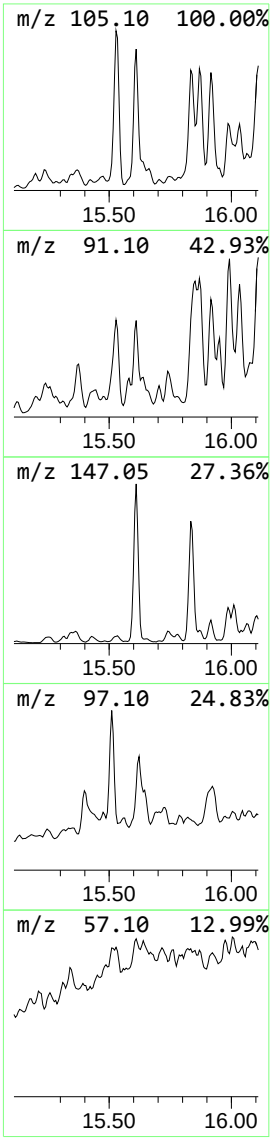
****

Peak Number 16 unknown15.610 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.610	62.43 ng	6849170	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Benzamidobicyclo(3.2.0)heptan-...	229	C14H15NO2	1000241-65-0	25
2	Fucose, cyclic ethylene mercaptal	240	C8H16O4S2	003650-70-2	23
3	4,5-Dihydro-4,4-dimethyl-2-pheny...	203	C12H13NO2	029637-55-6	16
4	Benzene, 1-(1-heptyldodecyl)-4-m...	358	C26H46	055191-36-1	12
5	Succinic acid, 2-fluorophenyl ph...	316	C18H17FO4	1000389-74-7	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

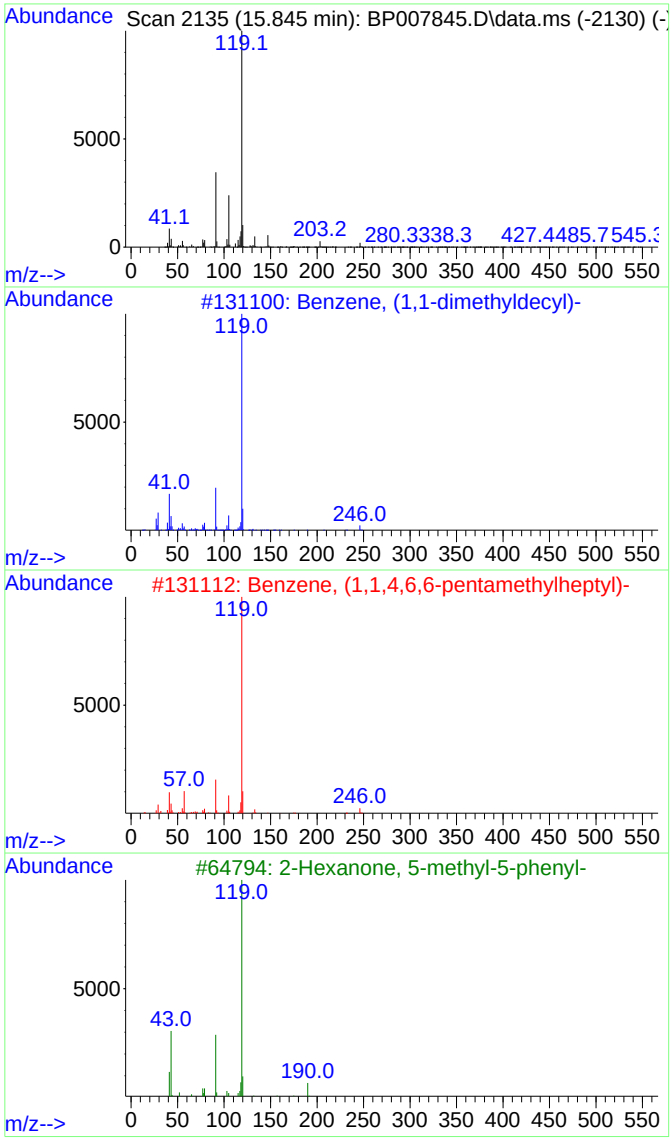
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

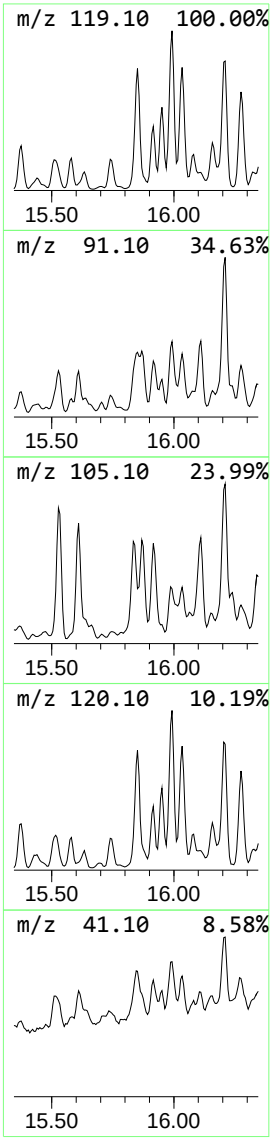
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 Benzene, (1,1-dimethyldecyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.845	100.37 ng	11011500	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	74
2	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	72
3	2-Hexanone, 5-methyl-5-phenyl-	190	C13H18O	014128-61-1	59
4	Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	59
5	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

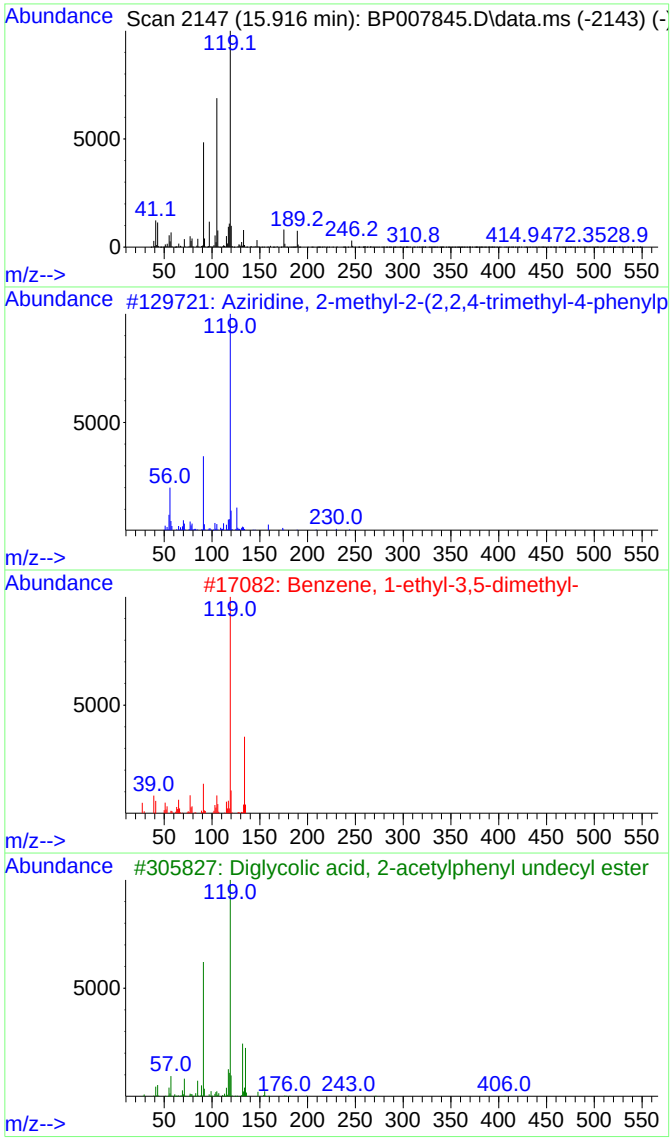
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

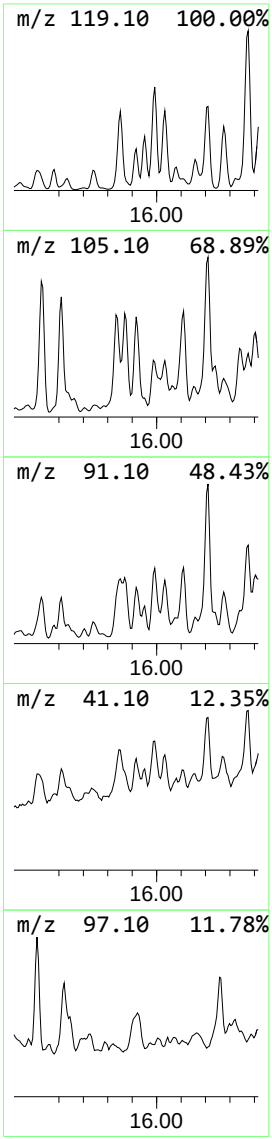
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Aziridine, 2-methyl-2-(2,2,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.916	50.87 ng	5580910	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aziridine, 2-methyl-2-(2,2,4-tri...	245	C17H27N	1000293-28-5	64
2	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	59
3	Diglycolic acid, 2-acetylphenyl ...	406	C23H34O6	1000382-72-7	59
4	Diglycolic acid, 2-acetylphenyl ...	392	C22H32O6	1000382-72-6	59
5	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

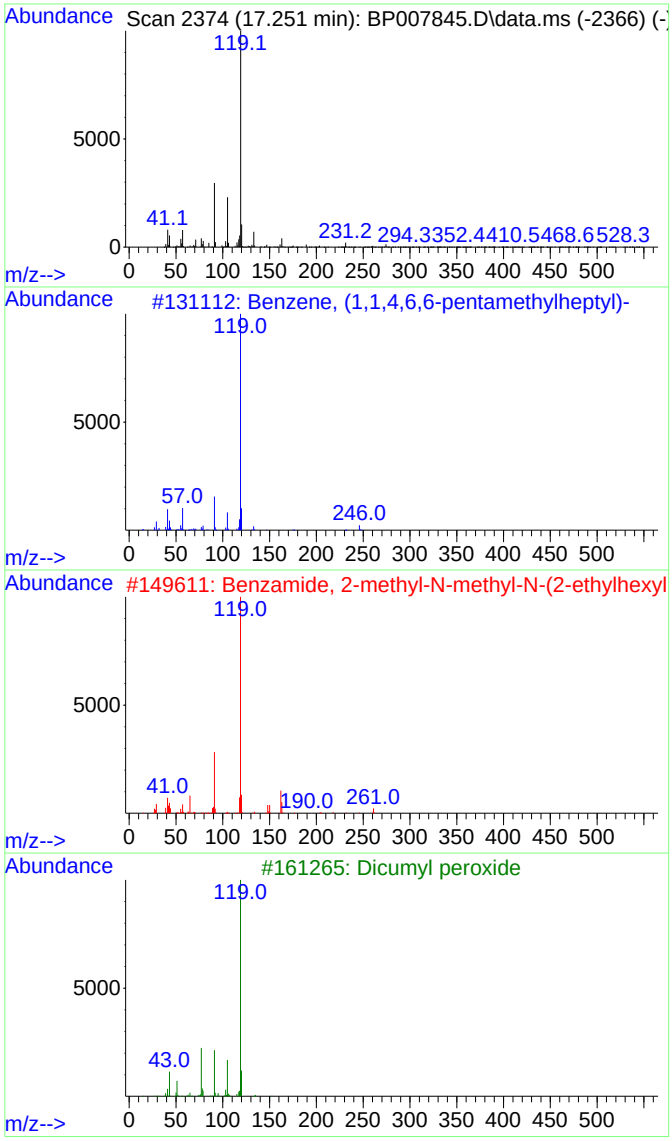
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

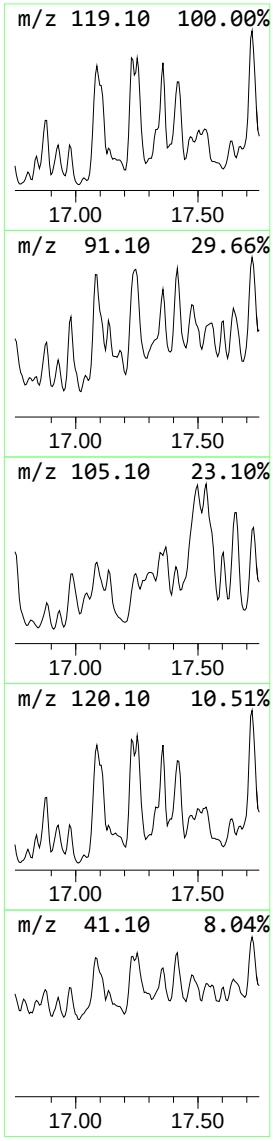
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Benzene, (1,1,4,6,6-pentame... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.251	20.00 ng	19893300	Phenanthrene-d10	17.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	64
2	Benzamide, 2-methyl-N-methyl-N-(...	261	C17H27NO	1000421-45-1	59
3	Dicumyl peroxide	270	C18H22O2	000080-43-3	59
4	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	59
5	2-Hexanone, 5-methyl-5-phenyl-	190	C13H18O	014128-61-1	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

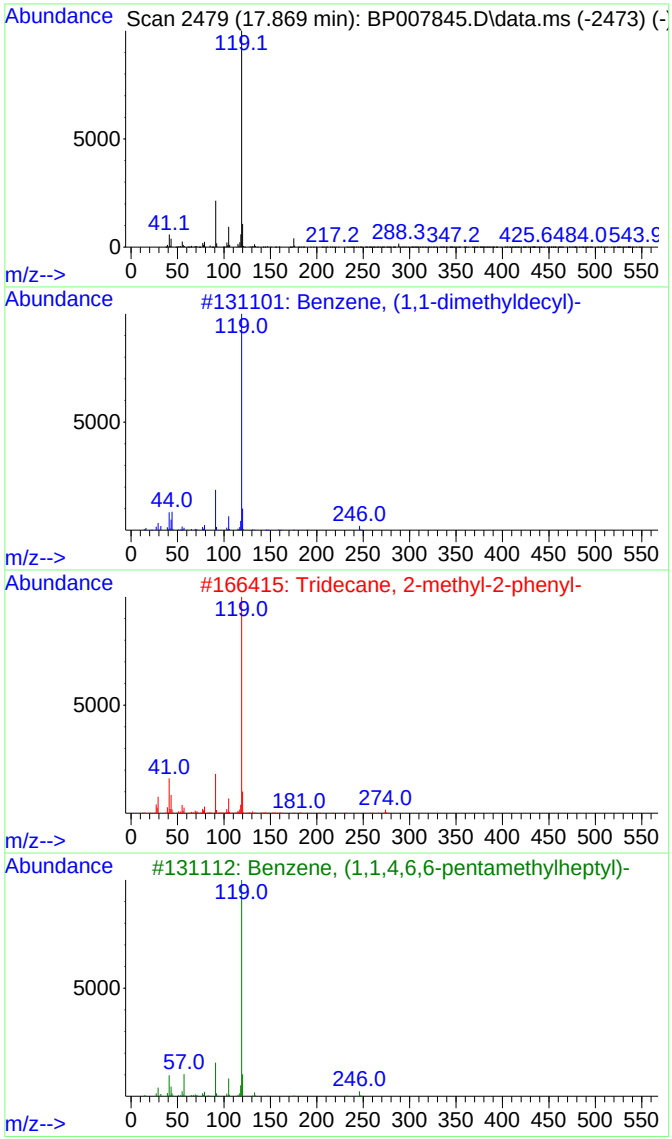
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

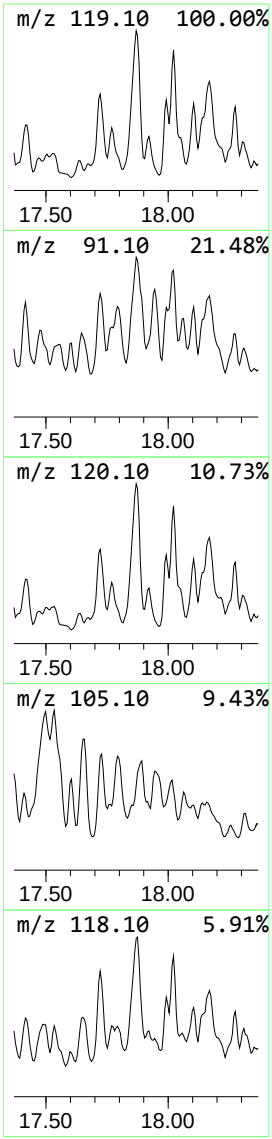
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 Tridecane, 2-methyl-2-phenyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.869	20.80 ng	20691700	Phenanthrene-d10	17.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	72
2	Tridecane, 2-methyl-2-phenyl-	274	C20H34	027854-41-7	72
3	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	72
4	Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	72
5	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110421\
Data File : BP007845.D
Acq On : 04 Nov 2021 13:31
Operator : CG/JU
Sample : M4438-03 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-20211101-WC-LM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.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
2-Pyrrolidinone...	8.181	37.0	ng	2145130	1	7.910	1160190	20.0
Heptyl isobutyl...	9.005	13.9	ng	807667	1	7.910	1160190	20.0
Benzene, (1,1-d...	9.175	21.8	ng	1266760	1	7.910	1160190	20.0
Cyclopentanecar...	11.969	35.2	ng	3034630	2	10.716	1724620	20.0
Cyclohexane, 1,...	12.110	16.1	ng	1385400	2	10.716	1724620	20.0
unknown12.328	12.328	18.4	ng	1584430	2	10.716	1724620	20.0
Thiophene, 3-et...	12.516	22.0	ng	1893580	2	10.716	1724620	20.0
Sulfurous acid,...	12.881	18.0	ng	1975040	3	14.557	2194120	20.0
2,4,4,6,6,8,8-H...	12.998	32.7	ng	3590610	3	14.557	2194120	20.0
unknown13.610	13.610	27.6	ng	3028590	3	14.557	2194120	20.0
Cyclohexanone, ...	13.722	17.8	ng	1952240	3	14.557	2194120	20.0
Benzoic acid, 2...	14.034	25.5	ng	2793320	3	14.557	2194120	20.0
Heneicosane, 5-...	14.740	15.1	ng	1661100	3	14.557	2194120	20.0
unknown14.981	14.981	16.7	ng	1836920	3	14.557	2194120	20.0
unknown15.528	15.528	60.5	ng	6635120	3	14.557	2194120	20.0
unknown15.610	15.610	62.4	ng	6849170	3	14.557	2194120	20.0
Benzene, (1,1-d...	15.845	100.4	ng	11011500	3	14.557	2194120	20.0
Aziridine, 2-me...	15.916	50.9	ng	5580910	3	14.557	2194120	20.0
Benzene, (1,1,4...	17.251	20.0	ng	19893300	4	17.316	19893300	20.0
Tridecane, 2-me...	17.869	20.8	ng	20691700	4	17.316	19893300	20.0